

Supplementary Material

Water-Mediated Formation of Hydride Derivates from Flexible Pd-Salan Complexes: A DFT Study

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Conformers of the Pd-Salen (PdSS) and Pd-Salan (PdHSS) complexes

In PdSS, the two enantiomers have a $\pm 26^\circ$ backbone bend defined by the C8–N1–N2–C9 dihedral, and they are connected by TS^{EI} which exhibits a planar chelate frame as well as a very low energy barrier (1.9 kcal mol⁻¹) that implies fast racemization. In the case of the HSS ligand, the flexibility of the palladium complexes is not only determined by the conformation of sp³ carbons of ethylene backbone but by two additional methylene (C7, C16) groups that connect the phenolate and amino groups of the ligand as well. Saturation of imine groups to amines also yields two nitrogen stereocenters in PdHSS, giving rise to (R,R) – (S,S) and (R,S) – (S,R) enantiomeric pairs (Fig. S1).

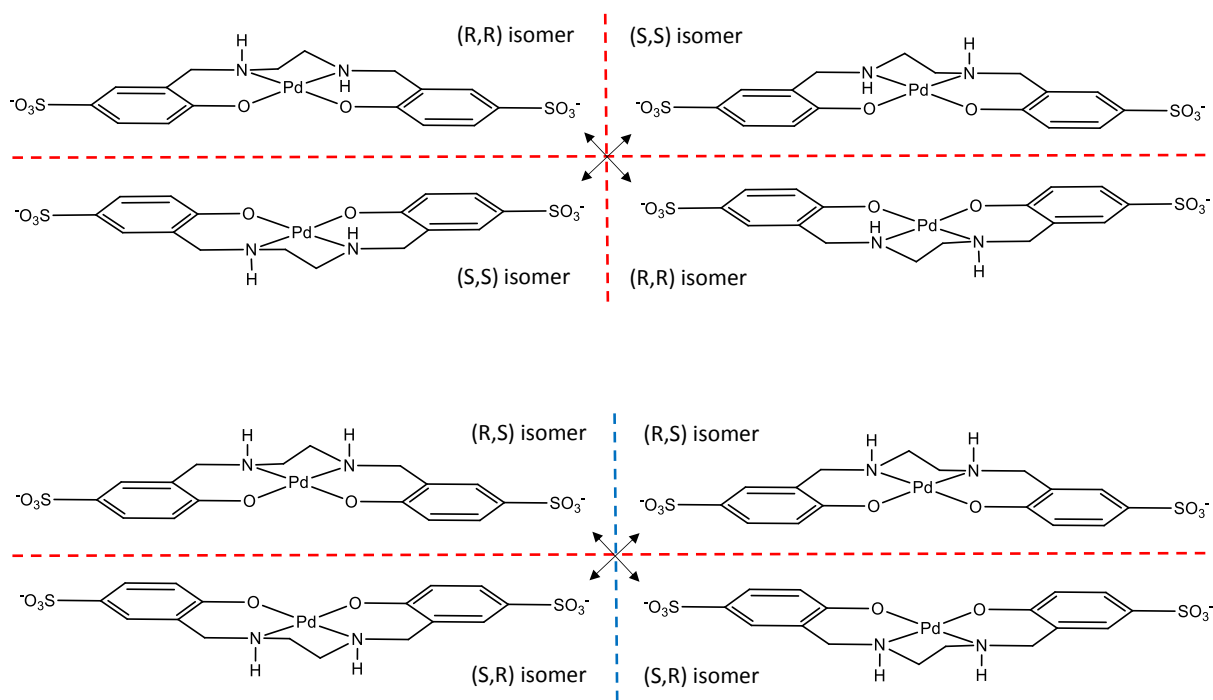


Fig. S1. Reflection signed as dashed line and rotation by 180° signed as narrows of the complexes show the relation among enantiomers. Red dashed lines represent blocked while the blue line shows free interconversion. Mirroring of (R,R) perpendicular or parallel to the plane of complex results an (S,S) isomer, however, (R,S) gives (S,R) isomer only in the case of parallel mirroring because free rotation of ethylene group i.e. ethylene inversion does not cause changes in stereocenters.

These are interconvertible by both parallel and perpendicular mirror planes, however, it is worth mentioning that EI of $(R,S)^\lambda$ results in a mirror image $(R,S)^\delta$ itself in which the backbone bend is $\pm 30^\circ$, and the relative energy is $1.7 \text{ kcal mol}^{-1}$. TS^{EI} of (R,S) isomers is at $5.7 \text{ kcal mol}^{-1}$ and has a symmetry mirror, while in case of the (R,R) and (S,S) diastereomers EI ($\Delta G^\ddagger = 12.3 \text{ kcal mol}^{-1}$) is non-symmetrical as the connected $(R,R)^\lambda$ and $(R,R)^\delta$ conformers have different free energies ($\Delta G = 7.3 \text{ kcal mol}^{-1}$) and backbone bend values ($+30^\circ$ and -27°), favoring the $(R,R)^\lambda$ form. Note that the C_2 -symmetric inverted $(R,R)^\delta$ has higher energy than the non-symmetric (R,S) isomers. In Fig. S2 the bottom representation of $(R,S)^\lambda$ and $(R,S)^\delta$ conformers show a volcano shape, and it can be observed that in this form the amino groups have more appropriate orientation at both equatorial sites resulting in lower energy in them than in the inverted $(R,R)^\delta$ isomer, see Table S2. Volcano-type geometry of TS^{EI} of (R,S) has also lower energy than $(R,R)^\delta$ enhancing these observations.

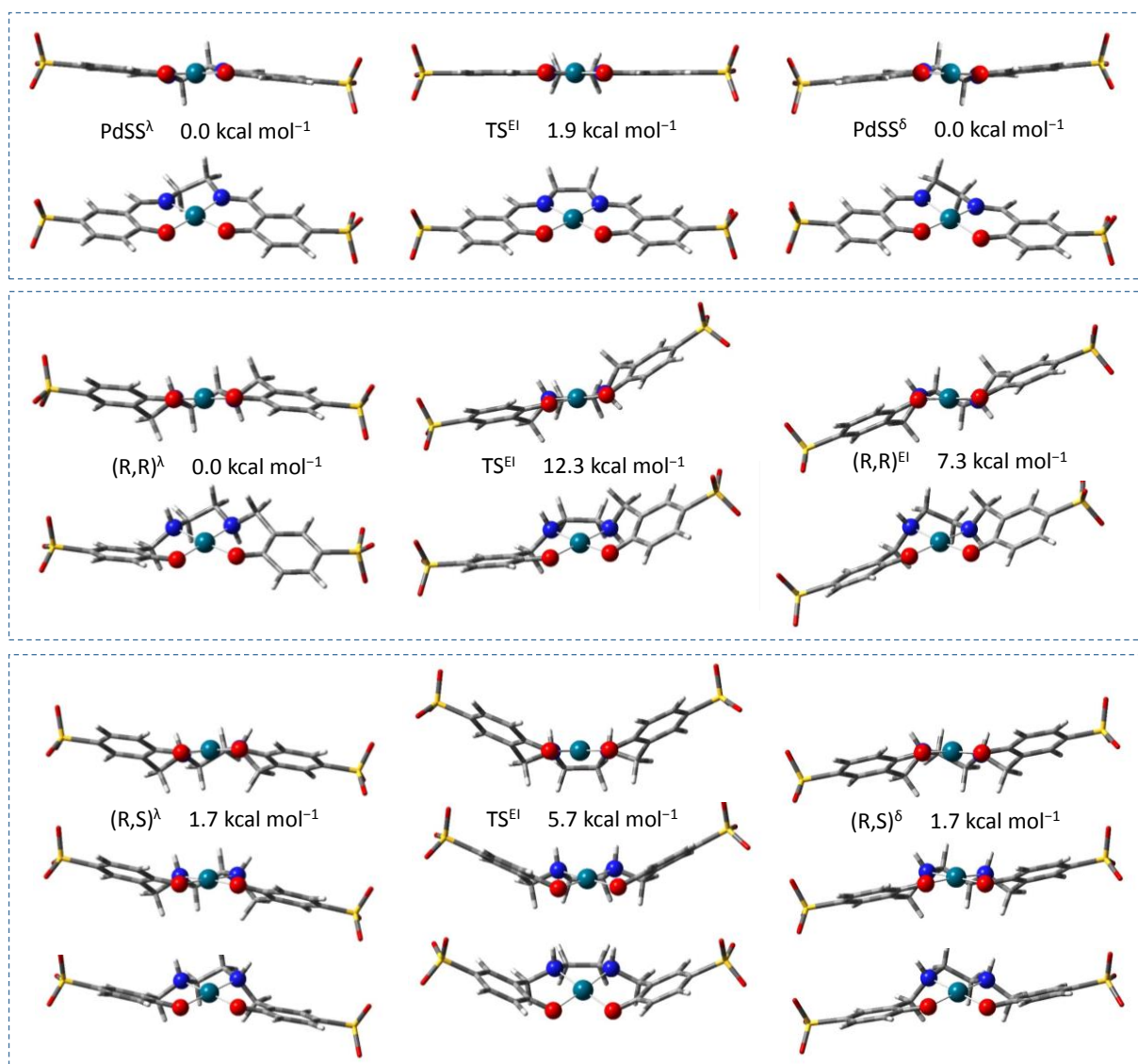


Fig. S2. The λ and δ helical isomers of the PdSS and (R,R) and (R,S) diastereomers of PdHSS in different orientations. Palladium, nitrogen, and oxygen atoms are indicated as grey, blue and red balls, respectively, while a tube representation is used for the rest of the molecule.

This is supported by the energetics as the half stepped (R,R) ^{λ ,hs} conformer in which one oxygen atom is out-of-plane at 5.1 kcal mol⁻¹ can be reached through a small, 7.3 kcal mol⁻¹ barrier. Note that these energy values are lower compared to ethylene inversion. On the other hand, the second arm rotation has a TS at 11.6 kcal mol⁻¹ and yields a less favored (10.5 kcal mol⁻¹) stepped (R,R) ^{λ ,s} conformer where a distorted geometry shows a transition between square planar and tetrahedral, see Fig. S3.

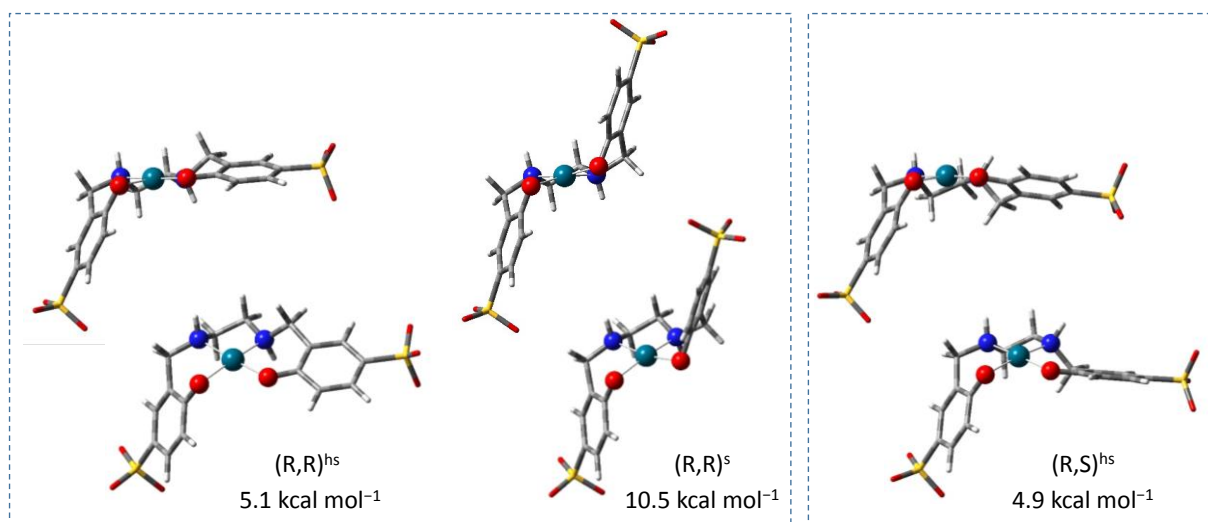


Fig. S3. The internal arm rotated (half stepped and stepped) conformers of the PdHSS in different orientations.

The $(R,R)^{E1}$ isomer, however, has two distorted equatorial arm conformations that cannot adopt a planar or stepped orientation due to steric strain that originates from the bond conformation between the amino nitrogen and ethylene carbon atoms. In the case of less stable (R,S) isomers ($1.7 \text{ kcal mol}^{-1}$) only half stepped $(R,S)^\lambda$ conformer ($4.9 \text{ kcal mol}^{-1}$) were found as a minimum. Considering the structural parameters, we found that the $N2-N1-O1-C5$ dihedral angle can be used to describe the internal arm rotation in PdHSS complexes. Surprisingly this dihedral angle for the (R,R) isomer is a bit larger than in PdSS ($+176^\circ$ vs. $+171^\circ$) while in $(R,R)^\lambda,hs$ is -115° but rotation affects also the other side where $N1-N2-O2-C14$ is -173° . Of course, due to the C_2 symmetry of $(R,R)^s$ these are equal like in the planar conformers (-110°). The $N1-O1-C2-C1$ dihedral angle describes the turn of the phenolic ring relative to the OONN square of the donor atoms which is 20° in (R,R) while in (R,S) isomers these are slightly different due to the non-symmetry ($\pm 21^\circ$ and $\pm 19^\circ$). $C1-C2-C11-C10$ dihedral angles define the rotation of the planes of phenolic rings relative to each other: it is $+1^\circ$ in PdSS, $+32^\circ$ in (R,R) and -5° in $(R,S)^\lambda$. Interconversion of diastereomers of HSS was also investigated, however, activation energies were very high predicting a blocked transition, see the following chapter.

Interconversion of (R,R) and (R,S) diastereomers

We found a pathway that connects diastereomers (R,R)^{hs} and (R,S)^λ in three steps by performing Pd–N dissociation, amino group inversion, and Pd–N coordination. All of them, however, involve high energy TS (31.1, 34.2 and 42.3 kcal mol⁻¹) and intermediate (32.6 and 32.7 kcal mol⁻¹) states, see Fig. S4. Note that TS1 has lower energy than I1 due to the flat PES. Also note that two intermediates are different in the chirality of the nitrogen atom while TS2 has a planar environment around nitrogen. During the process not only Pd–N1 distance but also Pd–C1 and Pd–C2 bonds changed, see Table S1 and Fig. S5.

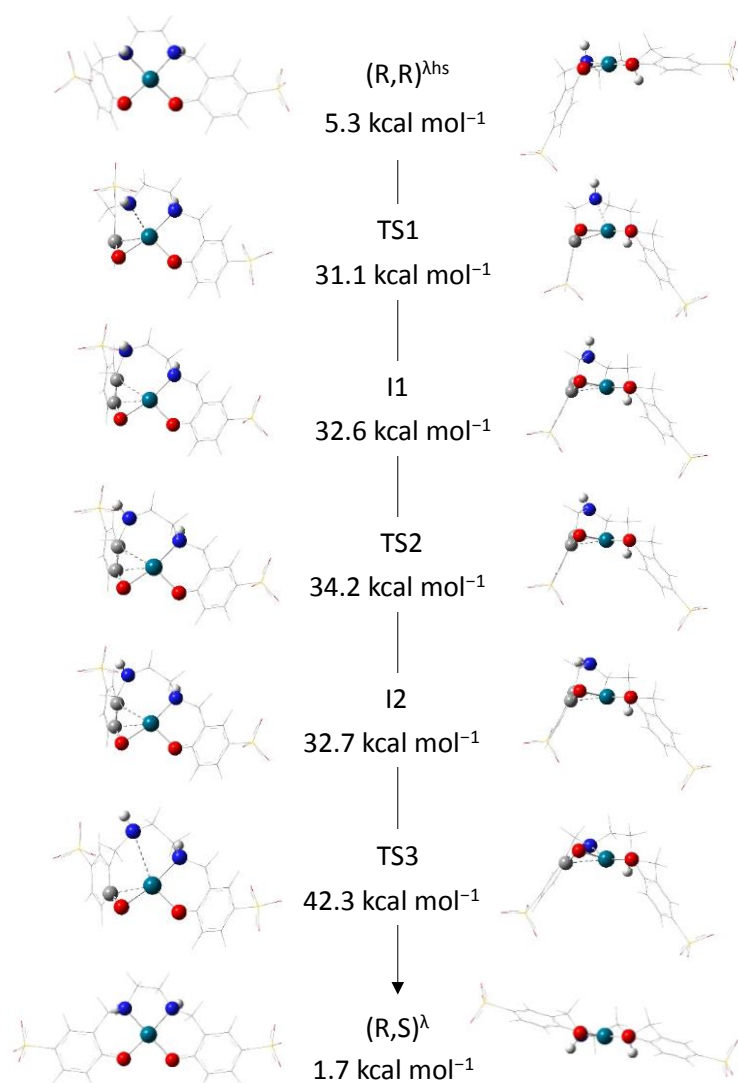


Fig. S4. Interconversion of diastereomers including nitrogen dissociation (TS1), nitrogen inversion (TS2), and nitrogen coordination (TS3) in different orientations. Note that TS1 has lower Gibbs free energy than that of I1 due to the flat PES.

Table S1. Changes in relevant bond lengths (pm) during interconversion of diastereomers.

| | Pd-O1 | Pd-N1 | Pd-C1 | Pd-C2 |
|----------------------|-------|-------|-------|-------|
| (R,R) ^{λhs} | 205 | 206 | 312 | 273 |
| TS1 | 209 | 269 | 221 | 237 |
| I1 | 209 | 357 | 223 | 231 |
| TS2 | 208 | 348 | 223 | 231 |
| I2 | 208 | 353 | 224 | 233 |
| TS3 | 204 | 309 | 238 | 259 |
| (R,S) ^λ | 203 | 206 | 330 | 295 |

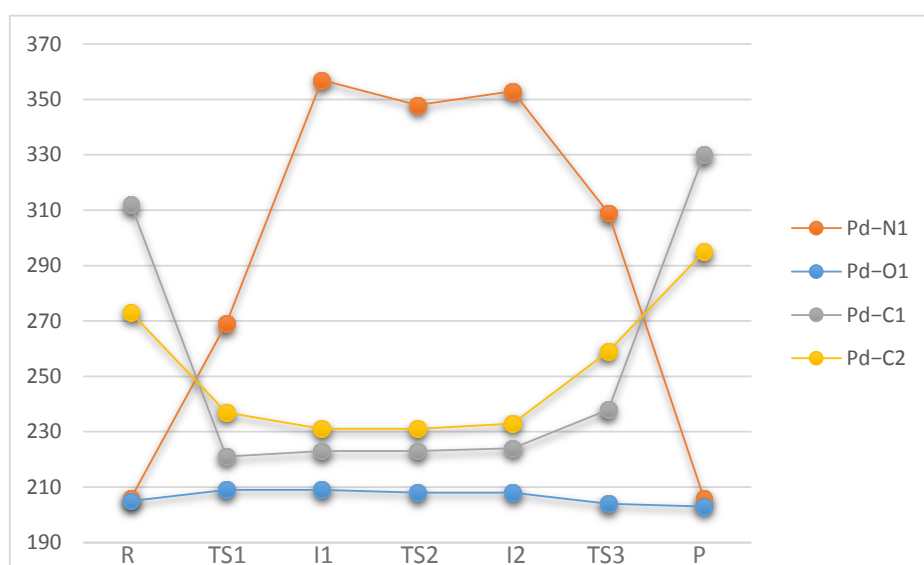


Fig. S5. Graphical representation of changes in relevant bond lengths (pm) during interconversion of diastereomers.

Coordinated water molecule in the saturated complex

We have also considered that during amino group inversion a water molecule can stabilize the vacancy differently, by creating an O^WNOO plane with typical values (212 pm for both) of $Pd-O^W$ and very short intramolecular $O^W-H\cdots NH$ bonds (168 pm for $(R,R)^W$ and 172 pm for $(R,S)^W$), however, we found that for both isomers ΔG^\ddagger is high as well: 34.8 and 29.1 kcal mol⁻¹, see Fig. S4. Reference structure here is a planar (R,R) complex to which one water molecule is bound by two H-bonds to oxygen atoms of phenolate arms. It can be seen that square planar geometries were slightly distorted in the products.

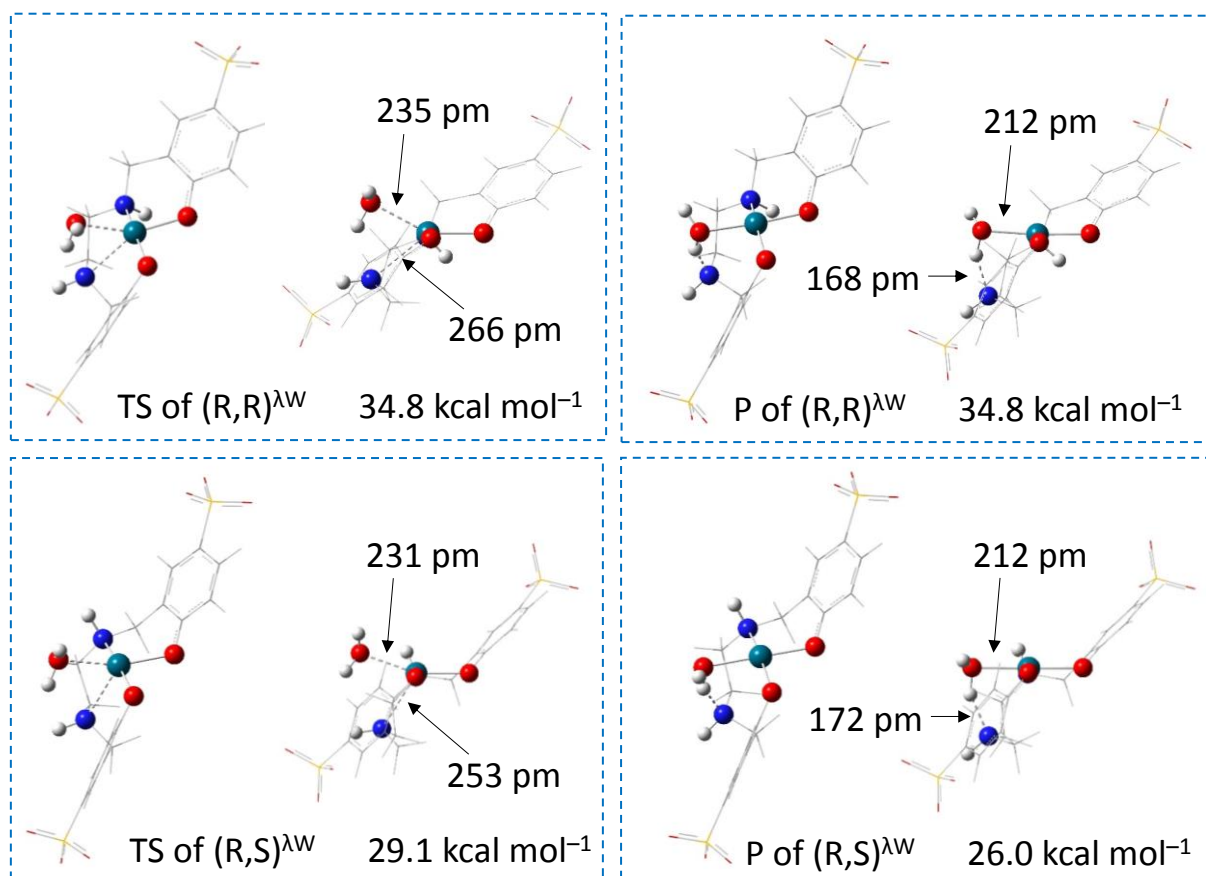


Fig. S6. Optimized structures of $(R,R)^\lambda$ and $(R,S)^\lambda$ isomers having a water molecule in the inner coordination sphere: TS means transition state, P means product.

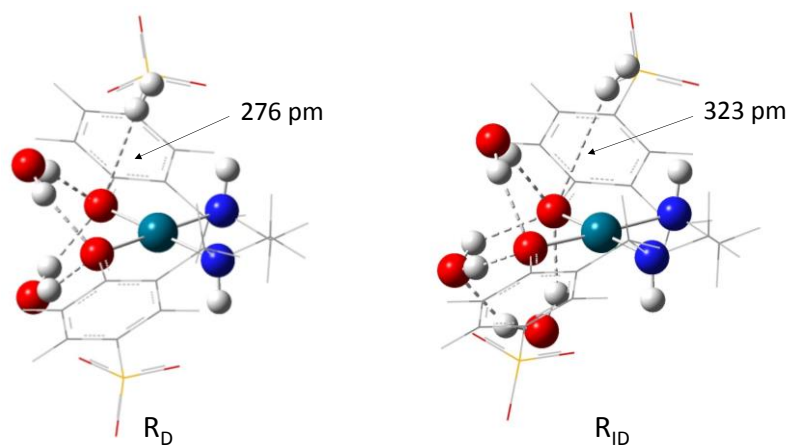


Fig. S7. Orientation of hydrogen and water molecules in the most stable reactant form set as a reference for direct and indirect mechanisms. As it can be seen a loosely bound H_2 is in both reactant forms.

Discussion of strain in sulfosalan diastereomers

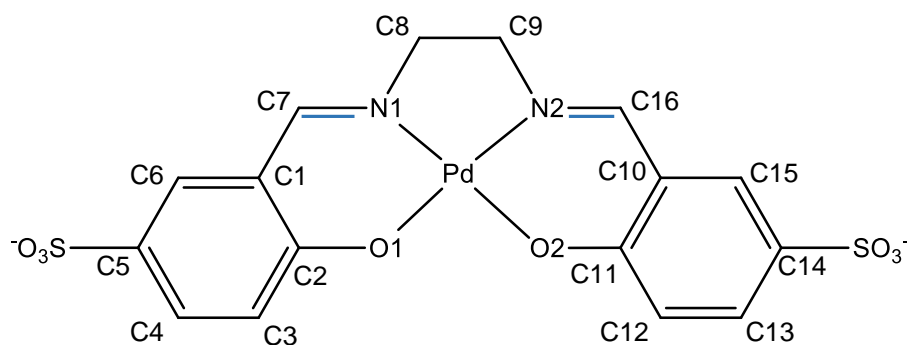
We optimized a fictive structure, namely the Pd(II)-dimethylamino complex [PdNH(Me)₂] to set it as a reference. We measured the angles of the amino group (α_i), and calculated the difference of the angles of the given structure and the reference one (Δ_i), finally we defined $\Delta_{\text{full}} \equiv \sum |\Delta_i|$ to obtain the strain in the chelated amino groups inside the complexes:

$$\alpha_1: \text{C7-N1-C8}; \alpha_2: \text{C7-N1-Pd}; \alpha_3: \text{Pd-N1-C8}$$

$$\alpha_4: \text{C9-N1-C16}; \alpha_5: \text{Pd-N1-C16}; \alpha_6: \text{C9-N1-Pd}$$

$$\Delta_i = \alpha_i(\text{PdHSS}) - \alpha_i(\text{PdNH}(\text{Me})_2)$$

$$\rightarrow \Delta_{\text{full}} \equiv \sum |\Delta_i|$$



In Table S3 it can be seen that (R,R) has the smallest strain compared to PdNH(Me)₂ while inverted (R,R)^{EI} the biggest, and the latter one has also a half eclipsed conformation along N–C_{eth} bonds (N1–C8 and N2–C9). These two structural properties set it 7.3 kcal mol⁻¹ higher in energy than the (R,R) conformer, while (R,S) diastereomers are only 1.7 kcal mol⁻¹ higher in energy due to the less strain of amino groups and that only one side has half eclipsed conformation in the central chelate.

Table S3. Analysis of strain around amino groups in the PdHSS complexes.

| | α_1 | α_2 | α_3 | α_4 | α_5 | α_6 | Δ_1 | Δ_2 | Δ_3 | Δ_4 | Δ_5 | Δ_6 | Δ_{full} |
|-----------------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------------------|
| (R,R) | 115,2 | 110,6 | 106,5 | 115,2 | 110,6 | 106,5 | 1,0 | 1,3 | -2,8 | 1,0 | 1,3 | -2,8 | 10,2 |
| (R,R) ^{EI} | 118,1 | 107,4 | 106,7 | 118,1 | 107,4 | 106,7 | 3,9 | -1,9 | -2,6 | 3,9 | -1,9 | -2,6 | 16,8 |
| (R,S) ^λ | 113,6 | 110,6 | 104,4 | 115,6 | 106,6 | 107,8 | -0,6 | 1,3 | -4,9 | 1,4 | -2,7 | -1,5 | 12,4 |
| PdNH(Me) ₂ | 114,2 | 109,3 | 109,3 | 114,2 | 109,3 | 109,3 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |

In Table S4 it can be concluded that the strain is increasing in TS1_{D1} and TS1_{D1}[▲] of (R,R) but in TS1_{D1}^λ and TS1_{D1}^{λ▲} the effect is larger setting the activation energies higher than in the first case. TS1_{D1}^{EI}, TS1_{D1}^{EI▲}, TS1_{D1}^δ, and TS1_{D1}^{δ▲} have similar strain around amino groups causing different effects for activation energies. The relative energy of the first two are closer to the non-inverted TS1s (~3.5 kcal mol⁻¹) than the difference between (R,R)^λ and (R,R)^δ (7.3 kcal mol⁻¹). On the other hand, TS1_{D1}^δ has 2.2 kcal mol⁻¹ higher energy than TS1_{D1} because despite the much smaller strain TS1_{D1}^δ has a weaker O^{W1}...H^{C16} H-bond than in TS1_{D1} (O^{W1}...H^{N2}). However, TS1_{D1}[▲] does not have O^{W1}...H^{N2} while TS1_{D1}^{δ▲} has a weak O^{W1}...H^{C16}, therefore, the latter one has 0.5 kcal mol⁻¹ lower energy than TS1_{D1}[▲].

Table S4. Analysis of strain around amino groups in the TS1s forms.

| | α_1 | α_2 | α_3 | α_4 | α_5 | α_6 | Δ_1 | Δ_2 | Δ_3 | Δ_4 | Δ_5 | Δ_6 | Δ_{full} | ΔG^\ddagger |
|---------------------------------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|-----------------|---------------------|
| TS1_{D1} | 110.3 | 117.2 | 108 | 115.3 | 112.7 | 106.6 | -3.9 | 7.9 | -1.3 | 1.1 | 3.4 | -2.7 | 20.3 | 19.2 |
| TS1_{D1}[▲] | 110.2 | 118.1 | 107.2 | 114.1 | 112.0 | 106.7 | -4.0 | 8.8 | -2.1 | -0.1 | 2.7 | -2.6 | 20.3 | 20.3 |
| TS1_{D1}^{EI} | 115.0 | 112.5 | 104.8 | 116.5 | 110.8 | 108.2 | 0.8 | 3.2 | -4.5 | 2.3 | 1.5 | -1.1 | 13.4 | 23.0 |
| TS1_{D1}^{EI▲} | 114.7 | 113.0 | 104.8 | 115.9 | 111.1 | 107.4 | 0.5 | 3.7 | -4.5 | 1.7 | 1.8 | -1.9 | 14.1 | 23.6 |
| TS1_{D1}^λ | 109.4 | 119.0 | 105.0 | 116.0 | 107.9 | 107.9 | -4.8 | 9.7 | -4.3 | 1.8 | -1.4 | -1.4 | 23.4 | 24.3 |
| TS1_{D1}^{λ▲} | 109.6 | 119.1 | 104.7 | 116.0 | 107.6 | 108.2 | -4.6 | 9.8 | -4.6 | 1.8 | -1.7 | -1.1 | 23.6 | 25.2 |
| TS1_{D1}^δ | 112.2 | 113.2 | 106.8 | 114.8 | 110.9 | 106.3 | -2.0 | 3.9 | -2.5 | 0.6 | 1.6 | -3.0 | 13.6 | 21.4 |
| TS1_{D1}^{δ▲} | 112.3 | 113.4 | 106.4 | 114.7 | 110.6 | 106.3 | -1.9 | 4.1 | -2.9 | 0.5 | 1.3 | -3.0 | 13.7 | 19.8 |
| PdNH(Me)₂ | 114.2 | 109.3 | 109.3 | 114.2 | 109.3 | 109.3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | |

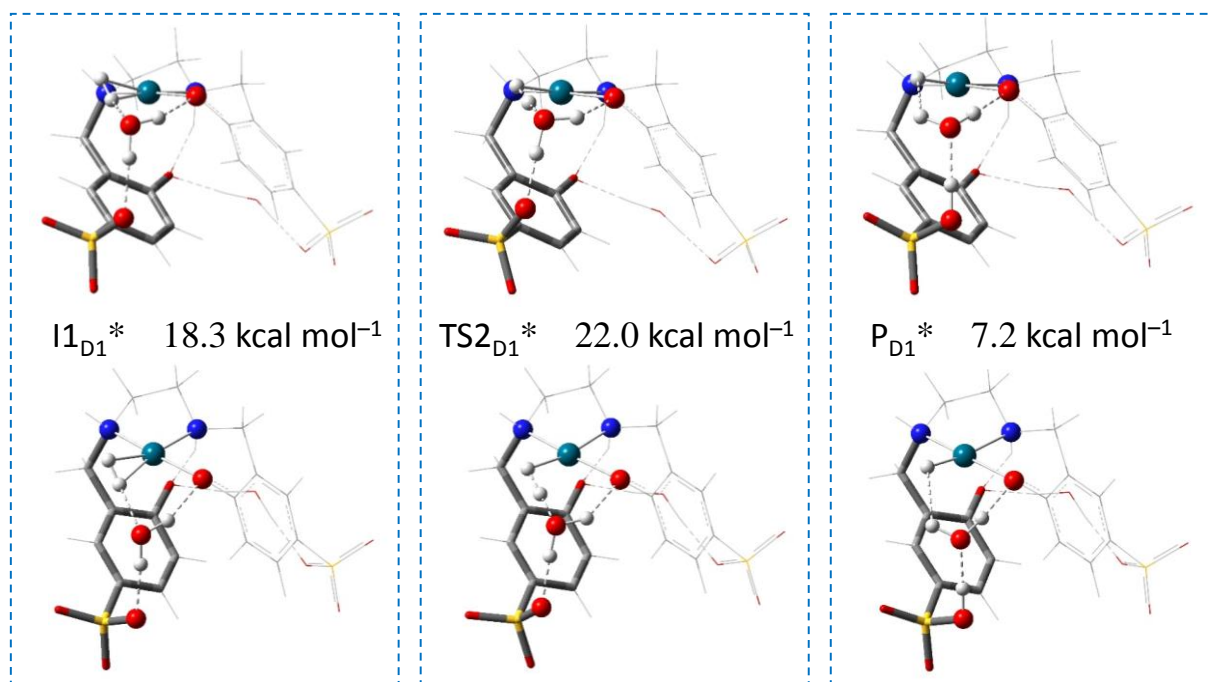


Fig. S8. The intermediate 1, the transition state, and the related product of hydrogen transfer to the sulfonate group. As can be seen, the phenolate arms are almost parallel to each other due to the separate H-bond networks of the water molecules which are bonded to the dissociated phenolate oxygen and the sulfonate group of the coordinated phenolate, and *vice versa*. Note that both $I1_{D1}^*$ is between $I1_{D1}$ and $I1_{D1}^\Delta$ in energy as $TS2_{D1}^*$ is between $TS2_{D1}^\Delta$ and $TS2_{D1}^W$. The path is endergonic showing a non-preferred proton transfer to the sulfonate group compared to the oxygen atom of the dissociated phenolate group. Even though the structure is strongly bent, it cannot be called as half stepped isomer since the N2–N1–O1–C5 dihedral angle is closer to $I1_{D1}$ than to $I1_{D1}^{hs}$ (109° vs. 146° or –119°). From $I1_{D1}^*$ a proton transfer can occur *via* water channel to the sulfonate group, however, it is endergonic (7.2 kcal mol⁻¹), but the activation barrier is not much higher (22.0 kcal mol⁻¹) than that of $TS2_{D1}^\Delta$, but lower than that of $TS2_{D1}^W$.

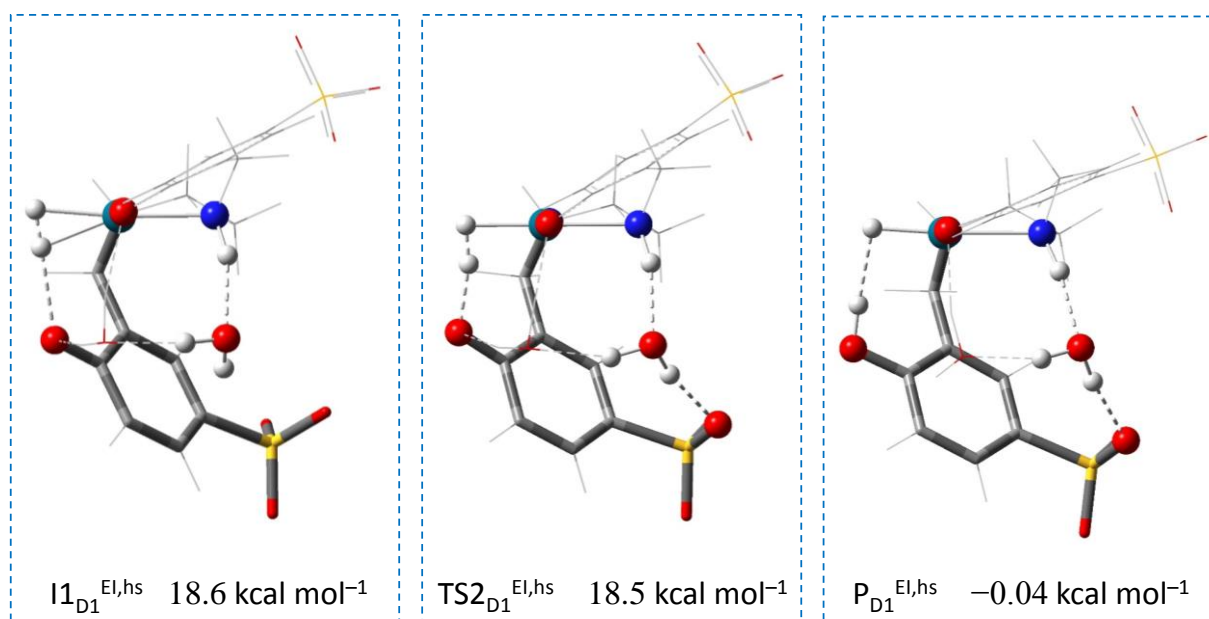
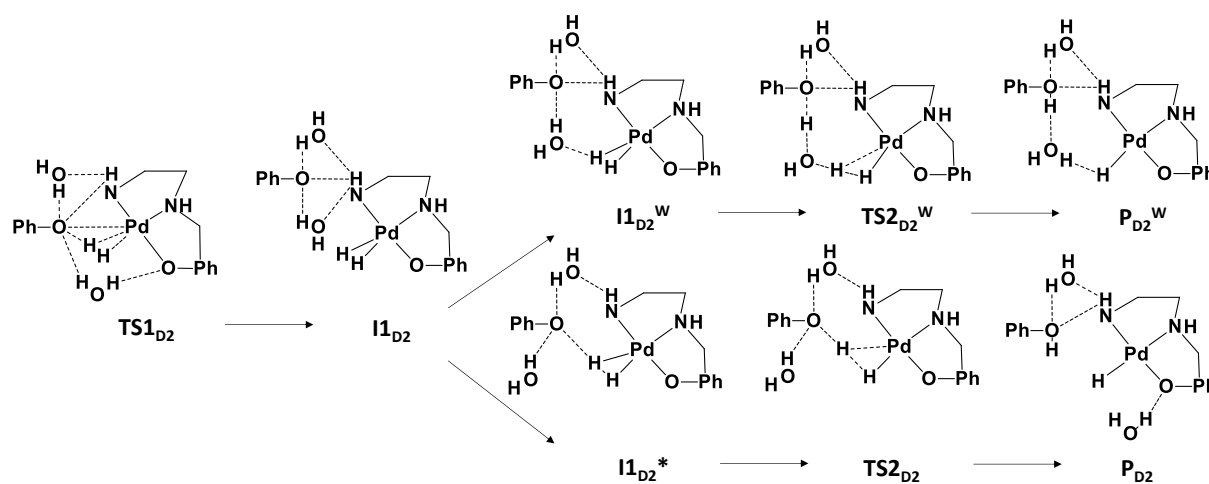


Fig. S9. The H-bond reorientation during proton transfer step as an effect of both arm rotation and ethylene inversion. Note that the $(R,R)^{EI}$ isomer itself does not have such conformers, however H_2 coordination and a consecutive EI in (R,R) yields the corresponding $I1_{D1}^{El,hs}$. From this intermediate, by following the reaction coordinate of H_2 dissociation ($TS1_{D1}^{El,hs}$), we were able to obtain the elusive reactant state, $(R,R)^{El,hs}$, which demonstrates of the stabilizing power of explicit water molecules through H-bonds.



Scheme S1. Possible pathways and H-bond networks in the D2 mechanism.

The apical form

In the apical form the main difference is the N1–Pd–H^H–H^P dihedral angle which is -6° where H^H is the hydrogen stayed at Pd as a hydride), in contrast to the almost perpendicular orientation found in the other I1 states (N1–Pd–H^H–H^P is -72°), see Fig. S11. This also affects the two Pd–H bond lengths, which are 178 pm for both bonds in I1_{D2} while I1_{D2}[^] exhibits longer distances: 180 (H^H) and 184 (H^P) pm. As the H₂ molecule is farther from the metal center, the H–H distance shrinks from 81.6 pm (I1_{D2}) to 80.9 pm (I1_{D2}[^]). This way the C1–H^P distance becomes short enough (233 pm) to allow for interaction between the hydrogen atom with a partial positive charge and the π system. This observation inspired us to check H-transfer to the nearest phenyl carbon atom (C1), see later.

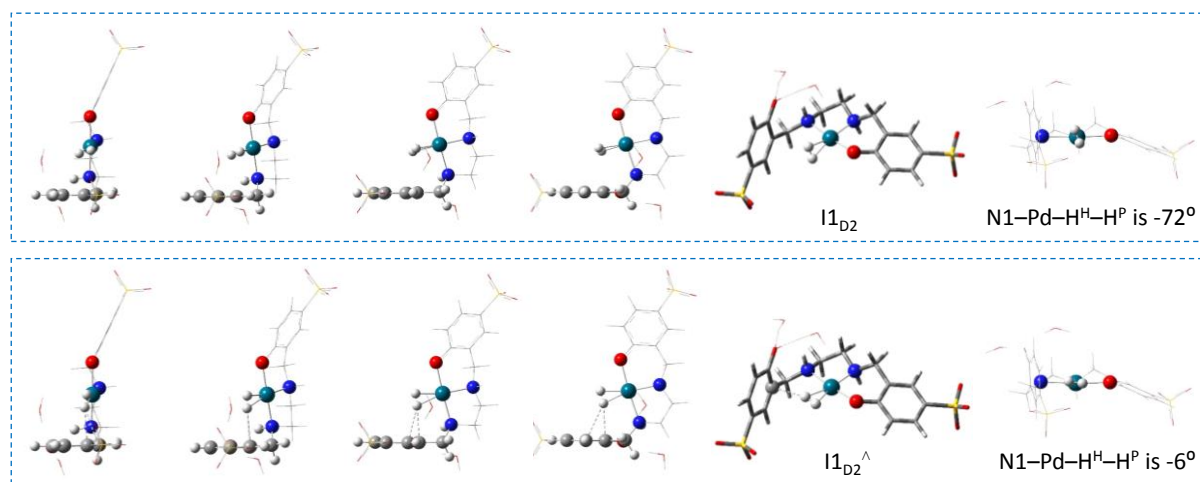


Fig. S10. Different orientations of “regular” and apical intermediate 1 of direct 2 (D2) mechanism.

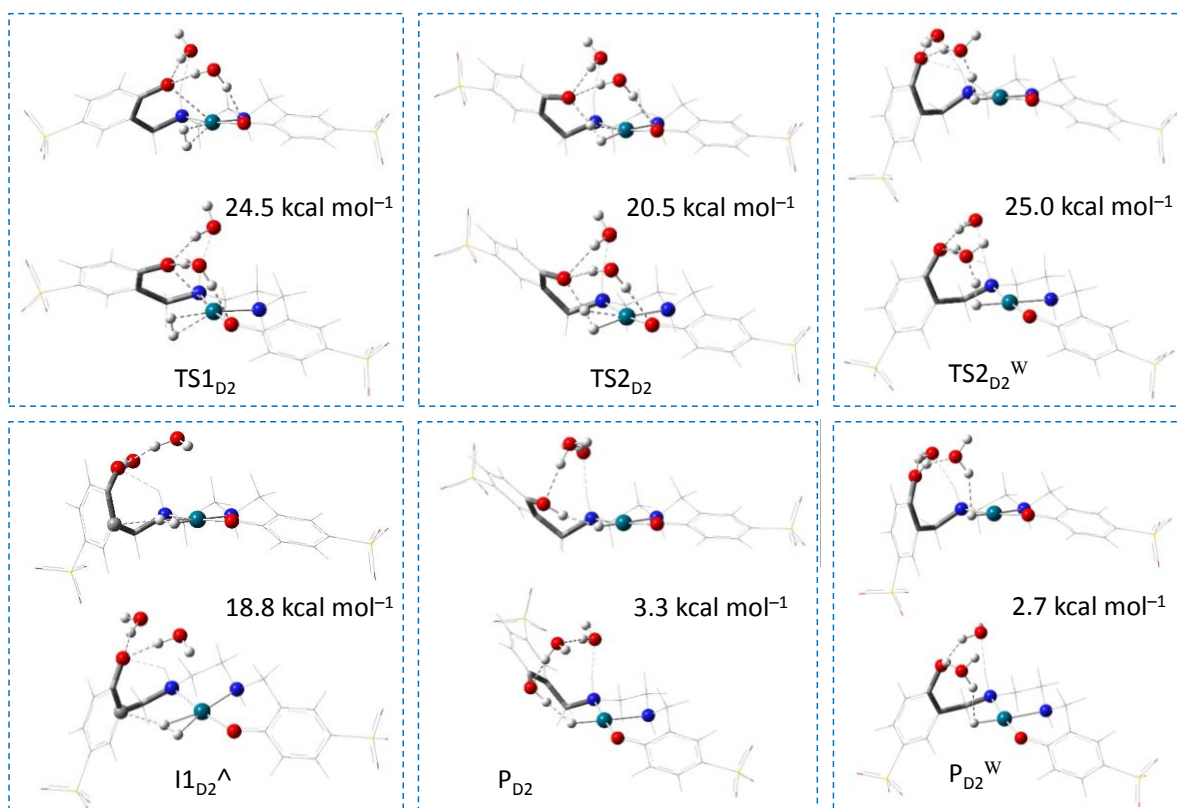


Figure S11. The most relevant stationary points of the direct 2 mechanisms in different orientations.

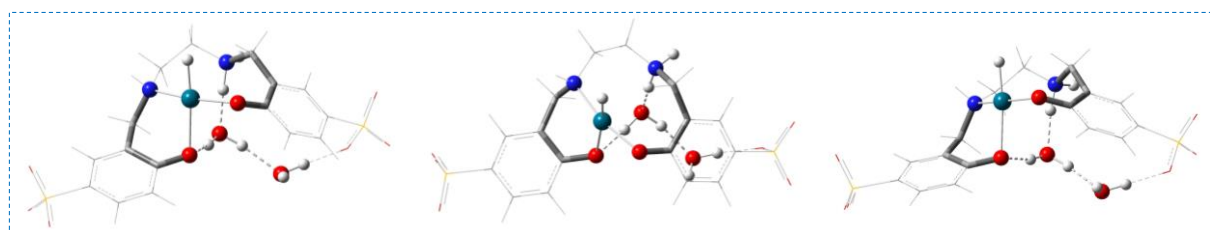


Fig. S12. Another type of monohydride complex in different orientations where protonated amino is dissociated instead of the phenolate arm.

Direct mechanism of the (R,S) diastereomer

Similar to the case of the (R,R) diastereomer, (R,S)^λ and (R,S)^δ provide two different scenarios similar to (R,R). This is due to having one planar equatorial and one distorted arm configurations analogously to the arm orientation in (R,R)^{EI}. The D1 approach of H₂ to (R,S)^λ is similar to the previously discussed (R,R) case, as the half of the complex accepting H₂ has almost the same equatorial arm structure. The difference is that the other non-planar arm has a methylene proton (H^{C16}) instead of an amino (H^{N2}) proton available for H-bonding with a water oxygen in the trigonal network. It can be concluded that the trigonal network has a positive effect only in those cases when O^{W1}...H^{N2}/H^{C16} H-bonds are short enough. For instance, in TS_{D1} it is 216 pm while in TS1_{D1}[▲] is 259 pm, and these differences are reflected in the relative energies as well (19.2 vs. 20.3 kcal mol⁻¹). In EI these relations are 220 vs. 237 pm and 23.0 and 23.6 kcal mol⁻¹, respectively. The TS_{D1}^λ-TS1_{D1}^{λ▲} relation offers similar differences: 226 vs. 240 pm and 24.3 and 25.2 kcal mol⁻¹. However, (R,S)^δ shows the benefit of trigonal network in terms of having one more H-bond: 239 vs. 238 pm and 21.4 and 19.8 kcal mol⁻¹. Note that the bond lengths of strongly covalent H-bonds are in the range of 120-150 pm while those of mostly electrostatic (moderate) ones are 150-220 pm. Over 220 pm H-bonds are weak electrostatic/dispersed type interactions [S1-S3]. As can be seen the δ-λ relation is opposite in (R,S). As it was discussed previously, EI is unfavored due to the N1^H-ethylene hydrogen repulsions causing 7.3 kcal mol⁻¹ higher relative energy in (R,R)^{EI} which is decreasing in TS1 forms to ~3.5 kcal mol⁻¹ due to the more appropriate amino group in TS_{D1}^{EI} and TS1_{D1}^{EI▲}, see Table S3 and the related discussion. In TS1_{D1}^λ and TS1_{D1}^{λ▲} the chemical environment of amino groups is less appropriate than in TS1_{D1}, therefore, their energy differences are larger (~5.0 kcal mol⁻¹) than the energy difference of saturated isomers (1.7 kcal mol⁻¹). On the other hand, (R,S)^δ shows similar effects such as (R,R)^δ, and together with the effect of trigonal network, TS_{D1} and TS1_{D1}^{δ▲} are very close energetically: 19.2 vs. 19.8 kcal mol⁻¹, see Table S2.

Table S2. Relative energies in kcal mol⁻¹ of the stationary points of the direct mechanism for the PdHSS complex.

| | (R,R) ^λ | (R,R) ^δ | (R,S) ^λ | (R,S) ^δ |
|----------------------------------|--------------------------|-------------------------|--------------------------|-------------------------|
| TS1 _{D1} | 19.2 | 23.0 | 24.3 | 21.4 |
| TS1 _{D1} [▲] | 20.3 | 23.6 | 25.2 | 19.8 |
| TS1 _{D1} ^{hs} | 20.7 | 20.7 | 23.2 | 23.1 |
| TS1 _{D1} ^{hs*} | 18.1^{**} | 24.6 | – | – |
| TS1 _{D1} ^s | 20.6 | n.c. | n.c. | n.c. |
| TS1 _{D2} | 24.5 | 34.7 | 28.4^{**} | 28.6 |
| TS1 _{D2} [*] | – | – | 26.9 | – |
| I _{D1} | 16.7 | 17.6 | – | 18.9 |
| I _{D1} [▲] | 19.2 | 18.4 | 22.6 | 19.3 |
| I _{D1} ^W | 19.5 | 19.8 | n.c. | n.c. |
| I _{D1} ^{hs} | 17.8 ^{Hr} | 18.6 | – | 21.3 |
| I _{D1} ^s | 18.4 | n.c. | n.c. | n.c. |
| I _{D2} | 18.2 | – | – | 19.6[▲] |
| I _{D2} ^W | 17.5 | 21.2 | – | – |
| TS2 _{D1} [▲] | 20.0 | 22.7 | 23.0 | 19.5 |
| TS2 _{D1} ^W | 26.2 | 24.5 | n.c. | n.c. |
| TS2 _{D1} ^{hs} | – | 18.5 | – | 19.1 |
| TS2 _{D1} ^s | 17.5^f | n.c. | n.c. | n.c. |
| TS2 _{D2} | 20.5^f | 24.2^f | – | 22.2[▲] |
| TS2 _{D2} ^W | 25.0 | 27.7 | – | n.c. |
| P _{D1} | 1.6 | -0.4 [▲] | 0.7 | 1.8 |
| P _{D1} ^W | -1.1 | -1.8 | n.c. | n.c. |
| P _{D1} ^{hs} | -2.0 | -0.04 | 2.7 | 1.4 |
| P _{D1} ^s | -0.2 | n.c. | n.c. | n.c. |
| P _{D2} | 3.3 | 5.5 ^{D1} | 6.5 | 5.4 |
| P _{D2} ^W | 2.7 | 4.7 | – | n.c. |

^{**} concerted process

^f it is a very flat PES where E_{el} proves that rel. energy of TS is higher than the minimum

^{Hr} H-bond reorientation causes concerted proton transfer → no TS2_{D1}^{hs}

^W water rearrangement

^{D1} D1 type product

n.c. not calculated

In the case of the (R,S) diastereomer, the arm opening towards the amino proton provides that water (W1) in H-bonding with the dissociated oxygen (O1) can also interact with not one but two amino protons as well. Note that this is due to both amino groups facing in the same direction in contrast to the antiparallel orientation in the (R,R) diastereomers. This dual amino interaction opens two possibilities only in the (R,S)^λ conformer; one is where W1 interacts with one amino proton (TS1_{D2}^λ), while the other (TS1_{D2}^{λ*}) contains two W1-amino H-bonds at a

slightly lower energy. In the second case, the dissociated phenolate is pulled towards the amino groups with more force through the water linker (331 vs. 287 pm) which creates a longer separation between the coordinated H₂ molecule (i.e. the H^P atom) and the O1 atom (217 vs. 240 pm). This effect can also be observed in the H₂ coordinated intermediate, where even the central chelate becomes distorted (the C8–N1–N2–C9 dihedral angle changed from -25° to 9°) resembling the structure of the other, δ conformation, see Fig. S13. In the case of the δ conformer, no two-H-bonds transition state (TS1_{D2} ^{δ *}) could be found. We observed that in TS1_{D2} ^{λ} the very short O1–H^P distance (217 pm) is an indication of a concerted process of substitution and coupled proton transfer. The same interaction in TS1_{D2} ^{δ} at 222 pm is slightly weaker and results in I1_{D2} ^{δ} where the phenolate arm is completely turned, however, it can rotate by Pd–N1–C7–C1 (I1_{D2} ^{δ *}) to shorten the O1···H^P bond to 215 pm from which proton transfer occurs in an almost barrierless process. In this case, the orientation of the phenolate arm is similar to the one found in the D1 mechanism, see Fig. S14.

[S1] Grabowski, S. J. *Hydrogen Bonding—New Insights*, Springer, **2006**.

[S2] Grunenberg, J. Direct Assessment of Interresidue Forces in Watson-Crick Base Pairs Using Theoretical Compliance Constants. *J. Am. Chem. Soc.* **2004**, *126*, 16310–16311.

[S3] Jeffrey, G. A. *An introduction to hydrogen bonding*, Oxford University Press, **1997**.

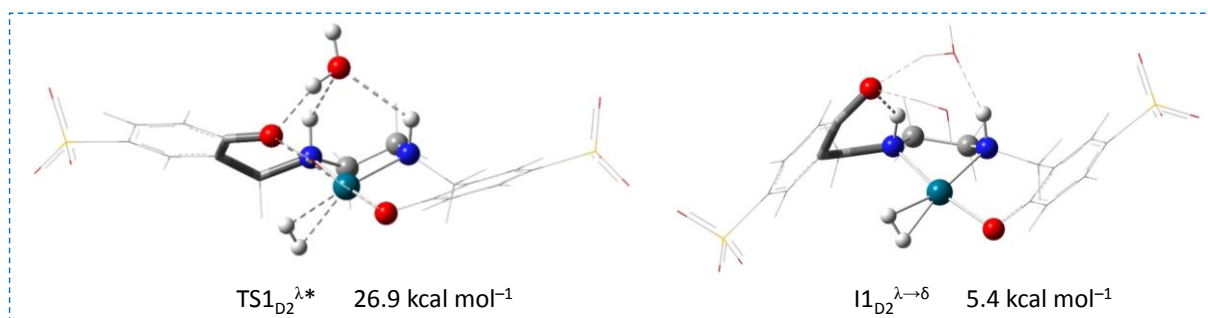


Fig. S13. The TS1 of (R,S) $^{\lambda}$ in D2 mechanism where both –NH groups have H-bond with one of the water molecules, and the I1 of that where the central chelate turned from λ to δ conformation. Dihedral angle C8–N1–N2–C9 changes from -25° to 9° .

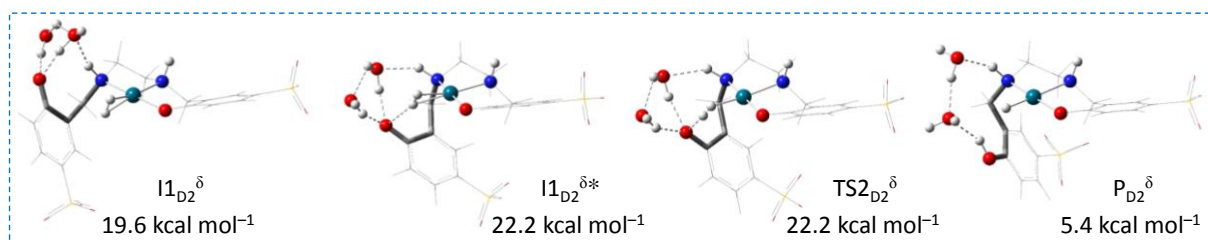


Fig. S14. The D2 mechanism of (R,S) $^{\delta}$ isomer from I1 in which the phenolate turned completely. In I1 $_{D2}^{\delta*}$ and TS2 $_{D2}^{\delta*}$ the phenolate rotated backward to indicate proton transfer, however, in this case, the proton transfer is similar to the D1 mechanism due to the orientation of the dissociated phenolate arm.

Structural parameters of TS1_D transition states

In general, it can be concluded that Pd–H bonds are the longest in TS1_{D1}, TS1_{D1}^{hs}, TS1_{D1}^s, TS1_{D1}^{El}, TS1_{D1}^{El,hs}, and TS1_{D1}^{λEl,hs} (~215-220 pm), TS1_{D1}^{λhs} and TS1_{D2}^{λ*} have a bit shorter (~205.5 and ~207.5 pm, respectively) while the rest of TS1's have Pd–H's ≤ 201 pm. Interestingly in some cases Pd–H^H is shorter than Pd–H^P (TS1_{D1}^{El,hs}, TS1_{D2}^{λ*} among those having “longer” Pd–H bonds and all others where distances are ≤ 201 pm). Of course, these parameters are strongly connected to H–H bonds where three groups have the following distance ranges: 76.3-76.7, 77.0-77.3, and 77.6-78.1 pm. Pd–O1 shows a similar trend to H^H–H^P bonds while H^P–O1 shows similarity to Pd–H bonds. However, N1–O1 does not correlate to these parameters directly but there is a trend that in TS1_{D1}'s is ~20-30 pm longer than in TS1_{D2}'s. All parameters are collected in Fig. S15. Some correlations also can be seen in Fig. S16 and Fig. S17 among angles and dihedral angles which are more obvious.

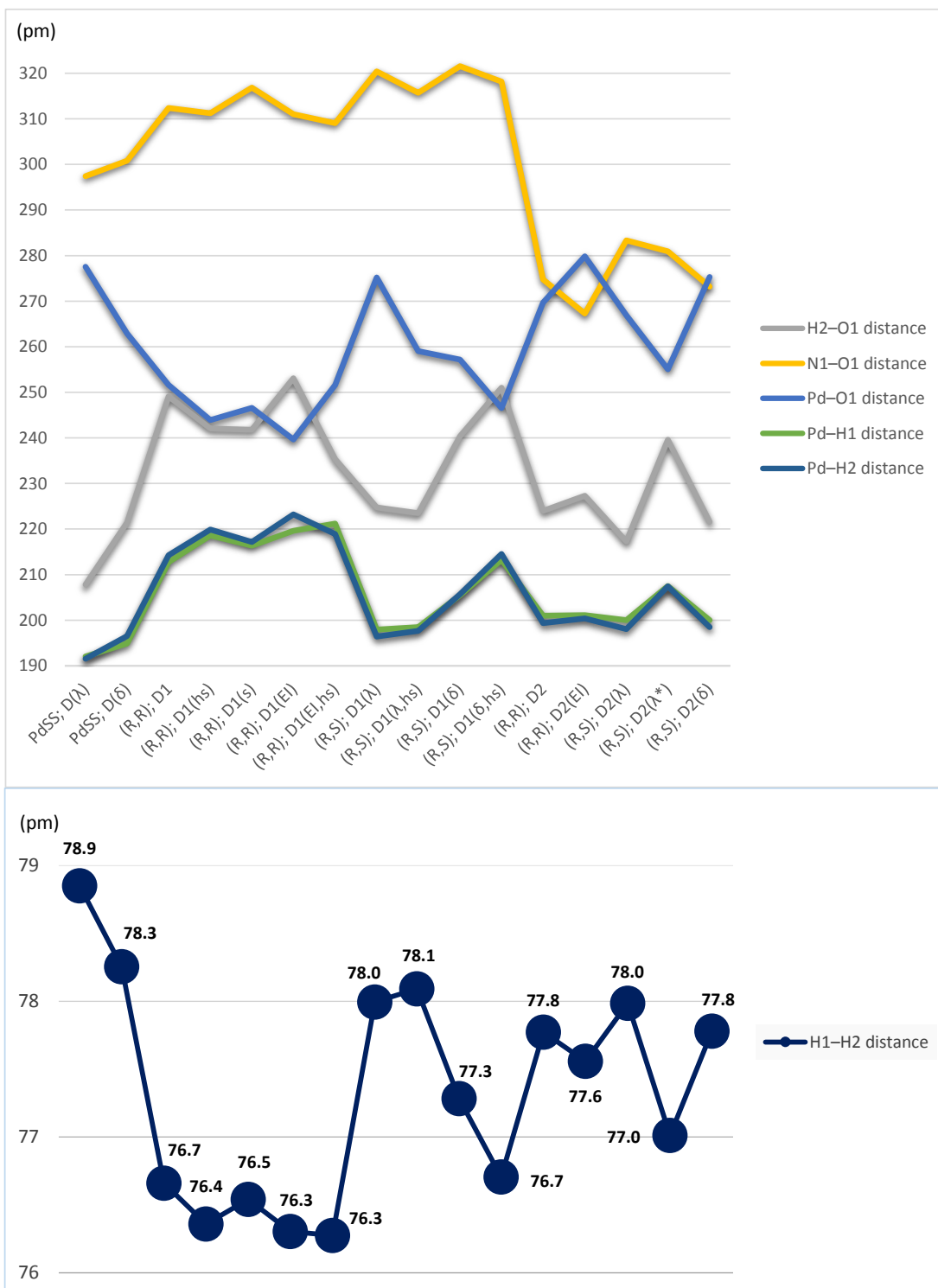


Fig. S15. Selected bond lengths of TS1D's.

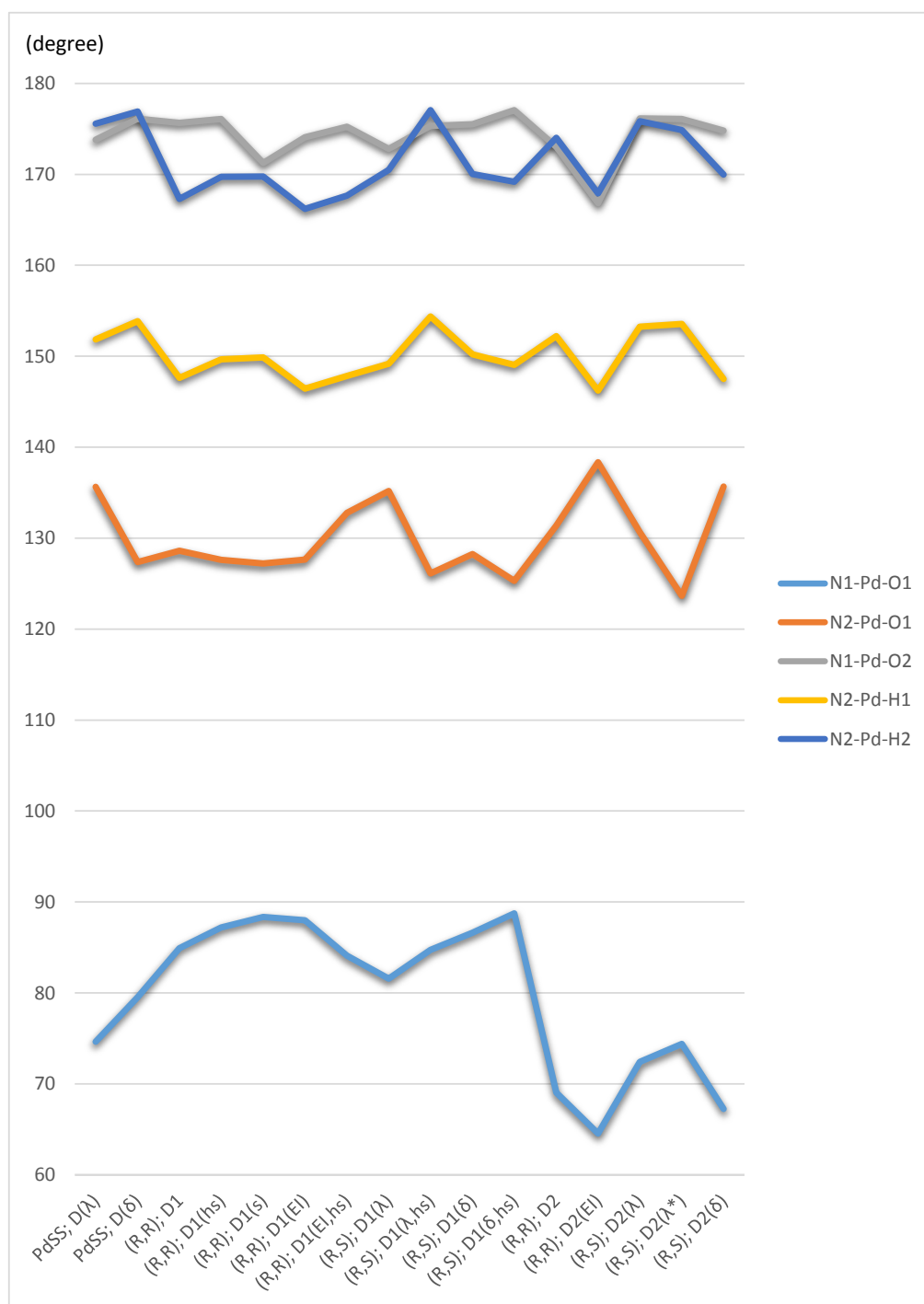


Fig. S16. Selected angles of TS_{1D}'s.

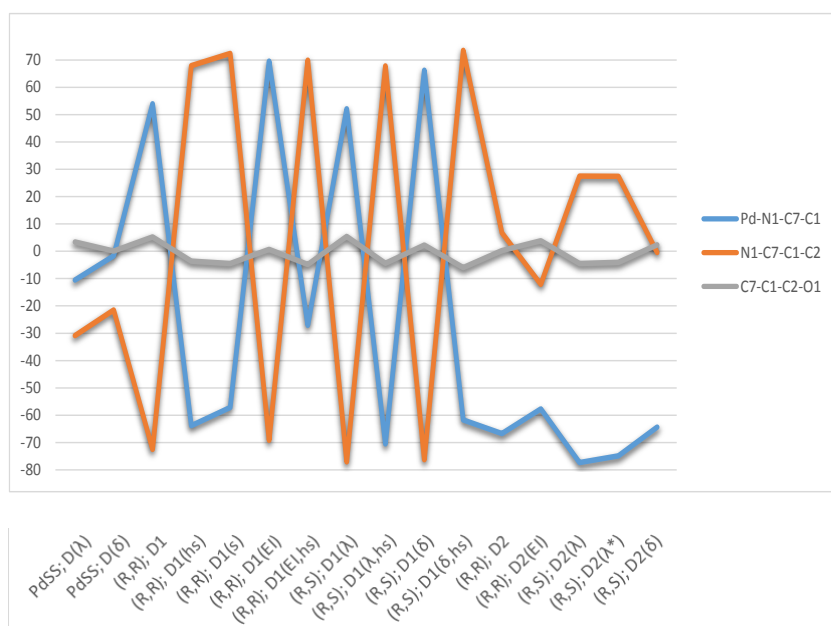


Fig. S17. Selected dihedral angles of TS_{1D}'s.

Concerted substitution and proton transfer processes without explicit water molecules

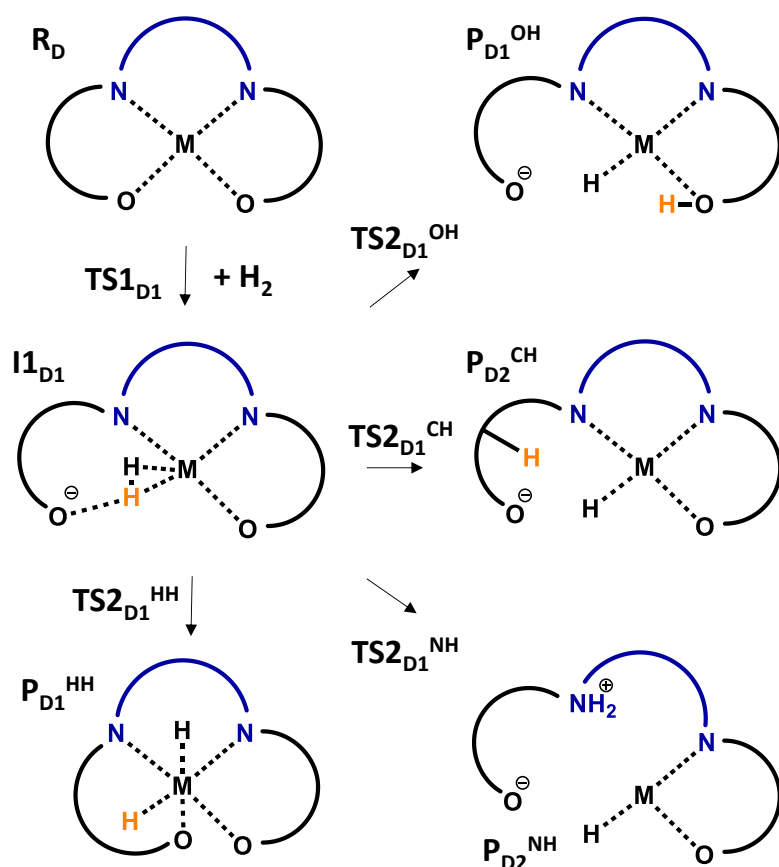
As was discussed in the main text, in several cases proton transfer takes place in concert with the substitution step called a concerted process. As it was mentioned, two water molecules bonded to O1 were taken into account because without them in most cases concerted processes (TS_{D1} , $\text{TS}_{\text{D1}}^{\text{hs}}$, $\text{TS}_{\text{D1}}^{\text{s}}$, $\text{TS}_{\text{D1}}^{\text{EI}}$, $\text{TS}_{\text{D1}}^{\text{EL,hs}}$) were found and only TS_{D2} gave intermediate I1 but all had high activation energies; especially large effect could be observed in the case of $\text{TS}_{\text{D1}}^{\text{s}}$ and $\text{TS}_{\text{D1}}^{\text{hs,EI}}$, see Table S5.

Table S5. Comparison of transition states without and with 2 water molecules of direct 2 mechanism. Energies are in kcal mol^{-1} .

| without water molecules | | with 2 water | |
|--|------|---|------|
| TS_{D1} | 22.3 | TS1_{D1} | 19.2 |
| $\text{TS}_{\text{D1}}^{\text{hs}}$ | 22.3 | $\text{TS1}_{\text{D1}}^{\text{hs}}$ | 18.1 |
| $\text{TS}_{\text{D1}}^{\text{s}}$ | 26.3 | $\text{TS1}_{\text{D1}}^{\text{s}}$ | 20.6 |
| $\text{TS}_{\text{D1}}^{\text{EI}}$ | 26.9 | $\text{TS1}_{\text{D1}}^{\text{EI}}$ | 23.0 |
| $\text{TS}_{\text{D1}}^{\text{EL,hs}}$ | 28.5 | $\text{TS1}_{\text{D1}}^{\text{EL,hs}}$ | 20.7 |
| TS1_{D2} | 28.4 | TS1_{D2} | 24.5 |
| TS2_{D2} | 24.3 | TS2_{D2} | 20.5 |

Minor pathways derived from intermediate 1

In I1 a hydrogen molecule is coordinated to the metal center therefore it was obvious to study the proton transfer step. We have investigated possible ways to get the hydride forms i.e. all potential proton acceptor have been taken into account in the case of (R,R): oxygen atom of dissociated, negatively charged phenolate (O1) arm which is the most relevant ($TS2_D$), oxygen of the coordinated phenolate arm ($TS2_D^{OH}$), the nitrogen of the dissociated phenolate arm ($TS2_D^{NH}$), C1 atom of the phenolic ring regarding the apical position of coordinated H_2 ($TS2_D^{CH}$), and homolytic dissociation of hydrogen bond ($TS2_D^{HH}$) have been studied as well, see Schemes S2. Moreover, $TS2$ was also studied *via* a water channel ($TS2_D^w$) which means an indirect proton transfer to the negatively charged oxygen of phenolate arm. $TS2_D$ and $TS2_D^w$ are the “default” deprotonation steps which are discussed in the main text.



Scheme S2. Possible minor pathways from intermediate 1.

Proton transfer to the coordinated phenolate arm ($\text{TS2}_{\text{D1}}^{\text{OH}}$) was checked in two cases: with two water molecules bound to O1 the $\Delta G^{\ddagger \text{e.s.}}$ (activation free energy of the elementary step) was very high ($19.9 \text{ kcal mol}^{-1}$) due to the unfavored steric condition i.e. direct transfer of proton distorts square planar geometry of $\text{NNH}^{\text{H}}\text{O}$ unit while taking into account one more water between coordinated H_2 and O2 ($\text{TS2}_{\text{D1}}^{\text{OH},3}$) the barrier decreases significantly ($\Delta G^{\ddagger \text{e.s.}} = 9.9 \text{ kcal mol}^{-1}$) giving a thermodynamically more exergonic elementary step ($\Delta G^{\text{e.s.}} = -0.8 \rightarrow -6.2 \text{ kcal mol}^{-1}$). In the case of inverted species, it is more preferred: $\Delta G^{\ddagger \text{e.s.}} = 7.0 \text{ kcal mol}^{-1}$ and $\Delta G^{\text{e.s.}} = -3.5 \rightarrow -8.9 \text{ kcal mol}^{-1}$. Note that in the manuscript the values calculated by 3 water were taken into account. Extending the system with two more water molecules we have built up an H-bond network by 5 water molecules in the case of (R,R) $^\lambda$ between O2 and sulfo group and, we have found that protonation of $-\text{SO}_3$ is preferred ($\Delta G = 2.2 \text{ kcal mol}^{-1}$).

Proton transfers to the nitrogen atom of the dissociated phenolate arm which has a huge activation barrier ($58.6 \text{ kcal mol}^{-1}$), while the product is also very unfavored ($31.8 \text{ kcal mol}^{-1}$) having a free coordination site. We checked proton transfer to the nitrogen from a coordinated water molecule as well, see the main text. TS2^{OH} , TS2^{NH} , and their products of (R,R) $^\lambda$ isomer can be seen in Fig. S18.

Formation of the *cis*-dihydride complex which is unsurprisingly not preferred due to unfavored oxidation state of the palladium(IV). In the case of I1_{D1} and $\text{I1}_{\text{D1}}^{\text{EI}}$ dissociated phenolate arm is coordinated to palladium in axial position forming an octahedral complex while starting from I1_{D2} and $\text{I1}_{\text{D2}}^{\text{EI}}$ on axial position a water molecule takes place in *cis*-dihydride products. TSs of *cis*-dihydride complex formation for (R,R) show high energy barriers that produce very unfavored—energetically very close to the TS—structures, see Table S6. For this reason, we did not study dihydride complex formation for (R,S) isomer.

The last minor pathway seems quite strange at first, however, APT charges confirm our finding, namely that proton transfer can occur also towards the C1 atom. In (R,R) C1 has a charge

-0.335 while in (R,S) it is -0.327. According to the orientation of phenolic ring relative to the coordinated hydrogen in $I1_{D2}^{\wedge}$ apical form, it is reasonable to check proton transfer to C1 while in other cases it seemed to be less trivial. C–O bond of the phenolic ring is changing after these processes. In general, typically C–O bond is shortening by 6 pm during D^{CH} processes and 4 pm elongation during dihydride formation, see Table S7. $TS2^{CH}$, $TS2^{HH}$, and their products of (R,R) $^{\lambda}$ isomer can be seen in Fig. S19. Of course, not only the C–O bond changes significantly during D^{CH} processes but also there is a change in bond orders (Table S8) due to the mesomeric structures drawn in Fig. S20.

Table S6. Relative energies in kcal mol⁻¹ of the stationary points of the minor pathways of direct mechanisms for the PdHSS complex. $TS2^{OH,3}$, and $P^{OH,3}$ means that the system was extended by one more water molecule.

| | (R,R) $^{\lambda}$ | (R,R) $^{\delta}$ | (R,S) $^{\lambda}$ | (R,S) $^{\delta}$ |
|-------------------|-------------------------|-------------------|--------------------|-------------------|
| $TS2_{D1}^{OH,3}$ | 28.4 | 25.0 | n.c. | n.c. |
| $TS2_{D1}^{CH}$ | 27.5 | 31.6 | 32.3 | 28.8 |
| $TS2_{D1}^{HH}$ | 37.2 | 36.4 | n.c. | n.c. |
| $TS2_{D2}^{CH}$ | 28.0 | 34.3 | 31.0 | 29.6 |
| $TS2_{D2}^{HH}$ | 39.1^f | 51.3 | n.c. | n.c. |
| $P_{D1}^{OH,3}$ | 12.4 | 9.2 | n.c. | n.c. |
| P_{D1}^{CH} | 20.6 | 17.6 | 21.2 | 18.9 |
| P_{D1}^{HH} | 36.6 ^f | 36.0 | n.c. | n.c. |
| P_{D2}^{CH} | 20.0 | 22.4 | 20.9 | 18.6 |
| P_{D2}^{HH} | 39.6 ^f | 51.0 | n.c. | n.c. |

^{n.c.} not calculated

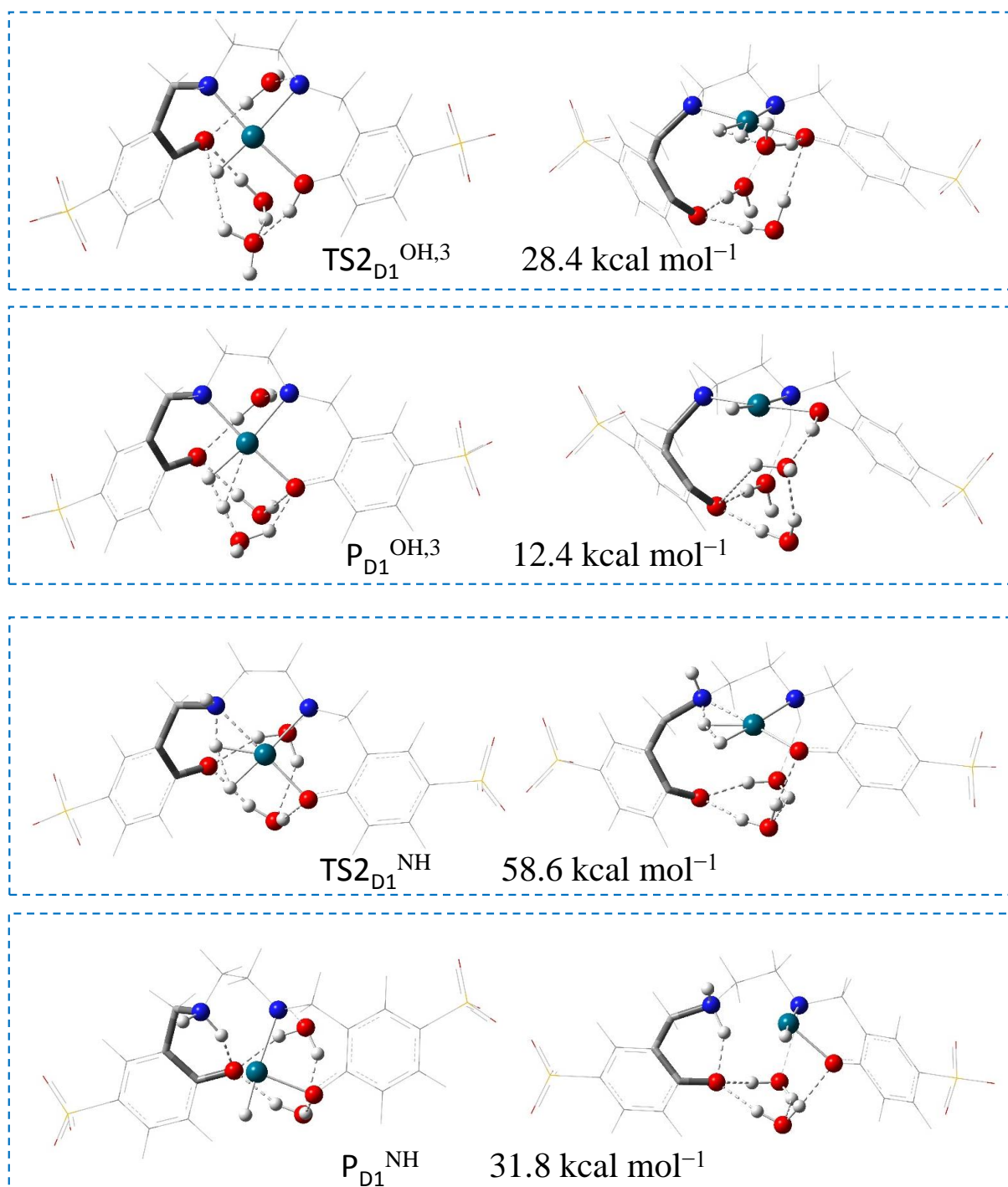


Fig. S18. The transition states and products of hydrogen transfer to the coordinated phenolate oxygen (O2), and to the nitrogen atom of the dissociated phenolate arm (N1) of the (R,R)^λ isomer.

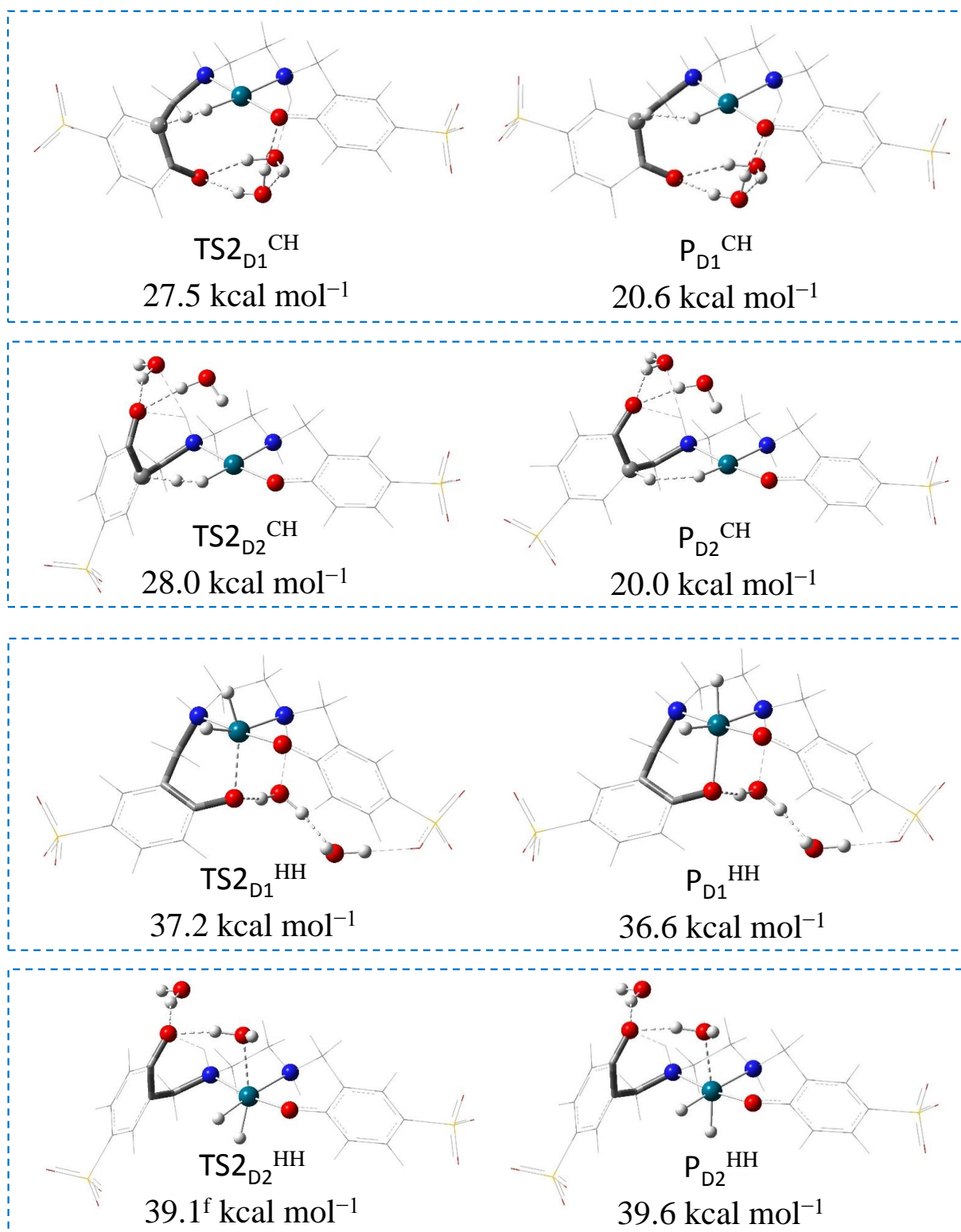


Fig. S19. The transition states and products of dihydride-complex formation (HH) and the H-transfer to the C1 atom (CH) of the (R,R)^λ isomer.

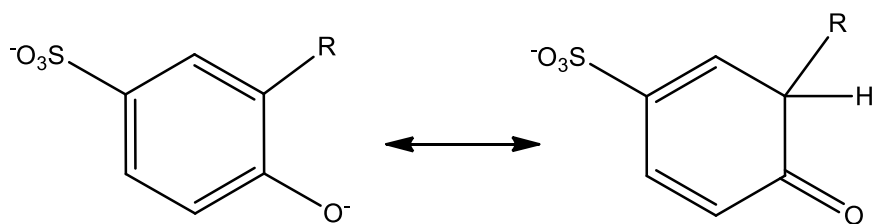


Fig. S20. Changes in bond orders after proton transfer to C1 atom of phenolic ring. R means the rest of the complex.

Table S7. Changes of C–O distances (pm) starting from the I1 after H-transfer to the phenolic C1 atom and the dihydride formation as well.

| Complex | Process | Change of C–O distance |
|--------------------|---|------------------------|
| (R,R) ^λ | I1 _{D1} →P _{D1} ^{CH} | 128→123 |
| (R,R) ^λ | I1 _{D1} →P _{D1} ^{HH} | 128→131 |
| (R,R) ^λ | I1 _{D2} →P _{D2} ^{CH} | 129→123 |
| (R,R) ^λ | I1 _{D2} →P _{D2} ^{HH} | 129→130 |
| (R,R) ^δ | I1 _{D1} →P _{D1} ^{CH} | 128→122 |
| (R,R) ^δ | I1 _{D1} →P _{D1} ^{HH} | 128→132 |
| (R,R) ^δ | I1 _{D2} →P _{D2} ^{CH} | 129→123 |
| (R,R) ^δ | I1 _{D2} →P _{D2} ^{HH} | 129→131 |
| (R,S) ^λ | I1 _{D1} →P _{D1} ^{CH} | 130→122 |
| (R,S) ^λ | I1 _{D2} →P _{D2} ^{CH} | 129→123 |
| (R,S) ^δ | I1 _{D1} →P _{D1} ^{CH} | 129→123 |
| (R,S) ^δ | I1 _{D2} →P _{D2} ^{CH} | 129→123 |

Table S8. Changes of distances (pm) of the phenolic ring during the D1^{CH} process in the case of (R,R)^λ complex. Most relevant changes are in bold.

| Bond | I1 _{D1} | P _{D1} ^{CH} |
|-------|------------------|-------------------------------|
| N1–C7 | 150 | 148 |
| C7–C1 | 148 | 152 |
| C1–C2 | 143 | 152 |
| C2–C3 | 142 | 145 |
| C3–C4 | 137 | 135 |
| C4–C5 | 140 | 144 |
| C5–C6 | 138 | 133 |
| C6–C1 | 139 | 148 |
| C3–O1 | 128 | 123 |

Table S9. Changes in bond lengths (pm) of donor atoms in the saturated and in the hydride product forms of (R,R) isomers.

| | Pd-H | Pd-N1 | Pd-N2 | Pd-O2 |
|--------------------------------|------|-------|-------|-------|
| (R,R) ^λ | – | 205 | 205 | 203 |
| (R,R) ^δ | – | 204 | 204 | 202 |
| P _{D1} | 157 | 209 | 216 | 205 |
| P _{D1} ^{EI▲} | 157 | 208 | 217 | 205 |
| P _{D2} | 157 | 210 | 217 | 205 |
| P _{D2} ^{EI} | 157 | 209 | 216 | 204 |

Experimental section

We examined the aqueous solution of $\text{Na}_2[\text{Pd}(\text{HSS})]$ in the presence of hydrogen gas at different pressures in terms of detecting the Pd-hydride species. Measurements were done by UV-Vis and ^1H -NMR spectroscopies.

UV-Vis spectroscopy:

We used the Analytik Jena Specord S 600 diode-line spectrophotometer. The UV-Vis spectrum of the PdHSS complex was recorded both in the presence and in absence of hydrogen gas. The intensity of the absorption spectrum of PdHSS was decreased by adding hydrogen gas (Fig. S23).

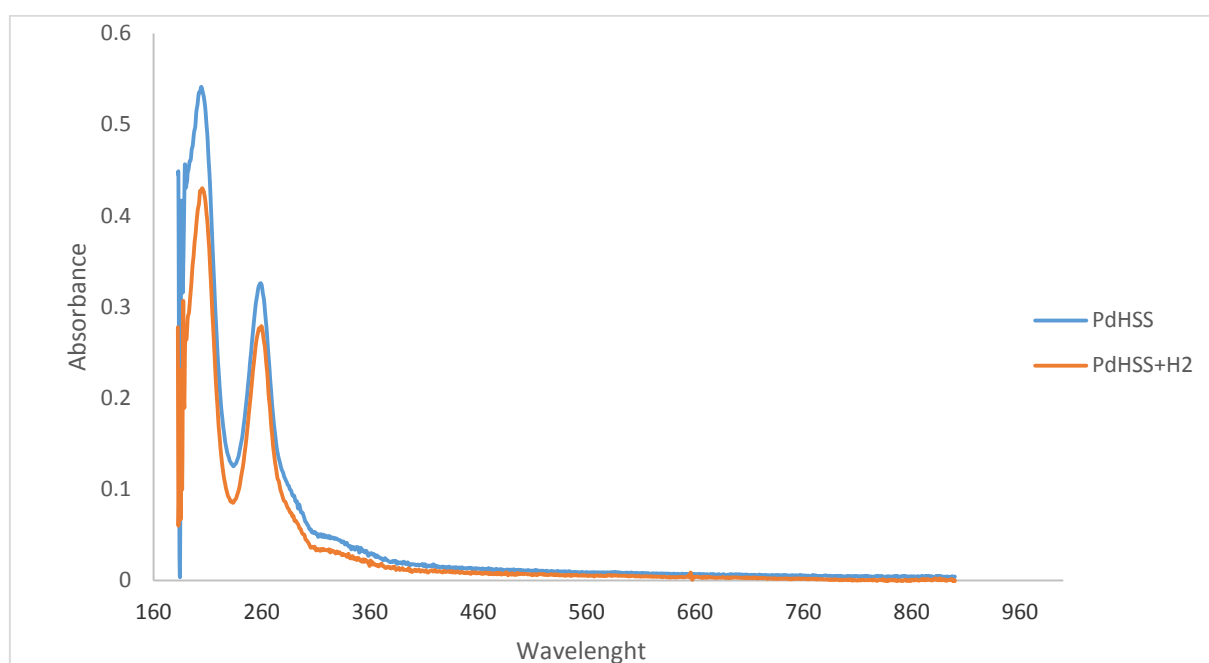


Fig. S21. UV-Vis spectra of $\text{Na}_2[\text{Pd}(\text{HSS})]$ dissolved in H_2O in the absence and presence of hydrogen.

¹H NMR:

¹H-NMR measurements were made on the BRUKER AVANCE DRX 360 at room temperature. The complex ¹H-NMR spectrum of Na₂[Pd(HSS)] was recorded in D₂O (Fig. S21), while the complex spectrum of Pd-hydride was recorded in H₂O. We used a pressure-resistant NMR tube "Wilmad® quick pressure valve" for my measurements at higher pressure at a constant temperature (25°C). During the preparation of the samples, all manipulations were done in an argon atmosphere. After the complete dissolution of the complex, the tube was filled with hydrogen gas (1 or 5 bar). Under 1 bar of hydrogen, no Pd-hydride complex could be identified, but at a pressure of 5 bar, a broad signal was observed in the hydride region. Although Figure 2 proves that a Pd-hydride complex is formed (chemical shift at -9.8 ppm in the hydride region), its exact structure cannot be determined. Based on the ¹H NMR spectrum, only one type of Pd hydride is formed under these conditions. Signal broadening may also result from a wide range of the chemical environment based on the different conformations of the flexibility of the dissociated phenolate arm, as shown in the DFT calculations. In presence of a substrate, no hydride signal could be identified even at 5 bar pressure.

It is worth mentioning that under 5 bar hydrogen in the stock solution (35 mM) of PdHSS a dark ring of a precipitate appeared on the wall of the NMR tube while the deep yellow color of the solution became pale yellow. We could not see similar precipitation in other case e.g. at lower concentration or even in the presence of substrate. DFT calculations showed high energy intermediates having palladium(0), which could form dimers in a thermodynamically very favored reaction. This can be an explanation for the experimental phenomenon that at higher concentration in presence of hydrogen a reaction can be occurred.

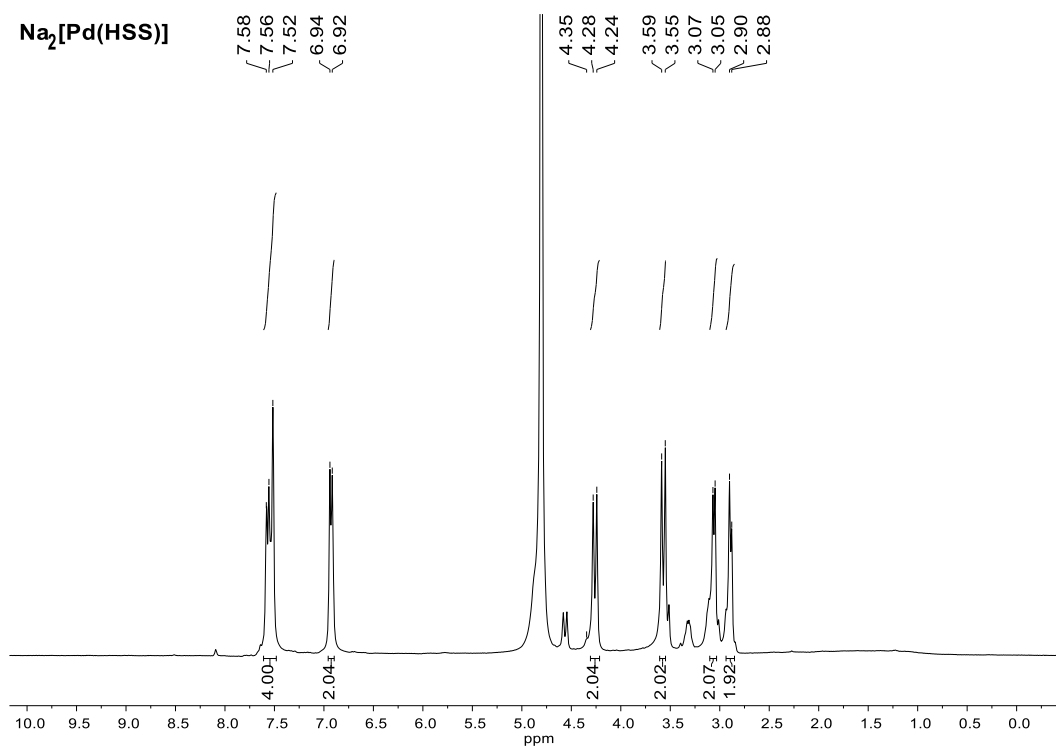


Fig. S22. ¹H NMR spectrum of Na₂[Pd(HSS)] (360 MHz, 298K, D₂O).

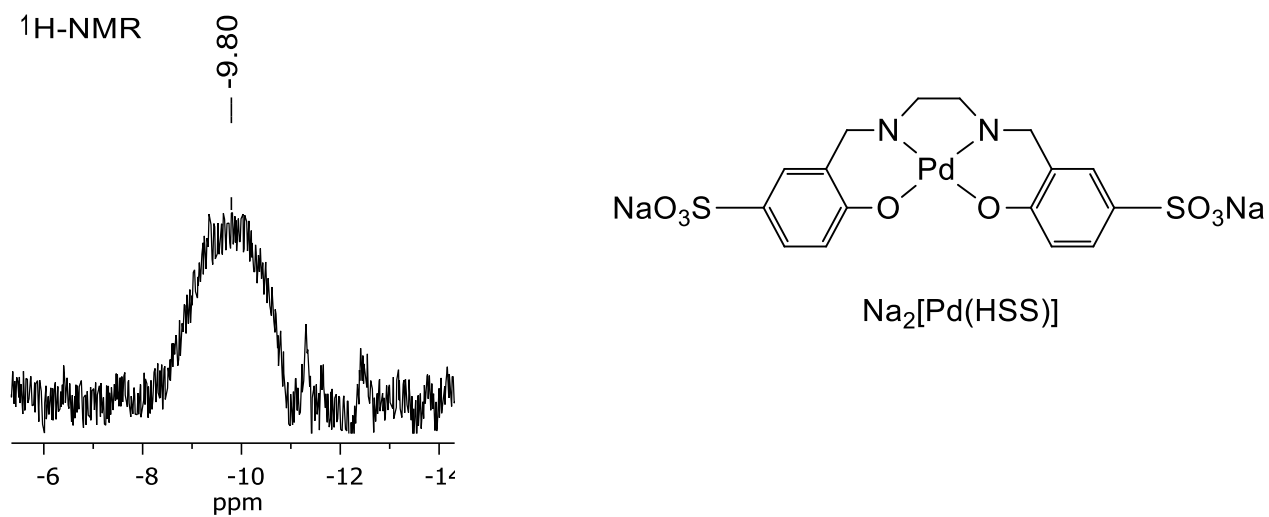


Fig. S23. The hydride region of the ¹H NMR spectrum of Na₂[Pd(HSS)] dissolved in H₂O under 5 bar H₂ (360 MHz, 298K, D₂O).

Simulated spectra (TDDFT and GIAO NMR)

TDDFT calculations showed very similar spectra for the PdHSS complex and its monohydride derivative, and it was found that the monohydride form had almost the same absorption bands with less intensity, which can also explain the experimental results. M06/TZVP/PCM was capable to predict the experimental spectra. We simulated the spectrum of the dihydride species as well, and it was found that a broad absorption appeared around 360 and 500 nm, which were not detected by UV-Vis measurements.

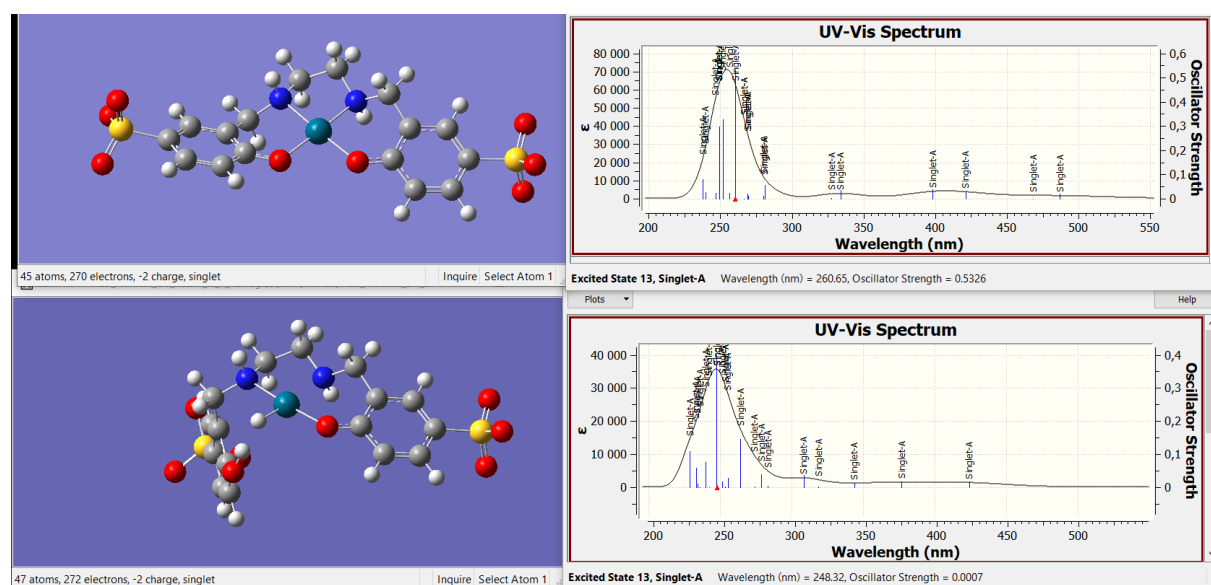


Fig. S24. Simulated UV-Vis spectra of the PdHSS complex (top) and the most favored monohydride form (bottom) at M06/TZVP/PCM theoretical level.

We performed GIAO NMR calculations to analyze the chemical shifts. We found that monohydride species showed in one case an excellent agreement with the experimental one (-9.2 ppm), however, another chemical shifts were a bit different. By using this method, we found that the unfavored dihydride species showed hydride signals around -2 and -3 ppm, which are quite far from the experimental data.

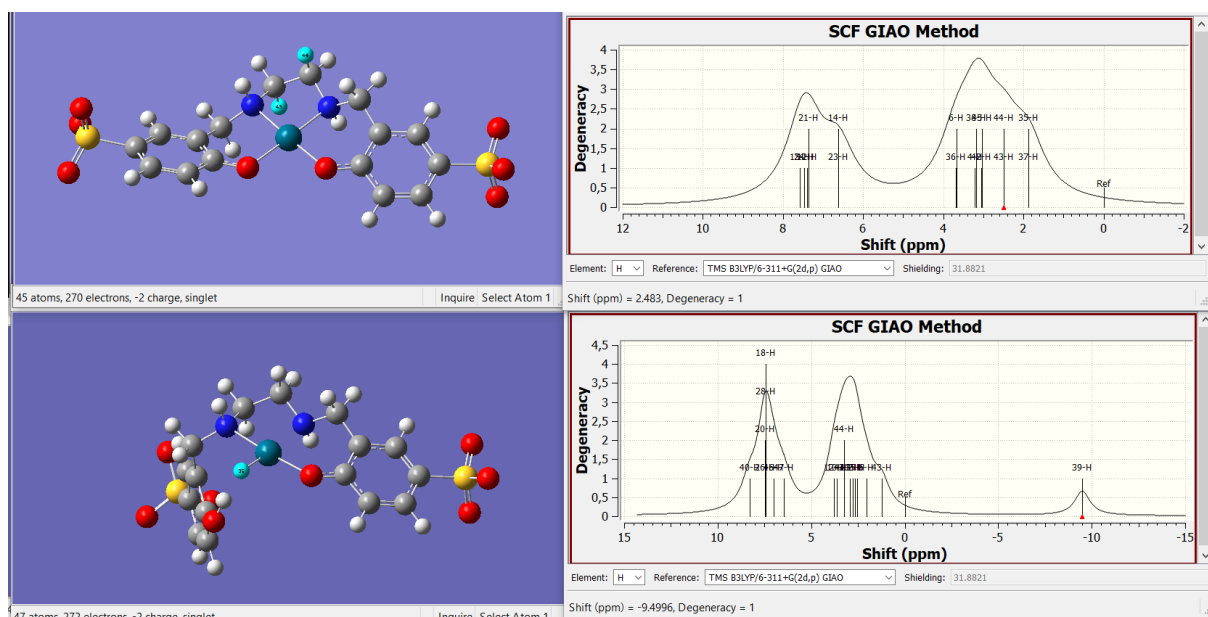


Fig. S25. Simulated spectra of the PdHSS complex (top) and the most favored monohydride form (bottom) at M06/TZVP/PCM theoretical level. Note that calculated chemical shifts are referred to the default B3LYP/6-311+G(d,p) theoretical level in vacuo. The calculated chemical shift of TMS at M06/TZVP/PCM, however; was -0.3 referred to the default B3LYP/6-311+G(d,p) theoretical level *in vacuo*. It means that the correct calculated value is -9.2 ppm for the hydride signal which is in very good agreement with the experimental one (-9.8 ppm).

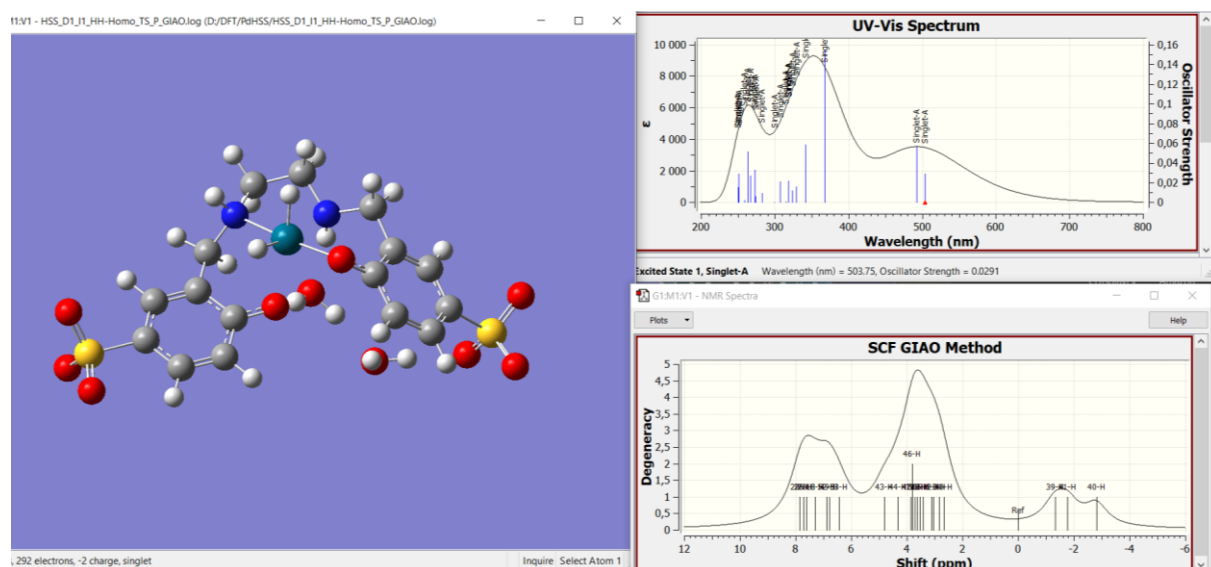


Fig. S26. The simulated UV-Vis and NMR spectra of the dihydride species (with two explicit water molecules) at M06/TZVP/PCM do not show agreement with the experimental data.

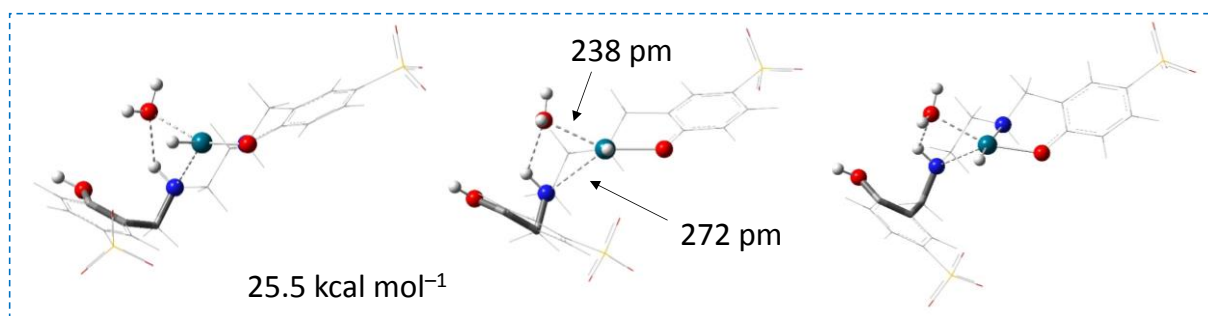


Fig. S27. The transition state of the amino group's substitution by water molecule in the hydride product in different orientations.

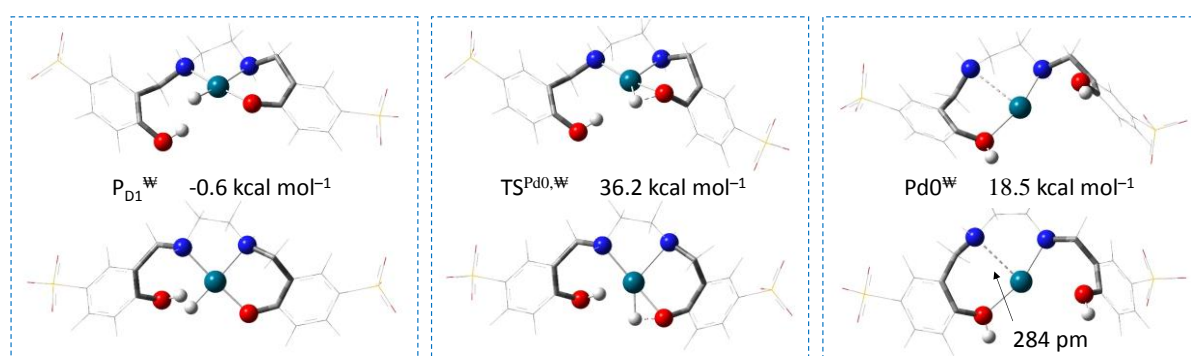


Fig. S28. Hydride transfer to the coordinated phenolate oxygen atom starting from the product of the D1 mechanism without explicit water molecules (^W). Structures are in different orientations while energies are referred to as the [(R,R)^λ + H₂] system where hydrogen has a similar orientation relative to the (R,R)^λ isomer as in Fig. S5. APT charges showed a tendency of decrease from positive to negative values (+0.917 → -0.015 → -0.028) proving the formation of Pd(0) to which one oxygen and one nitrogen were bonded weakly (224 pm and 215 pm, respectively) while two other donor atoms were far (Pd-N1 was 284 pm, Pd-O2 was 363 pm).

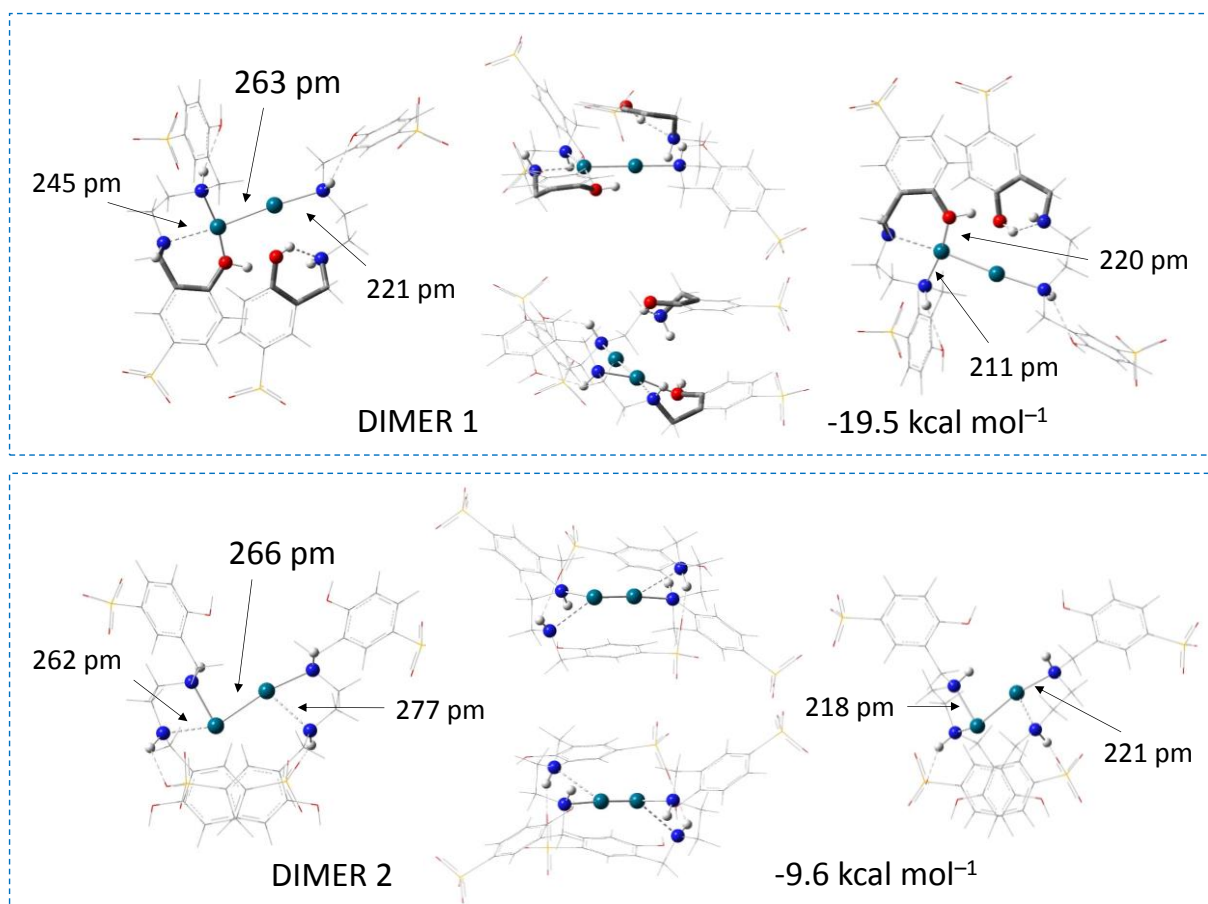


Fig. S29. Possible dimers of the product of Pd0^W. Relative Gibbs free energies are referred to as the sum of the energies of two separate Pd0^W complexes. Note that DIMER 2 had several imaginary frequencies of rotational modes.

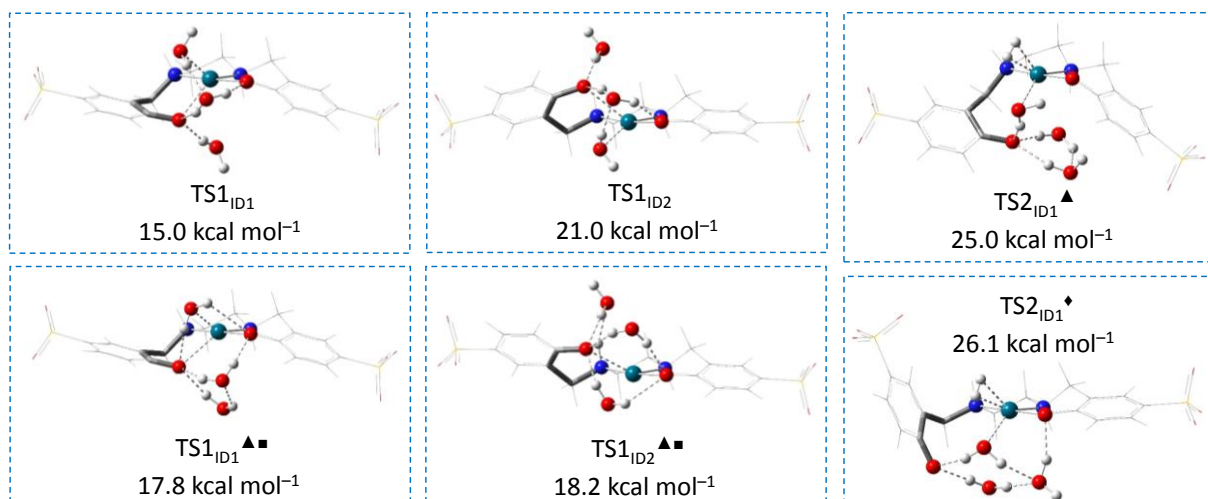


Fig. S30. Optimized TS1 structures of both ID1 and ID2 mechanisms, and the two TS2_{ID1}.

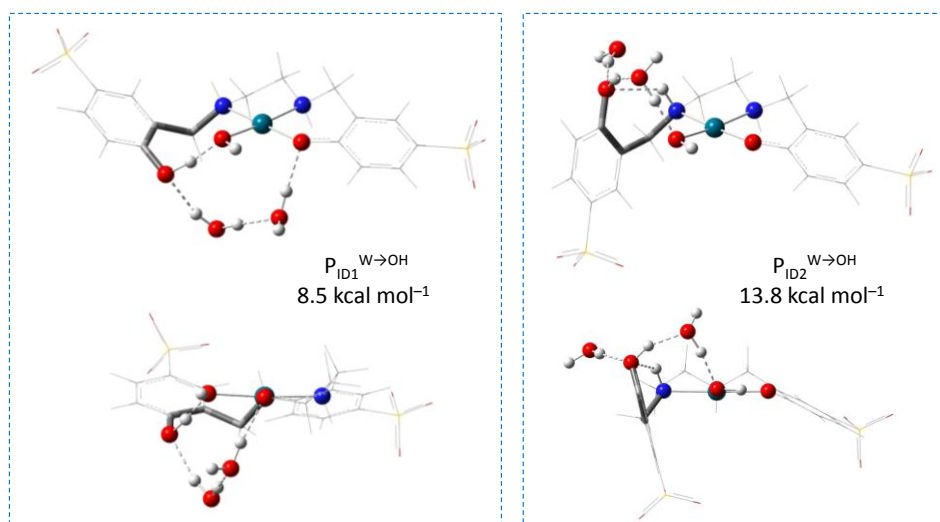


Fig. S31. Hydroxo complexes formed from $I1_{ID1}$ and $I1_{ID2}$ after proton transfer from the coordinated water molecule to the dissociated phenolate arm.

Indirect mechanism of the (R,S) diastereomer

In the case of (R,S)^λ the trigonal shape of ID1 stayed through the whole process while for (R,S)^δ TS2_{ID1} and TS3_{ID1} could not be found. The trigonal–diamond-shaped relation is less pronounced in (R,S)^λ while the inverted (R,R)^δ showed a square motif instead of diamond with energy identical to the trigonal isomer. In the case of (R,S)^δ only ID2[■] was studied because the equivalent (R,R)^δ showed a “fast” trigonal to square rearrangement similar to (R,R)^δ while the (R,S)^λ isomer behaves like (R,R)^λ. Table S10 shows all energies of the ID mechanisms.

Table S10. Relative energies in kcal mol⁻¹ of the stationary points of the indirect mechanism for the PdHSS complex.

| | (R,R) | (R,R) ^{EI} | (R,S) ^λ | (R,S) ^δ |
|-----------------------------------|-------------|-------------------------|-------------------------|--------------------|
| TS1 _{ID1} | 15.0 | n.c. | 21.0 | 17.0 |
| TS1 _{ID1} ^{▲■} | 17.8 | 20.5 | 22.7 | n.c. |
| TS1 _{ID1} ^{hs} | 13.3 | 20.4 | 17.3 | 17.3 |
| TS1 _{ID2} | 21.0 | 31.9 | 21.2 | – |
| TS1 _{ID2} ^{▲■} | 18.2 | 30.6 | 20.0 | 23.1 |
| I1 _{ID1} | 10.8 | n.c. | 17.7 | 11.3 |
| I1 _{ID1} ^{▲■} | 14.3 | 14.2 | 18.5 | n.c. |
| I1 _{ID1} ^{hs} | 4.7 | 8.1 | 16.4 | 11.5 |
| I1 _{ID2} | 10.2 | 11.4 | 9.2 | – |
| I1 _{ID2} ^{▲■} | 7.9 | 11.5 | 13.5 | 7.2 |
| TS2 _{ID1} [▲] | 25.0 | 25.4 | 29.8 | – |
| TS2 _{ID1} [♦] | 26.1 | 25.4[■] | 30.0 | 27.9 |
| TS2 _{ID2} ^{▲→■} | 22.7 | 24.8 | 24.8 | – |
| TS2 _{ID2} [■] | 19.8 | 25.2 | 20.8 | 20.2 |
| I2 _{ID1} [▲] | 16.6 | 17.4 | 16.2 | – |
| I2 _{ID1} [♦] | 20.1 | 19.1 [■] | 19.1 ^M | 18.6 |
| I2 _{ID2} ^{▲→■} | 18.2 | 16.7 | 17.8 | – |
| I2 _{ID2} [■] | 15.6 | 19.0 | 17.8 | 16.2 |
| TS3 _{ID1} [▲] | 25.5 | 25.1 | 27.1 | – |
| TS3 _{ID1} [♦] | 22.2 | 21.8[■] | 19.0^D | 24.9 |
| TS3 _{ID2} ^{▲→■} | 21.2 | 21.1 | 23.0 | – |
| TS3 _{ID2} [■] | 22.2 | 24.9 | 21.6 | 18.6 |
| P _{ID1} ^{▲/■} | -3.5 | -4.8 | 4.9 | – |
| P _{ID1} [♦] | -3.3 | -2.7 | -0.2 ^D | -2.8 |
| P _{ID2} ^{▲→■} | -1.5 | 1.2 | 1.4 | – |
| P _{ID2} [■] | -0.9 | 2.3 | 0.4 | -0.6 |

■ square motifs instead of diamond

♦ that it is an I1_{ID1}[♦]

^M coordinated H₂ seems to be in the middle of the diamond-shape “from above”

^D direct proton transfer to O1

Substituted derivatives of PdHSS (R,R) isomer

The six derivatives were investigated: (R,R)^λ-PhCl, (R,R)^λ-PhMe, (R,R)^λ-PhOMe, (R,R)^λ-Ph*t*Bu, (R,R)^λ-Me and (R,R)^λ-NMe. The calculated APT charges show agreements with chemical aspects in most cases compared to (R,R)^λ as reference, see Table S11. The methyl group on C7 influences the charge of C7, but slightly decreases the charge of C8 and Pd as well. The methyl group on N1, however, a bit surprisingly has only a significant effect on the nitrogen but barely increases the charge of Pd. Methyl group on C3 of phenyl ring shows the effect on C2 and not surprisingly on C3 the most but also on C1, C4, and C6. In the case of methoxy substituted *o*-vanillin based salan derivative, the partial charge of C3 changed sign while the rest of the atoms are similar to those of the methyl-substituted derivative. Interestingly, this effect is larger than in the chlorine derivative showing that the positive mesomeric effect has a large influence on atomic charges. *Tert*-butyl derivative shows similar charges to the methyl one predicting a larger effect on steric properties.

Table S11. APT charges of the (R,R)^λ and its substituted derivatives. Bold numbers show significant differences compared to the non-substituted form.

| Atom | (R,R) ^λ | (R,R) ^λ -Me _{C7} | (R,R) ^λ -NMe _{N1} | (R,R) ^λ -PhMe _{C3} | (R,R) ^λ PhOMe _{C3} | (R,R) ^λ PhCl _{C3} | (R,R) ^λ -PhtBu _{C3} |
|------|--------------------|---|--|---|---|--|--|
| Pd | 1.51 | 1.49 | 1.53 | 1.52 | 1.53 | 1.54 | 1.54 |
| N1 | -0.64 | -0.64 | -0.71 | -0.65 | -0.65 | -0.63 | -0.66 |
| O1 | -1.57 | -1.57 | -1.56 | -1.55 | -1.58 | -1.53 | -1.59 |
| C1 | -0.34 | -0.34 | -0.34 | -0.30 | -0.24 | -0.26 | -0.30 |
| C2 | 1.19 | 1.18 | 1.17 | 1.09 | 1.07 | 1.07 | 1.09 |
| C3 | -0.37 | -0.36 | -0.36 | -0.21 | 0.52 | 0.19 | -0.26 |
| C4 | 0.16 | 0.15 | 0.16 | 0.12 | -0.07 | 0.04 | 0.09 |
| C5 | -0.68 | -0.67 | -0.69 | -0.65 | -0.56 | -0.67 | -0.65 |
| C6 | 0.18 | 0.17 | 0.20 | 0.12 | 0.02 | 0.16 | 0.12 |
| C7 | 0.46 | 0.53 | 0.47 | 0.47 | 0.47 | 0.44 | 0.48 |
| C8 | 0.31 | 0.29 | 0.30 | 0.31 | 0.31 | 0.31 | 0.32 |

An interesting point is to compare the methyl-substituted derivatives since both electronic and atomic parameters are the same. We found that the most stable form is $(R,R)^\lambda$ -PhMe, followed by $(R,R)^\lambda$ -Me—where both methyl groups are axial i.e. almost perpendicular to the plane of the complex—has higher energy by 1.8 kcal mol⁻¹ while $(R,R)^\lambda$ -NMe is much less favored ($\Delta G = 14.1$ kcal mol⁻¹). Inverted forms are higher in energy by 6.7, 6.6, and 7.0 kcal mol⁻¹, respectively. Note that there are two other isomers of $(R,R)^\lambda$ -Me where methyl groups are both equatorial and axial-equatorial which are 4.8 and 2.5 kcal mol⁻¹ less favored than $(R,R)^\lambda$ -Me. All structures are represented in Fig. S29 and S30.

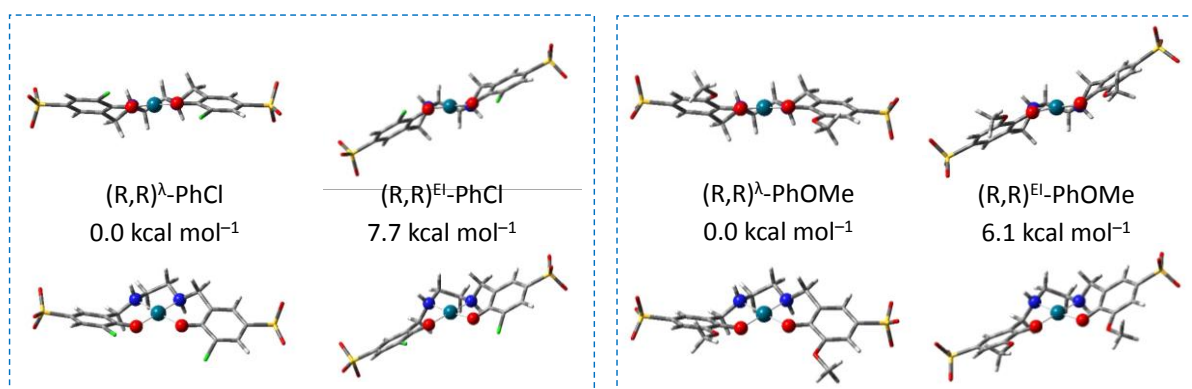


Fig. S32. Optimized structures of PdHSS derivatives: $(R,R)^\lambda$ isomer and the inverted form of chloro- and methoxy-substituted complexes.

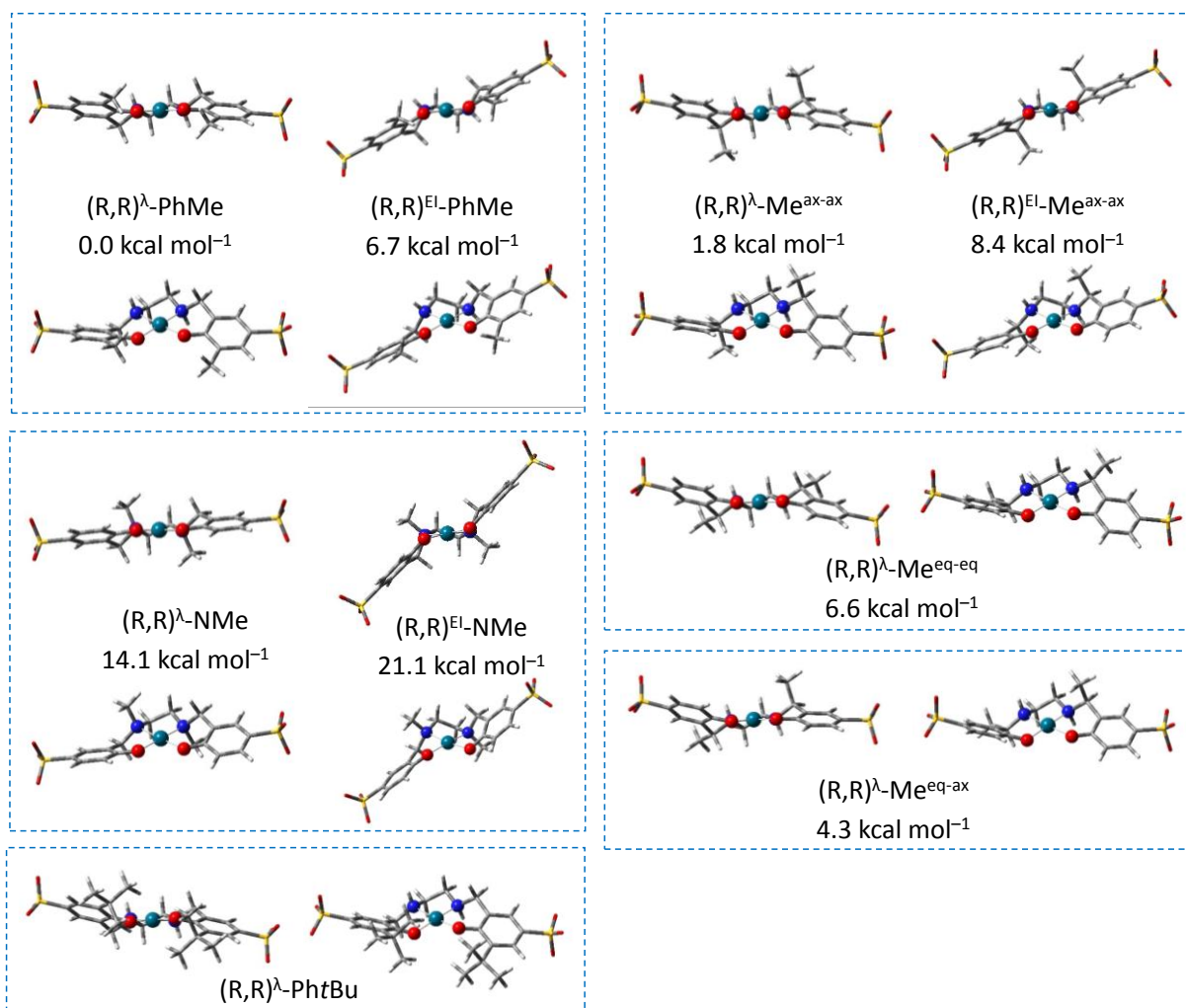


Fig. S33. Optimized structures of PdHSS derivatives: $(R,R)^\lambda$ isomer and the inverted form of methyl-substituted complexes at different positions, and $(R,R)^\lambda$ isomer of *tert*-butyl derivative. Energies are referred to as the most stable methyl-derivative. Superscript ax-ax, eq-eq and ax-eq refers to the position of the methyl groups at C7 and C16 atoms, respectively.

We studied four direct pathways (D1, D1^{hs}, D1^{El}, and D2) in the case of six (R,R)^λ derivatives. We found that (R,R)-NMe showed a preference for the D1 pathway but was very unfavored in the D2 pathway relative to the (R,R) due to the steric hindrance of a methyl group on the nitrogen atom. (R,R)-PhCl was favored in all cases, while (R,R)-PhOMe was unfavored in both pathways compared to (R,R), but only D2 was significantly worse than (R,R). (R,R)-Me, (R,R)-PhMe and (R,R)-Ph*t*Bu were less favored in D1 but more preferred in D2. All energies are in Table S12.

Only ID2 was studied due to the higher relative energies of ID1 in non-substituted forms. ID2 is unfavored for (R,R)-NMe like D2 but we did not study ID1 for this species, and for (R,R)-Ph*t*Bu there was no ID mechanism studied. On the other hand, the energy of TS1_{ID2}^{▲■} of (R,R)-PhCl and (R,R)-PhMe was smaller than TS1_{ID1}^{hs*} giving a relatively stable I1_{ID2}^{▲■}. Since water orientations can be changed easily, relative energies of I1_{ID2} of (R,R)-PhMe and I1_{ID2}[■] of (R,R)-PhCl can compete with arm rotated species regarding the population of species although the last proton transfer step (TS3_{ID2}[■] and TS3_{ID2}^{▲→■}) is higher in energy by 2.5-3.0 kcal mol⁻¹ than TS1_{ID1}^{hs*}. The results are collected in Table S13. The motifs of oxygen atoms showed transitions as follows: in (R,R)-Me ▲ stayed except the product, while in (R,R)-NMe neither ▲ nor ■ is relevant due to loss of -NH group and the larger steric effect of methyl group, however, in (R,R)-PhCl motifs were very similar to (R,R), in (R,R)-PhMe ▲ unit destroyed in the beginning but finally it turned to ■ not as fast as in (R,R)-PhOMe, see Table 14.

In addition, we found that (R,R)-PhCl showed lower activation barriers in every case, while (R,R)-PhOMe was less preferred in all cases. Other species did not show significant differences compared to (R,R)^λ, however, sterically substituents can play an important role in different reactions.

Table S12. Relative energies in kcal mol⁻¹ of the stationary points of the direct mechanism of the PdSS and the substituted PdHSS (R,R) complexes.

| | PdSS [*] ^λ and ^δ | (R,R) | (R,R) -Me | (R,R) -NMe | (R,R) -PhCl | (R,R) -PhMe | (R,R) -PhOMe | (R,R) -Ph <i>t</i> Bu |
|----------------------------------|--|--------------------------|-------------------------------------|--------------------------|--------------------|--------------------|--------------------------|--------------------------|
| TS1 _{D1} | – | 19.2 | 25.0 | – | c.p. | c.p. | c.p. | n.c. |
| TS1 _{D1} [▲] | 27.3^λ | 20.3 | – | 18.9 | 19.5 | 22.2 | 21.2 | 21.8 |
| TS1 _{D1} ^{EI▲} | 24.3^δ | 23.6 | 25.8 | 22.1 | 22.1 | 21.8 | 24.0 | n.c. |
| TS1 _{D1} ^{hs} | – | 20.7 | 21.2 | 21.6 | 19.2 | 19.7 | 19.6 | n.c. |
| TS1 _{D1} ^{hs*} | – | 18.1^{**} | 19.8 | – | 16.5 | 18.7 | 20.5^{**} | n.c. |
| TS1 _{D2} | * | 24.5 | 23.8^{**} | 33.1^{**} | 20.6 | 22.9 | 25.8 | 22.6 |
| I1 _{D1} | – | 16.7 → [▲] | 25.1 ^f → [▲] | – | n.c. | n.c. | n.c. | n.c. |
| I1 _{D1} [▲] | 27.8 ^{λ,f} | 19.2 | – | 19.9 ^f | 16.7 | 18.4 | 18.9 | 17.4 |
| I1 _{D1} ^{EI▲} | 23.8 ^δ | 18.4 | 23.2 | 21.3 | 16.9 | 17.1 | 21.0 | n.c. |
| I1 _{D1} ^{hs} | – | 17.8 ^{Hr} | 19.3 ^{Hr} | 19.9 | 15.9 ^{Hr} | 15.3 ^{Hr} | 19.3 ^{Hr} | n.c. |
| I1 _{D1} ^{hs*} | – | – | 16.5 | – | 14.1 | 15.7 | – | n.c. |
| I1 _{D2} | * | 18.2 | – | – | 16.8 | 17.5 | 20.8 | 21.4 |
| I1 _{D2} ^W | * | 17.5 | – | – | 17.8 | 18.3 | 20.5 | 21.4 |
| TS2 _{D1} [▲] | 27.9^λ | 20.0 | 24.0 | 18.9 | 18.1 | 19.8 | 20.8 | 19.7 |
| TS2 _{D1} ^{EI▲} | 24.3^δ | 22.7 | 27.0 | 21.6 | 21.4 | 21.7 | 23.5 | n.c. |
| TS2 _{D1} ^{hs} | – | – | – | 15.4^W | – | – | – | n.c. |
| TS2 _{D1} ^{hs*} | – | – | 16.5 | – | 13.9 | 15.9 | – | n.c. |
| TS2 _{D2} | * | 20.5 | – | – | 20.2 | 20.6 | 28.3 | 20.6 |
| TS2 _{D2} ^W | * | 25.0 | – | – | 23.0 | 25.0 | 27.8 | 25.4 |
| P _{D1} | 12.3 ^λ | 1.6 (-1.1) | 4.9 | 0.8 (-0.2) | -1.0 (0.4) | 1.3 (0.3) | 2.8 (0.04) | 0.2 |
| P _{D1} ^{EI} | 13.2 ^δ | -0.4 [▲] | 6.4 | 3.2 | 0.6 | 1.7 | 2.6 | n.c. |
| P _{D1} ^{hs} | – | – | – | -1.0 | – | – | – | n.c. |
| P _{D1} ^{hs*} | – | -2.0 | -0.3 | – | -0.9 | -2.0 | -1.4 | n.c. |
| P _{D2} | * | 3.3 | 6.3 | 1.0 ^W | 3.5 | 3.9 | 6.4 ^W | 2.8 ^W |
| P _{D2} ^W | * | 2.7 (1.6) | – | – | 1.5 (1.2) | 2.3 (0.5) | 4.2 (3.5) | 3.0 (-0.1) |

* there is only one direct and indirect mechanism

** concerted process

→[▲] in the next stationary point, there is a rearrangement to trigonal

^W water rearrangement

^W no water bridge → it is P_{D2}

^D direct proton transfer to O1

^f it is a very flat PES where E_{el} proves that rel. the energy of TS is higher than the minimum.

^{Hr} H-bond reorientation causes concerted proton transfer → no TS2_{D1}^{hs} and P_{D1}^{hs} ≡ P_{D1}^{hs*}

n.c. not calculated

c.p. convergence problem

Table S13. Relative energies in kcal mol⁻¹ of the stationary points of the indirect mechanism of the PdSS and the substituted PdHSS (R,R) complexes.

| | PdSS ^λ | PdSS ^δ | (R,R) ^λ | (R,R) ^λ -Me | (R,R) ^λ -NMe | (R,R) ^λ -PhCl | (R,R) ^λ -PhMe | (R,R) ^λ -PhOMe |
|-----------------------------------|-------------------|-------------------|--------------------|---------------------------|----------------------------|-----------------------------|-----------------------------|------------------------------|
| TS1 _{ID2} | 18.9 | 23.5 | 21.0 | 25.0 | – | 18.2 | 17.0 | 21.9 |
| TS1 _{ID2} ^{▲■} | 23.9 | 20.9 | 18.2 | 19.7 | 27.5 | 17.5 | 15.8 | n.c. |
| I1 _{ID2} | 18.1 | 22.3 | 10.2 | 21.2 | – | 6.4 | 4.8 | 13.1 |
| I1 _{ID2} ^{▲■} | 23.3 | 17.3 | 7.9 | 13.7 | 13.4 | 6.4 ^W | 6.4 ^W | n.c. |
| TS2 _{ID2} ^{▲→■} | – | – | 22.7 | 24.0 | 27.6[~] | 19.2 | 20.0 | 24.3 |
| TS2 _{ID2} [■] | – | – | 19.8 | 22.6 | – | 17.4 | 19.4 | 23.7 |
| I2 _{ID2} ^{▲→■} | – | – | 16.7 | 20.3 | 22.2 [~] | 14.9 | 16.9 | 18.1 |
| I2 _{ID2} [■] | – | – | 15.6 | 17.2 | – | 12.9 | 13.6 | 18.9 |
| TS3 _{ID2} ^{▲→■} | – | – | 21.2 | 24.3 | 27.9[~] | 19.1 | 21.7 | 21.5 |
| TS3 _{ID2} [■] | – | – | 22.2 | 24.3 | – | 19.4 | 21.8 | 25.2 |
| P _{ID2} ^{▲→■} | – | – | -1.5 | 1.1 | 3.6 [~] | 1.4 | -1.7 | 2.0 |
| P _{ID2} [■] | – | – | -0.9 | 0.5 | – | -1.4 | -1.6 | 2.9 |

[~] chain water orientation

^W water rearrangement

n.c. not calculated

Table 14. Representation of the changes in the H-bond networks during the ID2 mechanism. □ symbol represents the pseudo-square H-bond network which is a transition between trigonal and square motifs.

| | (R,R) ^λ | (R,R) ^δ | (R,S) ^λ | (R,R) ^λ -Me | (R,R) ^λ -PhCl | (R,R) ^λ -PhMe | (R,R) ^λ -PhOMe |
|-----------------------------------|--------------------|--------------------|--------------------|---------------------------|-----------------------------|-----------------------------|------------------------------|
| I1 _{ID2} ^{▲→■} | ▲ | ▲ | →▲ | →▲ | ▲ | ▲→□ | ▲→□ |
| TS2 _{ID2} ^{▲→■} | ▲ | ■ | ▲ | ▲ | ▲ | □ | □ |
| I2 _{ID2} ^{▲→■} | ▲ | ■ | ▲ | ▲ | ▲ | □ | ■ |
| TS3 _{ID2} ^{▲→■} | ▲→□ | ■ | ▲→□ | ▲ | ▲→□ | □ | ■ |
| P _{ID2} ^{▲→■} | □ | ■ | □ | ■ | □ | ■ | ■ |

Hydride formation in the reaction of PdSS and H₂

PdSS is analogous to the (R,S) isomers of PdHSS due to the equivalence of the λ and δ conformers, see Fig. 2. Checking the TS1_D structures, the most relevant structural parameters are the dihedral angles (β_1 , β_2 and β_3) of the phenolate arm involving the Pd–N1–C1–C7–C2–O1 unit: -11° , -31° and 3° for TS1_D of the PdSS ^{λ} and -2° , -22° and 0° for TS1_D of the PdSS ^{δ} showing smaller changes in them compared to the parameters of the PdSS complex: 0° , -5° and 0° , indicating that the δ pathway is the more favored. The whole process is strongly endergonic, PdSS hydride complexes are around 10-15 kcal mol⁻¹ higher in energy than PdHSS hydride complexes due to the non-bending phenolate arm of PdSS. On the other hand, activation barriers are closer energetically, especially δ conformers (1-2 kcal mol⁻¹), while λ isomers show somewhat larger differences (7-8 kcal mol⁻¹), see Table S11. TS1_{ID} showed much lower energies than TS1_D presuming the non-preference of hydrogen coordination in contrast to water coordination. However, during studying the second step of the ID mechanism for PdSS three different cases were found: 1) water left completely the inner coordination sphere, and TS went to the TS1 of direct mechanism; 2) dissociated phenolate stayed almost perpendicular to the central chelate resulting an sp³ nitrogen which is very unfavored for the imine group (ΔG is over 50 kcal mol⁻¹); 3) dissociated phenolate turned completely resulting high energy TS2 (ΔG is over 30 kcal mol⁻¹), however, this should be blocked in reality. Some structures are represented in Fig. S34.

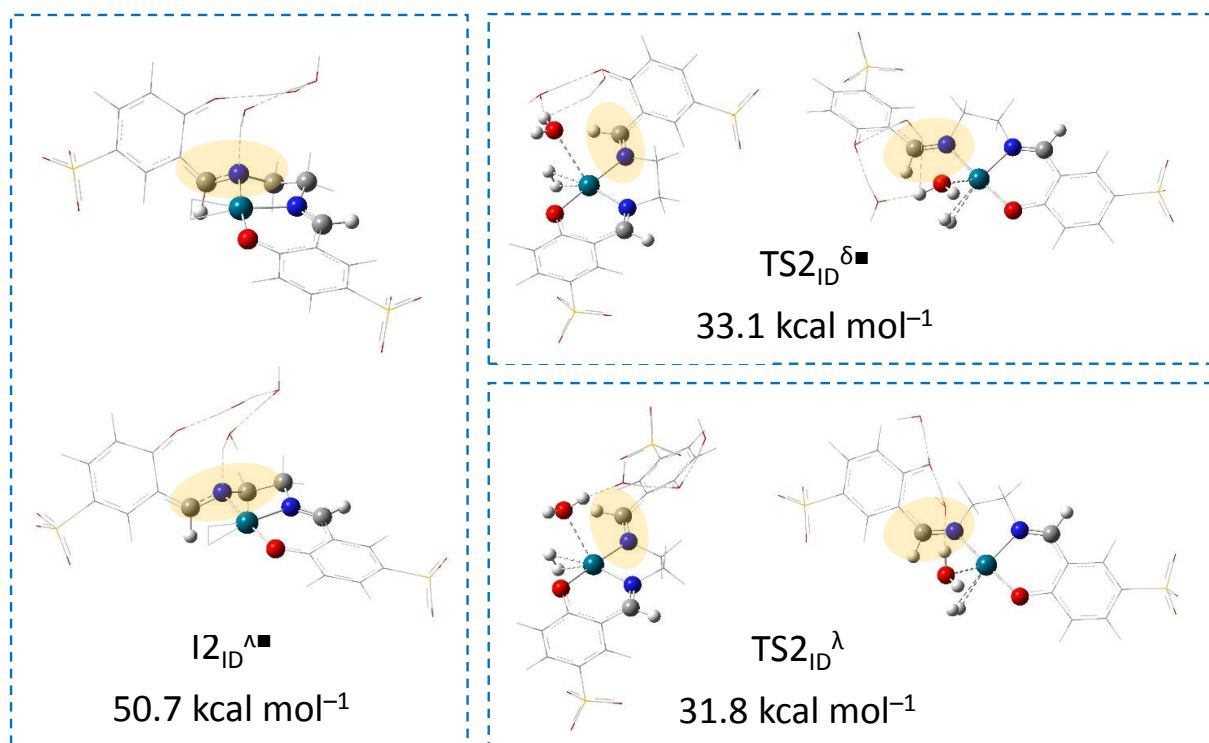


Fig. S34. Strange orientations of the imine group in the ID mechanism of PdSS. Shaded ovals show the sp^3 nitrogen in $I2_{ID}^{\lambda\delta}$, and the completely turned imine group in two cases of $TS2_{ID}$. The latter one should be blocked in the normal case due to the double bond of the imine group, however, these structures were found by optimizations generated from amino groups of the salan ligand.

Cartesian coordinates

Abbreviations:

RR – (R,R) isomer

RS – (R,S) isomer

EI – ethylene inversion

hs – half stepped

s – stepped

TS – transition state

R – reactant

P – product

I1 – intermediate 1 (\equiv TS1_P)

Htr – hydrogen transfer (proton transfer)

no2W – no explicit water molecules

noH2 – omitted non-coordinating H₂

D1, D2, ID1, ID2 – direct 1, direct 2, indirect 1, indirect 2

Hbond-reor – H-bond reorientation

W-reor – water reorientation

HH-Homo – hemolytic dissociation of coordinated hydrogen

CH, NH – H-transfer to carbon or nitrogen atom

HOphen – H-transfer to the coordinated phenolate oxygen

Number of atoms: 45

Name: RR

electronic energy: E(SCF) = -2254.86269581

ZPE corrected energy: E(ZPE) = -2254.538784

Gibbs free energy: E(G) = -2254.597371 a.u.

(Hartree)

| | | | |
|----|-------------|-------------|-------------|
| N | -1.38978800 | 1.76423500 | -0.07155300 |
| N | 1.38000700 | 1.76981800 | 0.06163800 |
| C | -2.48437700 | 1.42338100 | -1.00122000 |
| H | -3.12931100 | 2.29757100 | -1.14415100 |
| C | 2.47824900 | 1.42919600 | 0.98702400 |
| H | 2.00904000 | 1.19917600 | 1.95059100 |
| C | -3.29836300 | 0.27597800 | -0.48899400 |
| C | -2.69955100 | -0.95296600 | -0.10949000 |
| C | -4.67992100 | 0.41510000 | -0.42755200 |
| C | -3.56270800 | -1.99928000 | 0.28277200 |
| C | -5.49939200 | -0.62588700 | -0.03648600 |
| H | -5.13282900 | 1.36017300 | -0.71192000 |
| C | -4.92787200 | -1.84226500 | 0.32244000 |
| H | -3.10564100 | -2.94264800 | 0.56224800 |
| H | -5.56157600 | -2.66800800 | 0.63042200 |
| C | 3.29549500 | 0.28699500 | 0.46869600 |
| C | 2.70090400 | -0.94321400 | 0.08877800 |
| C | 4.67689000 | 0.43205200 | 0.40384400 |
| C | 3.56726900 | -1.98523000 | -0.30970900 |
| C | 5.49844100 | -0.60246000 | 0.00292100 |
| H | 5.12735100 | 1.37927500 | 0.68398400 |
| C | 4.93133300 | -1.82336500 | -0.34966400 |
| H | 3.11300500 | -2.92908000 | -0.59207700 |
| H | 5.56666900 | -2.64507000 | -0.66628200 |
| O | -1.41402500 | -1.19901200 | -0.11976300 |
| O | 1.41631600 | -1.19426800 | 0.10035100 |
| S | -7.27098300 | -0.40252300 | 0.10471100 |
| S | 7.27707500 | -0.40527400 | -0.07251400 |
| O | 7.66217500 | -0.69055700 | -1.48542600 |
| O | 7.84166400 | -1.40759400 | 0.87745900 |
| O | 7.55679700 | 1.00079100 | 0.33279900 |
| O | -7.58894900 | 0.85692700 | -0.62501100 |
| O | -7.55969600 | -0.31038500 | 1.56639400 |
| O | -7.88824600 | -1.60920700 | -0.51702800 |
| H | -1.78032700 | 1.85004300 | 0.86786000 |
| H | -2.01206500 | 1.19948900 | -1.96470600 |
| H | 1.76816000 | 1.86289600 | -0.87807900 |
| H | 3.11996500 | 2.30535200 | 1.13232800 |
| Pd | -0.00162000 | 0.25331600 | -0.00761800 |
| C | 0.63323500 | 3.00234300 | 0.39776100 |
| C | -0.64821000 | 3.00232200 | -0.39900900 |
| H | -1.25527200 | 3.88741200 | -0.19112100 |
| H | -0.43388900 | 2.98221200 | -1.47144000 |
| H | 0.41895900 | 2.97376600 | 1.47001800 |
| H | 1.23647200 | 3.89150400 | 0.19613400 |

53

RR_hs_TS2, E(SCF) = -2408.90328284, E(ZPE)

= -2408.512140, E(G) = -2408.573646 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.21011400 | -1.15248200 | -2.71782600 |
| H | -0.11470400 | -2.10670600 | -3.14342500 |
| H | 0.08929300 | -0.38165900 | -3.48439200 |
| C | 1.63173700 | -1.22936400 | -2.23323300 |
| H | 2.32960300 | -1.45785000 | -3.04380800 |
| H | 1.92644400 | -0.27469200 | -1.79103200 |
| N | 1.71717000 | -2.26082900 | -1.17061400 |
| N | -0.64907600 | -0.86597300 | -1.55279200 |
| C | 3.02878300 | -2.27073100 | -0.44856400 |
| H | 2.99925600 | -3.12890800 | 0.22579200 |
| C | -2.09089000 | -1.00790100 | -1.81519400 |
| H | -2.26650700 | -2.06599000 | -2.04360600 |
| C | 3.30834600 | -1.00879700 | 0.29542200 |
| C | 2.77565400 | -0.80137600 | 1.59534400 |
| C | 4.11262700 | -0.03801300 | -0.29094500 |
| C | 3.07178600 | 0.43776500 | 2.21635800 |
| C | 4.38458500 | 1.15985000 | 0.34180800 |
| H | 4.53062900 | -0.21631500 | -1.27822400 |
| C | 3.85936700 | 1.38970100 | 1.61105600 |
| H | 4.06628600 | 2.32689900 | 2.11893200 |
| C | -2.92012100 | -0.53939400 | -0.66167300 |
| C | -2.70795400 | -1.02289700 | 0.64683800 |

| | | | |
|----|-------------|-------------|-------------|
| C | -3.95167600 | 0.36231400 | -0.89731300 |
| C | -3.57496400 | -0.57866100 | 1.66320800 |
| C | -4.79931500 | 0.77979100 | 0.11453600 |
| H | -4.11088400 | 0.74135900 | -1.90192600 |
| C | -4.60043900 | 0.30131800 | 1.40467900 |
| H | -5.25598600 | 0.62440400 | 2.20713400 |
| O | 2.03952600 | -1.67797400 | 2.21317600 |
| O | -1.76301900 | -1.88072200 | 0.99248700 |
| S | 5.44608600 | 2.38736700 | -0.41617700 |
| S | -6.11690900 | 1.94821300 | -0.20378100 |
| O | -7.36518300 | 1.28197700 | 0.26586700 |
| O | -6.10418000 | 2.19472800 | -1.67221200 |
| O | -5.78929500 | 3.16474400 | 0.59361000 |
| O | 5.70683600 | 1.90699700 | -1.80234000 |
| O | 6.68036500 | 2.43849400 | 0.24071900 |
| O | 4.68474200 | 3.66929300 | -0.37732100 |
| H | 0.49195600 | -3.20498000 | 1.17456100 |
| H | 1.03604800 | -2.56322700 | 1.43881300 |
| H | 1.61182300 | -3.17590400 | -1.60977500 |
| H | 3.80946000 | -2.45275100 | -1.19580700 |
| H | -0.43867400 | 0.06816600 | -1.16575500 |
| H | -2.35069500 | -0.43313800 | -2.71103200 |
| Pd | -0.01579500 | -2.09040800 | -0.03553900 |
| H | 2.66587400 | 0.61126600 | 3.20842300 |
| H | -3.41087000 | -0.95830800 | 2.66656300 |
| H | 0.58332500 | -0.68934700 | 2.75842700 |
| O | -0.25264000 | -0.17842100 | 2.73617700 |
| H | -0.88048000 | -0.81698800 | 2.35585600 |
| H | 0.06110500 | 0.82606000 | 1.15926700 |
| O | 0.27717900 | 1.24979900 | 0.30267300 |
| H | 1.23333500 | 1.36763800 | 0.34331100 |

53

RR_hs_TS2, E(SCF) = -2408.90294216, E(ZPE)

= -2408.511744, E(G) = -2408.574045 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.22444700 | -1.13437100 | -2.73036500 |
| H | -0.09683200 | -2.08527300 | -3.16584700 |
| H | 0.09988000 | -0.35580100 | -3.48851700 |
| C | 1.64723600 | -1.21072100 | -2.24892000 |
| H | 2.34358900 | -1.43202400 | -3.06274100 |
| H | 1.94214000 | -0.25830600 | -1.80176500 |
| N | 1.73912400 | -2.24941400 | -1.19339600 |
| N | -0.63508200 | -0.86416000 | -1.56147500 |
| C | 3.04750500 | -2.24825800 | -0.46620300 |
| H | 3.03057700 | -3.11593900 | 0.19609500 |
| C | -2.07646400 | -0.99984900 | -1.82845700 |
| H | -2.25290700 | -2.05333600 | -2.07622200 |
| C | 3.30089700 | -0.99262300 | 0.29753000 |
| C | 2.75711100 | -0.81713000 | 1.60130100 |
| C | 4.08136900 | 0.00411800 | -0.26808100 |
| C | 3.02510500 | 0.41370900 | 2.24277100 |
| C | 4.32340000 | 1.20143500 | 0.38638300 |
| H | 4.50402600 | -0.15754100 | -1.25788300 |
| C | 3.79508700 | 1.39602300 | 1.65521900 |
| H | 3.98464500 | 2.33076300 | 2.17133400 |
| C | -2.90644400 | -0.55362800 | -0.66707100 |
| C | -2.70293900 | -1.07740000 | 0.63094400 |
| C | -3.92263300 | 0.36516100 | -0.87752400 |
| C | -3.57154500 | -0.66045100 | 1.65226600 |
| C | -4.76774400 | 0.76187800 | 0.14580500 |
| H | -4.06691400 | 0.77037600 | -1.87563200 |
| C | -4.58765700 | 0.24297100 | 1.41719200 |
| H | -5.24868100 | 0.55165300 | 2.21892700 |
| O | 2.03648300 | -1.72284400 | 2.19650900 |
| O | -1.76220600 | -1.95015800 | 0.94910100 |
| S | 5.36380900 | 2.43207800 | -0.39596300 |
| S | -6.03020000 | 1.99267200 | -0.18981300 |
| O | -5.29571400 | 3.25889000 | -0.47539300 |
| O | -6.86444500 | 2.06986800 | 1.04074700 |
| O | -6.78291100 | 1.49491600 | -1.37642000 |
| O | 4.76404000 | 2.68500400 | -1.73852700 |
| O | 6.72254400 | 1.82265000 | -0.49336400 |
| O | 5.32625900 | 3.62621300 | 0.49366700 |
| H | 0.50334800 | -3.25363600 | 1.12478900 |
| H | 1.03926600 | -2.61174100 | 1.40505500 |
| H | 1.64811200 | -3.16209700 | -1.64048600 |
| H | 3.83425500 | -2.40623200 | -1.21257400 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.42376700 | 0.06330400 | -1.15808400 |
| H | -2.33486200 | -0.40825300 | -2.71365600 |
| Pd | -0.00297800 | -2.11470300 | -0.06608800 |
| H | 2.61528600 | 0.56215000 | 3.23735200 |
| H | -3.41824600 | -1.07250900 | 2.64455300 |
| H | 0.57267400 | -0.77795200 | 2.75335300 |
| O | -0.27616200 | -0.28684800 | 2.76006900 |
| H | -0.89558900 | -0.92767800 | 2.37060500 |
| H | 0.01401600 | 0.76150700 | 1.20852100 |
| O | 0.19897600 | 1.22129300 | 0.36283000 |
| H | 1.14162000 | 1.41684500 | 0.40889000 |

47

RR_hs_D1_no2W_P, E(SCF) = -2256.04496876,
E(ZPE) = -2255.701944, E(G) = -2255.761853
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.14806800 | -1.05085000 | 2.60532900 |
| H | 0.17718200 | -2.01727400 | 3.00384400 |
| H | -0.07739000 | -0.31769900 | 3.41564700 |
| C | -1.56159700 | -1.13940200 | 2.08708200 |
| H | -2.27250900 | -1.36055600 | 2.88990500 |
| H | -1.85015600 | -0.18505300 | 1.63880600 |
| N | -1.64465200 | -2.17408500 | 1.02463900 |
| N | 0.73942400 | -0.71172600 | 1.48275100 |
| C | -2.96750500 | -2.19335600 | 0.33994400 |
| H | -2.95550800 | -3.05119900 | -0.33563600 |
| C | 2.17194700 | -0.92565900 | 1.73680800 |
| H | 2.29402300 | -1.99698900 | 1.94060300 |
| C | -3.31114200 | -0.93394400 | -0.39366000 |
| C | -2.87850700 | -0.68138000 | -1.70103100 |
| C | -4.16530900 | -0.01070600 | 0.20795600 |
| C | -3.31045000 | 0.46388500 | -2.36933800 |
| C | -4.57987200 | 1.12599800 | -0.45301000 |
| H | -4.52886200 | -0.19574800 | 1.21446400 |
| C | -4.15304200 | 1.36219400 | -1.75377900 |
| H | -4.48184400 | 2.25202600 | -2.28004900 |
| C | 3.00630400 | -0.49339600 | 0.57052200 |
| C | 2.82409600 | -1.05352100 | -0.72034500 |
| C | 4.01351800 | 0.44173900 | 0.77726100 |
| C | 3.71277900 | -0.63806200 | -1.73703700 |
| C | 4.86469200 | 0.83263600 | -0.23855900 |
| H | 4.14730100 | 0.87114100 | 1.76561800 |
| C | 4.71040900 | 0.27902700 | -1.50528300 |
| H | 5.37429900 | 0.57656800 | -2.31147900 |
| O | -2.09502600 | -1.52525300 | -2.40466100 |
| O | 1.92316000 | -1.95111400 | -1.03363100 |
| S | -5.68506400 | 2.30668300 | 0.33400800 |
| S | 6.15972500 | 2.03654900 | 0.04286400 |
| O | 5.87117500 | 3.17898400 | -0.87275900 |
| O | 7.43966400 | 1.35101000 | -0.30131000 |
| O | 6.07274400 | 2.41222800 | 1.48229700 |
| O | -5.97351800 | 1.75639700 | 1.68580400 |
| O | -6.88758000 | 2.37364200 | -0.54210200 |
| O | -4.93252400 | 3.59151200 | 0.37075900 |
| H | -0.33646200 | -3.14037200 | -1.13031400 |
| H | -1.50381500 | -2.04973700 | -1.82346200 |
| H | -1.54483600 | -3.08451600 | 1.47290600 |
| H | -3.73772900 | -2.38148500 | 1.09658600 |
| H | 0.59225200 | 0.25862000 | 1.20967200 |
| H | 2.48758500 | -0.38451700 | 2.63738900 |
| Pd | 0.12235900 | -2.05322500 | -0.07986000 |
| H | -2.96250500 | 0.62637500 | -3.38285600 |
| H | 3.57820700 | -1.07274000 | -2.72208000 |

47

RR_hs_D1_no2W_R, E(SCF) = -2256.02791272,
E(ZPE) = -2255.688640, E(G) = -2255.748215
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.38474400 | -2.62264900 | 1.83191800 |
| H | 0.69562600 | -3.57118200 | 1.38277300 |
| H | 0.73538500 | -2.61171000 | 2.86675000 |
| C | -1.11708100 | -2.47411200 | 1.74477600 |
| H | -1.62694900 | -3.26785000 | 2.29881300 |
| H | -1.44578700 | -1.51096900 | 2.14649100 |
| N | -1.47689500 | -2.51400500 | 0.31025000 |
| N | 1.01642800 | -1.53591600 | 1.04917600 |
| C | -2.90678100 | -2.28907500 | -0.02245700 |

| | | | |
|----|-------------|-------------|-------------|
| H | -3.10320200 | -2.90486800 | -0.90566300 |
| C | 2.41370700 | -1.77358400 | 0.64446000 |
| H | 2.39036200 | -2.60790100 | -0.06655100 |
| C | -3.25439900 | -0.86802700 | -0.33090200 |
| C | -2.58252600 | -0.20670200 | -1.39017100 |
| C | -4.29584600 | -0.23773500 | 0.33036100 |
| C | -3.04109200 | 1.06881500 | -1.76306600 |
| C | -4.71345000 | 1.02862000 | -0.04293000 |
| H | -4.80652600 | -0.74290900 | 1.14494500 |
| C | -4.08950900 | 1.67431200 | -1.10295800 |
| H | -4.42242200 | 2.66333900 | -1.46302100 |
| C | 3.03487700 | -0.54207300 | 0.05634700 |
| C | 2.40500700 | 0.22399000 | -0.95926100 |
| C | 4.29918100 | -0.17485600 | 0.50654100 |
| C | 3.12975600 | 1.31814400 | -1.48380000 |
| C | 4.98037100 | 0.90109800 | -0.02514900 |
| H | 4.77271700 | -0.75316000 | 1.29415200 |
| C | 4.38428600 | 1.64965300 | -1.03562400 |
| H | 4.90868700 | 2.49884900 | -2.49884900 |
| O | -1.56616700 | -0.75799300 | -2.02345900 |
| O | 1.21800600 | -0.00027900 | -1.46338600 |
| S | -6.06703100 | 1.84271400 | 0.80682700 |
| S | 6.60558400 | 1.36067600 | 0.56920500 |
| O | 6.47531700 | 2.75275900 | 1.08970700 |
| O | 7.51321900 | 1.28492400 | -0.61268200 |
| O | 6.95247800 | 0.37414600 | 1.63043100 |
| O | -6.47814700 | 0.92084000 | 1.90231300 |
| O | -7.13326300 | 2.04046800 | -0.21750100 |
| O | -5.52006400 | 3.13625100 | 1.30863800 |
| H | -0.31761200 | -3.92568600 | -2.55379700 |
| H | -0.83467300 | -3.38325900 | -2.54704400 |
| H | -1.21586000 | -3.43233700 | -0.04686400 |
| H | -3.53252900 | -2.67029600 | 0.79079100 |
| H | 0.97925900 | -0.67248600 | 1.59254500 |
| H | 2.99892400 | -2.09727400 | 1.51256800 |
| Pd | -0.16438400 | -1.20533700 | -0.59517500 |
| H | -2.53648300 | 1.56865800 | -2.58301500 |
| H | 2.65064700 | 1.89790300 | -2.26710300 |

47

RR_hs_D1_no2W_TS, E(SCF) = -2256.00216901,
E(ZPE) = -2255.663952, E(G) = -2255.722966
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.11185900 | -1.57337200 | 2.54474400 |
| H | 0.23209700 | -2.58565300 | 2.77417700 |
| H | 0.04521000 | -0.95007100 | 3.42925600 |
| C | -1.55070300 | -1.56985400 | -2.10673500 |
| H | -2.21752400 | -1.94521600 | 2.88779400 |
| H | -1.86925700 | -0.55514800 | 1.85168100 |
| N | -1.67367000 | -2.39138200 | 0.87864400 |
| N | 0.70011000 | -1.07635700 | 1.41153600 |
| C | -2.98998200 | -2.22516200 | 0.18762400 |
| H | -3.00886600 | -2.98721200 | -0.59623100 |
| C | 2.15812000 | -1.26191900 | 1.56820400 |
| H | 2.32938800 | -2.34344200 | 1.59182700 |
| C | -3.20668000 | -0.86738200 | -0.38301200 |
| C | -2.49537700 | -0.49819200 | -1.56813500 |
| C | -4.11848200 | 0.00057200 | 0.19905000 |
| C | -2.79393500 | 0.78924500 | -2.09947600 |
| C | -4.37152600 | 1.24889600 | -0.34327500 |
| H | -4.64724200 | -0.29953300 | 1.10043500 |
| C | -3.70517000 | 1.63045900 | -1.50849400 |
| H | -3.90487700 | 2.60547300 | -1.94453800 |
| C | 2.91780400 | -0.58849300 | 0.47128700 |
| C | 2.64025600 | -0.86894300 | -0.88639200 |
| C | 3.93920100 | 0.29586000 | 0.79613300 |
| C | 3.43982800 | -0.24214400 | -1.86277800 |
| C | 4.71357600 | 0.89209900 | -0.17910800 |
| H | 4.14616500 | 0.51636300 | 1.83866900 |
| C | 4.45886900 | 0.61453900 | -1.51804100 |
| H | 5.06124900 | 1.08005800 | -2.29192300 |
| O | -1.64183800 | -1.27719200 | -2.11833200 |
| O | 1.70840500 | -1.69783000 | -1.29913700 |
| S | -5.58691400 | 2.34371800 | 0.37251500 |
| S | 6.03186200 | 2.02913000 | 0.25083200 |
| O | 5.64203900 | 3.34798800 | -0.32655600 |
| O | 7.26530200 | 1.47822300 | -0.38011700 |

| | | | |
|----|-------------|-------------|-------------|
| O | 6.09427800 | 2.04185800 | 1.73864300 |
| O | -5.96126000 | 1.75013000 | 1.68890300 |
| O | -6.73482300 | 2.38652600 | -0.58377100 |
| O | -4.92599400 | 3.67605900 | 0.50648000 |
| H | -0.17860900 | -3.62973200 | -1.47536300 |
| H | -0.69439200 | -3.12044700 | -1.76644700 |
| H | -1.59002200 | -3.37251600 | 1.14521600 |
| H | -3.77434800 | -2.46278900 | 0.91576800 |
| H | 0.51049100 | -0.08165400 | 1.27386100 |
| H | 2.46550300 | -0.85284100 | 2.53686500 |
| Pd | 0.01574400 | -2.03559000 | -0.26800900 |
| H | -2.27204500 | 1.08844600 | -3.00369200 |
| H | 3.22606900 | -0.46166400 | -2.90303400 |

53

RR_hs_D1_TS1_02, E(SCF) = -2408.90203266,
E(ZPE) = -2408.510010, E(G) = -2408.571780
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.23088500 | -1.16133500 | -2.72093600 |
| H | -0.08929100 | -2.11304800 | -3.15341400 |
| H | 0.11479200 | -0.38369900 | -3.48149300 |
| C | 1.65111100 | -1.23595600 | -2.22957000 |
| H | 2.35462700 | -1.45586500 | -3.03907200 |
| H | 1.94331000 | -0.28331700 | -1.78411900 |
| N | 1.73562800 | -2.26998900 | -1.17330400 |
| N | -0.63243900 | -0.88139500 | -1.55608300 |
| C | 3.04632800 | -2.27283000 | -0.44406400 |
| H | 3.01651100 | -3.13303800 | 0.22760400 |
| C | -2.07010600 | -1.01562500 | -1.82681400 |
| H | -2.24834400 | -2.07073300 | -2.06791800 |
| C | 3.31460600 | -1.01219400 | 0.30326300 |
| C | 2.77665500 | -0.81469700 | 1.60381900 |
| C | 4.10958200 | -0.02906900 | -0.27922000 |
| C | 3.05833200 | 0.42912700 | 2.23233700 |
| C | 4.36761600 | 1.16770300 | 0.36154400 |
| H | 4.53255400 | -0.20196300 | -1.26279500 |
| C | 3.83387100 | 1.38918700 | 1.62573000 |
| H | 4.03008000 | 2.32762500 | 2.13865600 |
| C | -2.90404700 | -0.55409000 | -0.67252300 |
| C | -2.69916000 | -1.05221900 | 0.62858100 |
| C | -3.92999200 | 0.35941500 | -0.90554700 |
| C | -3.57210800 | -0.61539200 | 1.64519600 |
| C | -4.77161200 | 0.76647800 | 0.10653800 |
| H | -4.08288200 | 0.74772300 | -1.90754400 |
| C | -4.58761300 | 0.27589100 | 1.39355500 |
| H | -5.24797200 | 0.58899700 | 2.19638500 |
| O | 2.05074200 | -1.70089500 | 2.21989400 |
| O | -1.76305600 | -1.92009900 | 0.96804300 |
| S | 5.36312000 | 2.43856800 | -0.41048200 |
| S | -6.06725200 | 1.97682600 | -0.18993400 |
| O | -5.62641400 | 3.23483800 | 0.52565000 |
| O | -7.32341000 | 1.38548900 | 0.39997200 |
| O | -6.12889000 | 2.14305000 | -1.68427400 |
| O | 5.83390300 | 1.86805400 | -1.70788300 |
| O | 6.48110700 | 2.72122900 | 0.53769100 |
| O | 4.46208200 | 3.61578600 | -0.58855800 |
| H | 0.48462800 | -3.25968600 | 1.15357100 |
| H | 1.01650700 | -2.61975700 | 1.42217800 |
| H | 1.63925200 | -3.18395700 | -1.61480000 |
| H | 3.82778300 | -2.44776000 | -1.18684500 |
| H | -0.41904800 | 0.05017300 | -1.16168400 |
| H | -2.32322700 | -0.42806400 | -2.71917000 |
| Pd | -0.00633300 | -2.11712200 | -0.04814300 |
| H | 2.64975900 | 0.59285800 | 3.22170400 |
| H | -3.41336800 | -1.01162200 | 2.64648100 |
| H | 0.58498800 | -0.73238500 | 2.74865100 |
| O | -0.25099300 | -0.22979200 | 2.73256100 |
| H | -0.87959300 | -0.86598800 | 2.34966900 |
| H | 0.06612900 | 0.78521300 | 1.17126600 |
| O | 0.25845300 | 1.22524700 | 0.31478300 |
| H | 1.20360500 | 1.40966100 | 0.35528900 |

53

RR_hs_D1_TS1_P, E(SCF) = -2408.89557488,
E(ZPE) = -2408.505619, E(G) = -2408.570276
a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.13190200 | -0.93060100 | -2.61106500 |
|---|------------|-------------|-------------|

| | | | |
|----|-------------|-------------|-------------|
| H | -0.13961600 | -1.87475400 | -3.09257000 |
| H | 0.02036700 | -0.12944600 | -3.34710600 |
| C | 1.52745700 | -0.98057200 | -2.05396600 |
| H | 2.27697500 | -1.15592500 | -2.83129100 |
| H | 1.77141300 | -0.03696900 | -1.55967000 |
| N | 1.58090500 | -2.04902700 | -1.02692200 |
| N | -0.79535000 | -0.71850900 | -1.47935300 |
| C | 2.86152600 | -2.07624200 | -0.24581300 |
| H | 2.70851000 | -2.80090200 | 0.55743600 |
| C | -2.21932300 | -0.88994400 | -1.82195000 |
| H | -2.35386400 | -1.94201000 | -2.09796900 |
| C | 3.31281900 | -0.75583300 | 0.28187800 |
| C | 2.56151000 | -0.08732900 | 1.28711900 |
| C | 4.48960100 | -0.19863200 | -0.20091000 |
| C | 3.08416900 | 1.14298300 | 1.76234000 |
| C | 4.97072600 | 1.00395300 | 0.28424100 |
| H | 5.04973300 | -0.71457400 | -0.97581300 |
| C | 4.25655000 | 1.67220300 | 1.27591800 |
| H | 4.62832800 | 2.61700000 | 1.66232900 |
| C | -3.11810000 | -0.47961700 | -0.69976100 |
| C | -2.96095200 | -1.00704600 | 0.59839600 |
| C | -4.15165400 | 0.41448500 | -0.95334800 |
| C | -3.88565000 | -0.62261500 | -0.62253000 |
| C | -5.04820200 | 0.77841200 | 0.03139800 |
| H | -4.26815900 | 0.83068500 | -1.94902800 |
| C | -4.91276100 | 0.24980400 | 1.30938600 |
| H | -5.61361900 | 0.52927700 | 2.08965400 |
| O | 1.43826600 | -0.55399800 | 1.72163200 |
| O | -2.01585900 | -1.86150000 | 0.95098300 |
| S | 6.49574900 | 1.71078900 | -0.32931900 |
| S | -6.37859700 | 1.93429500 | -0.30500600 |
| O | -6.14235000 | 3.10130800 | 0.59213900 |
| O | -7.63785600 | 1.20964500 | 0.02906300 |
| O | -6.26906000 | 2.27872800 | -1.74945000 |
| O | 6.97878900 | 0.79181800 | -1.39914700 |
| O | 7.42438100 | 1.77856100 | 0.83789300 |
| O | 6.14678500 | 3.06707700 | -0.84606000 |
| H | 0.13904200 | -3.39557000 | 1.09890300 |
| H | 0.47076900 | -2.76702400 | 1.48648900 |
| H | 1.51284000 | -2.94702300 | -1.50642100 |
| H | 3.63215800 | -2.47849800 | -0.91221300 |
| H | -0.63797800 | 0.21162800 | -1.05131300 |
| H | -2.44145000 | -0.28867800 | -2.70910100 |
| Pd | -0.21926000 | -1.97461900 | 0.01739500 |
| H | 2.52135000 | 1.66131700 | 2.53356900 |
| H | -3.76508000 | -1.03858300 | 2.58115900 |
| H | 0.09446200 | -0.59167800 | 2.93362600 |
| O | -0.77019000 | -0.77119200 | 3.34800500 |
| H | -1.27561700 | -1.18695900 | 2.63169000 |
| H | 0.36112700 | 0.73553700 | 0.98757500 |
| O | -0.12925300 | 1.34970900 | 0.39828300 |
| H | 0.43401800 | 2.12344700 | 0.31399400 |

53

RR_hs_D1_TS1_R, E(SCF) = -2408.91153827,
E(ZPE) = -2408.521709, E(G) = -2408.586954
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.19764700 | -2.82819000 | -1.52722600 |
| H | -0.62762700 | -3.68790700 | -1.00411600 |
| H | -0.41527800 | -2.94234400 | -2.59205200 |
| C | 1.28787700 | -2.75347700 | -1.26578700 |
| H | 1.80008400 | -3.64894800 | -1.62979900 |
| H | 1.73118000 | -1.88210700 | -1.75842100 |
| N | 1.48130300 | -2.59211100 | -0.19354000 |
| N | -0.84672000 | -1.61229400 | -0.98584300 |
| C | 2.88367600 | -2.36131100 | 0.62878100 |
| H | 2.94219800 | -2.73835000 | 1.65302700 |
| C | -2.28041200 | -1.76221200 | -0.71239900 |
| H | -2.36953300 | -2.54323100 | 0.05294700 |
| C | 3.28496600 | -0.92190400 | 0.59965700 |
| C | 2.57904800 | -0.00446500 | 1.41295500 |
| C | 4.35697400 | -0.48843000 | -0.16220200 |
| C | 3.01839700 | 1.32701800 | 1.44996900 |
| C | 4.76575500 | 0.83464300 | -0.12185300 |
| H | 4.89159900 | -1.19031700 | -0.79462000 |
| C | 4.09810900 | 1.73861700 | 0.69419500 |
| H | 4.41939700 | 2.77506000 | 0.72599600 |

| | | | |
|----|-------------|--------------|-------------|
| C | -2.95576600 | -0.49209900 | -0.27334700 |
| C | -2.35176100 | 0.50561000 | 0.52517500 |
| C | -4.29340500 | -0.34351200 | -0.63674700 |
| C | -3.14392000 | 1.60413700 | 0.91754500 |
| C | -5.04923600 | 0.73482800 | -0.23046100 |
| H | -4.76250400 | -1.10327400 | -1.25449200 |
| C | -4.46294300 | 1.72159400 | 0.55428700 |
| H | -5.04389400 | 2.57996600 | 0.87617900 |
| O | 1.52303000 | -0.38991800 | 2.11359600 |
| O | -1.08942100 | 0.52270600 | 0.92271900 |
| S | 6.16030600 | 1.39873600 | -1.10223100 |
| S | -6.76948800 | 0.90053600 | -0.71000300 |
| O | -6.84701700 | 2.14682000 | -1.52482100 |
| O | -7.53479900 | 1.00938800 | 0.56491600 |
| O | -7.10330900 | -0.32475600 | -1.48734600 |
| O | 6.59904000 | 0.22479300 | -1.90654000 |
| O | 7.18992700 | 1.85166500 | -0.12301300 |
| O | 5.64285400 | 2.51862100 | -1.93930900 |
| H | -1.96271600 | -1.94960700 | 2.77354200 |
| H | -1.44926300 | -1.72441300 | 3.26988300 |
| H | 1.13845000 | -3.43261200 | 0.65645700 |
| H | 3.55623000 | -2.96341600 | 0.00927500 |
| H | -0.68465200 | -0.814464900 | -1.61446400 |
| H | -2.78168200 | -2.14057700 | -1.61114200 |
| Pd | 0.19276200 | -1.05517700 | 0.68203500 |
| H | 2.47624100 | 2.02841300 | 2.07586400 |
| H | -2.66729300 | 2.36923300 | 1.52205100 |
| H | 0.57032800 | 0.79588700 | 3.20545800 |
| O | -0.18290000 | 1.36809700 | 3.43862000 |
| H | -0.71234100 | 1.27114500 | 2.62914300 |
| H | -0.18136500 | 1.23181400 | -0.72574800 |
| O | 0.08794200 | 1.16036600 | -1.65743500 |
| H | 1.04915400 | 1.12349100 | -1.62307100 |

53

RR_hs_D1_TS1, E(SCF) = -2408.89143510,
E(ZPE) = -2408.501997, E(G) = -2408.565659
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.07325100 | -1.19466400 | -2.71119900 |
| H | -0.24769100 | -2.17609500 | -3.07216200 |
| H | -0.06973800 | -0.47193200 | -3.51952400 |
| C | 1.50408300 | -1.23102000 | -2.24395200 |
| H | 2.19096500 | -1.51537800 | -3.04634800 |
| H | 1.81092700 | -0.25144500 | -1.86765200 |
| N | 1.59492100 | -2.18891500 | -1.11712500 |
| N | -0.77266400 | -0.84646800 | -1.55181600 |
| C | 2.91528600 | -2.19780200 | -0.42576400 |
| H | 2.84965400 | -2.99025300 | 0.32520700 |
| C | -2.21549700 | -1.06771700 | -1.74512600 |
| H | -2.35440100 | -2.14896800 | -1.85436800 |
| C | 3.28311900 | -0.89066600 | 0.18873700 |
| C | 2.54753600 | -0.40379000 | 1.30077800 |
| C | 4.35441300 | -0.16525500 | -0.31521200 |
| C | 2.98146900 | 0.81779100 | 1.87165400 |
| C | 4.74759400 | 1.02966500 | 0.25840600 |
| H | 4.90162900 | -0.54422200 | -1.17346200 |
| C | 4.05101100 | 1.51696200 | 1.36178300 |
| H | 4.35673900 | 2.45293400 | 1.82018800 |
| C | -3.02653500 | -0.50124900 | -0.62172300 |
| C | -2.73936900 | -0.78943600 | 0.73076800 |
| C | -4.11721600 | 0.30372400 | -0.92977500 |
| C | -3.59994700 | -0.26381300 | 1.71359800 |
| C | -4.94719500 | 0.80865900 | 0.05088800 |
| H | -4.33154800 | 0.53828700 | -1.96766700 |
| C | -4.68532200 | 0.51432300 | 1.38346400 |
| H | -5.33071300 | 0.90472200 | 2.16403600 |
| O | 1.51037800 | -1.02689700 | 1.76873900 |
| O | -1.73185000 | -1.53486100 | 1.14365500 |
| S | 6.12280700 | 1.97039700 | -0.39641700 |
| S | -6.37113600 | 1.81500800 | -0.37073300 |
| O | -6.22586700 | 3.07689900 | 0.40932100 |
| O | -7.56442700 | 1.02436700 | 0.04788900 |
| O | -6.30177500 | 2.02696300 | -1.84306800 |
| O | 6.66156000 | 1.17802100 | -1.53776800 |
| O | 7.09854500 | 2.11184300 | 0.72381600 |
| O | 5.55947600 | 3.28628500 | -0.81968400 |
| H | 0.09290800 | -3.69131100 | 1.25721300 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.53042100 | -3.23861500 | 1.68932000 |
| H | 1.43508700 | -3.12799800 | -1.48430200 |
| H | 3.67370400 | -2.49108500 | -1.16014800 |
| H | -0.60069000 | 0.12541400 | -1.25646000 |
| H | -2.52321900 | -0.59832300 | -2.68647600 |
| Pd | -0.04318100 | -1.85439800 | 0.07991100 |
| H | 2.43102100 | 1.19385500 | 2.72988800 |
| H | -3.38436400 | -0.49380000 | 2.75160600 |
| H | 0.36729400 | -0.68715700 | 3.12567800 |
| O | -0.50520500 | -0.66216500 | 3.56409100 |
| H | -1.07568800 | -1.00046000 | 2.85375800 |
| H | 0.28780900 | 0.58597300 | 1.03599800 |
| O | -0.03539200 | 1.27210700 | 0.42709200 |
| H | 0.71005600 | 1.87459200 | 0.34011900 |

53

RR_hs_D1_TS2_P, E(SCF) = -2408.93222561,
E(ZPE) = -2408.538050, E(G) = -2408.601948
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.25585300 | -1.07447700 | -2.72922400 |
| H | -0.09976300 | -2.01471600 | -3.16390900 |
| H | 0.19344000 | -0.30628100 | -3.50797300 |
| C | 1.67356000 | -1.21853000 | -2.24088400 |
| H | 2.36336800 | -1.44866800 | -3.05882400 |
| H | 1.99852600 | -0.27944100 | -1.78660400 |
| N | 1.74857100 | -2.27268400 | -1.19395300 |
| N | -0.60363200 | -0.75954000 | -1.58206700 |
| C | 3.05897300 | -2.27486100 | -0.48168800 |
| H | 3.06387700 | -3.15341100 | 0.16609700 |
| C | -2.03748900 | -0.89758800 | -1.85030700 |
| H | -2.20575800 | -1.94887600 | -2.11944800 |
| C | 3.33258200 | -1.02148200 | 0.29240300 |
| C | 2.86946100 | -0.82035300 | 1.59644100 |
| C | 4.10490000 | -0.01705000 | -0.28931000 |
| C | 3.18844700 | 0.34987700 | 2.28299200 |
| C | 4.40471900 | 1.14828900 | 0.38523400 |
| H | 4.48909000 | -0.15543800 | -1.29541600 |
| C | 3.94405000 | 1.33334600 | 1.68212900 |
| H | 4.18003800 | 2.24493200 | 2.22054100 |
| C | -2.88213800 | -0.50049800 | -0.67721300 |
| C | -2.70383000 | -1.05926300 | 0.61001600 |
| C | -3.91317800 | 0.41017700 | -0.88512800 |
| C | -3.60392900 | -0.66792600 | 1.62348500 |
| C | -4.78252000 | 0.77422000 | 0.12409800 |
| H | -4.04848400 | 0.84225400 | -1.87191100 |
| C | -4.62253800 | 0.22555900 | 1.39095200 |
| H | -5.29809300 | 0.50366400 | 2.19400200 |
| O | 2.14115800 | -1.73491300 | 2.28228300 |
| O | -1.77188300 | -1.92926800 | 0.94918800 |
| S | 5.34616300 | 2.46140300 | -0.40983600 |
| S | -6.10865200 | 1.94443900 | -0.16386500 |
| O | -5.84821600 | 3.09684900 | 0.74678100 |
| O | -7.36833200 | 1.22548400 | 0.18480400 |
| O | -6.03074700 | 2.31437000 | -1.60475000 |
| O | 5.79646500 | 1.90598500 | -1.71367300 |
| O | 6.46734100 | 2.76822800 | 0.51958800 |
| O | 4.38923900 | 3.59385000 | -0.55066900 |
| H | 0.43548000 | -3.28161600 | 0.94409900 |
| H | 1.60660200 | -2.30248600 | 1.68087800 |
| H | 1.66895900 | -3.17784300 | -1.65568000 |
| H | 3.85096800 | -2.41209600 | -1.22656600 |
| H | -0.38495400 | 0.16609300 | -1.19494100 |
| H | -2.32367000 | -0.29557900 | -2.72227700 |
| Pd | -0.01260700 | -2.15645200 | -0.08518500 |
| H | 2.82133500 | 0.46930600 | 3.29643200 |
| H | -3.46289700 | -1.10177700 | 2.60851600 |
| H | 0.48914000 | -0.68903300 | 2.87730500 |
| O | -0.35059400 | -0.23833400 | 2.70650500 |
| H | -0.88115800 | -0.92076600 | 2.24923800 |
| H | 0.02848700 | 0.84449700 | 1.20227600 |
| O | 0.24758900 | 1.33126700 | 0.38258100 |
| H | 1.18290600 | 1.54139400 | 0.46895600 |

53

RR_hs_Hbond-reor_TS1_P, E(SCF) = -
2408.93222533, E(ZPE) = -2408.538049, E(G)
= -2408.601939 a.u.

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 0.25583800 | -1.07442800 | -2.72934200 | O | -6.52089600 | 0.88132300 | 1.71446200 |
| H | -0.09981100 | -2.01475800 | -3.16380800 | O | -6.91502600 | 2.27928700 | -0.30353800 |
| H | 0.19328700 | -0.30635200 | -3.50819900 | O | -5.23160600 | 2.97673300 | 1.37487900 |
| C | 1.67359100 | -1.21840200 | -2.24112400 | H | -0.27343200 | -4.19135000 | -2.46429800 |
| H | 2.36337000 | -1.44852000 | -3.05908900 | H | -0.79119700 | -3.64959600 | -2.45481600 |
| H | 1.99854900 | -0.27929900 | -1.78685100 | H | -1.24009100 | -3.59698300 | 0.11489500 |
| N | 1.74870900 | -2.27252500 | -1.19414900 | H | -3.55792200 | -2.76644500 | 0.84753000 |
| C | 3.05927400 | -2.27483800 | -0.48230000 | H | -2.58610600 | 1.23400200 | -2.80716000 |
| H | 3.06445400 | -3.15356200 | 0.16526200 | H | -1.23363000 | 1.88597100 | -0.91558700 |
| C | 3.33300600 | -1.02168600 | 0.29207800 | O | -0.30419000 | 2.03313400 | -0.69454300 |
| C | 2.87013600 | -0.27250800 | 1.59631400 | O | 0.17074000 | 1.31025700 | -1.15481500 |
| C | 4.10507100 | -0.01701300 | -0.28951400 | H | 0.02900800 | 1.50167600 | 1.02241600 |
| C | 3.18900500 | 0.34909400 | 2.28307200 | O | 0.30867700 | 1.10973200 | 1.87603600 |
| C | 4.40478100 | 1.14823100 | 0.38528400 | H | -0.40896400 | 1.28550500 | 2.48919800 |
| H | 4.48908400 | -0.15509200 | -1.12957200 | N | 0.96827300 | -1.58755000 | 1.07952600 |
| C | 3.94427100 | 1.33288600 | 1.68227900 | C | 2.37870400 | -1.82120000 | 0.74511300 |
| H | 4.18020100 | 2.24438000 | 2.22087900 | H | 2.41417300 | -2.72115300 | 0.11872600 |
| O | 2.14235400 | -1.73604500 | 2.28214200 | C | 3.00172400 | -0.63573400 | 0.06602600 |
| S | 5.34594100 | 2.46163200 | -0.40964600 | C | 2.37626400 | 0.07510500 | -0.98556600 |
| O | 5.79644100 | 1.90636500 | -1.71348500 | C | 4.27152200 | -0.24802100 | 0.48333300 |
| O | 6.46699000 | 2.76863900 | 0.51985600 | C | 3.08528800 | 1.14822000 | -1.56385100 |
| O | 4.38875900 | 3.59385700 | -0.55048400 | C | 4.95042300 | 0.79657500 | -0.11021300 |
| H | 0.43595100 | -3.28095500 | 0.94433300 | H | 4.75103800 | -0.78517600 | -1.29592200 |
| H | 1.60780500 | -2.30361900 | 1.68078100 | C | 4.34396700 | 1.50377200 | -1.14170400 |
| H | 1.66881600 | -3.17769500 | -1.65582100 | H | 4.86256500 | 2.33351500 | -1.61174400 |
| H | 3.85106900 | -2.41184700 | -1.22743300 | O | 1.17993800 | -0.17787400 | -1.48280500 |
| H | 2.82211500 | 0.46820900 | 3.29663200 | S | 6.58572200 | 1.27697100 | 0.44515900 |
| H | 0.48956800 | -0.68876600 | 2.87673600 | O | 6.45514600 | 2.67691400 | 0.94234900 |
| O | -0.35022000 | -0.23795500 | 2.70666200 | O | 7.46801500 | 1.18370800 | -0.75381900 |
| H | -0.88103700 | -0.92009300 | 2.24921300 | O | 6.95740300 | 0.31125000 | 1.51650100 |
| H | 0.02791200 | 0.84500100 | 1.20169200 | H | 0.85581900 | -0.65767100 | 1.51952600 |
| O | 0.24669800 | 1.33219300 | 0.38222900 | H | 2.93965300 | -2.04424400 | 1.66045500 |
| H | 1.18236400 | 1.54113300 | 0.46780400 | Pd | -0.18163400 | -1.40875900 | -0.59788300 |
| N | -0.60353000 | -0.75930700 | -1.58209200 | H | 2.59534300 | 1.69143700 | -2.36553500 |
| C | -2.03737600 | -0.89697100 | -1.85033500 | | | | |
| H | -2.20584500 | -1.94814000 | -2.11985000 | 53 | | | |
| C | -2.88211100 | -0.50023900 | -0.67715900 | RR_hs_Hbond-reor_TS1, E(SCF) = - | | | |
| C | -2.70369600 | -1.05907800 | 0.61002800 | 2408.89600734, E(ZPE) = -2408.506625, E(G) | | | |
| C | -3.91338100 | 0.41019200 | -0.88501100 | = -2408.569797 a.u. | | | |
| C | -3.60410100 | -0.66828600 | 1.62343900 | C | 0.14067500 | -1.26493500 | -2.62975000 |
| C | -4.78298000 | 0.77374600 | 0.12417300 | H | -0.21893600 | -2.23585600 | -2.98310600 |
| H | -4.04872700 | 0.84236000 | -1.87174600 | H | 0.01750800 | -0.54228200 | -3.44164200 |
| C | -4.62289700 | 0.22500900 | 1.39097000 | C | 1.57028600 | -1.35130000 | -2.17460600 |
| H | -5.29868300 | 0.50269000 | 2.19397600 | H | 2.23857100 | -1.67385300 | -2.97829800 |
| O | -1.77140100 | -1.92865700 | 0.94924000 | H | 1.91730900 | -0.37895600 | -1.81720700 |
| S | -6.10927400 | 1.94381800 | -0.16366100 | N | 1.63656100 | -2.29444200 | -1.03381900 |
| O | -5.84901200 | 3.09613500 | 0.74716100 | C | 2.96402400 | -2.31193300 | -0.35311500 |
| O | -7.36886900 | 1.22466400 | 0.18489300 | H | 2.90853200 | -3.11152400 | 0.38997000 |
| O | -6.03140800 | 2.31394400 | -1.60450500 | C | 3.31045800 | -1.00715200 | 0.27357800 |
| H | -0.38454500 | 0.16635600 | -1.19513600 | C | 2.61966400 | -0.60561400 | 1.44966600 |
| H | -2.32346300 | -0.29462000 | -2.72209800 | C | 4.27946500 | -0.19148300 | -0.29253900 |
| Pd | -0.01229700 | -2.15602400 | -0.08522100 | C | 3.00159800 | 0.63955600 | 2.01463900 |
| H | -3.46296600 | -1.10216500 | 2.60844100 | C | 4.61218600 | 1.02649900 | 0.27277500 |
| | | | | H | 4.78846400 | -0.50999400 | -1.19826000 |
| | | | | C | 3.96591800 | 1.43385600 | 1.43749000 |
| | | | | H | 4.22782800 | 2.38473200 | 1.89240600 |
| | | | | O | 1.68229500 | -1.32780100 | 1.97194600 |
| | | | | S | 5.85353500 | 2.08791700 | -0.45759100 |
| | | | | O | 6.33652300 | 1.38223700 | -1.67819600 |
| | | | | O | 6.91828500 | 2.25532700 | 0.57490000 |
| | | | | O | 5.16637100 | 3.37631600 | -0.76688600 |
| | | | | H | 0.10008500 | -3.76104900 | 1.27963400 |
| | | | | H | 0.55264100 | -3.31720500 | 1.70849000 |
| | | | | H | 1.45869900 | -3.23472800 | -1.38937200 |
| | | | | H | 3.71711800 | -2.58802400 | -1.09968000 |
| | | | | H | 2.50599800 | 0.95883300 | 2.92649600 |
| | | | | H | 0.51119300 | -0.18876200 | 2.58694600 |
| | | | | O | -0.26537500 | 0.41536100 | 2.65935300 |
| | | | | H | -0.97998900 | -0.19537100 | 2.41938800 |
| | | | | H | 0.00887000 | 1.16659300 | 0.96237300 |
| | | | | O | 0.18300500 | 1.46438500 | 0.04368900 |
| | | | | H | 1.13468400 | 1.61336500 | 0.02439200 |
| | | | | N | -0.68589100 | -0.87605600 | -1.46889200 |
| | | | | C | -2.12971900 | -1.06062100 | -1.68506500 |
| | | | | H | -2.28888700 | -2.13625900 | -1.82280200 |
| | | | | C | -2.96324800 | -0.51188900 | -0.57107400 |
| | | | | C | -2.70908800 | -0.82628800 | 0.78098700 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|--|--|--|
| 53 | | | | | | | |
| RR_hs_Hbond-reor_TS1_R, E(SCF) = - | | | | | | | |
| 2408.91518839, E(ZPE) = -2408.526553, E(G) | | | | | | | |
| = -2408.593225 a.u. | | | | | | | |
| C | 0.34484400 | -2.61088000 | 1.94227000 | | | | |
| H | 0.67200900 | -3.59429200 | 1.58875500 | | | | |
| H | 0.67735700 | -2.50064900 | 2.97808200 | | | | |
| C | -1.15612600 | -2.48529100 | 1.82178600 | | | | |
| H | -1.67336500 | -3.23022500 | 2.43322800 | | | | |
| H | -1.49183100 | -1.49054500 | 2.13185700 | | | | |
| N | -1.49544900 | -2.64929600 | 0.39010700 | | | | |
| C | -2.91778800 | -2.43104800 | 0.02520900 | | | | |
| H | -3.10600300 | -3.08613300 | -0.83080600 | | | | |
| C | -3.24798500 | -1.02284700 | -0.35530400 | | | | |
| C | -2.58892400 | -0.43921400 | -1.46921400 | | | | |
| C | -4.25830200 | -0.33179400 | 0.29132000 | | | | |
| C | -3.05696700 | 0.80704400 | -1.92656800 | | | | |
| C | -4.67226800 | 0.91401300 | -0.15382400 | | | | |
| H | -4.75510700 | -0.77772200 | 1.14795000 | | | | |
| C | -4.07672600 | 1.47426000 | -1.27527100 | | | | |
| H | -4.41306900 | 2.43960900 | -1.64066700 | | | | |
| O | -1.57778800 | -1.02890100 | -2.06748500 | | | | |
| S | -5.93665300 | 1.83210600 | 0.72824800 | | | | |

| | | | |
|----|-------------|-------------|-------------|
| C | -4.06067700 | 0.28001000 | -0.89122800 |
| C | -3.60424400 | -0.33471900 | 1.75157200 |
| C | -4.92472900 | 0.75007900 | 0.07694600 |
| H | -4.25245400 | 0.53220000 | -1.92940800 |
| C | -4.69355700 | 0.43233800 | 1.40990400 |
| H | -5.36539600 | 0.79612500 | 2.18090900 |
| O | -1.69400200 | -1.55009700 | 1.21445300 |
| S | -6.34920800 | 1.74959900 | -0.35919500 |
| O | -6.21408500 | 3.01423400 | 0.41828900 |
| O | -7.54252200 | 0.95585900 | 0.05298400 |
| O | -6.26864700 | 1.95724600 | -1.83148600 |
| H | -0.47568200 | 0.09547800 | -1.17999500 |
| H | -2.40888900 | -0.56605700 | -2.62262400 |
| Pd | -0.00217000 | -1.90976100 | 0.16079600 |
| H | -3.41024500 | -0.58813900 | 2.78888800 |

54

RR_hs_ID1_TS1_P_Htr_P, E(SCF) = -
 2484.18510541, E(ZPE) = -2483.784625, E(G)
 = -2483.850000 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.25965300 | -0.70931000 | 2.83028700 |
| H | 0.06360700 | -1.59955200 | 3.37903500 |
| H | -0.16247400 | 0.15129700 | 3.49901500 |
| C | -1.67651400 | -0.85825200 | 2.34031100 |
| H | -2.38598600 | -0.97981400 | 3.16392900 |
| H | -1.95942100 | 0.03471400 | 1.77871300 |
| N | -1.74407200 | -2.01373400 | 1.41270100 |
| N | 0.61393100 | -0.56449800 | 1.65089600 |
| C | -3.02069500 | -2.12433700 | 0.64999800 |
| H | -2.95011200 | -3.04953100 | 0.07545200 |
| C | 2.05024500 | -0.68190700 | 1.94447700 |
| H | 2.21072800 | -1.70140800 | 2.31555500 |
| C | -3.30943200 | -0.94528200 | -0.22694000 |
| C | -2.89289900 | -0.86517500 | -1.56464700 |
| C | -4.04621000 | 0.11589400 | 0.30095400 |
| C | -3.20261200 | 0.27962700 | -2.31022500 |
| C | -4.33608600 | 1.24210400 | -0.43882900 |
| H | -4.40273300 | 0.05848000 | 1.32513900 |
| C | -3.90850400 | 1.32388500 | -1.75882000 |
| H | -4.13261100 | 2.20527300 | -2.35042000 |
| C | 2.89978000 | -0.38794600 | 0.74617500 |
| C | 2.70592800 | -1.04538000 | -0.48986500 |
| C | 3.93717200 | 0.52903000 | 0.87391000 |
| C | 3.59403700 | -0.74504700 | -1.54130500 |
| C | 4.79923300 | 0.80182800 | -0.16953800 |
| H | 4.08404100 | 1.03709100 | 1.82172600 |
| C | 4.61979500 | 0.15855700 | -1.38839600 |
| H | 5.28775800 | 0.36931200 | -2.21767200 |
| O | -2.22427600 | -1.82405700 | -2.21899900 |
| O | 1.75683600 | -1.93023900 | -0.73343100 |
| S | -5.24412900 | 2.61705900 | 0.28063700 |
| S | 6.12651100 | 1.99514600 | 0.00883100 |
| O | 5.80868600 | 3.10576900 | -0.93452900 |
| O | 7.37486000 | 1.27260800 | -0.36918500 |
| O | 6.11054500 | 2.42204500 | 1.43556700 |
| O | -6.44681800 | 2.79900100 | -0.57901600 |
| O | -4.31386700 | 3.77905500 | 0.21635900 |
| O | -5.57382700 | 2.20491600 | 1.67161500 |
| H | -1.71059900 | -2.50707000 | -1.65349900 |
| H | -1.66085300 | -2.86747900 | 1.96427800 |
| H | -3.83391700 | -2.24467000 | 1.37435300 |
| H | 0.41316200 | 0.31886400 | 1.15943800 |
| H | 2.31565600 | 0.00536000 | 2.75599900 |
| Pd | 0.01617500 | -2.00135400 | 0.32200800 |
| H | -2.86899900 | 0.31772700 | -3.34164200 |
| H | 3.43926100 | -1.25177700 | -2.48855700 |
| H | -0.56095500 | -0.89011300 | -2.73739200 |
| O | 0.28237000 | -0.41877700 | -2.63944000 |
| H | 0.83563300 | -1.04827400 | -2.13947000 |
| H | -0.04493200 | 0.79987600 | -1.22909900 |
| O | -0.23114500 | 1.35168800 | -0.44226100 |
| H | -1.16690200 | 1.56618500 | -0.51547000 |
| O | -0.72704400 | -3.41799000 | -0.92030900 |
| H | -0.01259400 | -3.69176400 | -1.50468700 |

54

RR_hs_ID1_TS1_P_Htr_R, E(SCF) = -
 2484.18486562, E(ZPE) = -2483.783242, E(G)
 = -2483.846878 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.26465900 | -0.77583700 | 2.82272400 |
| H | 0.05518000 | -1.67005400 | 3.36605900 |
| H | -0.16239200 | 0.08271600 | 3.49274300 |
| C | -1.67535900 | -0.91338200 | 2.31899000 |
| H | -2.39210800 | -1.05148300 | 3.13331100 |
| H | -1.95675100 | -0.01213300 | 1.76990600 |
| N | -1.73626500 | -2.05101900 | 1.36883700 |
| N | 0.61459200 | -0.62329900 | 1.64597100 |
| C | -3.02068500 | -2.11979500 | 0.59782700 |
| H | -2.97280100 | -3.03195200 | 0.00071000 |
| C | 2.05323700 | -0.71185600 | 1.95023800 |
| H | 2.23260400 | -1.72696400 | 2.32300700 |
| C | -3.29312700 | -0.91811500 | -0.24654300 |
| C | -2.80146000 | -0.81852400 | -1.57755600 |
| C | -4.06222000 | 0.11333200 | 0.28528600 |
| C | -3.07300800 | 0.39172200 | -2.21792200 |
| C | -4.31947800 | 1.27269700 | -0.41929100 |
| H | -4.46399700 | 0.01554900 | 1.29040900 |
| C | -3.81275500 | 1.40681500 | -1.70999700 |
| H | -4.00395000 | 2.31527800 | -2.23568000 |
| C | 2.90432900 | -0.39229900 | 0.76143900 |
| C | 2.73071100 | -1.05418000 | -0.47336600 |
| C | 3.91625800 | 0.55174300 | 0.89289300 |
| C | 3.61320700 | -0.73767700 | -1.52305600 |
| C | 4.77306200 | 0.84347700 | -0.14949700 |
| H | 4.04624500 | 1.06668300 | 1.83942300 |
| C | 4.61622000 | 0.19110400 | -1.36661400 |
| H | 5.28166000 | 0.41749200 | -2.19377300 |
| O | -2.12438100 | -1.75075500 | -2.17148800 |
| O | 1.79874400 | -1.95978400 | -0.71205700 |
| S | -5.31649600 | 2.58581100 | 0.27747900 |
| S | 6.06967300 | 2.07101300 | 0.02941700 |
| O | 5.74898500 | 3.14655000 | -0.95228400 |
| O | 7.34252500 | 1.36702200 | -0.29791900 |
| O | 6.00755800 | 2.53468300 | 1.44304400 |
| O | -6.51310100 | 2.70940800 | -0.60563600 |
| O | -4.46571800 | 3.81104900 | 0.24391700 |
| O | -5.66007700 | 2.15427300 | 1.66172400 |
| H | -1.30629700 | -2.86722600 | -1.56928400 |
| H | -1.67175100 | -2.91503000 | -1.90766300 |
| H | -3.82477100 | -2.24910800 | 1.33154000 |
| H | 0.40019700 | 0.25581600 | 1.14663400 |
| H | 2.28730800 | -0.01761000 | 2.76474300 |
| Pd | 0.05019100 | -2.03513300 | 0.31095700 |
| H | -2.68941500 | 0.48315300 | -3.27950200 |
| H | 3.47525800 | -1.25070200 | -2.46939000 |
| H | -0.58253200 | -0.89033000 | -2.65266800 |
| O | 0.27737600 | -0.41820100 | -2.64952500 |
| H | 0.87422500 | -1.03479700 | -2.19272500 |
| H | -0.03794500 | 0.75690900 | -1.21164100 |
| O | -0.22746800 | 1.29315800 | -0.41339200 |
| H | -1.16767100 | 1.49281200 | -0.48594700 |
| O | -0.64665300 | -3.46309100 | -1.05550800 |
| H | 0.06385400 | -3.71169900 | -1.65798400 |

54

RR_hs_ID1_TS1_P_Htr_TS, E(SCF) = -
 2484.18420790, E(ZPE) = -2483.786472, E(G)
 = -2483.851873 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.24955000 | -0.76396200 | 2.83503300 |
| H | 0.07136000 | -1.66088600 | 3.37356800 |
| H | -0.14073900 | 0.09144200 | 3.50802100 |
| C | -1.66637900 | -0.89822900 | 2.34433000 |
| H | -2.37518500 | -1.03395100 | 3.16604600 |
| H | -1.95089800 | 0.00313700 | 1.79697200 |
| N | -1.73691100 | -2.03748800 | 1.39728200 |
| N | 0.62154800 | -0.61173900 | 1.65250900 |
| C | -3.02388600 | -2.12192500 | 0.63831100 |
| H | -2.97408300 | -3.04234900 | 0.05427900 |
| C | 2.06119100 | -0.72205000 | 1.94088300 |
| H | 2.23114700 | -1.74452700 | 2.29813600 |
| C | -3.30148000 | -0.93411500 | -0.22547900 |
| C | -2.83847600 | -0.85673800 | -1.56222500 |
| C | -4.05203900 | 0.11483100 | 0.30104900 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -3.12553100 | 0.32670800 | -2.28021300 | O | 7.34090600 | 1.36808300 | -0.29668500 |
| C | -4.31916200 | 1.25800500 | -0.42407300 | O | 6.00460000 | 2.53668600 | 1.44260600 |
| H | -4.43296800 | 0.04058500 | 1.31596600 | O | -6.51106400 | 2.71212300 | -0.60514200 |
| C | -3.84613600 | 1.35979700 | -1.72937000 | O | -4.46235300 | 3.81140000 | 0.24430000 |
| H | -4.04779700 | 2.25493700 | -2.30968500 | O | -5.65820600 | 2.15551000 | 1.66190400 |
| C | 2.90349900 | -0.39953100 | 0.74581900 | H | -1.30685200 | -2.86717100 | -1.56958600 |
| C | 2.70556000 | -1.03719800 | -0.49856500 | H | -1.67231100 | -2.91519600 | -1.90777100 |
| C | 3.93439500 | 0.52319300 | 0.88236100 | H | -3.82487500 | -2.24938800 | 1.33108700 |
| C | 3.58176200 | -0.71486100 | -1.55233400 | H | 0.40088800 | 0.25452600 | 1.14683400 |
| C | 4.78584100 | 0.81844400 | -0.16346600 | H | 2.28755900 | -0.02003400 | 2.76542600 |
| H | 4.08428600 | 1.01753600 | 1.83686900 | Pd | 0.05018900 | -2.03605000 | -0.31080100 |
| C | 4.60281900 | 0.19291300 | -1.39087800 | H | -2.68913400 | 0.48307900 | -3.27979900 |
| H | 5.26334300 | 0.42227300 | -2.22114000 | H | 3.47422300 | -1.25008700 | -2.46973600 |
| O | -2.16284700 | -1.80114100 | -2.16585100 | H | -0.58208100 | -0.89184500 | -2.65447200 |
| O | 1.75916400 | -1.92534100 | -0.74483800 | O | 0.27658000 | -0.49145300 | -2.64904300 |
| S | -5.26781300 | 2.60669500 | 0.27908900 | H | 0.87461400 | -1.03532800 | -2.19571200 |
| S | 6.10867700 | 2.01589200 | 0.02475300 | H | -0.03853800 | 0.75550100 | -1.21094300 |
| O | 5.78920300 | 3.12905500 | -0.91459000 | O | -0.22713500 | 1.29159300 | -0.41230300 |
| O | 7.36002700 | 1.29862700 | -0.35271500 | H | -1.16754800 | 1.49082200 | -0.48359900 |
| O | 6.08618600 | 2.43536700 | 1.45340900 | O | -0.64618200 | -3.46309500 | -1.05693500 |
| O | -6.46925300 | 2.76154200 | -0.59109500 | H | 0.06394100 | -3.71114200 | -1.66002200 |
| O | -4.37551800 | 3.80069800 | 0.22718800 | | | | |
| O | -5.60606200 | 2.19178900 | 1.66898600 | | | | |
| H | -1.44765300 | -2.70723800 | -1.56533700 | | | | |
| H | -1.65744500 | -2.90051100 | 1.93553600 | | | | |
| H | -3.82662300 | -2.24088500 | 1.37493400 | | | | |
| H | 0.41389200 | 0.27376200 | 1.16414100 | | | | |
| H | 2.31626600 | -0.04234500 | 2.76147400 | | | | |
| Pd | 0.02553900 | -2.00900500 | 0.30855800 | | | | |
| H | -2.76472400 | 0.39052000 | -3.30214200 | | | | |
| H | 3.42442400 | -1.20781600 | -2.50634300 | | | | |
| H | -0.61038100 | -0.87912300 | -2.67398700 | | | | |
| O | 0.23855900 | -0.39525100 | -2.64760100 | | | | |
| H | 0.83497000 | -1.01239400 | -2.18835300 | | | | |
| H | -0.06602100 | 0.78288700 | -1.20480200 | | | | |
| O | -0.24144400 | 1.32081300 | -0.40489700 | | | | |
| H | -1.17945300 | 1.53227900 | -0.46494400 | | | | |
| O | -0.73532900 | -3.38591200 | -1.03667800 | | | | |
| H | -0.04282600 | -3.65357600 | -1.65052400 | | | | |

54

RR_hs_ID1_TS1_R, E(SCF) = -2484.18181056,
E(ZPE) = -2483.783387, E(G) = -2483.851060
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.49156000 | 2.52568000 | -2.19340700 |
| H | 0.75766400 | 3.52184600 | -1.82595900 |
| H | 0.91946300 | 2.41023200 | -3.19346100 |
| C | -1.00766100 | 2.35057400 | -2.20713100 |
| H | -1.49004200 | 3.05927600 | -2.88595100 |
| H | -1.26932500 | 1.33679800 | -2.52796300 |
| N | -1.50331600 | 2.51957300 | -0.82365800 |
| N | 1.06094500 | 1.53200200 | -1.26090200 |
| C | -2.93548400 | 2.17308300 | -0.61812100 |
| H | -3.34948200 | 2.96999200 | 0.00583800 |
| C | 2.45356000 | 1.77793000 | -0.86106100 |
| H | 2.45884400 | 2.70887800 | -0.28119900 |
| C | -3.18527800 | 0.85343300 | 0.04780400 |
| C | -2.58079700 | 0.56552000 | 1.29525900 |
| C | -4.09016800 | -0.04248700 | -0.49864500 |
| C | -2.98861200 | -0.59057900 | 1.97936700 |
| C | -4.44744300 | -1.19951700 | 0.17509600 |
| H | -4.54098700 | 0.16623500 | -1.46412100 |
| C | -3.90992800 | -1.46055800 | 1.42741600 |
| H | -4.20382000 | -2.35588600 | 1.96635000 |
| C | 3.02433400 | 0.62776500 | -0.08610100 |
| C | 2.35077800 | 0.03796000 | 1.00945400 |
| C | 4.27700100 | 0.14599000 | -0.45206900 |
| C | 3.00125400 | -1.00933500 | 1.69210200 |
| C | 4.89571900 | -0.87755100 | 0.23705800 |
| H | 4.79030400 | 0.59116900 | -1.29861100 |
| C | 4.24480000 | -1.46086300 | 1.31811600 |
| H | 4.71705200 | -2.27103600 | 1.86483800 |
| O | -1.63960600 | 1.34048100 | 1.81191200 |
| O | 1.15856600 | 0.39028400 | 1.45101700 |
| S | -5.61653900 | -2.36310200 | -0.53505700 |
| S | 6.50088200 | -1.49973400 | -0.26539700 |
| O | 6.27991300 | -2.91641100 | -0.67692700 |
| O | 7.37601300 | -1.39088500 | 0.93738500 |
| O | 6.94740900 | -0.63262100 | -1.39108000 |
| O | -6.77291800 | -2.39939500 | 0.40504800 |
| O | -4.89977900 | -3.66818600 | -0.60337300 |
| O | -5.97027600 | -1.82044400 | -1.87552400 |
| H | -1.76651300 | 3.21709800 | 1.88143900 |
| H | -1.37770700 | 3.48696300 | -0.51563100 |
| H | -3.45296400 | 2.21161500 | -1.58083300 |
| H | 0.96323000 | 0.58464400 | -0.66120400 |
| H | 3.06423100 | 1.94964000 | -1.75495700 |
| Pd | -0.17970900 | 1.46855200 | 0.35233000 |
| H | -2.54536300 | -0.78847600 | 2.95013500 |
| H | 2.47733900 | -1.45975200 | -2.52906200 |
| H | -1.21801900 | -1.82218900 | 0.99090800 |
| O | -0.28324400 | -1.91861500 | 0.76576200 |
| H | 0.14966200 | -1.15306200 | 1.19518000 |
| H | 0.07668000 | -1.52458400 | -0.99285900 |
| O | 0.38499500 | -1.21184400 | -1.86812000 |

54

RR_hs_ID1_TS1_P, E(SCF) = -2484.18486645,
E(ZPE) = -2483.783254, E(G) = -2483.846873
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.26464500 | -0.77661500 | 2.82297900 |
| H | 0.05472000 | -1.67087200 | 3.36653000 |
| H | -0.16198300 | 0.08204300 | 3.49279600 |
| C | -1.67533600 | -0.91368500 | 2.31912900 |
| H | -2.39218700 | -1.05177700 | 3.13337100 |
| H | -1.95659800 | -0.01226300 | 1.77024400 |
| N | -1.73635100 | -2.05116500 | 1.36892400 |
| N | 0.61467900 | -0.62469400 | 1.64628200 |
| C | -3.02061700 | -2.11973700 | 0.59757900 |
| H | -2.97266000 | -3.03179000 | 0.00034900 |
| C | 2.05333500 | -0.71376900 | 1.95053700 |
| H | 2.23256700 | -1.72915100 | 2.32262900 |
| C | -3.29291100 | -0.91789900 | -0.24658600 |
| C | -2.80112900 | -0.81865500 | -1.57776900 |
| C | -4.06150600 | 0.11375800 | 0.28520800 |
| C | -3.07266000 | 0.39158700 | -2.26787000 |
| C | -4.31881300 | 1.27309200 | -0.41951900 |
| H | -4.46327400 | 0.01601500 | 1.29033800 |
| C | -3.81208700 | 1.40687700 | -1.71023900 |
| H | -4.00325400 | 2.31522800 | -2.27401300 |
| C | 2.90417000 | -0.39344500 | 0.76175600 |
| C | 2.73043100 | -1.05501000 | -0.47324900 |
| C | 3.91545300 | 0.55126900 | 0.89314800 |
| C | 3.61209300 | -0.73728000 | -1.52327000 |
| C | 4.77140700 | 0.84421000 | -0.14962600 |
| H | 4.04550000 | 1.06597500 | 1.83979900 |
| C | 4.61451600 | 0.19217300 | -1.36689600 |
| H | 5.27924700 | 0.41962400 | -2.19433900 |
| O | -2.12426600 | -1.75083900 | -2.17154600 |
| O | 1.79920000 | -1.96139600 | -0.71162500 |
| S | -5.31435200 | 2.58699200 | 0.27768100 |
| S | 6.06770200 | 2.07208200 | 0.02933500 |
| O | 5.74757500 | 3.14690500 | -0.95332300 |

H -0.29399100 -1.47640900 -2.49321800
O -1.68336400 4.15456200 1.62125100
H -2.39602400 4.61032900 2.07459800

54

RR_hs_ID1_TS1, E(SCF) = -2484.16655326,
E(ZPE) = -2483.767452, E(G) = -2483.833278
a.u.

C 0.02879400 -1.01568100 2.80441900
H 0.36377800 -1.99247700 3.16674000
H 0.20888700 -0.28285100 3.59566800
C -1.42382300 -1.06377900 2.40829100
H -2.06650500 -1.34150900 3.24906400
H -1.75463500 -0.09221100 2.03087300
N -1.55148300 -2.04138600 1.30510700
N 0.82484200 -0.68572600 1.60399100
C -2.90840800 -2.13523400 0.70870000
H -2.88868600 -3.01972800 0.06625900
C 2.26273900 -0.96598700 1.73143200
H 2.36336400 -2.05327000 1.82719500
C -3.30381800 -0.92224600 -0.05974200
C -2.66045000 -0.63755100 -1.28962100
C -4.30902300 -0.09249200 0.41619000
C -3.14214200 0.46959100 -2.02398900
C -4.72915000 1.01002700 -0.30499700
H -4.78075600 -0.31138800 1.37020700
C -4.14575500 1.27809300 -1.53888700
H -4.48282300 2.13067700 -2.12076900
C 3.05513200 -0.42807600 0.57999200
C 2.69371600 -0.66441600 -0.76562900
C 4.21639300 0.28589000 0.85630800
C 3.55650100 -0.18580600 -1.77174500
C 5.04475500 0.74653000 -0.14721100
H 4.49037400 0.47555600 1.88937000
C 4.70797300 0.50441300 -1.47336500
H 5.35014300 0.86087200 -2.27248800
O -1.65176000 -1.34377700 -1.72992800
O 1.60827200 -1.30184800 -1.16239000
S -6.00978800 2.09559000 0.31967400
S 6.51857100 1.69768300 0.22853000
O 6.25654000 3.07294200 -0.28545600
O 7.63279400 1.02414700 -0.49762100
O 6.67415800 1.65134200 1.70875400
O -7.11934400 2.04585500 -0.67670800
O -5.39130200 3.45046000 0.40644100
O -6.39965000 1.54984300 1.65008000
H -1.08377000 -3.05563300 -1.82671800
H -1.31008900 -2.96479900 1.66772200
H -3.62530300 -2.32107000 1.51627400
H 0.66947500 0.29761100 1.33181000
H 2.63217500 -0.52051300 2.66263600
Pd -0.02096400 -1.63209500 0.00143900
H -2.69012100 0.68081500 -2.98812600
H 3.28156200 -0.38176000 -2.80329300
H -0.60171100 -0.00275900 -2.41735700
O 0.12818800 0.64606600 -2.49459500
H 0.87787500 0.06744900 -2.27635500
H -0.01076700 1.41479100 -0.77936700
O -0.02072700 1.73832800 0.14597000
H -0.92334100 2.03285400 0.29579500
O -0.47770300 -3.72947400 -1.46004500
H 0.31484900 -3.67759800 -2.00317700

54

RR_hs_ID1_TS2, E(SCF) = -2484.18420790,
E(ZPE) = -2483.786472, E(G) = -2483.851873
a.u.

C -0.24955000 -0.76396200 2.83503300
H 0.07136000 -1.66088600 3.37356800
H -0.14073900 0.09144200 3.50802100
C -1.66637900 -0.89822900 2.34433000
H -2.37518500 -1.03395100 3.16604600
H -1.95089800 0.00313700 1.79697200
N -1.73691100 -2.03748800 1.39728200
N 0.62154800 -0.61173900 1.65250900
C -3.02388600 -2.12192500 0.63831100
H -2.97408300 -3.04234900 0.05427900

C 2.06119100 -0.72205000 1.94088300
H 2.23114700 -1.74452700 2.29813600
C -3.30148000 -0.93411500 -0.22547900
C -2.83847600 -0.85673800 -1.56222500
C -4.05203900 0.11483100 0.30104900
C -3.12553100 0.32670800 -2.28021300
C -4.31916200 1.25800500 -0.42407300
H -4.43296800 0.04058500 1.31596600
C -3.84613600 1.35979700 -1.72937000
H -4.04779700 2.25493700 -2.30968500
C 2.90349900 -0.39953100 0.74581900
C 2.70556000 -1.03719800 -0.49856500
C 3.93439500 0.52319300 0.88236100
C 3.58176200 -0.71486100 -1.55233400
C 4.78584100 0.81844400 -0.16459600
H 4.08428600 1.01753600 1.83686900
C 4.60281900 0.19291300 -1.39087800
H 5.26334300 0.42227300 -2.22114000
O -2.16284700 -1.80114100 -2.12459100
O 1.75916400 -1.92534100 -0.74483800
S -5.26781300 2.60669500 0.27908900
S 6.10867700 2.01589200 0.02475300
O 5.78920300 3.12905500 -0.91459000
O 7.36002700 1.29862700 -0.35271500
O 6.08618600 2.43536700 1.45340900
O -6.46925300 2.76154200 -0.59109500
O -4.37551800 3.80069800 0.22718800
O -5.60606200 2.19178900 1.66898600
H -1.44765300 -2.70723800 -1.56533700
H -1.65744500 -2.90051100 1.93553600
H -3.82662300 -2.24088500 -1.37493400
H 0.41389200 0.27376200 1.16414100
H 2.31626600 -0.04234500 2.76147400
Pd 0.02553900 -2.00900500 0.30855800
H -2.76472400 0.39052000 -3.30214200
H 3.42442400 -1.20781600 -2.50634300
H -0.61038100 -0.87912300 -2.67398700
O 0.23855900 -0.39525100 -2.64760100
H 0.83497000 -1.01239400 -2.18835300
H -0.06602100 0.78288700 -1.20480200
O -0.24144400 1.32081300 -0.40489700
H -1.17945300 1.53227900 -0.46494400
O -0.73532900 -3.38591200 -1.03667800
H -0.04282600 -3.65357600 -1.65052400

45

RR_hs_TS, E(SCF) = -2254.85239244, E(ZPE) =
-2254.528933, E(G) = -2254.585699 a.u.

N 1.36993600 2.47493600 0.05131700
N -1.30768300 1.90425300 0.60641700
C 2.78663800 2.09945600 0.28015800
H 3.40584900 2.86141100 -0.20482200
C -2.63702400 1.92484000 -0.03469600
H -2.50625400 2.43588100 -0.99584400
C 3.24002100 0.73454500 -0.17544500
C 2.63992200 -0.02321500 -1.20687800
C 4.40066300 0.26048500 0.42872500
C 3.28237700 -1.21818700 -1.59689500
C 5.00536700 -0.91466500 0.03099500
H 4.85635300 0.83439500 1.23064700
C 4.44088100 -1.65637500 -1.00120400
H 2.81792700 -1.78957700 -2.39354100
H 4.90690500 -2.58197500 -1.32433900
C -3.18721700 0.54370600 -0.20546000
C -2.45698900 -0.46436800 -0.88489500
C -4.46311700 0.26742600 0.27161400
C -3.09234200 -1.71266200 -1.06663200
C -5.05699300 -0.96507300 -0.83660000
H -5.01408000 1.04006400 0.79878600
C -4.36097700 -1.95854800 -0.59797200
H -2.53717500 -2.48224200 -1.59237200
H -4.81823900 -2.93127100 -0.75260100
O 1.53722400 0.31437800 -1.84011300
O -1.25303400 -0.31481500 -1.37524400
S 6.48865800 -1.51722100 0.83688900
S -6.70780900 -1.30489300 0.69103800
O -6.57775700 -2.47622000 1.60586900

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| O | -7.53121100 | -1.62008900 | -0.51280700 | N | -0.48461900 | -0.80248300 | -0.69741500 |
| O | -7.15547200 | -0.06862300 | 1.39201200 | C | 2.19986100 | 0.66668900 | 2.02527400 |
| O | 6.85042000 | -0.49670200 | 1.86001600 | H | 2.01888800 | 1.64940800 | 2.46656900 |
| O | 7.51275400 | -1.65141000 | -0.23929400 | C | -1.71820700 | -0.95319900 | -1.49223600 |
| O | 6.12318900 | -2.83477000 | 1.43382200 | H | -1.96588500 | -2.01544500 | -1.60861100 |
| H | 1.34050700 | 3.15168800 | -0.70921600 | C | 3.21090800 | 0.75170800 | 0.92465200 |
| H | 2.98302000 | 2.18743700 | 1.35165000 | C | 3.29053100 | 1.85348000 | 0.06436600 |
| H | -1.36455500 | 1.34250500 | 1.45672500 | C | 4.16301900 | -0.25770200 | 0.79249100 |
| H | -3.32619600 | 2.52654300 | 0.56855300 | C | 4.30952400 | 1.92590100 | -0.88409200 |
| Pd | 0.07640500 | 1.03469800 | -0.64033700 | C | 5.16028800 | -0.18855700 | -0.15775900 |
| C | -0.76100200 | 3.23865600 | 0.93828500 | H | 4.13171300 | -1.11355200 | 1.46038300 |
| C | 0.71034700 | 3.08904400 | 1.23130700 | C | 5.23858700 | 0.91550700 | -0.99681900 |
| H | 1.16987200 | 4.04934300 | 1.48061200 | H | 6.02593900 | 0.97905400 | -1.74038100 |
| H | 0.86082200 | 2.41069500 | 2.07510700 | C | -2.89337500 | -0.20981500 | -0.93753000 |
| H | -0.91828800 | 3.88244200 | 0.06810700 | C | -2.83610400 | 1.20546500 | -0.81361900 |
| H | -1.29270800 | 3.68170500 | 1.78501100 | C | -4.06137500 | -0.88105800 | -0.62862900 |

45

RR_hs, E(SCF) = -2254.85516463, E(ZPE) = -2254.531224, E(G) = -2254.589168 a.u.

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| N | -1.46052700 | -2.51791500 | 0.06267100 | H | -4.08931700 | -1.96414900 | -0.72133700 |
| N | 1.01061000 | -1.58855600 | 0.92100800 | C | -5.17012900 | 1.18473100 | -0.13004200 |
| C | -2.88578900 | -2.29427600 | -0.28577800 | H | -6.06195100 | 1.71659300 | 0.18205000 |
| H | -3.03865900 | -2.81522800 | -1.23563000 | O | 2.45701800 | 2.91417300 | 0.13157500 |
| C | 2.40744400 | -1.80597700 | 0.50405500 | O | -1.73829600 | 1.88950100 | -1.07313500 |
| H | 2.37930700 | -2.58146300 | -0.27048400 | S | 6.38933100 | -1.49363200 | -0.30656400 |
| C | -3.26469800 | -0.85790200 | -0.45074100 | S | -6.69033200 | -1.12303700 | 0.14614400 |
| C | -2.58790400 | -0.07137500 | -1.41700300 | O | -6.29025900 | -2.18890100 | 1.11005600 |
| C | -4.34078200 | -0.33079600 | 0.24448200 | O | -7.15231100 | -1.68599300 | -1.15665700 |
| C | -3.07759700 | 1.22292700 | -1.66582100 | O | -7.65260100 | -0.14563300 | 0.72705300 |
| C | -4.79336600 | 0.95337300 | -0.00858300 | O | 6.31536700 | -1.95102300 | -1.72189300 |
| H | -4.85336200 | -0.93694500 | 0.98503700 | O | 5.99037300 | -2.54106400 | 0.67168900 |
| C | -4.16013700 | 1.72535900 | -0.97505600 | O | 7.69349400 | -0.85222900 | 0.01978400 |
| H | -2.57023200 | 1.82097000 | -2.41527800 | H | -0.15755700 | 2.54840300 | 0.93545500 |
| H | -4.51590100 | 2.73010600 | -1.18175000 | H | 1.56717600 | 2.65964000 | 0.45203700 |
| C | 3.04577300 | -0.53890200 | 0.01761000 | H | 0.26610400 | 0.20961100 | 2.41879600 |
| C | 2.41872800 | 0.33370800 | -0.91086200 | H | 2.58897000 | 0.01788700 | 2.81820500 |
| C | 4.32976900 | -0.24881600 | 0.46886900 | H | 0.31362800 | -0.95596600 | -1.30909700 |
| C | 3.16039600 | 1.45807000 | -1.34068600 | H | -1.48189600 | -0.56005100 | -2.48564300 |
| C | 5.03112800 | 0.85309400 | 0.02456100 | Pd | -0.28912000 | 1.15953700 | 0.19305600 |
| H | 4.80465300 | -0.91423700 | 1.18339700 | H | 4.34640800 | 2.79573700 | -1.52959900 |
| C | 4.43219700 | 1.71429800 | -0.89007500 | H | -3.96893800 | 2.95422400 | -0.34154000 |
| H | 2.68195900 | 2.12248300 | -2.05229100 | | | | |
| H | 4.96987600 | 2.58697000 | -1.24785100 | | | | |
| O | -1.54385500 | -0.52344800 | -2.08271100 | | | | |
| O | 1.22088000 | 0.18594500 | -1.41732100 | | | | |
| S | -6.16856100 | 1.64728400 | 0.91022900 | | | | |
| S | 6.67591500 | 1.21508900 | 0.63377200 | | | | |
| O | 6.55643400 | 2.47303200 | 1.42783100 | | | | |
| O | 7.52984200 | 1.39231200 | -0.57648200 | | | | |
| O | 7.07841500 | 0.04433900 | 1.46266900 | | | | |
| O | -6.69621000 | 0.54312900 | 1.75964200 | | | | |
| O | -7.14995600 | 2.11585800 | -0.11037400 | | | | |
| O | -5.60250800 | 2.77375500 | 1.70826000 | | | | |
| H | -1.17398400 | -3.39905200 | -0.36160500 | | | | |
| H | -3.52237700 | -2.77692000 | 0.46281400 | | | | |
| H | 0.97654800 | -0.77063900 | 1.53062700 | | | | |
| H | 2.98536500 | -2.20391900 | 1.34571100 | | | | |
| Pd | -0.15645300 | -1.11375100 | -0.69588700 | | | | |
| C | 0.36789100 | -2.72972700 | 1.61317400 | | | | |
| C | -1.13348800 | -2.58468100 | 1.50365900 | | | | |
| H | -1.64783500 | -3.42227500 | 1.98448000 | | | | |
| H | -1.47955200 | -1.65732800 | 1.96956700 | | | | |
| H | 0.69502600 | -3.64369800 | 1.10771800 | | | | |
| H | 0.69603000 | -2.78858700 | 2.65364300 | | | | |

47

RR_s_D1_no2W_P, E(SCF) = -2256.03972409, E(ZPE) = -2255.696982, E(G) = -2255.757565 a.u.

| | | | | | | | |
|---|-------------|-------------|------------|---|-------------|-------------|-------------|
| C | -0.34866100 | -1.67977300 | 0.47403000 | H | -4.59976000 | -1.44239200 | -0.98167000 |
| H | -1.22826800 | -1.53912700 | 1.11041500 | C | -4.53710900 | 1.76576300 | 0.08269700 |
| H | -0.30970300 | -2.73720500 | 0.18812600 | H | -5.18482100 | 2.50608900 | 0.53915400 |
| C | 0.91906300 | -1.28780000 | 1.19684900 | O | 1.14537100 | 1.42942000 | 0.99427200 |
| H | 1.09864900 | -1.92270300 | 2.06949700 | O | -1.11771400 | 1.45006500 | -1.08597500 |
| H | 1.76971000 | -1.40780500 | 0.52022100 | S | 6.75434800 | 0.01592000 | -0.27271500 |
| N | 0.87285700 | 0.14192700 | 1.60266600 | S | -6.67134500 | 0.01540600 | 0.36211700 |

| | | | |
|----|-------------|-------------|-------------|
| O | -6.47751800 | -0.80440900 | 1.59475900 |
| O | -7.25133600 | -0.77944400 | -0.75796700 |
| O | -7.40818700 | 1.28329300 | 0.62254000 |
| O | 7.39460700 | 1.24731800 | -0.81210900 |
| O | 6.65215200 | -1.07763400 | -1.28229100 |
| O | 7.37090500 | -0.45009600 | 1.00314100 |
| H | -2.93243500 | -0.50065500 | 2.29272700 |
| H | -2.42933500 | -0.29888500 | 1.77326300 |
| H | 0.06608100 | -1.54070900 | 1.85197700 |
| H | 2.61681900 | -2.11572800 | 1.88979500 |
| H | -0.06341500 | -1.51102300 | -1.97180900 |
| H | -1.83559600 | -0.72391300 | -2.85169600 |
| Pd | 0.00631800 | 0.07568500 | -0.04986400 |
| H | 2.88321600 | 3.05351000 | -0.00456900 |
| H | -2.83399400 | 3.07205500 | -0.04356100 |

47

RR_s_D1_no2W_TS, E(SCF) = -2255.99687081,
E(ZPE) = -2255.657777, E(G) = -2255.716518
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.33633900 | -1.92165100 | -0.56348900 |
| H | 1.23371000 | -1.82167900 | -1.18007600 |
| H | 0.30062400 | -2.94342200 | -0.17306500 |
| C | -0.91669800 | -1.58633200 | -1.33098400 |
| H | -1.05867800 | -2.24876500 | -2.18819500 |
| H | -1.78925700 | -1.69176500 | -0.67962900 |
| N | -0.86575100 | -0.17013400 | -1.77097400 |
| N | 0.43550400 | -0.94681300 | 0.54483600 |
| C | -2.20345400 | 0.38315700 | -2.14005700 |
| H | -2.00020000 | 1.33525300 | -2.63809600 |
| C | 1.64041800 | -1.06009800 | 1.40698400 |
| H | 1.90741300 | -2.11691900 | 1.50595500 |
| C | -3.10648800 | 0.58275100 | -0.97357800 |
| C | -2.84422100 | 1.67813000 | -0.08735800 |
| C | -4.19831900 | -0.24568200 | -0.77554700 |
| C | -3.77464400 | 1.85404300 | 0.97433000 |
| C | -5.06945200 | -0.05246100 | 0.28609500 |
| H | -4.37261800 | -1.07018800 | -1.46312400 |
| C | -4.85471500 | 1.02006300 | 1.14942700 |
| H | -5.54031400 | 1.18336900 | 1.97503800 |
| C | 2.80896400 | -0.26441100 | 0.92718600 |
| C | 2.66448400 | 1.13926600 | 0.79975800 |
| C | 4.03711800 | -0.85562900 | 0.69979600 |
| C | 3.79932500 | 1.89805200 | 0.48853700 |
| C | 5.14625900 | -0.08492800 | 0.37992000 |
| H | 4.14068200 | -1.93258900 | 0.79645700 |
| C | 5.02501700 | 1.29255000 | 0.28341000 |
| H | 5.89842500 | 1.88878000 | 0.04401400 |
| O | -1.83220300 | 2.44756200 | -0.24053400 |
| O | 1.49319700 | 1.72606500 | 0.98281700 |
| S | -6.52295800 | -1.07567000 | 0.45293000 |
| S | 6.70359600 | -0.89166800 | -0.00612300 |
| O | 6.59621900 | -1.31408100 | -1.43291300 |
| O | 6.80663200 | -2.04949300 | 0.92524200 |
| O | 7.75990400 | 0.13395900 | 0.21333100 |
| O | -6.85851000 | -1.08998100 | 1.90665600 |
| O | -6.14876500 | -2.42272700 | -0.06960900 |
| O | -7.59607500 | -0.43342400 | -0.36665800 |
| H | 0.76800500 | 2.45425100 | -1.54558300 |
| H | 0.01559400 | 2.59407800 | -1.41052800 |
| H | -0.27132000 | -0.11904900 | -2.59811100 |
| H | -2.65793900 | -0.29790300 | -2.86920300 |
| H | -0.38804700 | -1.05488800 | 1.13669400 |
| H | 1.33407700 | -0.69626300 | 2.39138200 |
| Pd | 0.21335000 | 0.90287700 | -0.35277400 |
| H | -3.60515000 | 2.68329400 | 1.65475700 |
| H | 3.68959200 | 2.97414500 | 0.40973900 |

53

RR_s_D1_TS1_P, E(SCF) = -2408.89815999,
E(ZPE) = -2408.506301, E(G) = -2408.569326
a.u.

| | | | |
|---|-------------|-------------|------------|
| C | -0.31451800 | -1.84782300 | 0.87571400 |
| H | -1.19836900 | -1.78536000 | 1.51722000 |
| H | -0.25521200 | -2.86473100 | 0.47544100 |
| C | 0.95037900 | -1.48367100 | 1.61391900 |
| H | 1.12609500 | -2.13297500 | 2.47462200 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.80511300 | -1.58104600 | 0.93938900 |
| N | 0.88780500 | -0.06190000 | -2.04251600 |
| N | -0.45754600 | -0.86780900 | -0.21693100 |
| C | 2.22604100 | 0.53389300 | 2.36035000 |
| H | 2.02189200 | 1.50842100 | 2.80892700 |
| C | -1.61849200 | -1.02642400 | -1.12212300 |
| H | -1.82818900 | -2.09313700 | -1.24947900 |
| C | 3.12030600 | 0.66422400 | 1.17453700 |
| C | 2.98793100 | 1.77338300 | 0.28624600 |
| C | 4.10079800 | -0.29598400 | 0.95271500 |
| C | 3.88266600 | 1.80520400 | -0.81904000 |
| C | 4.94975100 | -0.23362800 | -0.13626900 |
| H | 4.20490800 | -1.12550800 | 1.64758200 |
| C | 4.83558700 | 0.83557000 | -1.02333800 |
| H | 5.49970300 | 0.89717700 | -1.88058500 |
| C | -2.85147200 | -0.29858200 | -0.69486800 |
| C | -2.79463800 | 1.10067300 | -0.52341400 |
| C | -4.06283600 | -0.96012100 | -0.57077900 |
| C | -3.98360400 | 1.79143500 | -0.25558200 |
| C | -5.22603800 | -0.26083300 | -0.29887800 |
| H | -4.10778500 | -2.03662100 | -0.70224600 |
| C | -5.18414000 | 1.11937200 | -0.15080200 |
| H | -6.09726400 | 1.66793800 | 0.05079300 |
| O | 2.10759900 | 2.70395900 | 0.43759100 |
| O | -1.64860700 | 1.76590200 | -0.61952400 |
| S | 6.18390800 | -1.49354200 | -0.43333700 |
| S | -6.79692100 | -1.11454600 | -0.11984700 |
| O | -7.71924100 | -0.47365300 | -1.09959700 |
| O | -7.22136300 | -0.88958600 | 1.29151500 |
| O | -6.52282600 | -2.54552700 | -0.42446200 |
| O | 6.07478800 | -2.45606200 | 0.69906000 |
| O | 7.49872000 | -0.78859800 | -0.47230600 |
| O | 5.83620100 | -2.10491100 | -1.75023300 |
| H | -0.25756200 | 2.50396400 | 1.54468200 |
| H | 0.50116400 | 2.50989700 | 1.17263200 |
| H | 0.32675200 | -0.01383000 | 2.89291100 |
| H | 2.69211300 | -0.10020100 | 3.12321400 |
| H | 0.39223600 | -0.87114500 | -0.80679300 |
| H | -1.28389100 | -0.63517400 | -2.08914600 |
| Pd | -0.29930600 | 0.96639600 | 0.68020400 |
| H | 3.79716400 | 2.64370100 | -1.50412400 |
| H | -3.93421400 | 2.86784600 | -0.13489100 |
| H | 1.21740800 | 2.71260500 | -1.20801700 |
| O | 0.74774900 | 2.46178200 | -2.03250400 |
| H | -0.17333400 | 2.32962400 | -1.75218000 |
| H | 1.33677100 | 0.70823900 | -2.17330000 |
| O | 1.61643700 | -0.23009500 | -2.10692900 |
| H | 2.51698600 | -0.17236200 | -1.76254200 |

53

RR_s_D1_TS1_R, E(SCF) = -2408.90850156,
E(ZPE) = -2408.519228, E(G) = -2408.585181
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.68543800 | -2.61742700 | -0.69773600 |
| H | -1.51976100 | -2.79084600 | -0.00972100 |
| H | -0.78966400 | -3.31033100 | -1.53844800 |
| C | 0.64565600 | -2.80573200 | 0.00074800 |
| H | 0.77428600 | -3.83121100 | 0.35718200 |
| H | 1.47183700 | -2.57740100 | -0.68105200 |
| N | 0.71737900 | -1.84451600 | 1.12555600 |
| N | -0.73705300 | -1.21751100 | -1.15560900 |
| C | 2.04375100 | -1.68689900 | 1.77793400 |
| H | 1.83678300 | -1.52322400 | 2.83905600 |
| C | -1.97389100 | -0.74380400 | -1.81769800 |
| H | -2.50302900 | -1.59502600 | -2.25747400 |
| C | 2.84562400 | -0.53974300 | 1.24882500 |
| C | 2.31598300 | 0.77542400 | 1.33978600 |
| C | 4.12040100 | -0.73901800 | 0.74753700 |
| C | 3.15230800 | 1.84449300 | 0.96892700 |
| C | 4.91128400 | 0.33068300 | 0.35705400 |
| H | 4.51835200 | -1.74635000 | 0.66848000 |
| C | 4.42592700 | 1.62490700 | 0.48157000 |
| H | 5.04703700 | 2.46629100 | 0.19030000 |
| C | -2.89326500 | 0.04277900 | -0.93701000 |
| C | -2.41164100 | 1.19305400 | -0.27015100 |
| C | 4.22934000 | -0.30657400 | -0.82865400 |
| C | -3.32743700 | 1.97547400 | 0.44781400 |

| | | | |
|----|-------------|-------------|-------------|
| C | -5.11167300 | 0.46824400 | -0.09466900 |
| H | -4.59728800 | -1.19697900 | -1.32929200 |
| C | -4.65714600 | 1.61724800 | 0.53794900 |
| H | -5.34681700 | 2.22936800 | 1.11050800 |
| O | 1.08579700 | 1.00489500 | 1.74974500 |
| O | -1.13081900 | 1.53668700 | -0.29711300 |
| S | 6.54782100 | 0.06899800 | -0.32987200 |
| S | -6.81801300 | -0.04077600 | 0.12422900 |
| O | -7.65082900 | 1.14600100 | -0.22143300 |
| O | -6.94190600 | -0.42202900 | 1.56165300 |
| O | -7.02716500 | -1.19009600 | -0.79908800 |
| O | 6.80505000 | -1.39435100 | -0.23024300 |
| O | 7.47691300 | 0.88311300 | 0.50456600 |
| O | 6.48156500 | 0.55262300 | -1.73927300 |
| H | -3.19274700 | -1.27869200 | 2.12764400 |
| H | -2.53148800 | -0.94819600 | 1.99411200 |
| H | 0.04931600 | -2.14413900 | 1.83460900 |
| H | 2.60540200 | -2.62210700 | 1.69088600 |
| H | 0.04343300 | -1.06199000 | -1.81255300 |
| H | -1.63557800 | -0.10624600 | -2.64237500 |
| Pd | -0.06573100 | -0.07365100 | 0.41239600 |
| H | 2.76518500 | 2.85340500 | 1.07941900 |
| H | -2.95545700 | 2.86390000 | 0.94649400 |
| H | 1.72992200 | 2.32787000 | -0.97233800 |
| O | 1.11105100 | 2.29904700 | -1.71335600 |
| H | 0.23792100 | 2.16558700 | -1.29217400 |
| H | 1.38282200 | 0.67921500 | -2.47126900 |
| O | 1.38716300 | -0.23328700 | -2.83161800 |
| H | 2.29279300 | -0.54180700 | -2.74560500 |

53

RR_s_D1_TS1, E(SCF) = -2408.89349032,
E(ZPE) = -2408.503249, E(G) = -2408.565954
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.37568700 | -2.17622900 | -0.22277800 |
| H | 1.25403900 | -2.27694900 | -0.86729500 |
| H | 0.32127100 | -3.05975700 | 0.42148200 |
| C | -0.89241100 | -2.01195200 | -1.02466900 |
| H | -1.07842900 | -2.86723900 | -1.67893400 |
| H | -1.74783400 | -1.91382600 | -0.35003000 |
| N | -0.80661500 | -0.76106700 | -1.81904800 |
| N | 0.52876000 | -0.95228000 | 0.58553500 |
| C | -2.11676900 | -0.26899200 | -2.33280200 |
| H | -1.87268200 | 0.53077000 | -3.03697000 |
| C | 1.73301600 | -0.85283000 | 1.44056600 |
| H | 2.01764200 | -1.85558700 | 1.77534900 |
| C | -3.02639400 | 0.22622300 | -1.26216100 |
| C | -2.73607900 | 1.46537700 | -0.62050200 |
| C | -4.15050100 | -0.50545300 | -0.90705600 |
| C | -3.68066700 | 1.91619900 | 0.33877400 |
| C | -5.02974500 | -0.05283800 | 0.06076700 |
| H | -4.34958700 | -1.45578500 | -1.39538100 |
| C | -4.79241000 | 1.17592900 | 0.67182900 |
| H | -5.48570300 | 1.54715700 | 1.42105100 |
| C | 2.89911400 | -0.16434500 | 0.80730500 |
| C | 2.74188600 | 1.16101400 | 0.34418000 |
| C | 4.14467400 | -0.76831300 | 0.75139100 |
| C | 3.86789800 | 1.84335700 | -0.13460600 |
| C | 5.24384300 | -0.07922200 | 0.26749100 |
| H | 4.27061000 | -1.78930300 | 1.09855200 |
| C | 5.10519400 | 1.23315400 | -0.16386800 |
| H | 5.96980700 | 1.77319100 | -0.53647600 |
| O | -1.66201500 | 2.13989600 | -0.87448700 |
| O | 1.55778400 | 1.76080800 | 0.35360200 |
| S | -6.47819100 | -0.99938100 | 0.51806400 |
| S | 6.85854300 | -0.86210100 | 0.18131000 |
| O | 7.76205300 | -0.01475500 | 1.01004200 |
| O | 7.23596200 | -0.85357100 | -1.26067300 |
| O | 6.67781000 | -2.23413200 | 0.72916300 |
| O | -6.37949900 | -2.28887300 | -0.22254500 |
| O | -7.65922900 | -0.18456400 | 0.10617800 |
| O | -6.40536700 | -1.17219200 | 1.99866900 |
| H | 0.95122900 | 1.75681700 | -2.43846500 |
| H | 0.27181500 | 2.09057400 | -2.32507100 |
| H | -0.20600800 | -0.94065300 | -2.62380500 |
| H | -2.59133500 | -1.08442800 | -2.89024300 |
| H | -0.29979200 | -0.82495800 | 1.19038000 |

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|----|-------------|-------------|-------------|
| H | 1.41611800 | -0.28507300 | 2.32220600 |
| Pd | 0.27242700 | 0.61803500 | -0.72866300 |
| H | -3.49591300 | 2.87192800 | 0.82035500 |
| H | 3.73935100 | 2.86356300 | -0.47933600 |
| H | -1.07280100 | 2.66872000 | 0.78333700 |
| O | -0.68516800 | 2.66723700 | 1.68597500 |
| H | 0.24813900 | 2.46488100 | 1.49986300 |
| H | -1.30298400 | 1.01134700 | 2.15124800 |
| O | -1.60176100 | 0.07997900 | 2.24758300 |
| H | -2.47182500 | 0.07703100 | 1.83006500 |

53

RR_s_D1_TS2_P, E(SCF) = -2408.92789024,
E(ZPE) = -2408.534336, E(G) = -2408.598990
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.35567100 | -1.60293100 | 1.16147200 |
| H | -1.27408600 | -1.38967600 | 1.71862200 |
| H | -0.30894800 | -2.68652000 | 0.99672200 |
| C | 0.87270400 | -1.14484800 | 1.91566200 |
| H | 0.98022500 | -1.65744200 | 2.87498700 |
| H | 1.75246300 | -1.38187400 | 1.31207200 |
| N | 0.85667600 | 0.33233800 | 2.12125700 |
| N | -0.38471100 | -0.85864500 | -0.10100000 |
| C | 2.21243300 | 0.91131200 | 2.34952200 |
| H | 2.05731000 | 1.93601100 | 2.69346500 |
| C | -1.50635600 | -1.12316600 | -1.01352900 |
| H | -1.73046300 | -2.19683800 | -1.04064300 |
| C | 3.10145200 | 0.87388200 | 1.14294700 |
| C | 3.08805000 | 1.86638600 | 0.15420200 |
| C | 4.00174400 | -0.17963900 | 0.99499800 |
| C | 3.97360700 | 1.80088200 | -0.91992900 |
| C | 4.85006700 | -0.26181100 | -0.09047000 |
| H | 4.04898400 | -0.95411900 | 1.75415700 |
| C | 4.84212600 | 0.73991200 | -1.05270500 |
| H | 5.51379500 | 0.68668900 | -1.90263800 |
| C | -2.75325200 | -0.35063400 | -0.70643100 |
| C | -2.72798800 | 1.06384000 | -0.71723300 |
| C | -3.95234200 | -1.01363800 | -0.49433700 |
| C | -3.94173100 | 1.74923100 | -0.55431100 |
| C | -5.13553800 | -0.31599900 | -0.31794100 |
| H | -3.97113000 | -2.09923500 | -0.48087300 |
| C | -5.12712000 | 1.07185900 | -0.35741900 |
| H | -6.05383600 | 1.62208800 | -0.22703000 |
| O | 2.26992300 | 2.94435100 | 0.17520400 |
| O | -1.60574000 | 1.75160900 | -0.88463700 |
| S | 5.90399300 | -1.70062500 | -0.32727400 |
| S | -6.68008600 | -1.17291200 | -0.00616700 |
| O | -7.63758900 | -0.68177500 | -1.03850900 |
| O | -7.08949400 | -0.78394000 | 1.37455300 |
| O | -6.38045200 | -2.62623100 | -0.13436800 |
| O | 5.83706200 | -2.46765700 | 0.94433600 |
| O | 7.26042600 | -1.16862200 | -0.62762500 |
| O | 5.29670100 | -2.42072800 | -1.48221600 |
| H | -0.24255200 | 2.63032600 | 1.23053900 |
| H | 1.43757500 | 2.75801300 | 0.66152800 |
| H | 0.30991600 | 0.52867000 | 2.95765500 |
| H | 2.69339400 | 0.36068600 | 3.16570400 |
| H | 0.48800000 | -1.01792200 | -0.61899100 |
| H | -1.14330500 | -0.84280700 | -2.00932200 |
| Pd | -0.29745600 | 1.17273400 | 0.60538600 |
| H | 3.94221500 | 2.59412800 | -1.65841400 |
| H | -3.91869700 | 2.83350300 | -0.57703800 |
| H | 1.19313200 | 2.47390000 | -1.80859500 |
| O | 0.74387500 | 1.87427500 | -2.41921300 |
| H | -0.15234000 | 1.78825900 | -2.03464600 |
| H | 1.56377900 | 0.20830800 | -2.19561500 |
| O | 1.83078500 | -0.71194700 | -1.99631700 |
| H | 2.75418600 | -0.65989000 | -1.72281500 |

53

RR_s_D1_TS2_R, E(SCF) = -2408.89815713,
E(ZPE) = -2408.506287, E(G) = -2408.569294
a.u.

| | | | |
|---|-------------|-------------|------------|
| C | -0.31460400 | -1.84910000 | 0.87110300 |
| H | -1.19882300 | -1.78788800 | 1.51222300 |
| H | -0.25466500 | -2.86541200 | 0.46936600 |
| C | 0.94969800 | -1.48550500 | 1.61059300 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.12497300 | -2.13571800 | 2.47069500 |
| H | 1.80495000 | -1.58180200 | 0.93659900 |
| N | 0.88636300 | -0.06425600 | 2.04085800 |
| N | -0.45758100 | -0.86765300 | -0.22016900 |
| C | 2.22419500 | 0.53115500 | 2.36088000 |
| H | 2.01962800 | 1.50512600 | 2.81049500 |
| C | -1.61881100 | -1.02528100 | -1.12529300 |
| H | -1.82859500 | -2.09183800 | -1.25368400 |
| C | 3.11964300 | 0.66310400 | 1.17611900 |
| C | 2.98854300 | 1.77375800 | 0.28956800 |
| C | 4.09996300 | -0.29710900 | 0.95360600 |
| C | 3.88436300 | 1.80716200 | -0.81473900 |
| C | 4.95019000 | -0.23310800 | -0.13434300 |
| H | 4.20315600 | -1.12784600 | 1.64715700 |
| C | 4.83711700 | 0.18748400 | -1.01981900 |
| H | 5.50208400 | 0.90042500 | -1.87628900 |
| C | -2.85155300 | -0.29785300 | -0.69675500 |
| C | -2.79457100 | 1.10127100 | -0.52410600 |
| C | -4.06273100 | -0.95953500 | -0.57198200 |
| C | -3.98326600 | 1.79177700 | -0.25461000 |
| C | -5.22570700 | -0.26048900 | -0.29832500 |
| H | -4.10781900 | -2.03594800 | -0.70419800 |
| C | -5.18371100 | 1.11956900 | -0.14919300 |
| H | -6.09663700 | 1.66794500 | 0.06089000 |
| O | 2.10835800 | 2.70445100 | 0.44161400 |
| O | -1.64852000 | 1.76646100 | -0.62071800 |
| S | 6.18299400 | -1.49392700 | -0.43325300 |
| S | -6.79643700 | -1.11440100 | -0.11872400 |
| O | -7.71903000 | -0.47385400 | -1.09844100 |
| O | -7.22057100 | -0.88912000 | 1.29268500 |
| O | -6.52214500 | -2.54540800 | -0.42304700 |
| O | 6.07457800 | -2.45657600 | 0.69909600 |
| O | 7.49827700 | -0.78999400 | -0.47389500 |
| O | 5.83286600 | -2.10471100 | -1.74980100 |
| H | -0.25826800 | 2.50326700 | 1.54341600 |
| H | 0.50160900 | 2.50894600 | 1.17300900 |
| H | 0.32448300 | -0.01736200 | 2.89076000 |
| H | 2.68958600 | -0.10380400 | 3.12343600 |
| H | 0.39198900 | -0.87006600 | -0.81034400 |
| H | -1.28440000 | -0.63308900 | -2.09200000 |
| Pd | -0.29958000 | 0.96575900 | 0.67882400 |
| H | 3.79976300 | 2.64680100 | -1.49851900 |
| H | -3.93382700 | 2.86808500 | -0.13301600 |
| H | 1.22096200 | 2.71477600 | -1.20652500 |
| O | 0.74984800 | 2.46449400 | -2.03026000 |
| H | -0.17136400 | 2.33573300 | -1.74901000 |
| H | 1.33806100 | 0.71077500 | -2.17190100 |
| O | 1.61849000 | -0.22742000 | -2.10708100 |
| H | 2.51766300 | -0.16980300 | -1.75912700 |

53

RR_s_D1_TS2, E(SCF) = -2408.89787105,
E(ZPE) = -2408.507248, E(G) = -2408.570853
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.32353600 | -1.88943700 | 0.88569500 |
| H | -1.21350200 | -1.81611100 | 1.51795400 |
| H | -0.26222100 | -2.91289400 | 0.50229300 |
| C | 0.93388000 | -1.52066400 | 1.63620500 |
| H | 1.10034500 | -2.16694000 | 2.50112600 |
| H | 1.79562800 | -1.62120900 | 0.97101300 |
| N | 0.86656000 | -0.09750500 | 2.05942800 |
| N | -0.45321000 | -0.92364500 | -0.21946700 |
| C | 2.19619600 | 0.49964800 | 2.40215700 |
| H | 1.98271200 | 1.46154500 | 2.87308700 |
| C | -1.61344200 | -1.07651900 | -1.12458500 |
| H | -1.84549400 | -2.14037700 | -1.23745500 |
| C | 3.09402800 | 0.66713000 | 1.22204800 |
| C | 2.79624900 | 1.79828800 | 0.36683500 |
| C | 4.06541100 | -0.29580100 | 0.96739500 |
| C | 3.87356300 | 1.86725500 | -0.72860000 |
| C | 4.91540000 | -0.20466100 | -0.11780900 |
| H | 4.16124600 | -1.14848100 | 1.63428600 |
| C | 4.81667000 | 0.89566400 | -0.96664300 |
| H | 5.48313800 | 0.98096000 | -1.81964200 |
| C | -2.83311100 | -0.31691300 | -0.71159700 |
| C | -2.75322600 | 1.08491100 | -0.56588200 |
| C | -4.05521700 | -0.95555200 | -0.57299800 |

| | | | |
|----|-------------|-------------|-------------|
| C | -3.93225100 | 1.79887700 | -0.31322100 |
| C | -5.20710900 | -0.23329500 | -0.31291900 |
| H | -4.11835800 | -2.03360400 | -2.68352700 |
| C | -5.14330400 | 1.14867400 | -0.19295200 |
| H | -6.04706600 | 1.71618200 | 0.00549600 |
| O | 2.09853000 | 2.74244200 | 0.53361500 |
| O | -1.59762100 | 1.73094500 | -0.66993400 |
| S | 6.12232700 | -1.47916800 | -0.47031400 |
| S | -6.78904200 | -1.05918900 | -0.10799200 |
| O | -7.71117500 | -0.41831900 | -1.08809100 |
| O | -7.19708000 | -0.80808700 | -0.39439600 |
| O | -6.54038200 | -2.49873100 | -0.39439600 |
| O | 6.01023900 | -2.47245400 | 0.63404600 |
| O | 7.44832000 | -0.79713700 | -0.50858100 |
| O | 5.73843600 | -2.04043900 | -1.79891500 |
| H | -0.12736300 | 2.45419600 | 1.45714200 |
| H | 0.68053000 | 2.45611000 | 1.09624000 |
| H | 0.28513900 | -0.04342200 | 2.89536600 |
| H | 2.66624200 | -0.14682000 | -0.15192600 |
| H | 0.39882500 | -0.93980000 | -0.80315800 |
| H | -1.26966100 | -0.70640600 | -2.09676900 |
| Pd | -0.27345100 | 0.92763700 | 0.65949600 |
| H | 3.79542900 | 2.72957300 | -1.38374200 |
| H | -3.86569300 | 2.87658100 | -0.21363200 |
| H | 1.24216400 | 2.73095300 | -1.20314400 |
| O | 0.79600100 | 2.44578500 | -2.02522900 |
| H | -0.12810600 | 2.30360300 | -1.75867500 |
| H | 1.38980300 | 0.68170800 | -2.13329000 |
| O | 1.65858600 | -0.26001100 | -2.08014400 |
| H | 2.55694500 | -0.22245700 | -1.72818100 |

45

RR_s_TS, E(SCF) = -2254.84558449, E(ZPE) =
-2254.521995, E(G) = -2254.578886 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.02506400 | 1.73939300 | 1.15573800 |
| N | 0.77831900 | 1.59808300 | -0.97139700 |
| C | -2.33603100 | 1.37655400 | 1.74982900 |
| H | -2.11632400 | 1.05681700 | 2.77248100 |
| C | 2.21360000 | 1.48902200 | -1.33444500 |
| H | 2.71200200 | 2.41472100 | -1.03654600 |
| C | -3.04928900 | 0.27823200 | 1.03041200 |
| C | -2.42318800 | -0.98878900 | 0.91027200 |
| C | -4.34410100 | 0.46005100 | 0.57294600 |
| C | -3.18241800 | -2.04450500 | 0.37389700 |
| C | -5.05950000 | -0.59035400 | 0.02294300 |
| H | -4.81644100 | 1.43446900 | 0.65678800 |
| C | -4.47613600 | -1.84866300 | -0.06112600 |
| H | -2.71235700 | -3.01934700 | 0.29878300 |
| H | -5.03904700 | -2.67677700 | -0.48085500 |
| C | 2.97482000 | 0.31985700 | -0.76637800 |
| C | 2.40634000 | -0.95661800 | -0.54014100 |
| C | 4.34014400 | 0.50138500 | -0.57751200 |
| C | 3.27620900 | -2.00257600 | -0.17006400 |
| C | 5.16864000 | -0.53998000 | -0.20635500 |
| H | 4.77524000 | 1.48325700 | -0.73813900 |
| C | 4.62861100 | -1.80592200 | -0.01219000 |
| H | 2.83482600 | -2.98034500 | -0.00835000 |
| H | 5.27117200 | -2.63227700 | 0.27561300 |
| O | -1.17839500 | -1.19328600 | 1.29033400 |
| O | 1.12338700 | -1.22645300 | -0.67053500 |
| S | -6.73162200 | -0.35435500 | -0.57917300 |
| S | 6.92446600 | -0.28639700 | 0.05303600 |
| O | 7.61396700 | -1.21086400 | -0.89315800 |
| O | 7.18335600 | -0.64251400 | -1.47821100 |
| O | 7.18628600 | 1.14976400 | -0.24287000 |
| O | -7.05843700 | 1.07832600 | -0.33500400 |
| O | -7.58716000 | -1.28822800 | 0.20891200 |
| O | -6.70158300 | -0.70546600 | -2.02877900 |
| H | -0.41701700 | 2.05927300 | 1.90818000 |
| H | -2.96673800 | 2.26975900 | 1.80917200 |
| O | 0.23072200 | 1.40958700 | -1.80927100 |
| H | 2.26591300 | 1.45133000 | -2.42751000 |
| Pd | -0.02054900 | 0.16764600 | 0.27148400 |
| C | 0.34923600 | 2.91726800 | -0.44435100 |
| C | -1.05003500 | 2.78863400 | 0.11342000 |
| H | -1.39719800 | 3.74141400 | 0.52463000 |
| H | -1.75905200 | 2.47469300 | -0.65892400 |

H 1.04677200 3.19496700 0.35091400
H 0.40173300 3.68463000 -1.22127100

45
RR_s, E(SCF) = -2254.84695611, E(ZPE) = -2254.522600, E(G) = -2254.580705 a.u.

N -0.77151100 1.47227500 1.16259600
N 0.77205100 1.47243600 -1.16340800
C -2.08768100 1.18243400 1.78693700
H -1.86307500 0.77842300 2.77827700
C 2.08817800 1.18219900 -1.78769300
H 2.63619700 2.11853900 -1.93188300
C -2.92273400 0.19567900 1.03444200
C -2.39895600 -1.09313400 0.75670400
C -4.23476200 0.49732700 0.70677100
C -3.26763200 -2.04330000 0.19150100
C -5.06346800 -0.45194400 0.13259100
H -4.62875000 1.48664600 0.91781200
C -4.57537800 -1.72920800 -0.11396500
H -2.87310000 -3.03412700 -0.00715000
H -5.22458900 -2.47880300 -0.55631200
C 2.92294900 0.19547500 -1.03488400
C 2.39904200 -1.09335400 -0.75738600
C 4.23478600 0.49719200 -0.70655100
C 3.26751000 -2.04348100 -0.19178200
C 5.06320600 -0.45198400 -0.13178600
H 4.62883100 1.48652700 -0.91739200
C 4.57506000 -1.72929100 0.11442900
H 2.87296200 -3.03435800 0.00659400
H 5.22408300 -2.47882200 0.55716900
O -1.14743400 -1.41543400 1.01994300
O 1.14764900 -1.41560700 -1.02121000
S -6.75179300 -0.05334800 -0.32307400
S 6.75138100 -0.05341200 0.32439100
O 7.60984200 -1.06365200 -0.35839000
O 6.81351700 -0.17205300 1.81037100
O 6.99302800 1.33567200 -0.15620000
O -6.99374000 1.33520100 0.15891400
O -7.60995200 -1.06444700 0.35875700
O -6.81395000 -0.17060400 -1.80917500
H -0.08193700 1.55109900 1.90845300
H -2.63551400 2.11890900 1.93094500
H 0.08262800 1.55196800 -1.90933000
H 1.86346300 0.77800600 -2.77893000
Pd -0.00000000 -0.04911100 -0.00069500
C 0.67753700 2.69660200 -0.33859500
C -0.67643600 2.69676800 0.33833700
H -0.81568700 3.59234300 0.95022800
H -1.48214500 2.66295500 -0.40213400
H 1.48324200 2.66208700 0.40185500
H 0.81720200 3.59238800 -0.95008200

47
RR_D1_TS1_R_no2W, E(SCF) = -2256.03651671, E(ZPE) = -2255.698398, E(G) = -2255.758486 a.u.

C 0.63738800 2.98376500 0.37845500
H 0.40617400 2.94222200 1.44679800
H 1.24260400 3.87581900 0.19713600
C -0.63155400 2.99088000 -0.43790900
H -1.24348400 3.87242300 -0.22929600
H -0.40190100 2.98218400 -1.50729400
N -1.37412000 1.74803000 -0.13331400
N 1.39138700 1.75613300 0.03999600
C -2.46095900 1.41296900 -1.07474000
H -3.10464500 2.28783500 -1.21846400
C 2.47253800 1.40480200 0.98134900
H 1.98555600 1.15760600 1.93176700
C -3.27543800 0.26623100 -0.56334900
C -2.67647300 -0.96686200 -0.20088900
C -4.65208500 0.42279100 -0.44738200
C -3.53584000 -2.00554600 0.21945800
C -5.46608600 -0.60516100 -0.01469000
H -5.10464600 1.37434600 -0.70830300
C -4.89631600 -1.83156400 0.31357500
H -5.52603500 -2.64852200 0.65278400
C 3.30392200 0.27427000 0.46037700

C 2.72185100 -0.95078700 0.04574000
C 4.68560800 0.42503300 0.42818500
C 3.60072800 -1.98216400 -0.35313700
C 5.52003400 -0.60008100 0.02937000
H 5.12544000 1.36810700 0.73768300
C 4.96481100 -1.81490200 -0.36115200
H 5.61023400 -2.62933600 -0.67580900
O -1.39187300 -1.21656300 -0.23691100
O 1.43827700 -1.20691600 0.02690600
S -7.23944100 -0.39161000 0.12751000
S 7.29755000 -0.38457200 -0.02340600
O 7.68457400 -0.49477000 -1.46045400
O 7.86907400 -1.48929600 0.79992800
O 7.56774300 0.96521200 0.54655400
O -7.51750500 1.02269700 -0.24842300
O -7.57559200 -0.69250200 1.54921900
O -7.84766900 -1.37459600 -0.81568400
H -2.69196400 0.37837300 2.92202400
H -2.98930200 0.07268000 0.23479000
H -1.77312800 1.82028700 0.80421000
H -1.98225500 1.19127200 -2.03531800
H 1.79709800 1.86217000 -0.89087500
H 3.10793900 2.28073400 1.24838300
Pd 0.01575400 0.23755800 -0.07461000
H -3.07841200 -2.95186200 0.48790700
H 3.15645900 -2.92240900 -0.66213700

53
RR_D1_TS1_R_REF, E(SCF) = -2408.92120538, E(ZPE) = -2408.532248, E(G) = -2408.598705 a.u.

C 0.62489000 3.14895100 0.35009000
H 0.38614100 3.12433800 1.41722600
H 1.23569200 4.03472700 0.15882700
C -0.63544000 3.14493700 -0.47714600
H -1.25093900 4.02753500 -0.28572400
H -0.39860800 3.11944700 -1.54448800
N -1.37998400 1.90615600 -0.15704500
N 1.37935100 1.91379100 0.03610600
C -2.47754700 1.57337500 -1.08842900
H -3.10401600 2.45847900 -1.24213100
C 2.45830000 1.58482000 0.98972800
H 1.96932000 1.33786100 1.93864300
C -3.31084100 0.45165400 -0.55348000
C -2.73551000 -0.78301500 -0.18394300
C -4.68516500 0.62740100 -0.43550400
C -3.59295500 -1.80282600 0.26685100
C -5.50720500 -0.38625500 0.01450500
H -5.12728000 1.58046000 -0.70758900
C -4.95266900 -1.61279600 0.36115300
H -5.58968200 -2.41636300 0.71714700
C 3.31162500 0.46457300 0.48322200
C 2.75648800 -0.76803600 0.07672200
C 4.69143300 0.63451700 0.45093400
C 3.63749300 -1.79016700 -0.32143500
C 5.53685600 -0.38260300 0.05596700
H 5.11919200 1.58433200 0.75579000
C 5.00059600 -1.60574200 -0.33019200
H 5.65666300 -2.41253400 -0.64121700
O -1.44157300 -1.04775200 -0.24833300
O 1.46264600 -1.03811200 0.06737800
S -7.28039000 -0.14991300 0.16044100
S 7.31480800 -0.14523600 0.00691700
O 7.70076300 -0.25126500 -1.44296390
O 7.89268100 -1.24407700 0.83180800
O 7.56519600 1.20713700 0.57754500
O -7.53976500 1.26590500 -0.22011100
O -7.61104700 -0.44176700 -1.58435000
O -7.89904100 -1.12953900 -0.77798100
H -1.77204000 1.98936700 0.78304300
H -2.00955200 1.32602900 -2.04739000
H 1.78824200 2.00320400 -0.89553100
H 3.07739600 2.47272600 1.15726000
Pd 0.00636800 0.39829100 -0.07356600
H -3.14884600 -2.75451100 0.54078600
H 3.20530800 -2.73988100 -0.62080400
H -0.80064100 -2.36418500 0.99287600

| | | | |
|---|-------------|-------------|-------------|
| H | -1.78116500 | 0.03626600 | 3.05751500 |
| H | -1.65939600 | -0.29641200 | 2.39620200 |
| O | -0.14175800 | -2.84211000 | 1.52405300 |
| H | 0.66846700 | -2.41522900 | 1.20468700 |
| H | -0.59644500 | -2.21445900 | -1.59536200 |
| O | 0.22403500 | -2.55884700 | -1.98022500 |
| H | 0.87381000 | -2.16914300 | -1.37193100 |

53

RR_D1_I1_CH-Homo_P, E(SCF) = -
2408.89449246, E(ZPE) = -2408.500952, E(G)
= -2408.565854 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.39468000 | 1.83608000 | 0.24568500 |
| N | -1.43303300 | 1.90480600 | 0.30007700 |
| C | 2.48191600 | 1.23928100 | 1.05325200 |
| H | 3.16862200 | 2.03421400 | 1.36444400 |
| C | -2.64360600 | 2.00311900 | -0.52005200 |
| H | -2.31824800 | 2.32028400 | -1.51921900 |
| C | 3.24332500 | 0.13120500 | 0.34031600 |
| C | 2.95398700 | -1.24946700 | 0.89760300 |
| C | 4.67125900 | 0.42565600 | 0.06838100 |
| C | 3.98597700 | -2.25147200 | 0.72912500 |
| C | 5.58503000 | -0.54523400 | 0.03809400 |
| H | 4.95232200 | 1.44869300 | -0.16178300 |
| C | 5.22820300 | -1.90863400 | 0.34289900 |
| H | 6.00277800 | -2.66678100 | 0.27645200 |
| C | -3.38283400 | 0.70149400 | -0.57974800 |
| C | -2.77671500 | -0.48135600 | -1.06854600 |
| C | -4.71554600 | 0.67267000 | -0.18471500 |
| C | -3.58278900 | -1.63515500 | -1.16062800 |
| C | -5.48010900 | -0.47441900 | -0.27630000 |
| H | -5.17538500 | 1.58011600 | 0.19469900 |
| C | -4.90274600 | -1.63761100 | -0.77263400 |
| H | -5.49192600 | -2.54584800 | -0.85379400 |
| O | 1.87212900 | -1.50637400 | 1.41343800 |
| O | -1.52665100 | -0.58145500 | -1.47179100 |
| S | 7.30742700 | -0.21173400 | -0.36667500 |
| S | -7.18988600 | -0.49713500 | 0.26119300 |
| O | -7.24702400 | -1.44526200 | 1.41198500 |
| O | -7.98165900 | -0.98125500 | -0.90666700 |
| O | -7.52140900 | 0.90279700 | 0.64824300 |
| O | 7.39736000 | 1.25120100 | -0.60094500 |
| O | 7.57254500 | -1.03027200 | -1.58017400 |
| O | 8.07034100 | -0.67556500 | 0.82306600 |
| H | 0.29799400 | -2.40994700 | 0.47295200 |
| H | 1.01501700 | -0.31678900 | -1.40751200 |
| H | 2.77102000 | 0.02291700 | -0.66202500 |
| O | -0.62154900 | -2.62457400 | 0.26038500 |
| H | -0.84725800 | -2.01787600 | -0.47175800 |
| H | 0.11579000 | -0.59701100 | 2.20469800 |
| O | -0.84552800 | -0.57029900 | 2.31428400 |
| H | -1.12021600 | -1.24309600 | 1.66845500 |
| H | 1.81685500 | 2.32820400 | -0.54151400 |
| H | 2.02075100 | 0.83739800 | 1.95695900 |
| H | -1.65071300 | 1.50485400 | 1.21433700 |
| H | -3.31128500 | 2.78469200 | -0.13496900 |
| Pd | -0.03546100 | 0.57602800 | -0.65040200 |
| H | 3.73764300 | -3.26813700 | 1.01058900 |
| H | -3.11999100 | -2.53825400 | -1.54603300 |
| C | -0.68148400 | 3.15503100 | 0.44215100 |
| C | 0.65337000 | 2.83641200 | 1.06426100 |
| H | -1.21890000 | 3.89363300 | 1.04830600 |
| H | 1.25706200 | 3.73706200 | 1.20515700 |
| H | 0.49584900 | 2.38867000 | 2.05028300 |
| H | -0.55060700 | 3.58074400 | -0.55820600 |

53

RR_D1_I1_CH_R, E(SCF) = -2408.89663065,
E(ZPE) = -2408.504482, E(G) = -2408.567994
a.u.

| | | | |
|---|-------------|------------|-------------|
| N | 1.55844100 | 2.21714200 | 0.11341500 |
| N | -1.16171300 | 2.01001500 | -0.18451500 |
| C | 2.54123500 | 1.94553700 | 1.21617600 |
| H | 3.26180300 | 2.77043400 | 1.21553700 |
| C | -2.33605500 | 1.77361800 | -1.04432600 |
| H | -1.97826600 | 1.83239400 | -2.07867500 |
| C | 3.21235100 | 0.62705300 | 1.09147700 |

| | | | |
|----|-------------|-------------|--------------|
| C | 2.62774300 | -0.49445900 | 1.75704200 |
| C | 4.34672600 | 0.48316500 | 0.30480500 |
| C | 3.25869400 | -1.74908500 | 1.53150000 |
| C | 4.92912700 | -0.75523000 | 0.11069400 |
| H | 4.77772100 | 1.35466400 | -0.18098700 |
| C | 4.37042000 | -1.87275500 | 0.73197500 |
| H | 4.81937300 | -2.84983800 | 0.57692000 |
| C | -3.00939100 | 0.47086600 | -0.76363700 |
| C | -2.29305300 | -0.74141700 | -0.79648800 |
| C | -4.38136100 | 0.45159000 | -0.53813300 |
| C | -3.01046000 | -1.93929200 | -0.62321900 |
| C | -5.06568000 | -0.73465400 | -0.36810000 |
| H | -4.93106500 | 1.38683100 | -0.50758400 |
| C | -4.37059900 | -1.93775100 | -0.41757500 |
| H | 4.90015200 | -2.87608700 | -0.28610800 |
| O | 1.57026500 | -0.39235100 | 2.47871100 |
| O | -0.98964200 | -0.83615700 | -0.99795200 |
| S | 6.39627600 | -0.94901200 | -0.89489800 |
| S | -6.85619600 | -0.75548700 | -0.145311200 |
| O | -7.01930700 | -1.40666600 | 1.25320200 |
| O | -7.41995500 | -1.55968100 | -1.18635100 |
| O | -7.27362700 | 0.66756400 | -0.09144500 |
| O | 6.69686200 | 0.39944500 | -0.45360300 |
| O | 6.04831600 | -1.94909800 | -1.94687200 |
| O | 7.46579800 | -1.44788400 | 0.01946800 |
| H | 0.31358400 | -1.57360600 | 2.00986100 |
| H | 1.46602000 | -0.53500200 | -1.23269000 |
| H | 1.79303700 | -0.43502500 | -0.49807200 |
| O | -0.50358800 | -2.02795400 | 1.70864600 |
| H | -0.56765700 | -1.80829700 | 0.76716600 |
| H | 0.04507200 | 0.61069100 | 2.52862400 |
| O | -0.91195900 | 0.82772800 | 2.49412200 |
| H | -1.28767700 | -0.05189800 | 2.33914400 |
| H | 2.08927100 | 2.43359400 | -0.73126200 |
| H | 1.97518800 | 1.98246700 | 2.14863600 |
| H | -1.38501300 | 1.85196000 | 0.81128700 |
| H | -3.04595900 | 2.59423400 | -0.89541700 |
| Pd | 0.30965600 | 0.64324600 | -0.50879000 |
| H | 2.82632600 | -2.62165500 | -0.10286300 |
| H | -2.45596500 | -2.87108100 | -0.65695700 |
| C | -0.55040600 | 3.34055600 | -0.38108600 |
| C | 0.69784000 | 3.38375300 | 0.45007800 |
| H | -1.25340500 | 4.12688100 | -0.09111600 |
| H | 1.24646800 | 4.31917600 | 0.32257200 |
| H | 0.43364600 | 3.29086500 | 1.50691600 |
| H | -0.33296800 | 3.45221900 | -1.44654900 |

53

RR_D1_I1_CH_TS, E(SCF) = -2408.87823538,
E(ZPE) = -2408.490032, E(G) = -2408.554836
a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.47344800 | 2.30669800 | 0.04886300 |
| N | -1.29274700 | 2.04855400 | -0.11158100 |
| C | 2.56177300 | 1.95965200 | 1.00900100 |
| H | 3.34198600 | 2.72405400 | 0.94608100 |
| C | -2.43541800 | 1.80128400 | -0.99956900 |
| H | -2.05538800 | 1.88009700 | -2.02583100 |
| C | 3.13389100 | 0.58791200 | 0.79079400 |
| C | 2.71345200 | -0.46273900 | 1.71613700 |
| C | 4.36548300 | 0.44130700 | 0.08061300 |
| C | 3.43119900 | -1.70268100 | 1.61961700 |
| C | 5.01805000 | -0.74703300 | 0.05745500 |
| H | 4.74781200 | 1.28033900 | -0.49275000 |
| C | 4.53139600 | -1.83027000 | -0.83266900 |
| H | 5.06357600 | -2.77644000 | 0.79840200 |
| C | -3.06763600 | 0.46691700 | -0.74838400 |
| C | -2.32317900 | -0.73498700 | -0.77514500 |
| C | -4.44192200 | 0.41486800 | -0.53786400 |
| C | -3.02903700 | -1.94411800 | -0.60783900 |
| C | -5.10884300 | -0.78267700 | -0.37400100 |
| H | -5.01003200 | 1.33946700 | -0.51270300 |
| C | -4.38977200 | -1.97192600 | -0.41278300 |
| H | -4.90122600 | -2.92092600 | -0.28443000 |
| O | 1.71067100 | -0.33071200 | 2.45558000 |
| O | -1.02029800 | -0.82165000 | -0.96279100 |
| S | 6.52654200 | -0.97784400 | -0.88795500 |
| S | -6.87892500 | -0.83621200 | -0.09503200 |

Pd -0.06905500 0.05715700 -0.19451500
H 3.98577800 -3.38879200 0.85429300
H -3.32566300 -2.94455400 -0.60717400

47

RR_D1_no2W_R, E(SCF) = -2256.03673917,
E(ZPE) = -2255.696978, E(G) = -2255.755845
a.u.

C -0.63740800 2.99602500 -0.35137400
H -0.41510700 2.96614500 -1.42237300
H -1.24266000 3.88506600 -0.15602400
C 0.63871600 2.99702600 0.45428000
H 1.24519900 3.88401400 0.25287500
H 0.41833400 2.97195800 1.52535700
N 1.38306300 1.76169900 0.12399600
N -1.38645700 1.76348900 -0.02029700
C 2.48612000 1.42006900 1.04302000
H 3.13032600 2.29489500 1.18486400
C -2.47179900 1.41727500 -0.95863400
H -1.98942400 1.18075200 -1.91457100
C 3.29554800 0.27824900 0.51172900
C 2.69347000 -0.95166600 0.14269700
C 4.67534000 0.42362400 0.41949300
C 3.55065300 -1.99148600 -0.28000600
C 5.48814300 -0.61013500 -0.00057400
H 5.13168400 1.36984300 0.69331500
C 4.91381900 -1.82933900 -0.34716700
H 5.54255200 -2.64975800 -0.67985200
C -3.29624400 0.27880800 -0.44347600
C -2.70747600 -0.94857100 -0.04597500
C -4.67822400 0.42522900 -0.39762400
C -3.57962400 -1.98690800 0.34920800
C -5.50565200 -0.60549500 0.00087200
H -5.12411600 1.37058400 -0.69105800
C -4.94395300 -1.82397700 0.37005700
H -5.58383900 -2.64296000 0.68450000
O 1.40953000 -1.20382200 0.18968600
O -1.42289500 -1.20093100 -0.03846000
S 7.26563300 -0.41389200 -0.10593100
S -7.28518700 -0.40714900 0.04893500
O -7.55770100 0.99902600 -0.36090900
O -7.69203800 -0.69207900 1.45581500
O -7.83593000 -1.40911500 -0.90949100
O 7.62735400 -0.70381700 -1.52387300
O 7.84464800 -1.41334300 0.83834300
O 7.55200100 0.99333100 0.29032700
H 0.85212200 0.87973900 -3.16402600
H 0.82272200 0.35706200 -2.62519700
H 1.76931500 1.85112100 -0.81739400
H 2.02343400 1.18839200 2.00921900
H -1.78617900 1.85819900 0.91439900
H -3.11119200 2.29250400 -1.11886100
Pd -0.00511900 0.24737900 0.06720000
H 3.09041900 -2.93428800 -0.55601900
H -3.12981200 -2.92873500 0.64504900

47

RR_D1_no2W_TS, E(SCF) = -2255.99924043,
E(ZPE) = -2255.662552, E(G) = -2255.723015
a.u.

C -0.61968500 3.08200300 -0.13518200
H -0.41906400 3.22797300 -1.19956800
H -1.22010500 3.92513700 0.21902800
C 0.65097100 2.93871900 0.65262900
H 1.28191500 3.82698800 0.57574800
H 0.41627500 2.79035300 1.71063700
N 1.39113200 1.73132200 0.20028900
N -1.37071600 1.81505800 0.00483000
C 2.36296300 1.28867700 1.24776000
H 2.96170200 2.16501400 1.52338800
C -2.55822300 1.70663200 -0.87122200
H -2.18519100 1.73967700 -1.90031800
C 3.24547100 0.16830900 0.83138400
C 2.70748300 -1.15717500 0.83342600
C 4.57529200 0.40102100 0.51331300
C 3.62225200 -2.19890000 0.50437200
C 5.42792800 -0.63953600 0.18794600

H 4.96194800 1.41627400 0.52597900
C 4.93711600 -1.94578400 0.19384900
H 5.60224500 -2.76764500 -0.05708800
C -3.33088600 0.46023600 -0.58914000
C -2.70528000 -0.80262000 -0.68496200
C -4.67898100 0.53914900 -0.26422800
C -3.49261100 -1.94805300 -0.45626200
C -5.43222300 -0.59932500 -0.05339400
H -5.15720200 1.51045600 -0.18471600
C -4.83127300 -1.84879400 -0.16057800
H -5.41812800 -2.74678200 0.00526300
O 1.47330300 -1.38528700 1.07590400
O -1.44076800 -0.97107300 -1.00526100
S 7.14517800 -0.34947700 -0.20751800
S -7.17572000 -0.49780200 -0.35703300
O -7.51072200 0.95292000 0.37414900
O -7.32019500 -1.14498600 1.69243700
O -7.88862700 -1.24868800 -0.71573700
O 7.36541800 -0.92257500 -1.56940300
O 7.94458400 -1.06554200 0.83189200
O 7.34086800 1.12847700 -0.16540000
H 1.19856300 -0.54709200 -1.63146400
H 1.17195300 -1.07282800 -1.56940300
H 1.91987800 1.96365600 -0.64142700
H 1.75324100 1.00417600 2.11029400
H -1.67064200 1.70352200 0.97532000
H -3.19405400 2.58477700 -0.71474000
Pd -0.01918400 0.32010000 -0.40592900
H 3.24155300 -3.21609800 0.50315100
H -3.00941000 -2.91571400 -0.54032100

56

RR_D1_TS1_3W_HOphen_P, E(SCF) = -
2485.35066686, E(ZPE) = -2484.932077, E(G) =
-2485.000464 a.u.

C -0.60844800 3.54866400 -0.28406000
H -0.30326600 3.73609300 -1.31908200
H -1.28032800 4.36197600 0.01713200
C 0.58856700 3.49822000 0.63636600
H 1.14161800 4.44047800 0.62683000
H 0.23870600 3.32410300 1.65725600
N 1.49260900 2.35917100 0.29289300
N -1.26764200 2.24037500 -0.23355300
C 2.28563200 1.91189100 1.48568300
H 3.01793000 2.69539700 1.71118100
C -2.36931500 2.03719800 -1.17479700
H -1.96823100 2.17094700 -2.18607100
C 2.93605500 0.59361200 1.27045600
C 2.23161000 -0.58550300 1.66260700
C 4.15305000 0.51090100 0.61704000
C 2.84245800 -1.82220100 1.31677900
C 4.71579200 -0.71334400 0.29169500
H 4.67219800 1.42231800 0.33080700
C 4.04575100 -1.88076400 0.64725100
H 4.47941100 -2.84539100 0.39778500
C -2.95676300 0.66566500 -0.99922100
C -2.23354700 -0.50565400 -1.25536600
C -4.25284000 0.52757800 -0.52967800
C -2.80096100 -1.75385700 -1.07115000
C -4.82589600 -0.72002200 -0.33589900
H -4.82999300 1.42199000 -0.31408100
C -4.10070900 -1.86332200 -0.60514200
H -4.55133100 -2.83654000 -0.45409700
O 1.10321500 -0.54609300 2.27688200
O -0.94444500 -0.41360000 -1.73375700
S 6.29026500 -0.82494100 -0.54600400
S -6.51979800 -0.81136000 0.27237100
O -6.82414000 -2.26013400 0.40660900
O -7.34545900 -0.12811100 -0.76118000
O -6.51151000 -0.08673900 1.57261300
O 6.69827900 0.57564500 -0.85596800
O 6.05349500 -1.64302000 -1.77282300
O 7.22635700 -1.50118600 0.40170600
H 0.03198800 -1.91323900 1.98147800
H 1.31686900 -2.14591000 -0.71436900
H 1.63922100 0.09139100 -1.07995300
O -0.58609100 -2.63167400 1.71754900

| | | | |
|----|-------------|-------------|-------------|
| H | -0.40118700 | -2.75267000 | 0.77712200 |
| H | -0.27216300 | 0.52136100 | 2.33782600 |
| O | -1.08163500 | 1.08184800 | 2.40090800 |
| H | -1.51884400 | 0.82148700 | 3.21389500 |
| H | 2.15709200 | 2.67011600 | -0.41396000 |
| H | 1.58302300 | 1.84805500 | 2.31826100 |
| H | -1.54691900 | 2.00843300 | 0.72571200 |
| H | -3.15679800 | 2.78821600 | -1.03476500 |
| Pd | 0.37011200 | 0.91895500 | -0.70652400 |
| O | 0.50221100 | -2.54904200 | -1.05557100 |
| H | -0.49246700 | -1.29430600 | -1.68868800 |
| H | 0.77746200 | -3.32088100 | -1.56014300 |
| H | -2.21860900 | -2.64264100 | -1.28793100 |
| H | 2.33239400 | -2.73624000 | 1.60956700 |

56

RR_D1_TS1_3W_HOphen_R, E(SCF) = -
2485.33423336, E(ZPE) = -2484.920272, E(G)
= -2484.990653 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.59939200 | 3.34521900 | -0.82489800 |
| H | -0.36466100 | 3.32152100 | -1.89238900 |
| H | -1.30980400 | 4.15906400 | -0.65061700 |
| C | 0.63472200 | 3.50519800 | 0.01531300 |
| H | 1.20065300 | 4.39885000 | -0.25449700 |
| H | 0.35181300 | 3.58587900 | 1.06699900 |
| N | 1.48643800 | 2.28851000 | -0.11405700 |
| N | -1.21109000 | 2.04740400 | -0.46707700 |
| C | 2.37546400 | 2.12986400 | 1.08561200 |
| H | 3.08271400 | 2.96648100 | 1.06956200 |
| C | -2.39749100 | 1.71179500 | -1.27500100 |
| H | -2.06071500 | 1.64886100 | -2.31570900 |
| C | 3.07490500 | 0.82033500 | 1.12379300 |
| C | 2.47914200 | -0.25181600 | 1.85557200 |
| C | 4.25531900 | 0.63555500 | 0.41533100 |
| C | 3.16318800 | -1.49778500 | 1.79977800 |
| C | 4.87874400 | -0.59666300 | 0.37177500 |
| H | 4.69188500 | 1.47002800 | -0.12761600 |
| C | 4.31943500 | -1.66421100 | 1.07598600 |
| H | 4.80497900 | -2.63559100 | 1.04887100 |
| C | -3.05067400 | 0.44509500 | -0.82893500 |
| C | -2.32393300 | -0.76236100 | -0.79389400 |
| C | -4.39546400 | 0.43935900 | -0.49664100 |
| C | -2.99983100 | -1.94091600 | -0.45847100 |
| C | -5.04709500 | -0.73554800 | -0.15798200 |
| H | -4.94936300 | 1.37407800 | -0.51578800 |
| C | -4.34550100 | -1.92954400 | -0.14802200 |
| H | -4.85719000 | -2.84853900 | 0.11345400 |
| O | 1.37043700 | -0.12518300 | 2.49524200 |
| O | -1.03134400 | -0.83817100 | -1.08980600 |
| S | 6.40290300 | -0.84250800 | -0.53159300 |
| S | -6.79395100 | -0.67335000 | 0.25831600 |
| O | -7.18605400 | -2.07050400 | 0.58793700 |
| O | -7.47969200 | -0.14428800 | -0.95482100 |
| O | -6.89881700 | 0.25418200 | 1.41994800 |
| O | 6.68704900 | 0.44567300 | -1.22576500 |
| O | 6.14706900 | -1.96798200 | -1.47801800 |
| O | 7.43743400 | -1.19219100 | 0.48634000 |
| H | 0.28806500 | -1.45342400 | 1.97534900 |
| H | 1.43164900 | -0.62753300 | -1.16803600 |
| H | 1.77267300 | -0.32924500 | -0.49217800 |
| O | -0.30042700 | -2.13705900 | 1.58937900 |
| H | -0.46398300 | -1.82827500 | 0.68808400 |
| H | -0.02212100 | 0.95265900 | 2.40318700 |
| O | -0.81329000 | 1.53588900 | 2.31592000 |
| H | -1.30745700 | 1.44292600 | 3.13285000 |
| H | 2.08523800 | 2.39544000 | -0.93383300 |
| H | 1.73183100 | 2.23892300 | 1.95924100 |
| H | -1.42128200 | 2.01382300 | 0.54334500 |
| H | -3.10998200 | 2.54071000 | -1.20757600 |
| Pd | 0.26914000 | 0.66383000 | -0.63836400 |
| O | 0.73165100 | -2.84858900 | -1.74664500 |
| H | -0.04879800 | -2.27647800 | -1.63544400 |
| H | 0.68786800 | -3.15976200 | -2.65337900 |
| H | -2.43570900 | -2.86835900 | -0.44606400 |
| H | 2.72921900 | -2.33113300 | 2.34371000 |

56

RR_D1_TS1_3W_HOphen, E(SCF) = -
2485.32038907, E(ZPE) = -2484.907124, E(G)
= -2484.974953 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.61538500 | 3.33534500 | -0.71648400 |
| H | -0.39798900 | 3.33080500 | -1.78858400 |
| H | -1.29632600 | 4.16925400 | -0.51464800 |
| C | 0.64113200 | 3.45871800 | 0.09984300 |
| H | 1.20640300 | 4.35749100 | -0.15631100 |
| H | 0.37748800 | 3.51579300 | 1.15836900 |
| N | 1.48929000 | 2.24259000 | -0.06757900 |
| N | -1.24507000 | 2.04639100 | -0.37918000 |
| C | 2.37981100 | 2.06501900 | 1.12754000 |
| H | 3.07849600 | 2.90973000 | 1.13322700 |
| C | -2.42710500 | 1.73968800 | -1.19629300 |
| H | -2.08890800 | 1.71328700 | -2.23898100 |
| C | 3.09303000 | 0.76418500 | 1.13872200 |
| C | 2.49590400 | -0.33442700 | 1.82449000 |
| C | 4.27565900 | 0.60958200 | 0.43317500 |
| C | 3.18909800 | -1.57190200 | 1.74048900 |
| C | 4.90868400 | -0.61862500 | 0.35305800 |
| H | 4.70913400 | 1.46429700 | -0.08027000 |
| C | 4.35158800 | -1.71016900 | 1.01862900 |
| H | 4.84362400 | -2.67455500 | 0.96547600 |
| C | -3.07874000 | 0.44987900 | -0.80995300 |
| C | -2.36893800 | -0.76946900 | -0.84922700 |
| C | -4.42155900 | 0.43910000 | -0.46798900 |
| C | -3.06034900 | -1.95433100 | -0.57335700 |
| C | -5.08757900 | -0.74298200 | -0.18609900 |
| H | -4.96380500 | 1.38032600 | -0.43329200 |
| C | -4.40262100 | -1.94436600 | -0.24731800 |
| H | -4.92350600 | -2.86964600 | -0.02985700 |
| O | 1.38386500 | -0.23157200 | 2.46582000 |
| O | -1.07632000 | -0.84242400 | -1.14995600 |
| S | 6.44261200 | -0.82469500 | -0.54024400 |
| S | -6.83096400 | -0.68237500 | 0.24159400 |
| O | -7.23218600 | -2.08769800 | 0.52338100 |
| O | -7.52111500 | -0.10628900 | -0.94788600 |
| O | -6.92451900 | 0.20405400 | 1.43615800 |
| O | 6.71174700 | 0.47939900 | -1.21681800 |
| O | 6.21763700 | -1.94233500 | -1.50507800 |
| O | 7.47993000 | -1.16976500 | 0.47792200 |
| H | 0.26509900 | -1.49934400 | 1.95902700 |
| H | 1.30589100 | -1.18758800 | -1.29340200 |
| H | 1.63115000 | -0.28591500 | -0.88483600 |
| O | -0.37699500 | -2.13626200 | 1.57337500 |
| H | -0.59773900 | -1.74567300 | 0.71811300 |
| H | 0.01088700 | 0.85884900 | 2.43026700 |
| O | -0.77835000 | 1.45160500 | 2.40217500 |
| H | -1.23295500 | 1.32574200 | 3.23740000 |
| H | 2.09040300 | 2.37196900 | -0.88118900 |
| H | 1.73497200 | 2.14731200 | 2.00361700 |
| H | -1.45588200 | 2.00026200 | 0.62671000 |
| H | -3.15212500 | 2.55728500 | -1.10975600 |
| Pd | 0.26494800 | 0.64806700 | -0.63476200 |
| O | 0.93302900 | -2.25642700 | -1.70741400 |
| H | -0.04254000 | -2.03201100 | -1.67743100 |
| H | 1.19913800 | -2.38056300 | -2.62752200 |
| H | -2.51072600 | -2.88946700 | -0.61425100 |
| H | 2.75669900 | -2.42566600 | 2.25413000 |

53

RR_D1_TS1_HOphen_P, E(SCF) = -
2408.89977060, E(ZPE) = -2408.506674, E(G)
= -2408.570492 a.u.

| | | | |
|---|-------------|------------|-------------|
| C | -1.38340500 | 1.49535100 | -2.04149500 |
| H | -1.80801100 | 0.48631500 | -2.06250600 |
| H | -2.02836200 | 2.13884900 | -2.65421000 |
| C | 0.02434700 | 1.51139200 | -2.59512700 |
| H | 0.05416200 | 1.11448900 | -3.61204600 |
| H | 0.37470600 | 2.54563300 | -2.62977900 |
| N | 0.98148000 | 0.76334100 | -1.72010900 |
| N | -1.32342200 | 1.94938200 | -1.64816400 |
| C | 2.36093900 | 1.34700900 | -1.80677100 |
| H | 2.73917800 | 1.14650200 | -2.81584300 |
| C | -2.59704900 | 2.01057300 | 0.07307200 |
| H | -3.35572900 | 2.53432500 | -0.52164700 |
| C | 3.27516800 | 0.81715700 | -0.76356400 |

| | | | |
|----|-------------|-------------|-------------|
| C | 3.37143300 | 1.51164800 | 0.47813700 |
| C | 3.96052500 | -0.36953600 | -0.96966500 |
| C | 4.18753300 | 0.90845400 | 1.47132500 |
| C | 4.74066900 | -0.93177800 | 0.02613600 |
| H | 3.87626500 | -0.87892300 | -1.92644000 |
| C | 4.84439200 | -0.28054100 | 1.25418800 |
| H | 5.45285500 | -0.71630000 | 2.04187900 |
| C | -3.13184400 | 0.66223200 | 0.46486500 |
| C | -2.45747500 | -0.17518700 | 1.35782600 |
| C | -4.34286300 | 0.21293500 | -0.03413400 |
| C | -2.97466300 | -1.39154100 | 1.75170800 |
| C | -4.87272200 | -1.01101800 | 0.34898400 |
| H | -4.88680100 | 0.84031300 | -0.73464300 |
| C | -4.19482500 | -1.81222200 | 1.24528700 |
| H | -4.61388200 | -2.76547000 | -0.34135400 |
| O | 2.75077500 | 2.61658500 | 0.71143600 |
| O | -1.22698100 | 0.25188600 | 1.83909300 |
| S | 5.62928600 | -2.45947000 | -0.23458500 |
| S | -6.45782300 | -1.45276400 | -0.36413500 |
| O | -6.26637600 | -1.50314200 | -1.81668900 |
| O | -7.43757200 | -0.50761300 | 0.12819600 |
| O | -6.71307300 | -2.88439600 | 0.20162800 |
| O | 5.29193500 | -2.90981000 | -1.61573600 |
| O | 5.15119300 | -3.40940400 | 0.81450200 |
| O | 7.07888900 | -2.13596200 | -0.07251400 |
| H | 1.72698500 | 2.50914400 | 2.13329000 |
| H | -0.90420300 | -0.34488400 | 2.52730000 |
| H | 1.16312300 | -0.53691300 | 0.58103100 |
| O | 1.10751100 | 2.43825800 | 2.89557800 |
| H | 0.24825200 | 2.29337800 | 2.48914500 |
| H | 1.47280400 | 3.48790300 | -0.02920000 |
| O | 0.70911700 | 3.98722800 | -0.41191600 |
| H | 0.78363600 | 4.88265100 | -0.07638000 |
| H | 1.04108700 | -0.19851100 | -2.05010500 |
| H | 2.24656500 | 2.42623200 | -1.69422200 |
| H | -0.84068700 | 2.85407100 | -0.59156900 |
| H | -2.41793900 | 2.60999900 | 0.97138100 |
| Pd | 0.10988700 | 0.52937100 | 0.15387500 |
| H | 4.26927800 | 1.41620300 | 2.42829100 |
| H | -2.42221500 | -2.01580700 | 2.44590500 |

53
RR_D1_TS1_HOphen_R, E(SCF) = -
2408.89373703, E(ZPE) = -2408.504002, E(G)
= -2408.569143 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -1.22721700 | 1.74051200 | -2.08075300 |
| H | -1.63969800 | 0.75315200 | -2.30484200 |
| H | -1.88085500 | 2.49310700 | -2.53389500 |
| C | 0.19305600 | 1.89682000 | -2.56991700 |
| H | 0.28663900 | 1.65862200 | -3.63007600 |
| H | 0.50473500 | 2.93404500 | -2.42829100 |
| N | 1.11545000 | 1.04951400 | -1.75493600 |
| N | -1.18170100 | 1.91304000 | -0.61518500 |
| C | 2.46458800 | 1.68117900 | -1.57467100 |
| H | 2.96337100 | 1.68003400 | -2.54983400 |
| C | -2.47589800 | 1.92287700 | 0.09943200 |
| H | -3.18969400 | 2.52484500 | -0.47238700 |
| C | 3.27164400 | 0.97803700 | -0.54154100 |
| C | 3.20366700 | 1.42277100 | 0.81422400 |
| C | 4.01079600 | -0.14554700 | -0.88622300 |
| C | 3.90799700 | 0.63414800 | 1.76507500 |
| C | 4.68102400 | -0.88573500 | 0.06972700 |
| H | 4.05563600 | -0.46470400 | -1.92454200 |
| C | 4.61820600 | -0.48636600 | 1.40419900 |
| H | 5.13691600 | -1.06681300 | 2.16174400 |
| C | -3.03804300 | 0.56684500 | 0.37308000 |
| C | -2.28563000 | -0.32998000 | 1.16567100 |
| C | -4.29761600 | 0.20484500 | -0.06389000 |
| C | -2.85711600 | -1.55463100 | 1.51769000 |
| C | -4.84441600 | -1.02348000 | 0.28458000 |
| H | -4.86814400 | 0.89617700 | -0.67857000 |
| C | -4.12754900 | -1.89450000 | 1.08691400 |
| H | -4.56345400 | -2.84864100 | 1.35870300 |
| O | 2.52433100 | 2.45147900 | 1.18285400 |
| O | -1.06019400 | -0.02259700 | 1.57767700 |
| S | 5.62108000 | -2.34309100 | -0.36469800 |
| S | -6.48215000 | -1.44538400 | -0.32359700 |

| | | | |
|----|-------------|-------------|-------------|
| O | -6.38940900 | -1.37210900 | -1.80943100 |
| O | -7.40024100 | -0.41556200 | 0.24018300 |
| O | -6.76586900 | -2.81714000 | 0.17767000 |
| O | 5.49353000 | -2.49182200 | -1.84447800 |
| O | 5.00352800 | -3.47493400 | 0.38601900 |
| O | 7.02407100 | -2.08108500 | 0.07058800 |
| H | 1.27321800 | 2.04237000 | 2.47714600 |
| H | 0.99840200 | -1.05792800 | 0.39117400 |
| H | 1.54431600 | -0.49273500 | 0.59294400 |
| O | 0.58569400 | 1.83704600 | 3.14269100 |
| H | -0.03768700 | 1.24524500 | 2.69577400 |
| H | 1.34104600 | 3.44615700 | 0.50205500 |
| O | 0.59928700 | 3.97194400 | 0.10624800 |
| H | 0.42834200 | 4.69925100 | 0.70824600 |
| H | 1.25106400 | 0.15960200 | -2.23390100 |
| H | 2.28622200 | 2.71699300 | -1.28281000 |
| H | -0.66981200 | 2.78588000 | -0.38591800 |
| H | -2.27935400 | 2.43888600 | 1.04523600 |
| Pd | 0.12210200 | 0.46904500 | 0.00366000 |
| H | 3.85754300 | 0.94509900 | 2.80431600 |
| H | -2.27736700 | -2.23336600 | 2.13317500 |

53
RR_D1_TS1_HOphen, E(SCF) = -2408.86058128,
E(ZPE) = -2408.472855, E(G) = -2408.537447
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 1.35020000 | 1.72776600 | 2.04913500 |
| H | 1.80285200 | 0.74058400 | 2.18072700 |
| H | 1.98721900 | 2.46291100 | 2.55291500 |
| C | -0.05953200 | 1.77525800 | 2.59346700 |
| H | -0.10093900 | 1.46068100 | 3.63732800 |
| H | -0.42807700 | 2.80188100 | 2.53657100 |
| N | -0.97886600 | 0.93868600 | 1.75747200 |
| N | 1.24781200 | 2.00865400 | 0.60810300 |
| C | -2.36296200 | 1.51259800 | 1.68809200 |
| H | -2.81893300 | 1.40300100 | 2.67807300 |
| C | 2.48287400 | 1.94541700 | -0.20055700 |
| H | 3.27005300 | 2.52785000 | 0.29021400 |
| C | -3.18649500 | 0.86753300 | 0.63120000 |
| C | -3.09927600 | 1.36070200 | -0.70447800 |
| C | -3.97241400 | -0.23456700 | 0.93041100 |
| C | -3.85787200 | 0.66624900 | -1.68217200 |
| C | -4.68856600 | -0.89512200 | -0.05293300 |
| H | 4.02424900 | -0.59736600 | 1.95370400 |
| C | -4.62456900 | -0.43120100 | -1.36580400 |
| H | -5.18410300 | -0.94300100 | -2.14378200 |
| C | 2.99373500 | 0.55553700 | -0.47538100 |
| C | 2.26741200 | -0.36457000 | -1.25408200 |
| C | 4.23776500 | 0.17086700 | -0.00628400 |
| C | 2.78986000 | -1.61362500 | -1.54374700 |
| C | 4.75793400 | -1.08430000 | -0.29225000 |
| H | 4.81404200 | 0.86703400 | 0.59688000 |
| C | 4.03901300 | -1.97529600 | -1.06500000 |
| H | 4.45309600 | -2.95173600 | -1.28446400 |
| O | -2.35553700 | 2.36264300 | -1.02811800 |
| O | 1.03172500 | -0.02910000 | -1.74103300 |
| S | -5.72740600 | -2.29587000 | 0.33965000 |
| S | 6.37707700 | -1.52053000 | 0.36932100 |
| O | 6.23906700 | -1.41337500 | 1.84787600 |
| O | 7.31727800 | -0.51389000 | -0.19495700 |
| O | 6.64695900 | -2.90546600 | -0.09815700 |
| O | -5.47215300 | -2.61378600 | 1.77392200 |
| O | -5.31166600 | -3.39687200 | -0.57915200 |
| O | -7.13402200 | -1.86019300 | 0.08756600 |
| H | -1.24761500 | 2.16168900 | -2.41014200 |
| H | 0.03489500 | -0.72050100 | -1.35253400 |
| H | -0.83740200 | -0.82595500 | -0.74578400 |
| O | -0.59352700 | 2.07599200 | -3.13786000 |
| H | 0.05184500 | 1.43549900 | -2.81488900 |
| H | -1.32824800 | 3.47207200 | -0.27868700 |
| O | -0.64473700 | 4.04986600 | 0.14648200 |
| H | -0.64018400 | 4.87462700 | -0.34318000 |
| H | -1.05050500 | 0.01060000 | 2.17185300 |
| H | -2.24087500 | 2.57738100 | 1.48533000 |
| H | 0.77523900 | 2.91445300 | 0.45343800 |
| H | 2.24018600 | 2.44546200 | -1.14348100 |
| Pd | -0.05212600 | 0.55744400 | -0.06914800 |

H -3.80061500 1.02335600 -2.70638300
H 2.20300700 -2.29792300 -2.14569800

53
RR_D1_TS1_non-trigo_P_TS2-went-to-trigo,
E(SCF) = -2408.89280439, E(ZPE) = -
2408.502285, E(G) = -2408.566820 a.u.

C -0.52092000 3.06852100 0.21910400
H -0.29274900 3.36459200 -0.80817700
H -1.07066000 3.88512800 0.69564200
C 0.72714200 2.72864700 0.98486100
H 1.40059800 3.58463700 1.06770000
H 0.46327300 2.41448000 1.99961200
N 1.42585800 1.57984000 0.34539000
N -1.34700300 1.84564100 1.16004800
C 2.37223000 0.94783500 1.31752200
H 2.90309000 1.76536100 1.81898500
C -2.52103300 1.92559700 -0.73453900
H -2.13050400 2.06434400 -1.74866200
C 3.36701900 0.00444000 0.72360100
C 3.04391400 -1.36015300 0.51905200
C 4.65712800 0.45715900 0.46373300
C 4.06754300 -2.21140600 -0.05574800
C 5.63688400 -0.39781900 -0.00044600
H 4.90699300 1.49995300 0.63717400
C 5.33631500 -1.74289000 -0.19725900
H 6.10563900 -2.41987700 -0.55631700
C -3.37036600 0.70103800 -0.61733000
C -2.83194200 -0.58226900 -0.85155300
C -4.71649400 0.83258000 -0.29911300
C -3.69819500 -1.68761100 -0.77426700
C -5.54910700 -0.26681000 -0.22897800
H -5.13047300 1.81830100 -0.11183500
C -5.03191500 -1.53357500 -0.47081100
H -5.67972100 -2.40288700 -0.41493200
O 1.82858900 -1.80847000 0.70524900
O -1.57055900 -0.80551800 -1.18047000
S 7.30064900 0.18412500 -0.32935800
S -7.28578200 -0.09024600 0.18814600
O -8.03970600 -0.67785800 -0.95584300
O -7.52041700 1.37066700 0.35357400
O -7.47978600 -0.85960800 1.45041800
O 7.29773100 1.64275000 -0.02773600
O 7.55943700 -0.11273200 -1.76793700
O 8.19311100 -0.59546300 0.57663300
H 0.35483500 -2.99807300 0.18714600
H 0.98934600 -0.73086100 -1.24319100
H 1.11810700 -1.06945700 -0.44186800
O -0.58628300 -3.20357100 0.06039000
H -0.92585500 -2.46669800 -0.47944700
H 0.48768300 -1.46015700 2.00809500
O -0.38163800 -1.51438400 2.44604700
H -0.84741300 -2.11784700 1.84833200
H 1.96830500 1.92090500 -0.44849800
H 1.75141900 0.45067900 2.06667600
H -1.66843200 1.60602300 1.10036100
H -3.10841000 2.81367900 -0.47827300
Pd -0.06807800 0.35086900 -0.45310000
H 3.82033500 -3.25606100 -0.10222000
H -3.28672900 -2.67276900 -0.96633500

53
RR_D1_TS1_P, E(SCF) = -2408.89607424,
E(ZPE) = -2408.506532, E(G) = -2408.572158
a.u.

C -0.55725600 3.33430800 -0.32038200
H -0.33155700 3.47904500 -1.38015800
H -1.25007400 4.12177500 -0.00836900
C 0.68477400 3.33207200 0.52275000
H 1.26132100 4.25179900 0.40806800
H 0.40808200 3.23270600 1.57503000
N 1.51736800 2.14492000 0.17970300
N -1.19072000 2.00793900 -0.17178000
C 2.42905900 1.79306600 1.31736400
H 3.14059600 2.61887300 1.42762200
C -2.38613400 1.82486600 -1.01382100
H -2.05507100 1.92961600 -2.05312900

C 3.12723600 0.49588100 1.12540400
C 2.51638800 -0.69534900 1.63092700
C 4.31769700 0.44166600 0.42072000
C 3.20806200 -1.90589600 1.36945700
C 4.94992400 -0.76559700 0.16643500
H 4.75518400 1.36686600 0.05027300
C 4.38569400 -1.93908300 0.65366000
H 4.88247900 -2.88302500 0.45574500
C -3.05276300 0.51090800 -0.77645400
C -2.33717900 -0.69597200 -0.93785300
C -4.39948100 0.47061500 -0.45378700
C -3.03828000 -1.90256000 -0.80181200
C -5.06988000 -0.73311500 -0.30968200
H -4.93865100 1.40491900 -0.32206900
C -4.38439200 -1.92227300 -0.49683900
H -4.90979700 -2.86423800 -0.38971300
O 1.38561800 -0.68686700 2.24723500
O -1.04991200 -0.75208600 -1.24415500
S 6.49611900 -0.77912400 -0.73455400
S -6.82203800 -0.71842500 0.08338600
O -7.20212100 -2.13999800 0.30794300
O -7.49963800 -0.11479600 -1.09998200
O -6.95709600 0.12431300 1.40632400
O 6.26274800 0.01954000 -1.97356400
O 6.79646600 -2.21144700 -1.01576400
O 7.50841600 -0.14149900 0.15911000
H 0.34638800 -1.94758300 -1.46619600
H 1.48828600 -0.40820800 -1.37630500
H 1.65958200 -0.53796100 -0.59447800
O -0.19822100 -2.56604900 0.93579800
H -0.42741700 -2.06241300 0.14021400
H 0.00642600 0.37698800 2.40424100
O -0.77588600 0.97747300 2.45177600
H -1.33489500 0.63351400 3.15164700
H 2.10135600 2.37443400 -0.62540300
H 1.80464000 1.75764700 2.21120100
H -1.39353000 1.80842400 0.82163200
H -3.08770100 2.63983600 -0.80603500
Pd 0.26098300 0.63742800 -0.56865800
H 2.76467200 -2.82522600 1.73950900
H -2.49118000 -2.82858700 -0.94051000

62
RR_D1_TS1_P_5W_HOphen, E(SCF) = -
2638.24169464, E(ZPE) = -2637.770557, E(G)
= -2637.841113 a.u.

C -0.82097400 3.71137900 -0.81754100
H -0.54321900 3.77766500 -1.87475400
H -1.52848600 4.52287400 -0.60741300
C 0.38787200 3.83792000 0.07760800
H 0.89161000 4.79842300 -0.05752200
H 0.05985100 3.78140900 1.11910600
N 1.34835500 2.71202800 -0.13161900
N -1.40803400 2.39126300 -0.57837000
C 2.26427400 2.56889500 1.05393400
H 3.04374700 3.33181500 0.95342900
C -2.54509100 2.03102400 -1.42719300
H -2.21029600 2.08124400 -2.46942600
C 2.84784200 1.21573900 1.24191700
C 2.19938400 0.32281600 2.15109700
C 3.98270800 0.82350000 0.55068800
C 2.80006700 -0.95836100 2.30768800
C 4.52276600 -0.44192200 0.71521900
H 4.45660600 1.51334700 -0.14321400
C 3.91953000 -1.33087600 1.60537000
H 4.33758700 -2.32518100 1.73664100
C -3.03360400 0.65448500 -1.08028300
C -2.24708300 -0.48042900 -1.28691500
C -4.28488800 0.48061300 -0.50346000
C -2.71174900 -1.74639200 -0.96305900
C -4.75006400 -0.77727700 -0.16698200
H -4.91569700 1.34437900 -0.32240600
C -3.96368100 -1.89419700 -0.39806200
H -4.32829000 -2.88223700 -0.13951600
O 1.13247200 0.63563300 2.79147300
O -0.99893300 -0.32433000 -1.83741400
S 5.89985800 -1.00254600 -0.26607300

| | | | |
|----|-------------|-------------|-------------|
| S | -6.37198600 | -0.99120500 | 0.58985300 |
| O | -6.10390100 | -1.52511600 | 1.95338200 |
| O | -7.08617400 | -1.96547200 | -0.27993500 |
| O | -6.99650700 | 0.35831800 | 0.59871600 |
| O | 6.34790500 | 0.15575200 | -1.08333600 |
| O | 5.34946300 | -2.11842900 | -1.12005400 |
| O | 6.93966900 | -1.51102500 | 0.66909600 |
| H | -0.02223600 | -0.73966100 | 2.54135100 |
| H | 1.20316700 | -2.51156400 | -2.18529100 |
| H | 1.58354900 | 0.27301500 | -1.13960500 |
| O | -0.77023300 | -1.30187600 | 2.24953900 |
| H | -0.38494500 | -1.90687100 | 1.59029200 |
| H | -0.46577600 | 1.42507600 | 2.38867600 |
| O | -1.42343900 | 1.46822300 | 2.18029300 |
| H | -1.60967000 | 0.52685900 | 2.02682100 |
| H | 1.93119600 | 2.94133300 | -0.93523000 |
| H | 1.66539600 | 2.81046800 | 1.93362700 |
| H | -1.64147900 | 2.26845600 | 0.41668100 |
| H | -3.36529500 | 2.74997800 | -1.31127700 |
| Pd | 0.27792600 | 1.09184500 | -0.88460500 |
| O | 0.52198300 | -3.11666900 | 0.48015300 |
| H | 1.41305100 | -2.81817300 | 0.23263600 |
| H | 0.11402600 | -3.27526200 | -0.38194400 |
| O | 0.23713000 | -2.59837200 | -2.34580200 |
| H | -0.56516300 | -1.19735000 | -2.05446500 |
| O | 2.62519700 | -2.14484500 | -1.21227200 |
| S | 3.60548100 | -2.24554600 | -1.23357700 |
| H | 0.12218900 | -3.00952600 | -3.20670900 |
| H | 2.49187400 | -1.21799000 | -0.95879800 |
| H | -2.08388600 | -2.61030400 | -1.14961600 |
| H | 2.33138800 | -1.65041400 | 3.00190800 |

62
RR_D1_TS1_P_5W_SO3-H, E(SCF) = -
2638.24158522, E(ZPE) = -2637.772533, E(G)
= -2637.844592 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.74964500 | 3.19014700 | -1.51857900 |
| H | -0.43847200 | 2.85914100 | -2.51523800 |
| H | -1.42722400 | 4.04230600 | -1.64989200 |
| C | 0.44394400 | 3.59016100 | -0.68735100 |
| H | 0.97712700 | 4.43644300 | -1.12963200 |
| H | 0.10235800 | 3.89551100 | 0.30593900 |
| N | 1.36249600 | 2.43546100 | -0.49116000 |
| N | -1.40655200 | 2.06126200 | -0.85421800 |
| C | 2.32259300 | 2.69702600 | 0.62325600 |
| C | 3.01337400 | 3.48468800 | 0.30112600 |
| H | -2.45394000 | 1.39830900 | -1.63338600 |
| H | -1.97394100 | 1.02706100 | -2.54804800 |
| C | 3.04524200 | 1.46728900 | 1.04215500 |
| C | 2.50998500 | 0.70132000 | 2.13243000 |
| C | 4.10630300 | 0.99732800 | 0.30269100 |
| C | 3.20115900 | -0.50678800 | 2.45190200 |
| C | 4.70999400 | -0.21775900 | 0.61376300 |
| H | 4.46493300 | 1.56813900 | -0.54996000 |
| C | 4.25080400 | -0.96749600 | 1.69909500 |
| H | 4.72089700 | -1.91606700 | 1.94145100 |
| C | -3.09759700 | 0.27429000 | -0.87538100 |
| C | -2.35766900 | -0.83074600 | -0.39815200 |
| C | -4.47561300 | 0.29589700 | -0.68800400 |
| C | -3.05671500 | -1.87781600 | 0.22726500 |
| C | -5.14141100 | -0.74219300 | -0.06527700 |
| H | -5.04822700 | 1.14532000 | -1.04735600 |
| C | -4.42301800 | -1.84151300 | 0.38863500 |
| H | -4.93745900 | -2.66209600 | 0.87895900 |
| O | 1.46221900 | 1.04927100 | 2.76457900 |
| O | -1.04329000 | -0.95592400 | -0.51097200 |
| S | 5.91479600 | -0.90284500 | -0.45577100 |
| S | -6.91951200 | -0.70496800 | 0.16682700 |
| O | -7.13901200 | -0.80688400 | 1.63828200 |
| O | -7.45081600 | -1.88921500 | -0.56787300 |
| O | -7.38664900 | 0.58938200 | -0.40319100 |
| O | 6.25469300 | 0.07759800 | -1.49150900 |
| O | 5.16447300 | -2.14486300 | -1.15277800 |
| O | 7.00002800 | -1.53169400 | 0.29786300 |
| H | 0.22669800 | -0.33105500 | 2.62182700 |
| H | 2.12620700 | -1.92207100 | -2.19240700 |
| H | 1.40492600 | -0.27315400 | -0.18966600 |

| | | | |
|----|-------------|-------------|-------------|
| O | -0.55562800 | -0.89570500 | 2.45762600 |
| H | -0.55511000 | -1.03717700 | 1.49675100 |
| H | -0.17474000 | 1.90532400 | 2.31979200 |
| O | -1.14234500 | 2.00660400 | 2.22385700 |
| H | -1.42167200 | 1.08023700 | 2.27592200 |
| H | 1.91221300 | 2.32102500 | -1.34278000 |
| H | 1.73662700 | 3.07875200 | 1.46102400 |
| H | -1.74660400 | 2.33659400 | 0.07053700 |
| H | -3.22521700 | 2.11569800 | -1.94210000 |
| Pd | 0.19675000 | 0.68915600 | -0.46002300 |
| O | 1.90736900 | -3.13146200 | 0.75850200 |
| H | 2.13502400 | -2.21231700 | 0.94756700 |
| H | 1.44233500 | -3.09293100 | -0.09519400 |
| O | 0.55306100 | -2.74801600 | -1.71019400 |
| H | -0.13669600 | -2.14217100 | -1.34652000 |
| O | 2.86324000 | -1.27790300 | -2.18563400 |
| H | 4.30537400 | -1.83405500 | -1.56884100 |
| H | 0.09308100 | -3.44485900 | -2.18356600 |
| H | 2.49742000 | -0.56597300 | -1.63457400 |
| H | -2.47609400 | -2.72181800 | 0.58657000 |
| H | 2.83095700 | -1.08798300 | 3.29131500 |

53
RR_D1_TS1_P_CH_P, E(SCF) = -2408.89449246,
E(ZPE) = -2408.500952, E(G) = -2408.565854
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.39468000 | 1.83608000 | 0.24568500 |
| N | -1.43303300 | 1.90480600 | 0.30007700 |
| C | 2.48191600 | 1.23928100 | 1.05325200 |
| H | 3.16862200 | 2.03421400 | 1.36444400 |
| C | -2.64360600 | 2.00311900 | -0.52005200 |
| H | -2.31824800 | 2.32028400 | -1.51921900 |
| C | 3.24332500 | 0.13120500 | 0.34031600 |
| C | 2.95398700 | -1.24946700 | 0.89760300 |
| C | 4.67125900 | 0.42565600 | 0.06838100 |
| C | 3.98597700 | -2.25147200 | 0.72912500 |
| C | 5.58503000 | -0.54523400 | 0.03809400 |
| H | 4.95232200 | 1.44869300 | -0.16178300 |
| C | 5.22820300 | -1.90863400 | 0.34289900 |
| H | 6.00277800 | -2.66678100 | 0.27645200 |
| C | -3.38283400 | 0.70149400 | -0.57974800 |
| C | -2.77671500 | -0.48135600 | -1.06854600 |
| C | -4.71554600 | 0.67267000 | -0.18471500 |
| C | -3.58278900 | -1.63515500 | -1.16062800 |
| C | -5.48010900 | -0.47441900 | -0.27630000 |
| H | -5.17538500 | 1.58011600 | 0.19469900 |
| C | -4.90274600 | -1.67263400 | -0.77263400 |
| H | -5.49192600 | -2.54584800 | -0.85379400 |
| O | 1.87212900 | -1.50637400 | 1.41343800 |
| O | -1.52665100 | -0.58145500 | -1.47179100 |
| S | 7.30742700 | -0.21173400 | -0.36667500 |
| S | -7.18988600 | -0.49713500 | 0.26119300 |
| O | -7.24702400 | -1.44526200 | 1.41198500 |
| O | -7.98165900 | -0.98125500 | -0.90666700 |
| O | -7.52140900 | 0.90279700 | 0.64824300 |
| O | 7.39736000 | 1.25120100 | -0.60094500 |
| O | 7.57254500 | -1.03027200 | -1.58017400 |
| O | 8.07034100 | -0.67556500 | 0.82306600 |
| H | 0.29799400 | -2.40994700 | 0.47295200 |
| H | 1.01501700 | -0.31678900 | -1.40751200 |
| H | 2.77102000 | 0.02291700 | -0.66202500 |
| O | -0.62154900 | -2.62457400 | 0.26038500 |
| H | -0.84725800 | -2.01787600 | -0.47175800 |
| H | 0.11579000 | -0.59701100 | 2.20469800 |
| O | -0.84552800 | -0.57029900 | 2.31428400 |
| H | -1.12021600 | -1.24309600 | 1.66845500 |
| H | 1.81685500 | 2.32820400 | -0.54151400 |
| H | 2.02075100 | 0.83739800 | 1.95695900 |
| H | -1.65071300 | 1.50485400 | 1.21433700 |
| H | -3.31128500 | 2.78469200 | -0.13496900 |
| Pd | -0.03546100 | 0.57602800 | -0.65040200 |
| H | 3.73764300 | -3.26813700 | 1.01058900 |
| H | -3.11999100 | -2.53825400 | -1.54603300 |
| C | -0.68148400 | 3.15503100 | 0.44215100 |
| C | 0.65337000 | 2.83641200 | 1.06426100 |
| H | -1.21890000 | 3.89363300 | 1.04830600 |
| H | 1.25706200 | 3.73706200 | 1.20515700 |

H 0.49584900 2.38867000 2.05028300
H -0.55060700 3.58074400 -0.55820600

53

RR_D1_TS1_P_CH_R, E(SCF) = -2408.89663065,
E(ZPE) = -2408.504482, E(G) = -2408.567994
a.u.

N 1.55844100 2.21714200 0.11341500
N -1.16171300 2.01001500 -0.18451500
C 2.54123500 1.94553700 1.21617600
H 3.26180300 2.77043400 1.21553700
C -2.33605500 1.77361800 -1.04432600
H -1.97826600 1.83239400 -2.07867500
C 3.21235100 0.62705300 1.09147700
C 2.62774300 -0.49445900 1.75704200
C 4.34672600 0.48316500 0.30480500
C 3.25869400 -1.74908500 1.53150000
C 4.92912700 -0.75523000 0.11069400
H 4.77772100 1.35466400 -0.18098700
C 4.37042000 -1.87275500 0.73197500
H 4.81937300 -2.84983800 0.57692000
C -3.00939100 0.47086600 -0.76363700
C -2.29305300 -0.74141700 -0.79648800
C -4.38136100 0.45159000 -0.53813300
C -3.01046000 -1.93929200 -0.62321900
C -5.06568000 -0.73465400 -0.36810000
H -4.93106500 1.38683100 -0.50758400
C -4.37059900 -1.93775100 -0.41757500
H -4.90015200 -2.87608700 -0.28610800
O 1.57026500 -0.39235100 2.47871100
O -0.98964200 -0.83615700 -0.99795200
S 6.39627600 -0.94901200 -0.89489800
S -6.83619600 -0.75548700 -0.07511200
O -7.01930700 -1.40666600 1.25320200
O -7.41995500 -1.55968100 -1.18635100
O -7.27362700 0.66756400 -0.09144500
O 6.69686200 0.39944500 -1.45390300
O 6.04831600 -1.94909800 -1.94687200
O 7.46579800 -1.44788400 0.01946800
H 0.31358400 -1.57360600 2.00986100
H 1.46602000 -0.53500200 -1.23269000
H 1.79303700 -0.43502500 -0.49807200
O -0.50358800 -2.02795400 1.70864600
H -0.56765700 -1.80829700 0.76716600
H 0.04507200 0.61069100 2.52862400
O -0.91195900 0.82772800 2.49412200
H -1.28767700 -0.05189800 2.33914400
H 2.08927100 2.43359400 -0.73126200
H 1.97518800 1.98246700 2.14863600
H -1.38501300 1.85196000 0.81128700
H -3.04595900 2.59423400 -0.89541700
Pd 0.30965600 0.64324600 -0.50879000
H 2.82632600 -2.62156500 2.01286300
H -2.45596500 -2.87108100 -0.65695700
C -0.55040600 3.34055600 -0.38108600
C 0.69784000 3.38375300 0.45007800
H -1.25340500 4.12688100 -0.09111600
H 1.24646800 4.31917600 0.32257200
H 0.43364600 3.29086500 1.50691600
H -0.33296800 3.45221900 -1.44654900

53

RR_D1_TS1_P_CH_TS, E(SCF) = -2408.87823538,
E(ZPE) = -2408.490032, E(G) = -2408.554836
a.u.

N 1.47344800 2.30669800 0.04886300
N -1.29274700 2.04855400 -0.11158100
C 2.56177300 1.95965200 1.00900100
H 3.34198600 2.72405400 0.94608100
C -2.43541800 1.80128400 -0.99956900
H -2.05538800 1.88009700 -2.02583100
C 3.13389100 0.58791200 0.79079400
C 2.71345200 -0.46273900 1.71613700
C 4.36548300 0.44130700 0.08061300
C 3.43119900 -1.70268100 1.61961700
C 5.01805000 -0.74703300 0.05745500
H 4.74781200 1.28033900 -0.49275000

C 4.53139600 -1.83027000 0.83266900
H 5.06357600 -2.77644000 0.79840200
C -3.06763600 0.46691700 -0.74838400
C -2.32317900 -0.73498700 -0.77514500
C -4.44192200 0.41486800 -0.53786400
C -3.02903700 -1.94411800 -0.60783900
C -5.10884300 -0.78267700 -0.37400100
H -5.01003200 1.33946700 -0.51270300
C -4.38977200 -1.97192600 -0.41278300
H -4.90122600 -2.92092600 -0.28443000
O 1.71067100 -0.33071200 2.45558000
O -1.02029800 -0.82165000 -0.96279100
S 6.52654200 -0.97784400 -0.88795500
S -6.87892500 -0.83621200 -0.09503200
O -7.06309900 -1.47031700 -1.24232800
O -7.43971700 -1.67017800 -1.19710100
O -7.34894200 0.57654200 -0.13706700
O 6.77405100 0.31168600 -1.58613300
O 6.24221200 -2.10764200 -1.58613300
O 7.57242900 -1.31562200 0.11764400
H 0.38594900 -1.60429500 1.94579200
H 1.52161800 -0.31160700 -0.86288000
H 2.20641400 0.06693900 -0.15205200
O -0.44276300 -2.00986400 1.63546500
H -0.51085400 -1.74218900 0.70220800
H 0.01503800 0.63903300 2.57919100
O -0.95502400 0.72449400 2.57944900
H -1.21660100 -0.17830600 2.33722100
H 1.89633200 2.60997000 -0.82878800
H 2.12123900 2.00410900 2.00700500
H -1.53293400 1.84968300 0.86741900
H -3.18537900 2.59067700 -0.86977900
Pd 0.25872500 0.70475200 -0.49876800
H 3.08757800 -2.52383700 2.23997700
H -2.45600300 -2.86529000 -0.63401800
C -0.69640900 3.38951400 -0.23470400
C 0.59207600 3.39493500 0.54678100
H -1.38091500 4.16348400 0.12818800
H 1.09697300 4.36233600 0.49422900
H 0.38236400 3.18203000 1.59887000
H -0.51244800 3.57654400 -1.29715900

53

RR_D1_TS1_P_HH-Homo P, E(SCF) = -
2408.86828520, E(ZPE) = -2408.477543, E(G) =
-2408.540305 a.u.

C -0.66186800 3.60059700 0.80748000
H -0.65351700 4.22344700 -0.09122100
H -1.26592900 4.11898800 1.56165300
C 0.73818800 3.39494500 1.34320700
H 1.26424400 4.34545400 1.43700500
H 0.67641400 2.95703100 2.34160300
N 1.55088400 2.44647600 0.50209900
N -1.22906400 2.29719600 0.45098500
C 2.30161700 1.47848600 1.37425300
H 3.09804300 2.03082200 1.88145000
C -2.50803900 2.33918500 -0.26616900
H -2.36543800 2.97095600 -1.15055900
C 2.83919000 0.27713300 0.68004900
C 1.90391300 -0.66510600 0.17895900
C 4.19575700 0.02347000 0.60210400
C 2.40103200 -1.85930700 -0.36167600
C 4.66322700 -1.15776200 0.04208100
H 4.90074000 0.75418400 0.99018200
C 3.76044100 -2.10105900 -0.42566200
H 4.13587000 -3.02286200 -0.85596900
C -2.92186300 0.95373700 -0.65710100
C -2.13167100 0.19161400 -1.55301700
C -4.08080400 0.40551200 -0.13732900
C -2.56857000 -1.09798900 -1.89171300
C -4.49949400 -0.86614800 -0.49725900
H -4.68001100 0.98849500 0.55650600
C -3.73738400 -1.62165400 -1.37365500
H -4.06232300 -2.62033800 -1.64439300
O 0.61657900 -0.40392900 0.20365500
O -1.03688000 0.65175100 -2.13579100
S 6.42865100 -1.47148700 0.00599800

| | | | |
|----|-------------|-------------|-------------|
| S | -5.90635500 | -1.59380700 | 0.33665200 |
| O | -5.35950300 | -2.05564300 | 1.65904700 |
| O | -6.36340400 | -2.72500300 | -0.50935100 |
| O | -6.91559500 | -0.51655800 | 0.49974400 |
| O | 6.83294200 | -1.71115500 | 1.42260400 |
| O | 7.05406100 | -0.24094700 | -0.55829800 |
| O | 6.61557700 | -2.66977200 | -0.85862600 |
| H | -2.32496500 | -2.11622800 | 0.96535100 |
| H | 0.28216900 | 2.72812400 | -1.76214100 |
| H | 1.41775300 | 1.14937500 | -1.88226600 |
| O | -2.59016800 | -2.05409400 | 1.88948200 |
| H | -3.56992100 | -2.04444400 | 1.85466100 |
| H | -0.32004200 | -0.14385200 | 1.69599600 |
| O | -0.93406100 | 0.16154800 | 2.39640300 |
| H | -1.61999200 | -0.53128000 | 2.40473500 |
| H | 2.22949800 | 2.97828900 | -0.03632800 |
| H | 1.58241400 | 1.15626300 | 2.13213700 |
| H | -1.31244300 | 1.68364900 | 1.27552300 |
| H | -3.28685000 | 2.80385900 | 0.35035900 |
| Pd | 0.30469200 | 1.48749500 | -0.87213600 |
| H | -1.95846800 | -1.67348100 | -2.57907600 |
| H | 1.68904400 | -2.58570500 | -0.73922500 |

53

RR_D1_TS1_P_HH-Homo_TS, E(SCF) = -
2408.86490895, E(ZPE) = -2408.476652, E(G) =
-2408.539385 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.64230500 | 3.61558400 | 0.75353400 |
| H | -0.61737300 | 4.20229700 | -0.16933900 |
| H | -1.25570100 | 4.16624100 | 1.47742500 |
| C | 0.74756200 | 3.42332800 | 1.31520000 |
| H | 1.27372700 | 4.37519300 | 1.39386800 |
| H | 0.67295900 | 3.00800000 | 2.32239000 |
| N | 1.56659500 | 2.45573300 | 0.50300200 |
| N | -1.21136600 | 2.30178000 | 0.43719800 |
| C | 2.29830300 | 1.49237100 | 1.39649900 |
| H | 3.10273800 | 2.04111700 | 1.89510200 |
| C | -2.48243200 | 2.33201900 | -0.29365800 |
| H | -2.32862000 | 2.95111700 | -1.18540900 |
| C | 2.81594000 | 0.27115400 | 0.72284200 |
| C | 1.86129200 | -0.67962400 | 0.26874600 |
| C | 4.16923900 | 0.01557400 | 0.60798400 |
| C | 2.34689900 | -1.88699900 | -0.26039900 |
| C | 4.62092500 | -1.17610400 | 0.05674000 |
| H | 4.88583900 | 0.75393400 | 0.95861300 |
| C | 3.70331200 | -2.12923900 | -0.36197700 |
| H | 4.06493700 | -3.06062100 | -0.78375700 |
| C | -2.89387500 | 0.94317300 | -0.67146300 |
| C | -2.09521200 | 0.17476400 | -1.55417700 |
| C | -4.05785400 | 0.39981600 | -0.15880300 |
| C | -2.52285600 | -1.12160400 | -1.87896400 |
| C | -4.47072100 | -0.87628000 | -0.50996500 |
| H | -4.66558400 | 0.98925100 | 0.52203200 |
| C | -3.69739300 | -1.64070600 | -1.36884700 |
| H | -4.01840700 | -2.64253600 | -1.63236800 |
| O | 0.58077900 | -0.41571500 | 0.32338300 |
| O | -1.00171800 | 0.63747300 | -2.13542700 |
| S | 6.38307000 | -1.49239200 | -0.02154000 |
| S | -5.89637500 | -1.58935900 | 0.30498000 |
| O | -5.37964100 | -2.03853600 | 1.64348900 |
| O | -6.34122600 | -2.72799400 | -0.53737800 |
| O | -6.90340200 | -0.50551200 | 0.43522400 |
| O | 6.82086900 | -1.74595800 | 1.38312400 |
| O | 6.99904100 | -0.25798100 | -0.58858300 |
| O | 6.54975800 | -2.68338000 | -0.90081600 |
| H | -2.34237600 | -2.05563600 | 1.03789100 |
| H | 0.67171100 | 2.51529600 | -1.98630800 |
| H | 1.42729800 | 1.34410200 | -1.99020000 |
| O | -2.62141300 | -1.98239100 | 1.95709500 |
| H | -3.60027700 | -1.98898500 | 1.90480000 |
| H | -0.34750200 | -0.07645600 | 1.78813400 |
| O | -0.97413000 | 0.24503500 | 2.47144600 |
| H | -1.66286200 | -0.44456600 | 2.47734800 |
| H | 2.25856900 | 2.97556500 | -0.02999700 |
| H | 1.57118800 | 1.19618800 | 2.15689100 |
| H | -1.30571100 | 1.71516700 | 1.28029700 |
| H | -3.26839100 | 2.80544400 | 0.30745900 |

| | | | |
|----|-------------|-------------|-------------|
| Pd | 0.33596300 | 1.48733300 | -0.88042100 |
| H | -1.90536300 | -1.70290800 | -2.55473500 |
| H | 1.62493800 | -2.62280200 | -0.59940600 |

53

RR_D1_TS1_P_EI_TS, E(SCF) = -2408.88980271,
E(ZPE) = -2408.499343, E(G) = -2408.562948
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.56187800 | 3.40271300 | -0.77266100 |
| H | 0.91282600 | 4.13478200 | -0.04330900 |
| H | 0.96520800 | 3.69315300 | -1.74636500 |
| C | -0.96568500 | 3.37618700 | -0.77391800 |
| H | -1.33862100 | 4.17489600 | -0.13428500 |
| H | -1.36790200 | 3.54632700 | -1.77516500 |
| N | -1.51832200 | 2.09151000 | -0.25549000 |
| N | 1.14461600 | 2.10296900 | -0.37530300 |
| C | -1.93264900 | 1.15441200 | -1.35339500 |
| H | -2.54671900 | 1.74031200 | -2.04629300 |
| C | 2.53052500 | 2.23584500 | 0.13008600 |
| H | 2.48041600 | 2.87097200 | 1.02063800 |
| C | -2.70879100 | -0.01315400 | -0.84990700 |
| C | -2.04607600 | -1.19674100 | -0.41728900 |
| C | -4.09585400 | 0.07393300 | -0.80802200 |
| C | -2.87773900 | -2.25048700 | 0.04624900 |
| C | -4.87166000 | -0.96977100 | -0.34220500 |
| H | -4.58732600 | 0.98160400 | -1.14872200 |
| C | -4.24696700 | -2.14208500 | -0.10870500 |
| H | -4.84819000 | -2.97098800 | 0.44333500 |
| C | 3.12975100 | 0.90430900 | 0.43223800 |
| C | 2.52699600 | 0.07150000 | 1.40170300 |
| C | 4.26679700 | 0.47781000 | -0.23016300 |
| C | 3.13319000 | -1.15916900 | 1.68487600 |
| C | 4.84436200 | -0.75005100 | 0.05737400 |
| H | 4.71276100 | 1.11951100 | -0.98533200 |
| C | 4.27773300 | -1.56344500 | -1.02387300 |
| H | 4.73418100 | -2.52072700 | 1.24753500 |
| O | -0.76075800 | -1.31785300 | -0.40733400 |
| O | 1.43523500 | 0.42279900 | 2.06621300 |
| S | -6.65656300 | -0.86211200 | -0.31494600 |
| S | 6.31247000 | -1.25607500 | -0.84522400 |
| O | 5.91985500 | -1.26020600 | -2.28326600 |
| O | 6.66135800 | -2.60813800 | -0.33051800 |
| O | 7.34929800 | -0.22874200 | -0.54262500 |
| O | -6.99469500 | 0.52954600 | -0.72876800 |
| O | -7.06914600 | -1.16652900 | 1.08708800 |
| O | -7.15326800 | -1.88827900 | -1.27906500 |
| H | -0.32047800 | -1.88319900 | 1.24411400 |
| H | -1.24528800 | 0.93431700 | 2.33270300 |
| H | -1.17067700 | 0.19691300 | 1.99307400 |
| O | -0.16861600 | -1.98017400 | 2.20925800 |
| H | 0.46493300 | -1.27119500 | 2.39964300 |
| H | 0.45168400 | -0.71820700 | -1.44133200 |
| O | 1.13207200 | -0.26563100 | -2.00111100 |
| H | 1.95753200 | -0.73149800 | -1.83964000 |
| H | -2.35754600 | 2.29938300 | 0.28253700 |
| H | -1.02806400 | 0.85458600 | -1.88564700 |
| H | 1.15159300 | 1.41663600 | -1.15234300 |
| H | 3.13033400 | 2.75720100 | -0.62384200 |
| Pd | -0.09315600 | 1.24041600 | 0.99670700 |
| H | -2.38902500 | -3.16227800 | 0.37671200 |
| H | 2.67943500 | -1.79718800 | 2.43524700 |

53

RR_D1_TS1_P, E(SCF) = -2408.89664961,
E(ZPE) = -2408.504639, E(G) = -2408.568155
a.u.

| | | | |
|---|-------------|------------|-------------|
| C | -0.54018200 | 3.33982500 | -0.41130400 |
| H | -0.31778800 | 3.43857500 | -1.47701200 |
| H | -1.24361100 | 4.13025400 | -0.13397600 |
| C | 0.70432000 | 3.39170000 | 0.42479100 |
| H | 1.25464200 | 4.32484200 | 0.28821300 |
| H | 0.43511800 | 3.31216400 | 1.48145300 |
| N | 1.56535100 | 2.21994900 | 0.10703000 |
| N | -1.15355700 | 2.01223400 | -0.20144100 |
| C | 2.54066900 | 1.96017000 | 1.21893500 |
| H | 3.26128800 | 2.78506100 | 1.21454000 |
| C | -2.32499500 | 1.76618000 | -1.06239300 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -1.96414400 | 1.81497100 | -2.09618800 | S | 6.36533600 | -0.96392400 | -0.90240700 |
| C | 3.21001700 | 0.63999300 | 1.10671000 | S | -6.82434300 | -0.75657200 | -0.07678300 |
| C | 2.62039500 | -0.47555900 | 1.77619900 | O | -7.01283900 | -1.40694600 | 1.25106300 |
| C | 4.33518600 | 0.48594000 | 0.31074800 | O | -7.40475100 | -1.56060400 | -1.18989700 |
| C | 3.23869300 | -1.73556300 | 1.54729000 | O | -7.26015500 | 0.66691900 | -0.09548000 |
| C | 4.90666500 | -0.75778000 | 0.11335100 | O | 6.66750700 | 0.38001800 | -1.47144100 |
| H | 4.76836900 | 1.35284900 | -0.18137900 | O | 6.00579700 | -1.96865600 | -1.94603300 |
| C | 4.34375300 | -1.86968700 | 0.73918300 | O | 7.43955100 | -1.46182100 | 0.00704000 |
| H | 4.78328700 | -2.85068100 | 0.58193400 | H | 0.31797800 | -1.54853700 | 2.03170700 |
| C | -2.99720500 | 0.46524600 | -0.77049000 | O | -0.49202500 | -2.01040000 | 1.72214700 |
| C | -2.28000100 | -0.74687100 | -0.79080800 | H | -0.54699200 | -1.79594500 | 0.77877200 |
| C | -4.36927500 | 0.44710900 | -0.54583400 | H | 0.04580200 | 0.63744000 | 2.53300700 |
| C | -2.99630300 | -1.94337600 | -0.60533600 | O | -0.91064200 | 0.85623400 | 2.48666400 |
| C | -5.05268200 | -0.73786000 | -0.36408800 | H | -1.28775900 | -0.02391900 | 2.33906400 |
| H | -4.91976600 | 1.38213600 | -0.52491500 | H | 2.10195900 | 2.42518900 | -0.74664700 |
| C | -4.35668200 | -1.94083900 | -0.40076100 | H | 1.96966600 | 2.00584800 | 2.14788100 |
| H | -4.88557200 | -2.87816100 | -0.25966200 | H | -1.38002400 | 1.86580300 | 0.79543800 |
| O | 1.56759100 | -0.36486900 | 2.50529500 | H | -3.03637100 | 2.58717400 | -0.92402100 |
| O | -0.97592800 | -0.84224800 | -0.99137000 | Pd | 0.31769100 | 0.63894000 | -0.50396300 |
| S | 6.36505800 | -0.96409400 | -0.90249100 | H | 1.69724700 | -0.54888700 | -0.45150700 |
| S | -6.82423000 | -0.75677900 | -0.07652400 | H | 2.80241700 | -2.60431700 | 2.03170500 |
| O | -7.01200400 | -1.40538300 | 1.25230500 | H | -2.44107100 | -2.87497900 | -0.62786600 |
| O | -7.40486100 | -1.56246300 | -1.18831600 | H | 1.54377700 | -0.44964700 | -1.24261800 |
| O | -7.26038600 | 0.66658900 | -0.09694500 | | | | |
| O | 6.66718300 | 0.37977200 | -1.47171700 | 53 | | | |
| O | 6.00496300 | -1.96884300 | -1.94591600 | RR_D1_TS1-trigo_R, E(SCF) = -2408.91864792, | | | |
| O | 7.43951600 | -1.46211500 | 0.00655800 | E(ZPE) = -2408.528541, E(G) = -2408.594095 | | | |
| H | 0.31811700 | -1.54903200 | 2.03250500 | a.u. | | | |
| H | 1.54375100 | -0.44969100 | -1.24263800 | C | -0.60546400 | 3.18723400 | -0.03440500 |
| H | 1.69734000 | -0.54868700 | -0.45155400 | H | -0.34123100 | 3.27722100 | -1.09211500 |
| O | -0.49128000 | -2.01104600 | 1.72156900 | H | -1.21961400 | 4.05013400 | 0.23547500 |
| H | -0.54643900 | -1.79433300 | 0.77873500 | C | 0.63608000 | 3.09038000 | 0.81623800 |
| H | 0.04603300 | 0.63662300 | 2.53223300 | H | 1.25730800 | 3.98571600 | 0.73164400 |
| O | -0.91024600 | 0.85649100 | 2.48685300 | H | 0.37576600 | 2.95447000 | 1.86961600 |
| H | -1.28859200 | -0.02319600 | 2.33987900 | N | 1.38144900 | 1.88886000 | 0.37988400 |
| H | 2.10203600 | 2.42558600 | -0.73665000 | N | -1.36880200 | 1.92808000 | 0.12611900 |
| H | 1.96937600 | 2.00578500 | 2.14775200 | C | 2.48898400 | 1.46715400 | 1.26289500 |
| H | -1.37990100 | 1.86585700 | 0.79544800 | H | 3.11755800 | 2.33256400 | 1.49915400 |
| H | -3.03646600 | 2.58723800 | -0.92386800 | C | -2.42306300 | 1.70351400 | -0.88386500 |
| Pd | 0.31770800 | 0.63914700 | -0.50407100 | H | -1.90970500 | 1.55153900 | -1.84023000 |
| H | 2.80288400 | -2.60415500 | 2.03256000 | C | 3.30726000 | 0.40882300 | 0.59340900 |
| H | -2.44096400 | -2.87494700 | -0.62874700 | C | 2.71285000 | -0.79156600 | 0.14699600 |
| | | | | C | 4.66911900 | 0.61110500 | 0.40724500 |
| | | | | C | 3.54230800 | -1.75479100 | -0.45392900 |
| | | | | C | 5.46424700 | -0.34959800 | -0.18710100 |
| | | | | H | 5.12236700 | 1.53978500 | 0.73863900 |
| | | | | C | 4.89323100 | -1.54266300 | -0.61373300 |
| | | | | H | 5.51047200 | -2.30151600 | -1.08404000 |
| | | | | C | -3.28866400 | 0.54103300 | -0.51001500 |
| | | | | C | -2.73644100 | -0.72716300 | -0.21760600 |
| | | | | C | -4.66803200 | 0.70999000 | -0.48110300 |
| | | | | C | -3.62552800 | -1.77899800 | 0.07703900 |
| | | | | C | -5.51959800 | -0.33801000 | -0.19216700 |
| | | | | H | -5.09064700 | 1.68653600 | -0.69503900 |
| | | | | C | -4.98837100 | -1.59365600 | 0.08150200 |
| | | | | H | -5.64803700 | -2.42354200 | 0.31457600 |
| | | | | O | 1.42795500 | -1.06809300 | 0.28501100 |
| | | | | O | -1.44804000 | -0.99547400 | -0.22813300 |
| | | | | S | 7.22102100 | -0.07821800 | -0.43537700 |
| | | | | S | -7.29928700 | -0.11622800 | -0.19885100 |
| | | | | O | -7.78222500 | -0.63199600 | 1.11402400 |
| | | | | O | -7.80470700 | -0.92594000 | -1.34506400 |
| | | | | O | -7.53183000 | 1.34446000 | -0.37237500 |
| | | | | O | 7.51070200 | 1.27477500 | 0.11488700 |
| | | | | O | 7.43880800 | -0.16875800 | -1.90755500 |
| | | | | O | 7.91075600 | -1.17070600 | 0.30826300 |
| | | | | H | 0.69527300 | -2.80045200 | -0.21275900 |
| | | | | O | -0.09006900 | -3.37170800 | -0.26461900 |
| | | | | H | -0.78100900 | -2.68448300 | -0.33699300 |
| | | | | H | 0.77381900 | -1.83989300 | 2.00223500 |
| | | | | O | 0.29350600 | -2.51765900 | 2.50317400 |
| | | | | H | -0.03139700 | -3.07863800 | 1.78228900 |
| | | | | H | 1.76873500 | 2.06462000 | -0.54933500 |
| | | | | H | 2.03280400 | 1.11788800 | 2.19553900 |
| | | | | H | -1.80396300 | 1.92231900 | 1.05025400 |
| | | | | H | -3.03593100 | 2.60689900 | -0.97517200 |
| | | | | Pd | -0.00460700 | 0.39888400 | 0.13423300 |

| | | | | | | | |
|---|-------------|-------------|-------------|--|--|--|--|
| 53 | | | | | | | |
| RR_D1_TS1-trigo_P, E(SCF) = -2408.89664951, | | | | | | | |
| E(ZPE) = -2408.504645, E(G) = -2408.568094 | | | | | | | |
| a.u. | | | | | | | |
| C | -0.54008400 | 3.33969700 | -0.41130900 | | | | |
| H | -0.31772100 | 3.43838400 | -1.47702400 | | | | |
| H | -1.24347200 | 4.13014600 | -0.13394700 | | | | |
| C | 0.70440900 | 3.39151000 | 0.42482400 | | | | |
| H | 1.25478000 | 4.32463500 | 0.28893000 | | | | |
| H | 0.43510400 | 3.31200000 | 1.48146700 | | | | |
| N | 1.56540000 | 2.21974300 | 0.10716700 | | | | |
| N | -1.15352300 | 2.01212500 | -0.20141500 | | | | |
| C | 2.54088600 | 1.96015100 | 1.21902200 | | | | |
| H | 3.26141100 | 2.78512300 | 1.21443600 | | | | |
| C | -2.32491700 | 1.76609700 | -1.06249100 | | | | |
| H | -1.96395300 | 1.81487400 | -2.09625000 | | | | |
| C | 3.21025700 | 0.64000600 | 1.10678500 | | | | |
| C | 2.62044800 | -0.47560000 | 1.77601400 | | | | |
| C | 4.33534300 | 0.48593400 | 0.31073200 | | | | |
| C | 3.23845700 | -1.73567600 | 1.54672100 | | | | |
| C | 4.90655300 | -0.75788000 | 0.11295300 | | | | |
| H | 4.76869600 | 1.35285800 | -0.18121500 | | | | |
| C | 4.34342400 | -1.86983300 | 0.73846600 | | | | |
| H | 4.78261700 | -2.85092100 | 0.58085400 | | | | |
| C | -2.99715800 | 0.46520200 | -0.77050600 | | | | |
| C | -2.28001000 | -0.74694500 | -0.79058100 | | | | |
| C | -4.36923400 | 0.44715900 | -0.54582000 | | | | |
| C | -2.99634500 | -1.94335900 | -0.60464400 | | | | |
| C | -5.05266500 | -0.73772300 | -0.36363000 | | | | |
| H | -4.91970200 | 1.38220400 | -0.52505700 | | | | |
| C | -4.35671700 | -1.94073900 | -0.40001100 | | | | |
| H | -4.88559900 | -2.87799800 | -0.25848300 | | | | |
| O | 1.56758400 | -0.36490500 | 2.50501500 | | | | |
| O | -0.97596300 | -0.84245700 | -0.99133600 | | | | |

| | | | |
|---|-------------|-------------|-------------|
| H | 1.21968000 | -1.15211300 | -2.46048000 |
| H | 3.08446500 | -2.67835000 | -0.79429900 |
| H | -3.19799500 | -2.75023800 | 0.30545500 |
| H | 0.92455000 | -0.54333200 | -2.78278600 |

53

RR_D1_TS1-trigo, E(SCF) = -2408.89041375,
E(ZPE) = -2408.501036, E(G) = -2408.566306
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.59044600 | 3.20848000 | 0.00098600 |
| H | -0.38294200 | 3.42893900 | -1.04945100 |
| H | -1.22017300 | 4.00876500 | 0.40073500 |
| C | 0.67488700 | 3.05401700 | 0.79168500 |
| H | 1.27716500 | 3.96550900 | 0.78341000 |
| H | 0.43455400 | 2.82231400 | 1.83404300 |
| N | 1.45563600 | 1.90589800 | 0.26185600 |
| N | -1.30467400 | 1.91606600 | 0.05044500 |
| C | 2.50878800 | 1.50143500 | 1.24226700 |
| H | 3.13329500 | 2.38093800 | 1.43453500 |
| C | -2.47099200 | 1.83843500 | -0.84972400 |
| H | -2.08115500 | 1.92847200 | -1.86930900 |
| C | 3.34150300 | 0.35308900 | 0.79991000 |
| C | 2.76078800 | -0.94155800 | 0.83869800 |
| C | 4.65543300 | 0.52726600 | 0.39494400 |
| C | 3.58146300 | -2.02814200 | 0.46076600 |
| C | 5.43271700 | -0.55648900 | 0.02424600 |
| H | 5.08968000 | 1.52261900 | 0.37148400 |
| C | 4.88602500 | -1.83640500 | 0.06122500 |
| H | 5.49369800 | -2.68733300 | -0.23274900 |
| C | -3.24810900 | 0.57886800 | -0.65014300 |
| C | -2.62328300 | -0.68209400 | -0.74319400 |
| C | -4.61518000 | 0.65119500 | -0.41174400 |
| C | -3.42805800 | -1.82982600 | -0.62104600 |
| C | -5.38494600 | -0.48840900 | -0.28990900 |
| H | -5.09458700 | 1.62142600 | -0.32795400 |
| C | -4.78403800 | -1.73583300 | -0.40504400 |
| H | -5.38207200 | -2.63685700 | -0.31446900 |
| O | 1.51647500 | -1.09772400 | 1.16066500 |
| O | -1.33313500 | -0.85473600 | -0.96967200 |
| S | 7.12114300 | -0.33853200 | -0.52980100 |
| S | -7.15436600 | -0.38573600 | -0.00528700 |
| O | -7.41433500 | -1.17997200 | 1.22877200 |
| O | -7.79398200 | -0.98502100 | -1.21134900 |
| O | -7.45936400 | 1.06245900 | 0.15647400 |
| O | 7.40392400 | 1.12101500 | -0.42831300 |
| O | 7.16278800 | -0.83926400 | -1.93523400 |
| O | 7.96904900 | -1.15914300 | 0.38341200 |
| H | 0.35505800 | -2.45426500 | 1.03290100 |
| O | -0.51341900 | -2.87505500 | 0.86759000 |
| H | -0.83619100 | -2.36137800 | 0.10858300 |
| H | 0.11590700 | -0.39219600 | 2.20788200 |
| O | -0.81650200 | -0.27871400 | 2.47413900 |
| H | -1.20919100 | -1.08350500 | 2.10689900 |
| H | 1.92237700 | 2.19584400 | -0.59899800 |
| H | 1.97564100 | 1.25702800 | 2.16582300 |
| H | -1.59530100 | 1.70680400 | 1.01095600 |
| H | -3.11638400 | 2.70370900 | -0.66215800 |
| Pd | 0.08141500 | 0.45879200 | -0.35859700 |
| H | 1.35618700 | -0.95714400 | -1.21950700 |
| H | 3.14754100 | -3.02332200 | 0.48369300 |
| H | -2.95168500 | -2.80040400 | -0.70949000 |
| H | 1.34703700 | -0.41077200 | -1.76150500 |

53

RR_D1_TS1, E(SCF) = -2408.89137538, E(ZPE)
= -2408.502675, E(G) = -2408.568142 a.u.

| | | | |
|---|-------------|------------|-------------|
| C | -0.64635200 | 3.27129700 | -0.32038700 |
| H | -0.43732500 | 3.45132400 | -1.37819200 |
| H | -1.28732200 | 4.08018300 | 0.04477700 |
| C | 0.61336600 | 3.16423700 | 0.49195700 |
| H | 1.21680400 | 4.07292100 | 0.43928800 |
| H | 0.35479100 | 2.98939500 | 1.54026600 |
| N | 1.40254800 | 1.98538900 | 0.04350200 |
| N | -1.33673200 | 1.97279700 | -0.20996700 |
| C | 2.38212800 | 1.58653700 | 1.09883500 |
| H | 3.03473800 | 2.44601100 | 1.28801000 |
| C | -2.55474900 | 1.83388900 | -1.02900100 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.23912900 | 1.90079100 | -2.07546100 |
| C | 3.18866400 | 0.38363200 | 0.75868200 |
| C | 2.54858200 | -0.88739100 | 0.77909800 |
| C | 4.53749700 | 0.48572800 | 0.47551500 |
| C | 3.35138200 | -2.01474400 | 0.51358000 |
| C | 5.30019400 | -0.64362700 | 0.20826900 |
| H | 5.00696700 | 1.46676800 | 0.46692700 |
| C | 4.69990600 | -1.89316600 | 0.23596000 |
| H | 5.30070000 | -2.77196600 | 0.02901400 |
| C | -3.25861800 | 0.54995800 | -0.73258500 |
| C | -2.58610300 | -0.68426600 | -0.88844900 |
| C | -4.57862300 | 0.56293400 | -0.31332600 |
| C | -3.30118600 | -1.86381100 | -0.63351100 |
| C | -5.26401800 | -0.61436000 | -0.06165900 |
| H | -5.08524100 | 1.51454000 | -0.17967300 |
| C | -4.62233200 | -1.83033400 | -0.23572700 |
| H | -5.15839700 | -2.75159900 | -0.03707900 |
| O | 1.26874200 | -0.98892900 | 0.98844300 |
| O | -1.33144600 | -0.77351200 | -1.29450800 |
| S | 7.04711600 | -0.45256600 | -0.13687800 |
| S | -6.99506200 | -0.54710900 | 0.40947400 |
| O | -7.30225000 | -1.86713400 | 1.02542900 |
| O | -7.75166900 | -0.30855000 | -0.85364400 |
| O | -7.11125200 | 0.58908200 | 1.36592700 |
| O | 7.13877900 | 0.49154000 | -1.28861900 |
| O | 7.55678300 | -1.81454900 | -0.46086200 |
| O | 7.65521300 | 0.11347700 | 1.10300400 |
| H | 0.50276300 | -2.46742400 | 0.29827500 |
| H | 1.40587500 | -0.32658200 | -2.02985100 |
| H | 1.42578300 | -0.87518900 | -1.49477200 |
| O | 0.00907800 | -3.08000600 | -0.28511400 |
| H | -0.52596300 | -2.45711600 | -0.80313800 |
| H | 0.00391200 | -0.06991400 | 1.98479100 |
| O | -0.69381300 | 0.52534500 | 2.33152000 |
| H | -1.10884200 | 0.05216800 | 3.05603500 |
| H | 1.92647500 | 2.23949700 | -0.79513600 |
| H | 1.78969400 | 1.40847800 | 2.00015100 |
| H | -1.54312000 | 1.76447000 | 0.77602500 |
| H | -3.22055100 | 2.67955500 | -0.82312100 |
| Pd | 0.06274800 | 0.52630500 | -0.61770100 |
| H | 2.88123500 | -2.99305000 | 0.52885100 |
| H | -2.78758200 | -2.81137900 | -0.75411300 |

53

RR_D1_TS2_P, E(SCF) = -2408.92171556,
E(ZPE) = -2408.528813, E(G) = -2408.596147
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.47946700 | -2.88643500 | 0.80942200 |
| H | 0.21845500 | -3.29029100 | -0.17384600 |
| H | 0.97338100 | -3.68451500 | 1.37408600 |
| C | -0.75550500 | -2.41163100 | 1.52842000 |
| H | -1.43486700 | -3.23931400 | 1.75166200 |
| H | -0.47514600 | -1.94729000 | 2.47916100 |
| N | -1.46025300 | -1.37130900 | 0.72986400 |
| N | 1.36636100 | -1.73354800 | 0.59853100 |
| C | -2.46210800 | -0.67601400 | 1.59200600 |
| H | -2.99757000 | -1.43725400 | 2.16167500 |
| C | 2.43226800 | -1.94926300 | -0.39025000 |
| H | 1.93362000 | -2.16404100 | -1.34366400 |
| C | -3.46025100 | 0.13500300 | 0.81997400 |
| C | -3.28640800 | 1.50236300 | 0.59430800 |
| C | -4.64045300 | -0.46298800 | 0.38767100 |
| C | -4.29294800 | 2.25047800 | -0.00359200 |
| C | -5.62680500 | 0.27638000 | -0.23427600 |
| H | -4.79974200 | -1.52417200 | 0.55506600 |
| C | -5.46228100 | 1.64289500 | -0.41374700 |
| H | -6.24272300 | 2.22687200 | -0.88932000 |
| C | 3.33125200 | -0.75576400 | -0.50136700 |
| C | 2.83680400 | 0.52622900 | -0.84084400 |
| C | 4.69626100 | -0.92888600 | -0.30137200 |
| C | 3.77301600 | 1.56900400 | -0.99202000 |
| C | 5.59300500 | 0.11160000 | -0.44904700 |
| H | 5.07308700 | -1.91158500 | -0.03493500 |
| C | 5.12034000 | 1.37150600 | -0.79684000 |
| H | 5.81362500 | 2.19780800 | -0.91929700 |
| O | -2.15404900 | 2.15444400 | 0.98092800 |
| O | 1.56844900 | 0.81143700 | -1.06568300 |

S -7.16904800 -0.50133100 -0.74743200
 S 7.34651500 -0.12431500 -0.15925400
 O 8.03490900 0.37419500 -1.38464600
 O 7.53665200 -1.58521400 0.06090600
 O 7.67671800 0.69219600 1.04509300
 O -6.94137000 -1.96658200 -0.63292900
 O -7.39759300 -0.04829200 -2.14655200
 O -8.20078600 0.00803800 0.19828600
 H 0.14269500 3.60750600 -0.38527400
 H -0.98687700 0.73779000 -0.88623400
 H -1.38216900 1.64498900 0.65812800
 O 0.88373500 3.21229900 0.08100600
 H 1.10799800 2.40054700 -0.42635100
 H -0.74693800 2.40190200 2.65531700
 O 0.21447600 2.36043700 2.69614700
 H 0.49330000 2.68942200 1.82038300
 H -1.96327500 -1.83296300 -0.02836300
 H -1.90547200 -0.05730100 2.29033500
 H 1.78263800 -1.45237500 1.48459500
 H 3.02670900 -2.83364000 -0.12916300
 Pd 0.03257800 -0.23126700 -0.19214300
 H -4.12947200 3.31124600 -0.15324500
 H 3.39486800 2.54873800 -1.26502100

53

RR_D1_TS2_R, E(SCF) = -2408.89334522,
 E(ZPE) = nofreq, E(G) = nofreq a.u.

C -0.53257000 3.10434100 0.22737900
 H -0.29952600 3.40529400 -0.79722900
 H -1.11536300 3.90277200 0.69479100
 C 0.70999400 2.79731700 1.01154600
 H 1.36805400 3.66527400 1.09151500
 H 0.43994500 2.48881900 2.02646300
 N 1.43357300 1.65361400 0.39089600
 N -1.32288300 1.85770200 0.15816900
 C 2.39256100 1.05940900 1.37782800
 H 2.95098500 1.89813400 1.80966600
 C -2.49939200 1.92486400 -0.73539400
 H -2.11050000 2.08599100 -1.74688100
 C 3.34462500 0.05535800 0.82128400
 C 2.97195200 -1.31513000 0.74042000
 C 4.62653400 0.45493800 0.45839600
 C 3.95834700 -2.22251700 0.28415300
 C 5.56200700 -0.45657800 0.00841000
 H 4.90634300 1.50202800 0.53550200
 C 5.21898400 -1.80482700 -0.07049500
 H 5.95426200 -2.52536600 -0.41667400
 C -3.32708800 0.68556200 -0.63673500
 C -2.76028300 -0.58194500 -0.88211400
 C -4.67836000 0.78677900 -0.32990100
 C -3.60205300 -1.70667500 -0.82461400
 C -5.48738000 -0.33061400 -0.28052700
 H -5.11429300 1.76165000 -0.13597600
 C -4.94153400 -1.58346400 -0.53203400
 H -5.57155600 -2.46646800 -0.49605200
 O 1.77210200 -1.71261500 1.02350900
 O -1.49022300 -0.77219000 -1.20271500
 S 7.21277100 0.05191500 -0.45840600
 S -7.23106700 -0.19603800 0.12475200
 O -7.96196900 -0.79752700 -1.02666400
 O -7.50025800 1.25839700 0.29257600
 O -7.41470600 -0.97356300 1.38335800
 O 7.25597800 1.53173600 -0.28761800
 O 7.38985800 -0.37318800 -1.87818000
 O 8.14368900 -0.66569400 0.46138300
 H 0.35959900 -2.82626300 0.49233400
 H 1.11010100 -0.61559000 -1.31760500
 H 1.11278900 -0.97537700 -0.56412300
 O -0.55740600 -3.08561700 0.28390100
 H -0.86785600 -2.40062600 -0.33296500
 H 0.35322500 -1.10200000 2.05713300
 O -0.55612800 -1.01761900 2.39843400
 H -1.01817800 -1.69889600 1.89039000
 H 1.97578600 1.99790600 -0.40276400
 H 1.77916400 0.62698200 2.17146600
 H -1.63042300 1.59165800 1.09757300
 H -3.09967500 2.79943200 -0.46406400

Pd -0.01883000 0.39659600 -0.44138300
 H 3.68475100 -3.27092000 0.22171700
 H -3.16910900 -2.68079100 -1.02505000

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RR_D1_TS2W_P, E(SCF) = -2408.92713948,
 E(ZPE) = -2408.534673, E(G) = -2408.600482
 a.u.

C -0.56481600 3.27713800 -0.23877200
 H -0.32118700 3.40613700 -1.29848200
 H -1.17277000 4.13776100 0.06758900
 C 0.68762600 3.20156900 0.59737100
 H 1.27417700 4.12144500 0.53055100
 H 0.40297300 3.06409600 1.64439500
 N 1.51931500 2.02164300 0.22016600
 N -1.28728800 2.01091600 -0.09516200
 C 2.39596200 1.63553300 1.36415200
 H 3.07113400 2.47088800 1.58278000
 C -2.41308200 1.82716400 -1.01147100
 H -2.00548700 1.88855200 -2.02881100
 C 3.17518700 0.39388000 1.09485800
 C 2.62898700 -0.86360500 1.38214700
 C 4.41370300 0.45948400 0.48019000
 C 3.32492000 -2.01675000 1.04633000
 C 5.10176900 -0.69419600 0.13460600
 H 4.84211500 1.43276900 0.25393000
 C 4.55451800 -1.93310700 0.41413100
 H 5.09793100 -2.83030200 0.14298800
 C -3.10222100 0.51469400 -0.78469400
 C -2.42141600 -0.72651600 -0.90695700
 C -4.45403200 0.51902600 -0.47692500
 C -3.17975500 -1.90036600 -0.74415300
 C -5.17242500 -0.65357400 -0.30077200
 H -4.96266500 1.47496300 -0.37834600
 C -4.52584500 -1.87019700 -0.44376500
 H -5.08249100 -2.79117400 -0.31226900
 O 1.41868700 -0.93407700 1.98552200
 O -1.13960100 -0.85780000 -1.18906900
 S 6.70509300 -0.54334500 -0.66762000
 S -6.92144000 -0.56705300 0.07902900
 O -7.03922900 0.30356300 1.28459400
 O -7.35741700 -1.96931300 0.33007600
 O -7.57656700 0.03686500 -1.11831900
 O 7.58059400 0.15338000 0.31636800
 O 6.46374000 0.26867800 -1.89293500
 O 7.14631200 -1.93321600 -0.96269400
 H 0.91034100 -1.69743700 1.61009800
 H 1.38926300 -0.40600100 -1.00422100
 H -0.45068200 -2.10475600 -0.07073200
 O -0.15047400 -2.65504500 0.68808200
 H 0.11280700 -3.50237400 0.32115800
 H -0.13461400 0.21245800 2.36482200
 O -0.92708100 0.74354600 2.54759400
 H -1.18683700 0.51249200 3.44259400
 H 2.12496200 2.28356200 -0.55628000
 H 1.74383000 1.50245700 2.22817800
 H -1.56984700 1.85837700 0.87530200
 H -3.14099400 2.64284200 -0.90757700
 Pd 0.23099000 0.55262500 -0.56396300
 H 2.88914200 -2.98287500 1.27808400
 H -2.66544600 -2.84985900 -0.85244000

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RR_D1_TS2W_R, E(SCF) = -2408.88989097,
 E(ZPE) = -2408.500369, E(G) = -2408.567585
 a.u.

C -0.58005700 3.33938000 0.00239700
 H -0.32980700 3.62037700 -1.02423800
 H -1.23199000 4.11313400 0.41945600
 C 0.64522200 3.14532600 0.84819000
 H 1.27599400 4.03653500 0.86608100
 H 0.34450000 2.92415500 1.87523000
 N 1.42116700 1.96849000 0.36430500
 N -1.28069800 2.04204400 -0.04148200
 C 2.30929900 1.47293400 1.46071700
 H 2.96353600 2.30775500 1.73943900
 C -2.51333800 2.03849000 -0.85326100

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | -2.21357600 | 2.28676400 | -1.87733300 | S | -6.90807400 | -0.69750800 | 0.36142000 |
| C | 3.10786900 | 0.27171800 | 1.10829000 | O | -7.28985500 | 0.67440200 | 0.79767200 |
| C | 2.58957300 | -1.01586600 | 1.44307300 | O | -6.85010900 | -1.67179700 | 1.48941600 |
| C | 4.34530300 | 0.40353000 | 0.50422600 | O | -7.73373300 | -1.19830300 | -0.77525500 |
| C | 3.42812000 | -2.12006400 | 1.14975500 | O | 7.50128300 | 0.63140400 | 0.37628700 |
| C | 5.12483800 | -0.70489200 | 0.20527100 | O | 6.54885500 | 0.17491500 | -1.86363200 |
| H | 4.71694000 | 1.40023200 | 0.27290200 | O | 7.53436500 | -1.67996000 | -3.53818900 |
| C | 4.65677100 | -1.96872200 | 0.54139000 | H | 0.82766700 | -2.16718400 | 0.68550000 |
| H | 5.27426100 | -2.83414300 | 0.32630200 | H | 1.18942300 | -0.48445900 | -1.26668200 |
| C | -3.20138000 | 0.71681700 | -0.78384800 | O | 0.78208300 | -1.27720400 | -0.83446900 |
| C | -2.51647000 | -0.43641300 | -1.22175100 | O | 0.48087900 | -2.40597000 | -3.25205000 |
| C | -4.50738700 | 0.61749600 | -0.32880000 | H | 1.01390100 | -3.13299900 | -0.59430800 |
| C | -3.20596500 | -1.66062600 | -1.21283000 | H | 0.02983500 | -0.32612100 | 2.17402700 |
| C | -5.16609300 | -0.59851800 | -0.32483100 | O | -0.76630600 | 0.23012500 | 2.32756500 |
| H | -5.03028700 | 1.59488700 | 0.01375600 | H | -1.15403300 | -0.09211000 | 3.14414900 |
| C | -4.51105800 | -1.73786300 | -0.77710900 | H | 2.03219400 | 2.13238800 | -0.41290500 |
| H | -5.02687500 | -2.69296900 | -0.77890600 | H | 1.61499800 | 1.07982400 | 2.27535600 |
| O | 1.41785000 | -1.17542500 | 1.95782200 | H | -1.50216700 | 1.67361400 | 0.95005200 |
| O | -1.28104500 | -0.39297800 | -1.68271400 | H | -3.21342500 | 2.84184600 | -0.39683400 |
| S | 6.70344100 | -0.47563300 | -0.60337200 | Pd | 0.03436700 | 0.59490200 | -0.68058600 |
| S | -6.85103500 | -0.73631500 | 0.27917300 | H | 3.20635400 | -3.21491600 | 1.23623200 |
| O | -7.28280400 | 0.64913100 | 0.61209100 | H | -2.81488200 | -2.50716900 | -1.63846300 |
| O | -6.78319900 | -1.62842600 | 1.47181400 | | | | |
| O | -7.63365000 | -1.33935600 | -0.83702100 | | | | |
| O | 7.45398900 | 0.51710900 | 0.22095800 | 53 | | | |
| O | 6.40254100 | 0.04656800 | -1.97016300 | RR_D1_TS2, E(SCF) = -2408.89280438, E(ZPE) | | | |
| O | 7.35499900 | -1.81617400 | -0.63067300 | = -2408.502288, E(G) = -2408.566827 a.u. | | | |
| H | 0.68667100 | -2.38538300 | 0.91772700 | C | -0.52091400 | 3.06853200 | 0.21917600 |
| H | 1.44440300 | -0.33383200 | -1.29459000 | H | -0.29279200 | 3.36461400 | -0.80811300 |
| H | 1.02760200 | -0.86908700 | -0.84080600 | H | -1.07063700 | 3.88513100 | 0.69574700 |
| O | 0.36204100 | -2.94968600 | 0.17946000 | C | 0.72719400 | 2.72866600 | 0.98486000 |
| H | 1.12298600 | -3.47766600 | -0.07323000 | H | 1.40065700 | 3.58465700 | 1.06763700 |
| H | 0.00951500 | -0.13624200 | 2.22465200 | H | 0.46339600 | 2.41450700 | 1.99963100 |
| O | -0.78126400 | 0.44149900 | 2.34653900 | N | 1.42586900 | 1.57985400 | 0.34535000 |
| H | -1.27488200 | 0.06332800 | 3.07729000 | N | -1.34699400 | 1.84565000 | 0.16015000 |
| H | 2.02302000 | 2.27260100 | -0.40261000 | C | 2.37226400 | 0.94782000 | 1.31743100 |
| H | 1.65699800 | 1.25487900 | 2.30763800 | H | 2.90314700 | 1.76532800 | 1.81889900 |
| H | -1.47630700 | 1.70810200 | 0.91371600 | C | -2.52108500 | 1.92564700 | -0.73434300 |
| H | -3.17660700 | 2.83158100 | -0.49215000 | H | -2.13063200 | 2.06449200 | -1.74848200 |
| Pd | 0.09419500 | 0.65176400 | -0.63081300 | C | 3.36703400 | 0.00442300 | 0.72347300 |
| H | 3.07718900 | -3.10939800 | 1.42981700 | C | 3.04397800 | -1.36019400 | 0.51901300 |
| H | -2.68518300 | -2.54377400 | -1.56550200 | C | 4.65713200 | 0.45716000 | 0.46357500 |
| | | | | C | 4.06766600 | -2.21147100 | 0.05589400 |
| | | | | C | 5.63695200 | -0.39784500 | -0.00041900 |
| | | | | H | 4.90695200 | 1.49997700 | 0.63693500 |
| | | | | C | 5.33644400 | -1.74295000 | -0.19706800 |
| | | | | H | 6.10582300 | -2.41996300 | -0.55595900 |
| | | | | C | -3.37040600 | 0.70107200 | -0.61720300 |
| | | | | C | -2.83199000 | -0.58222000 | -0.85151300 |
| | | | | C | -4.71654700 | 0.83260300 | -0.29902500 |
| | | | | C | -3.69826300 | -1.68755900 | -0.77435500 |
| | | | | C | -5.54916900 | -0.26678200 | -0.22900500 |
| | | | | H | -5.13053600 | 1.81830700 | -0.11167700 |
| | | | | C | -5.03199000 | -1.53353500 | -0.47093900 |
| | | | | H | -5.67982200 | -2.40283400 | -0.41977000 |
| | | | | O | 1.82865300 | -1.80855500 | 0.70518000 |
| | | | | O | -1.57060000 | -0.80548200 | -1.18039700 |
| | | | | S | 7.30068900 | 0.18413700 | -0.32941300 |
| | | | | S | -7.28585200 | -0.09027700 | 0.18810300 |
| | | | | O | -8.03973900 | -0.67797600 | -0.95586400 |
| | | | | O | -7.52055600 | 1.37063200 | 0.35347100 |
| | | | | O | -7.47983300 | -0.85961200 | 1.45039900 |
| | | | | O | 7.29780600 | 1.64273300 | -0.02764600 |
| | | | | O | 7.55933400 | -0.11258300 | -1.76804900 |
| | | | | O | 8.19321200 | -0.59554100 | 0.57643300 |
| | | | | H | 0.35469500 | -2.99805200 | 0.18702600 |
| | | | | H | 0.98933700 | -0.73087500 | -1.24307600 |
| | | | | H | 1.11813800 | -1.06949500 | -0.44173400 |
| | | | | O | -0.58643500 | -3.20347600 | 0.06027900 |
| | | | | H | -0.92600100 | -2.46653600 | -0.47947800 |
| | | | | O | 0.48789900 | -1.46044600 | 2.00809100 |
| | | | | H | -0.38137100 | -1.51449700 | 2.44617000 |
| | | | | H | -0.84739800 | -2.11776900 | 1.84846400 |
| | | | | H | 1.96829700 | 1.92091300 | -0.44855500 |
| | | | | H | 1.75148100 | 0.45064000 | 2.06659400 |
| | | | | H | -1.66833900 | 1.60600200 | 1.10048300 |
| | | | | H | -3.10846000 | 2.81369800 | -0.47795900 |
| | | | | Pd | -0.06808700 | 0.35089000 | -0.45306300 |

| | | | | | | | |
|---|-------------|-------------|-------------|--|--|--|--|
| 53 | | | | | | | |
| RR_D1_TS2W, E(SCF) = -2408.88026471, E(ZPE) | | | | | | | |
| = -2408.492151, E(G) = -2408.556385 a.u. | | | | | | | |
| C | -0.56910000 | 3.27955700 | 0.03347700 | | | | |
| H | -0.33914400 | 3.55985000 | -0.99861600 | | | | |
| H | -1.16949400 | 4.08138400 | 0.47663300 | | | | |
| C | 0.67821400 | 3.04312700 | 0.83813000 | | | | |
| H | 1.33355500 | 3.91718800 | 0.83804900 | | | | |
| H | 0.39998900 | 2.83909700 | 1.87532200 | | | | |
| N | 1.41508400 | 1.84192700 | 0.34600200 | | | | |
| N | -1.31380600 | 2.01285200 | -0.00146500 | | | | |
| C | 2.28332200 | 1.33622400 | 1.45259600 | | | | |
| H | 2.90652900 | 2.17884200 | 1.77711500 | | | | |
| C | -2.56012600 | 2.05200900 | -0.78461900 | | | | |
| H | -2.27703600 | 2.32246300 | -1.80849200 | | | | |
| C | 3.13822900 | 0.17423000 | 1.09554500 | | | | |
| C | 2.66801300 | -1.14210600 | 1.35263600 | | | | |
| C | 4.39637900 | 0.37712100 | 0.55438200 | | | | |
| C | 3.54372200 | -2.20217100 | 1.03367900 | | | | |
| C | 5.22848300 | -0.68785800 | 0.24178800 | | | | |
| H | 4.73836700 | 1.39562700 | 0.38061900 | | | | |
| C | 4.79245700 | -1.98180800 | 0.48772000 | | | | |
| H | 5.44539800 | -2.81510900 | 0.25281400 | | | | |
| C | -3.26164500 | 0.73435500 | -0.74342700 | | | | |
| C | -2.60677900 | -0.41355800 | -1.24506300 | | | | |
| C | -4.55512900 | 0.63615400 | -0.25383600 | | | | |
| C | -3.31651300 | -1.62825400 | -1.24734600 | | | | |
| C | -5.23351600 | -0.56964900 | -0.26769800 | | | | |
| H | -5.05431700 | 1.51938500 | 0.13280600 | | | | |
| C | -4.60825500 | -1.70350100 | -0.77348000 | | | | |
| H | -5.13716800 | -2.65155500 | -0.78665000 | | | | |
| O | 1.47357800 | -1.37471800 | 1.81729400 | | | | |
| O | -1.39284900 | -0.37723200 | -1.75117500 | | | | |
| S | 6.82658500 | -0.36922300 | -0.50119500 | | | | |

H 3.82050100 -3.25615200 -0.10196900
H -3.28679900 -2.67270400 -0.96650000

53

RR_D2_I1_P_CH_P, E(SCF) = -2408.89085396,
E(ZPE) = -2408.499749, E(G) = -2408.566870
a.u.

C 0.89252900 2.31599500 -1.58303800
H 0.79951900 3.03707600 -0.76372300
H 1.41174500 2.81388900 -2.40870400
C -0.47722500 1.85103900 -2.00397300
H -1.06205100 2.67883100 -2.41590800
H -0.40155600 1.06885900 -2.76610200
N -1.17708900 1.27776100 -0.82790100
N 1.64566900 1.15961100 -1.07943100
C -2.48082600 0.72125700 -1.22057400
H -2.29422600 -0.09137300 -1.92736500
C 2.82210700 1.49013900 -0.26446000
H 3.48266900 2.18174200 -0.80457100
C -3.30274900 0.18136100 -0.05706300
C -3.77131100 1.23357300 0.92053000
C -4.34451100 -0.77401400 -0.51158100
C -5.05829400 -0.104273900 1.54784000
C -5.54249600 -0.83381200 0.07014600
H -4.08833100 -1.46602500 -1.30767400
C -5.89558900 0.07542600 1.13159300
H -5.34208000 1.75152800 2.31671700
H -6.87611800 -0.02483400 1.58719400
C 3.58798900 0.26012000 0.11656700
C 2.98252100 -0.81359400 0.82147800
C 4.94095100 0.19868000 -0.19671100
C 3.81777300 -1.89217500 1.19282000
C 5.73103900 -0.87152800 0.17670000
H 5.39717700 1.02095800 -0.73951800
C 5.15605700 -1.92458000 0.88083600
H 3.35793100 -2.70897700 1.73943300
H 5.76387600 -2.77249600 1.18195600
O -3.05984800 2.20109800 1.19467400
O 1.72678100 -0.87402900 1.18614300
S -6.78710600 -2.03534000 -0.43133200
S 7.46612500 -0.94357000 -0.25896800
O 7.78935600 0.36294000 -0.89870000
O 7.60968100 -2.09735100 -1.19507800
O 8.20469700 -1.16278000 1.01882600
O -7.05264500 -2.83152400 0.79637600
O -6.17935700 -2.81994700 -1.53423000
O -7.95196500 -1.21117900 -0.85201400
H 2.44830700 2.02219900 0.62052900
H -3.05123900 1.49630400 -1.75069200
H 1.93537300 0.57089300 -1.85821900
H -1.37352000 2.06533200 -0.20549200
H -2.54886800 3.83612900 0.20285500
O -1.89944400 4.23781000 -0.38944300
H -2.41784200 4.65956600 -1.07908300
H -1.35573900 2.47193700 2.15470200
O -0.42544500 2.51221900 2.41878900
H -0.06206500 1.68851800 2.05947500
Pd 0.24080000 0.11318400 0.19070800
H -0.79451300 -0.57998900 1.14451400
H -2.59186400 -0.42143500 0.55180900

53

RR_D2_I1_P_CH_R, E(SCF) = -2408.89089601,
E(ZPE) = -2408.501899, E(G) = -2408.568804
a.u.

C 0.83023500 2.90175600 -1.00797700
H 0.64135300 3.40579100 -0.05471300
H 1.53238900 3.50185300 -1.59160800
C -0.46205400 2.65954500 -1.73273700
H -0.97932200 3.59804400 -1.95012000
H -0.29652400 2.11572800 -2.66785200
N -1.30371200 1.82331100 -0.85298300
N 1.41987300 1.57716900 -0.70327600
C -2.58196500 1.42166800 -1.48432600
H -2.35071400 0.78193300 -2.33971000
C 2.55675000 1.61381800 0.24446100
H 3.26062000 2.38599400 -0.08280200

C -3.48062900 0.72588100 -0.51812300
C -3.77350400 1.34603900 0.73111100
C -4.00378900 -0.52194500 -0.83110500
C -4.58865700 0.60905700 1.62640700
C -4.81024500 -1.20280800 0.06087200
H -3.76574400 -0.97990000 -1.78656000
C -5.09439800 -0.62714200 1.29848500
H -4.80970300 1.05966600 2.58895400
H -5.71856500 -1.16335000 2.00752900
C 3.24546800 0.29078100 0.30681900
C 2.52265200 -0.88035400 0.62203900
C 4.61199900 0.21546500 0.06913600
C 3.23520800 -2.09148000 0.70831500
C 5.29013700 -0.98385800 0.16211200
H 5.16370300 1.11519300 -0.18477800
C 4.59255000 -2.14156600 0.49003400
H 2.67756200 -2.98795000 0.95589600
H 5.11938000 -3.08788500 0.56370900
O -3.29707400 2.50544300 1.04776300
O 1.23214000 -0.90478300 0.87766700
S -5.47544300 -2.81802200 -0.32941400
S 7.05326000 -1.08101000 -0.15308700
O 7.49731400 0.31058700 -0.44167000
O 7.20681400 -1.99615400 -1.32007000
O 7.65807200 -1.64067500 1.08917200
O -4.91767900 -3.75339900 0.69114500
O -5.01897100 -3.13194400 -1.71275800
O -6.95868400 -2.69184900 -0.22246700
H 2.14441400 1.92449500 1.21098000
H -3.04435100 2.34173200 -1.86940300
H 1.73755800 1.14609600 -1.57420800
H -1.56890300 2.38964600 -0.03690300
H -2.93047100 3.98841800 0.16256600
H -2.49012500 4.74744300 -0.27556800
O -3.12763500 5.07389100 -0.91386800
H -1.79107000 2.75962000 1.98190000
O -0.86399400 2.95646500 2.23260300
H -0.49590000 2.10685500 2.49130500
Pd -0.07735100 0.37225100 0.00536200
H -1.68701600 -0.34522100 0.51833400
H -1.13215500 -0.89132700 0.73883900

53

RR_D2_I1_P_CH_TS, E(SCF) = -2408.87296568,
E(ZPE) = -2408.487448, E(G) = -2408.554027
a.u.

C 0.91061600 2.85455400 -1.31554200
H 0.81316700 3.45641400 -0.40590700
H 1.56639000 3.39132300 -2.00687400
C -0.44938200 2.59954800 -1.91469000
H -0.93642300 3.53285200 -2.21059900
H -0.37237100 1.95287000 -2.79370900
N -1.26051000 1.89677200 -0.89844100
N 1.49472400 1.55348500 -0.92871600
C -2.56128400 1.40765900 -1.39354100
H -2.37237300 0.79610600 -2.27910300
C 2.64280800 1.62936100 -0.00848000
H 3.38750000 2.33231000 -0.39973000
C -3.28375800 0.59851500 -0.35179000
C -3.67482600 1.26392300 0.88233400
C -4.00094700 -0.56662300 -0.76716200
C -4.55451900 0.53521600 1.74638200
C -4.86257700 -1.18874700 0.07452600
H -3.80412600 -0.99112700 -1.74677800
C -5.12875900 -0.63114600 1.34976900
H -4.79035900 0.98041500 2.70659000
H -5.81480100 -1.14936500 2.01315700
C 3.27399500 0.28553400 0.18770400
C 2.52503200 -0.83729600 0.62226600
C 4.64171700 0.15683700 -0.02772400
C 3.23009700 -2.04126100 0.84087600
C 5.30430700 -1.03406800 0.19344100
H 5.21086200 1.01671400 -0.36749600
C 4.58528700 -2.14030800 0.63441700
H 2.65761900 -2.89769600 1.18087100
H 5.09422700 -3.08282900 0.81234700
O -3.19872100 2.38278100 1.20629600

O 1.23703100 -0.84181800 0.86797400
S -5.70999000 -2.70001600 -0.39550500
S 7.06237300 -1.19108600 -0.11395800
O 7.54545700 0.17434600 -0.46269700
O 7.19813800 -2.15990000 -1.24068100
O 7.65531400 -1.71193700 1.15144700
O -5.30998300 -3.71056900 0.62288700
O -5.23477800 -3.02316500 -1.76672400
O -7.16137300 -2.37106600 -0.33453000
H 2.26000000 2.04601500 0.93170000
H -3.16137900 2.27508400 -1.69898200
H 1.77915000 1.04833200 -1.76810000
H -1.46218000 2.57214100 -0.15302800
H -2.80006700 3.99935400 0.40150900
O -2.22601000 4.65696500 -0.02888100
H -2.76669000 5.05824400 -0.71319800
H -1.62204300 2.62201000 2.18454400
O -0.71281400 2.73593100 2.51266600
H -0.28754700 1.89863900 2.29527700
Pd -0.05112000 0.46163900 -0.01590400
H -1.29063600 -0.38270300 0.70769600
H -2.13893100 -0.00736800 0.24420000

53
RR_D2_I1_P_HH-Homo_P, E(SCF) = -
2408.85798644, E(ZPE) = -2408.468827, E(G)
= -2408.535521 a.u.
C 0.89289800 2.93340600 -1.07927200
H 0.70870900 3.44908500 -0.13152800
H 1.53322000 3.57595000 -1.69053400
C -0.42162400 2.65394700 -1.77108800
H -0.94901400 3.58582200 -1.99448800
H -0.27211600 2.10096300 -2.70333500
N -1.25636700 1.83180700 -0.86808500
N 1.53901500 1.64699600 -0.78208300
C -2.59630200 1.50134300 -1.39666000
H -2.47531800 0.90537200 -2.30442400
C 2.61816500 1.65303500 0.21535400
H 3.37616300 2.40339200 -0.03717500
C -3.43524400 0.78189400 -0.38769800
C -3.47558600 1.22191700 0.96565200
C -4.17673100 -0.32109500 -0.78731300
C -4.29716000 0.48838700 1.85061900
C -4.97329200 -1.01386400 0.10607800
H -4.12877300 -0.65776900 -1.81881100
C -5.03127300 -0.59844400 1.43289300
H -4.32992500 0.81313000 2.88588200
H -5.65098000 -1.13971200 2.14139900
C 3.25557000 0.29620000 0.29112500
C 2.51384700 -0.86830900 0.60003000
C 4.62037500 0.18745600 0.05283300
C 3.20287100 -2.09284700 0.66475800
C 5.27660300 -1.02562200 0.13217100
H 5.19119800 1.07703600 -0.19456800
C 4.55958400 -2.17251200 0.44784100
H 2.62539900 -2.97925200 0.90302600
H 5.06580600 -3.13071500 0.50899700
O -2.76449600 2.22775600 1.39241300
O 1.22164900 -0.89353900 0.89377200
S -5.94559400 -2.42311700 -0.41909600
S 7.04006900 -1.15035000 -0.17771200
O 7.50433300 0.23126500 -0.48106400
O 7.18241200 -2.08113000 -1.33327800
O 7.63259400 -1.70363100 1.07310500
O -7.37550600 -2.01238100 -0.29315600
O -5.59674600 -3.53574900 0.51156100
O -5.54663000 -2.69934400 -1.82807500
H 2.16689200 1.99708600 1.17010500
H -3.05724700 2.45796000 -1.68435400
H 1.89355300 1.23967700 -1.64587200
H -1.46361500 2.39728000 -0.03427100
H -2.52231400 3.86768700 0.74985900
O -2.04672100 4.60442100 0.31310000
H -2.70218200 5.04604400 -0.23121200
H -1.19580400 1.81106700 1.95036600
O -0.22757500 1.59180200 1.88247700
H 0.00040600 1.04537400 2.64154900

Pd -0.06407900 0.35906600 -0.03314200
H -1.24007700 -0.57010800 0.32925200
H -0.17919300 -0.52367000 -1.25603300

53
RR_D2_I1_P_HH-Homo_R, E(SCF) = -
2408.89093254, E(ZPE) = -2408.502010, E(G)
= -2408.569715 a.u.
C 0.82810100 2.90082400 -1.00067800
H 0.63827200 3.39384100 -0.04199200
H 1.52336000 3.51231300 -1.58054900
C -0.46537300 2.65734300 -1.72451800
H -0.98833500 3.59566000 -1.92865400
H -0.29881700 2.12735200 -2.66748400
N -1.30111500 1.80414400 -0.85483000
N 1.42795400 1.57755300 -0.71065900
C -2.58679500 1.41982200 -1.48185000
H -2.37004000 0.78169500 -2.34234900
C 2.56112800 1.60298300 0.24153500
H 3.26778300 2.37711200 -0.07459700
C -3.48886300 0.73385100 -0.51125400
C -3.74605400 1.34517200 0.74777200
C -4.02978400 -0.50418200 -0.82154600
C -4.55492100 0.61583200 1.65244700
C -4.83164300 -1.18112000 0.08067400
H -3.81512900 -0.95997100 -1.78378700
C -5.08558600 -0.61171100 0.32604100
H -4.75025000 1.06238300 2.62254900
H -5.70561500 -1.14309600 2.04234200
C 3.24919600 0.27816200 0.29618600
C 2.52849200 -0.89918500 -0.59426900
C 4.61862200 0.20900300 0.07192900
C 3.24571000 -2.10735300 0.68101000
C 5.30094600 -0.98796800 0.16318800
H 5.16919700 1.11261200 -0.17028900
C 4.60532800 -2.15068800 0.47690600
H 2.68902300 -3.00764100 0.91651100
H 5.13540800 -3.09519000 0.55021900
O -3.24424500 2.49710100 1.06459800
O 1.23399100 -0.93593700 0.83161900
S -5.54298300 -2.77383100 -0.31830000
S 7.06729000 -1.07640800 -0.13644100
O 7.50788200 0.31796100 -0.41657700
O 7.23474700 -1.98714600 -1.30494300
O 7.66321400 -1.63763700 1.10935600
O -7.02344100 -2.59583000 -0.25086100
O -5.04633400 -3.72448200 -0.71989000
O -5.06387500 -3.11121700 -1.68864300
H 2.14652900 1.90469600 1.20991400
H -3.03863000 2.34827900 -1.86014200
H 1.75020600 1.15855300 -1.58599800
H -1.56540400 2.35318900 -0.02558000
H -2.89125100 3.98667500 0.19002400
O -2.45852200 4.75390900 -0.24181700
H -3.10257700 5.08450000 -0.87136600
H -1.74651300 2.73630300 1.99710200
O -0.82040400 2.92209400 2.26174700
H -0.46142400 2.06435300 2.50561800
Pd -0.06406700 0.34778300 -0.02965100
H -1.34441200 -0.48561000 0.88929400
H -1.32622700 -0.88929600 0.17985000

53
RR_D2_I1_P_HH-Homo_TS, E(SCF) = -
2408.85649233, E(ZPE) = -2408.469899, E(G)
= -2408.536421 a.u.
C 0.89490400 2.92314700 -1.07322600
H 0.68849300 3.45744600 -0.14080100
H 1.54697000 3.55361400 -1.68488700
C -0.40038400 2.61744300 -1.78876400
H -0.93104700 3.53767800 -2.04935500
H -0.22147900 2.04516100 -2.70416300
N -1.24664500 1.80433200 -0.88896300
N 1.53591200 1.64322000 -0.73968600
C -2.58045700 1.47023200 -1.42979500
H -2.45129400 0.85782700 -2.32548100
C 2.62626600 1.66452500 0.24521400

| | | | |
|----|-------------|-------------|-------------|
| H | 3.38029900 | 2.41135500 | -0.02862300 |
| C | -3.43282300 | 0.77280200 | -0.41644800 |
| C | -3.48422400 | 1.24061200 | 0.92730900 |
| C | -4.17006300 | -0.33845500 | -0.79962300 |
| C | -4.31381500 | 0.52530600 | 1.82014100 |
| C | -4.97542700 | -1.01217200 | 0.10072500 |
| H | -4.11303600 | -0.69673700 | -1.82347200 |
| C | -5.04443500 | -0.56981000 | 1.41828400 |
| H | -4.35507900 | 0.87076200 | 2.84841600 |
| H | -5.67072500 | -1.09619700 | 2.13227500 |
| C | 3.26448500 | 0.30815800 | 0.32354300 |
| C | 2.52099300 | -0.85363300 | 0.64013200 |
| C | 4.62532700 | 0.19394100 | 0.06792100 |
| C | 3.20480700 | -2.08139000 | 0.69566900 |
| C | 5.27650600 | -1.02269100 | 0.13853500 |
| H | 5.19705800 | 1.08075000 | -0.18712300 |
| C | 4.55849700 | -2.16678200 | 0.46173800 |
| H | 2.62618700 | -2.96552600 | 0.93950100 |
| H | 5.06130900 | -3.12724700 | 0.51513800 |
| O | -2.77864100 | 2.25616300 | 1.33709400 |
| O | 1.23222300 | -0.86844000 | 0.94818100 |
| S | -5.94303500 | -2.43197800 | -0.40318400 |
| S | 7.03492200 | -1.15611300 | -0.19759500 |
| O | 7.50028600 | 0.22237000 | -0.51277000 |
| O | 7.15520200 | -2.09136500 | -1.35198000 |
| O | 7.64368700 | -1.70774800 | 1.04607400 |
| O | -7.37429000 | -2.02056100 | -0.29498000 |
| O | -5.59981600 | -3.52595600 | 0.55153900 |
| O | -5.53462800 | -2.73533000 | -1.80393000 |
| H | 2.18700700 | 1.97108600 | 1.20094500 |
| H | -3.03535500 | 2.42223000 | -1.74193500 |
| H | 1.88119800 | 1.21117600 | -1.59595000 |
| H | -1.46506900 | 2.37164500 | -0.05785300 |
| H | -2.52688300 | 3.89059600 | 0.69179700 |
| O | -2.06886600 | 4.64142000 | 0.26018600 |
| H | -2.70594300 | 5.00611000 | -0.35789800 |
| H | -1.18911500 | 1.89303700 | 1.94025100 |
| O | -0.21587800 | 1.71018200 | 1.88845600 |
| H | 0.01811200 | 1.19235200 | 2.66495200 |
| Pd | -0.06200100 | 0.34142900 | -0.02093000 |
| H | -1.22676500 | -0.65421000 | 0.24574600 |
| H | -0.43301100 | -0.73534500 | -1.03674500 |

47
RR_D2_TS1_no2W_P, E(SCF) = -2256.00769361,
E(ZPE) = -2255.668911, E(G) = -2255.729857
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.83579300 | 3.26625100 | -0.70705200 |
| H | 0.71283400 | 3.73150600 | 0.27446800 |
| H | 1.53916300 | 3.86883300 | -1.28786300 |
| C | -0.48684700 | 3.11180800 | -1.40274600 |
| H | -0.97359200 | 4.07771700 | -1.56390000 |
| H | -0.34680600 | 2.64148000 | -2.38161800 |
| N | -1.34704200 | 2.22754500 | -0.59178100 |
| N | 1.37928400 | 1.90632300 | -0.48875700 |
| C | -2.53852600 | 1.75782600 | -1.33909000 |
| H | -2.20518700 | 1.11159800 | -2.15593500 |
| C | 2.57555000 | 1.85476500 | 0.38244500 |
| H | 3.31181600 | 2.57534500 | 0.01136600 |
| C | -3.50252000 | 1.05948500 | -0.44189500 |
| C | -3.84468300 | 1.69206800 | 0.79792800 |
| C | -4.05727100 | -0.15721100 | -0.80663900 |
| C | -4.77989500 | 0.99160100 | 1.61232900 |
| C | -4.96876900 | -0.80052900 | 0.01362300 |
| H | -3.77426900 | -0.61808600 | -1.74875300 |
| C | -5.32341700 | -0.21092200 | 1.22806600 |
| H | -5.05542000 | 1.44411300 | 2.56038000 |
| H | -6.03344700 | -0.71545300 | -1.87783700 |
| C | 3.16730700 | 0.48441100 | 0.40847100 |
| C | 2.38601200 | -0.62178200 | 0.80882600 |
| C | 4.50131400 | 0.30104800 | 0.06695000 |
| C | 3.01065100 | -1.88210700 | 0.86950000 |
| C | 5.09224200 | -0.94518100 | 0.13567300 |
| H | 5.09807700 | 1.15108800 | -0.24829400 |
| C | 4.33872900 | -2.03936700 | 0.54686900 |
| H | 2.40978700 | -2.72849400 | 1.18337900 |
| H | 4.79848600 | -3.02108600 | 0.60471600 |

| | | | |
|----|-------------|-------------|-------------|
| O | -3.31289900 | 2.79863600 | 1.15509400 |
| O | 1.12227300 | -0.53836500 | 1.16400100 |
| S | -5.69556400 | -2.36548200 | -0.44479700 |
| S | 6.81636100 | -1.18171600 | -0.29999900 |
| O | 6.82123500 | -2.14074900 | -1.44183900 |
| O | 7.46820100 | -1.74585300 | 0.91639500 |
| O | 7.33650600 | 0.16422900 | -0.66802800 |
| O | -5.31762600 | -3.33719900 | 0.62531200 |
| O | -5.12056800 | -2.72075200 | -1.77447600 |
| O | -7.17211800 | -2.14486300 | -0.49586900 |
| H | 2.24997600 | 2.18741800 | 1.37410300 |
| H | -2.99691000 | 2.65347700 | -1.78589500 |
| H | 1.61680000 | 1.48979300 | -1.39171000 |
| H | -1.76478600 | 2.73997000 | 0.21290300 |
| Pd | -0.14746300 | 0.77412700 | 0.28607900 |
| H | -1.28782500 | -0.14888900 | 1.29878300 |
| H | -1.70787100 | -0.08574200 | 0.60262400 |

47
RR_D2_TS1_no2W_R, E(SCF) = -2256.03571260,
E(ZPE) = -2255.696906, E(G) = -2255.757467
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.66993600 | 3.04417800 | -0.35191300 |
| H | -0.49109000 | 3.05837700 | -1.43091800 |
| H | -1.27021300 | 3.92173400 | -0.09678200 |
| C | 0.63518300 | 3.02192100 | 0.40384700 |
| H | 1.23192600 | 3.91699700 | 0.20970300 |
| H | 0.45156000 | 2.96445500 | 1.48068200 |
| N | 1.37505000 | 1.79952100 | 0.01585000 |
| N | -1.40053500 | 1.79553700 | -0.03988400 |
| C | 2.47669000 | 1.43303300 | 0.92540300 |
| H | 2.01204400 | 1.19433300 | 1.88890100 |
| C | -2.52663200 | 1.49099800 | -0.94404200 |
| H | -3.17805400 | 2.36854100 | -1.02395000 |
| C | 3.28878000 | 0.29187900 | 0.39366600 |
| C | 2.69632400 | -0.92047500 | -0.04453900 |
| C | 4.67382000 | 0.42035700 | 0.38596200 |
| C | 3.56834900 | -1.96042300 | -0.43873300 |
| C | 5.50035300 | -0.61188900 | -0.00941500 |
| H | 5.12259500 | 1.35394900 | 0.71103500 |
| C | 4.93435900 | -1.81507400 | -0.42013800 |
| H | 3.11523800 | -2.89100000 | -0.76370400 |
| H | 5.57267600 | -2.63662000 | -0.73071900 |
| C | -3.32080900 | 0.31770700 | -0.46024700 |
| C | -2.70822000 | -0.92348200 | -0.15158600 |
| C | -4.70209400 | 0.44562000 | -0.36309600 |
| C | -3.55705000 | -1.99041100 | 0.21781000 |
| C | -5.50648400 | -0.61495500 | 0.00274800 |
| H | -5.16673600 | 1.40011800 | -0.59075400 |
| C | -4.92157400 | -1.84409200 | 0.29131100 |
| H | -3.08877700 | -2.94177700 | 0.44714800 |
| H | -5.54351300 | -2.68565000 | 0.58106800 |
| O | 1.41146100 | -1.16121900 | -0.10057700 |
| O | -1.42253700 | -1.16357300 | -0.20490700 |
| S | 7.28147800 | -0.42248200 | -0.02686700 |
| S | -7.28462800 | -0.43776100 | -0.12537200 |
| O | -7.63023300 | -0.72985400 | 1.54709400 |
| O | -7.86177700 | -1.44436300 | -0.81231000 |
| O | -7.59034800 | 0.96598400 | -0.26889400 |
| O | 7.82099500 | -1.53669900 | 0.80534100 |
| O | 7.56013900 | 0.92235900 | 0.55072900 |
| O | 7.69525600 | -0.53604100 | -1.45624800 |
| H | -2.08737500 | 1.31373300 | -1.93267700 |
| H | 3.12566300 | 2.30220300 | 1.08080600 |
| H | -1.75759600 | 1.84818300 | 0.91510600 |
| H | 1.75589100 | 1.92376600 | -0.92308000 |
| Pd | -0.00941000 | 0.28748300 | -0.08408700 |
| H | 0.95861100 | -1.29431800 | 2.42828600 |
| H | 0.86882500 | -0.98487500 | 3.10597200 |

47
RR_D2_TS1_no2W, E(SCF) = -2255.99300938,
E(ZPE) = -2255.654464, E(G) = -2255.713286
a.u.

| | | | |
|---|------------|------------|-------------|
| C | 0.83190800 | 3.12553400 | -0.20563800 |
| H | 0.74137500 | 3.41336700 | 0.84538500 |
| H | 1.44446100 | 3.87538400 | -0.71314800 |

| | | | |
|----|-------------|-------------|-------------|
| C | -0.52395800 | 2.98595100 | -0.84340400 |
| H | -1.08231000 | 3.92588000 | -0.81224600 |
| H | -0.42651100 | 2.68774100 | -1.89198100 |
| N | -1.25808200 | 1.91674700 | -0.14061000 |
| N | 1.49164800 | 1.80211700 | -0.24477500 |
| C | -2.51317200 | 1.54041100 | -0.80450200 |
| H | -2.24847100 | 1.07046400 | -1.76080600 |
| C | 2.69892700 | 1.68549800 | 0.60157000 |
| H | 3.37712500 | 2.51384800 | 0.36932500 |
| C | -3.41596800 | 0.64504300 | 0.00195000 |
| C | -3.11985500 | 0.22917800 | 1.33575800 |
| C | -4.59395600 | 0.24629300 | -0.61370200 |
| C | -4.09534800 | -0.59947000 | 1.95866800 |
| C | -5.51989900 | -0.55174000 | 0.03136800 |
| H | -4.80023700 | -0.57073900 | -1.33046400 |
| C | -5.25968900 | -0.97447800 | 1.33400400 |
| H | -3.88351200 | -0.92735700 | 2.97205700 |
| H | -5.97870000 | -1.60362600 | 1.85082900 |
| C | 3.39762800 | 0.38231000 | 0.38647000 |
| C | 2.71796600 | -0.84273200 | 0.58353700 |
| C | 4.74035700 | 0.37625300 | 0.03043900 |
| C | 3.45591100 | -2.03362600 | 0.43503800 |
| C | 5.44104500 | -0.80568900 | -0.11108300 |
| H | 5.25684900 | 1.31734700 | -0.13068400 |
| C | 4.79073000 | -2.01642400 | 0.10294500 |
| H | 2.93451600 | -2.97145300 | 0.59287300 |
| H | 5.33511100 | -2.94946800 | -0.00496200 |
| O | -2.03362400 | 0.54676100 | 1.95094000 |
| O | 1.45394300 | -0.93425700 | 0.92584400 |
| S | -7.02255600 | -1.07765000 | -0.78175000 |
| S | 7.18036000 | -0.80740300 | -0.54956100 |
| O | 7.29081600 | -1.64595900 | -1.77749800 |
| O | 7.89320000 | -1.41097200 | 0.61326000 |
| O | 7.54886900 | 0.61680200 | -0.78107800 |
| O | -6.94557400 | -2.56603100 | -0.87827900 |
| O | -7.03139100 | -0.41399500 | -2.11715900 |
| O | -8.14931000 | -0.63269500 | 0.09143700 |
| H | 2.36121900 | 1.80802700 | 1.63644700 |
| H | -3.04612900 | 2.47018900 | -1.05283400 |
| H | 1.74339600 | 1.57677500 | -1.20873900 |
| H | -1.48025900 | 2.17706100 | 0.82516700 |
| Pd | 0.07509400 | 0.40825500 | 0.30807100 |
| H | -1.20306900 | -1.17305800 | 0.56732200 |
| H | -1.07017300 | -1.26749300 | -0.18636300 |

53
RR_D2_TS1_P_CH_P, E(SCF) = -2408.89085396,
E(ZPE) = -2408.499749, E(G) = -2408.566870
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.89252900 | 2.31599500 | -1.58303800 |
| H | 0.79951900 | 3.03707600 | -0.76372300 |
| H | 1.411174500 | 2.81388900 | -2.40870400 |
| C | -0.47722500 | 1.85103900 | -2.00397300 |
| H | -1.06205100 | 2.67883100 | -2.41590800 |
| H | -0.40155600 | 1.06885900 | -2.76610200 |
| N | -1.17708900 | 1.27776100 | -0.82790100 |
| N | 1.64566900 | 1.15961100 | -1.07943100 |
| C | -2.48082600 | 0.72125700 | -1.22057400 |
| H | -2.29422600 | -0.09137300 | -1.92736500 |
| C | 2.82210700 | 1.49013900 | -0.26446000 |
| H | 3.48266900 | 2.18174200 | -0.80257100 |
| C | -3.30274900 | 0.18136100 | -0.05706300 |
| C | -3.77131100 | 1.23357300 | 0.92053000 |
| C | -4.34451100 | -0.77401400 | -0.51158100 |
| C | -5.05829400 | 1.04273900 | 1.54784000 |
| C | -5.54249600 | -0.83381200 | 0.07014600 |
| H | -4.08833100 | -1.46602500 | -1.30767400 |
| C | -5.89558900 | 0.07542600 | 1.13159300 |
| H | -5.34208000 | 1.75152800 | 2.31671700 |
| H | -6.87611800 | -0.02483400 | 1.58719400 |
| C | 3.58798900 | 0.26012000 | 0.11656700 |
| C | 2.98252100 | -0.81359400 | 0.82147800 |
| C | 4.94095100 | 0.19868000 | -0.19671100 |
| C | 3.81777300 | -1.89217500 | 1.19282000 |
| C | 5.73103900 | -0.87152800 | 0.17670000 |
| H | 5.39717700 | 1.02095800 | -0.73951800 |
| C | 5.15605700 | -1.92458000 | 0.88083600 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.35793100 | -2.70897700 | 1.73943300 |
| H | 5.76387600 | -2.77249600 | 1.18195600 |
| O | -3.05984800 | 2.20109800 | 1.19467400 |
| O | 1.72678100 | -0.87402900 | 1.18614300 |
| S | -6.78710600 | -2.03534000 | -0.43133200 |
| S | 7.46612500 | -0.94357000 | -0.25896800 |
| O | 7.78935600 | 0.36294000 | -0.89870000 |
| O | 7.60968100 | -2.09735100 | -1.19507800 |
| O | 8.20469700 | -1.16278000 | 1.01882600 |
| O | -7.05264500 | -2.83152400 | 0.79637600 |
| O | -6.17935700 | -2.81994700 | -1.53423000 |
| O | -7.95196500 | -1.21179700 | -0.85201400 |
| H | 2.44830700 | 2.02219900 | 0.62052900 |
| H | -3.05123900 | 1.49630400 | -1.75069200 |
| H | 1.93537300 | 0.57089300 | -1.85821900 |
| H | -1.37352000 | 2.06533200 | -0.20549200 |
| H | -2.54886800 | 3.83512900 | 0.20285500 |
| O | -1.89944400 | 4.23781000 | -0.38944300 |
| H | -2.41784200 | 4.65956600 | -1.47908300 |
| H | -1.35573900 | 2.47193700 | 2.15470200 |
| O | -0.42544500 | 2.51221900 | 2.41878900 |
| H | -0.06206500 | 1.68851800 | 2.05947500 |
| Pd | 0.24080000 | 0.11318400 | 0.19070800 |
| H | -0.79451300 | -0.57998900 | 1.14451400 |
| H | -2.59186400 | -0.42143500 | 0.55180900 |

53
RR_D2_TS1_P_CH_R, E(SCF) = -2408.89089601,
E(ZPE) = -2408.501899, E(G) = -2408.568804
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.83023500 | 2.90175600 | -1.00797700 |
| H | 0.64135300 | 3.40579100 | -0.05471300 |
| H | 1.53238900 | 3.50185300 | -1.59160800 |
| C | -0.46205400 | 2.65954500 | -1.73273700 |
| H | -0.97932200 | 3.59804400 | -1.95012000 |
| H | -0.29652400 | 2.11572800 | -2.66785200 |
| N | -1.30371200 | 1.82331100 | -0.85298300 |
| N | 1.41987300 | 1.57716900 | -0.70327600 |
| C | -2.58196500 | 1.42166800 | -1.48432600 |
| H | -2.35071400 | 0.78193300 | -2.33971000 |
| C | 2.55675000 | 1.61381800 | 0.24446100 |
| H | 3.26062000 | 2.38599400 | -0.08280200 |
| C | -3.48062900 | 0.72588100 | -0.51812300 |
| C | -3.77350400 | 1.34603900 | 0.73111100 |
| C | -4.00378900 | -0.52194500 | -0.83110500 |
| C | -4.58865700 | 0.60905700 | 1.62640700 |
| C | -4.81024500 | -1.20280800 | 0.06087200 |
| H | -3.76574400 | -0.97990000 | -1.78656000 |
| C | -5.09439800 | -0.62714200 | 1.29848500 |
| H | -4.80970300 | 1.05966600 | 2.58895400 |
| H | -5.71856500 | -1.16335000 | 2.00752900 |
| C | 3.24546800 | 0.29078100 | 0.30681900 |
| C | 2.52265200 | -0.88035400 | 0.62203900 |
| C | 4.61199900 | 0.21546500 | 0.06913600 |
| C | 3.23520800 | -2.09148000 | 0.70831500 |
| C | 5.29013700 | -0.98385800 | -0.16211200 |
| H | 5.16370300 | 1.11519300 | -0.18477800 |
| C | 4.59255000 | -2.14156600 | 0.49003400 |
| H | 2.67756200 | -2.98795000 | 0.95589600 |
| H | 5.11938000 | -3.08788500 | 0.56370900 |
| O | -3.29707400 | 2.50544300 | 1.04776300 |
| O | 1.23214000 | -0.90478300 | 0.87766700 |
| S | -5.47544300 | -2.81802200 | -0.32941400 |
| S | 7.05326000 | -1.08101000 | -0.15308700 |
| O | 7.49731400 | 0.31058700 | -0.44167000 |
| O | 7.20681400 | -1.99615400 | -1.32007000 |
| O | 7.65807200 | -1.64067500 | 1.08917200 |
| O | -4.91767900 | -3.75339900 | 0.69114500 |
| O | -5.01897100 | -3.13194400 | -1.71275800 |
| O | -6.95868400 | -2.69184900 | -0.22246700 |
| H | 2.14441400 | 1.92449500 | 1.21098000 |
| H | -3.04435100 | 2.34173200 | -1.86940300 |
| H | 1.73755800 | 1.14609600 | -1.57420800 |
| H | -1.56890300 | 2.38964600 | -0.03690300 |
| H | -2.93047100 | 3.98841800 | 0.16256600 |
| O | -2.49012500 | 4.74744300 | -0.27556800 |
| H | -3.12763500 | 5.07398100 | -0.91386800 |

H -1.79107000 2.75962000 1.98190000
 O -0.86399400 2.95646500 2.23260300
 H -0.49590000 2.10685500 2.49130500
 Pd -0.07735100 0.37225100 0.00536200
 H -1.68701600 -0.34522100 0.51833400
 H -1.13215500 -0.89132700 0.73883900

53

RR_D2_TS1_P_CH_TS, E(SCF) = -2408.87296568,
 E(ZPE) = -2408.487448, E(G) = -2408.554027
 a.u.

C 0.91061600 2.85455400 -1.31554200
 H 0.81316700 3.45641400 -0.40590700
 H 1.56639000 3.39132300 -2.00687400
 C -0.44938200 2.59954800 -1.91469000
 H -0.93642300 3.53285200 -2.21059900
 H -0.37237100 1.95287000 -2.79370900
 N -1.26051000 1.89677200 -0.89844100
 N 1.49472400 1.55348500 -0.92871600
 C -2.56128400 1.40765900 -1.39354100
 H -2.37237300 0.79610600 -2.27910300
 C 2.64280800 1.62936100 -0.00848000
 H 3.38750000 2.33231000 -0.39973000
 C -3.28375800 0.59851500 -0.35179000
 C -3.67482600 1.26392300 0.88233400
 C -4.00094700 -0.56662300 -0.76716200
 C -4.55451900 0.53521600 1.74638200
 C -4.86257700 -1.18874700 0.07452600
 H -3.80412600 -0.99112700 -1.74677800
 C -5.12875900 -0.63114600 1.34976900
 H -4.79035900 0.98041500 2.70659000
 H -5.81480100 -1.14936500 2.01315700
 C 3.27399500 0.28553400 0.18770400
 C 2.52503200 -0.83729600 0.62226600
 C 4.64171700 0.15683700 -0.02772400
 C 3.23009700 -2.04126100 0.84087600
 C 5.30430700 -1.03406800 0.19344100
 H 5.21086200 1.01671400 -0.36749600
 C 4.58528700 -2.14030800 0.63441700
 H 2.65761900 -2.89769600 1.18087100
 H 5.09422700 -3.08282900 0.81234700
 O -3.19872100 2.38278100 1.20629600
 O 1.23703100 -0.84181800 0.86797400
 S -5.70999000 -2.70001600 -0.39550500
 S 7.06237300 -1.19108600 -0.11395800
 O 7.54545700 0.17434600 -0.46269700
 O 7.19813800 -2.15990000 -1.24068100
 O 7.65531400 -1.71193700 1.15144700
 O -5.30998300 -3.71056900 0.62287800
 O -5.23477800 -3.02316500 -1.76672400
 O -7.16137300 -2.37106600 -0.33453000
 H 2.26000000 2.04601500 0.93170000
 H -3.16137900 2.27508400 -1.69898200
 H 1.77915000 1.04833200 -1.76810000
 H -1.46218000 2.57214100 -0.15302800
 H -2.80006700 3.99935400 0.40150900
 O -2.22601000 4.65696500 -0.02888100
 H -2.76669000 5.05824400 -0.71319800
 H -1.62204300 2.62201000 2.18454400
 O -0.71281400 2.73593100 2.51266600
 H -0.28754700 1.89863900 2.29527700
 Pd -0.05112000 0.46163900 -0.01590400
 H -1.29063600 -0.38270300 0.70769600
 H -2.13893100 -0.00736800 0.24420000

53

RR_D2_TS1_P_HH-apical, E(SCF) = -
 2408.89089601, E(ZPE) = -2408.501899, E(G)
 = -2408.568804 a.u.

C 0.83023500 2.90175600 -1.00797700
 H 0.64135300 3.40579100 -0.05471300
 H 1.53238900 3.50185300 -1.59160800
 C -0.46205400 2.65954500 -1.73273700
 H -0.97932200 3.59804400 -1.95012000
 H -0.29652400 2.11572800 -2.66785200
 N -1.30371200 1.82331100 -0.85298300
 N 1.41987300 1.57716900 -0.70327600

C -2.58196500 1.42166800 -1.48432600
 H -2.35071400 0.78193300 -2.33971000
 C 2.55675000 1.61381800 0.24446100
 H 3.26062000 2.38599400 -0.08280200
 C -3.48062900 0.72588100 -0.51812300
 C -3.77350400 1.34603900 0.73111100
 C -4.00378900 -0.52194500 -0.83110500
 C -4.58865700 0.60905700 1.62640700
 C -4.81024500 -1.20280800 0.06087200
 H -3.76574400 -0.97990000 -1.78656000
 C -5.09439800 -0.62714200 1.29848500
 H -4.80970300 1.05966600 2.58895400
 H -5.71856500 -1.16335000 2.00752900
 C 3.24546800 0.29078100 0.30681900
 C 2.52265200 -0.88035400 0.62203900
 C 4.61199900 0.21546500 0.06913600
 C 3.23520800 -2.09148000 0.70831500
 C 5.29013700 -0.98385800 0.16211200
 H 5.11519300 -1.11519300 -0.84477800
 C 4.59255000 -2.14156600 0.49003400
 H 2.67756200 -2.98795000 0.95589600
 H 5.11938000 -3.08788500 0.56370900
 O -3.29707400 2.50544300 1.04776300
 O 1.23214000 -0.90478300 0.87766700
 S -5.47544300 -2.81802200 -0.32941400
 S 7.05326000 -1.08101000 -0.15308700
 O 7.49731400 0.31058700 -0.44167000
 O 7.20681400 -1.99615400 -1.32007000
 O 7.65807200 -1.64067500 1.08917200
 O -4.91767900 -3.75339900 0.69114500
 O -5.01897100 -3.13194400 -1.71275800
 O -6.95868400 -2.69184900 -0.22246700
 H 2.14441400 1.92449500 1.21098000
 H -3.04435100 2.34173200 -1.86940300
 H 1.73755800 1.14609600 -1.57420800
 H -1.56890300 2.38964600 -0.03690300
 H -2.93047100 3.98841800 0.16256600
 O -2.49012500 4.74744300 -0.27556800
 H -3.12763500 5.07389100 -0.91386800
 H -1.79107000 2.75962000 1.98190000
 O -0.86399400 2.95646500 2.23260300
 H -0.49590000 2.10685500 2.49130500
 Pd -0.07735100 0.37225100 0.00536200
 H -1.68701600 -0.34522100 0.51833400
 H -1.13215500 -0.89132700 0.73883900

53

RR_D2_TS1_P_HH-Homo P, E(SCF) = -
 2408.85798644, E(ZPE) = -2408.468827, E(G)
 = -2408.535521 a.u.

C 0.89289800 2.93340600 -1.07927200
 H 0.70870900 3.44908500 -0.13152800
 H 1.53322000 3.57595000 -1.69053400
 C -0.42162400 2.65394700 -1.77108800
 H -0.94901400 3.58582200 -1.99448800
 H -0.27211600 2.10096300 -2.70333500
 N -1.25636700 1.83180700 -0.86808500
 N 1.53901500 1.64699600 -0.78208300
 C -2.59630200 1.50134300 -1.39666000
 H -2.47531800 0.90537200 -2.30442400
 C 2.61816500 1.65303500 0.21535400
 H 3.37616300 2.40339200 -0.03717500
 C -3.43524400 0.78189400 -0.38769800
 C -3.47558600 1.22191700 0.96565200
 C -4.17673100 -0.32109500 -0.78731300
 C -4.29716000 0.48838700 1.85061900
 C -4.97329200 -1.01386400 0.10607800
 H -4.12877300 -0.65776900 -1.81881100
 C -5.03127300 -0.59844400 1.43289300
 H -4.32992500 0.81313000 2.88588200
 H -5.65098000 -1.13971200 2.14139900
 C 3.25557000 0.29620000 0.29112500
 C 2.51384700 -0.86830900 0.60003000
 C 4.62037500 0.18745600 0.05283300
 C 3.20287100 -2.09284700 0.66475800
 C 5.27660300 -1.02562200 0.13217100
 H 5.19119800 1.07703600 -0.19456800

| | | | |
|----|-------------|-------------|-------------|
| C | 4.55958400 | -2.17251200 | 0.44784100 |
| H | 2.62539900 | -2.97925200 | 0.90302600 |
| H | 5.06580600 | -3.13071500 | 0.50899700 |
| O | -2.76449600 | 2.22775600 | 1.39241300 |
| O | 1.22164900 | -0.89353900 | 0.89377200 |
| S | -5.94559400 | -2.42311700 | -0.41909600 |
| S | 7.04006900 | -1.15035000 | -0.17771200 |
| O | 7.50433300 | 0.23126500 | -0.48106400 |
| O | 7.18241200 | -2.08113000 | -1.33327800 |
| O | 7.63259400 | -1.70363100 | 1.07310500 |
| O | -7.37550600 | -2.01238100 | -0.29315600 |
| O | -5.59674600 | -3.53574900 | 0.51156100 |
| O | -5.54663000 | -2.69934400 | -1.82807500 |
| H | 2.16689200 | 1.94708600 | 1.17010500 |
| H | -3.05724700 | 2.45796000 | -1.68435400 |
| H | 1.89355300 | 1.23967700 | -1.64587200 |
| H | -1.46361500 | 2.39728000 | -0.03427100 |
| H | -2.52231400 | 3.86768700 | 0.74985900 |
| O | -2.04672100 | 4.60442100 | 0.31310000 |
| H | -2.70218200 | 5.04604400 | -0.23121200 |
| H | -1.19580400 | 1.81106700 | 1.95036600 |
| O | -0.22757500 | 1.59180200 | 1.88247700 |
| H | 0.00040600 | 1.04537400 | 2.64154900 |
| Pd | -0.06407900 | 0.35906600 | -0.03314200 |
| H | -1.24007700 | -0.57010800 | 0.32925200 |
| H | -0.17919300 | -0.52367000 | -1.25603300 |

53
RR_D2_TS1_P_HH-Homo_R, E(SCF) = -
2408.89093254, E(ZPE) = -2408.502010, E(G)
= -2408.569715 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.82810100 | 2.90082400 | -1.00067800 |
| H | 0.63827200 | 3.39384100 | -0.04199200 |
| H | 1.52336000 | 3.51231300 | -1.58054900 |
| C | -0.46537300 | 2.65734300 | -1.72451800 |
| H | -0.98833500 | 3.59566000 | -1.92865400 |
| H | -0.29881700 | 2.12735200 | -2.66748400 |
| N | -1.30111500 | 1.80414400 | -0.85483000 |
| N | 1.42795400 | 1.57755300 | -0.71065900 |
| C | -2.58679500 | 1.41982200 | -1.48185000 |
| H | -2.37004000 | 0.78169500 | -2.34234900 |
| C | 2.56112800 | 1.60298300 | 0.24153500 |
| H | 3.26778300 | 2.37711200 | -0.07459700 |
| C | -3.48886300 | 0.73385100 | -0.51125400 |
| C | -3.74605400 | 1.34517200 | 0.74777200 |
| C | -4.02978400 | -0.50418200 | -0.82154600 |
| C | -4.55492100 | 0.61583200 | 1.65244700 |
| C | -4.83164300 | -1.18112000 | 0.08067400 |
| H | -3.81512900 | -0.95997100 | -1.78378700 |
| C | -5.08558600 | -0.61171100 | 1.32604100 |
| H | -4.75025000 | 1.06238300 | 2.62254900 |
| H | -5.70561500 | -1.14309600 | 2.04234200 |
| C | 3.24919600 | 0.27816200 | 0.29618600 |
| C | 2.52849200 | -0.89918500 | 0.59426900 |
| C | 4.61862200 | 0.20900300 | 0.07192900 |
| C | 3.24571000 | -2.10735300 | 0.68101000 |
| C | 5.30094600 | -0.98796800 | 0.16318800 |
| H | 5.16919700 | 1.11261200 | -0.17028900 |
| C | 4.60532800 | -2.15068800 | 0.47690600 |
| H | 2.68902300 | -3.00764100 | 0.91651100 |
| H | 5.13540800 | -3.09519000 | 0.55021900 |
| O | -3.24424500 | 2.49710100 | 1.06459800 |
| O | 1.23399100 | -0.93593700 | 0.83161900 |
| S | -5.54298300 | -2.77383100 | -0.31830000 |
| S | 7.06729000 | -1.07640800 | -0.13644100 |
| O | 7.50788200 | 0.31796100 | -0.41657700 |
| O | 7.23474700 | -1.98714600 | -1.30494300 |
| O | 7.66321400 | -1.63763700 | 1.10935600 |
| O | -7.02344100 | -2.59583000 | -0.25086100 |
| O | -5.04633400 | -3.72448200 | 0.71989000 |
| O | -5.06387500 | -3.11121700 | -1.68864300 |
| H | 2.14652900 | 1.90469600 | 1.20991400 |
| H | -3.03863000 | 2.34827900 | -1.86014200 |
| H | 1.75020600 | 1.15855300 | -1.58599800 |
| H | -1.56540400 | 2.35318900 | -0.02558000 |
| H | -2.89125100 | 3.98667500 | 0.19002400 |
| O | -2.45852200 | 4.75390900 | -0.24181700 |

| | | | |
|----|-------------|-------------|-------------|
| H | -3.10257700 | 5.08450000 | -0.87136600 |
| H | -1.74651300 | 2.73630300 | 1.99710200 |
| O | -0.82040400 | 2.92209400 | 2.26174700 |
| H | -0.46142400 | 2.06435300 | 2.50561800 |
| Pd | -0.06406700 | 0.34778300 | -0.02965100 |
| H | -1.34441200 | -0.48561000 | 0.88929400 |
| H | -1.32622700 | -0.88929600 | 0.17985000 |

53
RR_D2_TS1_P_HH-Homo_TS, E(SCF) = -
2408.85649233, E(ZPE) = -2408.469899, E(G)
= -2408.536421 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.89490400 | 2.92314700 | -1.07322600 |
| H | 0.68849300 | 3.45744600 | -0.14080100 |
| H | 1.54697000 | 3.55361400 | -1.68488700 |
| C | -0.40038400 | 2.61744300 | -1.78876400 |
| H | -0.93104700 | 3.53767800 | -2.04935500 |
| H | -0.22147900 | 2.04516100 | -2.70416300 |
| N | -1.24664500 | 1.80433200 | -0.88896300 |
| N | 1.53591200 | 1.64322000 | -0.73968600 |
| C | -2.58045700 | 1.47023200 | -1.42979500 |
| H | -2.45129400 | 0.85782700 | -2.32548100 |
| C | 2.62626600 | 1.66525000 | 0.24521400 |
| H | 3.38029900 | 2.41135500 | -0.02862300 |
| C | -3.43282300 | 0.77280200 | -0.41644800 |
| C | -3.48422400 | 1.24061200 | 0.92730900 |
| C | -4.17006300 | -0.33845500 | -0.79962300 |
| C | -4.31381500 | 0.52530600 | 1.82014100 |
| C | -4.97542700 | -1.01217200 | 0.10072500 |
| H | -4.11303600 | -0.69673700 | -1.82347200 |
| C | -5.04443500 | -0.56981000 | 1.41828400 |
| H | -4.35507900 | 0.87076200 | 2.84841600 |
| H | -5.67072500 | -1.09619700 | 2.13227500 |
| C | 3.26448500 | 0.30815800 | 0.32354300 |
| C | 2.52099300 | -0.85363300 | 0.64013200 |
| C | 4.62532700 | 0.19394100 | 0.06792100 |
| C | 3.20480700 | -2.08139000 | 0.69566900 |
| C | 5.27650600 | -1.02269100 | 0.13853500 |
| H | 5.19705800 | 1.08075000 | -0.18712300 |
| C | 4.55849700 | -2.16678200 | 0.46173800 |
| H | 2.62618700 | -2.96552600 | 0.93950100 |
| H | 5.06130900 | -3.12724700 | 0.51513800 |
| O | -2.77864100 | 2.25616300 | 1.33709400 |
| O | 1.23222300 | -0.86844000 | 0.94818100 |
| S | -5.94303500 | -2.43197800 | -0.40318400 |
| S | 7.03492200 | -1.15611300 | -0.19759500 |
| O | 7.50028600 | 0.22237000 | -0.51277000 |
| O | 7.15520200 | -2.09136500 | -1.35198000 |
| O | 7.64368700 | -1.70774800 | 1.04607400 |
| O | -7.37429000 | -2.02056100 | -0.29498000 |
| O | -5.59981600 | -3.52595600 | 0.55153900 |
| O | -5.53462800 | -2.73533000 | -1.80393000 |
| H | 2.18700700 | 1.97108600 | 1.20094500 |
| H | -3.03535500 | 2.42223000 | -1.74193500 |
| H | 1.88119800 | 1.21117600 | -1.59595000 |
| H | -1.46506900 | 2.37164500 | -0.05785300 |
| H | -2.52688300 | 3.89059600 | 0.69179700 |
| O | -2.06886600 | 4.64142000 | 0.26018600 |
| H | -2.70594300 | 5.00611000 | -0.35789800 |
| H | -1.18911500 | 1.89303700 | 1.94025100 |
| O | -0.21587800 | 1.71018200 | 1.88845600 |
| H | 0.01811200 | 1.19235200 | 2.66495200 |
| Pd | -0.06200100 | 0.34142900 | -0.02093000 |
| H | -1.22676500 | -0.65421000 | 0.24574600 |
| H | -0.43301100 | -0.73534500 | -1.03674500 |

53
RR_D2_TS1_P, E(SCF) = -2408.89097398,
E(ZPE) = -2408.501515, E(G) = -2408.568374
a.u.

| | | | |
|---|-------------|------------|-------------|
| C | 0.83069000 | 2.89716800 | -1.00437700 |
| H | 0.63933500 | 3.39341300 | -0.04765300 |
| H | 1.52695300 | 3.50663000 | -1.58519500 |
| C | -0.46154600 | 2.65086000 | -1.72953400 |
| H | -0.98423600 | 3.58833900 | -1.93820100 |
| H | -0.29344200 | 2.11704700 | -2.67004300 |
| N | -1.29808500 | 1.80134500 | -0.85731100 |

| | | | |
|----|-------------|-------------|-------------|
| N | 1.43020600 | 1.57486800 | -0.70905900 |
| C | -2.58429200 | 1.41545800 | -1.48176300 |
| H | -2.36843900 | 0.77594800 | -2.34141100 |
| C | 2.56398700 | 1.60375200 | 0.24236100 |
| H | 3.27006900 | 2.37742800 | -0.07621100 |
| C | -3.48588500 | 0.73114000 | -0.50944200 |
| C | -3.74344300 | 1.34437400 | 0.74874600 |
| C | -4.03191000 | -0.50442500 | -0.82067700 |
| C | -4.55368100 | 0.61622900 | 1.65384500 |
| C | -4.83622500 | -1.17865100 | 0.08079300 |
| H | -3.81830700 | -0.96076300 | -1.78285000 |
| C | -5.08861100 | -0.60903300 | 1.32660500 |
| H | -4.74858500 | 1.06352400 | 2.62367800 |
| H | -5.71047600 | -1.13882000 | 2.04247700 |
| C | 3.25236000 | -0.27923100 | 0.29910800 |
| C | 2.53147600 | -0.89697700 | 0.60108200 |
| C | 4.62114500 | 0.20874900 | 0.07181200 |
| C | 3.24752100 | -2.10578300 | 0.68716100 |
| C | 5.30257200 | -0.96078200 | 0.16383400 |
| H | 5.17201000 | 1.11152000 | -0.17287500 |
| C | 4.60666800 | -2.15054000 | 0.47983900 |
| H | 2.69056400 | -3.00530500 | 0.92495000 |
| H | 5.13607500 | -3.09543400 | 0.55285200 |
| O | -3.24164500 | 2.49640700 | 1.06436100 |
| O | 1.23776300 | -0.93076400 | 0.84362100 |
| S | -5.55447600 | -2.76779700 | -0.32034900 |
| S | 7.06822900 | -1.07910100 | -0.14012600 |
| O | 7.50983400 | 0.31495400 | -0.42016700 |
| O | 7.23209200 | -1.98914000 | -1.30967500 |
| O | 7.66609500 | -1.64193800 | 1.10400100 |
| O | -5.06163900 | -3.72210100 | 0.71627200 |
| O | -5.07713300 | -3.10513300 | -1.69130900 |
| O | -7.03410400 | -2.58331600 | -0.25234700 |
| H | 2.14986600 | 1.90741300 | 1.21027200 |
| H | -3.03676900 | 2.34313500 | -1.86133900 |
| H | 1.75207400 | 1.15306200 | -1.58320900 |
| H | -1.56103900 | 2.35407300 | -0.03014000 |
| H | -2.88703500 | 3.98462800 | 0.18744800 |
| O | -2.45221900 | 4.74985800 | -0.24577400 |
| H | -3.09561000 | 5.08146200 | -0.87547000 |
| H | -1.74241100 | 2.73918600 | 1.99212200 |
| O | -0.81600500 | 2.92606700 | 2.25498100 |
| H | -0.45661600 | 2.06944200 | 2.50210500 |
| Pd | -0.06182500 | 0.34641400 | -0.02601000 |
| H | -1.43388900 | -0.41558000 | 0.83036800 |
| H | -1.23027900 | -0.96427100 | 0.26187100 |

53
RR_D2_TS1_R, E(SCF) = -2408.91628694,
E(ZPE) = -2408.527143, E(G) = -2408.594969
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.81178200 | 3.19529000 | 0.24738400 |
| H | 0.69358300 | 3.26757900 | 1.33248600 |
| H | 1.41126100 | 4.04607500 | -0.08850500 |
| C | -0.53200400 | 3.15793900 | -0.43517200 |
| H | -1.10705100 | 4.06782800 | -0.24643600 |
| H | -0.40134300 | 3.06324000 | -1.51745700 |
| N | -1.27231100 | 1.96209000 | 0.02962700 |
| N | 1.50262000 | 1.91684500 | -0.03869200 |
| C | -2.33622000 | 1.53785500 | -0.89197000 |
| H | -1.84027300 | 1.27674600 | -1.83502400 |
| C | 2.72108100 | 1.68027300 | 0.76320000 |
| H | 3.39352700 | 2.53951400 | 0.66503000 |
| C | -3.17294600 | 0.39656100 | -0.38758700 |
| C | -2.66204900 | -0.69788600 | 0.34535600 |
| C | -4.52347100 | 0.40713500 | -0.72858400 |
| C | -3.54783000 | -1.74214900 | 0.67677600 |
| C | -5.37158000 | -0.62670700 | -0.39163000 |
| H | -4.92587500 | 1.25203300 | -1.27894500 |
| C | -4.87415400 | -1.71360900 | 0.31867600 |
| H | -3.14288000 | -2.57753700 | 1.23883700 |
| H | -5.53063000 | -2.53369000 | 0.59246600 |
| C | 3.42489600 | 0.43093700 | 0.33712600 |
| C | 2.76018200 | -0.81737200 | 0.34418400 |
| C | 4.76577200 | 0.49284100 | -0.02242500 |
| C | 3.50915100 | -1.96244200 | 0.01313100 |
| C | 5.47660000 | -0.64429200 | -0.35370700 |

| | | | |
|----|-------------|-------------|-------------|
| H | 5.27212100 | 1.45291200 | -0.03648500 |
| C | 4.84069600 | -1.88081700 | -0.32359900 |
| H | 2.99830000 | -2.91923800 | 0.03009100 |
| H | 5.39254900 | -2.77986300 | -0.58050800 |
| O | -1.41998800 | -0.81507300 | 0.78167100 |
| O | 1.49395800 | -0.97346400 | 0.66475100 |
| S | -7.10426800 | -0.59941400 | -0.85640000 |
| S | 7.21326300 | -0.56009300 | -0.79278500 |
| O | 7.56154700 | 0.88765200 | -0.82521800 |
| O | 7.33127100 | -1.21775100 | -2.12585700 |
| O | 7.94009800 | -1.30906500 | 0.27282400 |
| O | -7.29621000 | -1.75801100 | -1.77558000 |
| O | -7.33407200 | 0.71375100 | -1.52001800 |
| O | -7.86878300 | -0.75255300 | 0.41456500 |
| H | 2.39583800 | 1.62955600 | 1.60838900 |
| H | -2.98939600 | 2.39265800 | -1.10313200 |
| H | 1.75364000 | 1.88490000 | -1.02777000 |
| H | -1.66082400 | 2.11748400 | 0.96924500 |
| H | -1.70386300 | 0.38518800 | 2.45755600 |
| O | -1.86977600 | 1.26918500 | 2.82185400 |
| H | -2.70687800 | 1.19628400 | 3.28775800 |
| H | -0.72062400 | -1.98832300 | 2.10347000 |
| O | 0.02842500 | -2.34786100 | -2.60598100 |
| H | 0.76575900 | -2.02606000 | 2.06014200 |
| Pd | 0.09488700 | 0.47099100 | 0.31109500 |
| H | -0.72359000 | -1.48145500 | -1.77078000 |
| H | -0.61544800 | -1.38799700 | -2.50711000 |

53
RR_D2_TS1, E(SCF) = -2408.88245414, E(ZPE)
= -2408.493473, E(G) = -2408.559644 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.79934100 | 2.99260300 | 0.04017800 |
| H | 0.66133600 | 3.05729100 | 1.12273900 |
| H | 1.40065900 | 3.84273400 | -0.28982100 |
| C | -0.53776400 | 2.93638100 | -0.64952000 |
| H | -1.12723200 | 3.83680600 | -0.45118800 |
| H | -0.42445700 | 2.83343900 | -1.73260300 |
| N | -1.23377400 | 1.73870400 | -0.13508600 |
| N | 1.50837100 | 1.72256800 | -0.23716100 |
| C | -2.54167400 | 1.50025600 | -0.75360400 |
| H | -2.35808700 | 1.22513600 | -1.79904700 |
| C | 2.62920100 | 1.42375300 | 0.68155700 |
| H | 3.26499300 | 2.31171400 | 0.76365200 |
| C | -3.42511900 | 0.47424200 | -0.08372100 |
| C | -3.04478800 | -0.36383500 | 0.99994000 |
| C | -4.70955300 | 0.37510400 | -0.61138900 |
| C | -4.02106300 | -1.27616200 | -1.47249600 |
| C | -5.63562900 | -0.52263500 | -0.12210300 |
| H | -4.99653100 | 1.01952000 | -1.43860300 |
| C | -5.28262000 | -1.35564700 | 0.93654700 |
| H | -3.72889000 | -1.92054100 | 2.29586200 |
| H | -6.00133800 | -2.06820700 | -1.32993200 |
| C | 3.44375000 | 0.26692600 | 0.19668600 |
| C | 2.85219800 | -0.97867800 | -0.10649800 |
| C | 4.82137500 | 0.41590800 | 0.08048000 |
| C | 3.69483900 | -2.03054600 | -0.50935000 |
| C | 5.62965700 | -0.63342200 | -0.30681900 |
| H | 5.27757400 | 1.37443100 | 0.30633600 |
| C | 5.05807700 | -1.86713600 | -0.59718100 |
| H | 3.23297500 | -2.98437900 | -0.73926800 |
| H | 5.68603000 | -2.69693600 | -0.90606900 |
| O | -1.86289800 | -0.34249400 | 1.54457400 |
| O | 1.55978800 | -1.23130100 | -0.01429400 |
| S | -7.28538700 | -0.62725500 | -0.80987000 |
| S | 7.40795000 | -0.43298200 | -0.44357200 |
| O | 7.69130100 | 0.98175800 | -0.07663600 |
| O | 7.74426200 | -0.74669900 | -1.86151200 |
| O | 7.99959600 | -1.41403800 | 0.51028800 |
| O | -7.45776300 | -2.04052800 | -1.25702100 |
| O | -7.33010000 | 0.34633800 | -1.93730900 |
| O | -8.21860800 | -0.27167100 | 0.29929500 |
| H | 2.18198400 | 1.24177400 | 1.66621500 |
| H | -3.07549400 | 2.46060900 | -0.78170400 |
| H | 1.86192100 | 1.73342800 | -1.19551200 |
| H | -1.34638800 | 1.86382600 | 0.87903500 |
| H | -1.28543900 | 0.94157700 | 2.55709500 |
| O | -0.87559100 | 1.80890400 | 2.77746700 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.41106400 | 2.18535200 | 3.47940400 |
| H | -0.62019200 | -1.48659300 | 2.21636200 |
| O | 0.20455100 | -1.95112100 | 2.45718000 |
| H | 0.77330700 | -1.82413200 | 1.68204600 |
| Pd | 0.13523600 | 0.19806700 | -0.18413600 |
| H | -1.11429600 | -1.35040700 | -0.31061700 |
| H | -0.97309700 | -1.22850000 | -1.06564200 |

53

RR_D2_TS2_P, E(SCF) = -2408.91851651,
E(ZPE) = -2408.525878, E(G) = -2408.593484
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.28514600 | -2.06001900 | 0.16899900 |
| H | 0.01585100 | -1.79522200 | 1.18754900 |
| H | -0.57568600 | -3.11541600 | 0.16780900 |
| C | 0.85637100 | -1.80908000 | -0.78331000 |
| H | 1.71869100 | -2.44223300 | -0.54248300 |
| H | 0.55410100 | -2.02600900 | -1.81212100 |
| N | 1.24159600 | -0.37910400 | -0.70373800 |
| N | -1.40858300 | -1.18771900 | -0.20827900 |
| C | 2.33004500 | -0.02073300 | -1.66263400 |
| H | 1.96719500 | 0.75149000 | -2.34273200 |
| C | -2.42831700 | -1.00611700 | 0.83350900 |
| H | -2.77538100 | -1.97797300 | 1.20660300 |
| C | 3.56153700 | 0.40787400 | -0.92856300 |
| C | 3.64566100 | 1.65893700 | -0.31578900 |
| C | 4.62090700 | -0.47991200 | -0.76641300 |
| C | 4.78078300 | 2.01715300 | 0.40422300 |
| C | 5.73890300 | -0.13288000 | -0.03486300 |
| H | 4.56864600 | -1.46265300 | -1.22416700 |
| C | 5.82087300 | 1.12373500 | 0.55004400 |
| H | 6.69827000 | 1.40013600 | 1.12478800 |
| C | -3.59807500 | -0.22030300 | 0.32469100 |
| C | -3.44490000 | 1.07578800 | -0.24483800 |
| C | -4.86702500 | -0.76251800 | 0.45658700 |
| C | -4.62222500 | 1.75256000 | -0.62531500 |
| C | -6.00509800 | -0.07379500 | 0.06784100 |
| H | -4.96750300 | -1.75623100 | 0.88676100 |
| C | -5.87421000 | 1.19729100 | -0.47060500 |
| H | -6.76131800 | 1.74091100 | -0.77608600 |
| O | 2.65537300 | 2.58792200 | -0.37261700 |
| O | -2.30655500 | 1.69879600 | -0.41357200 |
| S | 7.11244000 | -1.28105100 | 0.15867900 |
| S | -7.61226100 | -0.82948300 | 0.30058700 |
| O | -7.78349900 | -0.99579800 | 1.77424700 |
| O | -7.56223400 | -2.14078800 | -0.40998000 |
| O | -8.60100000 | 0.11440400 | -0.29237000 |
| O | 8.26195500 | -0.64419000 | -0.54193000 |
| O | 6.67181900 | -2.55334600 | -0.47322400 |
| O | 7.32792600 | -1.39675300 | 1.62732700 |
| H | -1.93091700 | -0.49594600 | 1.66850100 |
| H | 2.56057200 | -0.89445100 | -2.27632600 |
| H | -1.85471000 | -1.55077600 | -1.04925000 |
| H | 1.60740500 | -0.24423100 | 0.25236300 |
| H | 1.96709400 | 0.80150700 | 2.29333600 |
| O | 2.03087100 | -0.15049100 | 2.07490800 |
| H | 2.94097400 | -0.39364100 | 2.26669800 |
| H | 2.10338800 | 2.87750700 | 1.47698900 |
| O | 1.90794100 | 2.61425300 | 2.39067000 |
| H | 1.05511300 | 3.00871500 | 2.59192100 |
| Pd | -0.52614800 | 0.72036100 | -0.62967000 |
| H | 1.80941900 | 2.23525900 | -0.71937900 |
| H | 0.15865200 | 2.11718400 | -0.94029000 |
| H | -4.50837600 | 2.74337000 | -1.05287900 |
| H | 4.81611100 | 2.99845700 | 0.86402200 |

53

RR_D2_TS2_R, E(SCF) = -2408.88606086,
E(ZPE) = -2408.497089, E(G) = -2408.565143
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.42059100 | -1.95297200 | 1.08854600 |
| H | -0.15967100 | -1.40544100 | 1.99910200 |
| H | -0.80440300 | -2.93570400 | 1.37364400 |
| C | 0.76504700 | -2.04879300 | 0.16863900 |
| H | 1.59321000 | -2.59747900 | 0.62752400 |
| H | 0.49363300 | -2.55937900 | -0.75935100 |
| N | 1.18286200 | -0.67035200 | -0.16744700 |

| | | | |
|----|-------------|-------------|-------------|
| N | -1.46813100 | -1.17236300 | 0.38818000 |
| C | 2.26404600 | -0.59891100 | -1.20282500 |
| H | 1.88836200 | -0.00019200 | -2.03586400 |
| C | -2.58801100 | -0.73970700 | 1.25189400 |
| H | -2.96309400 | -1.60549100 | 1.80742800 |
| C | 3.53107800 | -0.02885800 | -0.65724100 |
| C | 3.52791200 | 1.31468100 | -0.19831400 |
| C | 4.69061200 | -0.78808500 | -0.61208200 |
| C | 4.75264000 | 1.83047400 | 0.28403900 |
| C | 5.87329400 | -0.25482100 | -0.13045200 |
| H | 4.67668000 | -1.81587500 | -0.96216900 |
| C | 5.89558100 | 1.06332900 | 0.31584400 |
| H | 6.82089400 | 1.48532700 | 0.69727100 |
| C | -3.69128400 | -0.13231900 | 0.44768000 |
| C | -3.44209300 | 0.96444600 | -0.41430900 |
| C | -4.97948900 | -0.62673900 | 0.57315500 |
| C | -4.53757100 | 1.52946000 | -1.08826400 |
| C | -6.04328800 | -0.05178100 | -0.10291500 |
| H | -5.15773800 | -1.47484400 | -1.22907500 |
| C | -5.81605400 | 1.03530200 | -0.93234200 |
| H | -6.64938600 | 1.48580200 | -1.45951500 |
| O | 2.43578600 | 2.02199300 | -0.18337600 |
| O | -2.25850600 | 1.50954200 | -0.59171000 |
| S | 7.37632900 | -1.22597800 | -0.07431400 |
| S | -7.68484800 | -0.74981000 | 0.09301200 |
| O | -7.97068000 | -0.72208000 | 1.55612200 |
| O | -7.60460500 | -2.14408200 | -0.44073500 |
| O | -8.59682600 | 0.12380300 | -0.69545100 |
| O | 8.36257300 | -0.51650000 | -0.94143800 |
| O | 7.01795300 | -2.57676400 | -0.59212600 |
| O | 7.80077200 | -1.24761100 | 1.35624300 |
| H | -2.16408300 | -0.03558800 | 1.97702000 |
| H | 2.43289400 | -1.60852600 | -1.58435200 |
| H | -1.84587900 | -1.73148500 | -0.37944700 |
| H | 1.51996400 | -0.23271700 | 0.70138300 |
| H | 1.83311400 | 1.62109100 | 1.51014500 |
| O | 1.52063900 | 1.05406200 | 2.24396200 |
| H | 2.24935400 | 1.02547400 | 2.86933200 |
| H | 2.40647400 | 3.67109700 | 0.46372900 |
| O | 2.33294500 | 4.54734400 | 0.90132300 |
| H | 1.54902100 | 4.47716400 | 1.45000300 |
| Pd | -0.54345300 | 0.44367300 | -0.47146100 |
| H | 0.71972600 | 1.74549000 | -0.87126500 |
| H | 0.05894400 | 1.84694400 | -1.35894400 |
| H | -4.34568900 | 2.37456500 | -1.74025400 |
| H | 4.76828500 | 2.85614900 | 0.63953600 |

53

RR_D2_TS2, E(SCF) = -2408.88499291, E(ZPE)
= -2408.497388, E(G) = -2408.566010 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.52791800 | -2.08323300 | 1.18152100 |
| H | -0.27155800 | -1.53232700 | 2.09159500 |
| H | -0.94971900 | -3.04873900 | 1.47273400 |
| C | 0.68225500 | -2.23737700 | 0.30048300 |
| H | 1.46306400 | -2.82891400 | 0.78745100 |
| H | 0.41610600 | -2.73502300 | -0.63638500 |
| N | 1.18351200 | -0.88311100 | -0.02388000 |
| N | -1.52398200 | -1.27766900 | 0.44127500 |
| C | 2.28423100 | -0.87464500 | -1.03535700 |
| H | 1.87968100 | -0.46134600 | -1.96318200 |
| C | -2.63314300 | -0.75648800 | 1.26488300 |
| H | -3.06681200 | -1.57565900 | 1.84859100 |
| C | 3.49939100 | -0.12692700 | -0.58154400 |
| C | 3.42035900 | 1.23330700 | -0.20554500 |
| C | 4.72648100 | -0.77862500 | -0.55853900 |
| C | 4.61446300 | 1.88008000 | 0.16879100 |
| C | 5.88417900 | -0.12188000 | -0.18714000 |
| H | 4.78180800 | -1.82502500 | -0.84180000 |
| C | 5.82149000 | 1.21761500 | 0.17931000 |
| H | 6.72556400 | 1.74113700 | 0.47456100 |
| C | -3.68951000 | -0.12647600 | 0.41448700 |
| C | -3.37439400 | 0.90973200 | -0.50150800 |
| C | -5.00407300 | -0.54307300 | 0.55164400 |
| C | -4.43699800 | 1.49346300 | -1.21471500 |
| C | -6.03203300 | 0.04877300 | -0.16396000 |
| H | -5.23059200 | -1.34499000 | -1.24959100 |
| C | -5.74067900 | 1.07583900 | -1.04840900 |

| | | | |
|----|-------------|-------------|-------------|
| H | -6.54491100 | 1.54064000 | -1.60750800 |
| O | 2.28047000 | 1.88820300 | -0.14766900 |
| O | -2.16683900 | 1.38538800 | -0.70272400 |
| S | 7.46238600 | -0.97243700 | -0.14190900 |
| S | -7.70656500 | -0.55656400 | 0.04862600 |
| O | -7.99362400 | -0.46671500 | 1.50924400 |
| O | -7.69910000 | -1.95677400 | -0.43817000 |
| O | -8.57203600 | 0.33585000 | -0.77097100 |
| O | 8.36896100 | -0.20245900 | -1.04163900 |
| O | 7.20043600 | -2.35633800 | -0.62604300 |
| O | 7.90805200 | -0.92866300 | 1.28094200 |
| H | -2.18814700 | -0.04551700 | 1.97111000 |
| H | 2.55993600 | -1.91112600 | -1.24688500 |
| H | -1.91674100 | -1.84163700 | -0.31431100 |
| H | 1.51677100 | -0.45916000 | 0.85289200 |
| H | 1.78731400 | 1.46179000 | 1.64421000 |
| O | 1.53777200 | 0.84338500 | 2.35549500 |
| H | 2.26464200 | 0.87049800 | 2.98314700 |
| H | 2.17281200 | 3.54205300 | 0.57597300 |
| O | 2.08771700 | 4.38008200 | 1.07309200 |
| H | 1.22672900 | 4.32506900 | 1.49303800 |
| Pd | -0.49013800 | 0.27924000 | -0.43655500 |
| H | 1.00107100 | 1.53461300 | -0.77519600 |
| H | 0.26895500 | 1.56593700 | -1.27643200 |
| H | -4.19613300 | 2.29171700 | -1.90840400 |
| H | 4.55758900 | 2.92427900 | 0.45866200 |

53
RR_D2_TS2W_P, E(SCF) = -2408.91825814,
E(ZPE) = -2408.526663, E(G) = -2408.594372
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.86355800 | 2.91275800 | -1.35291900 |
| H | 0.77081900 | 3.53064300 | -0.45313800 |
| H | 1.47717800 | 3.46503300 | -2.07301400 |
| C | -0.50002100 | 2.61711900 | -1.92153800 |
| H | -0.99460500 | 3.53381500 | -2.25772000 |
| H | -0.41106700 | 1.94401000 | -2.78004900 |
| N | -1.33239500 | 1.93842900 | -0.89785100 |
| N | 1.48624700 | 1.64153200 | -0.96154900 |
| C | -2.61572300 | 1.49946400 | -1.49162100 |
| H | -2.37946600 | 0.88022600 | -2.35995500 |
| C | 2.65834000 | 1.76225200 | -0.08416500 |
| H | 3.41093100 | 2.42440600 | -0.53105500 |
| C | -3.48992900 | 0.72421200 | -0.55913900 |
| C | -3.84912800 | 1.22050100 | 0.69167200 |
| C | -3.93438700 | -0.54212900 | -0.92068600 |
| C | -4.61226100 | 0.45575800 | 1.56533200 |
| C | -4.70021100 | -1.30067800 | -0.05609700 |
| H | -3.66096800 | -0.95331700 | -1.88651800 |
| C | -5.03344700 | -0.80650900 | 1.19643800 |
| H | -4.86468400 | 0.86558400 | 2.53728200 |
| H | -5.62627400 | -1.40549000 | 1.87930900 |
| C | 3.26929000 | 0.42464700 | 0.19929500 |
| C | 2.52483600 | -0.61466000 | 0.81731700 |
| C | 4.60869100 | 0.22051400 | -0.11076100 |
| C | 3.21456700 | -1.81229900 | 1.11430000 |
| C | 5.25294000 | -0.96569800 | 0.18417500 |
| H | 5.17175300 | 1.01660500 | -0.58858000 |
| C | 4.54343100 | -1.98634700 | 0.80859600 |
| H | 2.65037700 | -2.60426600 | 1.59572100 |
| H | 5.03877800 | -2.92278300 | 1.04757600 |
| O | -3.42507500 | 2.46588100 | 1.05998400 |
| O | 1.26572800 | -0.53785300 | 1.16579600 |
| S | -5.26844800 | -2.94554200 | -0.52180900 |
| S | 6.98084600 | -1.21197200 | -0.21338400 |
| O | 7.67413000 | -1.46007000 | 1.08507600 |
| O | 7.43567800 | 0.03998300 | -0.88188500 |
| O | 7.03260500 | -2.40153600 | -1.11288500 |
| O | -4.75333900 | -3.18335800 | -1.89661100 |
| O | -6.75491400 | -2.88274700 | -0.45376700 |
| O | -4.68619100 | -3.86771200 | 0.49185700 |
| H | 2.30733800 | 2.24329200 | 0.83761000 |
| H | -3.13641300 | 2.39424500 | -1.86162600 |
| H | 1.74737500 | 1.11802800 | -1.79525700 |
| H | -1.56745100 | 2.65408900 | -0.20466300 |
| H | -1.23176900 | 1.19189700 | 2.41158700 |
| H | -2.97948400 | 4.17588200 | 0.23191800 |

| | | | |
|----|-------------|-------------|-------------|
| O | -2.26670200 | 4.72575000 | -0.12538700 |
| H | -2.66318600 | 5.21752300 | -0.84846900 |
| H | -2.95037400 | 2.38974400 | 1.92164900 |
| O | -1.76696500 | 1.72382600 | 3.02907900 |
| H | -1.14707000 | 2.31910700 | 3.45986000 |
| Pd | -0.07479600 | 0.61335500 | 0.13449700 |
| H | -1.23936700 | -0.06284500 | 0.93831400 |

53
RR_D2_TS2W_R, E(SCF) = -2408.89027672,
E(ZPE) = -2408.501164, E(G) = -2408.568796
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.84000800 | 2.99399000 | -1.24092400 |
| H | 0.72069700 | 3.60060600 | -0.33838900 |
| H | 1.51284400 | 3.51973800 | -1.92332800 |
| C | -0.49158900 | 2.70488500 | -1.87140000 |
| H | -1.00292500 | 3.62408300 | -2.16854000 |
| H | -0.36623700 | 2.07771500 | -2.75924800 |
| N | -1.31817200 | 1.95710400 | -0.89774300 |
| N | 1.42563300 | 1.69623700 | -0.83502900 |
| C | -2.56747000 | 1.45553800 | -1.52313900 |
| H | -2.28271500 | 0.83036500 | -2.37292500 |
| C | 2.28457600 | 1.80404300 | -0.00280700 |
| H | 3.36023000 | 2.46271800 | -0.50713900 |
| C | -3.44471200 | 0.69661900 | -0.58692000 |
| C | -3.84137600 | 1.28768800 | 0.64326900 |
| C | -3.85058800 | -0.58804000 | -0.91707400 |
| C | -4.65151300 | 0.49703100 | 1.49426000 |
| C | -4.65002300 | -1.32969600 | -0.06516700 |
| H | -3.53004400 | -1.02819400 | -1.85667400 |
| C | -5.04773000 | -0.77476900 | 1.14864300 |
| H | -4.94898500 | 0.92905100 | 2.44524700 |
| H | -5.66733700 | -1.35359300 | 1.82749800 |
| C | 3.26252500 | 0.46574300 | 0.23765600 |
| C | 2.51224300 | -0.56261400 | 0.84843600 |
| C | 4.59117100 | 0.24269500 | -0.10088100 |
| C | 3.15966700 | -1.78311000 | 1.11573300 |
| C | 5.20548300 | -0.96368300 | 0.17205800 |
| H | 5.16501800 | 1.03053600 | -0.57847000 |
| C | 4.48271900 | -1.97718300 | 0.79184200 |
| H | 2.58193400 | -2.56817200 | 1.59075200 |
| H | 4.96082100 | -2.92747700 | 1.00844800 |
| O | -3.43277500 | 2.46232800 | 1.00711600 |
| O | 1.25570700 | -0.43289600 | 1.21900400 |
| S | -5.19985700 | -2.97605300 | -0.50046300 |
| S | 6.92646200 | -1.24621300 | -0.24912100 |
| O | 7.62564400 | -1.49963800 | 1.04340200 |
| O | 7.39167300 | -0.00602000 | -0.92942100 |
| O | 6.93539300 | -2.44045600 | -1.14132200 |
| O | -4.56045200 | -3.29739200 | -1.80801800 |
| O | -6.68859500 | -2.90532900 | -0.58760900 |
| O | -4.74625900 | -3.87306200 | 0.60298600 |
| H | 2.33942000 | 2.29011200 | 0.92986300 |
| H | -3.08560300 | 2.34072400 | -1.92109100 |
| H | 1.64797100 | 1.15266400 | -1.67154400 |
| H | -1.62458100 | 2.61728200 | -0.17346800 |
| H | -1.28035700 | 0.19346700 | 1.36566000 |
| H | -2.99170200 | 3.97039300 | 0.25835500 |
| O | -2.44256500 | 4.69795600 | -0.10782100 |
| H | -2.94435400 | 5.05633800 | -0.84305300 |
| H | -2.32560100 | 2.05034200 | 2.33588200 |
| O | -1.68660200 | 1.59822300 | 2.93190400 |
| H | -0.91164500 | 2.16603900 | 2.94379700 |
| Pd | -0.05433300 | 0.67130500 | 0.15339000 |
| H | -1.34226200 | -0.37643200 | 0.77191400 |

53
RR_D2_TS2W, E(SCF) = -2408.88087151, E(ZPE)
= -2408.493362, E(G) = -2408.558806 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.88343900 | -2.91099000 | -1.34424700 |
| H | -0.82288100 | -3.55099000 | -0.45843900 |
| H | -1.51099600 | -3.41536200 | -2.08493000 |
| C | 0.48740000 | -2.62181800 | -1.88597900 |
| H | 0.99795800 | -3.53986700 | -2.19042200 |
| H | 0.41727100 | -1.96464000 | -2.75824200 |
| N | 1.28683100 | -1.92001400 | -0.85289300 |
| N | -1.48407900 | -1.62828400 | -0.92735200 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.54096600 | -1.39827600 | -1.45137300 |
| H | 2.25651900 | -0.73814400 | -2.27444100 |
| C | -2.73027100 | -1.76981100 | -0.14851300 |
| H | -3.44247900 | -2.38568100 | -0.70907600 |
| C | 3.45025600 | -0.67354900 | -0.51451100 |
| C | 3.85029300 | -1.26162400 | 0.70918500 |
| C | 3.93409300 | 0.57163200 | -0.87711300 |
| C | 4.73161800 | -0.52132200 | 1.52524800 |
| C | 4.80953100 | 1.27239500 | -0.06319200 |
| H | 3.61900600 | 1.02358900 | -1.81478600 |
| C | 5.20727100 | 0.71488900 | 1.14692600 |
| H | 5.02735900 | -0.96195900 | 2.47259300 |
| H | 5.88609100 | 1.25980000 | 1.79607800 |
| C | -3.34282200 | -0.44364500 | 0.16683600 |
| C | -2.61155700 | 0.54140900 | 0.87071900 |
| C | -4.66578400 | -0.20096900 | -0.18268800 |
| C | -3.27892700 | 1.73723100 | 1.20552400 |
| C | -5.29668700 | 0.97961800 | 0.15801800 |
| H | -5.22355500 | -0.95745500 | -0.72606700 |
| C | -4.59409100 | 1.95033300 | 0.86422200 |
| H | -2.71808200 | 2.48938900 | 1.74967700 |
| H | -5.08186600 | 2.88124100 | 1.13648400 |
| O | 3.37180700 | -2.41067400 | 1.11530300 |
| O | -1.36778400 | 0.40252200 | 1.26816200 |
| S | 5.44880100 | 2.87609800 | -0.54245100 |
| S | -7.01336300 | 1.27366900 | -0.26565300 |
| O | -7.74003800 | 1.38957600 | 1.03202700 |
| O | -7.44828100 | 0.09828800 | -1.07042000 |
| O | -7.03291500 | 2.54867700 | -1.03868100 |
| O | 4.81176700 | 3.20487100 | -1.84871300 |
| O | 6.92887100 | 2.71417000 | -0.64459300 |
| O | 5.06087000 | 3.81875500 | 0.54725500 |
| H | -2.46181800 | -2.31935400 | 0.76133300 |
| H | 3.05571700 | -2.26459700 | -1.89403900 |
| H | -1.67472200 | -1.05972300 | -1.75319400 |
| H | 1.57887500 | -2.62208700 | -0.16532800 |
| H | 1.23184100 | -0.64548700 | 1.78538800 |
| H | 3.00475200 | -3.91600700 | 0.29776300 |
| O | 2.48889200 | -4.63766200 | -0.12322100 |
| H | 3.01564300 | -4.92869600 | -0.87079600 |
| H | 2.36482500 | -1.98239200 | 2.21499600 |
| O | 1.67052100 | -1.43361600 | 2.72956500 |
| H | 0.95626900 | -2.02410300 | 2.99730500 |
| Pd | -0.01793800 | -0.68258800 | 0.21655200 |
| H | 1.16633800 | 0.08409000 | 1.11030000 |

54

RR_ID1_I1_Htr_TS_R, E(SCF) = -2484.17255816, E(ZPE) = -2483.772566, E(G) = -2483.839864 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.26381700 | -2.49873000 | 0.79273200 |
| H | -0.01307000 | -2.86162100 | -0.20096700 |
| H | 0.69793900 | -3.33193900 | 1.35150800 |
| C | -0.91874900 | -1.90728900 | 1.50093500 |
| H | -1.70703600 | -2.64716400 | 1.66610000 |
| H | -0.61825100 | -1.51400500 | 2.47619400 |
| N | -1.44228300 | -0.76559100 | 0.70768300 |
| N | 1.25866000 | -1.41987200 | 0.61032000 |
| C | -2.45768000 | 0.01672100 | 1.49308300 |
| H | -2.78038300 | -0.62715400 | 2.31762500 |
| C | 2.34567400 | -1.77211300 | -0.32803100 |
| H | 1.87576000 | -1.88922300 | -1.31085100 |
| C | -3.64650600 | 0.41601100 | 0.68552300 |
| C | -3.76796900 | 1.74224200 | 0.18782200 |
| C | -4.64977700 | -0.51534500 | 0.45376100 |
| C | -4.95462600 | 2.05141700 | -0.51608800 |
| C | -5.78394700 | -0.18767000 | -0.26839000 |
| H | -4.54135700 | -1.52528800 | 0.84649200 |
| C | -5.93715500 | 1.11226500 | -0.73879300 |
| H | -6.83080200 | 1.37319800 | -1.29571800 |
| C | 3.43399600 | -0.74902400 | -0.34224000 |
| C | 3.15769500 | 0.61426700 | -0.57148100 |
| C | 4.75072600 | -1.16404200 | -0.17872000 |
| C | 4.24484600 | 1.50353900 | -0.65135600 |
| C | 5.80228000 | -0.27332300 | -0.25672200 |
| H | 4.96205800 | -2.21219000 | 0.00812500 |
| C | 5.54205200 | 1.06912900 | -0.50465500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 6.36077300 | 1.77838500 | -0.57243200 |
| O | -2.83261800 | 2.62604800 | 0.34691100 |
| O | 1.94284700 | 1.10469100 | -0.74093400 |
| S | -7.07982000 | -1.40528000 | -0.47911900 |
| S | 7.50129300 | -0.82505000 | -0.08406700 |
| O | 8.09944100 | 0.02439400 | 0.98481400 |
| O | 8.13741000 | -0.59602400 | -1.41303800 |
| O | 7.42997200 | -2.26521500 | 0.28649400 |
| O | -7.82254300 | -1.45394500 | 0.81559700 |
| O | -6.39053800 | -2.69295800 | -0.78169600 |
| O | -7.92452900 | -0.91810000 | -1.60614000 |
| H | 1.54419700 | 4.36505600 | -0.66118200 |
| O | 1.13577700 | 3.62160800 | -0.21178100 |
| H | 1.69116200 | 2.83104000 | -0.38466800 |
| H | -1.52770700 | 3.15881800 | -1.54713900 |
| O | -0.72717900 | 3.43916100 | 2.02774100 |
| H | -0.06128000 | 3.57324200 | 1.33689000 |
| H | -1.91630000 | -1.13886100 | -0.11650900 |
| H | -1.95298800 | 0.88239200 | -0.92502900 |
| H | 1.66906900 | -1.18429200 | 1.51571600 |
| H | 2.75743300 | -2.74517300 | -0.04050200 |
| Pd | 0.24213500 | 0.21806200 | -0.05412800 |
| O | -0.78887200 | 1.81366600 | -0.91346300 |
| H | -0.18925100 | 2.58366300 | -0.90070200 |
| H | -1.61149500 | 2.12059800 | -0.39799700 |
| H | -5.06313800 | 3.06314200 | -0.89413700 |
| H | 4.03685200 | 2.55152700 | -0.84060800 |

54

RR_ID1_I1_Htr_TS, E(SCF) = -2484.17169860, E(ZPE) = -2483.774934, E(G) = -2483.840971 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.43050700 | 2.85069000 | -0.02022300 |
| H | -0.20047700 | 3.09012800 | -1.06262500 |
| H | -0.93562400 | 3.71496300 | 0.42371900 |
| C | 0.80792700 | 2.49401800 | 0.75307100 |
| H | 1.52066700 | 3.32059000 | 0.80001700 |
| H | 0.52111900 | 2.23654500 | 1.77770700 |
| N | 1.45390200 | 1.28242600 | 0.17106600 |
| N | -1.29796900 | 1.66374900 | -0.00133800 |
| C | 2.31866900 | 0.64557200 | 1.20948600 |
| H | 2.74370200 | 1.45462700 | 1.81453500 |
| C | -2.49707000 | 1.76133200 | -0.84888400 |
| H | -2.14850600 | 1.85145900 | -1.88472200 |
| C | 3.44801800 | -0.18906000 | 0.69783000 |
| C | 3.34149300 | -1.57990100 | 0.57321500 |
| C | 4.67573900 | 0.41918300 | 0.44655000 |
| C | 4.47362800 | -2.32657600 | 0.24332900 |
| C | 5.78000600 | -0.32672300 | 0.08774600 |
| H | 4.77460200 | 1.49599000 | 0.54792400 |
| C | 5.68298600 | -1.70987800 | 0.00131400 |
| H | 4.37101400 | -3.40299400 | 0.16446400 |
| H | 6.55400100 | -2.29945100 | -0.26561000 |
| C | -3.40350700 | 0.58432000 | -0.66260500 |
| C | -2.93587600 | -0.73944600 | -0.82109900 |
| C | -4.74069300 | 0.80213500 | -0.35346300 |
| C | -3.85936600 | -1.78994600 | -0.66359600 |
| C | -5.63224700 | -0.24407300 | -0.21428100 |
| H | -5.10017700 | 1.81822900 | -0.22479500 |
| C | -5.18243900 | -1.55015200 | -0.37063500 |
| H | -3.49031800 | -2.80350500 | -0.78212200 |
| H | -5.87373700 | -2.37930200 | -0.25628200 |
| O | 2.16149500 | -2.20937400 | 0.73848600 |
| O | -1.69143000 | -1.06058600 | -1.11650000 |
| S | 7.36477300 | 0.46063000 | -0.23869100 |
| S | -7.35871100 | 0.05317100 | 0.17048700 |
| O | -7.62048300 | -0.66347300 | 1.45171800 |
| O | -8.13512600 | -0.52090900 | -0.96622200 |
| O | -7.50812600 | 1.53037200 | 0.28947500 |
| O | 7.72835600 | 0.05839500 | -1.62614000 |
| O | 8.30389100 | -0.08748100 | 0.77964700 |
| O | 7.13351100 | 1.92329100 | -0.09397700 |
| H | 0.21846700 | -2.19127900 | 1.50731900 |
| O | -0.74950600 | -2.15733400 | 1.56747500 |
| H | -1.04071600 | -2.01412700 | 0.65087400 |
| H | -2.15972800 | 3.32362600 | 3.22764900 |
| O | -1.46344200 | 0.39761100 | 2.57116500 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.23993600 | -0.51937600 | 2.31403400 |
| H | 2.04288900 | 1.56343900 | -0.61275200 |
| H | 1.66074900 | 0.06121400 | 1.85671300 |
| H | -1.56479700 | 1.42986400 | 0.96782400 |
| H | -3.04010800 | 2.68204100 | -0.60541200 |
| Pd | -0.11698400 | 0.10467000 | -0.59641800 |
| O | 1.02767300 | -1.42477200 | -1.28821800 |
| H | 0.39356200 | -2.02476100 | -1.69569100 |
| H | 1.61103100 | -1.96169000 | -0.12618500 |

54

RR_ID1_I1_Htr_P, E(SCF) = -2484.16993125,
E(ZPE) = -2483.771617, E(G) = -2483.840823
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.31525800 | -2.56308600 | 0.83675200 |
| H | 0.04892200 | -2.99249800 | -0.13308000 |
| H | 0.74794300 | -3.35717700 | 1.45191600 |
| C | -0.88307200 | -1.94401600 | 1.50034500 |
| H | -1.65569700 | -2.68513100 | 1.72257200 |
| H | -0.58663100 | -1.47621100 | 2.44372400 |
| N | -1.43202500 | -0.86748800 | 0.63445300 |
| N | 1.29532700 | -1.48588900 | 0.59452900 |
| C | -2.38495500 | 0.00000900 | 1.39439400 |
| H | -2.73948500 | -0.58328700 | 2.25065000 |
| C | 2.39893100 | -1.86190600 | -0.31109100 |
| H | 1.94041600 | -2.07468600 | -1.28342100 |
| C | -3.57596500 | 0.43575100 | 0.60150300 |
| C | -3.69073800 | 1.72851500 | 0.07735600 |
| C | -4.64071800 | -0.45071900 | 0.45013500 |
| C | -4.88221300 | 2.11509300 | -0.53916000 |
| C | -5.80056800 | -0.06824800 | -0.19053900 |
| H | -4.56646900 | -1.45516600 | 0.85825400 |
| C | -5.92849700 | 1.22826300 | -0.67430400 |
| H | -6.84640100 | 1.53565500 | -1.16454400 |
| C | 3.43694900 | -0.78801700 | -0.40602000 |
| C | 3.10808700 | 0.53770500 | -0.76431600 |
| C | 4.76649800 | -1.12068600 | -0.16978100 |
| C | 4.15951400 | 1.46158500 | -0.91131400 |
| C | 5.77991300 | -0.19356400 | -0.30552500 |
| H | 5.02016600 | -2.13554600 | 0.12003400 |
| C | 5.46918000 | 1.10693300 | -0.68525000 |
| H | 6.25889700 | 1.84281300 | -0.79963100 |
| O | -2.68553000 | 2.62052000 | 0.16216900 |
| O | 1.87965500 | 0.97030800 | -0.98827700 |
| S | -7.18107400 | -1.20837800 | -0.36919800 |
| S | 7.49017100 | -0.62996400 | 0.01441700 |
| O | 7.48454900 | -2.07102900 | 0.38976400 |
| O | 7.93644000 | 0.25943800 | 1.12505100 |
| O | 8.22336300 | -0.36028000 | -1.25549200 |
| O | -8.29307500 | -0.61583600 | 0.42587500 |
| O | -6.70757500 | -2.51264200 | 0.16784900 |
| O | -7.47941200 | -1.24686700 | -1.82784200 |
| H | 1.75109100 | 4.02874100 | 0.11233500 |
| O | 1.56827900 | 3.23669700 | 0.62310700 |
| H | 1.65867000 | 2.49263800 | -0.00591200 |
| H | -1.50917600 | 3.09686500 | 1.65188700 |
| O | -0.75328100 | 3.19242900 | 2.24975500 |
| H | 0.02471200 | 3.20460300 | 1.66293600 |
| H | -1.93977900 | -1.29917200 | -0.13851700 |
| H | -1.82173100 | 0.84964000 | 1.78523800 |
| H | 1.69059600 | -1.18415100 | 1.48592700 |
| H | 2.86041000 | -2.78915800 | 0.04577300 |
| Pd | 0.22773000 | 0.07255600 | -0.21901900 |
| O | -0.86514900 | 1.51199700 | -1.11266400 |
| H | -0.23814800 | 2.09131400 | -1.55743400 |
| H | -1.86331500 | 2.21859500 | -0.32911500 |
| H | -4.95366400 | 3.12588300 | -0.92455100 |
| H | 3.90267600 | 2.47543000 | -1.20001300 |

54

RR_ID1_I1_Htr_TS, E(SCF) = -2484.16990099,
E(ZPE) = -2483.773378, E(G) = -2483.842495
a.u.

| | | | |
|---|-------------|-------------|------------|
| C | 0.31241700 | -2.49127200 | 0.99054600 |
| H | 0.05311500 | -2.95953800 | 0.03680100 |
| H | 0.74405000 | -3.25905200 | 1.63871000 |
| C | -0.89252600 | -1.85036600 | 1.61998300 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.66334200 | -2.58572600 | 1.86622500 |
| H | -0.60673000 | -1.34099700 | 2.54499600 |
| N | -1.43833600 | -0.81558100 | 0.70347400 |
| N | 1.29231800 | -1.42251000 | 0.71072200 |
| C | -2.42609400 | 0.05954600 | 1.40897800 |
| H | -2.79496200 | -0.50306900 | 2.27292200 |
| C | 2.38743100 | -1.83034700 | -0.19167900 |
| H | 1.91948800 | -2.06946200 | -1.15345900 |
| C | -3.59959400 | 0.44949800 | 0.56805300 |
| C | -3.70824200 | 1.71729200 | -0.01889000 |
| C | -4.65231200 | -0.45335700 | 0.42906700 |
| C | -4.88563000 | 2.05904800 | -0.68965700 |
| C | -5.79538600 | -0.11451000 | -0.26417600 |
| H | -4.58176400 | -1.43668100 | 0.88653700 |
| C | -5.91954800 | 1.15653600 | -0.81284200 |
| H | -6.82383800 | 1.43071600 | -1.34632100 |
| C | 3.43491900 | -0.77019200 | -0.33115100 |
| C | 3.11741000 | 0.55518800 | -0.70047000 |
| C | 4.76678000 | -1.12388800 | -0.14113300 |
| C | 4.17939500 | 1.45826500 | -0.89612600 |
| C | 5.79097500 | -0.21822000 | -0.32833900 |
| H | 5.01309900 | -2.13902700 | 0.15404000 |
| C | 5.49000600 | 1.08205200 | -0.71644900 |
| H | 6.28796100 | 1.80148700 | -0.87076900 |
| O | -2.71654200 | 2.61951300 | 0.05334100 |
| O | 1.89133600 | 1.00894900 | -0.89200100 |
| S | -7.16468900 | -1.27137900 | -0.41509000 |
| S | 7.50560200 | -0.68975100 | -0.09565400 |
| O | 7.48483400 | -2.10320300 | 0.37186000 |
| O | 8.05367500 | 0.25332600 | 0.92067600 |
| O | 8.15520900 | -0.52582000 | -1.42785400 |
| O | -8.27902900 | -0.67677100 | 0.37584600 |
| O | -6.67513700 | -2.56099900 | 0.14309800 |
| O | -7.47153600 | -1.34035600 | -1.87092900 |
| H | 1.83527300 | 4.03704400 | 0.29717200 |
| O | 1.57546700 | 3.24194800 | 0.76835500 |
| H | 1.68369000 | 2.51139800 | 0.12733700 |
| H | -1.59254900 | 3.15933500 | 1.54117100 |
| O | -0.88669100 | 3.30028500 | 2.19012000 |
| H | -0.06268500 | 3.27148700 | 1.67143300 |
| H | -1.91932100 | -1.28525200 | -0.06474500 |
| H | -1.88742400 | 0.93023900 | 1.78794500 |
| H | 1.69435400 | -1.09568000 | 1.59006400 |
| H | 2.84491300 | -2.75016800 | 0.18880700 |
| Pd | 0.23045600 | 0.11559400 | -0.14228900 |
| O | -0.84260200 | 1.53825400 | -1.09143700 |
| H | -0.20611800 | 2.13024700 | -1.50500600 |
| H | -1.85835800 | 2.20611600 | -0.41017600 |
| H | -4.95518000 | 3.04976700 | -1.12460800 |
| H | 3.93097600 | 2.47156600 | -1.19413000 |

54

RR_ID1_TS1_Ntrigo-square_P, E(SCF) = -
2484.17714902, E(ZPE) = -2483.775953, E(G) =
-2483.841823 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.16385200 | 1.76780000 | 1.20979000 |
| H | -0.03065100 | 1.16608900 | 2.10260600 |
| H | 0.45094700 | 2.77248400 | 1.53033600 |
| C | -1.03802000 | 1.78827000 | 0.30466300 |
| H | -1.91385600 | 2.22487600 | 0.79430500 |
| H | -0.82494600 | 2.37463100 | -0.59305400 |
| N | -1.31518500 | 0.39839600 | -0.12382600 |
| C | -2.36185000 | 0.29518000 | -1.19047400 |
| H | -2.00579600 | -0.42162000 | -1.93407500 |
| C | -3.67835300 | -0.11920400 | -0.62668200 |
| C | -3.78282200 | -1.42634500 | -0.07876800 |
| C | -4.76425100 | 0.74304000 | -0.61683000 |
| C | -5.03926400 | -1.79881200 | -0.16540200 |
| C | -5.98030200 | 0.34715800 | -0.08707400 |
| H | -4.66602700 | 1.74320900 | -1.02957600 |
| C | -6.10977700 | -0.93297100 | 0.44481600 |
| H | -5.13641700 | -2.79653300 | 0.86693600 |
| H | -7.06223900 | -1.24743100 | 0.86147300 |
| O | -2.76673700 | -2.23483400 | -0.04606000 |
| S | -7.39511100 | 1.44346300 | -0.08525600 |
| O | -7.83932600 | 1.54343700 | 1.33594900 |
| O | -8.42591900 | 0.79617400 | -0.94967000 |

| | | | |
|----|-------------|-------------|-------------|
| O | -6.91375400 | 2.74259700 | -0.63470500 |
| H | -2.43006300 | 1.26559400 | -1.68555900 |
| H | -1.64793800 | -0.12687800 | 0.69005500 |
| O | -0.39582200 | -2.30439900 | -1.15293800 |
| H | -1.35208700 | -2.28689700 | -0.84379100 |
| H | -1.87152600 | -2.23965500 | 1.44464300 |
| O | -1.19144600 | -2.06094200 | 2.13632300 |
| H | -1.61500800 | -2.23213800 | 2.98065800 |
| H | 0.02962800 | -3.00428000 | -0.60930300 |
| H | 0.29554300 | -3.11126800 | 1.51633000 |
| O | 0.89554000 | -3.59306200 | 0.91622100 |
| H | 1.59883000 | -2.95674000 | 0.69814600 |
| Pd | 0.49717700 | -0.55160700 | -0.40096700 |
| N | 1.27396700 | 1.11923900 | 0.47152600 |
| C | 2.43712900 | 0.76696100 | 1.31735900 |
| H | 2.74794400 | 1.65147800 | 1.88341700 |
| C | 3.57709400 | 0.25602900 | 0.49798600 |
| C | 3.41838200 | -0.88469900 | -0.31811100 |
| C | 4.81488100 | 0.88182500 | 0.57340500 |
| C | 4.54350800 | -1.36412100 | -1.01078900 |
| C | 5.90607000 | 0.39686900 | -0.12119500 |
| H | 4.93358300 | 1.76366200 | 1.19440700 |
| C | 5.76698200 | -0.74078500 | -0.90819200 |
| H | 4.41861000 | -2.24502300 | -1.63071000 |
| H | 6.62103700 | -1.12880200 | -1.45434400 |
| O | 2.27658700 | -1.53537600 | -0.44188400 |
| S | 7.50929100 | 1.19475200 | -0.00239100 |
| O | 7.30317300 | 2.40968400 | 0.83344400 |
| O | 7.91175100 | 1.51129300 | -1.40262700 |
| O | 8.41403500 | 0.19524400 | 0.63476900 |
| H | 2.07781500 | 0.01782700 | 2.03264100 |
| H | 1.58992700 | 1.74077300 | -0.27500700 |

54
RR_ID1_TS1_Ntrigo-square_R, E(SCF) = -
2484.19017966, E(ZPE) = -2483.790938, E(G)
= -2483.858412 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.66548600 | 3.09015200 | 0.19345300 |
| H | 0.39364400 | 3.04602500 | 1.25221000 |
| H | 1.27192900 | 3.98384700 | 0.02755400 |
| C | -0.57624600 | 3.07917500 | -0.66283700 |
| H | -1.20586600 | 3.95286200 | -0.47199500 |
| H | -0.31816800 | 3.07117400 | -1.72613000 |
| N | -1.30553300 | 1.83194200 | -0.36163800 |
| C | -2.41659500 | 1.50929500 | -1.27086500 |
| H | -1.97404500 | 1.27509100 | -2.24584200 |
| C | -3.24253600 | 0.38029900 | -0.73477000 |
| C | -2.66252700 | -0.84642700 | -0.34470000 |
| C | -4.61909700 | 0.54422300 | -0.63041100 |
| C | -3.51631000 | -1.86433800 | 0.11902700 |
| C | -5.43851300 | -0.46960800 | -0.17438500 |
| H | -5.06687300 | 1.49038500 | -0.91717400 |
| C | -4.87853300 | -1.68594800 | 0.19747300 |
| H | -3.06183700 | -2.80579700 | 0.41417900 |
| H | -5.51197800 | -2.48885300 | 0.56117000 |
| O | -1.36785200 | -1.10991700 | -0.38735300 |
| S | -7.21506600 | -0.24664700 | -0.05625100 |
| O | -7.56710300 | -0.53595800 | 1.36328400 |
| O | -7.81178300 | -1.23454400 | -1.00051800 |
| O | -7.48053100 | 1.16566400 | -0.44624200 |
| H | -3.04936600 | 2.39451500 | -1.40063600 |
| H | -1.64089100 | 1.85706100 | 0.61401900 |
| O | 0.13435600 | -3.47796000 | -0.48556200 |
| H | -0.62640700 | -2.88710400 | -0.59961700 |
| H | -1.08114700 | 0.44793800 | 2.56192300 |
| O | -1.43288900 | 1.35723800 | 2.49568800 |
| H | -2.10750200 | 1.42485000 | 3.17537400 |
| H | 0.81179000 | -2.82447500 | -0.23872100 |
| H | -0.93247600 | -1.52238800 | 1.52784000 |
| O | -0.43885400 | -1.33527000 | 2.34500800 |
| H | 0.46773400 | -1.28704400 | 2.00345400 |
| Pd | 0.07886000 | 0.33862400 | -0.25877900 |
| N | 1.44066700 | 1.86486900 | -0.11293600 |
| C | 2.49238100 | 1.53494800 | 0.87288200 |
| H | 3.10886400 | 2.42120500 | 1.05825900 |
| C | 3.35231200 | 0.40901000 | 0.39294700 |
| C | 2.79310000 | -0.84386500 | 0.05670500 |

| | | | |
|---|------------|-------------|-------------|
| C | 4.72782400 | 0.58963400 | 0.31186100 |
| C | 3.66817800 | -1.87404400 | -0.33093200 |
| C | 5.56779100 | -0.43729700 | -0.07217400 |
| H | 5.15718600 | 1.55432500 | 0.56285200 |
| C | 5.02955000 | -1.67950200 | -0.38770800 |
| H | 3.23719400 | -2.83637400 | -0.58742000 |
| H | 5.68189300 | -2.49234600 | -0.69128600 |
| O | 1.49984900 | -1.10508300 | 0.11468500 |
| S | 7.34456200 | -0.20234500 | -0.15627300 |
| O | 7.58691300 | 1.22958400 | 0.17238700 |
| O | 7.73639900 | -0.55520700 | -1.55088200 |
| O | 7.92556700 | -1.13791700 | 0.84903100 |
| H | 1.97347200 | 1.28833800 | 1.80709400 |
| H | 1.87724300 | 1.96640500 | -1.03048800 |

54
RR_ID1_TS1_P, E(SCF) = -2484.16677466,
E(ZPE) = -2483.765781, E(G) = -2483.831654
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.54363600 | 3.10742800 | 0.14184500 |
| H | -0.37065700 | 3.39061000 | -0.89937300 |
| H | -1.08667800 | 3.91993600 | 0.63343100 |
| C | 0.74053200 | 2.79766300 | 0.85435200 |
| H | 1.41728800 | 3.65452400 | 0.86848400 |
| H | 0.52147800 | 2.53376900 | 1.89366100 |
| N | 1.40786700 | 1.61311000 | 0.24206600 |
| N | -1.34980200 | 1.86861000 | 0.13873000 |
| C | 2.32100500 | 1.00476800 | 1.26495400 |
| H | 2.84755200 | 1.84062000 | 1.74104400 |
| C | -2.58275500 | 1.95512300 | -0.67293700 |
| H | -2.25815600 | 2.14514100 | -1.70169600 |
| C | 3.33087500 | 0.02456500 | 0.76988400 |
| C | 3.01901000 | -1.35624400 | 0.67505100 |
| C | 4.62158200 | 0.46647100 | 0.49885700 |
| C | 4.06865800 | -2.23275900 | 0.31898200 |
| C | 5.62058900 | -0.41258900 | 0.12797600 |
| H | 4.85699800 | 1.52381700 | 0.58392400 |
| C | 5.33759300 | -1.77356700 | 0.05118900 |
| H | 6.12109300 | -2.47103700 | -0.22793500 |
| C | -3.41368800 | 0.71788900 | -0.56799600 |
| C | -2.88025800 | -0.54484600 | -0.90103600 |
| C | -4.74609800 | 0.82014100 | -0.18664200 |
| C | -5.73754100 | -1.65850800 | -0.86367600 |
| C | -5.56903900 | -0.28769800 | -0.15072300 |
| H | -5.15688100 | 1.78936200 | 0.07778200 |
| C | -5.05791100 | -1.53277100 | -0.49657400 |
| H | -5.70036800 | -2.40724600 | -0.37338800 |
| O | 1.80307100 | -1.79844400 | 0.84450000 |
| O | -1.62539900 | -0.73705200 | -1.27116900 |
| S | 7.28674800 | 0.15604000 | -0.20070200 |
| S | -7.29013500 | -0.15237600 | 0.33876300 |
| O | -7.44061000 | -1.02537500 | 1.53773200 |
| O | -8.08146100 | -0.64538700 | -0.82460900 |
| O | -7.52110500 | 1.28854200 | 0.63324000 |
| O | 7.24524900 | 1.64220600 | -0.10199100 |
| O | 7.62291700 | -0.32637900 | -1.57183100 |
| O | 8.14990900 | -0.47071900 | 0.84306400 |
| H | 0.16714200 | -2.85984700 | 0.51883600 |
| O | -0.78022900 | -3.01191100 | 0.37037000 |
| H | -1.04825800 | -2.31923600 | -0.25794700 |
| H | 0.45632700 | -1.14604300 | 2.00247500 |
| O | -0.38868800 | -0.97739300 | 2.46452000 |
| H | -0.97969500 | -1.58518900 | 1.99939600 |
| H | 1.97696700 | 1.92190800 | -0.54647300 |
| H | 1.67056100 | 0.56052800 | 2.02056800 |
| H | -1.59565300 | 1.61248000 | 1.09803300 |
| H | -3.16352400 | 2.82245400 | -0.34182300 |
| Pd | -0.11973300 | 0.42506500 | -0.58207900 |
| O | 1.12148800 | -0.99830900 | -1.50357600 |
| H | 0.56856900 | -1.56030300 | -2.06018800 |
| H | 1.38569300 | -1.52126400 | -0.68956600 |
| H | 3.83767100 | -3.29117100 | 0.25188600 |
| H | -3.32747000 | -2.62607300 | -1.13304600 |

54

RR_ID1_TS1_R, E(SCF) = -2484.18479236,
 E(ZPE) = -2483.785963, E(G) = -2483.855396
 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.82922700 | 3.32142300 | -0.35199900 |
| H | -0.72080200 | 3.41633500 | -1.43570500 |
| H | -1.43542600 | 4.15876200 | 0.00394300 |
| C | 0.51782500 | 3.28550900 | 0.32266800 |
| H | 1.08351600 | 4.20411500 | 0.15112300 |
| H | 0.39650700 | 3.16107000 | 1.40253400 |
| N | 1.27057200 | 2.10546900 | -0.17388900 |
| N | -1.50537700 | 2.03111700 | -0.08417400 |
| C | 2.35538500 | 1.67860800 | 0.72834600 |
| H | 2.99086300 | 2.54064400 | 0.95938600 |
| C | -2.70923700 | 1.78344300 | -0.90443800 |
| H | -2.36711700 | 1.71353200 | -1.94288200 |
| C | 3.20256200 | 0.57254000 | 0.17133200 |
| C | 2.67523900 | -0.55450800 | -0.49844700 |
| C | 4.57285700 | 0.62902500 | 0.41954400 |
| C | 3.56625200 | -1.58184300 | -0.86781900 |
| C | 5.42435000 | -0.39073000 | 0.05099400 |
| H | 4.98601600 | 1.49451800 | 0.92807000 |
| C | 4.91180700 | -1.50798400 | -0.59933000 |
| H | 5.57158200 | -2.31764500 | -0.89426200 |
| C | -3.43003100 | 0.54708500 | -0.46597200 |
| C | -2.77357000 | -0.69936300 | -0.37798600 |
| C | -4.78856300 | 0.62275900 | -0.17994800 |
| C | -3.53782900 | -1.82764300 | -0.03222600 |
| C | -5.51870700 | -0.49823800 | 0.16182300 |
| H | -5.29553700 | 1.58106600 | -0.23808200 |
| C | -4.88442500 | -1.73297000 | 0.23324800 |
| H | -5.44985400 | -2.62050600 | 0.49911700 |
| O | 1.40361700 | -0.74030200 | -0.79908700 |
| O | -1.48632200 | -0.88159100 | -0.62034100 |
| S | 7.18774200 | -0.28911600 | 0.36825200 |
| S | -7.26466200 | -0.37733400 | 0.55856900 |
| O | -7.37451300 | -0.69774400 | 2.01098200 |
| O | -7.94791200 | -1.38763300 | -0.29829100 |
| O | -7.66042600 | 1.02250500 | 0.24066900 |
| O | 7.39506000 | 0.96955900 | 1.13584600 |
| O | 7.83823200 | -0.26925800 | -0.97308000 |
| O | 7.53140600 | -1.51270200 | 1.14668500 |
| H | 0.79504400 | -2.33108500 | 0.07844600 |
| O | 0.19484200 | -2.72022000 | 0.73821000 |
| H | -0.62346500 | -2.24838400 | 0.50522300 |
| H | 2.51354400 | -1.09309100 | 2.11735900 |
| O | 1.73171200 | -1.25778100 | 2.65497100 |
| H | 1.14354500 | -1.77435000 | 2.07240400 |
| H | 1.66102500 | 2.31602700 | -1.09294500 |
| H | 1.87084000 | 1.36753700 | 1.66196600 |
| H | -1.77020700 | 1.99047300 | 0.90115800 |
| H | -3.37954200 | 2.64690000 | -0.83368200 |
| Pd | -0.08645100 | 0.59528100 | -0.40960800 |
| O | -0.08147400 | -2.14099100 | -2.74536800 |
| H | -0.79939500 | -1.86761700 | -2.15196700 |
| H | 0.68082400 | -1.73781500 | -2.30134700 |
| H | 3.14742900 | -2.44404500 | -1.37822400 |
| H | -3.03018000 | -2.78570000 | 0.01936300 |

54

RR_ID1_TS1_chain_P, E(SCF) = -
 2484.17191923, E(ZPE) = -2483.770893, E(G)
 = -2483.837182 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.66587800 | 3.39496700 | -0.13083900 |
| H | -0.52629700 | 3.63537800 | -1.18797500 |
| H | -1.30999300 | 4.16196100 | 0.31144800 |
| C | 0.64434000 | 3.29881000 | 0.59910100 |
| H | 1.24825700 | 4.19879400 | 0.47336400 |
| H | 0.44883500 | 3.17792100 | 1.66713400 |
| N | 1.40074900 | 2.08943500 | 0.15730200 |
| C | 2.19982800 | 1.55735400 | 1.31014100 |
| H | 2.87305400 | 2.36353300 | 1.62554800 |
| C | 2.96984300 | 0.31937500 | 1.02579500 |
| C | 2.34631700 | -0.94896900 | 1.19479300 |
| C | 4.29576300 | -0.40964200 | 0.62920900 |
| C | 3.16499600 | -2.08599600 | 0.96599100 |
| C | 5.05142900 | -0.72115200 | 0.37447900 |
| H | 4.75402400 | 1.38823200 | 0.51214900 |

| | | | |
|----|-------------|-------------|-------------|
| C | 4.47470500 | -1.97554700 | 0.56187100 |
| H | 5.06429200 | -2.87020900 | 0.38340900 |
| O | 1.09896600 | -1.08280800 | 1.50507700 |
| S | 6.77239400 | -0.60469900 | -0.09479100 |
| O | 6.93471800 | -1.46716700 | -1.30260400 |
| O | 7.56131500 | -1.11627900 | 1.06640900 |
| O | 7.03247100 | 0.83677700 | -0.37397600 |
| H | 0.48855100 | -2.19010900 | 0.26429000 |
| O | 0.31441400 | -2.59020300 | -0.62146200 |
| H | -0.45444100 | -2.09370600 | -0.95247800 |
| H | -0.15544900 | -0.02223400 | -2.08903800 |
| O | -0.86194300 | 0.60972800 | 2.36899000 |
| H | -1.36835000 | 0.16485100 | 3.05135500 |
| H | 2.05364600 | 2.34984600 | -0.58130500 |
| H | 1.48729200 | 1.48712400 | 2.11537600 |
| Pd | 0.06665000 | 0.77406900 | -0.77180600 |
| O | 1.56003400 | -0.44839700 | -1.68688000 |
| H | 1.43320100 | -0.41665600 | -2.64201700 |
| H | 1.31092100 | -1.36674000 | -1.40610400 |
| H | 2.71425500 | -3.06428000 | 1.10618300 |
| N | -1.31235100 | 2.06935000 | -0.05671300 |
| C | -2.58803000 | 1.99416300 | -0.79322600 |
| H | -2.35979900 | -2.23595000 | -1.83760900 |
| C | -3.23382100 | 0.65421000 | -0.66763200 |
| C | -2.55290300 | -0.50280600 | -1.09977800 |
| C | -4.52619200 | 0.54871300 | -0.17257100 |
| C | -3.23595000 | -1.73066000 | -1.04590100 |
| C | -5.17641000 | -0.66991500 | -0.12064000 |
| H | -5.04715500 | 1.43900800 | 0.16555600 |
| C | -4.52420700 | -1.81313000 | -0.56552700 |
| H | -5.02922700 | -2.77342300 | -0.53322900 |
| O | -1.32176000 | -0.48131800 | -1.57794900 |
| S | -6.83937800 | -0.80647500 | 0.53908700 |
| O | -6.72309500 | -1.64669200 | 1.76550700 |
| O | -7.64671600 | -1.46641900 | -0.52631200 |
| O | -7.28241000 | 0.58545500 | 0.82834700 |
| H | -1.44104500 | 1.76970500 | 0.92290300 |
| H | -3.26133200 | 2.76967700 | -0.41204200 |
| H | -2.72263300 | -2.61981500 | -1.39755200 |

54

RR_ID1_TS1_chain_R, E(SCF) = -
 2484.18200941, E(ZPE) = -2483.783296, E(G)
 = -2483.852596 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.68402500 | 3.08131100 | -0.48701800 |
| H | -0.41469300 | 3.00740100 | -1.54507900 |
| H | -1.30235500 | 3.97275800 | -0.35542700 |
| C | 0.55229900 | 3.12135600 | 0.37683700 |
| H | 1.16927500 | 3.99802000 | 0.16433800 |
| H | 0.28385900 | 3.14334300 | 1.43695700 |
| N | 1.31028100 | 1.87290600 | 0.13610000 |
| C | 2.37588700 | 1.57248200 | 1.11568300 |
| H | 2.99585100 | 2.46267300 | 1.26577300 |
| C | 3.22567100 | 0.43893800 | 0.63161200 |
| C | 2.66286800 | -0.81080000 | 0.29591200 |
| C | 4.59865500 | 0.62235700 | 0.51378000 |
| C | 3.52561900 | -1.83375200 | -0.13098100 |
| C | 5.42865100 | -0.39772600 | 0.09312300 |
| H | 5.03313200 | 1.58547500 | 0.76136300 |
| C | 4.88479900 | -1.63535700 | -0.22714000 |
| H | 5.52936500 | -2.44235300 | -0.56092700 |
| O | 1.36727700 | -1.08521600 | 0.38927900 |
| S | 7.20164800 | -0.15287400 | -0.05273000 |
| O | 7.53421400 | -0.45346100 | -1.47411400 |
| O | 7.82293400 | -1.12269500 | 0.89364800 |
| O | 7.45262100 | 1.26679500 | 0.31795900 |
| H | 0.79783700 | -2.29038000 | -0.90456800 |
| O | 0.22483200 | -2.60116300 | -1.63112400 |
| H | -0.63516000 | -2.28884900 | -1.29918100 |
| H | 0.94136000 | -1.26652000 | 2.19217600 |
| O | 0.73894400 | -1.19941800 | 3.14250900 |
| H | 0.90209100 | -2.07852800 | -2.49092800 |
| H | 1.73628100 | 1.91998800 | -0.79167200 |
| H | 1.87819000 | 1.34560700 | 2.06493500 |
| Pd | -0.07013500 | 0.35408700 | 0.06287400 |
| O | 0.96290500 | -0.38355100 | -3.24504900 |
| H | 0.45667800 | 0.33508200 | -2.85553900 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.69605900 | -1.17089000 | -2.73068300 |
| H | 3.09096100 | -2.79684500 | -0.37820100 |
| N | -1.44096500 | 1.85938200 | -0.13168000 |
| C | -2.52289300 | 1.48374300 | -1.06503000 |
| H | -2.04120600 | 1.19293400 | -2.00558000 |
| C | -3.36239200 | 0.38501800 | -0.49299900 |
| C | -2.78829100 | -0.83070300 | -0.05582700 |
| C | -4.73977300 | 0.55862600 | -0.41898400 |
| C | -3.65607700 | -1.83474000 | 0.41416600 |
| C | -5.56947500 | -0.44031000 | 0.04937700 |
| H | -5.17908400 | 1.49582400 | -0.74585500 |
| C | -5.01806400 | -1.64833500 | 0.46236600 |
| H | -5.66251400 | -2.44021100 | 0.83124100 |
| O | -1.49742500 | -1.09604700 | -0.08261600 |
| S | -7.34403800 | -0.20057000 | 0.15164400 |
| O | -7.68718000 | -0.30567600 | 1.59919000 |
| O | -7.95033400 | -1.29834200 | -0.65481900 |
| O | -7.60954300 | 1.15213100 | -0.41197900 |
| H | -1.85194400 | 1.98582000 | 0.79515100 |
| H | -3.14781800 | 2.35978000 | -1.26946500 |
| H | -3.21163800 | -2.76853900 | 0.74120100 |

54

RR_ID1_TS1_chain, E(SCF) = -2484.16227434,
E(ZPE) = -2483.763651, E(G) = -2483.830470
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.70050300 | 3.24010100 | -0.52520700 |
| H | -0.53164500 | 3.28946800 | -1.60387100 |
| H | -1.31052400 | 4.10169500 | -0.23479700 |
| C | 0.59748900 | 3.21048100 | 0.23555900 |
| H | 1.21173900 | 4.08928100 | 0.02715500 |
| H | 0.39527300 | 3.19636300 | 1.31009800 |
| N | 1.34384600 | 1.96297100 | -0.08045500 |
| C | 2.30229300 | 1.62624100 | 1.01174500 |
| H | 2.93782400 | 2.50263900 | 1.18251100 |
| C | 3.14727000 | 0.43080900 | 0.73498500 |
| C | 2.55394800 | -0.85831600 | 0.73184600 |
| C | 4.51100900 | 0.57417100 | 0.52773600 |
| C | 3.41755400 | -1.96466300 | 0.57090300 |
| C | 5.32664600 | -0.52741900 | 0.33620000 |
| H | 4.95499900 | 1.56546100 | 0.52255200 |
| C | 4.77057800 | -1.80209900 | 0.37302600 |
| H | 5.40688100 | -2.67180500 | 0.23935600 |
| O | 1.26610500 | -1.02245500 | 0.85144400 |
| S | 7.09134100 | -0.34389000 | 0.09496300 |
| O | 7.41748000 | -1.08785900 | -1.15653300 |
| O | 7.74092500 | -0.95129200 | 1.29399400 |
| O | 7.34337200 | 1.12053800 | -0.01808000 |
| H | 0.72136300 | -2.48104800 | -0.07541300 |
| O | 0.37732700 | -2.96328400 | -0.85835600 |
| H | -0.46566700 | -2.49482900 | -1.00117100 |
| H | 0.09617800 | -0.17225500 | 2.02923700 |
| O | -0.53824200 | 0.41100100 | 2.49346900 |
| H | -0.88643900 | -0.11178500 | 3.21943400 |
| H | 1.87196600 | 2.09144600 | -0.94483800 |
| H | 1.68853900 | 1.47854700 | 1.90543700 |
| Pd | -0.02226900 | 0.48427500 | -0.52755900 |
| O | 1.44513500 | -0.68415900 | -2.10500400 |
| H | 1.01748000 | -0.55825700 | -2.95718200 |
| H | 1.21827600 | -1.59953700 | -1.83666000 |
| H | 2.98247400 | -2.95929500 | 0.59235900 |
| N | -1.40843200 | 1.97539900 | -0.24456900 |
| C | -2.63288600 | 1.76170300 | -1.03900600 |
| H | -2.31872000 | 1.72549100 | -2.08786700 |
| C | -3.34980100 | 0.51552800 | -0.62831900 |
| C | -2.69694100 | -0.73661300 | -0.65667000 |
| C | -4.68756900 | 0.58245400 | -0.26073800 |
| C | -3.44494100 | -1.88116100 | -0.32835600 |
| C | -5.40358900 | -0.55535200 | 0.05754400 |
| H | -5.18771700 | 1.54532700 | -0.23228300 |
| C | -4.77525400 | -1.79473300 | 0.01466800 |
| H | -5.33136200 | -2.69275300 | 0.26525400 |
| O | -1.43494300 | -0.88896500 | -1.00373500 |
| S | -7.14071300 | -0.46577900 | 0.49812300 |
| O | -7.26044100 | -1.13028800 | 1.82715800 |
| O | -7.86864200 | -1.20576000 | -0.57255700 |
| O | -7.48159900 | 0.98317400 | 0.53789000 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.63232100 | 1.90857100 | 0.75299600 |
| H | -3.29573100 | 2.62622100 | -0.91860300 |
| H | -2.94008000 | -2.84147800 | -0.35322100 |

54

RR_ID1_TS1, E(SCF) = -2484.15962351, E(ZPE)
= -2483.759848, E(G) = -2483.826048 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.59770400 | 3.20641700 | -0.09422900 |
| H | -0.40429800 | 3.38099000 | -1.15564000 |
| H | -1.17540000 | 4.05096100 | 0.29278100 |
| C | 0.67674100 | 3.01218600 | 0.67558400 |
| H | 1.32678300 | 3.88828800 | 0.62270100 |
| H | 0.44571100 | 2.83452300 | 1.73027100 |
| N | 1.38765800 | 1.80279300 | 0.18012800 |
| N | -1.37169300 | 1.95164400 | 0.01621300 |
| C | 2.33597000 | 1.30182200 | 1.21844300 |
| H | 2.90205300 | 2.16373900 | 1.58968300 |
| C | -2.56741700 | 1.89336800 | -0.85041100 |
| H | -2.20428600 | 1.94934500 | -1.94910500 |
| C | 3.27523400 | 0.25414000 | 0.73340900 |
| C | 2.78991600 | -1.05101600 | 0.47575400 |
| C | 4.62383400 | 0.54381000 | 0.57484500 |
| C | 3.73162500 | -2.02661400 | 0.07964700 |
| C | 5.52092400 | -0.42823000 | 0.17193000 |
| H | 4.98757500 | 1.54740600 | 0.77487800 |
| C | 5.06512100 | -1.72127100 | -0.07015700 |
| H | 5.76639000 | -2.48924500 | -0.38278100 |
| C | -3.36780900 | 0.65718100 | -0.59882300 |
| C | -2.78400800 | -0.62024900 | -0.73279900 |
| C | -4.71044500 | 0.76616100 | -0.25885400 |
| C | -3.60339700 | -1.74691700 | -0.54155200 |
| C | -5.49601200 | -0.35409000 | -0.07103100 |
| H | -5.15836300 | 1.74850500 | -0.14669800 |
| C | -4.93580400 | -1.61642400 | -0.22038100 |
| H | -5.54742100 | -2.50099400 | -0.07498000 |
| O | 1.52025900 | -1.33418500 | 0.55697700 |
| O | -1.51725500 | -0.81269900 | -1.05845500 |
| S | 7.26056600 | -0.05805400 | -0.04118800 |
| S | -7.23535100 | -0.20988100 | 0.34807500 |
| O | -7.41077100 | -0.96914600 | 1.61861500 |
| O | -7.97765500 | -0.82630600 | -0.78850300 |
| O | -7.50157300 | 1.24730500 | 0.49625500 |
| O | 7.41453200 | -1.39322700 | 0.25898300 |
| O | 7.58105000 | -0.39449800 | -1.45889500 |
| O | 7.99189700 | -0.93122700 | 0.92303000 |
| H | 0.37804200 | -2.78913100 | 0.37144300 |
| O | -0.50560500 | -3.16223700 | 0.19560600 |
| H | -0.92102100 | -2.45558900 | -0.33042100 |
| H | 0.26255500 | -1.08019500 | 1.94065600 |
| O | -0.54600500 | -1.22336100 | 2.46726500 |
| H | -0.96132300 | -1.94354500 | 1.97291700 |
| H | 1.92552600 | 2.04561300 | -0.65306400 |
| H | 1.71279700 | 0.93495600 | 2.04039700 |
| H | -1.66220500 | 1.81286400 | 0.98631600 |
| H | -3.18316300 | 2.77970100 | -0.66223300 |
| Pd | -0.05374000 | 0.44955700 | -0.45334300 |
| O | 1.16317300 | -0.80649400 | -2.05001200 |
| H | 0.43802700 | -1.18760900 | -2.55936000 |
| H | 1.38410300 | -1.46813600 | -1.37041000 |
| H | 3.36687300 | -3.03107900 | -0.11409100 |
| H | -3.15912500 | -2.72975500 | -0.65647000 |

54

RR_ID1_TS2-diamond_R_noH2, E(SCF) = -
2484.17275648, E(ZPE) = -2483.772659, E(G)
= -2483.839679 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.28577000 | -2.52636700 | 0.66388100 |
| H | 0.00541200 | -2.85897600 | -0.33942800 |
| H | 0.72335100 | -3.37569900 | 1.19525700 |
| C | -0.89365300 | -1.95734800 | 1.39633200 |
| H | -1.68203900 | -2.70141700 | 1.54146500 |
| H | -0.58698600 | -1.59807200 | 2.38275300 |
| N | -1.41980800 | -0.78828600 | 0.64567600 |
| N | 1.27866700 | -1.44074300 | 0.51045100 |
| C | -2.41504200 | -0.01829900 | 1.47005600 |
| H | -2.71423800 | -0.67430000 | 2.29371600 |
| C | 2.36873300 | -1.76328700 | -0.43467100 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.32664900 | 0.71359300 | 2.71652100 |
| H | 1.73236800 | -0.39591400 | 2.04845500 |
| H | 2.87002200 | -2.43648400 | 1.22319000 |
| Pd | -0.09399000 | -0.06949800 | 0.32854000 |
| O | -1.11335800 | 3.22897700 | -0.99963900 |
| H | -0.25376500 | 3.47344800 | -0.62482400 |
| H | -1.70744100 | 3.15626200 | -0.21954100 |
| H | -4.26992900 | 3.11542600 | -0.82872000 |
| H | 3.16043600 | 1.95815300 | -2.07341800 |
| H | -1.41922800 | 0.37809500 | -0.75450400 |
| H | -1.06396800 | 1.11391400 | -0.65118100 |

54

RR_ID1_TS2-diamond_R_noH2, E(SCF) = -
2484.17275648, E(ZPE) = -2483.772659, E(G)
= -2483.839679 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.28577000 | -2.52636700 | 0.66388100 |
| H | 0.00541200 | -2.85897600 | -0.33942800 |
| H | 0.72335100 | -3.37569900 | 1.19525700 |
| C | -0.89365300 | -1.95734800 | 1.39633200 |
| H | -1.68203900 | -2.70141700 | 1.54146500 |
| H | -0.58698600 | -1.59807200 | 2.38275300 |
| N | -1.41980800 | -0.78828600 | 0.64567600 |
| N | 1.27866700 | -1.44074300 | 0.51045100 |
| C | -2.41504200 | -0.01829900 | 1.47005600 |
| H | -2.71423800 | -0.67430000 | 2.29371600 |
| C | 2.36873300 | -1.76328700 | -0.43467100 |
| H | 1.90344800 | -1.85206900 | -1.42243000 |
| C | -3.62635100 | 0.39248300 | 0.70332400 |
| C | -3.76187800 | 1.72386300 | 0.23155900 |
| C | -4.64200200 | -0.53604800 | 0.49490000 |
| C | -4.97541900 | 2.04847900 | -0.42383600 |
| C | -5.80003800 | -0.19312500 | -0.17323900 |
| H | -4.52995400 | -1.55097000 | 0.87018500 |
| C | -5.96459600 | 1.11602900 | -0.62443200 |
| H | -6.87955600 | 1.39467800 | -1.13934000 |
| C | 3.45174200 | -0.73470900 | -0.41169600 |
| C | 3.16752200 | 0.63437100 | -0.61854200 |
| C | 4.76478300 | -1.13980000 | -0.22880400 |
| C | 4.24648900 | 1.53039000 | -0.66526300 |
| C | 5.81406000 | -0.23753200 | -0.27638200 |
| H | 4.97197500 | -2.19333900 | -0.06124200 |
| C | 5.54795200 | 1.10382400 | -0.49790000 |
| H | 6.36818900 | 1.81124600 | -0.53999000 |
| O | -2.82340800 | 2.60727300 | 0.37187500 |
| O | 1.94897300 | 1.11208900 | -0.80041900 |
| S | -7.11633800 | -1.37860300 | -0.42995500 |
| S | 7.48854400 | -0.81901900 | 0.00564400 |
| O | 8.37737200 | 0.33367900 | -0.30619400 |
| O | 7.68131000 | -1.97395300 | -0.91631600 |
| O | 7.54166800 | -1.22345000 | 1.44012800 |
| O | -6.61975300 | -2.67670500 | 0.10805100 |
| O | -7.35728900 | -1.41438400 | -1.90218800 |
| O | -8.29611300 | -0.85424400 | 0.31935500 |
| H | 1.53588500 | 4.37028100 | -0.67854900 |
| O | 1.13783400 | 3.62006900 | -0.23105900 |
| H | 1.69056200 | 2.83253200 | -0.42617400 |
| H | -1.50278600 | 3.13455800 | 1.55833700 |
| O | -0.69678700 | 3.41099100 | 2.03194400 |
| H | -0.03908300 | 3.55216400 | 1.33474200 |
| H | -1.91055700 | -1.13238400 | -0.18131400 |
| H | -1.89863400 | 0.84133800 | 1.90049900 |
| H | 1.68793500 | -1.22792600 | 1.42195900 |
| H | 2.78310500 | -2.74295900 | -0.17476200 |
| Pd | 0.25586900 | 0.21030900 | -0.11088400 |
| O | -0.79394600 | 1.81532600 | -0.92215000 |
| H | -0.19857400 | 2.59179400 | -0.90595800 |
| H | -1.61191700 | 2.11196500 | -0.38999300 |
| H | -5.09507700 | 3.06716600 | -0.77901900 |
| H | 4.03490000 | 2.58026600 | -0.83990100 |

56

RR_ID1_TS2-diamond_R, E(SCF) = -
2485.34703198, E(ZPE) = -2484.931839, E(G)
= -2484.999870 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.28987700 | -2.48629800 | 0.85280600 |
| H | -0.01327000 | -2.85969300 | -0.12934600 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.73955500 | -3.31331700 | 1.40855100 |
| C | -0.87319400 | -1.88666000 | 1.58620700 |
| H | -1.65633100 | -2.62364000 | 1.78185400 |
| H | -0.54583700 | -1.48113000 | 2.54772300 |
| N | -1.41842800 | -0.75561200 | 0.79331600 |
| N | 1.27814500 | -1.40831300 | 0.63349700 |
| C | -2.41170200 | 0.03910300 | 1.59613900 |
| H | -2.72143900 | -0.59671000 | 2.43199600 |
| C | 2.34592900 | -1.76979400 | -0.32341000 |
| H | 1.85732300 | -1.89667300 | -1.29569100 |
| C | -3.60921600 | 0.43581800 | 0.80178900 |
| C | -3.72746400 | 1.75050900 | 0.28342000 |
| C | -4.60709300 | -0.50572300 | 0.57290900 |
| C | -4.90438600 | 2.04415600 | -0.44818300 |
| C | -5.73052000 | -0.19316100 | -0.16567100 |
| H | -4.50744900 | -1.50801900 | 0.98405900 |
| C | -5.87276300 | 1.09594200 | -0.67737800 |
| H | -6.75719700 | 1.35005200 | -1.25434500 |
| C | 3.43049700 | -0.74394500 | -0.36895100 |
| C | 3.14293900 | 0.61613300 | -0.62367600 |
| C | 4.74723100 | -1.14477500 | -0.20545500 |
| C | 4.22098100 | 1.50758200 | -0.73219300 |
| C | 5.79599200 | -0.24722800 | -0.31537000 |
| H | 4.95748600 | -2.19131300 | -0.00126500 |
| C | 5.52603900 | 1.08487700 | -0.58268600 |
| H | 6.34556800 | 1.78862300 | -0.67263200 |
| O | -2.79808100 | 2.64211100 | 0.43750000 |
| O | 1.92046000 | 1.08794700 | -0.79485800 |
| S | -6.99384800 | -1.41705500 | -0.50004600 |
| S | 7.47656500 | -0.82669200 | -0.06817700 |
| O | 8.35780600 | 0.32709100 | -0.39673600 |
| O | 7.65145600 | -1.97996700 | -0.99591900 |
| O | 7.55882700 | -1.23373800 | 1.36405400 |
| O | -6.62641600 | -2.62240600 | 0.29550600 |
| O | -6.95110400 | -1.66043300 | -1.97240200 |
| O | -8.28554900 | -0.80729500 | -0.06906500 |
| H | 1.53648100 | 4.35044600 | -0.75812400 |
| O | 1.12400500 | 3.61654600 | -0.29690800 |
| H | 1.67236400 | 2.81942900 | -0.46214500 |
| H | -1.45238600 | 3.18408400 | 1.58561200 |
| O | -0.63531200 | 3.47818500 | 2.02865200 |
| H | 0.00046000 | 3.60352300 | 1.30822000 |
| H | -1.91737000 | -1.13954300 | -0.01198800 |
| H | -1.89169700 | 0.90468700 | 2.00929300 |
| H | 1.70690200 | -1.15959500 | 1.52689800 |
| H | 2.76528800 | -2.73914900 | -0.03449600 |
| Pd | 0.24242000 | 0.21680500 | -0.03404500 |
| O | -0.81881500 | 1.78851700 | -0.89795700 |
| H | -0.21505000 | 2.55657700 | -0.94864300 |
| H | -1.60584500 | 2.12487600 | -0.34459400 |
| H | -5.00938400 | 3.04880100 | -0.84537700 |
| H | 4.00608800 | 2.55008700 | -0.94310700 |
| H | -2.91658300 | -0.51601900 | -2.33464500 |
| H | -2.82757200 | 0.14703600 | -1.99458500 |

56

RR_ID1_TS2-diamond, E(SCF) = -
2485.31772516, E(ZPE) = -2484.903831, E(G)
= -2484.972500 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.50844900 | 0.19690200 | 3.07044700 |
| H | 0.26285400 | -0.85926200 | 3.21968200 |
| H | 1.15072900 | 0.51441500 | 3.89345500 |
| C | -0.73492300 | 1.02414700 | 2.97148400 |
| H | -1.33197200 | 0.96045600 | 3.88489300 |
| H | -0.49566800 | 2.07442800 | 2.78494600 |
| N | -1.52003600 | 0.54848400 | 1.80795600 |
| N | 1.23934200 | 0.30159100 | 1.78619100 |
| C | -2.76416800 | 1.36338600 | 1.67214900 |
| H | -3.29906800 | 1.26190700 | 2.62435100 |
| C | 2.22519600 | -0.78574100 | 1.60941000 |
| H | 1.64736600 | -1.71236300 | 1.54346600 |
| C | -3.62164800 | 0.95066500 | 0.53053100 |
| C | -3.66298500 | 1.77113200 | -0.63531400 |
| C | -4.36543600 | -0.21367600 | 0.60857100 |
| C | -4.48233300 | 1.30500100 | -1.69441800 |
| C | -5.15032700 | -0.63982300 | -0.45156800 |
| H | -4.33137400 | -0.80765900 | 1.52056100 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -5.19834900 | 0.13059100 | -1.60816700 | O | 7.55613200 | 0.04314100 | 0.69751000 |
| H | -5.81217400 | -0.20217000 | -2.43809100 | O | -6.77678300 | -2.15144600 | 0.96194700 |
| C | 3.11491500 | -0.59224000 | 0.42647400 | O | -4.98381200 | -3.26468300 | -0.33299700 |
| C | 2.60565100 | -0.23893200 | -0.84075600 | O | -6.92338200 | -2.26144000 | -1.51615900 |
| C | 4.47621100 | -0.82159400 | 0.57161300 | H | 2.20943000 | 3.22218800 | -1.86779300 |
| C | 3.50725300 | -0.14240500 | -1.91342800 | O | 1.44065700 | 2.82873500 | -1.44846300 |
| C | 5.34514500 | -0.72935200 | -0.49951500 | H | 1.61715800 | 1.87370600 | -1.37422300 |
| H | 4.86203300 | -1.08851000 | 1.55119800 | H | -1.39530400 | 3.38940300 | 0.09669600 |
| C | 4.85315700 | -0.38397400 | -1.74831900 | O | -0.56860500 | 3.68657200 | 0.52547500 |
| H | 5.53540200 | -0.30511000 | -2.58874800 | H | 0.14119800 | 3.44159300 | -0.08688700 |
| O | -2.96776500 | 2.85307000 | -0.74485000 | H | -1.81031600 | -0.41563000 | 1.98856100 |
| O | 1.33729900 | 0.03828800 | -1.10100000 | H | -2.45234800 | 2.40078000 | 1.56689500 |
| S | -6.02771200 | -2.19385900 | -0.32788100 | H | 1.71134600 | 1.20543400 | 1.73626600 |
| S | 7.09714400 | -1.02546700 | -0.23913800 | H | 2.83464800 | -0.84425300 | 2.51849600 |
| O | 7.72812300 | -0.93195800 | -1.58595200 | Pd | -0.13129100 | 0.29008900 | 0.25488100 |
| O | 7.19556500 | -2.38815200 | 0.36107600 | O | -0.99920100 | 1.55635600 | -2.00860900 |
| O | 7.55613200 | 0.04314100 | 0.69751000 | H | -0.21564400 | 2.11111000 | -2.14058600 |
| O | -6.77678300 | -2.15144600 | 0.96194700 | H | -1.69377100 | 2.16517000 | -1.66895400 |
| O | -4.98381200 | -3.26468300 | -0.33299700 | H | -4.52484300 | 1.90845100 | -2.59771700 |
| O | -6.92338200 | -2.26144000 | -1.51615900 | H | 3.10546300 | 0.13375500 | -2.88336100 |
| H | 2.20943000 | 3.22218800 | -1.86779300 | H | -1.46979000 | -1.05211900 | -0.80105600 |
| O | 1.44065700 | 2.82873500 | -1.44846300 | H | -1.59269800 | -0.39351800 | -1.17230100 |
| H | 1.61715800 | 1.87370600 | -1.37422300 | | | | |
| H | -1.39530400 | 3.38940300 | 0.09669600 | | | | |
| O | -0.56860500 | 3.68657200 | 0.52547500 | | | | |
| H | 0.14119800 | 3.44159300 | -0.08688700 | | | | |
| H | -1.81031600 | -0.41563000 | 1.98856100 | | | | |
| H | -2.45234800 | 2.40078000 | 1.56689500 | | | | |
| H | 1.71134600 | 1.20543400 | 1.73626600 | | | | |
| H | 2.83464800 | -0.84425300 | 2.51849600 | | | | |
| Pd | -0.13129100 | 0.29008900 | 0.25488100 | | | | |
| O | -0.99920100 | 1.55635600 | -2.00860900 | | | | |
| H | -0.21564400 | 2.11111000 | -2.14058600 | | | | |
| H | -1.69377100 | 2.16517000 | -1.66895400 | | | | |
| H | -4.52484300 | 1.90845100 | -2.59771700 | | | | |
| H | 3.10546300 | 0.13375500 | -2.88336100 | | | | |
| H | -1.46979000 | -1.05211900 | -0.80105600 | | | | |
| H | -1.59269800 | -0.39351800 | -1.17230100 | | | | |

56

RR_ID1_TS2_H2-out-but-it-is-a-TS_P, E(SCF) = -2485.34090143, E(ZPE) = -2484.924637, E(G) = -2484.993712 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.57597300 | 3.13777300 | 0.09529500 |
| H | -0.40159000 | 3.40453800 | -0.95014300 |
| H | -1.13887600 | 3.94854200 | 0.56738800 |
| C | 0.70737100 | 2.86904600 | 0.82381900 |
| H | 1.37113400 | 3.73610100 | 0.81721800 |
| H | 0.48350300 | 2.63221700 | 1.86827000 |
| N | 1.39709300 | 1.67630800 | 0.25317700 |
| N | -1.35592100 | 1.88377500 | 0.11144400 |
| C | 2.31728200 | 1.12614300 | 1.30272400 |
| H | 2.86449400 | 1.98373500 | 1.71191800 |
| C | -2.59859200 | 1.94561100 | -0.68511000 |
| H | -2.28899500 | 2.14370900 | -1.71715800 |
| C | 3.29415600 | 0.09338300 | 0.85829700 |
| C | 2.91561400 | -1.27242800 | 0.81121100 |
| C | 4.60209700 | 0.46656200 | 0.57350900 |
| C | 3.91982700 | -2.20899000 | 0.47470900 |
| C | 5.55735300 | -0.47071600 | 0.23115100 |
| H | 4.88543700 | 1.51449900 | 0.61976900 |
| C | 5.20703900 | -1.81714500 | 0.18582200 |
| H | 5.95489300 | -2.55961100 | -0.07664400 |
| C | -3.40914700 | 0.69507300 | -0.57848100 |
| C | -2.85678500 | -0.55706100 | -0.91906600 |
| C | -4.74337100 | 0.77450000 | -0.19726700 |
| C | -3.69759400 | -1.68352900 | -0.89088600 |
| C | -5.54934100 | -0.34597600 | -0.16861700 |
| H | -5.16895500 | 1.73580500 | 0.07262500 |
| C | -5.01989100 | -1.58063100 | -0.52441300 |
| H | -5.64898900 | -2.46490400 | -0.50779000 |
| O | 1.68184600 | -1.64534500 | 1.00423600 |
| O | -1.59779100 | -0.73032600 | -1.28311000 |
| S | 7.22301300 | 0.01838800 | -0.20442500 |
| S | -7.27203000 | -0.24212800 | 0.32346100 |
| O | -7.40536400 | -1.11953500 | -1.52127100 |
| O | -8.05602300 | -0.74761900 | -0.83953100 |
| O | -7.52876800 | 1.19386500 | 0.62058200 |
| O | 7.30702100 | 1.48339800 | 0.05530600 |
| O | 7.38868600 | -0.32235400 | -1.64884900 |
| O | 8.13249400 | -0.78029700 | 0.66784900 |
| H | 0.09898900 | -2.70657200 | 0.78292800 |
| H | 4.11056300 | 0.16387700 | -2.63057800 |
| H | 3.59927900 | -0.02773900 | -2.11665400 |
| O | -0.84418400 | -2.88482100 | 0.62724200 |
| H | -1.08754300 | -2.28438800 | -0.09573900 |
| H | 0.28936400 | -0.76985500 | 1.94992100 |
| O | -0.55716000 | -0.47240800 | 2.34168700 |
| H | -1.15973200 | -1.15859200 | 2.02458200 |
| H | 1.97013300 | 1.97106400 | -0.53827500 |
| H | 1.67582400 | 0.74228600 | 2.09914700 |
| H | -1.57350600 | 1.61505900 | 1.07558900 |
| H | -3.19156600 | 2.80188700 | -0.34680900 |

56

RR_ID1_TS2-diamond, E(SCF) = -2485.31772516, E(ZPE) = -2484.903831, E(G) = -2484.972500 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.50844900 | 0.19690200 | 3.07044700 |
| H | 0.26285400 | -0.85926200 | 3.21968200 |
| H | 1.15072900 | 0.51441500 | 3.89345500 |
| C | -0.73492300 | 1.02414700 | 2.97148400 |
| H | -1.33197200 | 0.96045600 | 3.88489300 |
| H | -0.49566800 | 2.07442800 | 2.78494600 |
| N | -1.52003600 | 0.54848400 | 1.80795600 |
| N | 1.23934200 | 0.30159100 | 1.78619100 |
| C | -2.76416800 | 1.36338600 | 1.67214900 |
| H | -3.29906800 | 1.26190700 | 2.62435100 |
| C | 2.22519600 | -0.78574100 | 1.60941000 |
| H | 1.64736600 | -1.71236300 | 1.54346600 |
| C | -3.62164800 | 0.95066500 | 0.53053100 |
| C | -3.66298500 | 1.77113200 | -0.63531400 |
| C | -4.36543600 | -0.21367600 | 0.60857100 |
| C | -4.48233300 | 1.30500100 | -1.69441800 |
| C | -5.15032700 | -0.63982300 | -0.45156800 |
| H | -4.33137400 | -0.80765900 | 1.52056100 |
| C | -5.19834900 | 0.13059100 | -1.60816700 |
| H | -5.81217400 | -0.20217000 | -2.43809100 |
| C | 3.11491500 | -0.59224000 | 0.42647400 |
| C | 2.60565100 | -0.23893200 | -0.84075600 |
| C | 4.47621100 | -0.82159400 | 0.57161300 |
| C | 3.50725300 | -0.14240500 | -1.91342800 |
| C | 5.34514500 | -0.72935200 | -0.49951500 |
| H | 4.86203300 | -1.08851000 | 1.55119800 |
| C | 4.85315700 | -0.38397400 | -1.74831900 |
| H | 5.53540200 | -0.30511000 | -2.58874800 |
| O | -2.96776500 | 2.85307000 | -0.74485000 |
| O | 1.33729900 | 0.03828800 | -1.10100000 |
| S | -6.02771200 | -2.19385900 | -0.32788100 |
| S | 7.09714400 | -1.02546700 | -0.23913800 |
| O | 7.72812300 | -0.93195800 | -1.58595200 |
| O | 7.19556500 | -2.38815200 | 0.36107600 |

Pd -0.10741800 0.44869600 -0.58456400
H 3.63981800 -3.25713900 0.44008200
H -3.27274300 -2.64268700 -1.16766300
O 1.11956400 -1.02697000 -1.46353700
H 0.53741100 -1.58415400 -1.99608300
H 1.34613800 -1.52884600 -0.63424700

56

RR_ID1_TS2_H2-out-but-it-is-a-TS_R, E(SCF)
= -2485.35962080, E(ZPE) = -2484.944886,
E(G) = -2485.014147 a.u.

C -0.62292500 3.20509800 -0.09891800
H -0.35653100 3.26737000 -1.15794700
H -1.23846100 4.07380200 0.14713600
C 0.61549200 3.13027800 0.75786900
H 1.23871800 4.02160200 0.65092800
H 0.35251000 3.02157200 1.81363600
N 1.36086900 1.91620400 0.35469700
N -1.38710700 1.95021400 0.09288800
C 2.46597100 1.51906900 1.25212000
H 3.09918600 2.38880300 1.45670000
C -2.43200800 1.69383100 -0.91915900
H -1.91075100 1.51302500 -1.86583000
C 3.28348500 0.43382400 0.62339600
C 2.69676500 -0.78071700 0.21235300
C 4.64212300 0.63875100 0.41515900
C 3.52759700 -1.76663500 -0.34413800
C 5.43806900 -0.33544000 -0.15513600
H 5.09253100 1.58093000 0.70985100
C 4.87450400 -1.54872600 -0.53010200
H 5.49419700 -2.32178800 -0.97288600
C -3.30424600 0.54405300 -0.52042400
C -2.76798800 -0.71863400 -0.18768600
C -4.68354400 0.72234300 -0.51312600
C -3.66446900 -1.75849900 0.11534900
C -5.54465300 -0.31308600 -0.21134000
H -5.09712100 1.69550200 -0.75771000
C -5.02628200 -1.56469000 0.09885800
H -5.69495500 -2.38544500 0.33812200
O 1.40297400 -1.05177000 0.33656000
O -1.47296600 -0.99571300 -0.16713100
S 7.18812000 -0.05228200 -0.44536500
S -7.32347900 -0.07544200 -0.20947500
O -7.77510900 -0.41404000 1.17043600
O -7.85886800 -1.02165300 -1.22939000
O -7.54933600 1.35293700 -0.56311100
O 7.47908600 1.30534300 0.09134500
O 7.36922400 -0.14887700 -1.92172800
O 7.90031900 -1.13672800 0.28746500
H 0.55842300 -2.90026900 0.77342000
H 2.92236800 0.75718600 -2.81748000
H 2.73416700 0.24543000 -2.30248900
O -0.30832700 -3.22006700 1.06476500
H -0.88796300 -2.53959500 0.67150400
H 0.99839100 -1.10013200 2.37043000
O 0.55950200 -1.45970100 3.15483700
H 0.07654800 -2.20425200 2.76136200
H 1.74996000 2.06776100 -0.57840400
H 2.00930200 1.21270400 2.19949500
H -1.82813600 1.96927000 1.01409600
H -3.04342900 2.59391800 -1.04365100
Pd -0.02655500 0.42254000 0.15174200
H 3.07398900 -2.70869400 -0.63700900
H -3.25078800 -2.73099800 0.36130900
O 0.27269400 -2.07361100 -2.16591900
H -0.55932800 -1.79349900 -1.75370800
H 0.89721500 -1.87624900 -1.45215000

56

RR_ID1_TS2_H2-out-but-it-is-a-TS_v2_P,
E(SCF) = -2485.34045518, E(ZPE) = -
2484.923888, E(G) = -2484.991061 a.u.

C -0.56734400 3.13541600 0.22530500
H -0.39717500 3.44963400 -0.80781200
H -1.13225300 3.92151000 0.73517300
C 0.72054400 2.84006100 0.93569800
H 1.37983100 3.71004100 0.96512300

H 0.50405100 2.55433500 1.96939300
N 1.41296200 1.67919900 0.30546900
N -1.34082100 1.87846000 0.18750300
C 2.34931800 1.09165900 1.31875900
H 2.90781800 1.93343700 1.74521700
C -2.59194300 1.97049500 -0.59157100
H -2.29629100 2.22460700 -1.61577100
C 3.31259100 0.06499000 0.83141700
C 2.92234200 -1.29650400 0.75712600
C 4.62176600 0.43300900 0.54458700
C 3.91749600 -2.23568900 0.40217700
C 5.56640400 -0.50575100 0.17476500
H 4.91551100 1.47676600 0.61338100
C 5.20681600 -1.84956500 0.11669300
H 5.94834100 -2.59248300 -0.16719900
C -3.39063800 0.70890700 -0.54280700
C -2.83326400 -0.51616900 -0.96328300
C -4.71895200 0.75361200 -0.13658800
C -3.66668100 -1.64772800 -0.99699300
C -5.51630100 -0.37298700 -0.16419100
H -5.14683400 1.69340300 0.19772500
C -4.98444400 -1.57846000 -0.60615100
H -5.60712200 -2.46690700 -0.37715100
O 1.68421300 -1.66041500 0.93873500
O -1.57581900 -0.65870700 -1.34657100
S 7.25671100 -0.03597000 -0.18335400
S -7.22664300 -0.31417100 0.37738000
O -7.31357000 -1.23751100 1.54452000
O -8.03599800 -0.78783300 -0.78135300
O -7.49487600 1.10555600 0.73633700
O 7.30069000 1.45109100 -0.09908000
O 7.54578100 -0.54887500 -1.55444500
O 8.09951400 -0.70022400 0.85396900
H 0.10868000 -2.70863000 0.67377100
H 0.43310700 2.55969700 -3.31973100
H 0.34367500 1.89401300 -2.98400400
O -0.83396200 -2.88256500 0.50795800
H -1.07235300 -2.26336500 -0.20038800
H 0.28855300 -0.80413500 1.90557700
O -0.56642400 -0.52669100 2.29349900
H -1.15425900 -1.21630300 1.95607000
H 1.97377100 2.01645100 -0.47802400
H 1.71920700 0.68710500 2.11399100
H -1.54397000 1.55807500 1.13958200
H -3.18832800 2.80248400 -0.20259200
Pd -0.08884400 0.48460100 -0.58290500
H 3.62802500 -3.28048900 0.34925000
H -3.23899600 -2.58480400 -1.33779500
O 1.15227600 -0.94888400 -1.51834400
H 0.57910200 -1.48316200 -2.08301400
H 1.36780700 -1.48558800 -0.70902600

56

RR_ID1_TS2_H2-out-but-it-is-a-TS, E(SCF) =
-2485.33379349, E(ZPE) = -2484.918740, E(G)
= -2484.986129 a.u.

C 0.61076200 3.19482600 0.07847100
H 0.40995200 3.36893400 1.13856900
H 1.18831500 4.04106200 -0.30505500
C -0.65754700 2.99572800 -0.69981300
H -1.31106300 3.86948100 -0.65223600
H -0.41831600 2.81827100 -1.75269800
N -1.36810200 1.78390400 -0.20906300
N 1.38924400 1.94259800 -0.02726300
C -2.30224500 1.27770800 -1.25811800
H -2.86298200 2.13767700 -1.64167700
C 2.58240800 1.89013800 0.84334200
H 2.21567600 1.94398300 1.87367300
C -3.24876000 0.23490700 -0.77747200
C -2.76775100 -1.06647400 -0.49470900
C -4.59923100 0.52723800 -0.64273000
C -3.71482100 -2.03402000 -0.09246100
C -5.50246100 -0.43820700 -0.23945200
H -4.95948800 1.52806200 -0.86181100
C -5.04959700 -1.72462300 0.03889500
H -5.75345800 -2.48808200 0.35863900
C 3.38999400 0.65838800 0.59349800

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 2.81180400 | -0.62190900 | 0.72272400 | O | -7.47611000 | -1.75813800 | -0.65919400 |
| C | 4.73345600 | 0.77428100 | 0.25923100 | H | 0.59168700 | -2.05061800 | -1.47483200 |
| C | 3.63682000 | -1.74450200 | 0.53227600 | H | -1.44726600 | 0.43570500 | 1.95881600 |
| C | 5.52491100 | -0.34198500 | 0.07255700 | H | -1.46334800 | -0.11954000 | 1.36944300 |
| H | 5.17738900 | 1.75883400 | 0.15058100 | O | 1.54984600 | -2.17465300 | -1.60141600 |
| C | 4.96997500 | -1.60722700 | 0.21695800 | H | 1.90323700 | -2.21805700 | -0.70413300 |
| H | 5.58615500 | -2.48869900 | 0.07204200 | O | 0.13280300 | 0.06461300 | -1.95586300 |
| O | -1.49805000 | -1.35429400 | -0.56491900 | O | 0.93259900 | 0.51526900 | -2.30983200 |
| O | 1.54468400 | -0.82072100 | 1.04346000 | H | 1.57539600 | -0.21051800 | -2.28011700 |
| S | -7.23087300 | -0.03914100 | 0.00814000 | H | -2.16034100 | 2.58127600 | 0.33781700 |
| S | 7.26532000 | -0.18834300 | -0.33877600 | H | -1.56733900 | 1.23865700 | -2.18463200 |
| O | 7.45014600 | -0.94591700 | -1.60894300 | H | 1.32933200 | 1.77728800 | -0.98011300 |
| O | 8.00586700 | -0.80152100 | 0.80066800 | H | 3.17378000 | 2.93612000 | 0.18503100 |
| O | 7.52430000 | 1.27033600 | -0.48497600 | Pd | -0.19065700 | 1.04302700 | 0.82970600 |
| O | -7.41716000 | 1.33870200 | -0.52757400 | H | -2.53623300 | -3.07854000 | -0.52238800 |
| O | -7.46419600 | -0.12418700 | 1.48026400 | H | 2.49645600 | -2.23115400 | 1.96331300 |
| O | -8.00833100 | -1.06614000 | -0.74399700 | O | -0.16416800 | -2.46468200 | 1.20418500 |
| H | -0.34409000 | -2.80841600 | -0.38878000 | H | 0.30999300 | -1.72753500 | 1.62286000 |
| H | -4.17075500 | 0.40981400 | 2.66979000 | H | -0.47166500 | -2.07989900 | 0.36255400 |
| H | -3.65964000 | 0.20843900 | 2.15952500 | | | | |
| O | 0.54291700 | -3.17422200 | -0.21595600 | 54 | | | |
| H | 0.95496200 | -2.46552700 | 0.30995000 | RR_ID1_TS2-trigo_R_noH2, E(SCF) = - | | | |
| H | -0.23888200 | -1.09689700 | -1.95069300 | 2484.16689215, E(ZPE) = -2483.765923, E(G) | | | |
| O | 0.56820800 | -1.23490100 | -2.48082900 | = -2483.832717 a.u. | | | |
| H | 0.98896600 | -1.95433300 | -1.98998400 | C | -0.56273900 | 3.14211200 | 0.09163600 |
| H | -1.91813800 | 2.02769500 | 0.61620800 | H | -0.39495800 | 3.41372300 | -0.95365600 |
| H | -1.66860900 | 0.90672900 | -2.07009500 | H | -1.12649100 | 3.94868000 | 0.56980700 |
| H | 1.68347500 | 1.80328900 | -0.99622700 | C | 0.72583500 | 2.87590500 | 0.81181700 |
| H | 3.19394300 | 2.77977900 | 0.65716400 | H | 1.38500300 | 3.74658500 | 0.80659100 |
| Pd | 0.07605100 | 0.43603700 | 0.43858800 | H | 0.50956800 | 2.63123300 | 1.85612700 |
| H | -3.35369000 | -3.03562700 | 0.12176000 | N | 1.41781200 | 1.69096900 | 0.22869700 |
| H | 3.19647500 | -2.72953400 | 0.64351600 | N | -1.33767100 | 1.88488800 | 0.10704000 |
| O | -1.11354200 | -0.85503900 | 2.03281500 | C | 2.35776500 | 1.14598500 | 1.26260200 |
| H | -0.37423200 | -1.24676300 | 2.51301500 | H | 2.91253800 | 2.00586900 | 1.65664300 |
| H | -1.34450800 | -1.49504500 | 1.33496100 | C | -2.58249200 | 1.94365600 | -0.68614500 |
| | | | | H | -2.27628600 | 2.14424700 | -1.71873100 |
| 56 | | | | C | 3.32611400 | 0.10827300 | 0.80982700 |
| RR_ID1_TS2-trigo_P, E(SCF) = - | | | | C | 2.94795200 | -1.25854900 | 0.79351300 |
| 2485.33698722, E(ZPE) = -2484.920864, E(G) | | | | C | 4.62864100 | 0.47675100 | 0.49489400 |
| = -2484.987731 a.u. | | | | C | 3.94866300 | -2.20152600 | 0.46500700 |
| C | 0.55935600 | 3.54743900 | -0.18721500 | C | 5.57883700 | -0.46685800 | 0.15311900 |
| H | 0.38302700 | 3.94169000 | 0.81671600 | H | 4.91276600 | 1.52504900 | 0.52044700 |
| H | 1.21424800 | 4.24549900 | -0.71820900 | C | 5.23080800 | -1.81497900 | 0.14964900 |
| C | -0.72375900 | 3.33000900 | -0.94117000 | H | 5.97672600 | -2.56163000 | -0.10649000 |
| H | -1.33454200 | 4.23299200 | -0.97807800 | C | -3.38931100 | 0.69061300 | -0.57906000 |
| H | -0.49139000 | 3.04471600 | -1.96985400 | C | -2.83369000 | -0.56080300 | -0.91716700 |
| N | -1.49694400 | 2.20018800 | -0.33613500 | C | -4.72448300 | 0.76740000 | -0.20039100 |
| N | 1.21039100 | 2.22977800 | -0.05342500 | C | -3.67177800 | -1.68929300 | -0.88723800 |
| C | -2.28206200 | 1.48510700 | -1.39729600 | C | -5.52801200 | -0.35476300 | -0.17123700 |
| H | -2.98894000 | 2.21272500 | -1.81127400 | H | -5.15281500 | 1.72821000 | 0.06692200 |
| C | 2.48878700 | 2.23940900 | 0.67975800 | C | -4.99488300 | -1.58898100 | -0.52311900 |
| H | 2.27915300 | 2.62733200 | 1.68234400 | H | -5.62179800 | -2.47478900 | -0.50559700 |
| C | -2.99682600 | 0.26022500 | -0.94683000 | O | 1.71557100 | -1.62687200 | 1.00298700 |
| C | -2.29648400 | -0.97863200 | -0.90516000 | O | -1.57435500 | -0.73250500 | -1.28061300 |
| C | -4.34845000 | 0.31667400 | -0.63332600 | S | 7.25854300 | 0.00459600 | -0.24984000 |
| C | -3.05005200 | -2.12238600 | -0.54640700 | S | -7.25215700 | -0.25354300 | 0.31632900 |
| C | -5.04936200 | -0.81857800 | -0.27255400 | O | -7.38678900 | -1.12915000 | 1.51532100 |
| H | -4.87258900 | 1.26726900 | -0.68076800 | O | -8.03211900 | -0.76261200 | -0.84782900 |
| C | -4.38697100 | -2.04327300 | -0.23261500 | O | -7.51262000 | 1.18244400 | 0.61023600 |
| H | -4.93212600 | -2.94176900 | 0.04159000 | O | 7.29931300 | 1.49261500 | -0.18225800 |
| C | 3.09087200 | 0.87395100 | 0.72765300 | O | 7.51673400 | -0.52152600 | -1.62228500 |
| C | 2.39115900 | -0.17535600 | 1.35651700 | O | 8.12824600 | -0.64624000 | 0.77351800 |
| C | 4.33855500 | 0.63408700 | 0.17074200 | H | 0.13645300 | -2.69125300 | 0.78648700 |
| C | 3.01870900 | -1.42936000 | 1.45278000 | O | -0.80684500 | -2.87246800 | 0.63411800 |
| C | 4.92918700 | -0.61343400 | 0.25424800 | H | -1.05348100 | -2.27644600 | -0.09154100 |
| H | 4.86883600 | 1.43808900 | -0.32950400 | O | 0.32612500 | -0.74716200 | 1.94883700 |
| C | 4.26949200 | -1.64296200 | 0.91153500 | O | -0.52359700 | -0.45729800 | 2.33924100 |
| H | 4.73437600 | -2.62032800 | 0.99288700 | H | -1.11844200 | -1.15042200 | 2.02219300 |
| O | -1.02283800 | -1.05673000 | -1.13959000 | H | 1.97571700 | 1.99356600 | -0.57012900 |
| O | 1.18849400 | -0.01841200 | 1.88905600 | H | 1.73108700 | 0.76671300 | 2.07295700 |
| S | -6.78048200 | -0.73656600 | 0.17635900 | H | -1.55118100 | 1.61368800 | 1.07139800 |
| S | 6.56115300 | -0.91253200 | -0.43591500 | H | -3.17728000 | 2.79764300 | -0.34522600 |
| O | 6.41002400 | -2.09271600 | -1.33230100 | Pd | -0.08611700 | 0.45522700 | -0.59376900 |
| O | 7.44479900 | -1.19276000 | 0.73150400 | H | 3.66879800 | -3.25020600 | 0.45559900 |
| O | 6.93201300 | 0.33197100 | -1.16277400 | H | -3.24395400 | -2.64794800 | -1.16117300 |
| O | -7.21947700 | 0.65586700 | -0.12308700 | O | 1.14986400 | -1.01431300 | -1.47226400 |
| O | -6.84444800 | -1.06338600 | 1.63166700 | H | 0.57355900 | -1.57528300 | -2.00704400 |

H 1.37595900 -1.51463400 -0.64263600

56

RR_ID1_TS2-trigo_R, E(SCF) = -
2485.34044339, E(ZPE) = -2484.923608, E(G)
= -2484.990778 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.57055900 | 3.13912500 | -0.23782200 |
| H | 0.40955600 | 3.46011700 | 0.79475200 |
| H | 1.13444800 | 3.92039000 | -0.75628500 |
| C | -0.72354900 | 2.84519300 | -0.93725200 |
| H | -1.38062100 | 3.71689500 | -0.96439800 |
| H | -0.51486100 | 2.55629500 | -1.97168400 |
| N | -1.41490500 | 1.68747200 | -0.29979700 |
| N | 1.33964400 | 1.87945700 | -0.19920400 |
| C | -2.35451700 | 1.09839200 | -1.30962500 |
| H | -2.91585400 | 1.93951200 | -1.73360900 |
| C | 2.59865600 | 1.97365700 | 0.56646500 |
| H | 2.31552600 | 2.24261500 | 1.59030500 |
| C | -3.31446400 | 0.06857900 | -0.82257400 |
| C | -2.91895600 | -1.29145600 | -0.74922200 |
| C | -4.62620000 | 0.43062700 | -0.54002500 |
| C | -3.91110000 | -2.23541100 | -0.39868100 |
| C | -5.56814000 | -0.51276500 | -0.17502600 |
| H | -4.92434300 | 1.47310000 | -0.60901500 |
| C | -5.20308400 | -1.85514000 | -0.11747500 |
| H | -5.94253800 | -2.60166600 | 0.15700400 |
| C | 3.39221400 | 0.70847000 | 0.52750200 |
| C | 2.83304800 | -0.51105300 | 0.96140000 |
| C | 4.72084800 | 0.74663300 | 0.12146700 |
| C | 3.66462700 | -1.64372900 | 1.00571000 |
| C | 5.51668300 | -0.38060600 | 0.16108600 |
| H | 5.15042100 | 1.68243100 | -0.22178000 |
| C | 4.98260400 | -1.58085500 | 0.61451200 |
| H | 5.60365600 | -2.47007200 | 0.65462500 |
| O | -1.67894800 | -1.64959800 | -0.92483500 |
| O | 1.57613700 | -0.64852200 | 1.34802200 |
| S | -7.26223400 | -0.05095700 | 0.17573600 |
| S | 7.22735400 | -0.32886100 | -0.38026300 |
| O | 7.31225400 | -1.25748900 | -1.54336600 |
| O | 8.03509100 | -0.79954500 | 0.78079100 |
| O | 7.49952300 | 1.08854500 | -0.74547600 |
| O | -7.31258300 | 1.43593300 | 0.09191100 |
| O | -7.55534000 | -0.56582700 | 1.54523900 |
| O | -8.09708700 | -0.71859900 | -0.86582800 |
| H | -0.10872600 | -2.69967800 | -0.66628700 |
| H | -0.20567900 | 2.09156600 | 3.00906000 |
| H | -0.40036100 | 2.60449600 | 3.52055600 |
| O | 0.83366100 | -2.87501700 | -0.49993600 |
| H | 1.07248700 | -2.25427800 | 0.20693200 |
| H | -0.28608900 | -0.79518600 | -1.89971400 |
| O | 0.56903400 | -0.52067000 | -2.28954000 |
| H | 1.15514600 | -1.21239200 | -1.95334100 |
| H | -1.97283600 | 2.02798800 | 0.48416400 |
| H | -1.72609800 | 0.69579800 | -2.10729500 |
| H | 1.53208400 | 1.55178400 | -1.15116700 |
| H | 3.19531300 | 2.79775500 | 0.16142900 |
| Pd | 0.08784700 | 0.49411600 | 0.58666000 |
| H | -3.61743500 | -3.27907500 | -0.34660200 |
| H | 3.23516900 | -2.57654200 | 1.35589400 |
| O | -1.15314900 | -0.93317000 | 1.52962900 |
| H | -0.58146700 | -1.46530500 | 2.09777500 |
| H | -1.36705200 | -1.47360300 | 0.72270800 |

56

RR_ID1_TS2-trigo, E(SCF) = -2485.32088761,
E(ZPE) = -2484.907196, E(G) = -2484.974256
a.u.

| | | | |
|---|-------------|------------|-------------|
| C | 0.60585700 | 3.53131600 | -0.66946300 |
| H | 0.49342300 | 4.09041100 | 0.26652500 |
| H | 1.23006600 | 4.12668600 | -1.34558000 |
| C | -0.72032400 | 3.21121200 | -1.30839700 |
| H | -1.34206400 | 4.09985000 | -1.42478500 |
| H | -0.53861700 | 2.80051600 | -2.30295600 |
| N | -1.44586300 | 2.15514000 | -0.52866700 |
| N | 1.25459100 | 2.24792200 | -0.36032900 |
| C | -2.20843600 | 1.28885600 | -1.48854600 |
| H | -2.92043900 | 1.94161500 | -2.00126800 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.58882600 | 2.36150000 | 0.25218300 |
| H | 2.47988400 | 2.97588800 | 1.15150800 |
| C | -2.90834900 | 0.11376600 | -0.91090700 |
| C | -2.17839500 | -1.08919700 | -0.71523500 |
| C | -4.27784800 | 0.15211100 | -0.67551600 |
| C | -2.91689000 | -2.22518000 | -0.30379900 |
| C | -4.96551000 | -0.97125300 | -0.25192100 |
| H | -4.82780300 | 1.07355900 | -0.84453400 |
| C | -4.27263900 | -2.16623700 | -0.07573100 |
| H | -4.80587600 | -3.05615200 | 0.24637100 |
| C | 3.15149700 | 1.01836700 | 0.57087600 |
| C | 2.47781000 | 0.20245900 | 1.50785600 |
| C | 4.30517300 | 0.55317000 | -0.03780100 |
| C | 3.03765400 | -1.03860400 | 1.84508400 |
| C | 4.83589200 | -0.68238300 | 0.29460800 |
| H | 4.81384200 | 1.16772400 | -0.77429500 |
| C | 4.20426600 | -1.47444500 | 1.24502900 |
| H | 4.62605400 | -2.43746000 | 1.51385900 |
| O | -0.89305500 | -1.13713200 | -0.87023000 |
| O | 1.35324500 | 0.59228500 | 2.08423400 |
| S | -6.72905100 | -0.92400700 | 0.05199200 |
| S | 6.29053800 | -1.31338600 | -0.54673400 |
| O | 5.81008000 | -2.46714000 | -1.39613500 |
| O | 7.23242400 | -1.73002700 | 0.53116400 |
| O | 6.80401200 | -0.18860700 | -1.37268700 |
| O | -7.17129000 | 0.45546100 | -0.29519800 |
| O | -6.91169400 | -1.24244000 | -1.49831900 |
| O | -7.32577400 | -1.96485500 | -0.83202600 |
| H | 0.71949200 | -2.07912200 | -0.86030000 |
| H | -1.17039700 | 1.78048600 | 2.57228800 |
| H | -1.45767600 | 1.07681800 | 2.48817800 |
| O | 1.66593600 | -2.25605800 | -1.01991600 |
| H | 2.11012000 | -2.02645400 | -0.19140500 |
| H | 0.20235800 | -0.18317500 | -1.89552700 |
| O | 0.99457800 | 0.21443500 | -2.33043700 |
| H | 1.65715900 | -0.47337800 | -2.16282700 |
| H | -2.13043600 | 2.60967000 | 0.07471900 |
| H | -1.47915000 | 0.95241900 | -2.22887400 |
| H | 1.30466000 | 1.63759600 | -1.20267400 |
| H | 3.24744000 | 2.89192100 | -0.44236600 |
| Pd | -0.09572700 | 1.27561700 | 0.83920000 |
| H | -2.37141700 | -3.15638000 | -0.16059900 |
| H | 2.53484400 | -1.64960600 | 2.58564200 |
| O | -0.76566900 | -1.07625400 | -1.91471800 |
| H | 0.12100900 | -0.85925000 | 2.25248700 |
| H | -0.63175900 | -1.31659000 | 0.97768800 |

56

RR_ID1_TS3-diamond_P, E(SCF) = -
2485.37076044, E(ZPE) = -2484.951163, E(G)
= -2485.019382 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.49904000 | -2.42475900 | 2.01469800 |
| H | 0.17599000 | -3.14155200 | 1.25220100 |
| H | 1.05977000 | -2.98280000 | 2.77201900 |
| C | -0.69977100 | -1.74734600 | 2.62745300 |
| H | -1.32342500 | -2.46266600 | 3.17323900 |
| H | -0.37826100 | -0.97630500 | 3.33511000 |
| N | -1.49382300 | -1.07149200 | 1.57020400 |
| N | 1.32891400 | -1.41105700 | 1.35108400 |
| C | -2.60516200 | -0.28448000 | 2.16349500 |
| H | -3.16492200 | -0.94204700 | 2.84038900 |
| C | 2.26870900 | -1.94338500 | 0.35750700 |
| H | 1.65933400 | -2.41810400 | -0.42173800 |
| C | -3.51148800 | 0.25958900 | 1.10994300 |
| C | -3.43935300 | 1.59863900 | 0.70886000 |
| C | -4.39244000 | -0.58605500 | 0.45663400 |
| C | -4.22912500 | 2.05163400 | -0.34237200 |
| C | -5.17268900 | -0.13473900 | -0.59630100 |
| H | -4.46575700 | -1.62426300 | 0.77301800 |
| C | -5.08505200 | 1.18515600 | -0.99983800 |
| H | -5.69962400 | 1.53333300 | -1.82153800 |
| C | 3.14530400 | -0.87364100 | -0.22130200 |
| C | 2.62117000 | 0.27117800 | -0.87817400 |
| C | 4.52014600 | -1.04480500 | -0.15777800 |
| C | 3.53919200 | 1.15529300 | -1.47422500 |
| C | 5.40272700 | -0.14791700 | -0.73817000 |
| H | 4.91345000 | -1.92026300 | 0.35313500 |

| | | | |
|----|-------------|-------------|-------------|
| C | 4.90236800 | 0.95679400 | -1.40659000 |
| H | 5.58690400 | 1.65583900 | -1.87323300 |
| O | -2.60895000 | 2.42757800 | 1.37176700 |
| O | 1.33945800 | 0.55667300 | -1.00141400 |
| S | -6.29038500 | -1.28501500 | -1.41062600 |
| S | 7.16565900 | -0.44535900 | -0.60997500 |
| O | 7.82433600 | 0.66266300 | -1.35613700 |
| O | 7.40222100 | -1.78323400 | -1.22569900 |
| O | 7.48083000 | -0.43279200 | 0.84798300 |
| O | -7.22025800 | -1.76026600 | -0.34811800 |
| O | -5.42504400 | -2.37598500 | -1.94098300 |
| O | -6.97037000 | -0.50377300 | -2.47824800 |
| H | 1.75797000 | 3.60955800 | -0.40082700 |
| O | 0.96191500 | 3.10943700 | -0.20326400 |
| H | 1.08513000 | 2.21198200 | -0.59998300 |
| H | -0.81637200 | 2.31023200 | 2.20781800 |
| O | 0.09104400 | 2.51682100 | 2.47393300 |
| H | 0.53162600 | 2.69606500 | 1.62655000 |
| H | -1.91502700 | -1.79596800 | 0.98679000 |
| H | -2.16388200 | 0.50978300 | 2.76607600 |
| H | 1.84146400 | -0.87447900 | 2.04815700 |
| H | 2.89734400 | -2.72782500 | 0.79784000 |
| Pd | -0.10512600 | -0.18348600 | 0.27015200 |
| O | -1.51647200 | 4.30050500 | -0.18306100 |
| H | -0.61993500 | 3.92681800 | -0.31439800 |
| H | -2.36379000 | 3.19872000 | 0.80216700 |
| H | -4.17201800 | 3.09354100 | -0.63852200 |
| H | 3.13801500 | 2.01075400 | -2.00892100 |
| H | -1.18487900 | 0.60144700 | -0.54102400 |
| H | -1.84450400 | 4.52205500 | -1.05781700 |

56
RR_ID1_TS3-diamond, E(SCF) = -
2485.32714804, E(ZPE) = -2484.912246, E(G)
= -2484.978706 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.46785300 | -2.11839800 | 2.15068600 |
| H | 0.18321200 | -2.92022900 | 1.46311600 |
| H | 1.05088400 | -2.56224000 | 2.96183200 |
| C | -0.74947900 | -1.40866700 | 2.66454100 |
| H | -1.39652900 | -2.08267200 | 3.23280300 |
| H | -0.46687300 | -0.58077000 | 3.32220400 |
| N | -1.49388200 | -0.82367900 | 1.52093700 |
| N | 1.28188200 | -1.14971100 | 1.38776300 |
| C | -2.61096600 | 0.03209000 | 2.02338800 |
| H | -3.12887800 | -0.55499800 | 2.79267500 |
| C | 2.28998800 | -1.79529100 | 0.52438300 |
| H | 1.73157200 | -2.37300400 | -0.22090300 |
| C | -3.56559500 | 0.44771300 | 0.95911300 |
| C | -3.56208100 | 1.79044300 | 0.48211500 |
| C | -4.45755800 | -0.47802400 | 0.44346500 |
| C | -4.47254100 | 2.09080800 | -0.55836200 |
| C | -5.34275000 | -0.14525900 | -0.57065500 |
| H | -4.46212600 | -1.49121800 | 0.84336200 |
| C | -5.34161200 | 1.15050000 | -1.07026000 |
| H | -6.03006900 | 1.41154600 | -1.86647800 |
| C | 3.21778900 | -0.81563000 | -0.11898600 |
| C | 2.74411700 | 0.30436700 | -0.83751600 |
| C | 4.58366600 | -1.04958400 | -0.05308500 |
| C | 3.68653900 | 1.11934000 | -1.48552700 |
| C | 5.49627500 | -0.22597000 | -0.68960300 |
| H | 4.94217200 | -1.90653400 | 0.51098900 |
| C | 5.03971000 | 0.86182600 | -1.41528600 |
| H | 5.75060800 | 1.50573400 | -1.91981700 |
| O | -2.75201700 | 2.69020700 | 0.94145400 |
| O | 1.47105300 | 0.65431900 | -0.94927100 |
| S | -6.47171100 | -1.38818600 | -1.18986500 |
| S | 7.24842300 | -0.59408400 | -0.55752700 |
| O | 7.94890500 | 0.48151700 | -1.31117200 |
| O | 7.42787900 | -1.94423400 | -1.16350400 |
| O | 7.55719300 | -0.58206700 | 0.90077500 |
| O | -7.31292100 | -1.80182600 | -0.02784900 |
| O | -5.62217200 | -2.50885200 | -1.69138900 |
| O | -7.25995800 | -0.73157300 | -2.27073200 |
| H | 2.09066100 | 3.75010500 | -0.04191900 |
| O | 1.32973200 | 3.18026900 | 0.09472300 |
| H | 1.54112900 | 2.30904000 | -0.30442200 |
| H | -1.23044600 | 2.66664500 | 1.93933900 |

| | | | |
|----|-------------|-------------|-------------|
| O | -0.37445600 | 2.72087500 | 2.41034900 |
| H | 0.28053100 | 2.87349900 | 1.71269900 |
| H | -1.90832100 | -1.58724600 | 0.98308200 |
| H | -2.15409200 | 0.89565100 | 2.50717500 |
| H | 1.75015300 | -0.51287400 | 2.03329800 |
| H | 2.86839100 | -2.50840200 | 1.12187200 |
| Pd | -0.04147800 | -0.05019400 | 0.22543700 |
| O | -1.11093800 | 2.80341400 | -1.03775000 |
| H | -0.25884300 | 3.19276000 | -0.74987100 |
| H | -1.77017000 | 2.98761700 | -0.29898400 |
| H | -4.47230300 | 3.10600100 | -0.94465600 |
| H | 3.31640200 | 1.96675700 | -2.05380300 |
| H | -1.21435300 | 0.54150700 | -0.82733300 |
| H | -1.00665100 | 1.45429700 | -0.82454100 |

56
RR_ID1_TS3-diamond, E(SCF) = -
2485.32714804, E(ZPE) = -2484.912246, E(G)
= -2484.978706 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.46785300 | -2.11839800 | 2.15068600 |
| H | 0.18321200 | -2.92022900 | 1.46311600 |
| H | 1.05088400 | -2.56224000 | 2.96183200 |
| C | -0.74947900 | -1.40866700 | 2.66454100 |
| H | -1.39652900 | -2.08267200 | 3.23280300 |
| H | -0.46687300 | -0.58077000 | 3.32220400 |
| N | -1.49388200 | -0.82367900 | 1.52093700 |
| N | 1.28188200 | -1.14971100 | 1.38776300 |
| C | -2.61096600 | 0.03209000 | 2.02338800 |
| H | -3.12887800 | -0.55499800 | 2.79267500 |
| C | 2.28998800 | -1.79529100 | 0.52438300 |
| H | 1.73157200 | -2.37300400 | -0.22090300 |
| C | -3.56559500 | 0.44771300 | 0.95911300 |
| C | -3.56208100 | 1.79044300 | 0.48211500 |
| C | -4.45755800 | -0.47802400 | 0.44346500 |
| C | -4.47254100 | 2.09080800 | -0.55836200 |
| C | -5.34275000 | -0.14525900 | -0.57065500 |
| H | -4.46212600 | -1.49121800 | 0.84336200 |
| C | -5.34161200 | 1.15050000 | -1.07026000 |
| H | -6.03006900 | 1.41154600 | -1.86647800 |
| C | 3.21778900 | -0.81563000 | -0.11898600 |
| C | 2.74411700 | 0.30436700 | -0.83751600 |
| C | 4.58366600 | -1.04958400 | -0.05308500 |
| C | 3.68653900 | 1.11934000 | -1.48552700 |
| C | 5.49627500 | -0.22597000 | -0.68960300 |
| H | 4.94217200 | -1.90653400 | 0.51098900 |
| C | 5.03971000 | 0.86182600 | -1.41528600 |
| H | 5.75060800 | 1.50573400 | -1.91981700 |
| O | -2.75201700 | 2.69020700 | 0.94145400 |
| O | 1.47105300 | 0.65431900 | -0.94927100 |
| S | -6.47171100 | -1.38818600 | -1.18986500 |
| S | 7.24842300 | -0.59408400 | -0.55752700 |
| O | 7.94890500 | 0.48151700 | -1.31117200 |
| O | 7.42787900 | -1.94423400 | -1.16350400 |
| O | 7.55719300 | -0.58206700 | 0.90077500 |
| O | -7.31292100 | -1.80182600 | -0.02784900 |
| O | -5.62217200 | -2.50885200 | -1.69138900 |
| O | -7.25995800 | -0.73157300 | -2.27073200 |
| H | 2.09066100 | 3.75010500 | -0.04191900 |
| O | 1.32973200 | 3.18026900 | 0.09472300 |
| H | 1.54112900 | 2.30904000 | -0.30442200 |
| H | -1.23044600 | 2.66664500 | 1.93933900 |

56

RR_ID1_TS3-trigo_P, E(SCF) = -
 2485.37320671, E(ZPE) = -2484.953594, E(G)
 = -2485.019784 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.44164100 | 3.44320400 | 0.03456200 |
| H | 0.16764600 | 3.69177500 | 1.06548100 |
| H | 1.06349700 | 4.26225500 | -0.34827300 |
| C | -0.78686800 | 3.28061900 | -0.82534000 |
| H | -1.37786000 | 4.19937200 | -0.86161900 |
| H | -0.47302100 | 3.05184100 | -1.84766300 |
| N | -1.62507700 | 2.13616400 | -0.36217400 |
| N | 1.15829600 | 2.16678300 | 0.05279500 |
| C | -2.46520100 | 1.63049000 | -1.48658500 |
| H | -3.17672100 | 2.41435300 | -1.76961900 |
| C | 2.26736200 | 2.08899900 | 1.00066800 |
| H | 1.84883100 | 2.29045900 | 1.99517300 |
| C | -3.18407200 | 0.37105000 | -1.14571000 |
| C | -2.56672700 | -0.86626200 | -1.33801500 |
| C | -4.44142300 | 0.41057300 | -0.55885700 |
| C | -3.20541900 | -2.05419300 | -0.93889300 |
| C | -5.07036900 | -0.75134100 | -0.15205500 |
| H | -4.93264300 | 1.36613500 | -0.40292000 |
| C | -4.44797500 | -1.97747000 | -0.33847400 |
| H | -4.94177800 | -2.89028300 | -0.02227600 |
| C | 2.93218600 | 0.74578900 | 0.96872900 |
| C | 2.24126100 | -0.44085800 | 1.32019800 |
| C | 4.26527300 | 0.66612400 | 0.58878500 |
| C | 2.99169500 | -1.63055200 | 1.40895000 |
| C | 4.95942400 | -0.53140000 | 0.60443800 |
| H | 4.78364500 | 1.56958300 | 0.28189700 |
| C | 4.31707700 | -1.68449900 | 1.03947300 |
| H | 4.85874000 | -2.62397100 | 1.08194700 |
| O | -1.34133000 | -0.90682900 | -1.91726300 |
| O | 0.95084600 | -0.51518000 | 1.57677100 |
| S | -6.69616500 | -0.70352800 | 0.61885500 |
| S | 6.61406000 | -0.64800400 | -0.07083900 |
| O | 7.38387500 | -1.52489400 | 0.85552200 |
| O | 7.13940200 | 0.74368100 | -0.13378800 |
| O | 6.43687700 | -1.26254100 | -1.42062300 |
| O | -7.08159500 | 0.73246300 | 0.66890200 |
| O | -6.51491800 | -1.31115200 | 1.96670800 |
| O | -7.57985200 | -1.51739600 | -0.26173300 |
| H | 1.99457800 | -2.01257900 | -1.34239000 |
| H | -1.55295200 | -0.12585200 | 1.15671800 |
| H | 0.21981700 | -3.28594400 | -0.09692400 |
| O | 2.67321100 | -1.60842700 | -1.91322800 |
| H | 3.42651400 | -1.44985100 | -1.32974100 |
| H | 0.27503700 | 0.29145400 | -2.33679800 |
| O | 1.14158400 | 0.67958400 | -2.52948300 |
| H | 1.76115500 | -0.06380100 | -2.39468000 |
| H | -2.25664100 | 2.47064700 | 0.36433100 |
| H | -1.79872700 | 1.471139200 | -2.33510800 |
| H | 1.44847800 | 1.88896900 | -0.89136900 |
| H | 3.01369200 | 2.86925300 | 0.80039900 |
| Pd | -0.37400000 | 0.77690500 | 0.65236100 |
| H | -2.71283400 | -2.98921200 | -1.09895400 |
| H | 2.47408600 | -2.52857500 | 1.73059400 |
| O | 0.35921900 | -2.38298000 | -0.39626800 |
| H | 0.44232000 | -1.82565500 | 0.41278900 |
| H | -0.79548400 | -1.59816200 | -1.47759200 |

56
 RR_ID1_TS3-trigo_R, E(SCF) = -
 2485.33698702, E(ZPE) = -2484.920884, E(G)
 = -2484.987754 a.u.

| | | | |
|---|-------------|------------|-------------|
| C | 0.55913800 | 3.54748700 | -0.18732100 |
| H | 0.38298800 | 3.94170100 | 0.81665500 |
| H | 1.21395100 | 4.24553700 | -0.71841900 |
| C | -0.72410800 | 3.33009000 | -0.94106500 |
| H | -1.33489600 | 4.23307400 | -0.97777700 |
| H | -0.49190700 | 3.04488400 | -1.96981100 |
| N | -1.49718900 | 2.20020700 | -0.33599800 |
| N | 1.21020600 | 2.22979500 | -0.05364100 |
| C | -2.28215700 | 1.48505300 | -1.39720000 |
| H | -2.98912000 | 2.21258800 | -1.81117900 |
| C | 2.48893600 | 2.23964900 | 0.67897300 |
| H | 2.27978000 | 2.62812500 | 1.68144600 |
| C | -2.99675000 | 0.26004400 | -0.94685200 |

| | | | |
|----|-------------|-------------|-------------|
| C | -2.29630000 | -0.97876400 | -0.90547700 |
| C | -4.34835000 | 0.31632200 | -0.63323300 |
| C | -3.04980200 | -2.12267600 | -0.54706100 |
| C | -5.04919400 | -0.81908000 | -0.27278700 |
| H | -4.87256800 | 1.26688300 | -0.68049500 |
| C | -4.38670700 | -2.04373200 | -0.23315800 |
| H | -4.93181100 | -2.94234600 | 0.04076400 |
| C | 3.09089300 | 0.87417800 | 0.72736400 |
| C | 2.39123200 | -0.17466100 | 1.35706500 |
| C | 4.33840300 | 0.63388800 | 0.17025900 |
| C | 3.01869200 | -1.42866000 | 1.45392900 |
| C | 4.92893500 | -0.61363700 | 0.25436500 |
| H | 4.86861700 | 1.43755200 | -0.33059500 |
| C | 4.26931600 | -1.64269700 | 0.91246600 |
| H | 4.73413700 | -2.62050600 | 0.94280000 |
| O | -1.02263400 | -1.05670000 | -1.13989100 |
| O | 1.18876100 | -0.01713900 | 1.88987300 |
| S | -6.78025000 | -0.73718800 | 0.17638200 |
| S | 6.56065300 | -0.91335900 | -0.43613300 |
| O | 7.44453900 | -1.19344600 | 0.73113200 |
| O | 6.93163200 | 0.33080600 | -1.16350000 |
| O | 6.40900200 | -2.09378400 | -1.33211100 |
| O | -7.21956000 | 0.65502300 | -0.12364000 |
| O | -6.84394600 | -1.06333000 | 1.63185900 |
| O | -7.47579100 | -1.75930500 | -0.65856300 |
| H | 0.59299500 | -2.04913100 | -1.47295200 |
| H | -1.44719400 | 0.43590600 | 1.95956800 |
| H | -1.46401200 | -0.11888100 | 1.36985800 |
| O | 1.55125700 | -2.17208200 | -1.59997600 |
| H | 1.90497000 | -2.21644800 | -0.70287000 |
| H | 0.13238800 | 0.06516600 | -1.95767500 |
| O | 0.93218700 | 0.51587000 | -2.31147600 |
| H | 1.57558800 | -0.20931800 | -2.27917100 |
| H | -2.16068000 | 2.58125300 | 0.33788600 |
| H | -1.56737600 | 1.23878700 | -2.18452000 |
| H | 1.32880700 | 1.77733000 | -0.98037300 |
| H | 3.17375400 | 2.93603500 | 0.18355200 |
| Pd | -0.19072500 | 1.04334000 | 0.83002200 |
| H | -2.53589500 | -3.07879200 | -0.52330600 |
| H | 2.49656500 | -2.23010600 | 1.96513800 |
| O | -0.16350100 | -2.46415100 | 1.20321900 |
| H | 0.31056300 | -1.72751700 | 1.62277500 |
| H | -0.47245100 | -2.07807800 | 0.36269400 |

56
 RR_ID1_TS3-trigo, E(SCF) = -2485.32330780,
 E(ZPE) = -2484.908574, E(G) = -2484.973485
 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.56981400 | 3.54361600 | -0.55910500 |
| H | 0.45254500 | 4.07179000 | 0.39117000 |
| H | 1.17039200 | 4.17450100 | -1.22404700 |
| C | -0.76344800 | 3.22741200 | -1.18997700 |
| H | -1.39861000 | 4.11174800 | -1.25064900 |
| H | -0.59986900 | 2.87262900 | -2.21032000 |
| N | -1.46904000 | 2.12906400 | -0.44953000 |
| N | 1.24369700 | 2.26627900 | -0.28515300 |
| C | -2.12060900 | 1.20217400 | -1.43552100 |
| H | -2.79252100 | 1.81539600 | -2.04742800 |
| C | 2.55870000 | 2.37167000 | 0.36396400 |
| H | 2.41060000 | 2.91595400 | 1.30331200 |
| C | -2.87485700 | 0.05505500 | -0.85742600 |
| C | -2.21451400 | -1.16330600 | -0.54471900 |
| C | -4.25293700 | 0.15834100 | -0.70923200 |
| C | -3.02192000 | -2.22907600 | -0.08557800 |
| C | -5.01173300 | -0.89886000 | -0.24501500 |
| H | -4.75055600 | 1.08912500 | -0.96709300 |
| C | -4.38486600 | -2.10322100 | 0.05851200 |
| H | -4.97368200 | -2.94303000 | 0.41526000 |
| C | 3.14021600 | 1.01498900 | 0.60611200 |
| C | 2.49001100 | 0.11702200 | 1.47987300 |
| C | 4.31068500 | 0.62735200 | -0.02880400 |
| C | 3.11493300 | -1.11504900 | 1.74787600 |
| C | 4.88652500 | -0.60700300 | 0.21528100 |
| H | 4.79437900 | 1.30764000 | -0.72260900 |
| C | 4.29167700 | -1.47356200 | 1.12227700 |
| H | 4.74798400 | -2.43535300 | 1.33419100 |
| O | -0.91830400 | -1.29755300 | -0.62069100 |

| | | | |
|----|-------------|-------------|-------------|
| O | 1.33899200 | 0.38858100 | 2.06948900 |
| S | -6.79184900 | -0.77016800 | -0.09306400 |
| S | 6.36187200 | -1.13541100 | -0.66066200 |
| O | 7.34485800 | -1.51881800 | 0.39166300 |
| O | 6.79970500 | 0.03256300 | -1.47249900 |
| O | 5.93520300 | -2.29708600 | -1.49228100 |
| O | -7.13133300 | 0.65037900 | -0.38804300 |
| O | -7.11677300 | -1.16685800 | 1.30780000 |
| O | -7.35983100 | -1.72142700 | -1.09292100 |
| H | 0.73429400 | -2.29699100 | -0.82995400 |
| H | -1.36277000 | 0.65073200 | 1.86811500 |
| H | -1.02252900 | -0.30001100 | 1.89854100 |
| O | 1.68018400 | -2.44919500 | -1.00084000 |
| H | 2.12999000 | -2.18626800 | -0.18719800 |
| H | 0.22809000 | -0.32393800 | -1.64927200 |
| O | 0.96089000 | 0.08295200 | -2.16287700 |
| H | 1.64821200 | -0.59317500 | -2.07628500 |
| H | -2.20495900 | 2.53580800 | 0.12467900 |
| H | -1.32259700 | 0.84809400 | -2.08960600 |
| H | 1.32107500 | 1.68704300 | -1.13696000 |
| H | 3.23367500 | 2.96397300 | -0.26442500 |
| Pd | -0.12379900 | 1.24970800 | 0.88710700 |
| H | -2.52775100 | -3.16644600 | 0.15299300 |
| H | 2.64487400 | -1.78736900 | 2.45938500 |
| O | -0.59043000 | -1.48853100 | 1.99285100 |
| H | 0.32353100 | -1.20190200 | 2.21548800 |
| H | -0.58333000 | -1.66003000 | 1.00386200 |

54

RR_ID2_TS1_Ntrigo-square_P, E(SCF) = -
2484.17714902, E(ZPE) = -2483.775953, E(G)
= -2483.841823 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.16385200 | 1.76780000 | 1.20979000 |
| H | -0.03065100 | 1.16608900 | 2.10260600 |
| H | 0.45094700 | 2.77248400 | 1.53033600 |
| C | -1.03802000 | 1.78827000 | 0.30466300 |
| H | -1.91385600 | 2.22487600 | 0.79430500 |
| H | -0.82494600 | 2.37463100 | -0.59305400 |
| N | -1.31518500 | 0.39839600 | -0.12382600 |
| C | -2.36185000 | 0.29518000 | -1.19047400 |
| H | -2.00579600 | -0.42162000 | -1.93407500 |
| C | -3.67835300 | -0.11920400 | -0.62668200 |
| C | -3.78282200 | -1.42634500 | -0.07876800 |
| C | -4.76425100 | 0.74304000 | -0.61683000 |
| C | -5.03926400 | -1.79881200 | 0.45040200 |
| C | -5.98030200 | 0.34715800 | -0.08707400 |
| H | -4.66602700 | 1.74320900 | -1.02957600 |
| C | -6.10977700 | -0.93297100 | 0.44481600 |
| H | -5.13641700 | -2.79653300 | 0.86693600 |
| H | -7.06223900 | -1.24743100 | 0.86147300 |
| O | -2.76673700 | -2.23483400 | -0.04606000 |
| S | -7.39511100 | 1.44346300 | -0.08525600 |
| O | -7.83932600 | 1.54343700 | 1.33594900 |
| O | -8.42591900 | 0.79617400 | -0.94967000 |
| O | -6.91375400 | 2.74259700 | -0.63470500 |
| H | -2.43006300 | 1.26559400 | -1.68555900 |
| H | -1.64793800 | -0.12687800 | 0.69005500 |
| O | -0.39582200 | -2.30439900 | -1.15293800 |
| H | -1.35208700 | -2.28689700 | -0.84379100 |
| H | -1.87152600 | -2.23965500 | 1.44464300 |
| O | -1.19144600 | -2.06094200 | 2.13632300 |
| H | -1.61500800 | -2.23213800 | 2.98065800 |
| H | 0.02962800 | -3.00428000 | -0.60930300 |
| H | 0.29554300 | -3.11126800 | 1.51633000 |
| O | 0.89554000 | -3.59306200 | 0.91622100 |
| H | 1.59883000 | -2.95674000 | 0.69814600 |
| Pd | 0.49717700 | -0.55160700 | -0.40096700 |
| N | 1.27396700 | -1.11923900 | 0.47152600 |
| C | 2.43712900 | 0.76696100 | 1.31735900 |
| H | 2.74794400 | 1.65147800 | 1.88341700 |
| C | 3.57709400 | 0.25602900 | 0.49798600 |
| C | 3.41838200 | -0.88469900 | -0.31811100 |
| C | 4.81488100 | 0.88182500 | 0.57340500 |
| C | 4.54350800 | -1.36412100 | -1.01078900 |
| C | 5.90607000 | 0.39686900 | -0.12119500 |
| H | 4.93358300 | 1.76366200 | 1.19440700 |
| C | 5.76698200 | -0.74078500 | -0.90819200 |

54

RR_ID2_TS1_Ntrigo-square_R, E(SCF) = -
2484.19017966, E(ZPE) = -2483.790938, E(G)
= -2483.858412 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.66548600 | 3.09015200 | 0.19345300 |
| H | 0.39364400 | 3.04602500 | 1.25221000 |
| H | 1.27192900 | 3.98384700 | 0.02755400 |
| C | -0.57624600 | 3.07917500 | -0.66283700 |
| H | -1.20586600 | 3.95286200 | -0.47199500 |
| H | -0.31816800 | 3.07174700 | -1.72613000 |
| N | -1.30553300 | 1.83194200 | -0.36163800 |
| C | -2.41659500 | 1.50929500 | -1.27086500 |
| H | -1.97404500 | 1.27509100 | -2.24584200 |
| C | -3.24253600 | 0.38029900 | -0.73477000 |
| C | -2.66252700 | -0.84642700 | -0.34470000 |
| C | -4.61909700 | 0.54422300 | -0.63041100 |
| C | -3.51631000 | -1.86433800 | 0.11902700 |
| C | -5.43851300 | -0.46960800 | -0.17438500 |
| H | -5.06687300 | 1.49038500 | -0.91717400 |
| C | -4.87853300 | -1.68594800 | 0.19747300 |
| H | -3.06183700 | -2.80579700 | 0.41417900 |
| H | -5.51197800 | -2.48885300 | 0.56117000 |
| O | -1.36785200 | -1.10991700 | -0.38735300 |
| S | -7.21506600 | -0.24664700 | -0.05625100 |
| O | -7.56710300 | -0.53595800 | -1.03628400 |
| O | -7.81178300 | -1.23454400 | -1.00051800 |
| O | -7.48053100 | 1.16566400 | -0.44624200 |
| H | -3.04936600 | 2.39451500 | -1.40063600 |
| H | -1.64089100 | 1.85706100 | 0.61401900 |
| O | 0.13435600 | -3.47796000 | -0.48556200 |
| H | -0.62640700 | -2.88710400 | -0.59961700 |
| H | -1.08114700 | 0.44793800 | 2.56192300 |
| O | -1.43288900 | 1.35723800 | 2.49568800 |
| H | -2.10750200 | 1.42485000 | 3.17537400 |
| H | 0.81179000 | -2.82447500 | -0.23872100 |
| H | -0.93247600 | -1.52238800 | 1.52784000 |
| O | -0.43885400 | -1.33527000 | 2.34500800 |
| H | 0.46773400 | -1.28704400 | 2.00345400 |
| Pd | 0.07886000 | 0.33862400 | -0.25877900 |
| N | 1.44066700 | 1.86486900 | -0.11293600 |
| C | 2.49238100 | 1.53494800 | 0.87288200 |
| H | 3.10886400 | 2.42120500 | 1.05825900 |
| C | 3.35231200 | 0.40901000 | 0.39294700 |
| C | 2.79310000 | -0.84386500 | 0.05670500 |
| C | 4.72782400 | 0.58963400 | 0.31186100 |
| C | 3.66817800 | -1.87404400 | -0.33093200 |
| C | 5.56779100 | -0.43729700 | -0.07217400 |
| H | 5.15718600 | 1.55432500 | 0.56285200 |
| C | 5.02955000 | -1.67950200 | -0.38770800 |
| H | 3.23719400 | -2.83637400 | -2.58742000 |
| H | 5.68189300 | -2.49234600 | -0.69128600 |
| O | 1.49984900 | -1.10508300 | 0.11468500 |
| S | 7.34456200 | -0.20234500 | -0.15627300 |
| O | 7.58691300 | 1.22958400 | 0.17238700 |
| O | 7.73639900 | -0.55520700 | -1.55088200 |
| O | 7.92556700 | -1.13791700 | 0.84903100 |
| H | 1.97347200 | 1.28833800 | 1.80709400 |
| H | 1.87724300 | 1.96640500 | -1.03048800 |

54

RR_ID2_TS1_Ntrigo-square, E(SCF) = -
2484.15584797, E(ZPE) = -2483.757585, E(G)
= -2483.825427 a.u.

| | | | |
|---|-------------|------------|-------------|
| C | 0.59002500 | 2.80376800 | 0.50130300 |
| H | 0.33769000 | 2.61142700 | 1.54821200 |
| H | 1.12199900 | 3.75630600 | 0.44324700 |
| C | -0.65657500 | 2.79206800 | -0.34753900 |

| | | | | | | | |
|----|-------------|-------------|--------------|----|-------------|-------------|-------------|
| H | -1.35749300 | 3.57489000 | -0.04301800 | C | -2.64331900 | 0.38694500 | 1.00190400 |
| H | -0.41730000 | 2.94007300 | -1.40465700 | C | -4.65251800 | -0.30862800 | -0.16552100 |
| N | -1.26498200 | 1.45638800 | -0.18997700 | C | -3.31087700 | 1.58455500 | 1.58313000 |
| C | -2.45290600 | 1.19577400 | -1.02952800 | C | -5.28166700 | 0.87811000 | 0.15994500 |
| H | -2.08938800 | 0.82874300 | -1.99649400 | H | -5.19389800 | -1.04866300 | -0.74679800 |
| C | -3.43456300 | 0.25151000 | -0.39587000 | C | -4.60148000 | 1.82615100 | 0.91690400 |
| C | -3.03596600 | -0.94335700 | 0.25579100 | H | -2.76792300 | 2.32008800 | 1.91211800 |
| C | -4.78704000 | 0.56463300 | -0.48502800 | H | -5.08911700 | 2.76016200 | 1.17912200 |
| C | -4.05328400 | -1.76726600 | 0.78204500 | O | 3.73121900 | -2.43310600 | 0.66047800 |
| C | -5.76089300 | -0.26692700 | 0.03226200 | O | -1.41783300 | 0.21589300 | 1.43762200 |
| H | -5.09292100 | 1.48616300 | -0.97116000 | S | 4.83862800 | 3.25887700 | -0.57993600 |
| C | -5.38544500 | -1.44518600 | 0.66865400 | S | -6.94685100 | 1.23032000 | -0.40152800 |
| H | -3.74452100 | -2.67950900 | 1.28230100 | O | -7.73905600 | 1.53340600 | 0.82548600 |
| H | -6.14342700 | -2.10355400 | 1.08208400 | O | -7.41343800 | 0.00377200 | -1.10671400 |
| O | -1.77914700 | -1.28938000 | 0.40374400 | O | -6.83468400 | 2.41167000 | -1.88017600 |
| S | -7.50138600 | 0.13822900 | -0.10533800 | O | 3.52537700 | 3.94554800 | -0.42924500 |
| O | -8.03722800 | 0.12204000 | 1.28673000 | O | 5.32725800 | 3.26036500 | -1.98693800 |
| O | -8.10561100 | -0.93016600 | -0.95372600 | O | 5.85996600 | 3.72561600 | 0.39564900 |
| O | -7.56583700 | 1.48852700 | -0.73811300 | H | -2.49496900 | -2.45259100 | -0.57993500 |
| H | -2.95663300 | 2.14927200 | -1.22424400 | H | 2.90158600 | -2.01940500 | -2.12997600 |
| H | -1.51151800 | 1.33521900 | 0.80231600 | H | -1.66214500 | -1.23827500 | -1.64728900 |
| O | -0.55125600 | -1.62827500 | -1.88634400 | H | 1.74226500 | -2.58045800 | -0.13264600 |
| H | -1.13146500 | -1.18482100 | -1.13380100 | O | 1.31124000 | -0.02944100 | -1.80362700 |
| H | -1.34731000 | -0.38358400 | 1.98246800 | H | 1.97855200 | -1.23972500 | 2.50396700 |
| O | -1.21740200 | 0.40608700 | 2.54405500 | H | 3.63309300 | -3.89491100 | -0.54292900 |
| H | -1.87109200 | 0.33488800 | 3.24405200 | O | 3.29433000 | -4.55942000 | -1.16375300 |
| H | 0.23357400 | -2.18482100 | -1.820851000 | H | 3.93247200 | -4.57555700 | -1.88050700 |
| H | -0.59228000 | -2.50794300 | 1.15736200 | H | 0.76415200 | 0.53953000 | 2.15698900 |
| O | 0.25417400 | -2.93129300 | 1.38345900 | H | 3.39134500 | -2.47968500 | 1.59355500 |
| H | 0.90533400 | -2.42526800 | 0.87103700 | H | 2.47815400 | -1.99892700 | 2.92802900 |
| Pd | 0.25778200 | 0.09844600 | -0.39068000 | O | 1.81383600 | -2.61206300 | 3.25011700 |
| N | 1.45948900 | 1.69574000 | 0.04449300 | Pd | -0.05519800 | -0.81589800 | 0.34955600 |
| C | 2.52325200 | 1.29789200 | 0.99054800 | | | | |
| H | 3.06208600 | 2.19381800 | 1.31763900 | | | | |
| C | 3.48686900 | 0.33400900 | 0.36929500 | | | | |
| C | 3.05605400 | -0.86778400 | -0.23648500 | | | | |
| C | 4.84763200 | 0.61416000 | 0.43364400 | | | | |
| C | 4.03473400 | -1.75033600 | -0.72735800 | | | | |
| C | 5.79050500 | -0.26806800 | -0.05411400 | | | | |
| H | 5.18311000 | 1.54161200 | 0.88673100 | | | | |
| C | 5.37634700 | -1.46295500 | -0.63171300 | | | | |
| H | 3.69429900 | -2.67328400 | -1.18378300 | | | | |
| H | 6.11155000 | -2.16249200 | -1.01700200 | | | | |
| O | 1.79186500 | -1.22811200 | -0.35534700 | | | | |
| S | 7.54397300 | 0.10385300 | 0.02991600 | | | | |
| O | 7.65408400 | 1.42203400 | 0.71365100 | | | | |
| O | 8.01895800 | 0.13780500 | -1.38305300 | | | | |
| O | 8.15802300 | -1.01004700 | 0.80735500 | | | | |
| H | 2.01521800 | 0.87702500 | 1.86567100 | | | | |
| H | 1.89211400 | 1.95529500 | -0.84383400 | | | | |

54

RR_ID2_TS1_P_Htr_TS, E(SCF) = -
2484.15575059, E(ZPE) = -2483.759551, E(G)
= -2483.826668 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.87247700 | -3.05552600 | -1.25786300 |
| H | -0.80938100 | -3.68328800 | -0.36764400 |
| H | -1.49913700 | -3.56885100 | -1.99587200 |
| C | 0.48897200 | -2.75151400 | -1.81648100 |
| H | 1.04890200 | -3.65481000 | -2.06503700 |
| H | 0.38385700 | -2.15419300 | -2.72898200 |
| N | 1.26796600 | -1.93872100 | -0.84395000 |
| N | -1.48249500 | -1.77320500 | -0.85479100 |
| C | 2.30965800 | -1.17030000 | -1.56911900 |
| H | 1.79853900 | -0.45421000 | -2.21966200 |
| C | -2.76968800 | -1.92242600 | -0.14287900 |
| H | -3.46644300 | -2.48926100 | -0.77080500 |
| C | 3.29502900 | -0.46403600 | -0.69765300 |
| C | 3.94645100 | -1.15272800 | 0.35178500 |
| C | 3.60108900 | 0.86296900 | -0.94273300 |
| C | 4.90757000 | -0.45504500 | 1.09794600 |
| C | 4.54950800 | 1.53572300 | -0.18617500 |
| H | 3.08320900 | 1.38662500 | -1.74351600 |
| C | 5.20426000 | 0.86841100 | 0.83485000 |
| H | 5.40759700 | -0.98632300 | 1.90477200 |
| H | 5.94913800 | 1.39702300 | 1.42655100 |
| C | -3.36985400 | -0.60084000 | 0.22111600 |
| C | -2.66006200 | 0.29574400 | 1.05352100 |
| C | -4.64769000 | -0.27698900 | -0.21387100 |
| C | -3.30962100 | 1.48352300 | 1.44187700 |
| C | -5.26163000 | 0.89931000 | 0.17473800 |
| H | -5.18577800 | -0.96527500 | -0.85695200 |
| C | -4.58217900 | 1.78193400 | 1.01197500 |
| H | -2.76676100 | 2.16668500 | 2.08762400 |
| H | -5.05643200 | 2.70769300 | 1.31922200 |
| O | 3.62029700 | -2.39440600 | 0.65867800 |
| O | -1.45128300 | 0.06184000 | 1.51214900 |
| S | 4.90109000 | 3.25461100 | -0.55433100 |
| S | -6.90014900 | 1.32940300 | -0.41227500 |
| O | -7.71086000 | 1.60889200 | 0.80386900 |
| O | -7.38660300 | 0.14952800 | -1.18130400 |
| O | -6.72247300 | 2.54343300 | -1.26388300 |
| O | 3.61481300 | 3.98665000 | -0.37400300 |
| O | 5.37353400 | 3.28498700 | -1.96808400 |
| O | 5.95112400 | 3.67806100 | 0.41572800 |

54

RR_ID2_TS1_P_Htr_P, E(SCF) = -
2484.16346453, E(ZPE) = -2483.764248, E(G)
= -2483.832398 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.86267900 | -3.06619400 | -1.16766400 |
| H | -0.78039000 | -3.66351500 | -0.25533000 |
| H | -1.48775900 | -3.61613300 | -1.87843300 |
| C | 0.48993300 | -2.76786900 | -1.75092100 |
| H | 1.04007400 | -3.67589700 | -2.01039000 |
| H | 0.36777500 | -2.17421600 | -2.66226400 |
| N | 1.28874700 | -1.95182300 | -0.79846600 |
| N | -1.48153500 | -1.77847600 | -0.80056200 |
| C | 2.37140000 | -1.25956200 | -1.53800000 |
| H | 1.89377400 | -0.57432400 | -2.24196800 |
| C | -2.74397800 | -1.90979900 | -0.04600900 |
| H | -3.44845400 | -2.52623000 | -0.61584400 |
| C | 3.33713200 | -0.50615700 | -0.68202300 |
| C | 3.99667400 | -1.11973200 | 0.38319600 |
| C | 3.61726900 | 0.82209800 | -0.95372400 |
| C | 4.90250100 | -0.41393900 | 1.15656600 |
| C | 4.52533500 | 1.53053200 | -0.18147500 |
| H | 3.10679400 | 1.31746100 | -1.77495300 |
| C | 5.16723900 | 0.91688500 | 0.87835800 |
| H | 5.39382700 | -0.91925900 | 1.98109700 |
| H | 5.87323600 | 1.47973400 | 1.47677400 |
| C | -3.35566700 | -0.57886800 | 0.25147700 |

H -2.55850300 -2.52473700 0.74658900
H 2.83253000 -1.88357100 -2.22550900
H -1.62944200 -1.19045400 -1.67864800
H 1.78246800 -2.55834700 -0.21385100
O 1.25952400 -0.15891100 1.72472700
H 1.80814600 -1.06732200 2.33012800
H 3.54703800 -3.77319300 -0.45270600
O 3.29307700 -4.52525900 -1.02797900
H 3.83859800 -4.43102500 -1.81517300
H 0.70284000 0.35442600 2.31932800
H 2.99498200 -2.26888200 1.93893800
O 2.44351100 -1.91295200 2.76940500
H 1.91230800 -2.63257300 3.13622700
Pd -0.08445500 -0.88980500 0.36002700

54

RR_ID2_TS1_P, E(SCF) = -2484.16977318,
E(ZPE) = -2483.769483, E(G) = -2483.838116
a.u.

C 0.87789400 3.09186200 -1.06185100
H 0.76946500 3.65409400 -0.13073200
H 1.52907800 3.65968300 -1.73272500
C -0.45474700 2.80320200 -1.69141000
H -1.01704300 3.71503200 -1.91070000
H -0.30484700 2.26012400 -2.63028300
N -1.24945500 1.92970400 -0.79350700
N 1.49033400 1.78839100 -0.72418200
C -2.30850600 1.23138000 -1.56335700
H -1.81658400 0.52357200 -2.23599500
C 2.74500500 1.88856000 0.05581200
H 3.44390300 2.53855600 -0.48096000
C -3.31123100 0.53851300 -0.70340600
C -3.94374400 1.25190800 0.35114400
C -3.64172700 -0.77888900 -0.95284500
C -4.91815000 0.55962600 1.09731900
C -4.60542400 -1.43516400 -0.19799600
H -3.13600900 -1.31057400 -1.75574200
C -5.24395500 -0.75587500 0.82845500
H -5.40740600 1.09406500 1.90637200
H -5.99681600 -1.27031500 1.41555600
C 3.36462800 0.54914800 0.28697000
C 2.64618600 -0.45938900 0.96720100
C 4.66711800 0.30636100 -0.12883200
C 3.30376000 -1.67463300 1.23198800
C 5.29024000 -0.89793000 0.13588500
H 5.21488500 1.07782300 -0.66067000
C 4.60127100 -1.88925100 0.82583600
H 2.75227500 -2.44369100 1.76157400
H 5.08610100 -2.83738500 1.03727800
O -3.60066400 2.47549600 0.64726800
O 1.40971000 -0.30510600 1.38881000
S -4.98646800 -3.14487900 -0.56601000
S 6.96906600 -1.21295000 -0.41236200
O 7.74844000 -1.53017900 0.81868200
O 7.42398800 0.03626200 -1.08361600
O 6.88274600 -2.37550300 -1.34241700
O -3.72167300 -3.91010200 -0.35437700
O -5.42660400 -3.17628400 -1.99219800
O -6.06637000 -3.54251200 0.38152200
H 2.48025600 2.38322100 0.99645900
H -2.79872900 1.99052100 -2.19104600
H 1.68088800 1.27341500 -1.58580500
H -1.76018000 2.50674800 -0.11146700
O -1.29616800 -0.23311800 1.57169600
H -1.69545100 0.46508500 2.15917100
H -3.47776100 3.84996300 -0.43056300
O -3.23774600 4.62221500 -0.98876400
H -3.78167900 4.53875900 -1.77460200
H -0.71367200 -0.76687800 2.12969000
H -2.84259100 2.24811100 2.17285300
O -2.33807900 1.83166700 2.91615500
H -1.68654200 2.48019500 3.19397800
Pd 0.07474800 0.75976500 0.31627300

54

RR_ID2_TS1_R, E(SCF) = -2484.18275915,
E(ZPE) = -2483.783714, E(G) = -2483.851154
a.u.

C 0.84396400 3.27543600 -0.42650000
H 0.72325100 3.63785800 0.59857600
H 1.45381300 3.99808100 -0.97571000
C -0.49582900 3.06579500 -1.08377900
H -1.06475500 3.99591500 -1.15307600
H -0.35849300 2.68081300 -2.09862000
N -1.25048000 2.04483100 -0.32054000
N 1.52157200 1.96005100 -0.35517300
C -2.28812500 1.37321800 -1.11606800
H -1.76885000 0.86203500 -1.93613700
C 2.74363700 1.93552100 0.47474300
H 3.42033300 2.73280300 0.14900100
C -3.13944700 0.40934800 -0.34200000
C -2.66663800 -0.40389700 0.70986000
C -4.46369900 0.27665700 -0.75307800
C -3.56554400 -1.31861000 -1.29212400
C -5.32229100 -0.63420600 -0.17529200
H -4.83463700 0.90452700 -1.55720900
C -4.86573200 -1.43803400 0.86243100
H -3.19715000 -1.93032200 2.10954400
H -5.53215100 -2.15409400 1.33239900
C 3.42809400 0.61005500 0.37577200
C 2.74874700 -0.58181800 0.71575300
C 4.75339500 0.55335300 -0.03596100
C 3.46770100 -1.78991600 0.64548800
C 5.43738500 -0.64528000 -0.09821600
H 5.27091200 1.46925800 -0.30390800
C 4.78472200 -1.82294800 0.24621300
H 2.95140200 -2.70723800 0.91006300
H 5.31364600 -2.76971400 0.19752000
O -1.44981300 -0.35472100 1.23660800
O 1.49597700 -0.61705600 1.12451700
S -7.02659600 -0.77906800 -0.71903700
S 7.14806600 -0.71092900 -0.63398900
O 7.90303300 -1.33500700 0.49028300
O 7.55240100 0.69833700 -0.89503300
O 7.15859200 -1.55682100 -1.86174600
O -7.17880000 0.16937100 -1.85648800
O -7.86121800 -0.41354200 0.46112500
O -7.20396100 -2.20393200 -1.11968500
H 2.42733900 2.16149300 1.49899000
H -2.93395900 2.13166600 -1.57406400
H 1.76389200 1.65471900 -1.29914900
H -1.66549000 2.45404900 0.25756500
O -0.03329100 -2.19967800 -1.55739400
H -0.10367600 -2.50603400 -0.63332700
H -1.79313700 1.24142900 2.42127400
O -1.98226100 2.19007100 2.51415100
H -2.85694700 2.23594900 2.90885000
H 0.26228700 -1.28632300 -1.47128300
H -0.84626500 -2.14420200 1.38984400
O -0.15235200 -2.81125800 1.24211600
H 0.63290600 -2.23605300 1.32295000
Pd 0.09795800 0.68837000 0.39212500

54

RR_ID2_TS1_trigo-square, E(SCF) = -
2484.15380749, E(ZPE) = -2483.754641, E(G)
= -2483.821530 a.u.

C 0.52617300 2.71350200 0.80607600
H 0.25053200 2.40097600 1.81798000
H 1.04516100 3.67273700 0.87412400
C -0.69571900 2.79083400 -0.07491300
H -1.41316400 3.52993300 0.29249300
H -0.42581300 3.05615200 -1.10081400
N -1.29899900 1.44036800 -0.09738700
C -2.45060600 1.25549700 -1.01477700
H -2.04040100 0.93620100 -1.97867300
C -3.45610000 0.28977300 -0.46023900
C -3.07076000 -0.96912100 0.06966400
C -4.79849500 0.65207800 -0.46937000
C -4.09268300 -1.79642800 0.58332600
C -5.77807500 -0.18989300 0.01954600
H -5.09061400 1.61810800 -0.86971700

H 3.64125400 5.03227200 -0.57999700
 H -0.05896800 2.57576700 -1.64675200
 H -0.13373100 1.91946100 -2.14967700
 Pd -0.63182500 1.17952700 -0.64131700

54

RR_ID2_TS2_R_noH2, E(SCF) = -2484.17487234,
 E(ZPE) = -2483.774577, E(G) = -2483.841791
 a.u.

C -0.06061900 -0.86447000 1.59944400
 H -0.01692000 -0.11672000 2.39639500
 H -0.21283000 -1.84694700 2.05409600
 C 1.18683100 -0.81487100 0.76124100
 H 2.07830400 -1.03038200 1.35674100
 H 1.14007300 -1.54897700 -0.04998300
 N 1.27545300 0.53186100 0.15421600
 N -1.20362600 -0.51519500 0.72491000
 C 2.33090200 0.63721700 -0.88653900
 H 2.23997600 1.63204400 -1.32813800
 C -2.46551400 -0.23987700 1.44740800
 H -2.67042500 -1.07032400 2.13110500
 C 3.70789500 0.42419500 -0.34656300
 C 4.29838200 1.44880500 0.44465200
 C 4.39136100 -0.75648900 -0.59914900
 C 5.60701500 1.20224200 0.92829400
 C 5.66515300 -0.96748200 -0.10234700
 H 3.92226800 -1.53319100 -1.19732900
 C 6.27058500 0.02689100 0.66288000
 H 6.07564500 1.97768500 1.52645400
 H 7.27225300 -0.13059700 1.05272000
 C -3.61765700 -0.05831500 0.51117100
 C -3.57720700 0.91210400 -0.51915400
 C -4.76397700 -0.81998400 0.69092100
 C -4.73426600 1.08959700 -1.29935400
 C -5.88804200 -0.63008200 -0.09293100
 H -4.78765600 -1.56573200 1.47985800
 C -5.86622400 0.33224000 -1.09429100
 H -4.70421900 1.84318800 -2.07869000
 H -6.74549400 0.48847200 -1.70966000
 O 3.67836200 2.55074600 0.72225400
 O -2.53734500 1.67407300 -0.77013400
 S 6.56102000 -2.47567200 -0.45185900
 S -7.31208200 -1.70291800 0.09867200
 O -8.49537400 -0.88752800 -0.29421600
 O -7.33002700 -2.10988400 1.53158000
 O -7.08319200 -2.85639900 -0.82044900
 O 6.97715700 -3.02812500 0.87098400
 O 7.73471400 -2.08299500 -1.28758800
 O 5.61001300 -3.36597800 -1.17691200
 H -2.28136300 0.65331300 2.05447400
 H 2.09138600 -0.09556200 -1.66166400
 H -1.36562300 -1.27924600 0.06617800
 H 1.48550500 1.19135200 0.91767700
 O -0.11792300 2.76895300 -1.53157300
 H 0.54910000 3.35464600 -1.07613700
 H 2.51068800 2.49814600 2.02327400
 O 1.67174800 2.32005700 2.50641600
 H 1.10712300 3.06565700 2.28145700
 H -0.92972800 3.27569400 -1.65564500
 H 2.52852300 3.50980300 0.01543700
 O 1.75817600 4.08653100 -0.23472200
 H 2.12522800 4.89426200 -0.60044700
 Pd -0.64643000 1.09757100 -0.37522400

56

RR_ID2_TS2_R, E(SCF) = -2485.34856620,
 E(ZPE) = -2484.931949, E(G) = -2485.000056
 a.u.

C -0.04398500 -0.67808200 1.75534100
 H -0.00320800 0.11789200 2.50429200
 H -0.19012800 -1.63208500 2.26900300
 C 1.20050200 -0.67445800 0.91056100
 H 2.09552000 -0.84494900 1.51478300
 H 1.15467500 -1.46274100 0.15153100
 N 1.28049100 0.62881500 0.21297000
 N -1.18787200 -0.39005900 0.86038800
 C 2.28750300 0.64617500 -0.88040500

H 2.20328500 1.61929500 -1.36919600
 C -2.46757800 -0.12497000 1.55496900
 H -2.66581300 -0.94173900 2.25685000
 C 3.68149200 0.41130100 -0.39573200
 C 4.35397000 1.45437100 0.30000100
 C 4.29912200 -0.81495400 -0.59819900
 C 5.67302000 1.17687900 0.73805300
 C 5.58371800 -1.05505300 -0.14541100
 H 3.76928600 -1.60549000 -1.12300500
 C 6.26858200 -0.04465600 0.52577400
 C 6.20362900 1.96605200 1.26181400
 H 7.27912200 -0.22600000 0.88073000
 C -3.60191700 0.00380000 0.58891900
 C -3.56521600 0.96746200 -0.44766200
 C -4.72257500 -0.80140300 0.73835000
 C -4.70155000 1.09544800 -1.26641100
 C -5.82573600 -0.66117800 -0.08458900
 H -4.74388400 -1.54170800 1.53239000
 C -5.80855800 0.29476600 -1.66556000
 H -4.67540700 1.84424900 -2.05044500
 H -6.67208500 0.41130400 -1.73835000
 O 3.79918100 2.60008300 0.53535600
 O -2.54584800 1.76739100 -0.66556000
 S 6.37692100 -2.63871700 -0.39147500
 S -7.21558100 -1.78493600 0.06357300
 O -8.42089600 -0.99718700 -0.31851800
 O -7.23361000 -2.23177200 1.48431500
 O -6.94062700 -2.90282900 -0.88610900
 O 6.69639700 -3.15842000 0.97135500
 O 7.60954900 -2.37054800 -1.19010300
 O 5.39144900 -3.49007200 -1.11732600
 H -2.31636300 0.78897200 2.13944400
 H 1.98621100 -0.11741800 -1.60290400
 H -1.32265100 -1.18108700 0.22716100
 H 1.53624400 1.33226200 0.92111000
 O -0.13065500 2.83326800 -1.49402800
 H 0.59431300 3.40475300 -1.11504300
 H 2.68313200 2.65746300 1.88280600
 O 1.85994300 2.53160900 2.40838400
 H 1.32531200 3.30331400 2.19894000
 H -0.92551900 3.37212900 -1.58550800
 H 2.64765600 3.55746100 -0.17343200
 O 1.88705400 4.14743600 -0.42251900
 H 2.26117100 4.89210400 -0.89857600
 H -0.58200300 -0.93171300 -2.40823100
 H -0.47128100 -1.66743400 -2.31190900
 Pd -0.64872300 1.19539000 -0.28869000

56

RR_ID2_TS2-square_P, E(SCF) = -
 2485.33533111, E(ZPE) = -2484.919899, E(G)
 = -2484.989320 a.u.

C -0.11301100 -0.59738300 1.71528500
 H -0.09249700 0.23471600 2.42492600
 H -0.26935300 -1.52452700 2.27247200
 C 1.15042100 -0.63056900 0.90166800
 H 2.02757200 -0.78699600 1.53466600
 H 1.11859900 -1.44081500 0.16563800
 N 1.25606200 0.65322500 0.17347300
 N -1.24147700 -0.35964300 0.78525400
 C 2.34364500 0.68392900 -0.84301000
 H 2.35174600 1.70122000 -1.24325800
 C -2.52021600 -0.01133000 1.44295300
 H -2.72542200 -0.74763600 2.22693500
 C 3.68040500 0.31227000 -0.28720900
 C 4.37573500 1.24419300 0.54059500
 C 4.22240300 -0.93416700 -0.55108000
 C 5.61831400 0.81654100 1.06389300
 C 5.44491100 -1.31881900 -0.02030400
 H 3.67205600 -1.62557400 -1.18617600
 C 6.13969300 -0.43050100 0.79126500
 H 7.09458500 -0.73066000 1.20858100
 C -3.64609800 0.01831500 0.46172900
 C -3.57818300 0.83566300 -0.69211600
 C -4.78503400 -0.73457200 0.70330700
 C -4.69715200 0.86506200 -1.54166600
 C -5.87719000 -0.68269300 -0.14518300

| | | | |
|----|-------------|-------------|-------------|
| H | -4.82832000 | -1.36260100 | 1.58861400 |
| C | -5.82718100 | 0.12278200 | -1.27365100 |
| H | -6.68297500 | 0.16504400 | -1.93821400 |
| O | 3.90064200 | 2.41759100 | 0.80223600 |
| O | -2.55082900 | 1.59883300 | -0.99810100 |
| S | 6.11570800 | -2.92521800 | -0.43427400 |
| S | -7.29653900 | -1.73281700 | 0.17278000 |
| O | -6.92112000 | -3.08979800 | -0.32128300 |
| O | -8.42483400 | -1.13371600 | -0.59232200 |
| O | -7.50581500 | -1.70282800 | 1.64769500 |
| O | 7.33896200 | -3.09198300 | 0.40112300 |
| O | 6.41743200 | -2.88903800 | -1.89656700 |
| O | 5.05162100 | -3.91996500 | -0.10784700 |
| H | -1.38389800 | -1.19300100 | 0.21088100 |
| H | 1.42995400 | 1.39376400 | 0.87379400 |
| O | 0.65359300 | 4.26268100 | -0.07309800 |
| H | 1.54361400 | 4.42329200 | -0.46342700 |
| H | 2.50285700 | 2.72801000 | 1.81149200 |
| O | 1.58147500 | 2.77494900 | 2.15231200 |
| H | 1.14777800 | 3.41062400 | 1.55615700 |
| H | 0.18373500 | 5.09963600 | -0.10297600 |
| H | 3.55806100 | 3.60634800 | -0.33287800 |
| O | 3.22877200 | 4.35525500 | -0.89363000 |
| H | 3.47666000 | 4.14241200 | -1.79596900 |
| H | -0.07118200 | 2.70507800 | -1.15383500 |
| H | -0.15538500 | 2.19886200 | -1.80031700 |
| Pd | -0.65345800 | 1.13244400 | -0.48922300 |
| H | 2.05220200 | 0.00242800 | -1.64698200 |
| H | -2.36368200 | 0.95872900 | 1.92785300 |
| H | 6.16097500 | 1.51238200 | 1.69649200 |
| H | -4.64536300 | 1.49893100 | -2.42039400 |

54

RR ID2 TS2-square_R noH2, E(SCF) = -
2484.17153856, E(ZPE) = -2483.771479, E(G)
= -2483.839109 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.10406300 | -1.06964800 | 1.73318800 |
| H | -0.09799400 | -0.39044100 | 2.59007700 |
| H | -0.26585800 | -2.08651000 | 2.10199200 |
| C | 1.16901000 | -0.96113900 | 0.94079100 |
| H | 2.04435100 | -1.20814500 | 1.54626800 |
| H | 1.14145400 | -1.66035000 | 0.09942700 |
| N | 1.27456800 | 0.40660200 | 0.37871200 |
| N | -1.21916100 | -0.65422700 | 0.84916900 |
| C | 2.19684400 | 0.47742100 | -0.78879000 |
| H | 2.00587800 | 1.42960600 | -1.28461200 |
| C | -2.52090300 | -0.52202700 | 1.54246700 |
| H | -2.74838700 | -1.46663900 | 2.04799800 |
| C | 3.63670800 | 0.35762500 | -0.40741300 |
| C | 4.31230500 | 1.51053000 | 0.09613500 |
| C | 4.30685900 | -0.84665000 | -0.53976100 |
| C | 5.66911400 | 1.34245300 | 0.45337700 |
| C | 5.64145900 | -0.97242600 | -0.18202900 |
| H | 3.77755000 | -1.70924200 | -0.94014500 |
| C | 6.31743900 | 0.13254900 | 0.31840500 |
| H | 7.36080600 | 0.03062800 | 0.59724200 |
| C | -3.62838500 | -0.16556000 | 0.60436400 |
| C | -3.55828700 | 1.01411000 | -0.17881200 |
| C | -4.76042500 | -0.96086800 | 0.54332400 |
| C | -4.66993700 | 1.34500500 | -0.96934900 |
| C | -5.84426200 | -0.61493900 | -0.24831400 |
| H | -4.80304000 | -1.86665100 | 1.14268500 |
| C | -5.79576900 | 0.54727200 | -1.00141300 |
| H | -6.64586900 | 0.81689200 | -1.61789600 |
| O | 3.72229500 | 2.65733700 | 0.21901200 |
| O | -2.52275800 | 1.82342500 | -0.17522700 |
| S | 6.45948000 | -2.54989200 | -0.39471000 |
| S | -7.27987000 | -1.68996100 | -0.28025000 |
| O | -6.79841600 | -3.00066600 | -0.80443900 |
| O | -8.26540300 | -1.02984600 | -1.18038400 |
| O | -7.75177300 | -1.78473100 | 1.13106200 |
| O | 7.85729900 | -2.35830000 | 0.08544700 |
| O | 6.38735800 | -2.86514600 | -1.85239500 |
| O | 5.69427100 | -3.53362000 | 0.42768600 |
| H | -1.31961100 | -1.32852600 | 0.08839100 |
| H | 1.60442500 | 1.05772900 | 1.10562100 |
| O | -0.10311300 | 3.10299200 | -0.45892100 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.69611600 | 3.35912400 | -1.00113900 |
| H | 2.48665600 | 2.90574800 | 1.41236000 |
| O | 1.69173100 | 2.85883600 | 1.99252900 |
| H | 0.98121800 | 3.24847400 | 1.46804000 |
| H | -0.88143400 | 3.54374700 | -0.81879400 |
| H | 2.83698300 | 3.41200300 | -0.95796500 |
| O | 2.16110600 | 3.86148900 | -1.53616600 |
| H | 2.42482500 | 3.70473300 | -2.44576100 |
| Pd | -0.64660400 | 1.12723100 | 0.05817800 |
| H | 1.89536200 | -0.31684900 | -1.47604600 |
| H | -2.37866200 | 0.24414300 | 2.31234100 |
| H | 6.19741400 | 2.21020200 | 0.83638100 |
| H | -4.61700300 | 2.25232500 | -1.56112800 |

56

RR ID2 TS2-square_R, E(SCF) = -
2485.34471726, E(ZPE) = -2484.929911, E(G)
= -2485.000415 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.10453500 | -1.08706000 | 1.80506800 |
| H | -0.09753000 | -0.41456800 | 2.66693700 |
| H | -0.26742100 | -2.10671900 | 2.16586700 |
| C | 1.16755800 | -0.97587800 | 1.01058200 |
| H | 2.04521400 | -1.22477600 | -1.61186600 |
| H | 1.13533900 | -1.67470300 | 0.16917500 |
| N | 1.27372800 | 0.39210100 | 0.44743600 |
| N | -1.21845800 | -0.66358200 | 0.92323600 |
| C | 2.16049700 | 0.45366500 | -0.74886100 |
| H | 1.95265400 | 1.40126900 | -1.24649300 |
| C | -2.52571100 | -0.54445700 | 1.60911900 |
| H | -2.75656400 | -1.49744300 | 2.09698400 |
| C | 3.61323500 | 0.34435500 | -0.41697100 |
| C | 4.31319000 | 1.51948600 | -0.00597300 |
| C | 4.27516100 | -0.86812000 | -0.51465000 |
| C | 5.68353900 | 1.36347600 | 0.30299100 |
| C | 5.62177300 | -0.98271200 | -0.20131400 |
| H | 3.72954500 | -1.74702000 | -0.85199900 |
| C | 6.32207500 | 0.14492400 | 0.20716200 |
| H | 7.37548800 | 0.05294000 | 0.44911600 |
| C | -3.62353700 | -0.17328000 | 0.66504800 |
| C | -3.55007600 | 1.02777500 | -0.08488600 |
| C | -4.74480400 | -0.97882600 | 0.55905900 |
| C | -4.64910100 | 1.37017000 | -0.88751300 |
| C | -5.81534400 | -0.62263700 | -0.24643600 |
| H | -4.78935600 | -1.90139700 | 1.13209300 |
| C | -5.76449400 | 0.56070400 | -0.96561600 |
| H | -6.60477400 | 0.83761200 | -1.59228700 |
| O | 3.73338900 | 2.67443500 | 0.08100300 |
| O | -2.52058800 | 1.84376000 | -0.03839400 |
| S | 6.43044600 | -2.56956600 | -0.37866000 |
| S | -7.23327300 | -1.71620800 | -0.34799100 |
| O | -6.71964100 | -3.00037100 | -0.90629700 |
| O | -8.20827800 | -1.03964700 | -1.24739800 |
| O | -7.73541600 | -1.86794200 | 1.04771000 |
| O | 7.82158500 | -2.38243900 | 0.12241000 |
| O | 6.38131900 | -2.90479500 | -1.83306900 |
| O | 5.64285900 | -3.53517000 | -0.44373000 |
| H | -1.31255700 | -1.32620100 | 0.15146200 |
| H | 1.63261200 | 1.04115500 | 1.16314000 |
| O | -0.10018200 | 3.12775400 | -0.29378400 |
| H | 0.64464400 | 3.36600800 | -0.91579000 |
| H | 2.56861900 | 2.90847200 | 1.34850000 |
| O | 1.81781200 | 2.85197300 | 1.98419100 |
| H | 1.06857400 | 3.23231400 | 1.50808700 |
| H | -0.90193400 | 3.57906800 | -0.58435600 |
| H | 2.77290500 | 3.38628600 | -1.07090900 |
| O | 2.05698600 | 3.81497700 | -1.61535900 |
| H | 2.23684100 | 3.59792100 | -2.53306700 |
| H | -0.43638100 | 1.61780400 | -2.90614000 |
| H | -0.55533900 | 0.88691400 | -3.01708200 |
| Pd | -0.64564400 | 1.13222700 | 0.16679800 |
| H | 1.83732600 | -0.34653500 | -1.41958600 |
| H | -2.39066800 | 0.20991000 | 2.39167500 |
| H | 6.22993500 | 2.24801000 | 0.61567800 |
| H | -4.59451900 | 2.29422000 | -1.45268300 |

56

RR_ID2_TS2-square, E(SCF) = -2485.32733247,
 E(ZPE) = -2484.913832, E(G) = -2484.982660
 a.u.

| | | | |
|----|-------------|--------------|-------------|
| C | -0.06263300 | -0.96259500 | 1.51955800 |
| H | 0.00213200 | -0.23018000 | 2.32932900 |
| H | -0.22029000 | -1.95164400 | 1.95799600 |
| C | 1.17163100 | -0.91228800 | 0.66264400 |
| H | 2.06868700 | -1.15740300 | 1.23782500 |
| H | 1.09997400 | -1.62234600 | -0.16770700 |
| N | 1.27082300 | 0.44926400 | 0.09328300 |
| N | -1.21534100 | -0.158576300 | 0.67046900 |
| C | 2.33690600 | 0.59153100 | -0.93220700 |
| H | 2.23523700 | 1.60022500 | -1.33942800 |
| C | -2.46426200 | -0.30098200 | 1.40988800 |
| H | -2.67249100 | -1.13826200 | 2.08448200 |
| C | 3.70478000 | 0.38093800 | -0.36977800 |
| C | 4.28365200 | 1.41531900 | 0.42573400 |
| C | 4.38264800 | -0.80593300 | -0.58699000 |
| C | 5.57094400 | 1.15880000 | 0.95285700 |
| C | 5.63967700 | -1.02581300 | -0.04345000 |
| H | 3.91549600 | -1.58173000 | -1.19053400 |
| C | 6.23135300 | -0.02975800 | 0.72367300 |
| H | 7.21535500 | -0.20479800 | 1.14606800 |
| C | -3.61984100 | -0.09750100 | 0.48409000 |
| C | -3.57055800 | 0.88531300 | -0.53542600 |
| C | -4.76907900 | -0.85365100 | 0.65040300 |
| C | -4.71985200 | 1.07683500 | -1.32018400 |
| C | -5.89017600 | -0.64592500 | -0.13618400 |
| H | -4.79549000 | -1.61192300 | 1.42809700 |
| C | -5.86117500 | 0.32779100 | -1.12287200 |
| H | -6.74011500 | 0.49068500 | -1.73624400 |
| O | 3.66371200 | 2.52509400 | 0.66229800 |
| O | -2.52592300 | 1.64936700 | -0.76544400 |
| S | 6.49146900 | -2.55940900 | -0.39269100 |
| S | -7.32824400 | -1.69422000 | 0.09200900 |
| O | -6.93209300 | -3.04339300 | -0.40613900 |
| O | -8.41612500 | -1.07557900 | -0.71446300 |
| O | -7.61033000 | -1.69133700 | 1.55548200 |
| O | 7.66920500 | -2.59587500 | 0.52021100 |
| O | 6.88256500 | -2.50777600 | -1.83336300 |
| O | 5.51027700 | -3.64995400 | -0.11832400 |
| H | -1.39521800 | -1.33052700 | -0.00531900 |
| H | 1.47273800 | 1.09525400 | 0.87372600 |
| O | -0.02369700 | 3.47387200 | 0.22609000 |
| H | 0.73380900 | 3.88876500 | -0.25103400 |
| H | 2.37866400 | 2.54179000 | 1.87379600 |
| O | 1.53004300 | 2.36973700 | 2.33895100 |
| H | 0.87765200 | 2.88930900 | 1.84117600 |
| H | -0.77809500 | 4.06337100 | 0.14282500 |
| H | 2.89419000 | 3.60122100 | -0.36875500 |
| O | 2.31488300 | 4.26465400 | -0.82591300 |
| H | 2.53677500 | 4.22477900 | -1.75871200 |
| H | -0.10379200 | 2.39758600 | -2.01384200 |
| H | -0.19477900 | 1.72251200 | -2.36504500 |
| Pd | -0.63948400 | 1.04632200 | -0.43085100 |
| H | 2.11626200 | -0.12314300 | -1.72981100 |
| H | -2.26299100 | 0.58293200 | 2.02494200 |
| H | 6.02981600 | 1.93590700 | 1.55651200 |
| H | -4.68146100 | 1.83742400 | -2.09214000 |

56

RR_ID2_TS2, E(SCF) = -2485.32487816, E(ZPE)
 = -2484.910051, E(G) = -2484.978019 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.10560000 | -0.12699100 | 1.85550700 |
| H | -0.10755000 | 0.83687100 | 2.37229900 |
| H | -0.25593200 | -0.92200700 | 2.59079200 |
| C | 1.17523800 | -0.30060300 | 1.08755900 |
| H | 2.04102800 | -0.29117200 | 1.75601200 |
| H | 1.18263400 | -1.24875400 | 0.53952600 |
| N | 1.26481000 | 0.80141200 | 0.10308900 |
| N | -1.21623200 | -0.11526800 | 0.87804600 |
| C | 2.36269800 | 0.64747500 | -0.88699900 |
| H | 2.39488100 | 1.59339800 | -1.43834700 |
| C | -2.51963100 | 0.33052400 | 1.41729500 |
| H | -2.73245600 | -0.23078200 | 2.33359800 |
| C | 3.68793800 | 0.31710200 | -0.27912300 |
| C | 4.30233700 | 1.25076500 | 0.59940400 |

| | | | |
|----|-------------|-------------|-------------|
| C | 4.29417400 | -0.89916400 | -0.55454900 |
| C | 5.55396200 | 0.87768000 | 1.14768600 |
| C | 5.51759800 | -1.23327200 | 0.00025300 |
| H | 3.80397900 | -1.60864600 | -1.21569300 |
| C | 6.14503300 | -0.33034800 | 0.85559000 |
| H | 6.03707000 | 1.58021500 | 1.81977100 |
| H | 7.10407400 | -0.58539300 | -1.29707300 |
| C | -3.61604700 | 0.11616200 | 0.42477000 |
| C | -3.53284600 | 0.67150200 | -0.87392600 |
| C | -4.73493700 | -0.61988500 | 0.78741500 |
| C | -4.61832100 | 0.47057900 | -1.74581900 |
| C | -5.79236500 | -0.79864000 | -0.08566000 |
| H | -4.79301500 | -1.04771300 | 1.78377500 |
| C | -5.72659500 | -0.25035100 | -1.36050300 |
| H | -4.55407500 | 0.90340000 | -2.16890900 |
| H | -6.55350800 | -0.38916600 | -2.04886300 |
| O | 3.74134600 | 2.37640900 | 0.89771300 |
| O | -2.51835800 | 1.39097100 | -1.29940800 |
| S | 6.32470000 | -2.77057900 | -1.64963800 |
| S | -7.18687800 | -1.82813900 | 0.37552100 |
| O | -8.38088800 | -1.20585900 | -0.26215400 |
| O | -7.23796700 | -1.80658600 | 1.86378600 |
| O | -6.89050700 | -3.18531400 | -0.16960800 |
| O | 6.71010600 | -3.39926900 | 0.89841300 |
| O | 7.51785300 | -2.42381800 | -1.22852800 |
| O | 5.32304200 | -3.58527600 | -1.15597200 |
| H | -2.39839000 | 1.38462200 | 1.68909300 |
| H | 2.06124500 | -0.14018900 | -1.58324300 |
| H | -1.32979900 | -1.05097500 | 0.48345800 |
| H | 1.42529600 | 1.66157700 | 0.64325800 |
| O | -0.14712800 | 3.62574700 | -1.03241200 |
| H | 0.73817000 | 3.93003900 | -0.73508400 |
| H | 2.41198200 | 2.67703200 | 2.02813000 |
| O | 1.48668000 | 2.85564500 | 2.30469500 |
| H | 1.30237100 | 3.70761000 | 1.89324700 |
| H | -0.78255100 | 4.06340400 | -0.46011700 |
| H | 2.96281100 | 3.62309500 | 0.07907100 |
| O | 2.33643300 | 4.35233800 | -0.15529000 |
| H | 2.84435200 | 5.02447900 | -0.61383900 |
| H | -0.13585000 | 1.95793200 | -2.52640200 |
| H | -0.03275800 | 1.20920500 | -2.66386900 |
| Pd | -0.63173700 | 1.07728300 | -0.68138500 |

56

RR_ID2_TS3_P, E(SCF) = -2485.36142921,
 E(ZPE) = -2484.944439, E(G) = -2485.016482
 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.03601200 | -0.46375000 | 1.66194400 |
| H | -0.05394000 | 0.41364200 | 2.31624100 |
| H | -0.08790900 | -1.35495000 | 2.29649800 |
| C | 1.22999700 | -0.45886300 | 0.84281100 |
| H | 2.10666500 | -0.55981100 | 1.48969300 |
| H | 1.23364000 | -1.29514400 | 0.13540400 |
| N | 1.30429100 | 0.80013600 | 0.06009900 |
| N | -1.18734400 | -0.37056700 | 0.75416600 |
| C | 2.38828800 | 0.79735500 | -0.95587200 |
| H | 2.39094900 | 1.79116900 | -1.40661100 |
| C | -2.45439700 | 0.02108300 | 1.38506200 |
| H | -2.68701800 | -0.63967600 | 2.22994100 |
| C | 3.73240200 | 0.41960100 | -0.40489400 |
| C | 4.48177700 | 1.29047200 | 0.39196500 |
| C | 4.23365900 | -0.85957000 | -0.63288500 |
| C | 5.67469200 | 0.86085100 | 0.96827100 |
| C | 5.42339500 | -1.27730900 | -0.07282500 |
| H | 3.67067400 | -1.55040900 | -1.25288500 |
| C | 6.14445600 | -0.41500400 | 0.74194200 |
| H | 6.22572600 | 1.55826400 | 1.58855300 |
| H | 7.07660100 | -0.74100100 | 1.19072300 |
| C | -3.58634300 | -0.00212700 | 0.40398000 |
| C | -3.55848800 | 0.76786900 | -0.78875900 |
| C | -4.70866000 | -0.76641500 | 0.70159100 |
| C | -4.71253800 | 0.73354800 | -1.60415000 |
| C | -5.81888500 | -0.78648200 | -0.12049200 |
| H | -4.71961300 | -1.36112800 | 1.61005800 |
| C | -5.81669300 | -0.01854800 | -1.28028500 |
| H | -4.69682200 | 1.32964400 | -2.51076000 |
| H | -6.68325100 | -0.02149800 | -1.93471500 |

| | | | |
|----|-------------|-------------|-------------|
| O | 4.09315000 | 2.55512600 | 0.68848500 |
| O | -2.56841100 | 1.53030900 | -1.17830200 |
| S | 6.07124000 | -2.92437500 | -0.40028900 |
| S | -7.26441500 | -1.76188300 | 0.28726400 |
| O | -8.37765400 | -0.78811900 | 0.48742600 |
| O | -6.92459900 | -2.51393400 | 1.52806600 |
| O | -7.50315400 | -2.65382300 | -0.88505100 |
| O | 5.01207100 | -3.63254400 | -1.16793300 |
| O | 6.33071100 | -3.52399100 | 0.93770100 |
| O | 7.31993900 | -2.71059900 | -1.18419700 |
| H | -2.29880300 | 1.02777000 | 1.79396000 |
| H | 2.09886400 | 0.08977900 | -1.73608900 |
| H | -1.31658600 | -1.25699400 | 0.26980400 |
| H | 1.48075800 | 1.54442000 | 0.74490100 |
| O | 0.02032800 | 4.39591000 | 0.17057800 |
| H | 1.68655400 | 4.33200300 | -0.45961900 |
| H | 2.85339800 | 2.56364500 | 2.18079900 |
| O | 2.00692400 | 2.23699600 | 2.52462900 |
| H | 1.66636300 | 2.93288200 | 3.09165800 |
| H | -0.06664900 | 4.27428600 | 1.12058100 |
| H | 3.53688500 | 2.99702500 | 0.00215700 |
| O | 2.59568200 | 4.18359400 | -0.79628100 |
| H | 2.55571000 | 4.30230200 | -1.74797200 |
| H | -0.32776800 | 3.57155100 | -0.21948400 |
| H | -0.16582200 | 2.30688500 | -1.63226500 |
| Pd | -0.62926600 | 1.17458300 | -0.64081400 |

56
RR_ID2_TS3_R, E(SCF) = -2485.33181111,
E(ZPE) = -2484.916722, E(G) = -2484.987535
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.11037200 | -0.15323800 | 1.86473300 |
| H | -0.12431600 | 0.78504600 | 2.42632100 |
| H | -0.25419200 | -0.98116900 | 2.56376100 |
| C | 1.17370800 | -0.27950900 | 1.09479300 |
| H | 2.03677400 | -0.30575400 | 1.76548400 |
| H | 1.18564700 | -1.19699100 | 0.49701500 |
| N | 1.26790400 | 0.87422900 | 0.16970800 |
| N | -1.21752900 | -0.10862500 | 0.88338200 |
| C | 2.35697600 | 0.75451700 | -0.84051200 |
| H | 2.43586900 | 1.74115300 | -1.30773000 |
| C | -2.53163600 | 0.27841700 | 1.44324600 |
| H | -2.73667100 | -0.33783200 | 2.32479900 |
| C | 3.66560300 | 0.30716500 | -0.27293300 |
| C | 4.38160600 | 1.16962200 | 0.60155900 |
| C | 4.16026300 | -0.95193700 | -0.58262000 |
| C | 5.60880700 | 0.68020900 | 1.11299900 |
| C | 5.36469600 | -1.39702200 | -0.06823100 |
| H | 3.59727400 | -1.60163200 | -1.24689900 |
| C | 6.08486900 | -0.56948200 | 0.79057600 |
| H | 6.16899000 | 1.32928600 | 1.77897600 |
| H | 7.03096100 | -0.91247300 | 1.19964300 |
| C | -3.61918000 | 0.10334300 | 0.43371100 |
| C | -3.53979600 | 0.73226300 | -0.82912200 |
| C | -4.73042500 | -0.66744100 | 0.75144900 |
| C | -4.61963300 | 0.56248900 | -1.71688300 |
| C | -5.77763100 | -0.81863200 | -0.13625300 |
| H | -4.78384500 | -1.15838600 | 1.71815300 |
| C | -5.71955300 | -0.18998900 | -1.37559700 |
| H | -4.55659300 | 1.04799000 | -2.68457400 |
| H | -6.53639600 | -0.30598600 | -2.08109100 |
| O | 3.93956500 | 2.34227600 | 0.92285800 |
| O | -2.53867900 | 1.49316900 | -1.21681100 |
| S | 6.00082100 | -3.02303900 | -0.45995300 |
| S | -7.22373900 | -1.79022200 | 0.29298900 |
| O | -8.35790400 | -0.82394600 | 0.36242700 |
| O | -6.91888300 | -2.42292200 | 1.60605900 |
| O | -7.39032700 | -2.78067600 | -0.80848800 |
| O | 5.05703400 | -3.61308700 | -1.45165200 |
| O | 6.03389700 | -3.77884300 | 0.82738500 |
| O | 7.36895200 | -2.81103800 | -1.01800700 |
| H | -2.43250100 | 1.31699800 | 1.77724700 |
| H | 2.01406600 | 0.04630800 | -1.59972500 |
| H | -1.31052100 | -1.02500400 | 0.43994900 |
| H | 1.43664000 | 1.37533700 | 0.75317200 |
| O | 0.41121800 | 4.70757100 | -0.79399400 |
| H | 1.39096600 | 4.40298400 | -0.72043200 |

| | | | |
|----|-------------|------------|-------------|
| H | 2.65611200 | 2.62909200 | 2.02782100 |
| O | 1.75791900 | 2.65801100 | 2.43380800 |
| H | 1.56869500 | 3.58598100 | 2.58843100 |
| H | 0.08237600 | 4.46957300 | 0.10385000 |
| H | 3.47894700 | 3.57650300 | -0.11222200 |
| O | 3.14210000 | 4.35611500 | -0.62300200 |
| H | 3.62191900 | 4.35515700 | -1.45399800 |
| H | -0.08095100 | 2.64611600 | -1.50405100 |
| H | -0.15171700 | 2.03087700 | -2.05664000 |
| Pd | -0.64027000 | 1.18417500 | -0.59668700 |

56
RR_ID2_TS3-square_P, E(SCF) = -
2485.36512812, E(ZPE) = -2484.946515, E(G)
= -2485.015589 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.05314600 | -0.61698100 | 1.63075600 |
| H | -0.04398900 | 0.23182700 | 2.32223800 |
| H | -0.12009600 | -1.53263600 | 2.22796700 |
| C | 1.20106300 | -0.61193900 | 0.79227700 |
| H | 2.08692000 | -0.76691700 | 1.41620900 |
| H | 1.16603700 | -1.42035300 | 0.05383400 |
| N | 1.29778700 | 0.67375700 | 0.05848100 |
| N | -1.21343500 | -0.45637700 | -0.74315400 |
| C | 2.35752100 | 0.67774600 | -0.98054500 |
| H | 2.31083300 | 1.65355200 | -1.46544100 |
| C | -2.46457100 | -0.07018300 | 1.40873600 |
| H | -2.70528200 | -0.77085500 | 2.21838200 |
| C | 3.72469200 | 0.37610800 | -0.44014200 |
| C | 4.45719200 | 1.32316400 | 0.28985300 |
| C | 4.27143700 | -0.88962500 | -0.60652700 |
| C | 5.67328400 | 0.97330200 | 0.86332800 |
| C | 5.48961200 | -1.23066100 | -0.04454300 |
| H | 3.71787800 | -1.62904900 | -1.17918800 |
| C | 6.18991000 | -0.29794000 | 0.70072700 |
| H | 7.13968800 | -0.56977000 | 1.14510500 |
| C | -3.60362000 | -0.01243000 | 0.43737500 |
| C | -3.56967500 | 0.83783400 | -0.70335700 |
| C | -4.73376100 | -0.77653600 | 0.68689600 |
| C | -4.72439000 | 0.87500200 | -1.51190100 |
| C | -5.85216300 | -0.72040600 | -0.12869600 |
| H | -4.74883000 | -1.42276100 | 1.56079400 |
| C | -5.83895800 | 0.11269000 | -1.23818700 |
| H | -6.71149300 | 0.16284300 | -1.88027400 |
| O | 4.02386200 | 2.58753400 | 0.51702000 |
| O | -2.56898900 | 1.61340300 | -1.03709300 |
| S | 6.16211000 | -2.87558400 | -0.33429100 |
| S | -7.24790200 | -1.79114300 | 0.20421200 |
| O | -6.86336600 | -3.14579500 | -0.29325000 |
| O | -8.39766600 | -1.21163700 | -0.54627000 |
| O | -7.44473200 | -1.76886300 | 1.68229900 |
| O | 7.34149100 | -2.99452900 | 0.56416100 |
| O | 6.52161400 | -2.90654300 | -1.77980300 |
| O | 5.06649600 | -3.82500900 | 0.00478700 |
| H | -1.36648100 | -1.31580000 | 0.21869300 |
| H | 1.51466700 | 1.39096700 | 0.76477600 |
| O | 0.18955000 | 0.18952800 | 0.61781100 |
| H | 1.63495100 | 4.32116500 | -0.50198100 |
| H | 2.67417500 | 2.76280000 | 1.99297900 |
| O | 1.78004500 | 2.55396900 | 2.30159400 |
| H | 1.21640300 | 3.25275000 | 1.97244200 |
| H | -0.43952000 | 4.89333100 | 0.79526300 |
| H | 3.45860400 | 2.97254700 | -0.19270500 |
| O | 2.46324000 | 4.15830000 | -0.99311700 |
| H | 2.21712400 | 4.12880800 | -1.92107400 |
| H | -0.30327200 | 3.48694900 | 0.14857500 |
| H | -0.13356000 | 2.35196300 | -1.46223600 |
| Pd | -0.63315200 | 1.15606600 | -0.56851400 |
| H | 2.08007300 | -0.06465300 | -1.73245200 |
| H | -2.28180400 | 0.90895800 | 1.86979700 |
| H | 6.20985900 | 1.72600300 | 1.42926600 |
| H | -4.70460800 | 1.53114800 | -2.37593900 |

56
RR_ID2_TS3-square_R, E(SCF) = -
2485.33532050, E(ZPE) = -2484.919803, E(G)
= -2484.989116 a.u.

| | | | |
|---|-------------|-------------|------------|
| C | -0.11148900 | -0.62570400 | 1.69044700 |
|---|-------------|-------------|------------|

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -0.10116100 | 0.20159600 | 2.40589100 | H | 3.75973300 | -1.61833600 | -1.20577000 |
| H | -0.26539400 | -1.55758400 | 2.24031900 | C | 6.18538700 | -0.29199100 | 0.73997500 |
| C | 1.15774700 | -0.64455200 | 0.88549600 | H | 7.15142700 | -0.54733800 | 1.16120200 |
| H | 2.03142300 | -0.79908300 | 1.52383200 | C | -3.64229200 | -0.05445900 | 0.48100700 |
| H | 1.13732200 | -1.44951300 | 0.14334200 | C | -3.59747700 | 0.89355800 | -0.57388000 |
| N | 1.25908200 | 0.64531900 | 0.16765500 | C | -4.78151500 | -0.82244500 | 0.66473300 |
| N | -1.23611100 | -0.38878800 | 0.75526600 | C | -4.74770200 | 1.03068700 | -1.37335300 |
| C | 2.35554100 | 0.69318100 | -0.83856000 | C | -5.89870800 | -0.66907200 | -0.13969600 |
| H | 2.36052300 | 1.71455200 | -1.22846100 | H | -4.80410700 | -1.54827800 | 1.47324700 |
| C | -2.51771200 | -0.04526400 | 1.40944300 | C | -5.87547200 | 0.26564900 | -1.16423100 |
| H | -2.72331700 | -0.78385900 | 2.19117800 | H | -6.74977800 | 0.38842300 | -1.79363300 |
| C | 3.68952000 | 0.32409000 | -0.27470100 | O | 3.83131800 | 2.46246000 | 0.72013100 |
| C | 4.36985800 | 1.25009300 | 0.57183900 | O | -2.57505700 | 1.67588700 | -0.82954800 |
| C | 4.24257700 | -0.91520000 | -0.54876200 | S | 6.24672300 | -2.81575600 | -0.42143400 |
| C | 5.60999900 | 0.82513400 | 1.10236400 | S | -7.31514400 | -1.73158200 | 0.10834600 |
| C | 5.46242300 | -1.29816700 | -0.01067200 | O | -6.91105800 | -3.08300500 | -0.39859600 |
| H | 3.70327100 | -1.60247900 | -1.19767500 | O | -8.42591900 | -1.13551400 | -0.67980300 |
| C | 6.14269400 | -0.41565000 | 0.81924200 | O | -7.57607200 | -1.74433300 | 1.57630600 |
| H | 7.09553100 | -0.71447800 | 1.24214000 | O | 7.44869800 | -2.93194000 | -0.25123500 |
| C | -3.64225400 | -0.01493300 | 0.42662300 | O | 6.59040300 | -2.79014100 | -1.87454000 |
| C | -3.57279100 | 0.79937200 | -0.73047100 | O | 5.19920900 | -3.83276400 | -0.11166200 |
| C | -4.78349300 | -0.76153100 | 0.67110000 | H | -1.40599900 | -1.28754600 | 0.07592900 |
| C | -4.68954700 | 0.82517000 | -1.58188400 | H | 1.46863900 | 1.22690200 | 0.88055100 |
| C | -5.87502900 | -0.71288500 | -0.17998800 | O | 0.48011700 | 4.07123000 | -0.11547400 |
| H | -4.82488700 | -1.38782500 | 1.55838500 | H | 1.42601000 | 4.27915000 | -0.45025700 |
| C | -5.82474300 | 0.09029600 | -1.30839500 | H | 2.49036800 | 2.64004500 | 1.81719800 |
| H | -6.68028800 | 0.12724700 | -1.97328700 | O | 1.61109500 | 1.61109500 | 2.25697800 |
| O | 3.88357000 | 2.41672200 | 0.84310900 | H | 1.06842200 | 3.24144000 | 1.81682600 |
| O | -2.54432900 | 1.56035000 | -1.03831200 | H | -0.08826400 | 4.83864900 | -0.25438700 |
| S | 6.14701700 | -2.89522200 | -0.43742000 | H | 3.36249300 | 3.62048300 | -0.30766600 |
| S | -7.32672500 | -1.69333000 | 0.20775400 | O | 2.91442800 | 4.37881100 | -0.78265500 |
| O | -6.87658800 | -3.11502100 | 0.20120900 | H | 3.17269500 | 4.33311000 | -1.70618200 |
| O | -8.31985900 | -1.39168000 | -0.85969300 | H | 0.05292600 | 3.08098600 | -0.72360500 |
| O | -7.76908700 | -1.24679400 | 1.55973100 | H | -0.17099900 | 2.36739400 | -1.43063400 |
| O | 7.36598100 | -3.06254300 | 0.40408100 | Pd | -0.65818600 | 1.13228200 | -0.43285500 |
| O | 6.45776500 | -2.84135100 | -1.89726400 | H | 2.07867500 | -0.03820200 | -1.70619500 |
| O | 5.08759900 | -3.90051300 | -0.12859100 | H | -2.31422900 | 0.70543300 | 2.00562500 |
| H | -1.37362000 | -1.22106400 | 0.17822100 | H | 6.13391500 | 1.66909600 | 1.60585400 |
| H | 1.41988900 | 1.38207200 | 0.87497300 | H | -4.71683400 | 1.76341600 | -2.17259300 |
| O | 0.62783100 | 4.24394000 | -0.06275000 | | | | |
| H | 1.52158500 | 4.41602600 | -0.43939700 | | | | |
| H | 2.47265700 | 2.71415700 | 1.83781600 | | | | |
| O | 1.54688000 | 2.75577400 | 2.16698300 | | | | |
| H | 1.11659000 | 3.38955100 | 1.56631500 | | | | |
| H | 0.15209700 | 5.07769800 | -0.08848500 | | | | |
| H | 3.54344800 | 3.61515400 | -0.28283600 | | | | |
| O | 3.21478400 | 4.36692500 | -0.84015200 | | | | |
| H | 3.48044000 | 4.16744500 | -1.74051000 | | | | |
| H | -0.07421300 | 2.68719900 | -1.16866200 | | | | |
| H | -0.14649900 | 2.18229600 | -1.81732800 | | | | |
| Pd | -0.64835900 | 1.10934400 | -0.51189500 | | | | |
| H | 2.07581700 | 0.01798900 | -1.65194000 | | | | |
| H | -2.36483700 | 0.92376400 | 1.89755800 | | | | |
| H | 6.14145600 | 1.51569900 | 1.74920100 | | | | |
| H | -4.63497600 | 1.45247300 | -2.46476400 | | | | |

56

RR_ID2_TS3, E(SCF) = -2485.32400137, E(ZPE) = -2484.911100, E(G) = -2484.980424 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.07856200 | -0.42112000 | 1.75588300 |
| H | -0.08956200 | 0.45852300 | 2.40616800 |
| H | -0.18991700 | -1.31225000 | 2.38016600 |
| C | 1.19547200 | -0.45612400 | 0.95699400 |
| H | 2.06702000 | -0.54361200 | 1.61186200 |
| H | 1.20322200 | -1.31102400 | 0.27228700 |
| N | 1.27745300 | 0.78186900 | 0.14647500 |
| N | -1.20695600 | -0.29370600 | 0.81214000 |
| C | 2.36550600 | 0.75205000 | -0.87083900 |
| H | 2.39656700 | 1.75237900 | -1.31091600 |
| C | -2.49564100 | 0.06406100 | 1.43416200 |
| H | -2.70576000 | -0.62280100 | 2.26175300 |
| C | 3.69700900 | 0.35557500 | -0.31819700 |
| C | 4.39461900 | 1.24805200 | 0.54008800 |
| C | 4.22805600 | -0.89165900 | -0.61653200 |
| C | 5.63704300 | 0.79983500 | 1.05075500 |
| C | 5.44591500 | -1.29796900 | -0.10211900 |
| H | 3.68080800 | -1.56467800 | -1.27059300 |
| C | 6.14595100 | -0.44115200 | 0.74421500 |
| H | 6.18224800 | 1.47303200 | 1.70506500 |
| H | 7.10231900 | -0.75244300 | 1.15445100 |
| C | -3.61338300 | 0.01951100 | 0.44191600 |
| C | -3.56173600 | 0.77709400 | -0.75275400 |
| C | -4.73656400 | -0.74950900 | 0.72212500 |
| C | -4.68869800 | 0.73366800 | -1.60003000 |
| C | -5.82477100 | -0.77765800 | -0.12764500 |
| H | -4.76651400 | -1.33754300 | 1.63412400 |
| C | -5.79692900 | -0.02104600 | -1.29438900 |
| H | -4.65225700 | 1.32079500 | -2.51140500 |
| H | -6.64734600 | -0.03491800 | -1.96921900 |
| O | 3.92493100 | 2.41470800 | 0.85445700 |
| O | -2.55725200 | 1.54121800 | -1.11334700 |
| S | 6.11700200 | -2.91683300 | -0.46548900 |
| S | -7.27080200 | -1.77018000 | 0.24353400 |

56

RR_ID2_TS3-square, E(SCF) = -2485.32368204, E(ZPE) = -2484.910534, E(G) = -2484.978690 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.09205300 | -0.82021900 | 1.58240800 |
| H | -0.04492900 | -0.04972100 | 2.35842100 |
| H | -0.22304600 | -1.79025100 | 2.07072600 |
| C | 1.15200700 | -0.78405500 | 0.73710100 |
| H | 2.04174600 | -1.01249000 | 1.33025900 |
| H | 1.09108900 | -1.52098700 | -0.07093600 |
| N | 1.26263800 | 0.55888700 | 0.12255300 |
| N | -1.24221000 | -0.50622700 | 0.71178200 |
| C | 2.34282100 | 0.64857800 | -0.89751200 |
| H | 2.30691600 | 1.66450900 | -1.29621600 |
| C | -2.49634500 | -0.20913600 | 1.42921900 |
| H | -2.70990000 | -1.01231500 | 2.14336600 |
| C | 3.69622500 | 0.33548200 | -0.34488200 |
| C | 4.35713300 | 1.30461400 | 0.46527600 |
| C | 4.28507200 | -0.89417700 | -0.58634000 |
| C | 5.61765900 | 0.94044900 | 0.98842400 |
| C | 5.52093300 | -1.22250700 | -0.04826100 |

O -8.40844400 -0.81236800 0.36075600
O -6.97317800 -2.47646600 1.52094600
O -7.43348700 -2.69986900 -0.91153200
O 5.19956600 -3.53439400 -1.46516500
O 6.14148100 -3.65735700 0.83096500
O 7.49015300 -2.68735600 -1.00359300
H -2.36410200 1.06545000 1.86092300
H 2.05275900 0.05401100 -1.65211000
H -1.32047000 -1.16991000 0.30118300
H 1.45533700 1.54941000 0.80860000
O 0.26330800 4.20030300 -0.68567700
H 1.26900000 4.29064000 -0.61773200
H 2.68255700 2.53579100 2.04516600
O 1.81073600 2.44559400 2.49654000
H 1.51493500 3.34026300 2.67913700
H -0.10684800 4.29665600 0.20036000
H 3.28987700 3.58943800 -0.08081200
O 2.84246100 4.36176800 -0.52805900
H 3.31416500 4.52039900 -1.34877200
H -0.02649400 3.04122400 -1.13063800
H -0.15500000 2.24747600 -1.72800200
Pd -0.64132900 1.16871400 -0.55417800

47

RR_EI_hs_D1_TS1_no2W, E(SCF) = -
2255.99229261, E(ZPE) = -2255.654413, E(G)
= -2255.713092 a.u.
C -0.78821200 0.41664500 1.93756800
H -0.48784300 1.15567300 2.68664500
H -1.65011000 0.80859200 1.39425900
C -1.12980200 -0.89759800 2.58934000
H -0.30619700 -1.23153700 3.22412200
H -2.01263300 -0.78844800 3.22664700
N -1.35662600 -1.96076400 1.56933500
N 0.29652800 0.22918100 0.93959300
C -2.76912600 -2.15020900 1.11703500
H -2.79294900 -3.15542200 0.68581800
C 1.67712600 0.26503100 1.43649500
H 1.78675200 -0.53358800 2.17769800
C -3.23149100 -1.15723200 0.11063900
C -2.70876200 -1.25660700 -1.21640800
C -4.16182900 -0.18612400 0.44141900
C -3.22304500 -0.322304500 -2.16133500
C -4.62438200 0.71371500 -0.50455200
H -4.54147100 -0.12865100 1.45841100
C -4.14525800 0.63067800 -1.81150500
H -4.50753400 1.33053700 -2.55942600
C 2.69477600 0.13823600 0.33220700
C 2.46861100 -0.49768800 -0.91439700
C 3.95163500 0.67824000 0.59794200
C 3.54728400 -0.54694700 -1.82513000
C 4.98675300 0.60995300 -0.30812000
H 4.12444800 1.17117900 1.54997600
C 4.77527500 -0.00600200 -1.53802200
H 5.57959900 -0.06280000 -2.26458000
O -1.81771900 -2.13061300 -1.53139100
O 1.33468900 -1.02559600 -1.33225000
S -5.77488200 2.00957600 -0.06833400
S 6.59705900 1.30804600 0.05931900
O 6.84112600 2.34612500 -0.98304400
O 7.56085200 0.17395200 -0.03666700
O 6.50011500 1.87467300 1.43305700
O -6.20003600 1.73622200 1.33464100
O -6.90274700 1.91783200 -1.04248700
O -5.02685700 3.29617100 -0.20064500
H 0.49375400 -3.64697400 -0.18812600
H -0.05834300 -3.60564700 -0.71616900
H -1.06674500 -2.84089900 1.98946900
H -3.41445300 -2.13904800 2.00200700
H 0.19856900 0.93734500 0.21404500
H 1.83584100 1.21529900 1.96144000
Pd -0.03605700 -1.56706500 0.01887800
H -2.85358100 -0.39146300 -3.18039300
H 3.36464500 -1.03302800 -2.77727700

47

RR_EI_hs_D1_TS1_P_no2W, E(SCF) = -
2256.03958742, E(ZPE) = -2255.696361, E(G)
= -2255.756488 a.u.
C -0.90424600 0.17038900 1.57884100
H -0.67752200 0.89969200 2.36510900
H -1.64127200 0.62568200 0.91451600
C -1.47222600 -1.08238100 2.21601600
H -0.79356400 -1.44832900 2.98963600
H -2.42996900 -0.85959300 2.69922000
N -1.63443300 -2.19554100 1.23656100
N 0.29194900 -0.12531600 0.77091900
C -2.94869000 -2.23677900 0.53400200
H -2.94157600 -3.14622800 -0.07261400
C 1.58457800 -0.07898400 1.47326800
H 1.59476100 -0.90007000 2.01386000
C -3.25954700 -1.03274200 -0.29635900
C -2.73657800 -0.85074100 -1.58097500
C -4.12834600 -0.06641000 0.20637800
C -3.06471100 0.28854800 -2.31620000
C -4.44653200 1.06218400 -0.51945100
H -4.56386000 -0.19873800 1.19190400
C -3.90961700 1.24104400 -1.78788100
H -4.15620400 2.12762700 -2.36244400
C 2.73543400 -0.17710800 0.51190500
C 2.84442700 -1.19447800 -0.47583400
C 3.74818200 0.77106300 0.62552900
C 4.00581400 -1.18396400 -1.28450200
C 4.87053000 0.75213300 -0.17763600
H 3.65864000 1.55259600 1.37397900
C 4.99480300 -0.24206700 -1.14308500
H 5.86995700 -0.27052300 -1.78516900
O -1.94553200 -1.75550900 -2.20203800
O 1.98263400 -2.15199700 -0.70560300
S -5.57131100 2.30236700 0.14068100
S 6.15646200 1.98657600 -0.01219500
O 6.21997000 2.69525200 -1.32436400
O 7.41335300 1.23759900 0.28167500
O 5.73730600 2.87673400 1.10704100
O -5.94255300 1.83116300 1.50176800
O -6.72169400 2.33733000 -0.80437700
O -4.79728300 3.57432100 0.14852900
H -0.00836500 -3.71787400 -0.20497400
H -1.43363100 -2.28588600 -1.56248900
H -1.58262000 -3.06355100 1.76386600
H -3.73168600 -2.35538800 1.29093200
H 0.33255000 0.51739200 -0.01482600
H 1.67224000 0.85407900 2.04410800
Pd 0.13841800 -2.19879500 0.15168900
H -2.63906700 0.40252600 -3.30379100
H 4.08967900 -1.96330200 -2.03477900

53

RR_EI_hs_D1_TS1_P, E(SCF) = -2408.89759682,
E(ZPE) = -2408.506193, E(G) = -2408.569055
a.u.
C 0.94267300 0.03936300 -2.34169900
H 0.50961800 0.62735300 -3.15553700
H 1.71913800 0.64609000 -1.87165500
C 1.50781100 -1.25197600 -2.87146400
H 0.75379600 -1.77379500 -3.46529300
H 2.37090800 -1.06414500 -3.51778000
N 1.88632100 -2.17374500 -1.76128300
N -0.08222400 -0.22090500 -1.29982900
C 3.26877300 -2.01976700 -1.19228500
H 3.52487100 -3.00068200 -0.78600500
C -1.48004700 -0.28656400 -1.75432000
H -1.59106800 -1.17511600 -2.38742700
C 3.38723600 -0.98579700 -0.12321400
C 3.06924500 -1.33098400 1.22785300
C 3.78070500 0.30255100 -0.44251300
C 3.20408900 -0.29601800 2.19198700
C 3.85838800 1.29585700 0.51947900
H 4.02469300 0.54834500 -1.47377600
C 3.56645500 0.98536700 1.84475200
H 3.62795200 1.76088900 2.60219700
C -2.44622500 -0.28313200 -0.60152700
C -2.21533400 -0.95221700 0.62119700

| | | | | | | | |
|----------------------------------|--------------------|-------------|-------------|-----------------------------|----------------------|--------------|-------------|
| C | -3.63989900 | 0.41418600 | -0.77271300 | H | -2.16109900 | -1.70769000 | 1.35568600 |
| C | -3.21346800 | -0.88117800 | 1.61298300 | H | 1.55815700 | -1.60192600 | -1.59638500 |
| C | -4.60785800 | 0.45948000 | 0.20810300 | H | 3.11976100 | -2.51849600 | -0.02248800 |
| H | -3.82014700 | 0.93763200 | -1.70683700 | Pd | -0.00167600 | -0.23659900 | 0.11118300 |
| C | -4.38423500 | -0.18989700 | 1.41746700 | H | -3.10959200 | 2.95313000 | -0.61606000 |
| H | -5.13248000 | -0.15378000 | 2.20269000 | H | 3.12519700 | 2.89330600 | 0.89359300 |
| O | 2.67154800 | -2.50884100 | 1.56916000 | | | | |
| O | -1.13438500 | -1.64524600 | 0.93219400 | 53 | | | |
| S | 4.00534200 | 3.00039800 | 0.02448500 | RR_EI_hs_D1_TS1_R, E(SCF) = | -2408.90028282, | | |
| S | -6.12449800 | 1.38754800 | -0.02812900 | E(ZPE) = | -2408.510503, E(G) = | -2408.574884 | |
| O | -6.06636000 | 2.51804000 | 0.94300500 | a.u. | | | |
| O | -7.23321500 | 0.43783500 | 0.27398500 | C | 0.50866600 | -1.11203400 | -2.67814400 |
| O | -6.11411800 | 1.83917900 | -1.44694600 | H | -0.02544700 | -1.01508900 | -3.62793900 |
| O | 4.73142700 | 3.02059200 | -1.27226600 | H | 1.37249300 | -0.44116600 | -2.70945400 |
| O | 4.70709200 | 3.72176500 | 1.11825800 | C | 0.96269800 | -2.53262300 | -2.45919300 |
| O | 2.57851000 | 3.46435900 | -0.12456800 | H | 0.10883200 | -3.21352500 | -2.48459700 |
| H | 0.63157400 | -3.56240200 | 0.35087400 | H | 1.65939500 | -2.84276700 | -3.24338500 |
| H | 1.28590400 | -3.14664800 | 0.69586500 | N | 1.57810600 | -2.67028800 | -1.11352200 |
| H | 1.83112300 | -3.11876100 | -2.13355200 | N | -0.34031100 | -0.64310200 | -1.55073500 |
| H | 3.94575500 | -1.80520200 | -2.02587200 | C | 3.02145300 | -2.30789600 | -0.96591500 |
| H | 0.01521400 | 0.51653400 | -0.57850400 | H | 3.54122100 | -3.20703300 | -0.62469800 |
| H | -1.68452500 | 0.58406600 | -2.38712900 | C | -1.78417900 | -0.86664800 | -1.64313600 |
| Pd | 0.36868800 | -1.97499200 | -0.36297800 | H | -1.95498600 | -1.94949200 | -1.66829200 |
| H | 2.98623400 | -0.54467000 | 3.22594500 | C | 3.26225000 | -1.17096600 | -0.01507700 |
| H | -3.02089900 | -1.39437400 | 2.54924800 | C | 2.67310100 | -1.17265700 | 1.28124400 |
| H | 1.26930600 | -2.28848700 | 2.79091700 | C | 3.97167000 | -0.06448100 | -0.43472400 |
| O | 0.43343100 | -2.13875000 | 3.27350700 | C | 2.96739700 | -0.10480900 | 2.14431700 |
| H | -0.20464900 | -1.91621600 | 2.57617400 | C | 4.16287400 | 1.02486600 | 0.40472400 |
| H | 1.06547400 | 1.15157800 | 1.34881200 | H | 4.34846200 | -0.02529900 | -1.45357900 |
| O | 0.59534600 | 1.68209900 | 0.69308500 | C | 3.68325200 | 0.99059000 | 1.70340000 |
| H | 1.26630100 | 2.33290900 | 0.38991100 | H | 3.84116000 | 1.84151100 | 2.35650500 |
| | | | | C | -2.53878700 | -0.21506500 | -0.51135700 |
| 47 | | | | C | -2.03317500 | -0.01717300 | 0.79763400 |
| RR_EI_hs_D1_TS1_R_no2W, E(SCF) = | - | | | C | -3.84561300 | 0.17786400 | -0.79526600 |
| 2256.02516062, E(ZPE) = | -2255.686444, E(G) | | | C | -2.89184800 | 0.58326600 | 1.74445700 |
| = | -2255.747979 a.u. | | | C | -4.66683800 | 0.74690300 | 0.15377100 |
| C | 0.48608000 | -3.00521500 | 0.55507000 | H | -4.23379600 | 0.03223000 | -1.79875700 |
| H | 1.14873400 | -3.86779400 | 0.43801100 | C | -4.17765100 | 0.95424500 | 1.43945600 |
| H | -0.02874500 | -3.11091100 | 1.51184300 | H | -4.80882300 | 1.41006300 | 2.19582300 |
| C | -0.51210300 | -2.94857600 | -0.57593300 | O | 1.79104200 | -2.10080100 | 1.62446200 |
| H | 0.00342600 | -2.96741100 | -1.53870400 | O | -0.82305100 | -0.32476800 | 1.22489300 |
| H | -1.18049400 | -3.81410300 | -0.54032500 | S | 4.73660200 | 2.55640900 | -0.31646200 |
| N | -1.28848500 | -1.68297900 | -0.53888900 | S | -6.34951200 | 1.22867400 | -0.23299800 |
| N | 1.27426700 | -1.74689300 | 0.62944000 | O | -6.42954800 | 2.69197800 | 0.04402100 |
| C | -2.48837900 | -1.62809200 | 0.31278600 | O | -7.21916300 | 0.43289600 | 0.68096700 |
| H | -3.12482700 | -2.49570900 | 0.10398600 | O | -6.55856800 | 0.89573300 | -1.66951700 |
| C | 2.47531200 | -1.65231300 | -0.21320800 | O | 5.86298100 | 2.22063000 | -1.22569200 |
| H | 2.15374700 | -1.71816800 | -1.25880500 | O | 5.11744700 | 3.45067500 | 0.80608200 |
| C | -3.27075800 | -0.36567900 | 0.06094800 | O | 3.53748000 | 3.06189000 | -1.07123700 |
| C | -2.68168300 | 0.89990900 | -0.20927400 | H | -0.65130400 | -4.52309200 | 0.93023800 |
| C | -4.65850600 | -0.47152400 | 0.11584400 | H | -0.21975300 | -4.07617300 | 1.34963200 |
| C | -3.56242100 | 1.98979300 | -0.40639300 | H | 1.45963900 | -3.63060500 | -0.80451700 |
| C | -5.48870100 | 0.61285300 | -0.07283300 | H | 3.42483300 | -2.05751800 | -1.95051200 |
| H | -5.10744600 | -1.44106600 | 0.30940600 | H | -0.14057600 | 0.35575000 | -1.41011300 |
| C | -4.92661900 | 1.85810000 | -0.33846700 | H | -2.15242700 | -0.46341600 | -2.59436900 |
| H | -5.56531900 | 2.72102900 | -0.49907600 | Pd | 0.41446300 | -1.50582600 | 0.12546400 |
| C | 3.25409000 | -0.38896100 | 0.05279400 | H | 2.54097800 | -0.12809600 | 3.14164500 |
| C | 2.68015400 | 0.85633900 | 0.42965000 | H | -2.49365800 | 0.73765300 | 2.74229900 |
| C | 4.63520100 | -0.47669000 | -0.11245400 | H | 0.68922000 | -1.85508200 | 3.13572900 |
| C | 3.56708800 | 1.94513300 | 0.60610700 | O | -0.08426500 | -1.54299400 | 3.63860300 |
| C | 5.47081600 | 0.60488600 | 0.06427900 | H | -0.53247500 | -1.00969200 | 2.95968000 |
| H | 5.07504200 | -1.43113800 | -0.38662500 | O | 1.10314600 | 1.48180100 | 0.21039500 |
| C | 4.92267700 | 1.83143100 | 0.42872000 | O | 1.01382400 | 1.81450500 | -0.68962500 |
| H | 5.56496900 | 2.69386400 | 0.57663300 | H | 1.88350200 | 2.22091600 | -0.88272100 |
| O | -1.40056000 | 1.16549000 | -0.30844400 | | | | |
| O | 1.41107000 | 1.10474000 | 0.65409600 | 53 | | | |
| S | -7.27008700 | 0.45267400 | 0.02153300 | RR_EI_hs_D1_TS1, E(SCF) = | -2408.88993893, | | |
| S | 7.23967600 | 0.46671200 | -0.18077100 | E(ZPE) = | -2408.500578, E(G) = | -2408.565731 | |
| O | 7.86759200 | 0.95796000 | 1.07983100 | a.u. | | | |
| O | 7.56239000 | 1.33909100 | -1.34760400 | C | 0.88521200 | -0.25759800 | -2.49951800 |
| O | 7.51218100 | -0.97431500 | -0.44261800 | H | 0.42968600 | 0.23332600 | -3.36405700 |
| O | -7.54750700 | -0.99733000 | 0.22125400 | H | 1.70971500 | 0.37166500 | -2.15556200 |
| O | -7.79851100 | 0.97302200 | -1.27273400 | C | 1.36812600 | -1.63513300 | -2.86074400 |
| O | -7.69698900 | 1.28945400 | 1.18089900 | H | 0.55088700 | -2.22090000 | -3.28793500 |
| H | 1.09607200 | 0.16024500 | -3.33563400 | H | 2.17121700 | -1.58901300 | -3.60265300 |
| H | 0.97740400 | 0.05699300 | -2.61063400 | N | 1.82465000 | -2.35532700 | -1.64198500 |
| H | -1.57258300 | -1.45493600 | -1.48993000 | N | -0.08985900 | -0.32952700 | -1.38077300 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 3.22132800 | -2.05099800 | -1.18261000 | H | -5.15441300 | -0.08070900 | 2.12148600 |
| H | 3.60216300 | -2.98874700 | -0.77158000 | O | 2.61471600 | -2.29422400 | 1.90611400 |
| C | -1.50789000 | -0.40129500 | -1.75846900 | O | -1.39050300 | -2.07365100 | 0.80984800 |
| H | -1.67072800 | -1.34631900 | -2.28930900 | S | 4.01548400 | 3.05760100 | -0.13247900 |
| C | 3.31742300 | -0.97923000 | -0.14910700 | S | -5.92228400 | 1.63243900 | -0.06439400 |
| C | 2.82728200 | -1.26489900 | 1.16255300 | O | -5.77611500 | 2.69287200 | 0.97499000 |
| C | 3.82509300 | 0.26847000 | -0.45102300 | O | -7.14135300 | 0.79894300 | 0.14849200 |
| C | 2.99464600 | -0.25378500 | 2.14147900 | O | -5.81811400 | 2.16401400 | -1.45207700 |
| C | 3.90563900 | 1.26241900 | 0.51451000 | O | 4.79887600 | 2.94972000 | -1.38692600 |
| H | 4.15485900 | 0.48463600 | -1.46462800 | O | 4.67614500 | 3.84986400 | 0.93274100 |
| C | 3.49660900 | 0.98860600 | 1.81508100 | O | 2.59841500 | 3.49226200 | -0.37764400 |
| H | 3.56741300 | 1.76413900 | 2.57124200 | H | 0.64913400 | -3.64227300 | 0.33870500 |
| C | -2.42825800 | -0.25060100 | -0.57851200 | H | 2.06189200 | -2.77992600 | 1.25787900 |
| C | -2.15497000 | -0.76287000 | 0.71005300 | H | 1.99931200 | -3.28442700 | -1.89134200 |
| C | -3.63301500 | 0.41463600 | -0.79633800 | H | 4.01592800 | -1.87691200 | -1.74710800 |
| C | -3.12812800 | -0.58123700 | 1.71374700 | H | -0.06923700 | 0.41323300 | -0.63990100 |
| C | -4.57191000 | 0.57438800 | 0.19996100 | H | -1.71118400 | 0.24569500 | -2.52426300 |
| H | -3.84507600 | 0.82171400 | -1.78037100 | Pd | 0.31738700 | -2.23287400 | -0.29835300 |
| C | -4.31109700 | 0.07165200 | 1.47036800 | H | 2.96270400 | -0.23891900 | 0.37764400 |
| H | -5.03880400 | 0.19653800 | 2.26589900 | H | -3.23088200 | -1.60305300 | 2.43785800 |
| O | 2.23312900 | -2.38130500 | 1.42116400 | H | 0.86768900 | -1.78135300 | 2.96291200 |
| O | -1.05562600 | -1.39552200 | 1.07289500 | O | -0.02086500 | -1.47190400 | 3.18014800 |
| S | 4.19371300 | 2.94649200 | 0.01200300 | H | 4.19371300 | -1.71203200 | 2.39233300 |
| S | -6.11594700 | 1.43417900 | -0.10466500 | H | 1.01322600 | 1.33479100 | 1.28103600 |
| O | -6.12837900 | 2.59522500 | 0.83071700 | O | 0.56198900 | 1.78367500 | 0.55724800 |
| O | -7.19362000 | 0.45009200 | 0.20106900 | H | 1.23507100 | 2.40210000 | 0.20508900 |
| O | -6.08804900 | 1.84087900 | -1.53684700 | | | | |
| O | 5.09316300 | 2.90765900 | -1.17087900 | 53 | | | |
| O | 4.76745300 | 3.66568900 | 1.17957800 | RR_EI_hs_D1_TS2_R, E(SCF) = -2408.89759706, | | | |
| O | 2.82213700 | 3.46067400 | -0.34489700 | E(ZPE) = -2408.506201, E(G) = -2408.569135 | | | |
| H | -0.02286600 | -4.05051000 | 0.30256300 | a.u. | | | |
| H | 0.50540500 | -3.86146900 | 0.81926400 | C | 0.94288200 | 0.03938400 | -2.34139300 |
| H | 1.78910900 | -3.34989300 | -1.84986800 | H | 0.50992900 | 0.62739700 | -3.15527100 |
| H | 3.82074900 | -1.79636000 | -2.06259000 | H | 1.71925400 | 0.64611600 | -1.87119300 |
| H | 0.06505900 | 0.49407000 | -0.77298600 | C | 1.50814700 | -1.25190400 | -2.87119500 |
| H | -1.71629400 | 0.40596000 | -2.47071800 | H | 0.75426100 | -1.77357900 | -3.46531700 |
| Pd | 0.37751400 | -1.93867000 | -0.21909400 | H | 2.37143200 | -1.06402400 | -3.51724300 |
| H | 2.67007700 | -0.46818900 | 3.15477900 | N | 1.88628700 | -2.17389100 | -1.76108100 |
| H | -2.90617200 | -0.97826000 | 2.69885700 | N | -0.08215300 | -0.22103100 | -1.29971700 |
| H | 1.08677300 | -2.33472300 | 2.83016900 | C | 3.26865100 | -2.02029400 | -1.19179000 |
| O | 0.29729000 | -2.23973900 | 3.40140500 | H | 3.52431700 | -3.00123600 | -0.78529700 |
| H | -0.35694200 | -1.89165900 | 2.77492300 | C | -1.47992200 | -0.28651400 | -1.75433900 |
| H | 1.12045700 | 1.27351500 | 1.06692100 | H | -1.59094600 | -1.17490000 | -2.38767000 |
| O | 0.69326800 | 1.77932800 | 0.36306800 | C | 3.38726500 | -0.98614600 | -0.12290300 |
| H | 1.39718800 | 2.39354000 | 0.06100100 | C | 3.06928300 | -1.33090000 | 1.22824000 |
| | | | | C | 3.78083500 | 0.30210600 | -0.44261000 |
| 53 | | | | C | 3.20458100 | -0.29572900 | 2.19213000 |
| RR_EI_hs_D1_TS2_P, E(SCF) = -2408.92846899, | | | | C | 3.85870200 | 1.29564000 | 0.51907900 |
| E(ZPE) = -2408.534730, E(G) = -2408.598768 | | | | H | 4.02467000 | 0.54765500 | -1.47396100 |
| a.u. | | | | C | 3.56707400 | 0.98549100 | 1.84451900 |
| C | 0.94560100 | -0.17125000 | -2.30427200 | H | 3.62885200 | 1.76120600 | 2.60175400 |
| H | 0.54604900 | 0.32635600 | -3.19532500 | C | -2.44621200 | -0.28326800 | -0.60160500 |
| H | 1.68287200 | 0.50494800 | -1.86530300 | C | -2.21546900 | -0.95246000 | 0.62107400 |
| C | 1.59156400 | -1.47556700 | -2.71899000 | C | -3.63985500 | 0.41410200 | -0.77283700 |
| H | 0.88580700 | -2.06470400 | -3.30995700 | C | -3.21364300 | -0.88139200 | 1.61280800 |
| H | 2.47143000 | -1.28725200 | -3.34443800 | C | -4.60788800 | 0.45937600 | 0.20790800 |
| N | 1.96382200 | -2.32715200 | -1.55184600 | H | -3.81999200 | 0.93763000 | -1.70693400 |
| N | -0.10522300 | -0.37581300 | -1.29475300 | C | -4.38438900 | -0.19008500 | 1.41724100 |
| C | 3.29669100 | -2.06116700 | -0.94176400 | H | -5.13265000 | -0.15395300 | 2.20244700 |
| H | 3.59539000 | -2.99042700 | -0.45014700 | O | 2.67114100 | -2.50854100 | 1.56989400 |
| C | -1.47749400 | -0.53852300 | -1.79291700 | O | -1.13461100 | -1.64566100 | 0.93210200 |
| H | -1.53724900 | -1.49685800 | -2.32553000 | S | 4.00539600 | 3.00015400 | 0.02389400 |
| C | 3.34377600 | -0.92926800 | 0.03758100 | S | -6.12440800 | 1.38764900 | -0.02837400 |
| C | 3.03072200 | -1.10747400 | 1.39179400 | O | -6.06614600 | 2.51813100 | 0.94276600 |
| C | 3.74075900 | 0.33340400 | -0.38125800 | O | -7.23326700 | 0.43809300 | 0.27369200 |
| C | 3.18435400 | -0.05920700 | 2.29321400 | O | -6.11393700 | 1.83930900 | -1.44718100 |
| C | 3.82340800 | 1.39098000 | 0.50391800 | O | 4.72852200 | 3.02002600 | -1.27451800 |
| H | 3.99243700 | 0.49430600 | -1.42591300 | O | 4.71008500 | 3.72111000 | 1.11604600 |
| C | 3.56275300 | 1.19310300 | 1.85100600 | O | 2.57845200 | 3.46478500 | -0.12165600 |
| H | 3.64633500 | 2.02017500 | 2.54691800 | H | 0.63158900 | -3.56212800 | 0.35166800 |
| C | -2.46930600 | -0.46121900 | -0.66511900 | H | 1.28586200 | -3.14629200 | 0.69678200 |
| C | -2.34470100 | -1.20886800 | 0.53313200 | H | 1.83099600 | -3.11883800 | -2.13351600 |
| C | -3.55975800 | 0.39005800 | -0.81799700 | H | 3.94591400 | -1.80611900 | -2.02525400 |
| C | -3.33888700 | -1.03396500 | 1.51976000 | H | 0.01524900 | 0.51622100 | -0.57820400 |
| C | -4.53012800 | 0.52568500 | 0.15485700 | H | -1.68430800 | 0.58430500 | -2.38691800 |
| H | -3.65683200 | 0.96482100 | -1.73383100 | Pd | 0.36866100 | -1.97515500 | -0.36285200 |
| C | -4.40701100 | -0.18803300 | 1.34149800 | H | 2.98697300 | -0.54409500 | 3.22620800 |

| | | | |
|---|-------------|-------------|------------|
| H | -3.02116900 | -1.39464700 | 2.54906400 |
| H | 1.26785500 | -2.28571400 | 2.79152000 |
| O | 0.43212600 | -2.13467600 | 3.27385600 |
| H | -0.20599000 | -1.91352800 | 2.57606100 |
| H | 1.06566900 | 1.15054300 | 1.34985200 |
| O | 0.59546600 | 1.68094000 | 0.69407300 |
| H | 1.26615600 | 2.33216100 | 0.39129800 |

53
RR_EI_hs_D1_TS2, E(SCF) = -2408.89728057,
E(ZPE) = -2408.506858, E(G) = -2408.569275
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.92301500 | 0.00040800 | -2.37249300 |
| H | 0.48907300 | 0.56388100 | -3.20351500 |
| H | 1.69069800 | 0.62807700 | -1.91441600 |
| C | 1.50945400 | -1.29473100 | -2.87224300 |
| H | 0.76528000 | -1.83856700 | -3.45886700 |
| H | 2.37268400 | -1.10819900 | -3.51885800 |
| N | 1.89441900 | -2.19224600 | -1.74402300 |
| N | -0.10167700 | -0.24709900 | -1.32957400 |
| C | 3.27169700 | -2.02523400 | -1.17385400 |
| H | 3.53859300 | -3.00212000 | -0.76433300 |
| C | -1.49859800 | -2.35063200 | -1.77614400 |
| H | -1.59983700 | -1.26638500 | -2.37141200 |
| C | 3.37450600 | -0.98535000 | -0.10739900 |
| C | 3.05213000 | -1.31109100 | 1.24214000 |
| C | 3.76712300 | 0.30177900 | -0.43638900 |
| C | 3.19138400 | -0.27922000 | 2.20037700 |
| C | 3.84360600 | 1.30060800 | 0.51849000 |
| H | 4.01364600 | 0.53848600 | -1.46893900 |
| C | 3.55703500 | 1.00062000 | 1.84575200 |
| H | 3.62300300 | 1.77962100 | 2.59871800 |
| C | -2.45350000 | -0.31689900 | -0.61354400 |
| C | -2.21188800 | -0.95953800 | 0.62257500 |
| C | -3.64415600 | 0.38534100 | -0.78561900 |
| C | -3.19971700 | -0.85909300 | 1.62285500 |
| C | -4.60087400 | 0.45978000 | 0.20471600 |
| H | -3.83146300 | 0.88944500 | -1.72898200 |
| C | -4.36859900 | -0.16541400 | 1.42505800 |
| H | -5.10801900 | -0.10683300 | 2.21739700 |
| O | 2.64385100 | -2.49301100 | 1.60249500 |
| O | -1.13471400 | -1.65505300 | 0.93800200 |
| S | 4.00566800 | 3.00192300 | 0.00749800 |
| S | -6.11480800 | 1.39066300 | -0.03483100 |
| O | -6.05449700 | 2.52464700 | 0.93227000 |
| O | -7.22635800 | 0.44509500 | 0.27078200 |
| O | -6.10408800 | 1.83738800 | -1.45530400 |
| O | 4.75792500 | 3.00396900 | -1.27355700 |
| O | 4.68721900 | 3.73029100 | 1.10838400 |
| O | 2.58289600 | 3.46282500 | -0.17527600 |
| H | 0.77230900 | -3.46684300 | 0.43774100 |
| H | 1.45616100 | -3.02496100 | 0.79779700 |
| H | 1.83941500 | -3.14504000 | -2.09528500 |
| H | 3.95331400 | -1.80516700 | -2.00204100 |
| H | -0.01705200 | 0.50874800 | -0.62854800 |
| H | -1.72417100 | 0.48996200 | -2.44194900 |
| Pd | 0.38640000 | -1.97662400 | -0.34472000 |
| H | 2.97244400 | -0.52126400 | 3.23529900 |
| H | -2.99999700 | -1.35193100 | 2.56873200 |
| H | 1.21919100 | -2.22598600 | 2.86024000 |
| O | 0.37714700 | -2.03894400 | 3.31255400 |
| H | -0.24321100 | -1.86114200 | 2.58527100 |
| H | 1.03939700 | 1.17294000 | 1.30591200 |
| O | 0.57934300 | 1.69797900 | 0.63933100 |
| H | 1.25569000 | 2.34252600 | 0.33655200 |

53
RR_EI_hs_Hbond-reor_TS1_P, E(SCF) = -
2408.89540930, E(ZPE) = -2408.504584, E(G)
= -2408.569215 a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.88608000 | 0.34891900 | -1.94879500 |
| H | 0.56482300 | 1.12885800 | -2.64473300 |
| H | 1.66431900 | 0.77031800 | -1.30799200 |
| C | 1.39303700 | -0.85437400 | -2.69775500 |
| H | 0.65212300 | -1.17873300 | -3.43181300 |
| H | 2.31527200 | -0.62135000 | -3.23907000 |
| N | 1.61426400 | -2.00576500 | -1.77351600 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.98937600 | -2.13182100 | -1.18885800 |
| H | 3.03740700 | -3.14349100 | -0.77914700 |
| C | 3.32350700 | -1.13060600 | -0.13842100 |
| C | 2.92471200 | -1.36411800 | 1.21544100 |
| C | 4.03255200 | 0.01036000 | -0.47768700 |
| C | 3.30983800 | -0.36991400 | 2.15790800 |
| C | 4.36097500 | 0.97107900 | 0.46460800 |
| H | 4.33755200 | 0.16209500 | -1.51080100 |
| C | 3.99057500 | 0.77007000 | 1.79174600 |
| H | 4.25377400 | 1.51279500 | 2.53809000 |
| O | 2.24567600 | -2.39612500 | 1.57248200 |
| S | 5.09952400 | 2.51213300 | -0.05594800 |
| O | 5.95545100 | 2.18895300 | -1.23325100 |
| O | 5.87709000 | 3.02170500 | 1.10947300 |
| O | 3.95904900 | 3.40962900 | -0.41542100 |
| H | 0.18249400 | -3.65647200 | 0.05328800 |
| H | 0.78464300 | -3.28788900 | 0.48911400 |
| H | 1.46368100 | -2.85240900 | -2.31843100 |
| H | 3.69708200 | -2.02673900 | -2.00729700 |
| H | 3.03393900 | -0.53227700 | 3.19605400 |
| H | 0.90761600 | -1.73184200 | 2.59194400 |
| O | 0.13547100 | -1.24456200 | 2.95895200 |
| H | -0.60294600 | -1.52857200 | 2.39183100 |
| H | 0.35835900 | 0.34301700 | 2.05288200 |
| O | 0.48862700 | 1.11024400 | 1.45313300 |
| H | 1.44741900 | 1.22849200 | 1.44745900 |
| N | -0.24184400 | -0.02990100 | -1.05832300 |
| C | -1.59508100 | 0.08980100 | -1.61978500 |
| H | -1.69659600 | -0.65049900 | -2.42198900 |
| C | -2.66050600 | -0.06250500 | -0.56966000 |
| C | -2.57693600 | -0.96038100 | -0.51666100 |
| C | -3.79999500 | 0.72692400 | -0.70518300 |
| C | -3.65988200 | -1.01300000 | 1.41558400 |
| C | -4.85143100 | 0.65323600 | 0.18355200 |
| H | -3.86216200 | 1.42847800 | -1.53101600 |
| C | -4.77710900 | -0.22925100 | 1.25534400 |
| H | -5.59268400 | -0.29272500 | 1.96818900 |
| O | -1.56155700 | -1.76675300 | 0.78402400 |
| S | -6.33232000 | 1.63946600 | -0.05256300 |
| O | -6.64006300 | 2.23587300 | 1.27787400 |
| O | -7.38637600 | 0.68540700 | -0.50440000 |
| O | -5.99034900 | 2.65667800 | -1.08468800 |
| H | -0.16118100 | 0.53195600 | -0.19272800 |
| H | -1.69363200 | 1.07832900 | -2.08175800 |
| Pd | 0.04792000 | -1.93586100 | -0.41762600 |
| H | -3.58025300 | -1.70187500 | 2.24960700 |

53
RR_EI_hs_Hbond-reor_TS1, E(SCF) = -
2408.88489140, E(ZPE) = -2408.495165, E(G)
= -2408.559483 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67451300 | 0.44005000 | -2.12868400 |
| H | 0.34440900 | 1.17417100 | -2.87024900 |
| H | 1.51873300 | 0.86691300 | -1.58176600 |
| C | 1.07580200 | -0.84941400 | -2.79347900 |
| H | 0.27378600 | -2.20699700 | -3.44249400 |
| H | 1.96268400 | -0.70217300 | -3.41645800 |
| N | 1.32770500 | -1.91824600 | -1.78085000 |
| C | 2.74307100 | -2.13419000 | -1.37055800 |
| H | 2.77856900 | -3.16071300 | -0.99463600 |
| C | 3.22461300 | -1.19605500 | -0.32073300 |
| C | 2.73184100 | -1.34867900 | 1.00713300 |
| C | 4.14814800 | -0.21058600 | -0.62256300 |
| C | 3.33311500 | -0.53859000 | 1.99887000 |
| C | 4.65824100 | 0.62039500 | 0.36288800 |
| H | 4.49007700 | -0.09415900 | -1.64808200 |
| C | 4.25527600 | 0.43647800 | 1.68014600 |
| H | 4.67625300 | 1.06311400 | 2.45961300 |
| O | 1.77279200 | -2.18061800 | 1.29742400 |
| S | 5.69665200 | 2.00964600 | -0.07547200 |
| O | 6.43500800 | 1.60839100 | -1.30635000 |
| O | 6.59071400 | 2.24538000 | 1.09316400 |
| O | 4.76151800 | 3.15005200 | -0.31666200 |
| H | -0.44936700 | -3.91488500 | -0.07923100 |
| H | 0.09395600 | -3.89418800 | 0.44550400 |
| H | 1.00545900 | -2.79362800 | -2.18745500 |
| H | 3.37693300 | -2.07730600 | -2.26147800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.02392000 | -0.67502100 | 3.03013300 |
| H | 0.89862900 | -1.26076100 | 2.66212300 |
| O | 0.32875600 | -0.61221600 | 3.12585400 |
| H | -0.52329300 | -0.76676600 | 2.67999600 |
| H | 0.62579100 | 0.83842500 | 1.92214800 |
| O | 0.75733000 | 1.50985500 | 1.22087500 |
| H | 1.71216100 | 1.50864500 | 1.08525100 |
| N | -0.39869500 | 0.20229000 | -1.13109700 |
| C | -1.78028500 | 0.22225300 | -1.60960900 |
| H | -1.89499500 | -0.57657800 | -2.35074400 |
| C | -2.78242200 | 0.08412500 | -0.49321700 |
| C | -2.54602200 | -0.57494000 | 0.73602600 |
| C | -4.03826600 | 0.64135400 | -0.72813700 |
| C | -3.60813300 | -0.63416800 | 1.66253500 |
| C | -5.06060700 | 0.56338100 | 0.19138100 |
| H | -4.22009300 | 1.15545700 | -1.66712300 |
| C | -4.83646700 | -0.07786900 | 1.40539800 |
| H | -5.62959000 | -0.14214400 | 2.14337900 |
| O | -1.41029600 | -0.13255200 | 1.12367700 |
| S | -6.66784600 | 1.29085000 | -0.13448600 |
| O | -6.87405600 | 2.31876600 | 0.92573400 |
| O | -7.64586300 | 0.16980600 | -0.03314800 |
| O | -6.58939700 | 1.87332300 | -1.50265200 |
| H | -0.26612200 | 0.87279600 | -0.35957300 |
| H | -1.95821100 | 1.17112300 | -2.13127600 |
| Pd | 0.05314500 | -1.55011400 | -0.19968300 |
| H | -3.41486200 | -1.13909000 | 2.60306600 |

53

RR_EI_hs_Hbond-reor_TS2_P, E(SCF) = -
2408.93112050, E(ZPE) = -2408.537199, E(G)
= -2408.600997 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.84163700 | -0.54641100 | -2.40790200 |
| H | 0.37711200 | -0.20483900 | -3.34033300 |
| H | 1.60430400 | 0.19116700 | -2.14710700 |
| C | 1.45809800 | -1.90790100 | -2.63330000 |
| H | 0.70544900 | -2.59305800 | -3.03124600 |
| H | 2.27139600 | -1.84730200 | -3.36468200 |
| N | 1.95267500 | -2.52125600 | -1.36688200 |
| C | 3.32520600 | -2.11278700 | -0.94320200 |
| H | 3.76768200 | -2.98547600 | -0.45724200 |
| C | 3.39587700 | -0.93841000 | -0.01563200 |
| C | 3.30318800 | -1.09992000 | 1.37371300 |
| C | 3.62637900 | 0.33802300 | -0.51191300 |
| C | 3.48813800 | -0.01204100 | 2.22062800 |
| C | 3.74489000 | 1.42663700 | 0.33159700 |
| H | 3.73475700 | 0.48544700 | -1.58240600 |
| C | 3.68654200 | 1.25359500 | 1.70507100 |
| H | 3.80147600 | 2.10523700 | 2.36585800 |
| O | 3.09219500 | -2.30411400 | 1.95963300 |
| S | 3.81505200 | 3.08508300 | -0.35066600 |
| O | 4.33688900 | 2.95020300 | -1.73311300 |
| O | 4.68535700 | 3.87807800 | 0.55187700 |
| O | 2.38787800 | 3.54493700 | -0.31698200 |
| H | 0.79755700 | -3.45581500 | 0.86148300 |
| H | 2.38533600 | -2.78304100 | 1.48587900 |
| H | 1.98969600 | -3.52350600 | -1.52728000 |
| H | 3.91691500 | -1.90748000 | -1.84131700 |
| H | 3.44992900 | -0.18168800 | 3.29153800 |
| H | 1.08873600 | -0.05692200 | 2.76980700 |
| O | 0.18659700 | 0.22835800 | 2.58735200 |
| H | -0.24991000 | -0.56050800 | 2.20351600 |
| H | 0.30900700 | 1.42368700 | 1.12136500 |
| O | 0.22044800 | 1.85064600 | 0.24977600 |
| H | 1.01390400 | 2.40310400 | 0.11525900 |
| N | -0.13149800 | -0.57028100 | -1.30702800 |
| C | -1.52085600 | -0.86652700 | -1.67588400 |
| H | -1.57084000 | -1.91037800 | -2.01347300 |
| C | -2.45740400 | -0.61159100 | -0.52718800 |
| C | -2.22457900 | -1.07666900 | 0.79073100 |
| C | -3.60580800 | 0.13209100 | -0.78527000 |
| C | -3.18607800 | -0.76404600 | 1.77533700 |
| C | -4.53322900 | 0.41926000 | 0.19595600 |
| H | -3.78015300 | 0.50459200 | -1.79004900 |
| C | -4.31509200 | -0.03407500 | 1.49166500 |
| H | -5.03121100 | 0.19101000 | 2.27584500 |
| O | -1.18020000 | -1.77297600 | 1.19916200 |

| | | | |
|----|-------------|-------------|-------------|
| S | -6.00781300 | 1.37234000 | -0.16305200 |
| O | -5.97622900 | 2.53925800 | 0.76533400 |
| O | -7.15931400 | 0.46419100 | 0.11249500 |
| O | -5.91155000 | 1.76708200 | -1.59619100 |
| H | -0.09095700 | 0.32920300 | -0.80975100 |
| H | -1.82799000 | -0.24411000 | -2.52653200 |
| Pd | 0.41414500 | -2.18907200 | -0.00969500 |
| H | -2.99495800 | -1.12070200 | 2.78248700 |

53

RR_EI_hs_Hbond-reor_TS2_R, E(SCF) = -
2408.89725729, E(ZPE) = -2408.504925, E(G)
= -2408.566217 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.89620100 | 0.15364200 | -2.15586700 |
| H | 0.51178000 | 0.82731200 | -2.92694000 |
| H | 1.70544300 | 0.66819100 | -1.63429200 |
| C | 1.37479200 | -1.13369700 | -2.77202400 |
| H | 0.59122800 | -1.56013000 | -3.40242300 |
| H | 2.25045700 | -0.96301500 | -0.49651900 |
| N | 1.68695400 | -2.15196600 | -1.72641400 |
| C | 3.10363800 | -2.18645600 | -1.22791600 |
| H | 3.23812200 | -3.18744400 | -0.81212000 |
| C | 3.44104400 | -1.16550400 | -0.19659600 |
| C | 3.22680500 | -1.46124700 | 1.18363100 |
| C | 3.90802000 | 0.08284400 | -0.57670200 |
| C | 3.68719900 | -0.49045600 | 2.11508800 |
| C | 4.20399300 | 1.05703200 | 0.35971500 |
| H | 4.02348500 | 0.31755400 | -1.63253700 |
| C | 4.11503600 | 0.75007300 | 1.71661100 |
| H | 4.37170700 | 1.50568800 | 2.45302500 |
| O | 2.62384500 | -2.52489000 | 1.59109400 |
| S | 4.30544000 | 2.76411900 | -0.12422600 |
| O | 4.63352200 | 2.79445000 | -1.57519200 |
| O | 5.32898600 | 3.42278400 | 0.73230300 |
| O | 2.92173700 | 3.28833700 | 0.15766900 |
| H | 0.47097800 | -3.50293200 | 0.44639000 |
| H | 1.14828500 | -3.10419700 | 0.76432000 |
| H | 1.51316500 | -3.06330000 | -2.14458200 |
| H | 3.75525000 | -2.08923800 | -2.10317500 |
| H | 3.60103200 | -0.72964300 | 3.17081600 |
| H | 1.32942200 | -1.40535500 | 2.63422600 |
| O | 0.67683300 | -0.72851600 | 2.89129800 |
| H | -0.12818900 | -0.99704800 | 2.41286700 |
| H | 1.03777100 | 0.84512700 | 1.66281600 |
| O | 0.79667200 | 1.50346400 | 0.98597800 |
| H | 1.59537500 | 2.02559200 | 0.77699300 |
| N | -0.15351500 | -0.10988300 | -1.14090600 |
| C | -1.53972900 | -0.09191400 | -1.62404300 |
| H | -1.66327900 | -0.91927100 | -2.33318200 |
| C | -2.54605800 | -0.16141000 | -0.50858500 |
| C | -2.34896400 | -0.86733500 | 0.69803600 |
| C | -3.75471100 | 0.50182100 | -0.71204200 |
| C | -3.39365300 | -0.86476700 | 1.64364400 |
| C | -4.76575000 | 0.48184000 | 0.22376400 |
| H | -3.90936800 | 1.05381900 | -1.63421000 |
| C | -4.57721900 | -0.20590600 | -1.41799000 |
| H | -5.36232200 | -0.22310300 | 2.16699200 |
| O | -1.25732000 | -1.53361600 | 1.04090500 |
| S | -6.32065200 | 1.32791900 | -0.06623300 |
| O | -6.46831400 | 2.30447100 | 1.05053800 |
| O | -7.36823700 | 0.26714000 | -0.03307100 |
| O | -6.19461200 | 1.98007900 | -1.39878000 |
| H | -0.01883600 | 0.57782100 | -0.37725700 |
| H | -1.70059600 | 0.83470200 | -2.18657700 |
| Pd | 0.23145600 | -1.90706400 | -0.26946300 |
| H | -3.22735000 | -1.40684600 | 2.56814300 |

53

RR_EI_hs_Hbond-reor_TS2, E(SCF) = -
2408.89696459, E(ZPE) = -2408.506296, E(G)
= -2408.567922 a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.87147800 | 0.15485900 | -2.18160600 |
| H | 0.49134800 | 0.82096500 | -2.96182500 |
| H | 1.68579100 | 0.67079800 | -1.66831200 |
| C | 1.34481500 | -1.14215100 | -2.78450900 |
| H | 0.55779100 | -1.57364700 | -3.40706100 |
| H | 2.21770000 | -0.97988600 | -3.42411600 |

Pd -0.25154800 -1.77431900 0.37085200
H -3.73187000 -0.72881600 -3.12442300
H 3.17925100 -1.41595100 -2.53149700
H -1.35412100 -1.23864700 -2.60435000
O -0.64529600 -0.60952800 -2.80223100
H 0.11771000 -0.94761800 -2.29435000
H -0.88277900 0.98349900 -1.64985700
O -0.65451600 1.63742900 -0.96501300
H -1.44608000 2.18544500 -0.79839700
O -0.90761300 -3.52563000 -0.53684700
H -0.29899500 -3.77764400 -1.23944600

54

RR_EI_hs_ID1_TS1_P, E(SCF) = -
2484.18004149, E(ZPE) = -2483.778514, E(G)
= -2483.841517 a.u.

C -0.87257600 -0.36751300 -2.17749900
H -0.47166200 -1.05667000 -2.92638700
H -1.66859300 -0.88576700 -1.63977000
C -1.38670400 0.88533100 -2.83973000
H -0.61939800 1.29694800 -3.49944800
H -2.26697200 0.66843500 -3.45335000
N -1.69926600 1.94539000 -1.83789300
N 0.16871900 -0.04517600 -1.17000400
C -3.10588600 2.00014400 -1.32065500
H -3.23958800 3.01737200 -0.94571100
C 1.55962900 -0.07032500 -1.64166200
H 1.67549200 0.72140800 -2.39166000
C -3.43865200 1.02135800 -0.24421400
C -3.32376400 1.39383400 1.12756400
C -3.83650800 -0.26418800 -0.58072800
C -3.76639500 0.44088800 2.08257100
C -4.12985700 -1.20791500 0.38535300
H -3.90243800 -0.55004900 -1.62760000
C -4.11245200 -0.83815200 1.72839500
H -4.36532600 -1.57026800 2.48924400
C 2.55931200 0.07058100 -0.52456400
C 2.35353600 0.84060100 0.64234700
C 3.77575600 -0.58912800 -0.68884500
C 3.39227700 0.89086600 1.59303100
C 4.78436000 -0.50950000 0.24723500
H 3.93994300 -1.18619900 -1.58072500
C 4.58345900 0.23364800 1.40576800
H 5.36509300 0.29654600 2.15605100
O -2.82789200 2.51827300 1.53035900
O 1.25844700 1.52281300 0.93462900
S -4.17525900 -2.93680600 -0.03219700
S 6.35032100 -1.34904000 0.00475600
O 6.48710100 -2.29815500 1.14652800
O 7.38919300 -0.27939500 0.03087000
O 6.25366300 -2.03366100 -1.31404900
O -5.22373300 -3.58075700 0.80433800
O -2.79697400 -3.42159200 0.33100200
O -4.43675300 -3.02853300 -1.49383800
H -1.65646100 3.27763100 0.90872500
H -1.53472600 2.83950200 -2.29509600
H -3.77212000 1.86915400 -2.18081100
H 0.04080100 -0.69907700 -0.37682200
H 1.73815900 -1.02262400 -2.15452300
Pd -0.22293300 1.77845800 -0.40241000
H -3.74103600 0.73554100 3.12735400
H 3.21704600 1.47892600 2.48732700
H -1.38413100 1.38616700 2.55111400
O -0.69342800 0.74849800 2.79723200
H 0.08942900 1.04008500 2.29400300
H -0.96942100 -0.89220800 1.68932300
O -0.71500300 -1.58326700 1.05118400
H -1.50274200 -2.13348900 0.87395700
O -0.79934200 3.60863300 0.45513700
H -0.17906900 3.86557400 1.14666800

54

RR_EI_hs_ID1_TS1_R, E(SCF) = -
2484.17576132, E(ZPE) = -2483.776912, E(G)
= -2483.843910 a.u.

C 0.50887900 2.66565900 -1.39738600
H 1.19945700 3.46238900 -1.68951800

H -0.01383200 2.33844400 -2.29981600
C -0.47548000 3.16848700 -0.36834200
H 0.05509500 3.60788000 0.47945600
H -1.12318200 3.94132500 -0.79451900
N -1.28252300 2.04853700 0.17739200
N 1.25352600 1.48478000 -0.89575400
C -2.44092000 1.65657800 -0.60942800
H -3.11684000 2.46804300 -0.75601900
C 2.51632000 1.72257800 -0.18607400
H 2.28546500 2.23878500 0.75366800
C -3.20893500 0.48081300 0.02723800
C -2.67370700 -0.47329000 0.93510400
C -4.53883600 0.36244500 -0.35800100
C -3.52781300 -1.49920000 1.37991200
C -5.35531100 -0.65649000 -0.60942800
H -4.94850700 1.10039500 -1.04397500
C -4.84185300 -1.59499800 0.97856300
H -5.47579900 -2.39573500 1.34151600
C 3.26858700 0.43707400 0.43707400
C 2.65950200 -0.79943900 0.37837800
C 4.65572200 0.49381600 -0.06890800
C 3.50373000 -1.91193300 0.57715500
C 5.45837000 -0.60688500 0.14611100
H 5.12666400 1.43569600 -0.33369100
C 4.87000700 -1.82564800 0.46527700
H 5.48700100 -2.70350900 0.62842500
O -1.44781400 -0.46514400 1.43928100
O 1.36526200 -1.01464400 0.52467200
S -7.06230700 -0.72159700 -0.45279400
S 7.23976000 -0.51035400 -0.03032100
O 7.58644700 -1.39616000 -1.17942900
O 7.80362700 -1.00917200 1.25679100
O 7.55457400 0.92248400 -0.28747600
O -7.65599200 -1.92451600 0.19374400
O -7.00841000 -0.82553000 -1.93952600
O -7.68854900 0.55290200 0.00279600
H -1.60059400 0.88182300 2.74975700
H -1.58304900 2.27840700 1.13286100
H -2.08041400 1.32223900 -1.60247300
H 1.41057300 0.85357100 -1.69429100
H 3.14503400 2.39909000 -0.77714500
Pd -0.00880300 0.47400700 0.34282000
H -3.10756900 -2.22249400 2.07060500
H 3.02688300 -2.85438100 0.82569300
H -0.95969100 -2.34326800 -1.06833400
O -0.04224100 -2.46435700 -1.33050700
H 0.47662300 -2.10533900 -2.57922800
H 0.56180800 -1.19859100 -2.51496600
O 1.03702200 -0.47058800 -2.96456200
H 0.60034400 -0.34798300 -3.81005200
O -1.83917600 1.78383500 3.03605100
H -1.18440600 2.02656500 3.69502600

54

RR_EI_hs_ID1_TS1, E(SCF) = -2484.15234589,
E(ZPE) = -2483.753789, E(G) = -2483.821880
a.u.

C -0.51692500 -0.51756700 -2.27122900
H -0.14947200 -1.17547600 -3.06495900
H -1.37328600 -1.00327700 -1.79775500
C -0.91488500 0.82561900 -2.82537800
H -0.09208800 1.25894500 -3.39772400
H -1.76758900 0.72457200 -3.50233800
N -1.23356000 1.78191100 -1.72526400
N 0.51444200 -0.36163300 -1.21341900
C -2.66941400 1.96987800 -1.37858600
H -2.75315200 3.00303500 -1.03025000
C 1.91098300 -0.29869300 -1.64257600
H 2.01801700 0.56382700 -2.30985400
C -3.18851400 1.04899200 -0.32763800
C -2.71458600 1.18050500 1.00782400
C -4.16471800 0.11935900 -0.63435200
C -3.36439000 0.41126400 1.99166400
C -4.73857400 -0.67442100 0.34984300
H -4.49449400 0.02119300 -1.66612900
C 0.50726900 -0.34576800 -1.66806000
H -4.81432300 -1.10387400 2.44262100

C 4.63727200 -0.71987300 -0.48810800
H 4.53365500 0.11407800 1.47653600
C 4.17463200 -0.63174400 -1.80056800
H 4.55179600 -1.32472900 -2.54760200
C -2.71820300 -0.14257800 0.33259800
C -2.48146700 0.47389700 -0.92176600
C -3.97992200 -0.67016900 0.59993600
C -3.55522900 0.51639200 -1.83871200
C -5.01002600 -0.60865000 -0.31228300
H -4.16051500 -1.14794900 1.55821900
C -4.78831400 -0.01202000 -1.54988700
H -5.58840400 0.03895500 -2.28155000
O 1.81689900 2.10395000 -1.52976700
O -1.34210600 0.98892300 -1.34113800
S 5.84814800 -1.96430100 -0.06568600
S -6.62702700 -1.28919400 0.05856300
O -6.88065700 -2.32995000 -0.97879600
O -7.58035900 -0.14667900 -0.04288100
O -6.53550100 -1.84988600 1.43510000
O 6.09519900 -1.82481100 1.39831800
O 7.06090300 -1.66831900 -0.88591300
O 5.24015600 -3.28002100 -0.42594000
H -0.52402100 3.62942000 -0.35094200
H 0.15594700 3.56448700 -0.69599200
H 1.04328000 2.83446900 1.96985300
H 3.39141800 2.11944900 2.01410400
H -0.22737800 -0.95842000 0.23702700
H -1.87433800 -1.20174400 1.98152900
Pd 0.02482200 1.54037900 0.01003000
H 2.88200200 0.38096100 -3.17577000
H -3.36467800 0.98705100 -2.79703100

45
RR_EI_s_went-to-planar, E(SCF) = -
2254.85134243, E(ZPE) = -2254.527515, E(G)
= -2254.583677 a.u.
N -1.29976900 1.69181100 0.52840100
N 1.29934100 1.70502700 -0.54622200
C -2.47100600 1.60552600 -0.36011100
H -3.11093400 2.48228000 -0.20797500
C 2.46737900 1.60723300 0.34496200
H 2.10156200 1.63082800 1.37760100
C -3.26653200 0.35721500 -0.08119800
C -2.69084000 -0.90119000 0.24681300
C -4.65242400 0.46912500 -0.16515400
C -3.58172500 -1.98053900 0.45608600
C -5.49263400 -0.60417500 0.04129800
H -5.09216900 1.43376900 -0.40015800
C -4.94353900 -1.84332100 0.35810200
H -3.13907400 -2.93924800 0.70491200
H -5.59085300 -2.69750900 0.53081900
C 3.26586100 0.36290200 0.05572400
C 2.69498600 -0.89078200 -0.29809300
C 4.65032100 0.47271300 0.16298300
C 3.58882800 -1.96717700 -0.50881800
C 5.49386800 -0.59747300 -0.04717800
H 5.08611600 1.43442500 0.41652900
C 4.94896200 -1.83271000 -0.38554800
H 3.14999100 -2.92218900 -0.77776800
H 5.59763200 -2.68550600 -0.55969600
O -1.41438900 -1.16838100 0.38876600
O 1.42095700 -1.15538000 -0.46511800
S -7.27229900 -0.42953700 -0.05636600
S 7.26941400 -0.43296600 0.12098500
O 7.84998600 -0.93123800 -1.15937100
O 7.65394000 -1.28620900 1.28325900
O 7.53295600 1.01465000 0.35418400
O -7.53259200 0.99450400 -0.40825300
O -7.79507600 -0.79916900 1.29143300
O -7.72124800 -1.38125800 -1.11408400
H -1.61883300 1.50075200 1.47619400
H -2.10891600 1.64280800 -1.39364400
H 1.62209900 1.53227400 -1.49626200
H 3.10727400 2.48639300 0.20701100
Pd 0.00128700 0.21672000 -0.02418800
C 0.52120300 2.97080800 -0.54222500
C -0.52572400 2.95989500 0.54527300

H -0.05337500 3.02385300 1.52752800
H -1.19333500 3.82048000 0.44187300
H 1.18610500 3.83159000 -0.42423200
H 0.04850600 3.04962700 -1.52327300

53
RR_EI_D1_I1_CH_P, E(SCF) = -2408.89666390,
E(ZPE) = -2408.504164, E(G) = -2408.570579
a.u.
N 1.54288600 1.87755200 -0.03483400
N -1.16710500 1.52047900 0.65017300
C 2.32447500 1.34189700 1.09625700
H 3.10198700 2.06179600 1.37769000
C -2.39941500 1.85147000 -0.07303800
H -2.11412500 2.40982300 -0.97480300
C 2.93697900 -0.02636500 0.80282500
C 3.20722600 -0.75933300 2.10576900
C 4.07436900 0.04730500 -0.14937000
C 4.52140300 -1.33714400 -2.30003000
C 5.25323500 -0.50859600 0.12420900
H 3.92628600 0.55726600 -1.09719000
C 5.47982700 -1.21101100 1.36750300
H 6.46058700 -1.56948700 -1.53748900
C -3.19692200 0.62494500 -0.41423400
C -2.65417200 -0.49557700 -1.09009200
C -4.54276400 0.61126300 -0.05771900
C -3.52366800 0.16498500 -1.56948500
C -5.37249200 -0.45104700 -0.35552100
H -4.95900500 1.46516600 0.46774200
C -4.85064100 -1.55468100 -1.02102200
H -5.48887700 -2.39997800 -1.25887000
O 2.32243300 -0.86291600 2.94565900
O -1.40461100 -0.62859200 -1.48836600
S 6.63446700 -0.42068700 -1.02851700
S -7.09872100 -0.45086600 0.12665800
O -7.25990400 -1.59010300 1.07640500
O -7.87546900 -0.65233100 -1.13101400
O -7.35382700 0.87283900 0.76065200
O 6.14181900 0.34275900 -2.20174600
O 6.96096600 -1.84002100 -1.33032200
O 7.70949300 0.27314400 -0.26984300
H 0.29206500 -3.00518700 -0.00286600
H 1.07175700 -0.02484700 -1.90327700
H 2.13046000 -0.60674600 0.31377500
O -0.56845200 -2.64214300 0.22184100
H -0.78531900 -2.02472700 -0.50813400
H 0.40262900 -0.73263700 2.63646300
O -0.53761000 -0.79386000 2.40049100
H -0.55536700 -1.45713100 1.68443300
H 2.17814500 2.16546300 -0.77423000
H 1.65204200 1.22447300 1.94666500
H -1.33857900 0.82295300 1.37764000
H -3.02590000 2.52214600 0.52916100
Pd 0.11384100 0.57211500 -0.81196100
H 4.69648600 -1.86232000 3.23167900
H -3.09870000 -2.42399300 -1.89483200
C -0.43327100 2.65986300 1.22546600
C 0.73769400 3.06826000 0.35463200
H -0.08874000 2.36802100 2.22014400
H 0.38283400 3.52265400 -0.57276600
H 1.36365000 3.80242400 0.87436800
H -1.09327600 3.52175100 1.36727800

53
RR_EI_D1_I1_CH_R, E(SCF) = -2408.89566946,
E(ZPE) = -2408.504076, E(G) = -2408.567621
a.u.
N 1.61089700 2.08971200 -0.16288300
N -1.08347600 1.75263800 0.29766400
C 2.40474500 1.89939100 1.09195800
H 3.06894700 2.76622300 1.18625200
C -2.26424900 1.80963900 -0.58801100
H -1.92333800 2.10456600 -1.58728500
C 3.16261700 0.61823100 1.04127700
C 2.63729000 -0.54123100 1.68772800
C 4.32578200 0.54637400 0.28537100
C 3.35723000 -1.75064900 1.47595000

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 4.99744300 | -0.64819300 | 0.10745200 | O | 6.64331900 | 0.35915600 | -1.84911100 |
| H | 4.71792300 | 1.44417500 | -0.18698400 | O | 6.22053400 | -2.09197600 | -1.85762200 |
| C | 4.49609500 | -1.80257200 | 0.70898700 | O | 7.61204200 | -1.08625400 | -0.07188300 |
| H | 5.01288400 | -2.74784700 | 0.56834400 | H | 0.57556400 | -1.65370000 | 2.19668800 |
| C | -3.00911400 | 0.50824700 | -0.58823700 | H | 1.51394400 | -0.47147400 | -0.92701800 |
| C | -2.36407300 | -0.73632200 | -0.74070500 | H | 2.18143100 | -0.03246000 | -0.20249700 |
| C | -4.39149400 | 0.53831600 | -0.42840800 | O | -0.25464400 | -2.11758600 | 1.99401300 |
| C | -3.15386800 | -1.90065100 | -0.73326500 | H | -0.47217300 | -1.84481100 | 1.08151400 |
| C | -5.14870400 | -0.61467000 | -0.43583600 | H | 0.10968900 | 0.57288900 | 2.81983100 |
| H | -4.89281100 | 1.49232500 | -0.29772400 | O | -0.86045900 | 0.55852900 | 2.91112700 |
| C | -4.51963500 | -1.84517400 | -0.58501600 | H | -1.04703300 | -0.38045100 | 2.74457700 |
| H | -5.10411100 | -2.75963300 | -0.58316200 | H | 2.02798300 | 2.20685200 | -1.24650800 |
| O | 1.56814000 | -0.52557200 | 2.40019400 | H | 1.90696400 | 2.12231000 | 1.67987500 |
| O | -1.06158600 | -0.90910700 | -0.89870500 | H | -1.43595200 | 1.38795300 | 1.23496400 |
| S | 6.48967500 | -0.74316000 | -0.87332100 | H | -3.04953000 | 2.55675200 | -0.32598600 |
| S | -6.92432300 | -0.55813200 | -0.18003600 | Pd | 0.26915800 | 0.52239400 | -0.43088800 |
| O | -7.16216000 | -1.20305700 | 1.14315500 | H | 3.31038000 | -2.30805700 | 2.39448300 |
| O | -7.52161000 | -1.33269300 | -1.30443000 | H | -2.64400400 | -2.92687900 | -0.29125500 |
| O | -7.29722600 | 0.88510200 | -0.19905300 | C | 3.11622000 | 3.11622000 | 0.29120200 |
| O | 6.73918100 | 0.63427300 | -1.38558700 | C | 0.60829900 | 3.36443300 | -0.33570300 |
| O | 6.20586000 | -1.72379000 | -1.96266400 | H | -0.22429200 | 3.10059800 | 1.63167300 |
| O | 7.56589100 | -1.22301000 | 0.04365900 | H | 0.25229200 | 3.51892900 | -1.35651300 |
| H | 0.40988800 | -1.81114200 | 1.85679000 | H | 1.16655000 | 4.25652600 | -0.03486800 |
| H | 1.34990500 | -0.42597700 | -1.66796700 | H | -1.28851400 | 3.92622500 | 0.50066500 |
| H | 1.68356200 | -0.56544800 | -0.93943700 | | | | |
| O | -0.37687900 | -2.31761600 | 1.56043500 | 53 | | | |
| H | -0.54299400 | -1.99672900 | 0.65931800 | RR_EI_D1_I1_HH-Homo_P, E(SCF) = - | | | |
| H | -0.01476700 | 0.21676200 | 2.66080900 | 2408.86759576, E(ZPE) = -2408.476181, E(G) | | | |
| O | -0.99351800 | 0.30589800 | 2.70575000 | = -2408.541414 a.u. | | | |
| H | -1.26775900 | -0.59454500 | 2.47103000 | C | -0.40405200 | 2.87584300 | 1.03248200 |
| H | 2.27553600 | 2.15128800 | -0.93292100 | H | -1.10626400 | 3.69522100 | 1.21744700 |
| H | 1.71037700 | 1.90215600 | 1.93262100 | H | 0.13160300 | 2.70476100 | 1.96870200 |
| H | -1.32155000 | 1.26146800 | 1.17946700 | C | 0.55598500 | 3.28169700 | -0.06758600 |
| H | -2.93113700 | 2.59912900 | -0.22700800 | H | 0.01398200 | 3.57876400 | -0.96710600 |
| Pd | 0.30528100 | 0.53168500 | -0.56465100 | H | 1.16815200 | 4.13075400 | 0.25139500 |
| H | 2.96972700 | -2.64905100 | 1.94789800 | N | 1.44302800 | 2.14064100 | -0.43735900 |
| H | -2.64538400 | -2.85233500 | -0.84675700 | N | -1.11759900 | 1.63243900 | 0.69482200 |
| C | -0.46655300 | 3.05871400 | 0.65616500 | C | 2.51748500 | 1.90979600 | 0.57803400 |
| C | 0.75998100 | 3.30739200 | -0.17948300 | H | 3.20188500 | 2.76177300 | 0.52879800 |
| H | -0.21792200 | 3.01274700 | 1.71840500 | C | -2.40986700 | 1.82219000 | 0.03020700 |
| H | 0.48447900 | 3.49482300 | -1.21952700 | H | -2.23220000 | 2.37467000 | -0.90049400 |
| H | 1.32222000 | 4.17215500 | 0.18611300 | C | 3.25098200 | 0.62569400 | 0.41425600 |
| H | -1.19386800 | 3.86313100 | 0.52830800 | C | 2.54939400 | -0.57548700 | 0.65320900 |
| | | | | C | 4.60505400 | 0.59788600 | 0.11678100 |
| | | | | C | 3.26976700 | -1.78050800 | 0.61655600 |
| | | | | C | 5.29086900 | -0.60246500 | 0.06850900 |
| | | | | H | 5.13897100 | 1.52459200 | -0.06910200 |
| | | | | C | 4.61826700 | -1.79143100 | 0.33044000 |
| | | | | H | 5.15876600 | -2.73258500 | 0.30049400 |
| | | | | C | -3.13512100 | 0.52977500 | -0.23404100 |
| | | | | C | -2.53185800 | -0.66450200 | -0.68802300 |
| | | | | C | -4.51706100 | 0.54606400 | -0.04471800 |
| | | | | C | -3.36612700 | -1.77395400 | -0.93748000 |
| | | | | C | -5.31250600 | -0.55043700 | -0.29725700 |
| | | | | H | -4.98842500 | 1.45662600 | 0.31235700 |
| | | | | C | -4.72421900 | -1.72889500 | -0.74109400 |
| | | | | H | -5.33195700 | -2.60568900 | -0.93938600 |
| | | | | O | 1.25527200 | -0.55902900 | 0.89550300 |
| | | | | O | -1.23933700 | -0.89357700 | -0.88663300 |
| | | | | S | 7.04396300 | -0.65334500 | -0.30966700 |
| | | | | S | -7.08298500 | -0.50237000 | -0.00992200 |
| | | | | O | -7.33578300 | -1.44006600 | 1.12150000 |
| | | | | O | -7.71099000 | -0.96446000 | -1.28023700 |
| | | | | O | -7.40954800 | 0.91161500 | 0.32281700 |
| | | | | O | 7.44670700 | 0.75278300 | -0.58973200 |
| | | | | O | 7.17800600 | -1.54577900 | -1.49660300 |
| | | | | O | 7.70770200 | -1.21806500 | 0.90058100 |
| | | | | H | 0.31237400 | -2.13459500 | -1.14070400 |
| | | | | H | -0.40034000 | 1.20554900 | -1.94770300 |
| | | | | H | 0.99879200 | -0.08831900 | -1.82337400 |
| | | | | O | -0.48868900 | -2.69213000 | 1.18328700 |
| | | | | H | -0.94283200 | -2.38389600 | 0.38433600 |
| | | | | H | 0.18662400 | -0.26961400 | 2.42066700 |
| | | | | O | -0.69243700 | -0.30423000 | 2.84130800 |
| | | | | H | -1.01733700 | -1.15770300 | 2.51132200 |
| | | | | H | 1.88982600 | -2.34759400 | -1.32812700 |
| | | | | H | 2.02662000 | 1.92831800 | 1.55416600 |

H -1.23970900 1.05830900 1.53746600
H -3.05252200 2.46031700 0.64920800
Pd 0.15987500 0.54151100 -0.69752200
H -2.88931000 -2.68270600 -1.29031600
H 2.73620200 -2.70584600 0.80978500

53

RR_EI_D1_I1_HH-Homo_TS, E(SCF) = -
2408.86487992, E(ZPE) = -2408.475689, E(G)
= -2408.540653 a.u.

C -0.40434400 2.87192500 1.04009000
H -1.11288100 3.68469100 1.23115400
H 0.13351900 2.69866100 1.97447500
C 0.54829200 3.28635800 -0.06083000
H 0.00109800 3.57093300 -0.96148200
H 1.15058000 4.14527400 0.25137500
N 1.44723300 2.15318900 -0.42453600
N -1.10941200 1.62505600 0.69561100
C 2.51618500 1.92736700 0.59937000
H 3.20373600 2.77664700 0.54281100
C -2.38859100 1.81532700 0.00406900
H -2.19022700 2.34974700 -0.93325200
C 3.24324000 0.63880800 0.45138300
C 2.53802100 -0.55321800 0.73424800
C 4.58892500 0.59759400 0.12056800
C 3.25480500 -1.76337600 0.70138900
C 5.26755500 -0.67734900 0.07771900
H 5.12332900 1.51735200 -0.09678600
C 4.59432700 -1.78730700 0.37839800
H 5.12882300 -2.73218300 0.35205400
C -3.12008600 0.52613100 -0.25091200
C -2.51574900 -0.66761600 -0.70248700
C -4.50107600 0.54157100 -0.05754900
C -3.34701300 -1.78005700 -0.94708400
C -5.29446500 -0.55788300 -0.30494100
H -4.97327100 1.45244900 0.29741100
C -4.70479900 -1.73635800 -0.74695900
H -5.31166800 -2.61468800 -0.94115200
O 1.25536300 -0.52093600 1.00647100
O -1.22317500 -0.88845800 -0.90438200
S 7.01007900 -0.67538900 -0.33932700
S -7.06514300 -0.51212200 -0.01845200
O -7.31909700 -1.45942900 1.10461800
O -7.69197300 -0.96349900 -1.29325800
O -7.39193400 0.89902300 0.32587800
O 7.41579100 0.72390400 -0.64945500
O 7.11384000 -1.58607700 -1.51577800
O 7.69928200 -1.22672800 0.86338400
H 0.31241100 -2.07864500 1.18362100
H -0.09527000 0.97378700 -2.16606900
H 0.92654900 0.01208400 -1.96159500
O -0.47344600 -2.66138300 1.19455500
H -0.90874000 -2.36543400 0.38090400
H 0.14694700 -0.25110700 2.47971200
O -0.74319400 -0.28794500 2.87823700
H -1.06038900 -1.13864300 2.53499500
H 1.90418300 2.37000800 -1.30780400
H 2.02126000 1.95725400 1.57272800
H -1.24934900 1.05654300 1.53964200
H -3.03564300 2.46900000 0.60209600
Pd 0.16879400 0.55064300 -0.71040100
H -2.86918400 -2.68894800 -1.29802200
H 2.72293300 -2.68235600 0.92755400

47

RR_EI_D1_no2W_P, E(SCF) = -2256.04030958,
E(ZPE) = -2255.697406, E(G) = -2255.757055
a.u.

C 0.46877900 2.59089100 -0.83707600
H 1.05396000 3.51527800 -0.78101200
H 0.09122900 2.51396500 -1.85908100
C -0.68431100 2.66285900 0.13868900
H -0.31884600 2.84034100 1.15231600
H -1.35386800 3.48844100 -0.12695200
N -1.43549300 1.38045000 0.16723000
N 1.31110200 1.40925800 -0.58053800
C -2.29283100 1.17506000 -1.03094600

H -2.79569700 2.12198700 -1.26065900
C 2.43605600 1.59823900 0.35169200
H 2.01533100 1.78683700 1.34765900
C -3.32332800 0.11232400 -0.81454100
C -3.08098800 -1.23583400 -1.09435400
C -4.58459400 0.47840300 -0.35131800
C -4.10183300 -2.17244600 -0.95574500
C -5.58720500 -0.45643600 -0.19470400
H -4.79246200 1.52046200 -0.12818900
C -5.34758900 -1.78765700 -0.50920000
H -6.13674800 -2.52324800 -0.39498400
C 3.34067700 0.40003600 0.35280200
C 2.87489500 -0.91907300 0.60443000
C 4.69444900 0.61057900 0.11046400
C 3.84178700 -1.95191800 0.61433300
C 5.61382900 -0.41967000 0.12446500
H 5.04495900 1.61796200 -0.09252200
C 5.17446000 -1.71484900 0.38179900
H 5.88400900 -2.53661100 -0.39504400
O -1.89001000 -1.68853900 -1.55486200
O 1.63726100 -1.26907100 0.84675600
S -7.21702100 0.02329400 0.39975000
S 7.34973800 -0.12339300 -0.19774400
O 7.48593000 1.34453500 -0.42274400
O 7.68941200 -0.92840100 -1.40690400
O 8.08226700 -0.59314300 1.01429000
O -7.14369500 1.48713100 0.65302700
O -7.43769800 -0.77791500 1.63556100
O -8.16286900 -0.33732100 -0.69283000
H -0.88142200 -0.97538800 1.29350200
H -1.15780800 -1.19793100 -1.13341000
H -2.04831300 1.39338100 0.97971100
H -1.64714100 0.93453400 -1.87827100
H 1.68241900 1.05999800 -1.45864900
H 3.01513100 2.48824600 0.07417500
Pd 0.05988700 -0.03361800 0.47801500
H -3.88640300 -3.20790700 -1.19211300
H 3.48583800 -2.95750300 0.81272000

47

RR_EI_D1_no2W_R, E(SCF) = -2256.02482726,
E(ZPE) = -2255.685832, E(G) = -2255.746445
a.u.

C 0.51508200 2.95836600 -0.58539900
H 1.18176900 3.81973200 -0.48295600
H 0.03500300 3.02638300 -1.56356500
C -0.52321900 2.96237000 0.51056400
H -0.04293300 3.03236500 1.48902600
H -1.18770500 3.82507700 0.40495300
N -1.30231700 1.69749700 0.51153200
N 1.29224300 1.69184700 -0.57941000
C -2.47051200 1.60009800 -0.37942400
H -3.11178700 2.47797100 -0.23981400
C 2.47066300 1.61203600 0.29864400
H 2.11951000 1.66803200 1.33494600
C -3.26631400 0.35377900 -0.09131800
C -2.69373900 -0.89725100 0.26925400
C -4.65047900 0.46006000 -0.20359800
C -3.58575900 -1.97526500 0.47926900
C -5.49172000 -0.61300900 0.00067600
H -5.08783600 1.41911600 -0.46499000
C -4.94608400 -1.84381600 0.35335900
H -5.59352600 -2.69818900 0.52413600
C 3.26151400 0.35661900 0.03646600
C 2.68672400 -0.90128300 -0.29496800
C 4.64617100 0.46293100 0.14387900
C 3.57730900 -1.98408900 -0.48659300
C 5.48580200 -0.61510500 -0.03944900
H 5.08526600 1.42665700 0.38448000
C 4.93807500 -1.85191500 -0.36683700
H 5.58411200 -2.71017300 -0.52249700
O -1.41914100 -1.15830100 0.44024200
O 1.41159600 -1.16597100 -0.45564100
S -7.27023300 -0.43290100 -0.10953400
S 7.26474600 -0.43351500 0.06137500
O 7.51203600 0.93540700 0.59492300
O 7.77776400 -0.61470000 -1.32858500

O 7.73616500 -1.51003000 0.97959900
O -7.51594100 0.93557800 -0.64492500
O -7.78982100 -0.61411300 1.27790300
O -7.73627900 -1.51014400 -1.02974800
H 0.60449200 0.66208800 3.31499700
H 0.19324100 0.23093900 2.85888400
H -1.62655500 1.52352500 1.46142900
H -2.10540300 1.62562300 -1.41223400
H 1.60282600 1.50285100 -1.53044900
H 3.11235300 2.48400900 0.12723700
Pd -0.00274500 0.21310700 -0.02148600
H -3.14555900 -2.92853600 0.75212900
H 3.13520400 -2.94210900 -0.73900400

47

RR_EI_D1_no2W_TS, E(SCF) = -2255.99590859,
E(ZPE) = -2255.657201, E(G) = -2255.715585
a.u.

C -0.43400200 2.73953700 0.73810800
H -1.07428900 3.62173800 0.65676000
H 0.01376600 2.74686700 1.73290900
C 0.63235600 2.74606100 -0.32387800
H 0.18707600 2.82295500 -1.31786500
H 1.30762600 3.59684500 -0.18975600
N 1.38887600 1.46985000 -0.27755300
N -1.25091700 1.50111000 0.63146500
C 2.39285200 1.37330900 0.82827300
H 2.92788700 2.32858800 0.87832500
C -2.45284000 1.59390600 -0.21950700
H -2.11441500 1.77670500 -1.24504400
C 3.35138900 0.25533200 0.60101200
C 2.89904600 -1.09433000 0.74515300
C 4.66756700 0.53104400 0.25854300
C 3.87621300 -2.10616400 0.52257400
C 5.58716000 -0.48284900 0.05623000
H 4.99193500 1.56304900 0.15842500
C 5.17520500 -1.80908500 0.18823800
H 5.89152800 -2.61028100 0.02732600
C -3.32217800 0.37274000 -0.11763700
C -2.82400800 -0.94805200 -0.01212500
C -4.69964700 0.57694500 -0.15667400
C -3.76558600 -1.99981600 0.03406400
C -5.59699700 -0.46811500 -0.11253000
H -5.08348100 1.59004900 -0.22466000
C -5.11809500 -1.77091200 -0.01283800
H -5.81237800 -2.60431700 0.02833200
O 1.68804500 -1.38651900 1.04348700
O -1.55955700 -1.30017700 0.06594400
S 7.28181000 -0.12886300 -0.38445100
S -7.36571700 -0.17947900 -0.14601900
O -7.54143200 1.29342800 -0.28105800
O -7.89101600 -0.71186000 1.14444100
O -7.88066100 -0.93937200 -1.32147300
O 7.40842400 1.35695000 -0.40043700
O 7.50245600 -0.74036500 -1.72947400
O 8.13271600 -0.76922600 0.66299700
H 0.64466400 -1.07935300 -1.69441000
H 0.97691500 -1.41626500 -1.07615400
H 1.89983400 1.36761700 -1.15337600
H 1.83740800 1.24271600 1.76084400
H -1.54470300 1.21814900 1.56486400
H -3.03417700 2.46961900 0.09138800
Pd -0.06306600 0.00367800 -0.13709100
H 3.55609600 -3.13858900 0.62691500
H -3.37586700 -3.00869100 0.11405600

56

RR_EI_D1_TS1_3W_HOphen_P, E(SCF) = -
2485.34634246, E(ZPE) = -2484.928777, E(G)
= -2484.999404 a.u.

C -0.47086900 3.22984400 0.13131500
H -1.13021500 4.05289100 -0.16138200
H -0.27254700 3.35121800 1.19938500
C 0.82110300 3.31320500 -0.65499600
H 0.61189400 3.36242000 -1.72613500
H 1.38357200 4.21174600 -0.37620900
N 1.64993900 2.09900700 -0.43120100

N -1.13436400 1.92528900 -0.04855000
C 2.31156100 2.05159500 0.90695500
H 2.95170800 2.93919400 0.98510200
C -2.28273100 1.88150500 -0.96451900
H -1.91546900 1.99403800 -1.99131500
C 3.08725800 0.79176900 1.06292700
C 2.50382900 -0.31102100 1.75194400
C 4.32287200 0.66991800 0.44569500
C 3.24346700 -1.52460400 1.72714300
C 5.01772700 -0.52723600 0.44918600
H 4.75573800 1.52707100 -0.06552800
C 4.46029000 -1.62959900 1.09500200
H 4.99375200 -2.57611400 1.09918000
C -3.04011600 0.59335500 -0.78662500
C -2.48247700 -0.66581100 -1.01859900
C -4.35644200 0.63720600 -0.33803100
C -3.21533600 -1.82841400 -0.82050300
C -5.09370800 -0.51466000 -0.14424000
H -4.81858300 1.59842300 -1.50425700
C -4.52243300 -1.75351300 -0.38535700
H -5.09570400 -2.66053200 -0.22884900
O 1.37119700 -0.23767500 2.35721800
O -1.18680200 -0.76589900 -1.464139100
S 6.62161300 -0.67919400 -0.32267700
S -6.80738100 -0.43894500 0.41024800
O -7.60291400 -1.02258300 -0.70468600
O -7.09466300 1.00003200 0.64859800
O -6.85867500 -1.26443000 1.64726900
O 6.88576900 0.62433000 -0.99725500
O 6.51625800 -1.81716200 -1.28390700
O 7.59304800 -0.96667700 -0.77529200
H 0.26633400 -1.49775500 1.92296300
H 0.58613500 -3.33146000 -1.55414800
H 1.49318200 -0.32412600 -1.46669500
O -0.49885000 -2.03277900 1.59993000
H -0.56199500 -1.78384600 0.67188000
H -0.19420300 0.58847500 2.52756800
O -1.16731500 0.71572600 2.57362800
H -1.48283200 -0.17905800 2.38386300
H 2.38820300 2.08039900 -1.13143900
H 1.53559900 2.11777600 1.67076100
H -1.41068200 1.57002600 0.87437400
H -2.96494300 2.71782200 -0.771068800
Pd 0.35531400 0.55679800 -0.85506900
O -0.30402100 -3.19664300 -1.89485200
H -0.91167800 -1.69480200 -1.69788900
H -0.30095000 -3.55551300 -2.78724900
H -2.74733900 -2.78955400 -1.00470000
H 2.81163100 -2.38244800 2.23518700

56

RR_EI_D1_TS1_3W_HOphen_R, E(SCF) = -
2485.33260107, E(ZPE) = -2484.917449, E(G)
= -2484.985227 a.u.

C -0.46715200 3.24383500 0.13276200
H -1.20405000 4.00864300 -0.12107800
H -0.17759000 3.40347100 1.17343400
C 0.72594400 3.32109600 -0.77920600
H 0.41519000 3.28598900 -1.82549600
H 1.28894300 4.24582100 -0.62038400
N 1.59361300 2.13866400 -0.53749500
N -1.08808100 1.89203100 0.06012800
C 2.44143300 2.22325500 0.69679400
H 3.11003500 3.08170300 0.56735900
C -2.27213900 1.76489700 -0.81133600
H -1.93881200 1.86053600 -1.85107500
C 3.19297300 0.95316400 0.89764700
C 2.68265300 -0.03983000 1.78825200
C 4.32727400 0.70884000 0.13377700
C 3.38046400 -1.28085800 1.79958500
C 4.98137500 -0.50782300 0.18144900
H 4.70855300 1.48268400 -0.52860500
C 4.49123800 -1.50660900 1.02278900
H 4.99221800 -2.46974900 1.06134100
C -3.01561800 0.48555900 -0.55962500
C -2.37838600 -0.76139500 -0.41687200
C -4.40456400 0.54142700 -0.48062700

| | | | |
|----|-------------|-------------|-------------|
| C | -3.16910300 | -1.89998200 | -0.18764800 |
| C | -5.16651500 | -0.59007500 | -0.27887300 |
| H | -4.90716100 | 1.49793100 | -0.58491200 |
| C | -4.54025100 | -1.82092900 | -0.12504600 |
| H | -5.12979300 | -2.71565800 | 0.04586500 |
| O | 1.64270500 | 0.14050300 | 2.51964800 |
| O | -1.06503400 | -0.95865900 | -0.48133000 |
| S | 6.45025400 | -0.81541500 | -0.79037600 |
| S | -6.95757400 | -0.49527900 | -0.17834800 |
| O | -7.46742100 | -1.44244400 | -1.20945500 |
| O | -7.30972100 | 0.92281100 | -0.46192100 |
| O | -7.30816500 | -0.91869900 | 1.20693800 |
| O | 6.64927300 | 0.39713300 | -1.63433100 |
| O | 6.16705500 | -2.04088600 | -1.59396100 |
| O | 7.55996100 | -1.02962800 | 0.18507000 |
| H | 0.46892100 | -1.22661100 | 2.37797400 |
| H | 1.36377500 | -0.66092800 | -1.38306900 |
| H | 1.70572700 | -0.60685700 | -0.64595000 |
| O | -0.33711700 | -1.77004300 | 2.23649300 |
| H | -0.53676100 | -1.64761400 | 1.29533800 |
| H | 0.05377700 | 0.94608500 | 2.67832800 |
| O | -0.92310400 | 1.03597500 | 2.73616400 |
| H | -1.19022000 | 0.10299400 | 2.73766600 |
| H | 2.22533800 | 2.03483200 | -1.33064800 |
| H | 1.78276600 | 2.41928700 | 1.54371200 |
| H | -1.31648500 | 1.59751500 | 1.02764900 |
| H | -2.94188600 | 2.60689000 | -0.60927900 |
| Pd | 0.30341900 | 0.52572900 | -0.53920800 |
| O | 0.24533300 | -3.39358400 | -0.90172500 |
| H | -0.29458500 | -2.58511700 | -0.85555100 |
| H | 0.11366100 | -3.72716200 | -1.79182000 |
| H | -2.66015300 | -2.85172400 | -0.06966300 |
| H | 3.00182500 | -2.05749300 | 2.45795500 |

56

RR_EI_D1_TS1_3W_HOphen, E(SCF) = -
 2485.32031818, E(ZPE) = -2484.906657, E(G) =
 -2484.974146 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.49750800 | 3.15488800 | 0.26763600 |
| H | -1.21327100 | 3.95031200 | 0.04466900 |
| H | -0.21381700 | 3.26276000 | 1.31706100 |
| C | 0.71078400 | 3.26502500 | -0.62737800 |
| H | 0.41053400 | 3.28469000 | -1.67721200 |
| H | 1.27587100 | 4.17893200 | -0.41569900 |
| N | 1.57157700 | 2.06862500 | -0.43798100 |
| N | -1.13383700 | 1.82424600 | 0.12273500 |
| C | 2.36170700 | 2.08186400 | 0.83397700 |
| H | 3.00024600 | 2.97315600 | 0.80771700 |
| C | -2.30764900 | 1.76147500 | -0.76589500 |
| H | -1.95639600 | 1.88279200 | -1.79758600 |
| C | 3.15822400 | 0.83242800 | 0.97519500 |
| C | 2.64140600 | -0.25066800 | 1.74636900 |
| C | 4.34194200 | 0.69783400 | 0.26511900 |
| C | 3.39685500 | -1.45509200 | 1.71301500 |
| C | 5.04956500 | -0.49129900 | 0.25768400 |
| H | 4.72021000 | 1.53892700 | -0.31121700 |
| C | 4.56122700 | -1.57200000 | 0.99145800 |
| H | 5.10535400 | -2.51241500 | 0.98879400 |
| C | -3.07394900 | 0.48417900 | -0.57793100 |
| C | -2.46270000 | -0.78543400 | -0.59204200 |
| C | -4.45133700 | 0.56144900 | -0.39318200 |
| C | -3.26841400 | -1.92202000 | -0.41524600 |
| C | -5.22919700 | -0.56748200 | -0.23432600 |
| H | -4.93296100 | 1.53411200 | -0.37149800 |
| C | -4.62988800 | -1.82062500 | -0.24635700 |
| H | -5.22986900 | -2.71467500 | -0.11232800 |
| O | 1.55084600 | -0.17240800 | 2.42225200 |
| O | -1.16062400 | -0.98939100 | -0.75985000 |
| S | 6.59093100 | -0.65432000 | -0.63190200 |
| S | -7.00963000 | -0.44336100 | -0.03441300 |
| O | -7.59685500 | -1.07042400 | -1.25319900 |
| O | -7.30967600 | 1.01069400 | 0.07406000 |
| O | -7.33328300 | -1.20217000 | 1.20646400 |
| O | 6.76051800 | 0.60744400 | -1.40858600 |
| O | 6.44284500 | -1.85557200 | -1.50645600 |
| O | 7.65542800 | -0.84310700 | 0.39879000 |
| H | 0.38501500 | -1.48488500 | 2.09567500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.15087100 | -1.37483100 | -1.37162900 |
| H | 1.52933900 | -0.42024200 | -1.27332100 |
| O | -0.41555800 | -2.02173100 | 1.90000100 |
| H | -0.64330400 | -1.77744900 | 0.98999800 |
| H | -0.00868100 | 0.63798300 | 2.66400500 |
| O | -0.98077200 | 0.74709500 | 2.76348300 |
| H | -1.27801400 | -0.17025000 | 2.66891100 |
| H | 2.23834100 | 2.02280800 | -1.20635300 |
| H | 1.65928700 | 2.18343500 | 1.66207800 |
| H | -1.37722200 | 1.48058900 | 1.06357900 |
| H | -2.97113600 | 2.60590500 | -0.54904200 |
| Pd | 0.27493600 | 0.47931900 | -0.61634400 |
| O | 0.72418100 | -2.50778300 | -1.49914200 |
| H | -0.23377200 | -2.27275800 | -1.35031100 |
| H | 0.83299900 | -2.82401900 | -2.40521200 |
| H | -2.78090700 | -2.89189500 | -0.41714200 |
| H | 3.01645200 | -2.29714700 | 2.28452200 |

53

RR_EI_D1_TS1_HOphen_P, E(SCF) = -
 2408.90156463, E(ZPE) = -2408.508691, E(G) =
 -2408.575405 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.48371400 | 2.94590300 | 1.00208900 |
| H | -1.13826500 | 3.82281700 | 0.98426900 |
| H | -0.28064000 | 2.72832100 | 2.05388700 |
| C | 0.80541100 | 3.26369200 | 0.27324100 |
| H | 0.59383000 | 3.63985700 | -0.73016800 |
| H | 1.37259100 | 4.03106000 | 0.81239100 |
| N | 1.63085000 | 2.03712000 | 0.11258300 |
| N | -1.15718000 | 1.76711800 | 0.42585700 |
| C | 2.29330500 | 1.58901300 | 1.37261800 |
| H | 2.92963300 | 2.41507300 | 1.71457200 |
| C | -2.31589500 | 2.03026600 | -0.43856400 |
| H | -1.96129200 | 2.47684200 | -1.37478800 |
| C | 3.07572800 | 0.34356100 | 1.15181500 |
| C | 2.50281900 | -0.91618400 | 1.49174300 |
| C | 4.31835900 | 0.41572300 | 0.53990400 |
| C | 3.25978000 | -2.06473500 | 1.13356000 |
| C | 5.03102900 | -0.72528000 | -0.21506100 |
| H | 4.74435800 | 1.38753800 | 0.30108000 |
| C | 4.48336000 | -1.97216700 | 0.51294600 |
| H | 5.03169700 | -2.87426100 | 0.25591300 |
| C | -3.07300000 | 0.75589000 | -0.69018100 |
| C | -2.53651400 | -0.33371000 | -1.37463000 |
| C | -4.36660600 | 0.62121700 | -0.19699400 |
| C | -3.26113400 | -1.49614200 | -1.57927900 |
| C | -5.10007900 | -0.53214500 | -0.39762700 |
| H | -4.81650400 | 1.44347800 | 0.34896800 |
| C | -4.54843100 | -1.59650900 | -1.09121400 |
| H | -5.12022200 | -2.50409700 | -1.24879500 |
| O | 1.36327400 | -1.02899600 | 2.07758500 |
| O | -1.25174400 | -0.24170800 | -1.87452200 |
| S | 6.63376900 | -0.63296800 | -0.56946400 |
| S | -6.78534100 | -0.67830200 | 0.22714100 |
| O | -6.77350700 | -1.87508200 | 1.11056800 |
| O | -7.63196900 | -0.86223100 | -0.98307500 |
| O | -7.05912400 | 0.58974400 | 0.95241200 |
| O | 6.92035600 | 0.81725100 | -0.76555400 |
| O | 6.51145100 | -1.37704400 | -1.85883500 |
| O | 7.59796000 | -1.29048100 | 0.36284400 |
| H | 0.28000300 | -2.11255200 | 1.29489900 |
| H | -1.04709600 | -0.96906100 | -2.47459900 |
| H | 1.47844000 | 0.08623800 | -1.62943700 |
| O | -0.48847200 | -2.56610300 | 0.86991700 |
| H | -0.43055700 | -2.30885200 | -0.05443800 |
| H | -0.22326000 | -0.30491600 | 2.46357200 |
| O | -1.20135300 | -0.22957300 | 2.50526500 |
| H | -1.46462800 | -1.01632600 | -2.00441700 |
| H | 2.36777700 | 2.23024400 | -0.56256900 |
| H | 1.51542900 | 1.42261000 | 2.11794600 |
| H | -1.42924600 | 1.13671900 | 1.18947100 |
| H | -2.99356300 | 2.75344100 | 0.03030500 |
| Pd | 0.33201300 | 0.71240900 | -0.77753400 |
| H | 2.83560500 | -3.03609300 | 1.37239500 |
| H | -2.80869600 | -2.32480300 | -2.11439200 |

53

RR_EI_D1_TS1_HOphen R, E(SCF) = -
 2408.89544370, E(ZPE) = -2408.504400, E(G)
 = -2408.569891 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.46237100 | 3.01702400 | 0.70298000 |
| H | -1.19058900 | 3.82703800 | 0.62214500 |
| H | -0.15395100 | 2.95972300 | 1.74886400 |
| C | 0.71836100 | 3.26241500 | -0.19685100 |
| H | 0.39000700 | 3.43370700 | -1.22411800 |
| H | 1.29131000 | 4.13650700 | 0.12773100 |
| N | 1.57916600 | 2.05042900 | -0.20369700 |
| N | -1.10536300 | 1.71804500 | 0.36973800 |
| C | 2.45572100 | 1.90703200 | 1.00293000 |
| H | 3.11606800 | 2.78145700 | 1.02532600 |
| C | -2.29345000 | 1.78503400 | -0.50329300 |
| H | -1.95915300 | 2.07759900 | -1.50551500 |
| C | 3.22659300 | 0.63504500 | 0.94591400 |
| C | 2.69338400 | -0.53443000 | 1.56688600 |
| C | 4.40349200 | 0.57766300 | 0.21179700 |
| C | 3.42798600 | -1.71804600 | 1.36973800 |
| C | 5.08870400 | -0.61131900 | 0.04345700 |
| H | 4.79511000 | 1.48140300 | -0.24907100 |
| C | 4.58578600 | -1.77246200 | 0.62970900 |
| H | 5.11490300 | -2.71198000 | 0.49664200 |
| C | -3.05379800 | 0.49194700 | -0.50142000 |
| C | -2.42547200 | -0.76455900 | -0.62260600 |
| C | -4.43996200 | 0.54505900 | -0.38325600 |
| C | -3.23334500 | -1.91688500 | -0.61161100 |
| C | -5.21457800 | -0.59581800 | -0.39302400 |
| H | -4.93024500 | 1.50795800 | -0.27901600 |
| C | -4.60149700 | -1.83834100 | -0.50510200 |
| H | -5.20021400 | -2.74352300 | -0.50123700 |
| O | 1.59799000 | -0.52620600 | 2.23675900 |
| O | -1.12369400 | -0.96343700 | -0.75228600 |
| S | 6.61341100 | -0.68608000 | -0.88749800 |
| S | -7.00312100 | -0.50431400 | -0.27205300 |
| O | -7.37621700 | -1.34757000 | 0.89880300 |
| O | -7.52253800 | -1.05501900 | -1.55664200 |
| O | -7.32893900 | 0.93596900 | -0.08206800 |
| O | 6.83431700 | 0.68260600 | -1.43514200 |
| O | 6.40055800 | -1.70958900 | -1.95326800 |
| O | 7.67277800 | -1.09837900 | 0.08064800 |
| H | 0.44210200 | -1.86509100 | 1.87442000 |
| H | 1.27835800 | -0.51119900 | -1.60338200 |
| H | 1.62761300 | -0.63655000 | -0.88018100 |
| O | -0.36570900 | -2.37514000 | 1.64776800 |
| H | -0.59463500 | -2.05846900 | 0.75820900 |
| H | 0.03553800 | 0.20572900 | 2.67433200 |
| O | -0.93845600 | 0.27183800 | 2.78285300 |
| H | -1.20487500 | -0.63524900 | 2.56377400 |
| H | 2.19355800 | 2.09525600 | -1.01564500 |
| H | 1.81477000 | 1.93518100 | 1.88491400 |
| H | -1.33686600 | 1.23787100 | 1.25872700 |
| H | -2.94906200 | 2.58141600 | -0.13615300 |
| Pd | 0.26055100 | 0.47523900 | -0.49687800 |
| H | 3.03608300 | -2.64134700 | 1.82524000 |
| H | -2.73648500 | -2.87780200 | -0.69511200 |

53

RR_EI_D1_TS1_HOphen, E(SCF) = -
 2408.85515586, E(ZPE) = -2408.467403, E(G)
 = -2408.532774 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.43599000 | 2.99290000 | -1.11416300 |
| H | -1.17289800 | 3.62508900 | -1.61813800 |
| H | 0.12707300 | 3.63291500 | -0.43165700 |
| C | 0.47876700 | 2.33721000 | -2.12056300 |
| H | -0.10006400 | 1.78125700 | -2.86108500 |
| H | 1.07535800 | 3.08482500 | -2.65280300 |
| N | 1.36615800 | 1.36377400 | -1.42955300 |
| N | -1.10318600 | 1.96022900 | -0.28983100 |
| C | 2.52466000 | 2.00905900 | -0.73527000 |
| H | 3.12096300 | 2.51282300 | -1.50461400 |
| C | -2.38266500 | 1.48799200 | -0.82599700 |
| H | -2.22785800 | 1.27185600 | -1.88953200 |
| C | 3.33134700 | 1.01304300 | 0.01959400 |
| C | 2.98880100 | 0.73012000 | 1.37465800 |
| C | 4.35120800 | 0.32126900 | -0.61605000 |
| C | 3.74291300 | -0.29185700 | 2.01184600 |

| | | | |
|----|-------------|-------------|-------------|
| C | 5.06284900 | -0.66984000 | 0.03722000 |
| H | 4.59801000 | 0.55422400 | -1.64885700 |
| C | 4.74557600 | -0.97163000 | 1.36073900 |
| H | 5.29698600 | -1.75132900 | 1.87908000 |
| C | -3.04268800 | 0.27463800 | -0.19333700 |
| C | -2.46727600 | -0.78190800 | 0.52700800 |
| C | -4.41081000 | 0.17955300 | -0.46902300 |
| C | -3.24289900 | -1.87437500 | 0.92136300 |
| C | -5.16932200 | -0.89894200 | -0.07662300 |
| H | -4.89567300 | 0.97906000 | -1.02056400 |
| C | -4.58370900 | -1.94168800 | 0.62895800 |
| H | -5.17558000 | -2.79356000 | 0.94494800 |
| O | 2.03804600 | 1.34293500 | 1.98539900 |
| O | -1.17373900 | -0.80050500 | 0.97404600 |
| S | 6.38725400 | -1.55277400 | -0.77551800 |
| S | -6.92638700 | -0.98455600 | -0.46797800 |
| O | -7.61555200 | -1.09228200 | 0.84679600 |
| O | -7.08006200 | -2.20801200 | -1.30200500 |
| O | -7.24451800 | 0.27032700 | -1.19883000 |
| O | 6.43929700 | -1.03199200 | -2.17178600 |
| O | 6.02651300 | -3.00074500 | -0.71319400 |
| O | 7.62955100 | -1.25402100 | -0.00189600 |
| H | 0.90114100 | 0.43970900 | 2.98598500 |
| H | -0.21765300 | -1.38838300 | 0.38510500 |
| H | 0.74996100 | -1.30223500 | -0.10277000 |
| O | 0.09649900 | 0.11814600 | 3.45410700 |
| H | -0.42128400 | -0.30877900 | 2.75767100 |
| H | 0.63024000 | 2.47704000 | 2.05784100 |
| O | -0.27049400 | 2.76474300 | 2.31672900 |
| H | -0.51180300 | 2.05164000 | 2.92929300 |
| H | 1.74784400 | 0.72195400 | -2.12142800 |
| H | 2.12358800 | 2.76702700 | -0.05953800 |
| H | -1.17628200 | 2.30097800 | 0.67920600 |
| H | -3.10014900 | 2.31576100 | -0.78510700 |
| Pd | 0.10786400 | 0.28665300 | -0.18285800 |
| H | 3.49484700 | -0.52779600 | 3.04296000 |
| H | -2.75206100 | -2.66284700 | 1.48000500 |

53

RR_EI_D1_TS1_non-trigo_P, E(SCF) = -
 2408.89484593, E(ZPE) = -2408.504790, E(G)
 = -2408.570625 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.47475300 | 2.93788500 | 0.72818000 |
| H | -1.17554400 | 3.77098800 | 0.64451300 |
| H | -0.19977700 | 2.84516600 | 1.78022200 |
| C | 0.73599600 | 3.17062700 | -0.13486700 |
| H | 0.43968800 | 3.40232700 | -1.16013800 |
| H | 1.33898100 | 4.00221200 | 0.24318800 |
| N | 1.54525000 | 1.92443400 | -0.18109300 |
| N | -1.14824300 | 1.66605700 | 0.34513400 |
| C | 2.34499300 | 1.66562400 | 1.05758600 |
| H | 2.96862900 | 2.55076200 | 1.22707500 |
| C | -2.36417000 | 1.80023200 | -0.48357000 |
| H | -2.05348500 | 2.12664200 | -1.48284700 |
| C | 3.17631300 | 0.43793700 | 0.91428500 |
| C | 2.64397200 | -0.82667000 | 1.31345900 |
| C | 4.43296800 | 0.52518800 | 0.33952300 |
| C | 3.46985400 | -1.95472200 | 1.08105200 |
| C | 5.21022200 | -0.60309600 | 0.12354800 |
| H | 4.81342700 | 1.50208300 | 0.04611900 |
| C | 4.71723800 | -1.84529900 | 0.50447500 |
| H | 5.32445300 | -2.72831100 | 0.33731800 |
| C | -3.15011700 | 0.52482000 | -0.50960800 |
| C | -2.55091700 | -0.72597400 | -0.78408000 |
| C | -4.51485200 | 0.57949800 | -0.26617000 |
| C | -3.36873500 | -1.86593100 | -0.79276800 |
| C | -5.30714100 | -0.55498300 | -0.29860300 |
| H | -4.97132900 | -1.54127900 | -0.04782700 |
| C | -4.72598500 | -1.78447100 | -0.56224900 |
| H | -5.34243700 | -2.67561300 | -0.57949200 |
| O | 1.46991300 | -0.95174700 | 1.82681700 |
| O | -1.26967500 | -0.90553600 | -1.05889300 |
| S | 6.84117900 | -0.42167500 | -0.58913300 |
| S | -7.07062500 | -0.39846800 | 0.00118600 |
| O | -7.61789900 | -1.78201000 | -0.04711000 |
| O | -7.59144600 | 0.47305600 | -1.09087100 |
| O | -7.20239000 | 0.23546900 | 1.34392400 |

O 6.66515000 0.38644300 -1.83183100
O 7.32994800 -1.80330800 -0.86150200
O 7.66854100 0.29217600 0.42920100
H 0.47942800 -2.27016400 1.13485900
H 1.18375400 -0.39003900 -1.85660800
H 1.40965200 -0.74642000 -1.16129700
O -0.10221600 -2.89585800 0.65368900
H -0.54607800 -2.33235200 0.00054800
H 0.13029800 -0.13147500 2.44917500
O -0.69768500 0.33109200 2.72768700
H -1.16147800 -0.27012900 3.31362400
H 2.20783000 1.99824600 -0.95202000
H 1.64899600 1.56858100 1.89205700
H -1.35611700 1.15004100 1.21708500
H -2.98826200 2.59418200 -0.06112800
Pd 0.16716200 0.44144600 -0.63505400
H 3.08349400 -2.92600900 1.37560100
H -2.89871200 -2.82184000 -0.99873600

53
RR_EI_D1_TS1_non-trigo, E(SCF) = -
2408.88568435, E(ZPE) = -2408.496951, E(G)
= -2408.561997 a.u.
C -0.43906500 2.89490800 0.67053200
H -1.09078700 3.77068600 0.61460900
H -0.00276200 2.86971300 1.67058300
C 0.63487600 2.95696700 -0.38158100
H 0.18935100 3.05462800 -1.37391500
H 1.29695600 3.81312000 -0.21930100
N 1.41158600 1.68990200 -0.37711400
N -1.23535500 1.64931900 0.51413600
C 2.42303300 1.57308700 0.71437800
H 3.00203700 2.50273300 0.74371400
C -2.48377700 1.76317000 -0.24788800
H -2.21562900 2.04244200 -1.27338800
C 3.33044800 0.41006300 0.47852800
C 2.81634200 -0.91346400 0.56268500
C 4.66305000 0.61775200 0.16896000
C 3.70955200 -1.97236100 0.31428900
C 5.52474700 -0.44760800 -0.05254400
H 5.04211300 1.63527000 0.10994200
C 5.03894600 -1.74453600 0.01692000
H 5.71410300 -2.57334100 -0.16477000
C -3.31220700 0.50895300 -0.20506600
C -2.78484200 -0.80302400 -0.20453400
C -4.69517500 0.67897200 -0.20184000
C -3.69836100 -1.87838300 -0.20729700
C -5.56703500 -0.38794100 -0.21265800
H -5.10372500 1.68451000 -0.19050300
C -5.05710000 -1.68200600 -0.21349100
H -5.73066700 -2.53302800 -0.21400100
O 1.56391600 -1.14209500 0.84422100
O -1.50690600 -1.12869000 -0.19084700
S 7.24011100 -0.11262000 -0.45082900
S -7.34327300 -0.14028500 -0.22144600
O -7.55451400 1.33226500 -0.15838500
O -7.86130800 -0.85602200 0.97973000
O -7.83139500 -0.74480700 -1.49459500
O 7.22630600 0.61868800 -1.75168500
O 7.90969400 -1.44022300 -0.53963900
O 7.76533500 0.72991900 0.66270700
H 0.72759800 -2.74790500 0.65655600
H 0.95415800 -0.83677800 -2.15357400
H 0.98233400 -1.37614600 -1.61979400
O 0.03049200 -3.40086700 0.45106700
H -0.69827400 -2.81526100 0.18972700
H 0.56511600 -0.38121500 2.23713600
O -0.04154500 0.16977400 2.77280200
H -0.17979900 -0.30995800 3.59243900
H 1.91616500 1.62268700 -1.26044500
H 1.88036200 1.48049100 1.65910300
H -1.41171100 1.25704400 1.44452600
H -3.07601300 2.58834700 0.16532800
Pd -0.01308700 0.20085600 -0.29525100
H 3.32101000 -2.98494500 0.36925700
H -3.28417000 -2.88137200 -0.20381200

53
RR_EI_D1_TS1_P_CH_P, E(SCF) = -
2408.89666390, E(ZPE) = -2408.504164, E(G)
= -2408.570579 a.u.
N 1.54288600 1.87755200 -0.03483400
N -1.16710500 1.52047900 0.65017300
C 2.32447500 1.34189700 1.09625700
H 3.10198700 2.06179600 1.37769000
C -2.39941500 1.85147000 -0.07303800
H -2.11412500 2.40982300 -0.97480300
C 2.93697900 -0.02636500 0.80282500
C 3.20722600 -0.75933300 2.10576900
C 4.07436900 0.04730500 -0.14937000
C 4.52140300 -1.33714400 2.30003000
C 5.25323500 -0.50859600 0.12420900
H 3.92628600 0.55726600 -1.09719000
C 5.47982700 -1.21101100 1.36750300
H 6.46058700 -1.64579400 1.53489100
C -3.19692200 0.62494500 -0.41423400
C -2.65417200 -0.49557700 -1.09009200
C -4.54276400 0.61126300 -0.05771900
C -3.52366800 -1.56948500 -1.37776600
C -5.37249200 -0.45104700 -0.35552100
H -4.95900500 1.46516600 0.46774200
C -4.85064100 -1.55468100 -1.02102200
H -5.48887700 -2.39997800 -1.25887000
O 2.32243300 -0.86291600 2.95465900
O -1.40461100 -0.62859200 -1.48836600
S 6.63446700 -0.42068700 -1.02851700
S -7.09872100 -0.45086600 0.12665800
O -7.25990400 -1.59010300 -1.07640500
O -7.87546900 -0.65233100 -1.13101400
O -7.35382700 0.87283900 0.76065200
O 6.14181900 0.34275900 -2.20174600
O 6.96096600 -1.84002100 -1.33032200
O 7.70949300 0.27314400 -0.26984300
H 0.29206500 -3.00518700 -0.00286600
H 1.07175700 -0.02484700 -1.90327700
H 2.13046000 -0.60674600 0.31377500
O -0.56845200 -2.64214300 0.22184100
H -0.78531900 -2.02472700 -0.50813400
H 0.40262900 -0.73263700 2.63646300
O -0.53761000 -0.79386000 2.40049100
H -0.55536700 -1.45713100 1.68443300
H 2.17814500 2.16546300 -0.77423000
H 1.65204200 1.22447300 1.94666500
H -1.33857900 0.82295300 1.37764000
H -3.02590000 2.52214600 0.52916100
Pd 0.11384100 0.57211500 -0.81196100
H 4.69648600 -1.86232000 3.23167900
H -3.09870000 -2.42399300 -1.89483200
C -0.43327100 2.65986300 1.22546600
C 0.73769400 3.06826000 0.35463200
H -0.08874000 2.36802100 2.22014400
H 0.38283400 3.52265400 -0.57276600
H 1.36365000 3.80242400 0.87436800
H -1.09327600 3.52175100 1.36727800

53
RR_EI_D1_TS1_P_CH_R, E(SCF) = -
2408.89566946, E(ZPE) = -2408.504076, E(G)
= -2408.567621 a.u.
N 1.61089700 2.08971200 -0.16288300
N -1.08347600 1.75263800 0.29766400
C 2.40474500 1.89939100 1.09195800
H 3.06894700 2.76622300 1.18625200
C -2.26424900 1.80963900 -0.58801100
H -1.92333800 2.10456600 -1.58728500
C 3.16261700 0.61823100 1.04127700
C 2.63729000 -0.54123100 1.68772800
C 4.32578200 0.54637400 0.28537100
C 3.35723000 -1.75064900 1.47595000
C 4.99744300 -0.64819300 0.10745200
H 4.71792300 1.44417500 -0.18698400
C 4.49609500 -1.80257200 0.70898700
H 5.01288400 -2.74784700 0.56834400
C -3.00911400 0.50824700 -0.58823700

| | | | |
|----|-------------|-------------|-------------|
| C | -2.36407300 | -0.73632200 | -0.74070500 |
| C | -4.39149400 | 0.53831600 | -0.42840800 |
| C | -3.15386800 | -1.90065100 | -0.73326500 |
| C | -5.14870400 | -0.61467000 | -0.43583600 |
| H | -4.89281100 | 1.49232500 | -0.29772400 |
| C | -4.51963500 | -1.84517400 | -0.58501600 |
| H | -5.10411100 | -2.75963300 | -0.58316200 |
| O | 1.56814000 | -0.52557200 | 2.40019400 |
| O | -1.06158600 | -0.90910700 | -0.89870500 |
| S | 6.48967500 | -0.74316000 | -0.87332100 |
| S | -6.92432300 | -0.55813200 | -0.18003600 |
| O | -7.16216000 | -1.20305700 | 1.14315500 |
| O | -7.52161000 | -1.33269300 | -1.30443000 |
| O | -7.29722600 | 0.88310200 | -0.19905300 |
| O | 6.73918100 | 0.67327300 | -1.36458700 |
| O | 6.20586000 | -1.72379000 | -1.96266400 |
| O | 7.56589100 | -1.22301000 | 0.04365900 |
| H | 0.40988800 | -1.81114200 | 1.85679000 |
| H | 1.34990500 | -0.42597700 | -1.66796700 |
| H | 1.68356200 | -0.56544800 | -0.93943700 |
| O | -0.37687900 | -2.31761600 | 1.56043500 |
| H | -0.54299400 | -1.99672900 | 0.65931800 |
| H | -0.01476700 | 0.21676200 | 2.66080900 |
| O | -0.99351800 | 0.30589800 | 2.70575000 |
| H | -1.26775900 | -0.59454500 | 2.47103000 |
| H | 2.27553600 | 2.15128800 | -0.93292100 |
| H | 1.71037700 | 1.90215600 | 1.93262100 |
| H | -1.32155000 | 1.26146800 | 1.17946700 |
| H | -2.93113700 | 2.59912900 | -0.22700800 |
| Pd | 0.30528100 | 0.53168500 | -0.56465100 |
| H | 2.96972700 | -2.64905100 | 1.94789800 |
| H | -2.64538400 | -2.85233500 | -0.84675700 |
| C | -0.46655300 | 3.05871400 | 0.65616500 |
| C | 0.75998100 | 3.30739200 | -0.17948300 |
| H | -0.21792200 | 3.01274700 | 1.71840500 |
| H | 0.48447900 | 3.49482300 | -1.21952700 |
| H | 1.32222000 | 4.17215500 | 0.18611300 |
| H | -1.19386800 | 3.86313100 | 0.52830800 |

53
RR_EI_D1_TS1_P_CH_TS, E(SCF) = -
2408.87228888, E(ZPE) = -2408.484435, E(G)
= -2408.548325 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.49908500 | 2.17615600 | -0.37614100 |
| N | -1.19114000 | 1.80507600 | 0.32761500 |
| C | 2.46155300 | 2.01547600 | 0.74650200 |
| H | 3.20743600 | 2.81538100 | 0.69127500 |
| C | -2.33895400 | 1.76329100 | -0.58560000 |
| H | -1.97470700 | 1.97729700 | -1.59821900 |
| C | 3.11313100 | 0.65749800 | 0.68616000 |
| C | 2.79940800 | -0.32155900 | 1.72303800 |
| C | 4.31383700 | 0.50912800 | -0.07407000 |
| C | 3.57903900 | -1.52889700 | 1.68866000 |
| C | 5.03182800 | -0.64112100 | -0.03109100 |
| H | 4.61997700 | 1.31094700 | -0.74016200 |
| C | 4.64371400 | -1.67433800 | 0.85760200 |
| H | 5.22226300 | -2.59333700 | 0.87513200 |
| C | -3.04224100 | 0.43436900 | -0.50133100 |
| C | -2.37368500 | -0.81394200 | -0.43957000 |
| C | -4.43480600 | 0.45260500 | -0.48064900 |
| C | -3.16649900 | -1.97736100 | -0.34896700 |
| C | -5.18572900 | -0.70220300 | -0.41264600 |
| H | -4.95227100 | 1.40654000 | -0.51944400 |
| C | -4.53907900 | -1.93093800 | -0.33830800 |
| H | -5.11621900 | -2.84780400 | -0.27155200 |
| O | 1.84137500 | -0.18238300 | 2.51880700 |
| O | -1.06743800 | -1.00819200 | -0.46365500 |
| S | 6.49784800 | -0.87914000 | -1.03855300 |
| S | -6.97738700 | -0.64682400 | -0.39022400 |
| O | -7.39049200 | -1.27523200 | 0.89800100 |
| O | -7.42346000 | -1.43875700 | -1.57264200 |
| O | -7.34870900 | 0.79275400 | -0.48041500 |
| O | 6.64331900 | 0.35915600 | -1.84911100 |
| O | 6.22053400 | -2.09197600 | -1.85762200 |
| O | 7.61204200 | -1.08625400 | -0.07188300 |
| H | 0.57556400 | -1.65370000 | 2.19668800 |
| H | 1.51394400 | -0.47147400 | -0.92701800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.18143100 | -0.03246000 | -0.20249700 |
| O | -0.25464400 | -2.11758600 | 1.99401300 |
| H | -0.47217300 | -1.84481100 | 1.08151400 |
| H | 0.10968900 | 0.57288900 | 2.81983100 |
| O | -0.86045900 | 0.55852900 | 2.91112700 |
| H | -1.04703300 | -0.38045100 | 2.74457700 |
| H | 2.02798300 | 2.20685200 | -1.23650800 |
| H | 1.90696400 | 2.12231000 | 1.67987500 |
| H | -1.43595200 | 1.38795300 | 1.23496400 |
| H | -3.04953000 | 2.55675200 | -0.32598600 |
| Pd | 0.26915800 | 0.52239400 | -0.43088800 |
| H | 3.31038000 | -2.30805700 | 2.39448300 |
| H | -2.64400400 | -2.92687900 | -0.29125500 |
| C | -0.55824700 | 3.11622000 | 0.59120200 |
| C | 0.60829900 | 3.36443300 | -0.33570300 |
| H | -0.22429200 | 3.10059800 | 1.63167300 |
| H | 0.25229200 | 3.51892900 | -1.35651300 |
| H | 1.16655000 | 4.25652600 | -0.03486800 |
| H | -1.28851400 | 3.92622500 | 0.50066500 |

53
RR_EI_D1_TS1_P_HH-Homo_P, E(SCF) = -
2408.86759576, E(ZPE) = -2408.476181, E(G)
= -2408.541414 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.40405200 | 2.87584300 | 1.03248200 |
| H | -1.10626400 | 3.69522100 | 1.21744700 |
| H | 0.13160300 | 2.70476100 | 1.96870200 |
| C | 0.55598500 | 3.28169700 | -0.06758600 |
| H | 0.01398200 | 3.57876400 | -0.96710600 |
| H | 1.16815200 | 4.13075400 | 0.25139500 |
| N | 1.44302800 | 2.14064100 | -0.43735900 |
| N | -1.11759900 | 1.63243900 | 0.69482200 |
| C | 2.51748500 | 1.90979600 | 0.57803400 |
| H | 3.20188500 | 2.76177300 | 0.52879800 |
| C | -2.40986700 | 1.82219000 | 0.03020700 |
| H | -2.23220000 | 2.37467000 | -0.90049400 |
| C | 3.25098200 | 0.62569400 | 0.41425600 |
| C | 2.54939400 | -0.57548700 | 0.65320900 |
| C | 4.60505400 | 0.59788600 | 0.11678100 |
| C | 3.26976700 | -1.78050800 | 0.61655600 |
| C | 5.29086900 | -0.60246500 | 0.06850900 |
| H | 5.13897100 | 1.52459200 | -0.06910200 |
| C | 4.61826700 | -1.79143100 | 0.33044000 |
| H | 5.15876600 | -2.73258500 | 0.30049400 |
| C | -3.13512100 | 0.52977500 | -0.23404100 |
| C | -2.53185800 | -0.66450200 | -0.68802300 |
| C | -4.51706100 | 0.54606400 | -0.04471800 |
| C | -3.36612700 | -1.77395400 | -0.93748000 |
| C | -5.31250600 | -0.55043700 | -0.29725700 |
| H | -4.98842500 | 1.45662600 | 0.31235700 |
| C | -4.72421900 | -1.72889500 | -0.74109400 |
| H | -5.33195700 | 2.60568900 | -0.93938600 |
| O | 1.25527200 | -0.55902900 | 0.89550300 |
| O | -1.23933700 | -0.89357700 | -0.88663300 |
| S | 7.04396300 | -0.65334500 | -0.30966700 |
| S | -7.08298500 | -0.50237000 | -0.00992200 |
| O | -7.33578300 | -1.44006600 | 1.12150000 |
| O | -7.71099000 | -0.96446000 | -1.28023700 |
| O | -7.40954800 | 0.91161500 | 0.32281700 |
| O | 7.44670700 | 0.75278300 | -0.58973200 |
| O | 7.17800600 | -1.54577900 | -1.49660300 |
| O | 7.70770200 | -1.21806500 | 0.90058100 |
| H | 0.31237400 | -2.13459500 | 1.14070400 |
| H | -0.40034000 | 1.20554900 | -1.94770300 |
| H | 0.99879200 | -0.08831900 | -1.82337400 |
| O | -0.48868900 | -2.69213000 | 1.18328700 |
| H | -0.94283200 | -2.38389600 | 0.38433600 |
| H | 0.18662400 | -0.26961400 | 2.42066700 |
| O | -0.69243700 | -0.30423000 | 2.84130800 |
| H | -1.01733700 | -1.15770300 | 2.51132200 |
| H | 1.88982600 | 2.34759400 | -1.32812700 |
| H | 2.02662000 | 1.92831800 | 1.55416600 |
| H | -1.23970900 | 1.05830900 | 1.53746600 |
| H | -3.05252200 | 2.46031700 | 0.64920800 |
| Pd | 0.15987500 | 0.54151100 | -0.69752200 |
| H | -2.88931000 | -2.68270600 | -1.29031600 |
| H | 2.73620200 | -2.70584600 | 0.80978500 |

53
RR_EI_D1_TS1_P_HH-Homo_TS, E(SCF) = -
2408.86487992, E(ZPE) = -2408.475689, E(G)
= -2408.540653 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.40434400 | 2.87192500 | 1.04009000 |
| H | -1.11288100 | 3.68469100 | 1.23115400 |
| H | 0.13351900 | 2.69866100 | 1.97447500 |
| C | 0.54829200 | 3.28635800 | -0.06083000 |
| H | 0.00109800 | 3.57093300 | -0.96148200 |
| H | 1.15058000 | 4.14527400 | 0.25137500 |
| N | 1.44723300 | 2.15318900 | -0.42453600 |
| N | -1.10941200 | 1.62505600 | 0.69561100 |
| C | 2.51618500 | 1.92756700 | 0.59937000 |
| H | 3.20373600 | 2.77664700 | 0.54281100 |
| C | -2.38859100 | 1.81532700 | 0.00406900 |
| H | -2.19022700 | 2.34974700 | -0.93325200 |
| C | 3.24324000 | 0.63880800 | 0.45138300 |
| C | 2.53802100 | -0.53821800 | 0.73424800 |
| C | 4.58892500 | 0.59759400 | 0.12056800 |
| C | 3.25480500 | -1.76337600 | 0.70138900 |
| C | 5.26755500 | -0.60734900 | 0.07771900 |
| H | 5.12332900 | 1.51735200 | -0.09678600 |
| C | 4.59432700 | -1.78730700 | 0.37839800 |
| H | 5.12882300 | -2.73218300 | 0.35205400 |
| C | -3.12008600 | 0.52613100 | -0.25091200 |
| C | -2.51574900 | -0.66761600 | -0.70248700 |
| C | -4.50107600 | 0.54157100 | -0.05754900 |
| C | -3.34701300 | -1.78005700 | -0.94708400 |
| C | -5.29446500 | -0.55788300 | -0.30494100 |
| H | -4.97327100 | 1.45244900 | 0.29741100 |
| C | -4.70479900 | -1.73635800 | -0.74695900 |
| H | -5.31166800 | -2.61468800 | -0.94115200 |
| O | 1.25536300 | -0.52093600 | 1.00647100 |
| O | -1.22317500 | -0.88845800 | -0.90438200 |
| S | 7.01007900 | -0.67538900 | -0.33932700 |
| S | -7.06514300 | -0.51212200 | -0.01845200 |
| O | -7.31909700 | -1.45942900 | 1.10461800 |
| O | -7.69197300 | -0.96349900 | -1.29325800 |
| O | -7.39193400 | 0.89902300 | 0.32587800 |
| O | 7.41579100 | 0.72390400 | -0.64945500 |
| O | 7.11384000 | -1.58607700 | -1.51577800 |
| O | 7.69928200 | -1.22672800 | 0.86338400 |
| H | 0.31241100 | -2.07864500 | 1.18362100 |
| H | -0.09527000 | 0.97378700 | -2.16606900 |
| H | 0.92654900 | 0.01208400 | -1.96159500 |
| O | -0.47344600 | -2.66138300 | 1.19455500 |
| H | -0.90874000 | -2.36543400 | 0.38090400 |
| H | 0.14694700 | -0.25110700 | 2.47971200 |
| O | -0.74319400 | -0.28794500 | 2.87823700 |
| H | -1.06038900 | -1.13864300 | 2.53499500 |
| H | 1.90418300 | 2.37000800 | -1.30780400 |
| H | 2.02126000 | 1.95725400 | 1.57272800 |
| H | -1.24934900 | 1.05654300 | 1.53964200 |
| H | -3.03564300 | 2.46900000 | 0.60209600 |
| Pd | 0.16879400 | 0.55064300 | -0.71040100 |
| H | -2.86918400 | -2.68894800 | -1.29802200 |
| H | 2.72293300 | -2.68235600 | 0.92755400 |

53
RR_EI_D1_TS1-trigo_R, E(SCF) = -
2408.90651223, E(ZPE) = -2408.517537, E(G)
= -2408.585767 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.58191300 | 3.03852500 | 0.91831100 |
| H | -1.25372200 | 3.90072800 | 0.96152200 |
| H | -0.07519300 | 2.96355600 | 1.88205700 |
| C | 0.42299600 | 3.20424300 | -0.19327300 |
| H | -0.08224800 | 3.40569900 | -1.13983600 |
| H | 1.08817100 | 4.04736500 | 0.01384000 |
| N | 1.20796900 | 1.95603900 | -0.38695700 |
| N | -1.35675000 | 1.78065200 | 0.75053900 |
| C | 2.40675100 | 1.76708000 | 0.44587400 |
| H | 3.03542300 | 2.66294400 | 0.38724700 |
| C | -2.54459400 | 1.81650600 | -0.11960000 |
| H | -2.20236400 | 2.00366300 | -1.14362400 |
| C | 3.20891100 | 0.57131200 | 0.00165200 |
| C | 2.65059500 | -0.63362600 | -0.49409400 |

| | | | |
|----|-------------|-------------|-------------|
| C | 4.59361300 | 0.67285800 | 0.12422000 |
| C | 3.54088800 | -1.67761800 | -0.82573600 |
| C | 5.43831900 | -0.36554600 | -0.20176900 |
| H | 5.02654100 | 1.59899600 | 0.48989400 |
| C | 4.90092700 | -1.55514500 | -0.68218600 |
| H | 5.55390300 | -2.38074500 | -0.94687100 |
| C | -3.33766400 | 0.53994400 | -0.01980600 |
| C | -2.76790300 | -0.74591000 | 0.15296200 |
| C | -4.72206400 | 0.65665200 | -0.12587600 |
| C | -3.64827800 | -1.84825100 | 0.20021700 |
| C | -5.55704100 | -0.43882900 | -0.08273500 |
| H | -5.16310000 | 1.64147900 | -0.24608800 |
| C | -5.00883400 | -1.70589300 | 0.08490400 |
| H | -5.65379000 | -2.57786400 | 0.12644600 |
| O | 1.36802900 | -0.69735300 | -0.69474400 |
| O | -1.48401500 | -1.01651500 | 0.29361200 |
| S | 7.21780100 | -0.19977500 | -0.04965300 |
| S | -7.33691600 | -0.26022900 | -0.20309000 |
| O | -7.88620500 | -0.78659000 | -0.08087500 |
| O | -7.75093500 | -1.08646300 | -1.37327900 |
| O | -7.59503000 | 1.19373300 | -0.39580900 |
| O | 7.45930600 | 1.16222400 | 0.50191800 |
| O | 7.76197700 | -0.37562600 | -1.42702500 |
| O | 7.65103100 | -1.28820700 | 0.87267200 |
| H | 0.68262800 | -2.60112100 | -0.49812600 |
| H | 1.10951000 | 0.70972400 | -3.47270100 |
| H | 1.51624900 | 0.26565500 | -3.02623800 |
| O | 0.09382400 | -3.22893900 | -0.03999100 |
| H | -0.68064200 | -2.65375000 | 0.11295500 |
| H | 1.54683100 | -1.36618800 | 1.98364000 |
| O | 1.37913300 | -2.25396500 | 2.31452700 |
| H | 0.93588500 | -2.69283400 | 1.56385200 |
| H | 1.49492400 | 1.90862100 | -1.36354700 |
| H | 2.07758400 | 1.67118400 | 1.48690000 |
| H | -1.65313800 | 1.46339200 | 1.67182000 |
| H | -3.18061400 | 2.66067000 | 0.17039800 |
| Pd | -0.06568300 | 0.40494800 | -0.01750400 |
| H | 3.10638100 | -2.59825300 | -1.20245400 |
| H | -3.20569700 | -2.83043600 | 0.33250300 |

53
RR_EI_D1_TS1-trigo, E(SCF) = -
2408.88581177, E(ZPE) = -2408.496518, E(G)
= -2408.561022 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.42632200 | 2.76173000 | 1.20686900 |
| H | -1.07493800 | 3.63607400 | 1.30808100 |
| H | 0.06996500 | 2.60580900 | 2.16691700 |
| C | 0.58078800 | 2.96371000 | 0.10686100 |
| H | 0.07819300 | 3.17266300 | -0.83973000 |
| H | 1.24039400 | 3.80748600 | 0.33120200 |
| N | 1.37297600 | 1.71984500 | -0.08345300 |
| N | -1.23827000 | 1.54663600 | 0.93502600 |
| C | 2.49172300 | 1.53752500 | 0.88756800 |
| H | 3.06850200 | 2.46847000 | 0.91898400 |
| C | -2.47668300 | 1.75879500 | 0.18135200 |
| H | -2.20336400 | 2.22029800 | -0.77415500 |
| C | 3.37478900 | 0.39973800 | 0.49414600 |
| C | 2.88632600 | -0.93150100 | 0.57462700 |
| C | 4.66383600 | 0.64582700 | 0.04275700 |
| C | 3.76435300 | -1.96660900 | 0.18409400 |
| C | 5.50291700 | -0.39050700 | -0.32556300 |
| H | 5.02938200 | 1.66669600 | -0.01567000 |
| C | 5.04207800 | -1.70183900 | -0.25459100 |
| H | 5.69490300 | -2.51846600 | -0.54828300 |
| C | -3.28511300 | 0.50653200 | -0.02916000 |
| C | -2.76270700 | -0.80512300 | -0.06868000 |
| C | -4.65138900 | 0.69255300 | -0.23457500 |
| C | -3.66069700 | -1.86560100 | -0.31037600 |
| C | -5.50688400 | -0.35852800 | -0.47939200 |
| H | -5.05873900 | 1.69835900 | -0.20104400 |
| C | -5.00289400 | -1.65505200 | -0.50703800 |
| H | -5.66665100 | -2.49416000 | -0.68890800 |
| O | 1.67574700 | -1.18955800 | 0.97352800 |
| O | -1.50033400 | -1.14767000 | 0.12437500 |
| S | 7.16131100 | -0.07462700 | -0.92519500 |
| S | -7.26062100 | -0.08924400 | -0.74482300 |
| O | -7.95605400 | -0.84442400 | 0.33627700 |

O -7.55310200 -0.64008700 -2.09913700
O -7.47030600 1.38216300 -0.65545900
O 7.36888400 1.39677200 -0.81469900
O 7.18834100 -0.55919200 -2.33649200
O 8.07529000 -0.85808200 -0.04432400
H 0.60221800 -2.61086200 1.49373100
H 0.60093900 -0.68940900 -1.92550900
H 1.03596400 -1.12485200 -1.47454600
O -0.24633200 -3.01657400 1.75549100
H -0.86732300 -2.56184600 1.16025500
H 0.69376100 -0.49766600 2.50905400
O -0.07291800 -0.38889400 3.10215200
H -0.49844400 -1.25218600 2.99059100
H 1.78782700 1.74392800 -1.01405700
H 2.04728000 1.38816200 1.87539700
H -1.42996700 1.06923300 1.82000600
H -3.09213400 2.48848800 0.72193400
Pd -0.01827800 0.19064300 -0.01110700
H 3.39743500 -2.98651000 0.24079400
H -3.24681700 -2.86826100 -0.33191700

53
RR_EI_D1_TS2-trigo_P, E(SCF) = -
2408.92766297, E(ZPE) = -2408.533361, E(G)
= -2408.599324 a.u.
C 0.41512300 -2.62109800 1.23133200
H 1.03533800 -3.52026200 1.31100700
H 0.10514600 -2.36062600 2.24582600
C -0.79412600 -2.91595500 0.37149100
H -0.48445400 -3.29492200 -0.60502900
H -1.42730000 -3.67409000 0.84651900
N -1.57077100 -1.67310400 0.12586600
N 1.18566600 -1.48803500 0.69645700
C -2.31390100 -1.20598000 1.32488700
H -2.86661500 -2.05723900 1.74188600
C 2.33038900 -1.82660800 -0.15524800
H 1.93676600 -2.27207200 -1.07872100
C -3.26804400 -0.10918700 0.97377400
C -2.98783600 1.24854900 1.17478900
C -4.47734800 -0.45144500 0.38147400
C -3.90853400 2.21278200 0.77667100
C -5.38820700 0.51008000 -0.01662200
H -4.71164900 -1.50368100 0.23629900
C -5.10011100 1.85002900 0.18113600
H -5.81541800 2.60294100 -0.12753900
C 3.18155400 -0.62056800 -0.43803300
C 2.66519500 0.60525800 -0.92941200
C 4.54961900 -0.73088700 -0.20506100
C 3.58284400 1.65398400 -1.15792800
C 5.42630100 0.30696900 -0.45078600
H 4.94591900 -1.66671600 0.17714600
C 4.93032900 1.51592600 -0.92529600
H 5.60432600 2.34525100 -1.11583500
O -1.85765300 1.71262100 1.74828800
O 1.40222100 0.86256600 -1.20129900
S -6.93817000 -0.01403600 -0.76518600
S 7.17593500 0.14673200 -0.09971300
O 7.40745200 -1.29168400 0.21176600
O 7.44529100 1.04090300 1.06444900
O 7.88493600 0.59739400 -1.33191500
O -7.67304300 1.23624100 -1.09526500
O -7.61979700 -0.84111800 0.26965600
O -6.55493700 -0.80553000 -1.96741200
H -0.21657900 2.72742600 0.82362300
H -1.13948100 0.39857400 -1.53864000
H -1.23576200 1.02094000 2.04931000
O 0.74938600 2.69409300 0.79092300
H 0.94458300 2.17688300 -0.01837300
H 0.77647100 0.81417900 3.52807200
O 0.55280800 0.60330200 2.61755800
H 0.84045400 1.37332500 2.08076200
H -2.25200600 -1.86144000 -0.60616200
H -1.58373200 -0.90279700 2.07810400
H 1.47314300 -0.88612600 1.46764900
H 2.95219900 -2.59240400 0.32631400
Pd -0.14037500 -0.34151900 -0.25333800
H -3.66427400 3.25527100 0.94530000

H 3.17889200 2.59090800 -1.52882900
53
RR_EI_D1_TS2-trigo_R, E(SCF) = -
2408.89522238, E(ZPE) = -2408.504210, E(G)
= -2408.569403 a.u.
C 0.45093300 -3.00217100 0.72629600
H 1.17550900 -3.81615600 0.65297300
H 0.14295200 -2.93328200 1.77162600
C -0.73120900 -3.25080600 -0.17049500
H -0.40440000 -3.43074800 -1.19674500
H -1.30649700 -4.12070400 0.16104800
N -1.58864600 -2.03622700 -0.18610500
N 1.09924800 -1.70922200 0.38069700
C -2.46656800 -1.88454600 1.01747400
H -3.13110500 -2.75558700 1.04277900
C 2.28440900 -1.78766700 -0.49547000
H 1.94595500 -2.08450000 -1.49500400
C -3.23201700 -0.60920800 -0.95265800
C -2.68684700 0.56563000 1.56153200
C -4.40938100 -0.54956000 0.22735200
C -3.41261500 1.76737100 1.35679900
C -5.09236400 0.64548500 0.05468900
H -4.80217600 -1.46063900 -0.22164700
C -4.57872700 1.80532700 0.62263600
H -5.10946400 2.74063600 0.47919000
C 3.05021700 -0.49787800 -0.50276400
C 2.42667600 0.76015200 -0.63185600
C 4.43612200 -0.55560900 -0.38357400
C 3.23890400 1.90946600 -0.62878100
C 5.21495500 0.58225600 -0.40055900
H 4.92278100 -1.51963900 -0.27297400
C 4.60672000 1.82630900 -0.52119500
H 5.20909600 2.72906000 -0.52329600
O -1.58775900 0.54956100 2.22544600
O 1.12549900 0.96300200 -0.76238900
S -6.60970400 0.66093000 -0.89228300
S 7.00296200 0.48548600 -0.27540800
O 7.32408500 -0.95564300 -0.08404900
O 7.37573100 1.32813500 0.89601900
O 7.52688600 1.03422300 -1.55893400
O -7.06239200 2.08048700 -0.92168400
O -7.56287200 -0.23629700 -0.17369200
O -6.26396400 0.13568900 -2.24677000
H -0.42922700 1.88319900 1.86002800
H -1.28038800 0.51537600 -1.60239600
H -1.62825400 0.64782200 -0.87979000
O 0.38042500 2.39000900 1.63196500
H 0.60746900 2.07021100 0.74306000
H -0.02718200 -0.18164000 2.67631000
O 0.94658100 -0.24675900 2.78539400
H 1.21242600 0.65852100 2.55768400
H -2.20152700 -2.08497500 -0.99896800
H -1.82815800 -1.91085200 1.90135700
H 1.33645200 -1.22381200 1.26527400
H 2.93743000 -2.58482900 -0.12541300
Pd -0.26421500 -0.46727800 -0.49120300
H -3.01290000 2.67456000 1.80109400
H 2.74575900 2.87169500 -0.71887100

53
RR_EI_D1_TS2W_P, E(SCF) = -2408.92762104,
E(ZPE) = -2408.535005, E(G) = -2408.601502
a.u.
C -0.47868400 2.98543100 0.68772200
H -1.13637600 3.85192900 0.56034700
H -0.21073600 2.94737000 1.74653400
C 0.76450600 3.17052300 -0.16009500
H 0.49179000 3.38618900 -1.19564100
H 1.35851500 4.01200200 0.21562100
N 1.57766600 1.92842000 -0.18142000
N -1.18031500 1.73232600 0.36702900
C 2.29818700 1.66787100 1.09513600
H 2.91462800 2.54335200 1.33220300
H -2.32676800 1.82793300 -0.54512900
H -1.94622500 2.09230800 -1.54052700
C 3.14959300 0.44547900 0.97092700

| | | | |
|----|-------------|-------------|-------------|
| C | 2.66047300 | -0.82385800 | 1.28821300 |
| C | 4.41985600 | 0.55158600 | 0.41643700 |
| C | 3.43229000 | -1.95390700 | 1.03001700 |
| C | 5.18318300 | -0.57115000 | 0.16013200 |
| H | 4.81622900 | 1.53132600 | 0.16670400 |
| C | 4.68312800 | -1.83030200 | 0.45982600 |
| H | 5.27924600 | -2.71379400 | 0.25779300 |
| C | -3.10568400 | 0.54135900 | -0.56892400 |
| C | -2.51701600 | -0.72156400 | -0.83392400 |
| C | -4.47241800 | 0.60654400 | -0.31151100 |
| C | -3.36287200 | -1.85112800 | -0.83031300 |
| C | -5.27778500 | -0.51493200 | -0.31918900 |
| H | -4.92594900 | 1.56989500 | -0.09878100 |
| C | -4.71057300 | -1.75698500 | -0.57886900 |
| H | -5.33015900 | -2.64840300 | -0.58267600 |
| O | 1.43642800 | -0.94907000 | 1.85302000 |
| O | -1.24518000 | -0.93610100 | -1.10167800 |
| S | 6.82093200 | -0.43031700 | -0.57314400 |
| S | -7.03313100 | -0.40819400 | 0.02225900 |
| O | -7.32318200 | 1.03245800 | 0.26674200 |
| O | -7.27022300 | -1.26076700 | 1.22366800 |
| O | -7.71999400 | -0.94151200 | -1.19014800 |
| O | 7.06705700 | 1.02671300 | -0.74396900 |
| O | 6.74138300 | -1.16817700 | -1.86458400 |
| O | 7.74915200 | -1.07392700 | 0.39757200 |
| H | 0.95803900 | -1.73183700 | 1.47421900 |
| H | 1.25673500 | -0.37214500 | -1.53375100 |
| H | -0.51653900 | -2.18913400 | -0.07923600 |
| O | -0.11012100 | -2.73954000 | 0.62981300 |
| H | 0.19846200 | -3.54413100 | 0.20638400 |
| H | -0.05077600 | -0.07557400 | 2.58359300 |
| O | -0.94538000 | 0.23586500 | 2.79908600 |
| H | -0.96472500 | 0.33976000 | 3.75288700 |
| H | 2.27749400 | 2.01568400 | -0.91490700 |
| H | 1.55661500 | 1.55433100 | 1.88605200 |
| H | -1.46257400 | 1.28364600 | 1.24067400 |
| H | -2.99690400 | 2.64029600 | -0.23475300 |
| Pd | 0.21394300 | 0.44777800 | -0.69345100 |
| H | 3.03445500 | -2.93056300 | 1.28503100 |
| H | -2.90488500 | -2.81425400 | -1.03301700 |

53
RR_EI_D1_TS2W_R, E(SCF) = -2408.88927924,
E(ZPE) = -2408.500170, E(G) = -2408.567171
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.44709300 | 2.92100800 | 0.55298600 |
| H | -1.10010400 | 3.78885600 | 0.44780400 |
| H | -0.16186400 | 2.85458900 | 1.60462200 |
| C | 0.76366300 | 3.06202400 | -0.33164900 |
| H | 0.46467400 | 3.31050900 | -1.35237400 |
| H | 1.43143800 | 3.84910800 | 0.03432200 |
| N | 1.47486300 | 1.75964800 | -0.38064000 |
| N | -1.19419700 | 1.67882000 | 0.20590800 |
| C | 2.16130300 | 1.42012300 | 0.90466400 |
| H | 2.69815300 | 2.32074300 | 1.22673100 |
| C | -2.50698000 | 1.90236300 | -0.43857500 |
| H | -2.31275500 | 2.31182600 | -1.43704500 |
| C | 3.10383100 | 0.27714200 | 0.76312600 |
| C | 2.61860000 | -1.05406900 | 0.88677600 |
| C | 4.45043000 | 0.52175100 | 0.52922800 |
| C | 3.58225100 | -2.08900500 | 0.76269600 |
| C | 5.35944200 | -0.51298500 | 0.40620600 |
| H | 4.80381800 | 1.54624900 | 0.44891600 |
| C | 4.91146000 | -1.82656900 | 0.52736000 |
| H | 5.61980600 | -2.64561400 | 0.44150600 |
| C | -3.31981300 | 0.64807800 | -0.47785600 |
| C | -2.80521700 | -0.53975600 | -1.04050200 |
| C | -4.61424200 | 0.66142000 | 0.02778500 |
| C | -3.64047000 | -1.67295000 | -1.07077100 |
| C | -5.42103100 | -0.45796600 | -0.02624200 |
| H | -5.00984500 | 1.57288600 | 0.46493500 |
| C | -4.92535800 | -1.63224100 | -0.58188400 |
| H | -5.55051400 | -2.51865200 | -0.62363400 |
| O | 1.36985200 | -1.32628300 | 1.07350900 |
| O | -1.60829400 | -0.65255300 | -1.57330200 |
| S | 7.09158100 | -0.19798600 | 0.08891900 |
| S | -7.09181400 | -0.43070600 | 0.62597200 |

| | | | |
|----|-------------|-------------|-------------|
| O | -7.33961100 | 0.97042800 | 1.06550300 |
| O | -7.10762900 | -1.40570600 | -1.75460400 |
| O | -7.97423700 | -0.85421900 | -0.49902300 |
| O | 7.25697500 | 1.28299900 | 0.12285600 |
| O | 7.38123200 | -0.78145700 | -1.25474300 |
| O | 7.84622500 | -0.89100700 | 1.17412400 |
| H | 1.01877000 | -2.47318300 | -0.20892700 |
| H | 0.96651400 | -0.27738400 | -2.24621000 |
| H | 0.91941500 | -0.90260800 | -1.71608800 |
| O | 0.94874000 | -2.94136100 | -1.07321200 |
| H | 1.82148400 | -3.31725300 | -1.21367000 |
| H | 0.04865900 | -0.60811800 | 1.89897600 |
| O | -0.77931400 | -0.19626200 | 2.24855700 |
| H | -0.70440300 | -0.19507600 | 3.20469000 |
| H | 2.19346400 | 1.80905100 | -1.10108700 |
| H | 1.39069900 | 1.19977300 | 1.64526200 |
| H | -1.30941100 | 1.11217500 | 1.06286900 |
| H | -3.05084500 | 2.66433700 | 0.12916200 |
| Pd | -0.03725400 | 0.45383600 | -0.97768800 |
| H | 3.23766600 | -3.11279000 | 0.87887500 |
| H | -3.23822300 | -2.58294600 | -1.50221000 |

53
RR_EI_D1_TS2W, E(SCF) = -2408.88125564,
E(ZPE) = -2408.493412, E(G) = -2408.559740
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.42899400 | 2.86244000 | 0.58976900 |
| H | -1.05331800 | 3.75274700 | 0.49003000 |
| H | -0.14624400 | 2.78425500 | 1.64167200 |
| C | 0.79276300 | 2.98071400 | -0.28753000 |
| H | 0.50538800 | 3.24227600 | -1.30844500 |
| H | 1.47221100 | 3.75368500 | 0.08865500 |
| N | 1.48104400 | 1.66644700 | -0.34371400 |
| N | -1.20436700 | 1.64803200 | 0.23052200 |
| C | 2.13292600 | 1.30276000 | 0.95133700 |
| H | 2.63871000 | 2.20330900 | 1.32169300 |
| C | -2.50149400 | 1.90138600 | -0.42661100 |
| H | -2.28762500 | 2.31039100 | -1.42181000 |
| C | 3.11419200 | 0.19073600 | 0.80365400 |
| C | 2.69097900 | -1.15853500 | 0.90612200 |
| C | 4.44984200 | 0.49034400 | 0.56423500 |
| C | 3.68491700 | -2.15309500 | 0.74582400 |
| C | 5.39604800 | -0.50541600 | 0.41148400 |
| H | 4.76292800 | 1.52889400 | 0.49880600 |
| C | 5.00189800 | -1.83689300 | 0.50262100 |
| H | 5.73910900 | -2.62580400 | 0.38621300 |
| C | -3.33204600 | 0.65781300 | -0.48678800 |
| C | -2.84032300 | -0.53006600 | -1.07688400 |
| C | -4.62099000 | 0.68222900 | 0.03246000 |
| C | -3.70095100 | -1.64659400 | -1.11670000 |
| C | -5.44838500 | -0.42233900 | -0.02859700 |
| H | -4.99647600 | 1.59328400 | 0.48818000 |
| C | -4.97783300 | -1.59524400 | -0.60896300 |
| H | -5.61701700 | -2.47146500 | -0.65707000 |
| O | 1.44660200 | -1.49390700 | 1.09364500 |
| O | -1.65331100 | -0.65857700 | -1.62127000 |
| S | 7.11322400 | -0.11573300 | 0.08280800 |
| S | -7.10732000 | -0.37960400 | 0.64873400 |
| O | -7.33313400 | 1.02118100 | 1.10248100 |
| O | -7.12010700 | -1.36209200 | -1.77174100 |
| O | -8.01465200 | -0.78451900 | -0.46389700 |
| O | 7.21652800 | 1.36998500 | 0.13086700 |
| O | 7.41128300 | -0.67410500 | -1.26893400 |
| O | 7.90281400 | -0.78835000 | 1.15514900 |
| H | 1.07484100 | -2.28171900 | -0.16972100 |
| H | 0.92566500 | -0.44406700 | -2.06946000 |
| O | 0.84220500 | -1.31372500 | -1.62557900 |
| O | 0.89468100 | -2.53102500 | -1.14883900 |
| H | 1.67886800 | -2.98499100 | -1.47957200 |
| H | 0.06174200 | -0.75476100 | 1.85447900 |
| O | -0.76523800 | -0.34598600 | 2.20295600 |
| H | -0.76920300 | -0.50863000 | 3.14816500 |
| H | 2.21266100 | 1.71321800 | -1.05028400 |
| H | 1.34826700 | 1.04030700 | 1.66223700 |
| H | -1.34182900 | 1.07522500 | 1.07370600 |
| H | -3.04690900 | 2.66999200 | 0.13207300 |
| Pd | -0.05327600 | 0.40971300 | -0.99267800 |

H 3.37657800 -3.19122800 0.83162800
H -3.32009800 -2.55622600 -1.56852900

53

RR_EI_D1_TS2-trigo, E(SCF) = -
2408.88840050, E(ZPE) = -2408.498505, E(G)
= -2408.562501 a.u.

C -0.37666500 2.70080400 0.75317300
H -0.98241300 3.60916300 0.78748800
H -0.00851800 2.51903600 1.76467500
C 0.77034200 2.86386500 -0.21048900
H 0.40379000 3.15458800 -1.19738500
H 1.46619100 3.63464400 0.13709700
N 1.47571300 1.56401700 -0.37084500
N -1.21392100 1.53579100 0.36369300
C 2.32304600 1.18784200 0.80027000
H 2.82442500 2.09840400 1.14793800
C -2.47531400 1.83592200 -0.33992100
H -2.21513000 2.20975800 -1.33702700
C 3.35098700 0.14573300 0.48518300
C 3.00793000 -1.22149300 0.35318200
C 4.68349200 0.53310900 0.38206600
C 4.04964900 -2.14250500 0.13601700
C 5.68488500 -0.39139100 0.16026700
H 4.95056800 1.58038900 0.48664600
C 5.36259500 -1.73934500 0.04510200
H 6.14802000 -2.46992900 -0.12244100
C -3.36644400 0.63014100 -0.39021100
C -2.91178500 -0.64477700 -0.79479000
C -4.70120200 0.79080300 -0.03049800
C -3.84396000 -1.70124900 -0.81839000
C -5.59858900 -0.25613000 -0.07372000
H -5.05336800 1.76593300 0.29108800
C -5.16090000 -1.51398300 -0.47118200
H -5.85629100 -2.34673700 -0.50260200
O 1.75714000 -1.62758400 0.40210000
O -1.68019900 -0.93332200 -1.17614400
S 7.40240500 0.11205300 0.03592600
S -7.31594500 -0.02729100 0.38984200
O -8.11448200 -0.40347700 -0.81161100
O -7.45536000 1.40938400 0.75602700
O -7.55265400 -0.94748500 1.53878700
O 7.41304400 1.59153300 0.20466300
O 7.85580400 -0.32394700 -1.31593800
O 8.11710000 -0.60488900 1.13051300
H 0.26152400 -2.91376700 0.34674800
H 0.89913900 -0.85055800 -1.66989800
H 1.14880200 -1.14253700 -0.83766200
O -0.68642900 -3.12319700 0.33239400
H -1.05639300 -2.48963700 -0.30965700
H 0.40892800 -1.00651600 1.75292900
O -0.46307000 -0.87207500 2.16675000
H -0.94394900 -1.63776400 1.81508200
H 2.08827200 1.62942300 -1.18164400
H 1.65923500 0.85761700 1.60200900
H -1.41062400 0.96782300 1.19395800
H -2.99792100 2.64324800 0.18386500
Pd -0.07744300 0.24383100 -0.77741400
H -3.48659300 -2.67742300 -1.12990800
H 3.78325100 -3.18983700 0.04084500

53

RR_EI_D2_I1_CH_P, E(SCF) = -2408.88781935,
E(ZPE) = -2408.495623, E(G) = -2408.563043
a.u.

C -0.53693300 1.45189800 2.26125700
H -1.20084600 1.99499000 2.94341400
H 0.04081300 0.75368100 2.87088000
C 0.38341300 2.42898300 1.56492500
H -0.19294100 3.19425500 1.03936000
H 1.02343500 2.93924600 2.29358300
N 1.21174400 1.74877400 0.53995100
N -1.30796300 0.65809300 1.28789700
C 2.34414500 1.00153100 1.11186000
H 1.94502800 0.25454200 1.80115500
C -2.59393500 1.23445000 0.85929600
H -3.17987700 1.54586100 1.73379000

C 3.16296700 0.29468200 0.04356100
C 4.03960200 1.22263500 -0.76108500
C 3.82182100 -0.95501700 0.50132300
C 5.20377000 0.64214400 -1.39758800
C 4.96736600 -1.36942400 -0.04129200
H 3.31155100 -1.56552900 1.23954000
C 5.64771600 -0.57434600 -1.03480000
H 5.75021900 1.26508100 -2.09593500
H 6.55856200 -0.97191800 -1.47244400
C -3.39337700 0.24842700 0.05724200
C -2.87692900 -0.42294700 -1.08559600
C -4.70573800 0.01074200 0.45376800
C -3.75836300 -1.29622800 -1.76814700
C -5.54061100 -0.84615800 -0.23549900
H -5.09394000 0.52109800 -1.30201000
C -5.05270600 -1.50585300 -1.35953100
H -3.36656200 -1.80505300 -2.64286500
H -5.69459300 -2.18506000 -1.91256300
C 3.75109400 2.40877100 1.46895400
O -1.67170700 -0.30033900 -1.57480600
S 5.72893700 -2.93277700 0.42616600
S -7.21932300 -1.14704100 0.30551900
O -7.44988000 -0.24470900 1.48693600
O -7.28438200 -2.59240800 0.67367700
O -8.09326500 -0.82593900 -0.86074100
O 5.78634000 -3.71183200 -0.83959700
O 4.84274800 -3.52888400 -1.45658300
O 7.07470100 -2.55829000 0.93719800
H -2.37587700 2.14161600 0.28092400
H 2.97625700 1.68730900 1.69073900
H -1.48687400 -0.26510400 1.67127400
H 1.56596700 2.47436200 -0.08802400
H 3.60442300 3.86000000 0.38547500
O 3.08181600 4.53896500 0.83941700
H 3.69735900 5.24283400 1.05826700
H 1.93183300 3.81730500 -1.88293600
O 1.29662900 4.20384300 -1.27206600
H 1.85312100 4.58581000 -0.56963000
Pd -0.16480300 -0.64548300 -0.56769500
H 0.66628700 0.79431000 -1.88958400
H 2.42129000 -0.04938300 -0.71586900

53

RR_EI_D2_I1_CH_TS, E(SCF) = -2408.86444925,
E(ZPE) = -2408.478036, E(G) = -2408.543973
a.u.

C 0.54113700 1.95629900 -2.33815800
H 1.27019500 2.57483700 -2.87174500
H -0.04756600 1.42107200 -3.08621200
C -0.35598000 2.81707500 -1.48100900
H 0.23972500 3.44693200 -0.81553700
H -0.96342100 3.48441000 -2.10035900
N -1.22021600 1.98284200 -0.61377800
N 1.22338900 0.92615200 -1.52075400
C -2.53013000 1.57379100 -1.15944700
H -2.36294000 1.04616500 -2.10135800
C 2.44612700 1.31907800 -0.80296600
H 3.13173400 1.82893000 -1.49019900
C -3.24154700 0.67917400 -0.17751800
C -3.72262800 1.28447200 1.05464200
C -3.84124800 -0.53167900 -0.63960300
C -4.56832600 0.46587400 1.87310300
C -4.67502700 -1.24297700 0.16040200
H -3.57282700 -0.91599100 -1.61910100
C -5.02901600 -0.73602700 1.43535900
H -4.87334300 0.86766200 2.83311600
H -5.69026100 -1.32345000 2.06568900
C 3.13886200 0.11905900 -0.21268100
C 2.46446900 -0.97869300 0.38898900
C 4.53081500 0.11426400 -0.26485400
C 3.26925500 -2.01826500 0.91316600
C 5.28595400 -0.91218500 0.26146600
H 5.04443800 0.94629100 -0.73699500
C 4.63989000 -1.99212300 0.85567500
H 2.75159100 -2.85368100 1.37255300
H 5.21857500 -2.81179300 1.27020600
O -3.34233200 2.42689300 1.41642600

O 1.16728800 -1.14400500 0.50156700
 S -5.37363000 -2.81075200 -0.36437100
 S 7.07432700 -0.89405700 0.17369400
 O 7.44383900 0.37758800 -0.50893200
 O 7.46024500 -2.10512700 -0.60774000
 O 7.55610300 -0.95714700 1.58443000
 O -4.89963200 -3.81037300 0.63313600
 O -4.85160600 -3.05288800 -1.73546800
 O -6.84983700 -2.61723400 -0.31984700
 H 2.16116600 2.04729800 -0.03337600
 H -3.12078200 2.47417000 -1.37024600
 H 1.44568800 0.13095500 -2.11462100
 H -1.38393000 2.51175200 0.24912300
 H -3.17139700 4.03482200 0.55188500
 O -2.68115700 4.80587300 0.20726100
 H -3.28592600 5.54978500 0.24836800
 H -1.57137300 3.08763600 2.22423100
 O -0.80970100 3.61309900 1.93762100
 H -1.23787400 4.33507000 1.44731100
 Pd -0.12067000 0.33134400 -0.03484100
 H -1.24072100 -0.12823700 1.10475100
 H -2.08461400 0.12125100 0.50076500

53

RR_EI_D2_I1_P_HH-Homo_P, E(SCF) = -
 2408.84061993, E(ZPE) = -2408.450943, E(G)
 = -2408.517471 a.u.

C 0.58831100 2.44068000 -2.10120900
 H 1.26576500 3.23710300 -2.42783500
 H -0.01000400 2.13412400 -2.96299900
 C -0.31532100 2.94883400 -1.00461400
 H 0.27731900 3.36359600 -0.18512700
 H -0.95254800 3.75414700 -1.37796000
 N -1.16172500 1.86830700 -0.42887100
 N 1.33313800 1.24951400 -1.65571000
 C -2.59154100 1.85032900 -0.80061200
 H -2.69961700 1.57865200 -1.85358000
 C 2.51594800 1.44296000 -0.82040400
 H 3.24506100 2.08078600 -1.33471700
 C -3.33602800 0.90351000 0.09336100
 C -3.02696200 0.82026200 1.48327400
 C -4.32450100 0.09604400 -0.45050400
 C -3.76836300 -0.10882900 2.24624200
 C -5.04247400 -0.78992200 0.33137800
 H -4.54200800 0.15534400 -1.51295400
 C -4.75385300 -0.89114400 1.68896600
 H -3.53353400 -0.18466500 3.30320400
 H -5.30703800 -1.59181200 2.30733700
 C 3.17607900 0.13187500 -0.45809600
 C 2.52512700 -1.11688100 -0.28667300
 C 4.55458200 0.19715800 -0.24952800
 C 3.31835200 -2.22075600 0.09655800
 C 5.30254900 -0.89695800 0.12181400
 H 5.06266700 1.14703000 -0.38873400
 C 4.67248200 -2.12475900 0.29303600
 H 2.80700300 -3.16829000 0.22559900
 H 5.24646000 -3.00001300 0.57998700
 O -2.08923800 1.54169100 2.04106900
 O 1.24209800 -1.40877600 -0.47279100
 S -6.31046700 -1.83762600 -0.37701100
 S 7.07218600 -0.76727800 0.38498000
 O 7.69297500 -1.75531100 -0.54294300
 O 7.29587000 -1.11659000 1.81723000
 O 7.43474300 0.64108300 0.06574800
 O -7.56239200 -1.53586700 0.37681300
 O -5.85225800 -3.24216100 -0.16513800
 O -6.39756500 -1.46763400 -1.81782900
 H 2.20666000 1.97917700 0.08427200
 H -2.95852900 2.87889300 -0.67532000
 H 1.58989900 0.69120000 -2.46446600
 H -1.22276200 2.01662300 0.59233300
 H -2.34308300 3.30913500 1.88750500
 O -2.38493100 4.25128900 1.62134600
 H -3.31470000 4.41583600 1.44963000
 H -0.33755500 0.96822100 2.05724600
 O 0.54390200 0.83870200 1.62975700
 H 1.01497200 0.17394900 2.14329700

Pd -0.07185000 0.10932100 -0.45698100
 H -1.17341200 -0.75036100 0.20615800
 H -0.75526100 -0.42956100 -1.69122100

53

RR_EI_D2_I1_P_HH-Homo_TS, E(SCF) = -
 2408.83859613, E(ZPE) = -2408.450760, E(G)
 = -2408.516899 a.u.

C 0.57077200 2.44103100 -2.11307100
 H 1.25066400 3.23327700 -2.44471300
 H -0.04166700 2.14366200 -2.96795900
 C -0.30997400 2.94241700 -0.99711600
 H 0.29986500 3.33055300 -0.17712800
 H -0.94238900 3.76291100 -1.34514400
 N -1.15969100 1.86015000 -0.42932200
 N 1.31516700 1.24117400 -1.68348400
 C -2.59209400 1.85731300 -0.78863100
 H -2.71299300 1.59257000 -1.84218800
 C 2.52870600 1.43453300 -0.89422300
 H 3.25075400 2.04034800 -1.45514500
 C -3.33405800 0.91077900 0.10777500
 C -3.00989700 0.81939700 1.49421700
 C -4.32600500 0.10487100 -0.43164400
 C -3.74323200 -0.11624200 2.25810200
 C -5.03514500 -0.78748100 0.35128300
 H -4.55283800 0.16969700 -1.49188400
 C -4.73277100 -0.89661600 1.70536500
 H -3.49760700 -0.19944200 3.31209800
 H -5.27825400 -1.60271000 2.32445500
 C 3.17764200 0.12566700 -0.50613800
 C 2.52189900 -1.12074000 -0.33910700
 C 4.55064800 0.19242600 -0.26595700
 C 3.30198000 -2.21893700 0.08555300
 C 5.28785500 -0.89872800 0.13456800
 H 5.06298700 1.14028400 -0.40379100
 C 4.65216300 -2.12341000 0.30809400
 H 2.78559700 -3.16361100 0.21506900
 H 5.21839800 -2.99505000 0.62022000
 O -2.06771300 1.53716100 2.04616600
 O 1.24749400 -1.41305100 -0.57334700
 S -6.31018900 -1.83035400 -0.35057000
 S 7.05400300 -0.77101600 0.42292300
 O 7.68533900 -1.76012800 -0.49664900
 O 7.25760200 -1.12040000 1.85801900
 O 7.42246300 0.63669300 0.10792000
 O -7.55742200 -1.52490600 0.40978300
 O -5.85618600 -3.23681600 -0.14190000
 O -6.40386800 -1.45952100 -1.79086400
 H 2.25977200 2.00519600 0.00209600
 H -2.94984300 2.88812800 -0.65470900
 H 1.54010400 0.67651400 -2.47939500
 H -1.21099900 1.99705300 0.59403600
 H -2.32122600 3.30271000 1.90593700
 O -2.37344700 4.24880800 1.65512000
 H -3.30523000 4.40558100 1.48713800
 H -0.24533400 1.02762600 2.04829200
 O 0.62989800 0.95338500 1.60399100
 H 1.16062400 0.34739300 2.13080600
 Pd -0.07502200 0.09539600 -0.48947400
 H -1.20255600 -0.80204400 0.11094900
 H -1.03037900 -0.66370000 -1.40357200

53

RR_EI_D2_TS1_P, E(SCF) = -2408.88659474,
 E(ZPE) = -2408.496421, E(G) = -2408.563627
 a.u.

C 0.32164400 2.08677400 -2.27710900
 H 1.07979800 2.66954100 -2.80543800
 H -0.23507500 1.51902700 -3.02364500
 C -0.59703000 2.97537800 -1.48415200
 H -0.03350600 3.61092600 -0.79733200
 H -1.17557000 3.63037000 -2.14331500
 N -1.50290300 2.13404000 -0.66623500
 N 0.97663400 1.10077300 -1.37199400
 C -2.65242700 1.56792200 -1.42680900
 H -2.25851000 1.04188500 -2.29876500
 C 2.28524700 1.51814200 -0.82066200

H -1.23787400 4.33507000 1.44731100
Pd -0.12067000 0.33134400 -0.03484100
H -1.24072100 -0.12823700 1.10475100
H -2.08461400 0.12125100 0.50076500

53

RR_EI_D2_TS1_P_HH-Homo_P, E(SCF) = -
2408.84061993, E(ZPE) = -2408.450943, E(G)
= -2408.517471 a.u.

C 0.58831100 2.44068000 -2.10120900
H 1.26576500 3.23710300 -2.42783500
H -0.01000400 2.13412400 -2.96299900
C -0.31532100 2.94883400 -1.00461400
H 0.27731900 3.36359600 -0.18512700
H -0.95254800 3.75414700 -1.37796000
N -1.16172500 1.86830700 -0.42887100
N 1.33313800 1.24951400 -1.65571000
C -2.59154100 1.85032900 -0.80061200
H -2.69961700 1.57865200 -1.85358000
C 2.51594800 1.44296000 -0.82040400
H 3.24506100 2.08078600 -1.33471700
C -3.33602800 0.90351000 0.09336100
C -3.02696200 0.80262600 1.48327400
C -4.32450100 0.09604400 -0.45050400
C -3.76836300 -0.10882900 2.24624200
C -5.04247400 -0.78992200 0.33137800
H -4.54200800 0.15534400 -1.51295400
C -4.75385300 -0.89114400 1.68896600
H -3.53353400 -0.18466500 3.30320400
H -5.30703800 -1.59181200 2.30733700
C 3.17607900 0.13187500 -0.45809600
C 2.52512700 -1.11688100 -0.28667300
C 4.55458200 0.19715800 -0.24952800
C 3.31835200 -2.22075600 0.09655800
C 5.30254900 -0.89695800 0.12181400
H 5.06266700 1.14703000 -0.38873400
C 4.67248200 -2.12475900 0.29303600
H 2.80700300 -3.16829000 0.22559900
H 5.24646000 -3.00001300 0.57998700
O -2.08923800 1.54169100 2.04106900
O 1.24209800 -1.40877600 -0.47279100
S -6.31046700 -1.83762600 -0.37701100
S 7.07218600 -0.76727800 0.38498000
O 7.69297500 -1.75531100 -0.54294300
O 7.29587000 -1.11659000 1.81723000
O 7.43474300 0.64108300 0.06574800
O -7.56239200 -1.53586700 0.37681300
O -5.85225800 -3.24216100 -0.16513800
O -6.39756500 -1.46763400 -1.81782900
H 2.20666000 1.97917700 0.08427200
H -2.95852900 2.87889300 -0.67532000
H 1.58989900 0.69120000 -2.46446600
H -1.22276200 2.01662300 0.59233300
H -2.34308300 3.30913500 1.88750500
O -2.38493100 4.25128900 1.62134600
H -3.31470000 4.41583600 1.44963000
H -0.33755500 0.96822100 2.05724600
O 0.54390200 0.83870200 1.62975700
H 1.01497200 0.17394900 2.14329700
Pd -0.07185000 0.10932100 -0.45698100
H -1.17341200 -0.75036100 0.20615800
H -0.75526100 -0.42956100 -1.69122100

53

RR_EI_D2_TS1_P_HH-Homo_TS, E(SCF) = -
2408.83859613, E(ZPE) = -2408.450760, E(G)
= -2408.516899 a.u.

C 0.57077200 2.44103100 -2.11307100
H 1.25066400 3.23327700 -2.44471300
H -0.04166700 2.14366200 -2.96795900
C -0.30997400 2.94241700 -0.99711600
H 0.29986500 3.33055300 -0.17712800
H -0.94238900 3.76291100 -1.34514400
N -1.15969100 1.86015000 -0.42932200
N 1.31516700 1.24117400 -1.68348400
C -2.59209400 1.85731300 -0.78863100
H -2.71299300 1.59257000 -1.84218800

C 2.52870600 1.43453300 -0.89422300
H 3.25075400 2.04034800 -1.45514500
C -3.33405800 0.91077900 0.10777500
C -3.00989700 0.81939700 1.49421700
C -4.32600500 0.10487100 -0.43164400
C -3.74323200 -0.11624200 2.25810200
C -5.03514500 -0.78748100 0.35128300
H -4.55283800 0.16969700 -1.49188400
C -4.73277100 -0.89661600 1.70536500
H -3.49760700 -0.19944200 3.31209800
H -5.27825400 -1.60271000 0.32445500
C 3.17764200 0.12566700 -0.50613800
C 2.52189900 -1.12074000 -0.33910700
C 4.55064800 0.19242600 -0.26595700
C 3.30198000 -2.21893700 0.08555300
C 5.28785500 -0.89872800 0.13456800
H 5.06298700 1.14028400 -0.40379100
C 4.65216300 -2.12341000 0.30809400
H 2.78559700 -3.16861100 0.31506900
H 5.21839800 -2.99505000 0.62022000
O -2.06771300 1.53716100 2.04616600
O 1.24749400 -1.41305100 -0.57334700
S -6.31018900 -1.83053400 -0.35057000
S 7.05400300 -0.77101600 0.42292300
O 7.68533900 -1.76012800 -0.49664900
O 7.25760200 -1.12040000 1.85801900
O 7.42246300 0.63669300 0.10792000
O -7.55742200 -1.52490600 0.40978300
O -5.85618600 -3.23681600 -0.14190000
O -6.40386800 -1.45952100 -1.79086400
H 2.25977200 2.00519600 0.00209600
H -2.94984300 2.88812800 -0.65470900
H 1.54010400 0.67651400 -2.49739500
H -1.21099900 1.99705300 0.59403600
H -2.32122600 3.30271000 1.90593700
O -2.37344700 4.24880800 1.65512000
H -3.30523000 4.40558100 1.48713800
H -0.24533400 1.02762600 2.04829200
O 0.62989800 0.95338500 1.60399100
H 1.16062400 0.34739300 2.13080600
Pd -0.07502200 0.09539600 -0.48947400
H -1.20255600 -0.80204400 0.11094900
H -1.03037900 -0.66370000 -1.40357200

53

RR_EI_D2_TS1_R, E(SCF) = -2408.90928749,
E(ZPE) = -2408.520952, E(G) = -2408.587993
a.u.

C 0.55476700 3.00920600 -0.87627400
H 1.23766400 3.86219100 -0.92896300
H 0.00582400 2.96556600 -1.81894500
C -0.40062500 3.16101200 0.28185400
H 0.14666900 3.32712400 1.21240700
H -1.05609300 4.02303600 0.12524900
N -1.19817800 1.92500000 0.47412000
N 1.31742000 1.73666700 -0.77117400
C -2.41033900 1.77912300 -0.33720900
H -2.11359100 1.78570700 -1.39282700
C 2.54562900 1.74725400 0.04238100
H 3.17689800 2.58777500 -0.26836900
C -3.19089700 0.52918200 -0.01203500
C -2.64512900 -0.66344700 0.51673900
C -4.55137000 0.56892600 -0.31187000
C -3.51399000 -1.75440200 0.71340700
C -5.37814400 -0.51654000 -0.11939500
H -4.97796700 1.48345400 -0.71315700
C -4.85153700 -1.69114700 0.40487400
H -3.08745400 -2.66308400 1.12582200
H -5.49140900 -2.55229600 0.56734100
C 3.32074400 0.46440900 -0.10493300
C 2.72771200 -0.81540400 -0.24854700
C 4.70961100 0.56583000 -0.07053800
C 3.59345600 -1.92710800 -0.34489200
C 5.52954200 -0.53871200 -0.15858500
H 5.16766500 1.54524900 0.02884500
C 4.95938400 -1.79966200 -0.29916500
H 3.13322700 -2.90407800 -0.45378000

C -5.38494500 -1.44732500 -0.30388100
H -3.77308000 -2.83374700 -0.56082100
H -6.15163900 -2.21547200 -0.29104000
O 2.19262400 -2.07998100 0.42817700
O -1.80853800 -1.28556400 -0.65318400
S 7.46365300 0.59448900 -0.09577200
S -7.45908400 0.33690200 0.04288200
O -7.87985400 -0.27104900 1.34027500
O -8.17921300 -0.26422100 -1.11807200
O -7.50753400 1.82206000 0.05424000
O 7.94175300 0.23659700 -1.46017400
O 8.30556700 0.00115100 0.98011500
O 7.22858000 2.05286200 0.07975700
H 0.46603400 -2.34750100 1.39283500
O -0.47162200 -2.46699500 1.61584500
H -0.94867000 -2.25060100 0.79277400
H -0.89446900 0.08293000 3.63604900
O -1.40770100 -0.15454000 2.86057400
H -1.02588400 -0.99639800 2.53433900
H 2.04190400 1.12353900 -1.22916700
H 1.65170100 0.33165000 1.52946200
H -1.46411900 0.93241100 1.33383200
H -2.89706400 2.55254000 0.08679000
Pd -0.18298000 -0.09180700 -0.61051300
O 0.88440100 -1.48402600 -1.62817200
H 0.25111800 -2.14082200 -1.93544000
H 1.64697900 -1.92283000 -0.43639200

54

RR_EI_ID1_I1_Htr_R, E(SCF) = -
2484.17061470, E(ZPE) = -2483.773765, E(G)
= -2483.839740 a.u.

C -0.28775800 2.47845800 0.71258700
H -0.83507600 3.42460700 0.70986400
H 0.11671400 2.33792600 1.71831300
C 0.82178600 2.49796300 -0.30639000
H 0.42761100 2.72691100 -1.29885800
H 1.57225300 3.25385900 -0.05302600
N 1.44142700 1.14963500 -0.38051800
N -1.20671700 1.34335900 0.45203100
C 2.29914100 0.80874100 0.80161400
H 2.65685700 1.74990800 1.23404300
C -2.42184800 1.65703800 -0.31668500
H -2.11318100 1.92848100 -1.33353000
C 3.47769500 -0.04182900 0.44782200
C 3.36531100 -1.44048200 0.29766500
C 4.72256300 0.56623700 0.30570700
C 4.53655900 -2.17232200 0.03725600
C 5.85517700 -0.17318700 0.03039300
H 4.81309200 1.64199800 0.42313400
C 5.75956900 -1.55424500 -0.09757100
H 4.44496900 -3.24841800 -0.06401300
H 6.64893500 -2.14117600 -0.30508900
C -3.40831400 0.52101500 -0.30413000
C -3.04642200 -0.84140800 -0.42675500
C -4.75618500 0.85165700 -0.18531100
C -4.07854500 -1.80136400 -0.40957700
C -5.74921300 -0.10536400 -0.19172000
H -5.04028600 1.89512900 -0.08820500
C -5.40092200 -1.44760200 -0.29631100
H -3.78862800 -2.84305300 -0.49434500
H -6.17046000 -2.21293400 -0.29009500
O 2.20557900 -2.06947600 0.38835300
O -1.81674000 -1.30218400 -0.56031400
S 7.45978600 0.61388600 -0.13929400
S -7.47616800 0.34484400 -0.02076400
O -7.92758000 -0.24115500 1.27484500
O -8.17207500 -0.26612900 -1.18933600
O -7.51904400 1.83333300 -0.03016100
O 7.93970500 0.26989500 -1.50836000
O 8.31615200 0.02016700 0.92715600
O 7.22468200 2.07234000 0.04659500
H 0.61836200 -2.27358900 1.38077100
O -0.29719700 -2.41342000 1.69044500
H -0.84798000 -2.26393100 0.90238300
H -0.90564600 0.13726800 3.67835000
O -1.36639200 -0.14185000 2.88400200

H -0.91904800 -0.96205500 2.58552600
H 2.02378000 1.10295500 -1.21470300
H 1.66899000 0.31591300 1.54610400
H -1.46264400 0.92227200 1.35814100
H -2.90047600 2.54131600 0.11918700
Pd -0.19756200 -0.10845700 -0.55969600
O 0.88143500 -1.57070600 -1.53330100
H 0.28111400 -2.27942000 -1.78800500
H 1.53797700 -1.90194000 -0.63055200

54

RR_EI_ID1_I1_Htr_TS, E(SCF) = -
2484.17012128, E(ZPE) = -2483.773705, E(G)
= -2483.839328 a.u.

C -0.28672500 2.47761200 0.71213300
H -0.83063100 3.42605400 0.71076400
H 0.11912200 2.33698000 1.71744800
C 0.82346400 2.49893300 -0.30754100
H 0.42918400 2.73047500 -1.29932900
H 1.57338000 3.25480900 -0.05197500
N 1.44448500 1.15149700 -0.38776500
N -1.20684000 1.34511900 0.45248300
C 2.29842500 0.80872100 0.79295300
H 2.66047600 1.74560700 1.22893800
C -2.41908000 1.65934400 -0.31952500
H -2.10737700 1.92745500 -1.33647800
C 3.47791300 -0.04434000 0.44061800
C 3.38096000 -1.43748200 0.29339700
C 4.72373400 0.56434100 0.30272200
C 4.54237700 -2.17554200 0.04698900
C 5.85744600 -0.17728500 0.03995000
H 4.81357000 1.64017500 0.41693800
C 5.76789200 -1.55767700 -0.08122100
H 4.44859000 -3.25137700 -0.04960100
H 6.65939900 -2.14431500 -0.27788600
C -3.40569800 0.52300500 -0.30845200
C -3.04491000 -0.83936500 -0.44123700
C -4.75283100 0.85302600 -0.18001000
C -4.07807200 -1.79859700 -0.42187300
C -5.74675200 -0.10331100 -0.18591000
H -5.03588000 1.89613600 -0.07603700
C -5.39963600 -1.44518800 -0.29865100
H -3.78917100 -2.84003400 -0.51392200
H -6.16937700 -2.21033900 -0.29166500
O 2.20904300 -2.08408600 0.39362800
O -1.81721900 -1.30063300 -0.58759700
S 7.46481700 0.61360600 -0.12324600
S -7.47231400 0.34672000 -0.00329000
O -7.91653200 -0.24312700 1.29315900
O -8.17565000 -0.26036400 -1.16958800
O -7.51525100 1.83532000 -0.00777900
O 7.94612500 0.26685900 -1.48991100
O 8.31194500 0.01880200 0.94840800
O 7.22460500 2.07046700 0.06091100
H 0.55070100 -2.32016500 1.39015200
O -0.37548900 -2.44629800 1.66060000
H -0.89341700 -2.25915800 0.85660200
H -0.88154300 0.10862900 3.66671100
O -1.37538600 -0.15258300 2.88627800
H -0.95989600 -0.98251300 2.57060500
H 2.02449000 1.10707500 -1.22350000
H 1.66847800 0.31490800 1.53757200
H -1.46586400 0.92635500 1.35756600
H -2.90018600 2.54498200 0.11134400
Pd -0.19379700 -0.10684500 -0.57414700
O 0.87738800 -1.52761800 -1.56609900
H 0.25760700 -2.20959500 -1.84494500
H 1.61980300 -1.91447100 -0.49913300

54

RR_EI_ID1_TS1_Ntrigo-square_R, E(SCF) = -
2484.17496141, E(ZPE) = -2483.776427, E(G)
= -2483.844453 a.u.

C 0.54837800 3.09671800 -0.74512700
H 1.22984600 3.95230400 -0.74093500
H 0.01553200 3.10147900 -1.69789000
C -0.42622700 3.18283500 0.40320000

H 0.46603400 -2.34750100 1.39283500
O -0.47162200 -2.46699500 1.61584500
H -0.94867000 -2.25060100 0.79277400
H -0.89446900 0.08293000 3.63604900
O -1.40770100 -0.15454000 2.86057400
H -1.02588400 -0.99639800 2.53433900
H 2.04190400 1.12353900 -1.22916700
H 1.65170100 0.33165000 1.52946200
H -1.46411900 0.93241100 1.33383200
H -2.89706400 2.55254000 0.08679000
Pd -0.18298400 -0.09180700 -0.61051300
O 0.88440100 -1.48402600 -1.62817200
H 0.25111800 -2.14082200 -1.93544000
H 1.64697900 -1.92283000 -0.43639200

54

RR_EI_ID1_TS1_P_Htr_R, E(SCF) = -
2484.17061470, E(ZPE) = -2483.773765, E(G)
= -2483.839740 a.u.

C -0.28775800 2.47845800 0.71258700
H -0.83507600 3.42460700 0.70986400
H 0.11671400 2.33792600 1.71831300
C 0.82178600 2.49796300 -0.30639000
H 0.42761100 2.72691100 -1.29885800
H 1.57225300 3.25385900 -0.05302600
N 1.44142700 1.14963500 -0.38051800
N -1.20671700 1.34335900 0.45203100
C 2.29914100 0.80874100 0.80161400
H 2.65685700 1.74990800 1.23404300
C -2.42184800 1.65703800 -0.31668500
H -2.11318100 1.92848100 -1.33353000
C 3.47769500 -0.04182900 0.44782200
C 3.36531100 -1.44048200 0.29766500
C 4.72256300 0.56623700 0.30570700
C 4.53655900 -2.17232200 0.03075600
C 5.85517700 -0.17318700 0.03039300
H 4.81309200 1.64199800 0.42313400
C 5.75956900 -1.55424500 -0.09757100
H 4.44496900 -3.24841800 -0.06401300
H 6.64893500 -2.14117600 -0.30508900
C -3.40831400 0.52101500 -0.30413000
C -3.04642200 -0.84140800 -0.42675500
C -4.75618500 0.85165700 -0.18531100
C -4.07854500 -1.80136400 -0.40957700
C -5.74921300 -0.10536400 -0.19172000
H -5.04028600 1.89512900 -0.08820500
C -5.40092200 -1.44760200 -0.29631100
H -3.78862800 -2.84305300 -0.49434500
H -6.17046000 -2.21293400 -0.29009500
O 2.20557900 -2.06947600 0.38835300
O -1.81674000 -1.30218400 -0.56031400
S 7.45978600 0.61388600 -0.13929400
S -7.47616800 0.34484400 -0.02076400
O -7.92758000 -0.24115500 1.27484500
O -8.17207500 -0.26612900 -1.18933600
O -7.51904400 1.83333300 -0.03016100
O 7.93970500 0.26989500 -1.50836000
O 8.31615200 0.02016700 0.92715600
O 7.22468200 2.07234000 0.04659500
H 0.61836200 -2.27358900 1.38077100
O -0.29719700 -2.41342000 1.69044500
H -0.84798000 -2.26393100 0.90238300
H -0.90564600 0.13726800 3.67835000
O -1.36639200 -0.14185000 2.88400200
H -0.91904800 -0.96205500 2.58552600
H 2.02378000 1.10295500 -1.21470300
H 1.66899000 0.31591300 1.54610400
H -1.46264400 0.92227200 1.35814100
H -2.90047600 2.54131600 0.11918700
Pd -0.19756200 -0.10845700 -0.55969600
O 0.88143500 -1.57070600 -1.53330100
H 0.28111400 -2.27942000 -1.78800500
H 1.53797700 -1.90194000 -0.63055200

54

RR_EI_ID1_TS1_P_Htr_TS, E(SCF) = -
2484.17012128, E(ZPE) = -2483.773705, E(G)
= -2483.839328 a.u.

C -0.28672500 2.47761200 0.71213300
H -0.83063100 3.42605400 0.71076400
H 0.11912200 2.33698000 1.71744800
C 0.82346400 2.49893300 -0.30754100
H 0.42918400 2.73047500 -1.29932900
H 1.57338000 3.25480900 -0.05197500
N 1.44448500 1.15149700 -0.38776500
N -1.20684000 1.34511900 0.45248300
C 2.29842500 0.80782100 0.79295300
H 2.66047600 1.74560700 1.22893800
C -2.41908000 1.65934400 -0.31952500
H -2.10737700 1.92745500 -1.33647800
C 3.47791300 -0.04434000 0.44061800
C 3.38096000 -1.43748200 0.29339700
C 4.72373400 0.56434100 0.30272200
C 4.54237700 -2.17554200 0.04269800
C 5.85744600 -0.17728500 0.03995000
H 4.81357000 1.64017500 0.41693800
C 5.76789200 -1.55767700 -0.08122100
H 4.44859000 -3.25137700 -0.04960100
H 6.65939900 -2.14431500 -0.27788600
C -3.40569800 0.52300500 -0.30845200
C -3.04491000 -0.83936500 -0.44123700
C -4.75283100 0.85302600 -0.18001000
C -4.07807200 -1.79859700 -0.42187300
C -5.74675200 -0.10331100 -0.18591000
H -5.03588000 1.89613600 -0.07603700
C -5.39963600 -1.44518800 -0.29865100
H -3.78917100 -2.84003400 -0.51392200
H -6.16937700 -2.21033900 -0.29166500
O 2.20904300 -2.08408600 0.39362800
O -1.81721900 -1.30063300 -0.58759700
S 7.46481700 0.61360600 -0.12324600
S -7.47231400 0.34672000 -0.00329000
O -7.91653200 -0.24312700 1.29315900
O -8.17565000 -0.26364400 -1.16958800
O -7.51525100 1.83532000 -0.00777900
O 7.94612500 0.26685900 -1.48991100
O 8.31194500 0.01880200 0.94840800
O 7.22460500 2.07046700 0.06091100
H 0.55070100 -2.32016500 1.39015200
O -0.37548900 -2.44629800 1.66060000
H -0.89341700 -2.25915800 0.85660200
H -0.88154300 0.10862900 3.66671100
O -1.37538600 -0.15258300 2.88627800
H -0.95989600 -0.98251300 2.57060500
H 2.02449000 1.10707500 -1.22350000
H 1.66847800 0.31490800 1.53757200
H -1.46586400 0.92635500 1.35756600
H -2.90018600 2.54498200 0.11134400
Pd -0.19379700 -0.10684500 -0.57414700
O 0.87738800 -1.52761800 -1.56609900
H 0.25760700 -2.20959500 -1.84494500
H 1.61980300 -1.91447100 -0.49913300

54

RR_EI_ID1_TS1_P, E(SCF) = -2484.16828613,
E(ZPE) = -2483.766884, E(G) = -2483.831820
a.u.

C 0.37062100 -2.81089600 0.61080300
H 0.98998200 -3.70879500 0.57128900
H 0.02916300 -2.69702900 1.64136700
C -0.79748400 -2.92587500 -0.33410100
H -0.45516500 -3.19062100 -1.33680300
H -1.50023400 -3.69419300 0.00520100
N -1.47120700 -1.60525000 -0.43010000
N 1.18780100 -1.61089000 0.26856000
C -2.23724900 -1.24750300 0.80522700
H -2.73229200 -2.16232800 1.15257700
C 2.49245400 -1.88963900 -0.36646000
H 2.28560900 -2.28779600 -1.36644900
C -3.26132800 -0.18075700 0.59285400
C -2.88835700 1.18875000 0.53842400
C -4.60013800 -0.54265400 0.49405500

H 1.15828300 -1.62941000 -1.38028900
H 3.53550300 -2.93639700 -0.32563900
H -3.46274500 -2.80379200 -0.19806600

56

RR_EI_ID1_TS2-diamond_P, E(SCF) = -
2485.33309409, E(ZPE) = -2484.916265, E(G)
= -2484.983770 a.u.

C 0.38572000 -2.56964700 1.39700100
H 1.04826700 -3.41504500 1.59546100
H -0.05857500 -2.26947400 2.34719000
C -0.67122900 -2.92935200 0.39064200
H -0.21889200 -3.26709700 -0.54394400
H -1.31852900 -3.72930400 0.76256700
N -1.47327000 -1.71282100 0.09359700
N 1.17210200 -1.41274100 0.89365400
C -2.46232800 -1.40844400 1.17519200
H -2.98184300 -2.34753500 1.39906100
C 2.40376500 -1.78906900 0.18283000
H 2.10639700 -2.34943700 -0.71136500
C -3.43525700 -0.35641200 0.78257200
C -3.10625300 1.01187600 1.01378300
C -4.64469000 -0.70864000 0.20896500
C -4.08051700 1.96484000 0.62339600
C -5.57114500 0.25337800 -0.16631000
H -4.87246200 -1.76186800 0.05427300
C -5.27918200 1.59428700 0.05164400
H -6.00682800 2.34562300 -0.23619000
C 3.28732300 -0.63057500 -0.16770200
C 2.80802000 0.62477500 -0.58395300
C 4.66310000 -0.84511000 -0.12104500
C 3.74627400 1.60792000 -0.95238100
C 5.56551500 0.13134700 -0.48286200
H 5.04051900 -1.80695900 0.21177900
C 5.09893100 1.37172300 -0.90266800
H 5.79871900 2.15036100 -1.18806000
O -1.97697100 1.36296900 1.52455300
O 1.53310300 0.99269500 -0.63493400
S -7.12164600 -0.26395400 -0.89138100
S 7.33439600 -0.17154800 -0.42750700
O 7.50103600 -1.53445700 0.14725400
O 7.89944300 0.90213600 0.43763200
O 7.80503700 -0.07182200 -1.83856800
O -7.81065100 -1.09514600 0.14064200
O -6.77026500 -1.06060300 -2.10455100
O -7.86602000 0.98584200 -1.21685600
H 2.20182500 3.40542200 1.35750700
O 1.36494500 2.94032300 1.27713800
H 1.47641700 2.30610800 0.53728400
H -0.48568100 0.80604800 2.40081500
O 0.41935200 0.67714000 2.75800000
H 0.86908400 1.49334100 2.48067100
H -2.00746100 -1.87778400 -0.75849200
H -1.90531400 -1.10634300 2.06337200
H 1.35787600 -0.77213600 1.67838800
H 2.96674700 -2.48107600 0.81801600
Pd -0.01746900 -0.25932600 -0.30598600
O -1.05594300 3.18586600 -0.25960300
H -0.19447800 3.45356100 0.08834900
H -1.41297100 2.63153900 0.47205000
H -3.85555100 3.01356900 0.79345600
H 3.36249800 2.56927000 -1.27812800
H -1.01783800 0.48123600 -1.58416900
H -0.97697400 1.08699500 -1.03336600

54

RR_EI_ID1_TS2-diamond_R_noh2, E(SCF) = -
2484.16664672, E(ZPE) = -2483.767069, E(G)
= -2483.832465 a.u.

C 0.19501400 -2.20952500 1.05867500
H 0.65773500 -3.19643600 1.13580200
H -0.20126900 -1.94785500 2.04157600
C -0.90319100 -2.19719700 0.03064900
H -0.52612300 -2.50558800 -0.94673300
H -1.71251500 -2.87838000 0.31224500
N -1.41493100 -0.80841300 -0.10561300
N 1.21990700 -1.18427400 0.71267600

C -2.33354200 -0.37008600 1.00789000
H -2.54572900 -1.24698300 1.62663200
C 2.35362000 -1.66624500 -0.10882200
H 1.95478100 -1.92753700 -1.09486100
C -3.60816900 0.19067100 0.47167300
C -3.64896000 1.53353400 -0.00015000
C -4.74106500 -0.60588100 0.41671100
C -4.88655200 1.99713100 -0.49394300
C -5.93944400 -0.11956300 -0.08207600
H -4.68708900 -1.62918400 0.78252500
C -6.00452900 1.19031000 -0.53708000
H -6.94488200 1.56809700 -0.92345500
C 3.45892200 -0.65359000 -0.19343200
C 3.23931800 0.71840700 -0.44310200
C 4.76570400 -1.11105800 -0.04504300
C 4.36073300 1.56353300 -0.54212000
C 5.85050800 -0.26623600 -0.15279400
H 4.94170900 -2.16241400 0.15943900
C 5.64165300 1.08496600 -0.40393800
H 6.48704100 1.76039500 -0.48674500
O -2.60394700 2.30598200 0.02818200
C 2.05482300 1.28583000 -0.59680000
S -7.37092800 -1.19538900 -0.12327100
S 7.52716500 -0.87933800 0.03121800
O 7.40478000 -2.33888600 0.29840500
O 8.11434900 -0.12322800 1.17414900
O 8.21063100 -0.57714200 -1.25861200
O -7.61821300 -1.61325600 1.28804800
O -6.99593000 -2.34973200 -0.99172800
O -8.48336200 -0.38181900 -0.68976700
H 2.19854100 3.88402500 1.32485700
O 1.44362800 3.55212300 0.83336900
H 1.77247800 2.77385600 0.33925900
H -1.53216000 2.57333600 1.47595600
O -0.90764600 2.70965200 2.21503000
H -0.08685900 3.01045400 1.78864000
H -1.94758500 -0.75304400 -0.97296400
H -1.79957000 0.35825700 1.62139200
H 1.60106000 -0.79901900 1.57541100
H 2.74593800 -2.58608500 0.33765500
Pd 0.31146900 0.31112300 -0.33451600
O -0.66020000 1.76089200 -1.46271900
H -0.08839900 2.52346100 -1.60583500
H -1.46674700 2.05695700 -0.89485700
H -4.93341700 3.02248300 -0.84689900
H 4.17943700 2.61563400 -0.73692400

56

RR_EI_ID1_TS2-diamond, E(SCF) = -
2485.31969602, E(ZPE) = -2484.905052, E(G)
= -2484.973613 a.u.

C 0.36465300 -2.42368800 1.46707800
H 1.01357400 -3.27480000 1.68408300
H -0.06716600 -2.09021800 2.41175300
C -0.70531600 -2.78950500 0.47782100
H -0.26556800 -3.15042400 -0.45406500
H -1.36082100 -3.57257100 0.87146400
N -1.48672100 -1.56348400 0.17158200
N 1.16921200 -1.29795900 0.92075800
C -2.41770900 -1.20904900 1.28782400
H -2.88710800 -2.14634700 1.61129700
C 2.41188000 -1.73485800 0.26456800
H 2.12276800 -2.36060000 -0.58789300
C -3.45574700 -0.21644200 0.90191600
C -3.26896400 1.15586900 1.24027900
C -4.60823300 -0.63776100 0.25895200
C -4.31816300 2.03701800 0.87845900
C -5.60771400 0.25707800 -0.09106400
H -4.73196000 -1.69519500 0.02931000
C -5.45464400 1.60048000 0.23247500
H -6.23775600 2.30087700 -0.03641800
C 3.31951300 -0.62105900 -0.15642500
C 2.86483600 0.58051000 -0.72849900
C 4.69048700 -0.82944400 -0.02448600
C 3.82211500 1.51778800 -1.16181800
C 5.61246900 0.09980600 -0.45577300
H 5.04895700 -1.74939300 0.42631400

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C 5.17036300 1.28586100 -1.03016000
H 5.88628100 2.02648800 -1.37169800
O -2.19159100 1.58638800 1.80424400
O 1.59489200 0.93132900 -0.87604500
S -7.08235400 -0.34993600 -0.90154000
S 7.37569900 -0.18447000 -0.27256000
O 7.51322400 -1.52709000 0.35535400
O 7.87555700 0.92062700 0.59406000
O 7.93851000 -0.12376000 -1.65144000
O -7.74995600 -1.26537700 0.07160800
O -6.61959900 -1.07545600 -2.12174700
O -7.90588400 0.85098300 -1.22050000
H 1.96176200 3.68624000 0.88037600
O 1.26240700 3.02866500 0.85043700
H 1.53523300 2.36245400 0.18843200
H -0.54764400 1.03539500 2.37580300
O 0.39850300 0.93884600 2.61970600
H 0.80404100 1.71409000 2.19624300
H -2.06060300 -1.70545600 -0.65240400
H -1.82066500 -0.82299000 2.11404100
H 1.34049300 -0.61235600 1.66915400
H 2.95402400 -2.38078600 0.96379500
Pd 0.01089800 -0.20039500 -0.36546400
O -1.08139000 2.13671500 -0.59086000
H -0.32324100 2.72584400 -0.47791700
H -1.45427800 2.07681900 0.32073200
H -4.19668400 3.08749300 1.12598800
H 3.45790200 2.43811900 -1.60668700
H -0.81004100 -0.16959000 -2.43262900
H -1.13009700 0.46001800 -2.14393900
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56
RR_EI_ID1_TS2-trigo_P, E(SCF) = -
2485.33517604, E(ZPE) = -2484.919121, E(G)
= -2484.986403 a.u.
C 0.40903600 3.14645800 -1.08447900
H 1.04834100 4.02724200 -1.01331100
H 0.31233000 2.90146300 -2.14459100
C -0.93457500 3.43471600 -0.45604700
H -0.80586900 3.99497900 0.47157300
H -1.56673300 4.02428700 -1.12809700
N -1.61094200 2.16234000 -0.09683300
N 1.06997500 1.98810700 -0.41459800
C -2.14940900 1.40129300 -1.26667700
H -2.80661800 2.08699800 -1.81377800
C 2.40684000 2.24495800 0.16752800
H 2.27214000 2.88273500 1.04688400
C -2.89876000 0.17894900 -0.85464700
C -2.21359000 -1.04649100 -0.62444900
C -4.27810800 0.25109700 -0.70040900
C -3.00476300 -2.15594500 -0.24003000
C -5.01853200 -0.85177900 -0.32046400
H -4.79221600 1.19063800 -0.88590000
C -4.36869800 -2.06211300 -0.09252900
H -4.94465100 -2.93498400 0.20055800
C 3.08326700 0.95174100 0.49440800
C 2.50008100 0.05008400 1.41478500
C 4.28116000 0.62062200 -0.11479000
C 3.19303400 -1.13081300 1.72075600
C 4.94458800 -0.55850500 0.19041100
H 4.71465600 1.30723900 -0.83695400
C 4.40131700 -1.43013000 1.11789200
H 4.92828800 -2.34656100 1.35874000
O -0.92375200 -1.15089000 -0.72848700
O 1.34800800 0.28203800 2.02115300
S -6.79447800 -0.75645600 -0.11834300
S 6.49604800 -0.92698600 -0.63593000
O 6.17828900 -0.95713800 -2.09134600
O 6.93476800 -2.24523800 -0.10347100
O 7.41929100 0.18674800 -0.27827000
O -7.17816600 0.63701300 -0.48143100
O -7.06546800 -1.07758800 1.31378000
O -7.37130100 -1.77713200 -1.04142800
H 0.66866700 -2.23692500 -0.81788700
H -1.25620100 0.87120700 2.38156300
H -1.28444900 0.15873300 1.98585800
O 1.60614100 -2.43617700 -0.99397000
```

```
H 2.05883500 -2.23910700 -0.16401200
H 0.13978800 -0.40406000 -1.90961000
O 0.93400900 -0.04413100 -2.36880200
H 1.58294600 -0.74065000 -2.18228200
H -2.40174900 2.37837100 0.50888300
H -1.31238100 1.15712300 -1.92181600
H 1.17225300 1.23689800 -1.12481600
H 3.00787500 2.79848500 -0.56086300
Pd -0.17008600 1.15930300 0.99565000
H -2.49492800 -3.09927000 -0.06746000
H 2.75692000 -1.80875500 -2.44715900
O -0.21470100 -2.12107600 1.85783200
H 0.40042700 -1.41633500 2.11830900
H -0.46636300 -1.87203800 0.94810700
```

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54
RR_EI_ID1_TS2-trigo_R_noH2, E(SCF) = -
2484.16810187, E(ZPE) = -2483.766790, E(G)
= -2483.832604 a.u.
C -0.38307200 2.80328100 0.58780000
H -1.00581200 3.69852800 0.54255200
H -0.04139500 2.69710600 1.61907100
C 0.78475300 2.91647300 -0.35767000
H 0.44180100 3.17407900 -1.36201400
H 1.48471300 3.68928600 -0.02283700
N 1.46297200 1.59764200 -0.44554100
N -1.19589100 1.59792600 0.25304700
C 2.22979100 1.25011900 0.79247600
H 2.72040700 2.16912900 1.13497100
C -2.50097800 1.86822600 -0.38482100
H -2.29539100 2.25702700 -1.38860900
C 3.25872700 0.18673600 0.58740100
C 2.89137100 -1.18447500 0.53800900
C 4.59647000 0.55356800 0.49274300
C 3.93763200 -2.12592400 0.40019000
C 5.59430500 -0.39143300 0.35087600
H 4.87138200 1.60350300 0.53706300
C 5.25510800 -1.74089200 0.31069800
H 6.03500000 -2.48926500 0.20470200
C -3.37401500 0.65012500 -0.40645600
C -2.92487400 -0.60196900 -0.89060600
C -4.67713600 0.76623200 0.05439400
C -3.83474900 -1.67131000 -0.90232100
C -5.55782500 -0.30193300 0.03277300
H -5.01434400 1.72494500 0.43949900
C -5.12963300 -1.52744100 -0.45047400
H -5.81565800 -2.36665500 -0.46226200
O 1.64634500 -1.56412700 0.57703500
O -1.70476600 -0.83781300 -1.33974600
S 7.31794200 0.08382600 0.25121300
S -7.22779000 -0.07329500 0.64976600
O -7.08233400 0.37655300 2.06365700
O -7.89275000 -1.39916400 0.52439000
O -7.84465300 0.97250500 -0.21595000
O 7.34155500 1.57297900 0.30215400
O 7.82354600 -0.46047100 -1.04311400
O 7.98847200 -0.54782800 1.42510300
H 0.15377700 -2.75355800 0.46640900
O -0.78556500 -2.98882900 0.37306200
H -1.11644700 -2.36942800 -0.30023000
H 0.28386700 -0.83805400 1.67542000
O -0.56870000 -0.63372800 2.11379700
H -1.09616300 -1.40211800 1.85195300
H 2.12485200 1.61951000 -1.22000200
H 1.51017600 0.95998500 1.56030600
H -1.33025100 1.03090900 1.10071500
H -3.01044500 2.65964900 0.17445900
Pd -0.11545700 0.33398600 -0.91692600
H 3.66540100 -3.17604500 0.36591900
H -3.48305300 -2.62702600 -1.27712700
O 1.08235900 -1.07000400 -1.96187300
H 0.52937700 -1.67354300 -2.47264500
H 1.36390100 -1.54418600 -1.13515800
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56

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RR_EI_ID1_TS2-trigo_R, E(SCF) = -
2485.34097154, E(ZPE) = -2484.924593, E(G)
= -2484.992298 a.u.
C 0.39328100 2.74637400 -0.78368800
H 1.01728000 3.64209500 -0.78932800
H 0.05404000 2.58065700 -1.80792700
C -0.77667100 2.91483500 0.15059400
H -0.43525500 3.22194900 1.14156200
H -1.47038400 3.67434900 -0.22514700
N -1.46435100 1.60632800 0.30247900
N 1.20246100 1.56101900 -0.37957700
C -2.24256300 1.20865800 -0.91283800
H -2.73607800 2.11265300 -1.28921300
C 2.49235900 1.85989100 0.27504400
H 2.26607600 2.28319100 1.26057400
C -3.26869300 0.15492500 -0.65264000
C -2.90005700 -1.21399700 -0.55992400
C -4.60334100 0.52684600 -0.53792800
C -3.94363100 -2.14868600 -0.36469600
C -5.59768400 -0.41114900 -0.33687500
H -4.87908700 1.57486700 -0.61325400
C -5.25800500 -1.75866100 -0.25491400
H -6.03557800 -2.50131500 -0.10188900
C 3.36862600 0.64629600 0.35750100
C 2.91135400 -0.59215600 0.86840500
C 4.68357900 0.75383100 -0.07144700
C 3.82456500 -1.65661600 0.93750600
C 5.56812200 -0.30788900 0.01060900
H 5.02741900 1.70191300 -0.47642200
C 5.13065900 -1.52087000 0.51690000
H 5.82046500 -2.35505500 0.57549900
O -1.65621600 -1.59588500 -0.60635700
O 1.68150600 -0.82005700 1.29435200
S -7.31567400 0.07041300 -0.18949000
S 7.24607700 -0.10147100 -0.59253500
O 7.12405100 0.15972700 -2.05569300
O 7.94730900 -1.37828700 -0.28564900
O 7.80754400 1.06545000 0.14615200
O -7.34698900 1.55200600 -0.34586200
O -7.75522900 -0.37930700 1.16373100
O -8.04001400 -0.64401100 -1.28085800
H -0.16275800 -2.79153600 -0.44187000
H 0.56228100 2.15878200 3.58297600
H -0.10236800 1.82510700 3.49128900
O 0.77586200 -3.02468700 -0.33705600
H 1.10549900 -2.38167200 0.31480900
H -0.27489000 -0.90557200 -1.71202700
O 0.58354900 -0.73012400 -2.15093100
H 1.09816600 -1.49472100 -1.85375900
H -2.12047600 1.66834800 1.08018600
H -1.53018300 0.88511300 -1.67375700
H 1.35639000 0.96000400 -1.19995500
H 3.01093800 2.63338900 -0.30068100
Pd 0.10245400 0.34671000 0.82407200
H -3.67099200 -3.19721700 -0.29812300
H 3.46651400 -2.60173700 1.33261500
O -1.10698000 -1.00745400 1.92311000
H -0.55634800 -1.58797400 2.46237500
H -1.38335100 -1.51750600 1.11710600

56
RR_EI_ID1_TS2-trigo_R, E(SCF) = -
2485.32167841, E(ZPE) = -2484.907288, E(G)
= -2484.973723 a.u.
C 0.37640100 2.94481300 -1.43394800
H 1.00287900 3.83533800 -1.50015000
H 0.22704600 2.57313500 -2.45055700
C -0.93821400 3.28660700 -0.77075500
H -0.76756000 3.93247400 0.09246800
H -1.60800500 3.80644000 -1.46392100
N -1.57568800 2.04458300 -0.26353300
N 1.08660900 1.88516000 -0.66262400
C -2.11103000 1.16937800 -1.34971500
H -2.73835200 1.80370100 -1.98777500
C 2.45137700 2.22460600 -0.20043700
H 2.36103900 3.00644100 0.56229100
C -2.90320500 0.01695600 -0.83158000

C -2.25432800 -1.18800100 -0.45145500
C -4.28467100 0.13033300 -0.73466900
C -3.07926700 -2.23656500 0.02016900
C -5.06073000 -0.91043500 -0.26069300
H -4.77052200 1.05437400 -1.03582100
C -4.44542600 -2.10328500 0.11069700
H -5.04784200 -2.92788300 0.48043200
C 3.14813800 1.00311600 0.30803600
C 2.61845900 0.28779200 1.40765200
C 4.30167500 0.54709700 -0.30470200
C 3.31214900 -0.83997600 1.86939300
C 4.96957500 -0.57782800 0.15942200
H 4.69304900 1.08520900 -1.16375200
C 4.47924700 -1.26247200 1.25809100
H 5.00466800 -2.13799000 1.62099800
O -0.96274900 -1.31857400 -0.49398400
O 1.51161400 0.65374800 2.02416400
S -6.84365200 -0.77316900 -0.17252800
S 6.48629600 -1.09000800 -0.68721000
O 6.15939500 -1.15675600 -2.10896400
O 6.83740300 -2.41247000 -0.07241700
O 7.48752400 -0.02983800 -0.34757900
O -7.16626200 0.64967200 0.48907900
O -7.21989100 -1.15771200 1.21916000
O -7.38397600 -1.72838000 -1.18436600
H 0.59737000 -2.33297900 -0.25269200
H -0.85280700 2.05839200 2.80745600
H -1.36973500 1.50055400 2.77809600
O 1.53281300 -2.59332500 -0.35208700
H 1.99448100 -2.18837000 0.39293300
H 0.14720300 -0.75434900 -1.70878900
O 0.95684400 -0.48116700 -2.20199300
H 1.59808100 -1.12800000 -1.86985900
H -2.36444600 2.30286100 0.32825800
H -1.26685900 0.83207500 -1.95185800
H 1.15656700 1.03639000 -1.25715800
H 3.01324900 2.63981000 -1.04386000
Pd -0.06487900 1.25995700 0.92777900
H -2.59329800 -3.16156600 0.31616500
H 2.90895900 -1.36991600 2.72671800
O -0.76600100 -0.92538400 2.26177000
H 0.16124700 -0.79221900 2.51031600
H -0.73532900 -1.25723300 1.34107200

56
RR_EI_ID1_TS3-diamond_P, E(SCF) = -
2485.36826880, E(ZPE) = -2484.949324, E(G)
= -2485.018468 a.u.
C 0.43333400 -2.38025100 1.73403200
H 1.05630400 -3.24387900 1.99341500
H 0.02869000 -1.98494000 2.66897800
C -0.68441600 -2.81458200 0.81422400
H -0.27846900 -3.25149500 -0.10073500
H -1.30847100 -3.57336400 1.29884700
N -1.51148500 -1.64576400 0.41437900
N 1.23011400 -1.31229500 -1.11350500
C -2.47711400 -1.25173400 1.47624600
H -2.99660000 -2.15636200 1.81468100
C 2.34808700 -1.77139000 0.28700500
H 1.92463300 -2.32797000 -0.55934900
C -3.46608400 -0.26119200 0.96065600
C -3.24571000 1.11365100 1.08271500
C -4.59499200 -0.70046500 0.28687900
C -4.14359200 2.01386000 0.52113100
C -5.49020200 0.19845000 -0.27084400
H -4.77558300 -1.76901500 0.19719200
C -5.25821900 1.55773000 -0.16102800
H -5.96035800 2.25783500 -0.59749200
C 3.22656200 -0.65217500 -0.19934300
C 2.74685600 0.57644400 -0.71211900
C 4.60148400 -0.87549300 -0.17142800
C 3.69956500 1.51132900 -1.17150800
C 5.51121200 0.05256100 -0.63450300
H 4.97607300 -1.81358300 0.22672300
C 5.05053000 1.26434800 -1.13482100
H 5.75244300 2.00832400 -1.49796000
O -2.15961900 1.54503700 1.76563500
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O 1.48260600 0.96047100 -0.77896400
S -6.92427100 -0.43436000 -1.15596800
S 7.27575900 -0.25543100 -0.55821200
O 7.43071600 -1.65609700 -0.07645800
O 7.82556700 0.75113900 0.39577600
O 7.78684700 -0.05573400 -1.94495700
O -7.61106400 -1.34806400 -0.20123400
O -6.37479800 -1.15238900 -2.34021500
O -7.73837600 0.75637300 -1.51869400
H 2.23411500 3.45052400 1.03805400
O 1.42999900 2.92534200 1.05943800
H 1.50764900 2.25848100 0.33472700
H -0.34047600 0.96961100 2.62774400
O 0.57488700 0.97054000 2.94291400
H 0.97902100 1.69824900 2.43823500
H -2.05827700 -1.91073900 -0.40237600
H -1.91868500 -0.85312100 2.32274000
H 1.53639300 -0.65538700 1.83219700
H 2.96661900 -2.48281200 0.84972100
Pd -0.09148000 -0.23453900 -0.20971700
O -1.09761300 3.30818900 0.03311000
H -0.19899700 3.45144700 0.38737000
H -1.81882200 2.35478500 1.31520000
H -3.95982700 3.07747800 0.62633800
H 3.32069200 2.44957600 -1.56529500
H -1.06801100 0.48047500 -1.21704600
H -0.98324300 2.57274700 -0.58779200

56

RR_EI_ID1_TS3-diamond, E(SCF) = -
2485.32783557, E(ZPE) = -2484.912858, E(G)
= -2484.979460 a.u.
C 0.36290600 -2.48247000 1.33862900
H 0.98086400 -3.36766300 1.50747200
H -0.04776700 -2.18239400 2.30413700
C -0.73758200 -2.77215300 0.35427300
H -0.32651300 -3.10992100 -0.59943100
H -1.40902500 -3.55100000 0.72995500
N -1.49227600 -1.51615800 0.10458800
N 1.19187500 -1.36130400 0.83263800
C -2.38690900 -1.16172500 1.25163800
H -2.83014800 -2.09888000 1.60997100
C 2.39751300 -1.78881100 0.10581600
H 2.06182200 -2.30678100 -0.80078800
C -3.45483400 -0.20078200 0.86473600
C -3.25797600 1.19316000 1.06991500
C -4.63328300 -0.67202700 0.30960000
C -4.30749600 2.04593300 0.65519200
C -5.64490900 0.19265100 -0.07905000
H -4.76483100 -1.74486200 0.17904900
C -5.47225900 1.55912000 0.09890000
H -6.26210100 2.23664000 -0.20549200
C 3.33203400 -0.66444300 -0.22279700
C 2.90790800 0.58268100 -0.72238500
C 4.69607000 -0.90153300 -0.07032100
C 3.89451500 1.52438200 -1.07671300
C 5.64478200 0.03725600 -0.41681200
H 5.02803000 -1.85520100 0.32787900
C 5.23559300 1.26346200 -0.92691600
H 5.97059200 2.01075100 -1.20786300
O -2.16599600 1.66915800 1.57899900
O 1.64963400 0.96862600 -0.87978200
S -7.15689900 -0.48015800 -0.76161500
S 7.39581300 -0.28215700 -0.18627600
O 7.49947400 -1.69329700 0.27662400
O 7.85753100 0.70149600 0.83494100
O 8.02611700 -0.05548900 -1.51770900
O -7.76293000 -1.31591100 0.31700300
O -6.75339100 -1.29860500 -1.94298600
O -8.00272800 0.68986600 -1.13040000
H 1.98875200 3.77863500 0.70099000
O 1.30035200 3.10885500 0.70192000
H 1.58059800 2.40275700 0.07691400
H -0.53942000 1.12777800 2.23950300
O 0.39429900 1.00951600 2.51454800
H 0.83701000 1.76656700 2.10053100
H -2.08934300 -1.65318900 -0.70937100

H -1.77054500 -0.74796200 2.04956200
H 1.42904800 -0.73555700 1.60780600
H 2.93472900 -2.52615700 0.71228800
Pd 0.02431700 -0.16293700 -0.39488600
O -1.13669900 2.76941100 -0.50616400
H -0.27326400 3.14321300 -0.23355200
H -1.55884900 2.49593900 0.37156900
H -4.17180100 3.11440000 0.79563800
H 3.55880900 2.47443000 -1.48010300
H -0.94476600 0.69431700 -1.48640700
H -0.92203100 1.51131600 -1.00341400

56

RR_EI_ID1_TS3-trigo_P, E(SCF) = -
2485.37337961, E(ZPE) = -2484.954350, E(G)
= -2485.021855 a.u.
C 0.36259700 2.99941500 -0.97323700
H 1.01070900 3.88184700 -0.94936300
H 0.13255000 2.80991800 -2.02520300
C -0.90954000 3.28992800 -0.20200300
H -0.67367200 3.66248900 0.79717600
H -1.50275800 4.05373400 -0.71849800
N -1.70609700 2.04985200 -2.01797500
N 1.06022800 1.81136100 -0.45354900
C -2.36746600 1.58179900 -1.26521200
H -3.00956100 2.38752400 -1.64066200
C 2.20887300 2.04913400 0.42772100
H 1.83558300 2.47510100 1.36820200
C -3.17183200 0.35088500 -1.00098600
C -2.61422800 -0.92353500 -1.11541500
C -4.47359500 0.46949800 -0.52842700
C -3.34703600 -2.04479600 -0.73708400
C -5.20065700 -0.64451000 -0.15533600
H -4.92578400 1.45284900 -0.43875500
C -4.63165100 -1.90617900 -0.25086300
H -5.20001500 -2.78189600 0.04417500
C 2.97572500 0.77767900 0.66285700
C 2.38990700 -0.39491500 1.20391900
C 4.31994300 0.75430400 0.30524500
C 3.23192300 -1.50666800 1.41975000
C 5.11669500 -0.35853700 0.49767400
H 4.76410800 1.64183600 -0.13464500
C 4.56260600 -1.49921100 1.06708800
H 5.17485000 -2.37970000 1.23421100
O -1.35838000 -1.05634900 -1.60830600
O 1.12143800 -0.53899400 1.52846300
S -6.88197500 -0.48750200 0.46751100
S 6.82502300 -0.38367800 -0.04661500
O 6.87076700 -1.35228000 -1.18093500
O 7.62454100 -0.84570400 1.12378400
O 7.14744900 1.00980000 -0.46090900
O -7.19374300 0.96659200 0.43642800
O -6.84919800 -1.05179400 1.84550000
O -7.72713900 -1.28956400 -0.45995200
H 1.78760500 -2.46027900 -1.12246900
H -1.39935800 0.02236800 1.72449700
H 0.03295800 -3.41507700 0.39067400
O 2.49223300 -2.15201800 -1.72231800
H 3.21234300 -1.90197800 -1.13017200
H 0.17839800 -0.24427900 -2.53302100
O 1.07513300 0.04364600 -2.76065700
H 1.64178900 -0.70600500 -2.49227000
H -2.43679300 2.23539800 0.66544200
H -1.59491000 1.39725100 -2.01125200
H 1.33923100 1.22601000 -1.24811500
H 2.88562800 2.79285800 -0.01272100
Pd -0.34048900 0.71079600 0.79230800
H -2.89461000 -3.02627600 -0.83371000
H 2.78330600 -2.39379500 1.85597300
O 0.24960700 -2.58207900 -0.03705400
H 0.48814800 -1.93983200 0.67553800
H -0.87021500 -1.75281800 -1.11137500

56

RR_EI_ID1_TS3-trigo_R, E(SCF) = -
2485.33517311, E(ZPE) = -2484.918489, E(G)
= -2484.985028 a.u.

C 2.58767200 -0.56250400 0.75493400
C 4.56791200 0.26217100 -0.36855200
C 3.39529800 -1.58036800 1.30417200
C 5.33801600 -0.73645500 0.18973700
H 5.04370700 0.97961300 -1.02999100
C 4.73880600 -1.66734600 1.03257000
H 2.91347800 -2.29928400 1.95776200
H 5.33105100 -2.46273500 1.47366000
O -3.81992800 2.45743400 0.77760700
O 1.31633000 -0.57177700 1.08428700
S -4.68216000 -3.22724400 -0.60286700
S 7.08433800 -0.88581900 -0.18634000
O 7.78191200 -0.93058600 1.13082500
O 7.43931000 0.31523500 -0.99237000
O 7.23070600 -2.16049600 -0.94740300
O -3.76095800 -3.54352800 -1.73114800
O -6.12156100 -3.34192200 -0.98320100
O -4.36754900 -3.99803200 0.63583200
H 2.29601600 2.34410800 0.02375100
H -2.90729800 2.28885900 -1.92651800
H 1.30769700 0.33738500 -1.85311900
H -1.87943600 2.52710700 0.17138300
O -1.17153000 0.13685400 1.97817000
H -1.61221700 0.89425200 2.45476300
H -3.67540000 3.87004200 -0.25770300
O -3.44389100 4.67233700 -0.77489900
H -4.02058700 4.64867700 -1.54099900
H -0.54349300 -0.27237300 2.58621000
H -3.08664600 2.40634900 2.29216400
O -2.51344000 2.14637800 3.06019100
H -2.05206800 2.94145800 3.33694300
Pd -0.04314400 0.66905600 0.29164800

54
RR_EI_ID2_TS1_R, E(SCF) = -2484.17440886,
E(ZPE) = -2483.775979, E(G) = -2483.845003
a.u.
C 0.60425800 2.91123600 -1.21171600
H 1.29780900 3.73892300 -1.38649600
H 0.04755100 2.74609000 -2.13600100
C -0.33751800 3.23357400 -0.07755300
H 0.22114400 3.52139500 0.81588900
H -0.98646500 4.07289500 -0.34583400
N -1.14356200 2.04469100 0.29256400
N 1.35484500 1.65606000 -0.93473200
C -2.36841100 1.80525600 -0.47485700
H -2.09260700 1.68490500 -1.52903000
C 2.59985700 1.77835000 -0.15515600
H 3.23021700 2.55418600 -0.60432700
C -3.14638200 0.60616200 0.00969900
C -2.60931100 -0.49637500 0.71232600
C -4.50215000 0.59857200 -0.31429900
C -3.48279500 -1.54512000 1.05914800
C -5.33210100 -0.444856800 0.02103400
H -4.92121900 1.44352800 -0.85232600
C -4.81547900 -1.53018700 0.72510800
H -3.06371400 -2.38075700 1.61035000
H -5.45801500 -2.35846500 1.00552000
C 3.36584500 0.48268600 -0.11362400
C 2.76639100 -0.79873900 -0.02627000
C 4.75548900 0.57754000 -0.13378400
C 3.62461000 -1.91713000 0.04615100
C 5.56926400 -0.53218100 -0.05514100
H 5.21943900 1.55586800 -0.21505900
C 4.99172800 -1.79436700 0.03507500
H 3.15832600 -2.89488300 0.11372500
H 5.61923500 -2.67829700 0.09058200
O -1.34383200 -0.62497100 1.11400400
O 1.47332700 -1.05040900 -0.02035000
S -7.08188300 -0.41139100 -0.38073900
S 7.35520300 -0.37893200 -0.07119400
O 7.82544500 -0.93274700 1.23177900
O 7.64394000 1.07427300 -0.22299200
O 7.82386500 -1.19052400 -1.23116500
O -7.28474400 0.79617200 -1.22770500
O -7.79266300 -0.33253000 0.92762600
O -7.36000200 -1.68555100 -1.10197600

H 2.32932300 2.12320200 0.84928800
H -3.00955300 2.69330100 -0.41607200
H 1.58388500 1.21433500 -1.82323500
H -1.37529500 2.09653700 1.29337100
O -1.40296600 -2.22493000 -2.14157800
H -1.05157100 -2.59209900 -1.30740800
H -1.28673600 0.48292300 2.67680100
O -1.28273700 1.36430400 3.09208900
H -2.00643300 1.35870700 3.72318000
H -1.33836200 -1.27306600 -2.02099800
H -0.77991700 -2.38305100 0.82552800
O -0.30152900 -3.08261900 0.34261000
H 0.54534800 -2.62596200 0.17838800
Pd 0.09088900 0.43851500 0.10445000

54
RR_EI_ID2_TS1, E(SCF) = -2484.13719522,
E(ZPE) = -2483.737802, E(G) = -2483.803576
a.u.
C 0.65761700 3.45231000 -0.11552500
H 1.30082900 4.21388100 0.33722600
H 0.26322000 3.85212400 -1.05116300
C -0.47854400 3.08062000 0.80778300
H -0.12974200 2.98980300 1.83940400
H -1.23454200 3.86762600 0.78755700
N -1.08342900 1.77156800 0.42722400
N 1.46163600 2.26372800 -0.49244500
C -2.52274700 1.76012200 0.13347700
H -2.65793900 2.11543500 -0.89485100
C 2.43817300 1.74302500 0.47284000
H 3.12071400 2.55321300 0.75642300
C -3.19217400 0.41801700 0.32680900
C -2.51755500 -0.82222300 0.50915200
C -4.58131900 0.43978800 0.28170300
C -3.32855500 -1.98026500 0.59668100
C -5.34122400 -0.70989800 0.38014400
H -5.09279900 1.39020200 0.15095200
C -4.70101600 -1.93478600 0.53931500
H -2.81325100 -2.92840400 0.72235200
H -5.28327100 -2.84820500 0.61432700
C 3.23867400 0.59663500 -0.09794700
C 2.80881600 -0.27585500 -1.13037800
C 4.49283500 0.39201600 0.47475200
C 3.68386200 -1.31539100 -1.51303600
C 5.32454600 -0.63370900 0.08235800
H 4.83155500 1.06467300 1.25724400
C 4.91220200 -1.49616700 -0.92753100
H 3.34526300 -1.97649800 -2.30438600
H 5.55756700 -2.30636900 -1.25170800
O -1.22177600 -0.94430900 0.58818300
O 1.66492900 -0.21204400 -1.79771500
S -7.12964400 -0.64303600 0.36887800
S 6.93135200 -0.87373700 0.84271800
O 6.88465600 -2.22444100 1.47307500
O 7.08856400 0.22622000 1.83382100
O 7.92130500 -0.80249300 -0.26993100
O -7.49393900 0.76429800 0.03924200
O -7.56912900 -1.04513600 1.73822400
O -7.57507600 -1.61660300 -0.67075300
H 1.88964100 1.43429100 1.36954500
H -3.01701500 2.49347900 0.78387300
H 1.94966600 2.47313200 -1.36173000
H -0.92328700 1.15167700 1.22529200
O -1.29971700 -0.42158500 -2.22569100
H -1.00785200 -1.34187000 -2.04586300
H -0.27052800 -0.46709600 1.96368500
O 0.23028100 0.15543200 2.53789100
H -0.01992700 -0.05499900 -3.44013800
H -1.03015500 -0.23674300 -3.13134200
H -0.39626900 -2.16095800 -0.37194700
O 0.00276100 -2.59846000 -1.16100300
H 0.78245200 -2.05516100 -1.35734500
Pd 0.15079200 0.78838300 -0.91332600

56

O -2.52548500 1.59943800 -0.96234100
S 6.20623300 -2.74386100 -0.32127700
S -7.25318600 -1.70024000 0.36748400
O -8.18552700 -0.76666100 1.06332100
O -6.79889800 -2.82229200 1.23528900
O -7.79186500 -2.16035000 -0.94512000
O 6.51358700 -3.30974000 1.02673600
O 7.44249400 -2.51601900 -1.12702100
O 5.17503800 -3.53120700 -1.05573300
H -1.88204100 -0.14261800 1.75011400
H 1.96766000 -0.00811700 -1.49201900
H -1.26575800 -1.13116800 -0.92593200
H 1.55104800 1.65486900 0.91036700
O -0.28733100 3.31224300 -0.80592900
H 0.60748600 3.68971700 -0.58272600
H 2.70024500 2.84164900 2.00526700
O 1.81577200 2.89765000 2.43001800
H 1.46480500 3.73461200 2.10899200
H -0.95797400 3.85816200 -0.38300100
H 2.83679700 3.62303000 -0.03260000
O 2.11215600 4.26525900 -0.26235500
H 2.47737300 4.89177900 -0.89066400
H -0.89388800 -0.17304700 -3.17584100
H -0.22919100 -0.50939400 -3.25834100
Pd -0.62235800 1.28200100 -0.40467900

56

RR_EI_ID2_TS2-square_P, E(SCF) = -
2485.32916379, E(ZPE) = -2484.912919, E(G)
= -2484.983796 a.u.
C 0.20926300 -1.40654800 0.39590500
H -0.04411400 -2.23331500 1.06380700
H 0.72373600 -1.82944200 -0.46915700
C 1.07160100 -0.38710000 1.08542400
H 0.59701000 -0.01819700 1.99836600
H 2.03982300 -0.81489400 1.36330200
N 1.25850900 0.78602300 0.19682600
N -1.03621600 -0.75745900 -0.10557100
C 2.26356100 0.60763200 -0.89217000
H 2.24129800 1.53636300 -1.46849500
C -2.18871300 -0.79231800 0.82263900
H -2.30897400 -1.81706300 1.18857400
C 3.63386500 0.32045300 -0.37565900
C 4.36554700 1.36854700 0.25502700
C 4.17373900 -0.95172100 -0.48799700
C 5.65348100 1.03332700 0.74181900
C 5.43286500 -1.24478900 0.00917000
H 3.59510600 -1.73711600 -0.96888200
C 6.17263300 -0.23567100 0.61976600
H 7.15962700 -0.46244000 1.01041100
C -3.46202100 -0.35409900 0.16155100
C -3.54527300 0.76804900 -0.70064400
C -4.61336100 -1.07725100 0.44448500
C -4.80983400 1.09842100 -1.22267700
C -5.84584900 -0.72620300 -0.07521300
H -4.54025900 -1.94317700 1.09741100
C -5.93898400 0.37187100 -0.91667300
H -6.90190100 0.64790300 -1.33101700
O 3.88335200 2.55839800 0.39053900
O -2.54097500 1.53656600 -1.06485500
S 6.15152700 -2.86496400 -0.23153200
S -7.28670200 -1.70987000 0.34270200
O -6.99820300 -3.08917500 -0.14564100
O -8.43299400 -1.07117200 -0.36100800
O -7.40725000 -1.65037100 1.82788900
O 6.93053200 -2.79676700 -1.50472900
O 5.00845700 -3.81887900 -0.31746900
O 7.02560500 -3.10801400 0.95213800
H -1.31835100 -1.20580400 -0.97612500
H 1.56178200 1.56141100 0.80556700
O 0.36089000 4.58483300 0.89638400
H 1.03703200 4.68327300 0.19144900
H 2.74568400 2.79918600 1.75193300
O 1.92348000 2.70715800 2.27907900
H 1.35893200 3.44727500 1.99325700
H 0.05476900 5.46687800 1.11870200
H 2.95160800 3.60120400 -0.54276500

O 2.36159500 4.31193900 -0.90052100
H 2.28561700 4.16515700 -1.84533500
H -0.37864200 2.98966500 -0.32439000
H -0.23437200 2.80515800 -1.11368900
Pd -0.64595900 1.22319200 -0.47917600
H 1.91592600 -0.19214400 -1.55035800
H -1.93163200 -0.16746900 1.68525200
H 6.22631900 1.81885500 1.22501600
H -4.86618000 1.95819500 -1.88122000

54

RR_EI_ID2_TS2-square_R_noH2, E(SCF) = -
2484.16952264, E(ZPE) = -2483.768457, E(G)
= -2483.834166 a.u.
C 0.11557800 -1.58319500 0.25162500
H -0.16573300 -2.48486400 0.80075300
H 0.56815000 -1.90152500 -0.68887200
C 1.07615200 -0.73720200 1.04494800
H 0.66980100 -0.51021700 2.03360400
H 2.02970100 -1.25715800 1.18544100
N 1.27715400 0.55395700 0.34674600
N -1.10209900 -0.79051800 -0.09032000
C 2.21004700 0.49008900 -0.81730000
H 2.04671800 1.40406100 -1.39184800
C -2.24982600 -0.96324600 0.83164000
H -2.41117600 -2.03465500 0.98979500
C 3.63716100 0.36664400 -0.40047800
C 4.30496900 1.52340700 0.09310200
C 4.29869000 -0.85077300 -0.48509800
C 5.65761900 1.35669200 0.47946800
C 5.61866300 -0.97767500 -0.09127000
H 3.77568900 -1.72280100 -0.86978000
C 6.29535600 0.14085400 0.39067900
H 7.33292100 0.04901300 0.69923100
C -3.50801300 -0.35547600 0.28505000
C -3.56170500 0.95296100 -0.26336700
C -4.67228200 -1.10792900 0.35347800
C -4.81260800 1.42809600 -0.69836200
C -5.89141900 -0.61425400 -0.07686300
H -4.62238000 -2.11404000 0.76196400
C -5.95617100 0.66533200 -0.60682800
H -6.90766000 1.05463700 -0.95077000
C 3.71640800 2.67225500 0.19340500
O -2.53479800 1.76130100 -0.39288200
S 6.48082900 -2.53995800 -0.22215300
S -7.34391600 -1.66204500 0.01818300
O -7.07674000 -2.81716900 -0.88737000
O -8.48581700 -0.82089300 -0.43571500
O -7.45832000 -2.07903500 1.44540800
O 7.55648900 -2.34075800 -1.23861400
O 5.46302600 -3.54235300 -0.64862500
O 7.03715200 -2.82187300 1.13386100
H -1.41331000 -1.05511000 -1.02377300
H 1.64521400 1.23255000 1.02646000
O -0.19002200 3.24339700 0.07118600
H 0.53504500 3.56070100 -0.54434500
H 2.61120700 2.91795900 1.54312000
O 1.86522400 2.81152700 2.17524800
H 1.11389200 3.24889700 1.75467200
H -0.99637100 3.73652400 -0.12269100
H 2.67132500 3.46436900 -0.81257100
O 1.93467700 3.97906100 -1.24257700
H 2.04545200 3.89195000 -2.19194200
Pd -0.63516700 1.19256800 -0.08575600
H 1.90448400 -0.34745100 -1.44823000
H -1.95919500 -0.53147400 1.79554600
H 6.18367400 2.22981900 0.85303900
H -4.84727400 2.42904300 -1.11464000

56

RR_EI_ID2_TS2-square_R, E(SCF) = -
2485.34294310, E(ZPE) = -2484.926224, E(G)
= -2484.993793 a.u.
C 0.11168600 -1.59702300 0.26756500
H -0.16992600 -2.50431600 0.80713000
H 0.56236800 -1.90550600 -0.67714400
C 1.07466000 -0.76091000 1.06832500

O -6.88935200 -2.72613700 1.34630300
O 6.96701900 -3.01914100 1.06115900
O 7.75399300 -2.08528000 -1.09241900
O 5.66604900 -3.42972800 -1.01630000
H -1.91733500 -0.08095700 1.65320200
H 2.03602100 -0.33351800 -1.59224200
H -1.35900500 -1.31238100 -0.93753500
H 1.54198000 1.57188400 0.56949400
O -0.33046300 3.41938300 0.66063000
H 0.42491400 3.85533900 0.21474200
H 2.42162000 2.59320000 2.08373200
O 1.56321700 2.61788700 2.56652500
H 1.70580300 2.19404200 3.41504300
H 0.06524600 3.12736100 1.49984200
H 2.66038100 3.62453400 -0.20158600
O 2.02895500 4.31174600 -0.52168100
H 2.13391500 4.34733200 -1.47507300
H -0.30546100 2.91585700 -1.67401900
H -0.09709000 2.39254900 -2.19749700
Pd -0.65090700 1.12845000 -0.66820400

56

RR_EI_ID2_TS3_P, E(SCF) = -2485.36054101,
E(ZPE) = -2484.942400, E(G) = -2485.012302
a.u.

C 0.27940300 -1.13677900 0.54878900
H 0.09283200 -1.89942200 1.31309200
H 0.81115900 -1.62933600 -0.26900500
C 1.12487300 -0.02947400 1.12969300
H 0.63634200 0.41545700 1.99993700
H 2.09047400 -0.42322700 1.46573400
N 1.31192700 1.07038800 0.14805200
N -0.98231900 -0.60730300 0.00292500
C 2.27485400 0.78196100 -0.94775300
H 2.32899000 1.69317400 -1.54632900
C -2.11196400 -0.52846300 0.94357800
H -2.23387100 -1.48486300 1.46789200
C 3.62398500 0.33254400 -0.46996600
C 4.52376100 1.20597900 0.15644400
C 3.98382300 -1.00307600 -0.58782200
C 5.72252500 0.72583900 0.66753100
C 5.18361400 -1.47694600 -0.08611900
H 3.30273700 -1.69058600 -1.08268800
C 6.05245300 -0.61198100 0.55456600
H 6.39336700 1.42750600 1.14966600
H 6.98863700 -0.98850000 0.94951000
C -3.39371700 -0.19093700 0.23585700
C -3.52468300 0.90093500 -0.66566600
C -4.50454900 -0.98298600 0.51207400
C -4.80604300 1.12037600 -1.22619200
C -5.74217900 -0.74025800 -0.04901500
H -4.39818300 -1.82204000 1.19292000
C -5.88795600 0.33002400 -0.92660900
H -4.90556300 1.95536000 -1.91191300
H -6.85362400 0.53519200 -1.37894100
O 4.27356800 2.52665000 0.34173800
O -2.58007900 1.73060200 -1.02482700
S 5.56822400 -3.22703300 -0.25881300
S -7.16204900 -1.75785200 0.34147600
O -6.66964500 -2.83307100 1.24842200
O -7.66592500 -2.28314900 -0.96142300
O -8.14915300 -0.85234600 1.00004600
O 4.49304700 -3.94376300 0.48190500
O 6.91606200 -3.40635700 0.34316500
O 5.53512600 -3.49874900 -1.72233900
H -1.86012900 0.22186900 1.70344700
H 1.83788500 0.01394700 -1.58892900
H -1.27101200 -1.17095400 -0.79126600
H 1.65480500 1.86693800 0.68874800
O 0.77952000 4.59231700 0.93664400
H 1.96648700 4.42884600 -0.41676800
H 3.26729200 2.80827200 1.98807700
O 2.37338600 2.81722100 2.36792900
H 2.44826600 2.51120300 3.27507600
H 1.23827800 4.08802400 1.63277900
H 3.68368000 2.94592100 -0.32932000
O 2.67872100 4.16334300 -1.03782700

H 2.28444200 4.15505700 -1.91340700
H 0.09679000 3.98512600 0.61006700
H -0.33289700 2.96376100 -0.88148600
Pd -0.62477100 1.46364600 -0.52673300

56

RR_EI_ID2_TS3_R, E(SCF) = -2485.33012380,
E(ZPE) = -2484.915237, E(G) = -2484.986869
a.u.

C 0.23698400 -1.37258900 0.42631100
H -0.00171400 -2.16761500 1.13692600
H 0.79455700 -1.82262500 -0.39728200
C 1.03670500 -0.27895900 1.07619400
H 0.51349700 0.14127300 1.93814000
H 2.00347700 -0.65454000 1.42609600
N 1.22885400 0.82995100 0.10874200
N -1.01681800 -0.80530900 -0.14428000
C 2.29672100 0.60668600 -0.90851000
H 2.31201100 1.51465400 -1.51909700
C -2.17606300 -0.79147100 0.77221300
H -2.29324700 -1.79444100 1.19619900
C 3.63392200 0.33432900 -0.30164000
C 4.23413700 1.33794700 0.51240500
C 4.27150800 -0.87374300 -0.51687100
C 5.50423000 1.04167000 1.05180800
C 5.52196900 -1.13153100 0.02808100
H 3.78657000 -1.62839400 -1.13306500
C 6.13157700 -0.16546700 0.81660400
H 5.97978200 1.79849100 1.66799100
H 7.10822300 -0.37087200 1.24149100
C -3.45225800 -0.39732900 0.08688400
C -3.53493900 0.61243600 -0.89928000
C -4.61495400 -1.05140400 0.48859600
C -4.81155200 0.91895300 -1.41762400
C -5.84975200 -0.73311300 -0.03406000
H -4.55198000 -1.83687600 1.23535400
C -5.94357200 0.26560500 -0.99862800
H -4.86655200 1.69643200 -2.17154400
H -6.90867400 0.52307500 -1.42325500
O 3.63291100 2.46242600 0.74813600
O -2.52781100 1.29348600 -1.40367700
S 6.29805400 -2.71481600 -0.27965700
S -7.33551000 -1.58055900 0.50408300
O -6.88875500 -2.63141300 1.45999600
O -7.95473400 -2.13946100 -0.73185900
O -8.19067200 -0.53882200 1.14299100
O 5.40487200 -3.74216100 0.33360600
O 7.63834000 -2.65281400 0.36946000
O 6.37917900 -2.85811900 -1.76317100
H -1.92993000 -0.11935500 1.60199600
H 1.98802000 -0.21452600 -1.55946600
H -1.27531400 -1.33227100 -0.97717000
H 1.50640400 1.65333800 0.64967700
O 0.20348200 4.21834600 0.72257900
H 1.00271300 4.43232900 0.20071200
H 2.56035100 2.63188300 2.07706600
O 1.67789100 2.65856800 2.51770500
H 1.81276700 2.48427000 3.45093800
H 0.55946500 3.75437100 1.50086900
H 3.03813400 3.67062500 -0.29819500
O 2.57193100 4.43031900 -0.72407800
H 2.55573600 4.23920200 -1.66436600
H -0.34179800 2.91979900 -0.64073800
H -0.37357400 2.69146300 -1.44082800
Pd -0.65967200 1.13932300 -0.69367200

56

RR_EI_ID2_TS3-square_P, E(SCF) = -
2485.35927122, E(ZPE) = -2484.941075, E(G)
= -2485.010485 a.u.

C 0.27337100 -1.21832300 0.44770800
H 0.08386400 -2.01595400 1.17457200
H 0.79759100 -1.67419500 -0.39615300
C 1.12728600 -0.14493500 1.07649300
H 0.64727500 0.25960700 1.97088300
H 2.09315200 -0.55793700 1.38723100
N 1.31554900 1.00154600 0.15047200

O 7.82085200 -2.03992800 -0.93997200
H -1.95873400 -0.12763200 1.57996500
H 2.01988900 -0.35259800 -1.54969700
H -1.37800200 -1.42087200 -0.97493300
H 1.49945500 1.52244700 0.62154100
O 0.25770500 4.01535000 0.34880900
H 1.13000700 4.31213100 -0.02535200
H 2.24544000 2.59103100 2.15045800
O 1.31150800 2.68267600 2.45388000
H 1.32270600 2.88963800 3.39051900
H 0.49134300 3.60370900 1.21606300
H 3.13215600 3.66227900 -0.08364800
O 2.75073400 4.46815900 -0.51469400
H 2.93201400 4.38131300 -1.45347500
H -0.15885900 3.06133600 -0.49354700
H -0.36357500 2.60887400 -1.30608800
Pd -0.67941900 1.06919200 -0.72232900

45

RR_EI_TS, E(SCF) = -2254.84365766, E(ZPE) = -2254.519815, E(G) = -2254.577768 a.u.

N -1.33949200 1.79020600 0.23852700
N 1.38054100 1.93863000 -0.40496000
C -2.59540300 1.67687000 -0.53811100
H -3.26033900 2.50533800 -0.27087200
C 2.41750200 1.54329100 0.56868600
H 1.90659700 1.34318200 1.51776000
C -3.30004200 0.38038200 -0.27412200
C -2.63769800 -0.87347800 -0.31345200
C -4.66860600 0.42297200 -0.02468600
C -3.42587700 -2.02982200 -0.11375500
C -5.41234200 -0.72344300 0.16690100
H -5.17287800 1.38390300 0.01469900
C -4.77765100 -1.96138200 0.11772800
H -2.91761000 -2.98757800 -0.14841400
H -5.35032900 -2.87129100 0.26916500
C 3.22640400 0.36711400 0.09502200
C 2.69195700 -0.72724500 -0.63521000
C 4.57750700 0.36289100 0.43409700
C 3.58096500 -1.77500300 -0.97193100
C 5.41712600 -0.67808000 0.09861800
H 4.98907300 1.20582600 0.98110300
C 4.90554600 -1.75934200 -0.61382700
H 3.16806600 -2.60862200 -1.52996100
H 5.55374000 -2.58517800 -0.89027000
O -1.36018500 -1.05280000 -0.53010300
O 1.45349500 -0.85817700 -1.04221300
S -7.17251400 -0.64875400 0.48815400
S 7.14576500 -0.67115900 0.56812400
O 7.91698700 -0.83821800 -0.69800100
O 7.32430100 -1.82887900 1.49252100
O 7.39206400 0.64117800 1.22911300
O -7.53650700 0.79589200 0.47166800
O -7.37510300 -1.28223500 1.82365600
O -7.82315400 -1.42482100 -0.60738000
H -1.54643200 1.50183300 1.19312600
H -2.32399800 1.80057900 -1.59268900
H 1.82161200 1.98157200 -1.32102200
H 3.09179400 2.39026500 0.73868300
Pd 0.01333600 0.43367100 -0.45706800
C 0.71652200 3.25024900 -0.14951600
C -0.75287900 3.16283200 0.28067300
H -0.87525900 3.54710600 1.29371100
H -1.35180800 3.79900400 -0.37250500
H 1.29466400 3.78994800 0.60360900
H 0.78694200 3.82362700 -1.07317400

45

RR_EI, E(SCF) = -2254.85138138, E(ZPE) = -2254.527456, E(G) = -2254.585693 a.u.

N -1.30238100 1.69186000 0.52938200
N 1.30237000 1.69186200 -0.52934900
C -2.46569800 1.59826400 -0.36868700
H -3.10608800 2.47707100 -0.23087200
C 2.46566900 1.59820500 0.36876400
H 2.09436500 1.62505900 1.39933000
C -3.26518800 0.35342800 -0.08543600

C -2.69444600 -0.90202200 0.26260300
C -4.64960400 0.46513600 -0.18786100
C -3.58875700 -1.97823800 -1.47238100
C -5.49325000 -0.60636900 0.01547000
H -5.08535600 1.42729400 -0.44030200
C -4.94942900 -1.84130900 0.35626400
H -3.15004500 -2.93476000 0.73614700
H -5.59872200 -2.69437300 0.52655700
C 3.26519600 0.35341600 0.08545900
C 2.69444400 -0.90207100 -0.26247500
C 4.64961300 0.46516200 0.18775200
C 3.58874900 -1.97829100 -0.47221500
C 5.49325900 -0.60635600 -0.01556800
H 5.08537700 1.42734200 0.44008900
C 4.94943100 -1.84131900 -0.35623500
H 3.15004400 -2.93483500 -0.73591000
H 5.59872500 -2.69438700 -0.52650800
O -1.41983000 -1.16862200 0.42136900
O 1.41982800 -1.16865400 -0.42118000
S -7.27175400 -0.41965500 -0.08164200
S 7.27176300 -0.41964200 0.08150300
O 7.78270100 -0.60238500 -1.30901400
O 7.74795800 -1.49304800 -0.10010200
O 7.51642600 0.95098200 0.61188100
O -7.51640900 0.95093300 -0.61213200
O -7.78268700 -0.60227500 1.30889200
O -7.74795200 -1.49313700 -1.00106200
H -1.62995300 1.51045900 1.47616400
H -2.09443800 1.62524100 -1.39926700
H 1.62996600 1.51046000 -1.47612100
H 3.10604200 2.47704600 0.23108100
Pd -0.00000800 0.20986400 0.00003500
C 0.52699300 2.95917200 -0.54034600
C -0.52697700 2.95914800 0.54039600
H 0.06095800 3.03109900 1.52515200
H -1.19291900 3.81949600 0.42509300
H 1.19294400 3.81950000 -0.42495100
H 0.06101800 3.03118000 -1.52511700

53

RR_D1_I1*_Htr_TS_P, E(SCF) = -2408.92078753, E(ZPE) = -2408.527147, E(G) = -2408.587203 a.u.

N -2.62802000 -2.46866900 0.67579200
N -0.04689900 -2.66868600 -0.22559600
C -2.82547700 -1.47862300 1.79209000
H -3.85602300 -1.12662700 -1.71337800
C 1.01589300 -2.66211400 -1.23124200
H 0.59261000 -3.04494700 -2.16660300
C -1.90695400 -0.29409000 1.73261700
C -0.52392200 -0.41733500 2.09483200
C -2.39430000 0.90615700 1.25412400
C 0.27918100 0.75646000 1.96267300
C -1.57128700 2.01815000 1.12619700
H -3.43527200 0.97996500 0.95335800
C -0.22072400 1.93424700 1.47707800
H 1.33000000 0.67895000 2.22861000
H 0.42736900 2.79813400 1.36374900
C 1.50196100 -1.25212800 -1.36640100
C 0.66333200 -0.25061400 -1.92011900
C 2.71269000 -0.89520700 -0.80693900
C 1.15788800 1.06146100 -1.97237200
C 3.14442400 0.42319500 -0.80069700
H 3.31694400 -1.66231000 -0.33032800
C 2.37021400 1.40081700 -1.40023600
H 0.53849200 1.82807500 -2.42618800
H 2.71217200 2.42977400 -1.39867200
O -0.01962800 -1.52611300 2.47408200
O -0.54785300 -0.51824100 -2.38409600
S -2.18649000 3.49831600 0.42289000
S 4.62032600 0.82454300 0.12228800
O 4.81407300 2.29343500 -0.00145500
O 5.73180000 0.02742500 -0.46728400
O 4.32029100 0.40329100 1.53166800
O -1.43516000 3.63477900 -0.99239600
O -1.72237900 4.66557400 1.17502400
O -3.62379500 3.35165500 0.16686200

H 1.80639600 -1.65285800 2.44418500
H -3.03126900 -0.80705800 -1.45721900
H -2.99328500 1.23644300 -2.20893500
O 2.76324800 -1.85666900 2.40640000
H 3.20234800 -1.06278000 2.05604000
H -3.54583000 -2.79125700 0.39010100
H -2.72726600 -2.01217100 2.74266400
H 0.29777000 -2.27736600 0.66041800
H 1.84398800 -3.32244100 -0.94095000
Pd -1.70858600 -1.49537700 -0.94307200
C -0.71345000 -3.94105300 0.05148000
H -1.12160000 -4.32445700 -0.88916000
H -0.01972800 -4.69448200 0.44771800
C -1.81037600 -3.66804500 1.05914200
H -2.45903100 -4.53811100 1.17164700
H -1.35532200 -3.44643200 2.02489000
O -2.17656900 1.62704400 -2.53956600
H -1.70638100 2.86892700 -1.58785100
H -1.54585400 0.86101800 -2.55104600

53

RR_D1_I1*_Htr_TS, E(SCF) = -2408.89553786,
E(ZPE) = -2408.504697, E(G) = -2408.563711
a.u.

N -2.31474900 -2.65797500 0.73074800
N 0.22232400 -2.65907500 -0.15094500
C -2.68033900 -1.65892500 1.80140600
H -3.75043600 -1.46937000 1.69942900
C 1.37154300 -2.61249700 -1.06669600
H 1.07053300 -3.09298800 -2.00317000
C -1.94061500 -0.36090600 1.68531200
C -0.54155600 -0.28868300 1.97564900
C -2.61575400 0.75605400 1.21934700
C 0.08261300 0.97203100 1.77473500
C -1.96604200 1.96338900 1.01775400
H -3.67422100 0.67936900 0.98312400
C -0.60293300 2.05898300 1.28741100
H 1.14814400 1.04452800 1.97855800
H -0.08712100 2.99877100 1.11513200
C 1.76328200 -1.18303000 -1.25788900
C 0.86648300 -0.29696200 -1.90004100
C 2.92895600 -0.69409100 -0.70173800
C 1.24674900 1.04353400 -2.04162400
C 3.25323500 0.65138500 -0.79435700
H 3.58701800 -1.37204000 -0.16586200
C 2.41742200 1.51693000 -1.47917600
H 0.57391600 1.72324200 -2.55540800
H 2.67966100 2.56615400 -1.55418900
O 0.13080000 -1.32085400 2.34712600
O -0.30958700 -0.70825400 -2.35417700
S -2.81749700 3.30682600 0.22165100
S 4.65389800 1.25603800 0.14024600
O 4.87998700 2.65962100 -0.29154200
O 5.79297300 0.34752400 -0.16115100
O 4.22500600 1.16155000 1.57529600
O -2.55483900 3.13612200 -1.25881000
O -2.21839600 4.57113600 0.71915800
O -4.26178000 3.15445700 0.53602700
H 1.92842900 -1.12783300 2.53814000
H -2.95462500 -1.09859900 -1.38587500
H -2.71004500 -0.27075100 -1.78959600
O 2.89694600 -1.14406400 2.68679200
H 3.25821700 -0.34956300 2.25880900
H -3.17290600 -3.07831100 0.38778400
H -2.51700900 -2.13858800 2.77093200
H 0.44904900 -2.16345800 0.73216600
H 2.20479500 -3.18331000 -0.64061300
Pd -1.42587500 -1.66452000 -0.88554300
C -0.30153100 -3.98848300 0.19840700
H -0.66349300 -4.46924800 -0.71452900
H 0.48536600 -4.61889400 0.62778500
C -1.40909200 -3.75858600 1.19927700
H -1.98445800 -4.66758000 1.37654800
H -0.97310500 -3.42499400 2.14070800
O -2.48397900 0.81012000 -2.51803500
H -2.51400300 1.66286700 -1.99729600
H -1.54048400 0.57232100 -2.66869400

53

RR_D1_I1*_Htr_TS_R, E(SCF) = -
2408.90183946, E(ZPE) = -2408.509268, E(G)
= -2408.569479 a.u.

N -2.39394700 -2.62769300 0.73645100
N 0.11480600 -2.67410800 -0.17598300
C -2.71162000 -1.60107800 1.79863400
H -3.77269200 -1.36697200 1.69548000
C 1.27090000 -2.64054000 -1.08944600
H 0.96873000 -3.11533700 -2.02778500
C -1.91564700 -0.33672900 1.67557100
C -0.52072600 -0.32480400 1.98018200
C -2.53809700 0.81316500 1.20628600
C 0.15402600 0.91751500 1.82767700
C -1.83782000 1.99458700 1.03532600
H -3.59470200 0.78626200 0.95245000
C -0.47979300 2.03495200 1.34673700
H 1.21506900 0.94603900 2.06063900
H 0.07908500 2.95575700 1.20560600
C 1.68511500 -1.21666400 -1.26666800
C 0.79076800 -0.31524400 -1.88823000
C 2.85930200 0.744627600 -0.71446800
C 1.16699200 1.02794300 -2.00030800
C 3.18742500 0.59898800 -0.78727700
H 3.51384000 -1.43559600 -0.18861500
C 2.34815500 1.80140600 -1.44326200
H 0.48534600 1.72120700 -2.48328500
H 2.61166300 2.53302300 -1.49311900
O 0.10884600 -1.39519100 2.32506400
O -0.38655000 -0.72220500 -2.34821600
S -2.60465300 3.41321100 0.27594100
S 4.61722700 1.16682200 0.12873500
O 4.77210100 2.61202100 -0.17771800
O 5.76726600 0.33464600 -0.31692800
O 4.26746900 0.91770400 1.56618100
O -2.02068400 3.49802800 -1.10952600
O -2.23158000 4.60234700 1.08891700
O -4.06748100 3.14248600 0.24774900
H 1.92516100 -1.33258700 2.45439700
H -3.12518400 -1.23755400 -1.49102000
H -2.77533400 -0.50096800 -1.54527300
O 2.89636900 -1.43050800 2.53816100
H 3.28572000 -0.62132000 2.16594300
H -3.27015400 -3.02820800 0.41486300
H -2.56719300 -2.08098900 2.77101600
H 0.35224900 -2.18580200 0.71338600
H 2.08724200 -3.22559400 -0.65164800
Pd -1.49915700 -1.65760700 -0.89754800
C -0.42382800 -4.00020000 0.17819400
H -0.80389700 -4.47514500 -0.72981700
H 0.36611200 -4.63502400 0.59354300
C -1.51097000 -3.75115700 1.19561700
H -2.10727900 -4.64582500 1.37381300
H -1.05545100 -3.43002800 2.13207900
O -2.41075500 1.20720600 -2.63764800
H -2.23312000 2.00703800 -2.10163100
H -1.57629900 0.70701500 -2.66759700

47

RR_both-HOphen_ch-2_TS, E(SCF) = -
2255.97696293, E(ZPE) = -2255.639006, E(G)
= -2255.700794 a.u.

C -0.56653000 3.12031600 0.03415400
H -0.23683800 3.23403300 -1.00445100
H -0.92535300 4.10405000 0.36635700
C 0.60095800 2.70049900 0.91277200
H 1.31130900 3.52586000 1.03234300
H 0.22098500 2.45325300 1.90967000
N 1.31171200 1.49365600 0.41079300
N -1.58484400 2.08316900 0.07884700
C 2.16659900 0.91296800 1.47020000
H 2.72756900 1.71667100 1.96500800
C -2.56556700 1.95597800 -0.99794000
H -2.02312700 2.01049200 -1.94789700
C 3.13330000 -0.10120700 0.94620200
C 2.78667400 -1.44735200 0.79005700

C 4.43837800 0.28564600 0.65466600
C 3.74610200 -2.37489800 0.39397600
C 5.38162100 -0.63477700 0.24227000
H 4.73030200 1.32462600 0.77479800
C 5.03716400 -1.97382200 0.12074100
H 5.78000300 -2.69939700 -0.19320900
C -3.28840800 0.63602000 -0.86213500
C -2.70450700 -0.60131800 -1.20930000
C -4.55932300 0.62862800 -0.30364300
C -3.40375800 -1.78396300 -0.97714100
C -5.24462800 -0.55289900 -0.07502600
H -5.02846500 1.57052700 -0.03587100
C -4.66281100 -1.76520800 -0.40926700
H -5.19583500 -2.69337300 -0.23033600
O 1.54503000 -1.91541900 1.06897500
O -1.51223400 -0.66910700 -1.86243500
S 7.06853300 -0.12943900 -0.12803800
S -6.88907300 -0.54527200 0.65406700
O -7.22329800 0.88339400 0.90342100
O -6.77619300 -1.34617200 1.90556500
O -7.77749800 -1.18703100 -0.35564800
O 7.28143800 -0.47091800 -1.56221900
O 7.93327600 -0.92839400 0.78440600
O 7.12503000 1.33261700 0.14084100
H -0.36648000 -1.12954000 -1.38771300
H 0.87079400 -1.30652200 0.69062600
H 1.92568000 1.78392600 -0.34894200
H 1.50136800 0.47036300 2.21707700
H -2.03689400 2.04272400 0.98630700
H -3.30502300 2.76891100 -1.00029300
Pd -0.17306700 0.28466500 -0.59220100
H 3.44900400 -3.41245800 0.29438300
H -2.93335800 -2.71981900 -1.25820100

47

RR_both-HOphen_ch-2, E(SCF) = -
2256.00970477, E(ZPE) = -2255.665625, E(G)
= -2255.728943 a.u.

N -1.71518100 1.99741600 0.13618900
N 1.35953100 1.60051700 0.67531600
C -2.28242500 1.52340900 -1.11890200
H -2.88377400 2.28713900 -1.63866200
C 2.32232600 1.30749300 1.75580700
H 1.74968200 1.01753500 2.63830600
C -3.14618500 0.31859700 -0.86866100
C -2.66263400 -0.99582100 -0.87272900
C -4.48423100 0.50505200 -0.55774400
C -3.49845500 -2.06407600 -0.59155900
C -5.32432900 -0.55946700 -0.26691200
H -4.87939000 1.51802100 -0.55236900
C -4.83157100 -1.84938700 -0.28510200
H -3.09828500 -3.07319000 -0.60710100
H -5.48707200 -2.68196500 -0.06161500
C 3.27171700 0.22379000 1.35714600
C 3.12028300 -1.08866900 1.80873600
C 4.32302500 0.50885400 0.49566700
C 3.99982900 -2.08237700 1.38838600
C 5.19243700 -0.47857700 0.07036600
H 4.46651600 1.52658200 0.14388900
C 5.03189500 -1.77960400 0.52278100
H 3.86808800 -3.09770400 1.74985300
H 5.71391500 -2.55815100 0.19848000
O -1.34751300 -1.22877100 -1.19421600
O 2.10612500 -1.35535500 2.66347400
S -7.05669600 -0.23167200 0.09773100
S 6.57346900 -0.08836500 -1.01378700
O 6.47866100 -1.04871000 -2.14839300
O 7.79841100 -0.29542500 -0.19032000
O 6.37960900 1.32813000 -1.42625200
O -7.05133000 0.73500600 1.23037300
O -7.65288400 -1.54779200 0.45164600
O -7.62158000 0.35116000 -1.15137100
H -2.45065100 2.32711900 0.75071200
H -1.44869300 1.26290000 -1.77803500
H 1.89901900 1.90574000 -0.13482200
H 2.88385700 2.21935900 2.00985200
Pd 0.24382600 -0.04008400 -0.15944300

C 0.46610900 2.71511200 1.05534600
C -0.63724700 2.97210900 0.04321800
H -0.99916700 3.99950400 0.18316100
H -0.21057500 2.93712800 -0.96517000
H 0.01658200 2.46282200 2.02108400
H 1.05941600 3.62906800 1.20123600
H 2.11066300 -2.28948000 2.89803500
H -1.18421300 -2.17806400 -1.24071500

50

RR_D1_ts2_P_1W_NH-dissoc W-coord NH-W-
substl_TS, E(SCF) = -2332.44011482, E(ZPE)
= -2332.074006, E(G) = -2332.137078 a.u.

C 0.57779000 -3.09823400 0.78194200
H 0.39792100 -3.56295600 -0.19401900
H 1.31749700 -3.71854000 1.30446900
C -0.70363200 -3.03267100 1.58241900
H -1.02490500 -4.05253300 1.84357200
H -0.51019600 -2.51468600 2.51043100
N -1.71573300 -2.28453200 0.86110200
N 1.10074900 -1.74947800 0.55239200
C -2.90128800 -1.94817800 1.63661200
C 2.35917300 -1.70759600 -0.19547200
H 2.12452900 -1.98479100 -1.23296300
C 3.03488300 -0.36583200 -0.11822100
C 2.34038000 0.87901900 -0.13084000
C 4.42155400 -0.36343700 -0.04910500
C 3.12759600 2.05155700 -0.07011900
C 5.16456200 0.80388200 -0.00499100
H 4.94044100 -1.31925700 -0.02922200
C 4.50187200 2.02325300 -0.00983700
H 5.07166700 2.94454600 0.03274200
O 1.04525400 1.05207300 -0.17009500
H -1.16756600 0.53465800 -1.33916900
H -1.98293900 -2.78129300 0.01542700
H -3.42099400 -2.84662000 2.00586000
H 1.24370700 -1.29999900 1.45592800
H 3.05408000 -2.47076700 0.18157200
Pd -0.26555900 -0.47282400 -0.56614600
H 2.59739200 2.99830500 -0.07692400
O -1.30898400 -2.08686200 -1.96967800
H -1.95320500 -1.57624100 -2.47242300
H -0.64570600 -2.35696000 -2.61421200
H -2.58132000 -1.37637500 2.51354900
S 6.94955700 0.70513100 0.08869700
C -3.81758900 -1.11024100 0.80137800
C -4.56163300 -1.69030000 -0.22652200
C -3.86425900 0.26781300 0.95297800
C -5.34214900 -0.90550600 -1.06870200
C -4.63618400 1.05288500 0.11597500
H -3.27634200 0.74047700 1.73313100
C -5.37422700 0.46528100 -0.90033400
H -5.91458100 -1.37550600 -1.86250800
H -5.97683000 1.07949300 -1.56089000
S -4.66263200 2.84240600 0.29079600
O -4.47647100 -3.03627700 -0.36901000
H -5.02357300 -3.32744500 -1.10631400
O -3.79058000 3.15388700 1.45525100
O -6.09042400 3.20522400 0.51443000
O -4.13362800 3.37415400 -0.99694800
O 7.44303800 2.11092800 0.05632300
O 7.38475800 -0.08948300 -1.09740800
O 7.26449100 0.01181700 1.37280000

53

RR_D1_ts2_P_NH-dissoc W-coord W-out-to-
sulfo (P_D1_W2), E(SCF) = -2408.89891027,
E(ZPE) = -2408.506428, E(G) = -2408.574852
a.u.

C -0.41925100 1.73322000 -0.06715000
H 0.00504700 1.71041500 -1.07695100
H -0.92966400 2.69897400 0.04170200
C 0.67368900 1.62160000 0.97923300
H 0.99875200 2.62389800 1.28175300
H 0.25633100 1.15237600 1.87786100
N 1.81909300 0.82237900 0.53670300
N -1.40648900 0.64992600 0.04706200

| | | | | | | | |
|----|-------------|--------------|-------------|--|-------------|-------------|--------------|
| C | 2.57208700 | 0.24054600 | 1.65454500 | C | -5.42291200 | 0.72350500 | -1.48855500 |
| H | 2.85157500 | 1.00616500 | 2.39097800 | H | -6.12909700 | 0.96224900 | -2.27804000 |
| C | -2.57687400 | 0.86398800 | -0.82526400 | O | 1.96636500 | 2.19266400 | -2.15306500 |
| H | -2.28647200 | 0.56092100 | -1.84023500 | O | -2.33701400 | 2.03740500 | -0.19642900 |
| C | 3.80735100 | -0.41171200 | 1.11593000 | S | 6.85867100 | -1.10772600 | -0.83174000 |
| C | 3.81353000 | -1.71258600 | 0.60390400 | S | -7.12267800 | -1.36124500 | -0.89976600 |
| C | 4.94379000 | 0.36132900 | 0.94745100 | O | -7.03102400 | -2.14908300 | 0.06889900 |
| C | 4.93482000 | -2.21267400 | -0.04408600 | O | -7.09531600 | -1.81356400 | -2.32165200 |
| C | 6.04236200 | -0.11652400 | 0.25756400 | O | -8.27532400 | -0.45359900 | -0.62321400 |
| H | 4.94073600 | 1.37995000 | 1.32518600 | O | 8.00917900 | -0.20194100 | -1.06561800 |
| C | 6.04298000 | -1.40887700 | -0.23789100 | O | 6.77376300 | -2.23830300 | -1.79139400 |
| H | 6.90585300 | -1.77746300 | -0.77917200 | O | 6.76709900 | -1.57132500 | 0.59342700 |
| C | -3.79446500 | 0.13168700 | -0.34392100 | H | -0.24562000 | 3.14953100 | 0.67710600 |
| C | -3.76557100 | -1.22063400 | 0.08216100 | H | 1.19479800 | 1.85230400 | -0.66007600 |
| C | -5.00023500 | 0.36391900 | -0.32338400 | H | 2.69553400 | -1.14879600 | -1.14805200 |
| C | -4.99025000 | -1.79399700 | 0.50027400 | H | 0.82327000 | -0.17592300 | -0.60940800 |
| C | -6.18125900 | 0.23960200 | 0.08450500 | H | -1.34400200 | -1.01534100 | 0.38703400 |
| H | -5.01611600 | 1.86562200 | -0.63778500 | H | -3.08074900 | -1.15628000 | 2.16411400 |
| C | -6.16764000 | -1.408810100 | 0.56246100 | Pd | -0.64449100 | 1.66423000 | 0.87727300 |
| H | -7.08671100 | -1.56385600 | 0.83119800 | H | 4.27174200 | 3.00341200 | -1.70950000 |
| O | 2.72869400 | -2.53362800 | 0.66121300 | H | -4.11393200 | 2.35377500 | -1.94871500 |
| O | -2.71017200 | -1.98995700 | 0.13485400 | O | 1.06641900 | 1.40939600 | 1.96948400 |
| S | 7.36931300 | 1.03684300 | -0.10113900 | H | 1.55864800 | 0.22388300 | 1.58719400 |
| S | -7.71828700 | 1.15607900 | 0.11621700 | H | 1.66438100 | 2.15543200 | 1.87559100 |
| O | -7.40332300 | 2.51919400 | -0.39723700 | O | 4.39704000 | -1.64057400 | 2.10460700 |
| O | -8.16520400 | 1.16276700 | 1.54031100 | H | 4.52950100 | -2.27445000 | 2.81270700 |
| O | -8.66374800 | 0.40919900 | -0.76478100 | H | 5.23283800 | -1.63017600 | 1.59431800 |
| O | 8.37150800 | 0.29227500 | -0.90196800 | | | | |
| O | 7.88094800 | 1.52138900 | 1.20660200 | 53 | | | |
| O | 6.69519800 | 2.12626200 | -0.88215200 | RR_D1_ts2_P_NH2-dissoc_OH-coord_W-out-to- | | | |
| H | -0.61204400 | -2.92274000 | -0.89397600 | sulfo_H-bonded (P_D1_OH), E(SCF) = - | | | |
| H | 2.07097900 | -2.19902700 | 1.28403400 | 2408.90476009, E(ZPE) = -2408.510802, E(G) | | | |
| H | 2.46193800 | 1.41526300 | 0.00118000 | = -2408.576738 a.u. | | | |
| H | 1.91004300 | -0.45735400 | 2.18284000 | C | -0.47687800 | 0.36873300 | 2.56555700 |
| H | -1.73913800 | 0.63617900 | 1.01019400 | H | -0.22324600 | 1.38326300 | 2.88749400 |
| H | -2.81333100 | 1.93516500 | -0.87390600 | H | -1.04216700 | -0.09571000 | 3.38382600 |
| Pd | -0.86250600 | -1.44626200 | -0.48806100 | C | 0.77073100 | -0.46222600 | 2.40012200 |
| H | 4.90818600 | -3.22870000 | -0.41993200 | H | 1.25457800 | -0.55371400 | 3.37314900 |
| H | -4.96544100 | -2.82940600 | 0.82353900 | H | 0.53114400 | -1.47345500 | 2.06122600 |
| O | 1.05183400 | -1.01813100 | -1.21571100 | N | 1.78390900 | 0.10887000 | 1.46851800 |
| H | 1.40268100 | -0.31459700 | -0.56685800 | N | -1.31677000 | 0.45103300 | 1.36226500 |
| H | 1.60763600 | -1.79792300 | -1.08099000 | C | 1.69762500 | -0.35060500 | 0.03851700 |
| O | 3.87961200 | 2.42979100 | -1.06513800 | H | 1.49585700 | -1.42290400 | 0.05281800 |
| H | 3.71446200 | 3.21929400 | -1.58481500 | C | -2.74418200 | 0.62467800 | 1.71546500 |
| H | 4.85218800 | 2.34731400 | -1.01966400 | H | -2.85462200 | 1.64341200 | 2.10720900 |
| | | | | C | 2.99464300 | -0.07303300 | -0.64720600 |
| | | | | C | 3.25770900 | 1.10457600 | -1.36722700 |
| | | | | C | 4.01848500 | -0.98827200 | -0.46199000 |
| | | | | C | 4.52315400 | 1.28454900 | -1.92771400 |
| | | | | C | 5.29067700 | -0.75242400 | -0.94102300 |
| | | | | H | 3.81539900 | -1.89407600 | 0.10385800 |
| | | | | C | 5.54253200 | 0.38182000 | -1.69512700 |
| | | | | H | 6.54020700 | 0.56300000 | -2.07767600 |
| | | | | C | -3.64509300 | 0.38198300 | 0.55051800 |
| | | | | C | -3.61425800 | 1.24071100 | -0.57541700 |
| | | | | C | -4.54408600 | -0.67624800 | -0.58894100 |
| | | | | C | -4.54758200 | 0.99274800 | -1.60738000 |
| | | | | C | -5.43813300 | -0.90363600 | -0.44107500 |
| | | | | H | -4.56143000 | -1.33236500 | 1.45430500 |
| | | | | C | -5.43465700 | -0.05607900 | -1.54496400 |
| | | | | H | -6.13597900 | -0.22387000 | -2.35684700 |
| | | | | O | 2.34036700 | 2.06130000 | -1.56965300 |
| | | | | O | -2.80888500 | 2.25872800 | -0.69231400 |
| | | | | S | 6.59228100 | -1.85309200 | -0.38935800 |
| | | | | S | -6.56762100 | -2.29102500 | -0.40353400 |
| | | | | O | -6.41777600 | -2.91424400 | 0.94201900 |
| | | | | O | -6.14499400 | -3.19929600 | -1.51081500 |
| | | | | O | -7.92924000 | -1.72470800 | -1.623266700 |
| | | | | O | 7.86351700 | -1.32086300 | -0.93718600 |
| | | | | O | 6.24805100 | -3.21429100 | -0.87428200 |
| | | | | O | 6.51854900 | -1.75341000 | 1.10775600 |
| | | | | H | -0.69590200 | 3.58059300 | -0.75613300 |
| | | | | H | 2.73075400 | -0.12202200 | 1.82675500 |
| | | | | H | 0.84928300 | 0.16097500 | -0.42122000 |
| | | | | H | -1.24573700 | -0.42324200 | 0.84291500 |
| | | | | H | -3.01234200 | -0.06563100 | 2.52617400 |
| | | | | Pd | -0.90696800 | 2.29260900 | 0.07192300 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 4.70149100 | 2.18642400 | -2.50190800 | H | -0.06158900 | 0.07236600 | 2.87790700 |
| H | -4.53532400 | 1.65740300 | -2.46499500 | N | -1.66302600 | -0.85255600 | 1.88227000 |
| O | 1.05105000 | 2.48251000 | 0.67782700 | N | 1.33211900 | -1.42201500 | 1.24854700 |
| H | 1.66122800 | 1.15933300 | 1.42032700 | C | -2.37715600 | 0.46159900 | 1.75644100 |
| H | 1.79570900 | 2.23372200 | -0.74368800 | H | -2.88797500 | 0.67907300 | 2.69417000 |
| O | 4.29993600 | -0.75418800 | 2.55376200 | C | 2.67632100 | -1.03738100 | 1.73163400 |
| H | 4.63110900 | -0.41764400 | 3.38930900 | H | 3.15695600 | -1.95315700 | 2.09359500 |
| H | 5.08496700 | -1.07510700 | 2.06336800 | C | -3.31155400 | 0.38928500 | 0.59047400 |
| H | 1.20227500 | 3.38221100 | 0.97649700 | C | -2.83290200 | -0.13211500 | -0.63801500 |

53

RR_D1_ts2_P_NH2-Htr-to-Ophen_TS_R
(P_D1_W2), E(SCF) = -2408.89414136, E(ZPE)
= -2408.502420, E(G) = -2408.570947 a.u.

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -0.62358000 | 1.70121200 | 2.46350700 | H | -4.98442200 | 1.22290800 | 1.64896700 |
| H | -0.20186700 | 2.70674800 | 2.36038500 | C | -5.02086300 | 0.28738900 | -1.59719800 |
| H | -1.30289900 | 1.72884500 | 3.32270800 | H | -5.69430400 | 0.25200700 | -2.49359500 |
| C | 0.46778300 | 0.70087700 | 2.75755000 | C | 3.49360400 | -0.40867400 | 0.65403400 |
| H | 0.93851300 | 0.94600500 | 3.72092200 | C | 3.88264700 | -1.18930600 | -0.45794100 |
| H | 0.02292800 | -0.29612600 | 2.86710400 | C | 3.88955700 | 0.91684500 | 0.74487000 |
| N | 1.44173400 | 0.63733400 | 1.67859400 | C | 4.72238700 | -0.59346300 | -1.41737900 |
| N | -1.36961500 | 1.34115400 | 1.24607400 | C | 4.69600100 | 1.48854700 | -0.22407200 |
| C | 2.43686800 | -0.41668100 | 1.85093900 | H | 3.57374400 | 1.51617300 | 1.59388900 |
| H | 3.04747200 | -0.27984400 | 2.75465400 | C | 5.11971600 | 0.72143700 | -1.30388000 |
| C | -2.83183000 | 1.46616400 | 1.39553900 | H | 5.76066200 | 1.16263000 | -1.06113400 |
| H | -3.08272400 | 2.53363700 | 1.37051200 | O | -1.59682700 | -0.56856000 | -0.74658200 |
| C | 3.31866000 | -0.54596100 | 0.64291800 | O | 3.51944600 | -2.44829400 | -0.59084600 |
| C | 2.77009800 | -0.48573600 | -0.64455400 | S | -7.16279900 | 1.38275700 | -0.25471800 |
| C | 4.67820100 | -0.79404500 | 0.77269300 | S | 5.18089900 | 3.21193500 | -0.12893300 |
| C | 3.57143500 | -0.69222400 | -1.76260600 | O | 4.63903400 | 3.72448000 | 1.16069200 |
| C | 5.47278300 | -1.00214600 | -0.33960100 | O | 4.57017300 | 3.87508000 | -1.31800800 |
| H | 5.12662800 | -0.83607600 | 1.76028100 | O | 6.67155800 | 3.22512300 | -0.17953200 |
| C | 4.91766300 | -0.95563300 | -1.61092800 | O | -7.27045800 | 2.52400800 | -1.20868100 |
| H | 5.54299900 | -1.11734500 | -2.48240600 | O | -7.34862600 | 1.79261500 | 1.16497000 |
| C | -3.53632100 | 0.70415800 | 0.32058500 | O | -8.02821800 | 0.23382700 | -0.64828700 |
| C | -3.37139300 | 1.06234800 | -1.03708900 | H | 1.65659900 | -3.56154300 | -1.86000100 |
| C | -4.33706500 | -0.37908200 | 0.65435300 | H | -0.31755800 | 0.62674900 | -0.47849600 |
| C | -4.05916400 | 0.30097600 | -2.00438700 | O | 0.35093800 | 1.11114200 | 0.05303400 |
| C | -5.00493400 | -1.11005700 | -0.31289900 | H | 1.04255700 | 1.38743400 | -0.55458500 |
| H | -4.45423400 | -0.65447400 | 1.69816100 | H | -2.33807100 | -1.58681800 | 2.09879500 |
| C | -4.85683200 | -0.76507800 | -1.65172400 | H | -1.58615000 | 1.20250000 | 1.60311300 |
| H | -5.37362200 | -1.33504000 | -2.41749700 | H | 0.92196500 | -0.56036200 | 0.86690300 |
| O | 1.45169300 | -0.23690200 | -0.83252800 | H | 2.58901700 | -0.34650000 | 2.58201000 |
| O | -2.65728800 | 2.08540000 | -1.43975900 | Pd | 1.49623700 | -2.69230700 | -0.58329800 |
| S | 7.23317500 | -1.32672700 | -0.16897500 | H | -3.36899400 | -0.57228300 | -2.66376400 |
| S | -5.97895800 | -2.54833800 | 0.12747400 | H | 5.03637900 | -1.19687000 | -2.26266200 |
| O | -7.25759300 | -2.42840200 | -0.63051200 | H | -1.35677400 | -1.01427600 | 0.89007200 |
| O | -6.16838200 | -2.48388600 | 1.60394100 | O | -0.60247200 | -2.97395200 | -0.67870700 |
| O | -5.17866600 | -3.73378100 | -0.30040600 | H | -0.84231100 | -3.61619500 | -1.35286200 |
| O | 7.51511300 | -1.30322200 | 1.29179100 | H | -1.05719100 | -2.11455200 | -0.90808300 |
| O | 7.91702800 | -0.23298600 | -0.91496200 | | | | |
| O | 7.45557900 | -2.66416900 | -0.78693500 | | | | |
| H | -0.62173300 | 3.38940700 | -1.85146000 | | | | |
| H | -0.19868100 | -1.34670900 | -0.53614100 | | | | |
| O | -0.95983300 | -1.47080600 | 0.04978700 | | | | |
| H | -1.72938900 | -1.47829400 | -0.52838900 | | | | |
| H | 1.89395400 | 1.54297300 | 1.57720700 | | | | |
| H | 1.88027900 | -1.35420000 | 1.99021000 | | | | |
| H | -1.17404800 | 0.36248500 | 1.01176300 | | | | |
| H | -3.14771200 | 1.07991100 | 2.37354200 | | | | |
| Pd | -0.87374400 | 2.53705300 | -0.58262700 | | | | |
| H | 3.11697700 | -0.63893800 | -2.74536100 | | | | |
| H | -3.93533300 | 0.58004800 | -3.04546500 | | | | |
| H | 1.12694000 | 0.17992400 | 0.01466500 | | | | |
| O | 1.05325500 | 3.18929700 | 0.10159500 | | | | |
| H | 1.02146300 | 4.13293100 | 0.29989500 | | | | |
| H | 1.68252900 | 3.10243200 | -0.62499400 | | | | |

53

RR_D1_ts2_P_NH2-Htr-to-Ophen_TS_P
(P_D1_W3), E(SCF) = -2408.89543893, E(ZPE)
= -2408.500598, E(G) = -2408.566024 a.u.

| | | | | | | | |
|---|-------------|-------------|------------|---|-------------|-------------|-------------|
| C | 0.48779000 | -1.94435400 | 2.33823900 | H | 5.56283500 | -0.32773200 | -2.46705300 |
| H | -0.03753400 | -2.84455500 | 2.00145800 | C | -3.47703200 | 0.38262300 | 0.63135500 |
| H | 1.12692400 | -2.25063200 | 3.16848400 | C | -3.88912400 | 1.14910800 | -0.48191400 |
| C | -0.51328600 | -0.92208000 | 2.83138100 | C | -3.84984200 | -0.94871500 | 0.73436000 |
| H | -0.90510500 | -1.16820000 | 3.81688500 | C | -4.72564700 | 0.53210700 | -1.43106600 |

C -4.65400200 -1.54079900 -0.22425500
 H -3.51904100 -1.53701000 1.58548900
 C -5.09886400 -0.78887100 -1.30610500
 H -5.73774400 -1.24618700 -2.05549000
 O 1.59374700 0.65916900 -0.54243800
 O -3.55349800 2.41442200 -0.62509500
 S 7.13620100 -1.41208900 -0.32409900
 S -5.10525400 -3.27223800 -0.11351600
 O -4.55290100 -3.76277800 1.18029400
 O -4.48204800 -3.93383800 -1.29705000
 O -6.59535400 -3.31552800 -0.16324100
 O 7.18224100 -2.55976800 -1.27394600
 O 7.38352800 -1.81320800 1.08795700
 O 7.99110600 -0.27402500 -0.76687300
 H -1.72601900 3.58683200 -1.89162300
 H 0.31294600 -0.68342900 -0.42826000
 O -0.32845800 -1.16390900 0.12727700
 H -1.00761100 -1.49517400 -0.46684200
 H 2.25964800 1.72217700 2.06510700
 H 1.75209700 -1.15106100 1.86207100
 H -0.90382200 0.59589300 0.84225100
 H -2.55736500 0.34792100 2.55235700
 Pd -1.53911500 2.71781500 -0.61701200
 H 3.24701000 0.55602800 -2.57115000
 H -5.05748800 1.12461000 -2.27722100
 H 1.40497600 0.92354000 0.73654800
 O 0.55051000 3.08131200 -0.72859200
 H 0.76080700 3.66706200 -1.46169700
 H 1.03719700 2.23193100 -0.88358500

53

RR_Pd0_1, E(SCF) = -2408.88038964, E(ZPE) =
 -2408.483892, E(G) = -2408.550375 a.u.
 C 0.66381400 3.07130300 0.32436800
 H 0.39220600 3.22776200 1.37206200
 H 1.35879900 3.85878500 0.03234700
 C -0.53969800 3.11951000 -0.58013900
 H -1.00029900 4.10605300 -0.52784400
 H -0.25699000 2.93332000 -1.61911800
 N -1.55833100 2.10281000 -0.22430300
 N 1.36642900 1.77222900 0.24265000
 C -2.78470200 2.11654600 -1.09892300
 H -3.39488200 2.98051300 -0.83679800
 C 2.64341200 1.72209800 1.03092500
 H 2.33365900 1.77736700 2.08014300
 C -3.49920900 0.81746500 -0.94497200
 C -2.72671900 -0.36732700 -1.06832600
 C -4.86330400 0.75794500 -0.71309200
 C -3.40682400 -1.59687400 -0.94938000
 C -5.50422400 -0.46394500 -0.61381000
 H -5.43980600 1.67258100 -0.61502500
 C -4.76616900 -1.63942400 -0.73264500
 H -5.27023400 -2.59762400 -0.64830100
 C 3.41537900 0.48691400 0.72499200
 C 2.90175700 -0.79368300 1.06663500
 C 4.64899800 0.60333200 0.09348400
 C 3.72231500 -1.90870500 0.75577800
 C 5.41651800 -0.50495900 -0.20250100
 H 5.02381900 1.58802100 -0.16978500
 C 4.93879700 -1.77072400 0.13469300
 H 5.53330900 -2.64971800 -0.09627100
 O -1.43836700 -0.29366500 -1.25072900
 O 1.74905200 -1.00223500 1.61921100
 S -7.26644900 -0.56559600 -0.30650800
 S 6.99403100 -0.35160900 -1.03257200
 O 7.23570100 1.10935100 -1.19949000
 O 6.84603600 -1.06718800 -2.33388600
 O 7.99625000 -1.00805000 -0.14281700
 O -7.76322900 0.83871800 -0.27535200
 O -7.41627300 -1.26299200 1.00416600
 O -7.83595700 -1.35942100 -1.43393200
 H -0.30214300 -1.62342400 -0.78489200
 H 0.75744100 1.02763000 0.69428000
 O 0.51598200 -2.14883800 -0.65791100
 H 0.84122200 -1.87452300 0.22083500
 H 0.16712600 0.21044900 -2.20709300
 O 1.13692300 0.23660300 -2.12432500

H 1.30184600 -0.62924100 -1.70628100
 H -1.82781400 2.17258600 0.75927800
 H -2.40334300 2.24954900 -2.11643100
 H 1.50890900 1.44957600 -0.73674200
 H 3.21571600 2.61759300 0.78515000
 Pd -0.12877700 -0.10649800 2.14876700
 H -2.82810800 -2.51147600 -1.03641000
 H 3.34071200 -2.89121900 1.01579300
 H -1.19519400 1.11924300 -0.40733000

53

RR_Pd0_2, E(SCF) = -2408.89362433, E(ZPE) =
 -2408.496977, E(G) = -2408.566715 a.u.
 C 0.59537400 2.85048000 0.81611300
 H 0.33573900 2.73730900 1.87309100
 H 1.28562900 3.68919200 0.72357100
 C -0.63579500 3.07726300 -0.02354100
 H -1.11970800 3.99896100 0.32959100
 H -0.35617400 3.24599300 -1.06987900
 N -1.52678900 1.92927100 0.02877400
 N 1.31052100 1.61522000 0.42031600
 C -2.81434900 2.16978700 -0.62786100
 H -3.38388000 2.97386200 -0.14259100
 C 2.50613900 1.32128900 1.27534100
 H 2.08681700 1.00495300 2.24010500
 C -3.63098000 0.91468100 -0.68922500
 C -3.04836900 -0.26917300 -1.15365400
 C -4.97323500 0.90066200 -0.33851100
 C -3.80408300 -1.42744800 -1.28317700
 C -5.72764900 -0.25129900 -0.46885900
 H -5.44263800 1.80734800 0.02893500
 C -5.14246800 -1.41746100 -0.94271800
 H -5.73499500 -2.32055200 -1.04274200
 C 3.37974200 0.27952100 0.67054700
 C 2.85983800 -1.00251100 0.35812100
 C 4.71261300 0.57456500 0.41214400
 C 3.75545800 -1.93722000 -0.21370300
 C 5.56406100 -0.36283000 -0.13957900
 H 5.09908400 1.56079800 0.65108100
 C 5.07093000 -1.62550500 -0.46134400
 H 5.73082300 -2.36604800 -0.90349800
 O -1.74244500 -0.29760600 -1.51217600
 O 1.61271300 -1.33709300 0.51836300
 S -7.46701600 -0.27134500 -0.00645900
 S 7.27915300 0.02296500 -0.47978700
 O 7.50567400 1.40117200 0.03989900
 O 7.43960700 -0.07214900 -1.96067600
 O 8.08373000 -1.00804100 0.23856600
 O -7.80593000 1.12705600 0.37285900
 O -7.56759600 -1.22672500 1.13255900
 O -8.19716600 -0.74501800 -1.21536000
 H -0.28312000 -1.48642800 -1.91913200
 H 0.66719400 0.79675700 0.56125200
 O 0.66442700 -1.67847800 -1.98347900
 H 0.96104000 -1.71542300 -1.04572200
 H 1.12275400 1.34253700 -3.00832400
 O 1.58837700 0.92491200 -2.27979200
 H 1.29169100 -0.01329300 -2.27176700
 H -1.68953300 1.65102400 0.99562300
 H -2.58907400 2.51218200 -1.64688500
 H 1.54659900 1.59935900 -0.59308400
 H 3.05062000 2.25619800 1.41638300
 Pd -0.03151700 -0.84328900 1.79699400
 H -3.32353700 -2.32851500 -1.64693600
 H 3.36169300 -2.91822200 -0.46142000
 H -1.30206800 0.45283900 -1.03973800

53

RR_Pd0_3, E(SCF) = -2408.89804154, E(ZPE) =
 -2408.503174, E(G) = -2408.571127 a.u.
 C 0.59881900 2.46869500 -1.99786400
 H 0.29789300 3.39257500 -1.49304200
 H 1.20128300 2.76215500 -2.87027700
 C -0.60330000 1.71768200 -2.51921400
 H -1.15166800 2.38781600 -3.19928600
 H -0.26469800 0.86602100 -3.12383600
 N -1.46105000 1.19912800 -1.46767800

N 1.41678900 1.67367400 -1.06659400
C -2.71365100 0.63775600 -1.96191800
H -3.37004200 1.39255700 -2.41840600
C 2.80090600 2.18554700 -1.03080200
H 2.76463100 3.22010400 -0.68552200
C -3.44229400 -0.10511500 -0.88137800
C -2.74428900 -0.98671500 -0.04635200
C -4.81542500 0.01376400 -0.72163900
C -3.42266500 -1.74636600 0.90002300
C -5.48955300 -0.74126200 0.22105600
H -5.37313200 0.69689900 -1.35408300
C -4.79174400 -1.62543400 1.03203600
H -5.32029800 -2.21736000 1.77172400
C 3.67043800 1.34970300 -0.14526500
C 4.09736300 1.79133400 1.10923300
C 4.06413100 0.08672000 -0.56965600
C 4.86254600 0.96077700 1.92317900
C 4.83378500 -0.73432000 0.23368000
H 3.75685700 0.67393000 -1.54977600
C 5.22527900 -0.29933400 1.49070000
H 5.82946000 -0.93865600 2.12505900
O -1.40372400 -1.13408300 -0.16117800
O 3.75656800 0.37530200 1.49785900
S -7.26816200 -0.57865900 0.43368800
S 5.30748600 -2.38094800 -0.31335400
O 4.99423700 -2.43622000 -1.76681800
O 4.48779200 -3.32537700 0.49779800
O 6.76405200 -2.49672900 -0.02332800
O -7.72328500 0.36346700 -0.62463300
O -7.46144800 -0.04619100 1.81218300
O -7.81973600 -0.95310700 0.27109700
H 0.20635800 -1.60994800 0.90396200
O 1.17338600 -1.55803300 0.97377200
H 1.31786600 -0.59318900 1.08772600
H 0.47628200 -1.63762700 -2.13084600
O 1.32398700 -1.28958800 -1.83864800
H 1.37215000 -1.52841500 -0.89161300
H -1.63312400 1.90860300 -0.75756400
H -2.44393700 -0.06603500 -2.76252300
H 1.43954800 0.70946400 -1.41739700
H 3.21399500 2.19158500 -2.05170700
Pd 0.57553600 1.55632400 0.93727800
H -2.85620000 -2.42282300 1.52992500
H 5.18001700 1.31706600 2.89847900
H -1.06642000 -0.30454500 -0.60564100
H 4.11247400 3.22223400 2.37465100

94

DIMER_1, E(SCF) = -4512.063487, E(ZPE) = -
4511.376499, E(G) = -4511.473209 a.u.
N 1.75103400 -0.87852200 2.34984300
N 2.71060900 1.49300900 0.76502300
C 0.88474200 -1.41904600 3.37763100
H 1.45707600 -1.80618900 4.23991000
C 3.45288900 1.89688000 -0.44526700
H 2.77352300 2.49880500 -1.05346600
C 0.02009700 -2.50771300 2.81847200
C 0.52409500 -3.80377100 2.69014200
C -1.28191500 -2.26152400 2.39737200
C -0.26929300 -4.82697200 2.18250900
C -2.08514500 -3.28615600 1.91625600
H -1.69377800 -1.26138400 2.49292800
C -1.57272400 -4.56933500 1.80415800
H 0.14266600 -5.82782700 2.09017300
H -2.19603500 -5.37407000 1.42819700
C 4.72517400 2.65027600 -0.18146300
C 4.67542100 3.93955700 0.35114400
C 5.96805100 2.08834000 -0.43258100
C 5.84249400 4.64697100 0.61154500
C 7.13369600 2.78660900 -0.17191100
H 6.02784000 1.08149700 -0.83351600
C 7.07028500 4.06996000 0.34861500
H 5.78321400 5.65012700 1.02149700
H 7.98209500 4.61983100 0.55461500
O 1.79379600 -4.02659800 3.10428100
O 3.44537000 4.45458700 0.59874900
S -3.82071300 -3.01395200 1.51617200

S 8.74400100 2.06306600 -0.51856100
O 9.50555400 2.15011700 0.75910300
O 9.33716200 2.90572300 -1.59505800
O 8.48179300 0.66387100 -0.94974700
O -4.10507500 -1.58532800 1.82723700
O -4.56901200 -3.95602200 2.39892100
O -3.98303100 -3.34973000 0.07348000
H 2.13680100 -1.61821800 1.76206700
H 0.25057300 -0.60882500 3.76391600
H 2.47025400 2.33842700 1.27951900
H 3.67265000 0.98587200 -1.00991200
Pd 0.71207200 0.60209400 0.22976800
C 3.52380800 0.63110900 1.63735100
C 2.75031900 0.05232900 2.80166200
H 3.46584100 -0.39993300 3.51146100
H 2.25206100 0.86687600 3.34964400
H 3.90870900 -0.18995800 1.01823300
H 4.39456100 1.18196600 2.01640600
H 3.52067800 5.34538800 0.95690900
H 2.04595400 -4.93635700 2.91337500
N -2.78182300 -1.46656200 -2.54902700
N -2.36905400 0.98030100 -0.88162800
C -1.92663300 -2.18243900 -3.148318700
H -2.47924600 -2.60327800 -4.33597600
C -2.72838900 1.78521300 0.30573600
H -1.79410700 1.95042400 0.85399100
C -1.16659300 -3.25029900 -2.76333700
C -1.77528500 -4.46134800 -2.42761000
C 0.12656800 -3.01616500 -2.32563100
C -1.08667500 -5.41878800 -1.69399700
C 0.82046700 -3.97289000 -1.60020700
H 0.60836900 -2.07253000 -2.56906400
C 0.20861000 -5.17074600 -1.27332100
H -1.57467800 -6.35568000 -1.44288300
H 0.75215800 -5.91461000 -0.70308800
C -3.41333500 3.08028700 -0.02749300
C -2.73622400 4.07282500 -0.73878700
C -4.73999700 3.30624100 0.31104800
C -3.36984200 5.25924300 -1.08807900
C -5.37619100 4.48486100 -0.03576700
H -5.29291400 2.54268400 0.84904800
C -4.69027200 5.46334700 -0.73798500
H -2.82392800 6.01703700 -1.64119300
H -5.18831000 6.38710400 -1.01264500
O -3.04344500 -4.65167300 -2.85967200
O -1.45026300 3.81675500 -1.08377300
S 2.47985600 -3.61132000 -1.01807100
S -7.09555600 4.77691100 0.40487500
O -7.80475500 5.01301100 -0.88391000
O -7.08532400 5.98345900 1.27865700
O -7.55144100 3.54809500 1.10826100
O 3.15784700 -2.89971100 -2.13683900
O 3.09118700 -4.93177100 -0.69627000
O 2.33098400 -2.74639400 0.18839800
H -3.56612900 -2.03435700 -2.24837800
H -1.21162600 -1.46053600 -3.88976600
H -1.67860900 1.51344300 -1.40948300
H -3.37725300 1.17612200 0.94077600
Pd -1.38444200 -
O.91258900 -0.40503700
C -3.53317700 0.72516900 -1.74681200
C -3.18360900 -0.13175500 -2.94339400
H -4.03109800 -0.11751900 -3.64456100
H -2.33979800 0.33162700 -3.46918500
H -4.29706700 0.23209400 -1.13365600
H -3.96306500 1.67135200 -2.10334500
H -1.08014700 4.55762100 -1.57548500
H -3.38428500 -5.48585000 -2.52024600

94

DIMER_2, E(SCF) = -4512.079355, E(ZPE) = -
4511.388688, E(G) = -4511.488943 a.u.
N 1.13588600 -2.11392100 1.92812200
N 3.44565200 -0.93371000 0.34408400
C 0.23963700 -2.62983300 2.95310800
H 0.32318100 -3.72008200 -3.08396000
C 4.47938100 -0.82968600 -0.70721800

| | | | | | |
|---------------|-------------|-------------|---|-------------|-------------|
| H 4.39866600 | 0.17358200 | -1.13349200 | S -7.28463100 | -2.58795500 | -1.59645900 |
| C -1.18005300 | -2.25519600 | 2.64817400 | O 9.21011300 | -4.60085400 | 0.30810700 |
| C -1.49559500 | -0.92546400 | 2.32070800 | O 10.05981100 | -3.20626300 | -1.55555800 |
| C -2.20609400 | -3.18158100 | 2.71456900 | O 7.96443000 | -4.51164300 | -1.84153700 |
| C -2.81038800 | -0.56604700 | 2.04946800 | O -1.54422700 | 7.36116600 | 2.72490600 |
| C -3.52248300 | -2.81197400 | 2.47599600 | O 0.16045500 | 9.09489700 | 2.20331700 |
| H -1.97234100 | -4.21141700 | 2.97160200 | O -1.76355900 | 8.75048400 | 0.67820100 |
| C -3.82507000 | -1.50477800 | 2.13670800 | O -7.45865600 | -3.98888700 | -1.12917400 |
| H -3.01760600 | 0.46229200 | 1.77025000 | O -7.79933400 | -1.57804100 | -0.62813200 |
| H -4.85212800 | -1.22938200 | 1.92539900 | O -7.79190900 | -2.36385000 | -2.97877400 |
| C 5.88412200 | -1.08787100 | -0.24233400 | O -6.09384800 | -3.37731200 | 2.35451600 |
| C 6.48907400 | -0.22412200 | 0.67231100 | O -4.69640400 | -4.57587000 | 4.02259800 |
| C 6.61365000 | -2.17377400 | -0.70426900 | O -4.47226800 | -5.11384000 | 1.61646000 |
| C 7.79218600 | -0.44287000 | 1.10346700 | | | |
| C 7.91308000 | -2.39350100 | -0.28247000 | | | |
| H 6.16051500 | -2.86117700 | -1.41166800 | 59 | | |
| C 8.50281100 | -1.52670700 | 0.62503700 | RR-Me_hs_D1_TS1_P, E(SCF) = -2487.48641050, | | |
| H 8.24532000 | 0.24128800 | 1.81410800 | E(ZPE) = -2487.040346, E(G) = -2487.107800 | | |
| H 9.52093100 | -1.69710100 | 0.95828900 | a.u. | | |
| O -0.54443000 | 0.02937600 | 2.29024000 | C 0.14933700 | -1.11285300 | -2.39152500 |
| O 5.74796500 | 0.82489800 | 1.10929100 | H -0.04258600 | -2.10418200 | -2.80560500 |
| H 0.86073300 | -2.45325600 | 1.00840100 | H 0.02614200 | -0.37861800 | -3.19278600 |
| H 0.54583900 | -2.17620900 | 3.90645600 | C 1.52352400 | -1.04356900 | -1.78540000 |
| H 3.69391400 | -0.27339500 | 1.07945300 | H 2.30633800 | -1.23646400 | -1.52725900 |
| H 4.21674500 | -1.53606200 | -1.49976700 | H 1.70107400 | -0.05113600 | -1.36503100 |
| Pd 1.53175700 | -0.17304700 | -0.46557600 | N 1.58967700 | -2.02459300 | -0.67402800 |
| C 3.40037600 | -2.28113800 | 0.93016200 | N -0.82404300 | -0.85041200 | -1.30898100 |
| C 2.54080100 | -2.39128400 | 2.16821700 | C 2.87252400 | -1.98027600 | -1.98073900 |
| H 2.68205900 | -3.40903700 | 2.56691300 | H 2.61317900 | -2.47839300 | 1.07698900 |
| H 2.91078700 | -1.70452300 | 2.94147800 | C -2.25526800 | -1.05403800 | -1.65141500 |
| H 3.03671100 | -2.96636900 | 0.15500400 | C 3.29230300 | -0.57402700 | 0.46230900 |
| H 4.41080600 | -2.61576000 | 1.20438200 | C 2.50583300 | 0.18227900 | 1.37898300 |
| H 6.25467500 | 1.36020700 | 1.72951600 | C 4.42407400 | -0.00586500 | -0.10856300 |
| H 0.30906400 | -0.41390500 | 2.05316300 | C 2.94984300 | 1.49603000 | 1.67741500 |
| N -0.93609600 | 1.40709200 | -2.25829500 | C 4.82457200 | 1.28139800 | 0.20131200 |
| N -0.39706600 | 2.65271100 | -1.24069400 | H 5.02793100 | -0.56629800 | -0.81384800 |
| C -3.25659700 | 0.33736300 | -3.19499900 | C 4.07637300 | 2.03355000 | 1.10233700 |
| H -4.04854600 | 0.61484200 | -3.90682400 | H 4.38677000 | 3.04426300 | 1.35109300 |
| C 0.09992600 | 3.18380600 | 0.04768500 | C -3.11461500 | -0.46480100 | -0.56652900 |
| H 0.96887000 | 2.57114300 | 0.31429800 | C -2.94623000 | -0.81103200 | -0.79080700 |
| C -3.69266600 | -0.89107800 | -2.44218200 | C -4.13636100 | 0.40468100 | -0.92690900 |
| C -2.81183000 | -1.72345100 | -1.73854700 | C -3.84021400 | -0.26129300 | 1.72775100 |
| C -5.04207000 | -1.20362000 | -2.38490700 | C -5.00677900 | 0.92759400 | 0.00911700 |
| C -3.27146000 | -2.81897900 | -1.03103200 | H -4.26569500 | 0.67569500 | -1.97034500 |
| C -5.50940900 | -2.30208900 | -1.67830300 | C -4.85282200 | 0.58960400 | 1.34774400 |
| H -5.74557700 | -0.57610700 | -2.92451200 | H -5.52902200 | 0.99481800 | 2.09373800 |
| C -4.62528100 | -3.10830700 | -0.98848200 | O 1.41447700 | -0.28345700 | 1.89071900 |
| H -2.56951600 | -3.43687500 | -0.47751600 | O -2.02305600 | -1.64014100 | 1.25092800 |
| H -4.97123000 | -3.95341900 | -0.40317500 | S 6.27948000 | 2.00644900 | -0.54633600 |
| C 0.45347100 | 4.64057500 | 0.01353500 | S -6.30466700 | 2.06856500 | -0.47410600 |
| C 1.50005700 | 5.08315600 | -0.79925300 | O -5.93917400 | 3.38238700 | 0.12979500 |
| C -0.23585700 | 5.57729000 | 0.76784300 | O -7.56619600 | 1.51445800 | 0.09437700 |
| C 1.85200400 | 6.42543000 | -0.83934500 | O -6.29539500 | 2.09130600 | -1.96280400 |
| C 0.11363900 | 6.91700700 | 0.73420500 | O 6.87654300 | 0.94751200 | -1.40928200 |
| H -1.05307600 | 5.25542900 | 1.40652400 | O 7.17221000 | 2.40541900 | 0.58141800 |
| C 1.15422000 | 7.34268900 | -0.07513100 | O 5.80354400 | 3.18741400 | -1.32666300 |
| H 2.67406300 | 6.74760700 | -1.47086000 | H 0.13646300 | -3.13076800 | 1.63285600 |
| H 1.42897900 | 8.39122100 | -0.09706600 | H 0.47026100 | -2.45883200 | 1.92776900 |
| O -1.46109300 | -1.45713100 | -1.78451900 | H 1.53634400 | -2.96020900 | -1.08100800 |
| O 2.14369000 | 4.13973500 | -1.53227100 | H -0.70143600 | 0.12093400 | -0.97158000 |
| H -3.74221800 | 1.62516600 | -1.68122100 | H -2.43427900 | -0.47800900 | -2.56912600 |
| H -2.35535300 | 0.13477200 | -3.78390600 | Pd -0.22597000 | -1.87887900 | 0.34606700 |
| H 0.35499800 | 2.76284400 | -1.92043600 | H 2.35772000 | 2.07424300 | 2.38126300 |
| H -0.67140300 | 2.99867800 | 0.79997200 | H -3.71193700 | -0.53447300 | 2.76971600 |
| Pd | -0.84061300 | | H 0.07901400 | -0.22268900 | 3.12371700 |
| 0.58918300 | -1.29991700 | | O -0.77573200 | -0.38933100 | 3.56263200 |
| C -1.59575400 | 3.37907300 | -1.72790100 | H -1.28887800 | -0.84925600 | 2.87885300 |
| C -2.34447300 | 2.61966800 | -2.80776500 | H 0.24851600 | 0.88234700 | 1.04084700 |
| H -3.08698100 | 3.28857300 | -3.26542900 | O -0.29133200 | 1.40219800 | 1.40716100 |
| H -1.64797800 | 2.32771400 | -3.60143800 | H 0.21883100 | 2.19942500 | 0.24067700 |
| H -2.25624000 | 3.52417600 | -0.86502700 | C -2.58193000 | -2.51128800 | -1.91741000 |
| H -1.31965700 | 4.37502400 | -2.09330500 | H -1.99770300 | -2.92849200 | -2.73907700 |
| H 2.83783800 | 4.54164000 | -2.06603600 | H -2.41467500 | -3.11646700 | -1.02348700 |
| H -0.96521800 | -2.08743600 | -1.24313200 | H -3.63573200 | -2.58691300 | -2.18991400 |
| S 8.86120300 | -3.79489100 | -0.89520700 | C 3.91511400 | -2.82258600 | -0.57038100 |
| S -0.83590200 | 8.12860500 | 1.66524800 | H 4.83632800 | -2.85697000 | 0.01269200 |
| S -4.80297600 | -4.06534000 | 2.62592300 | H 3.55710100 | -3.84800100 | -0.68585700 |
| | | | H 4.15826900 | -2.43549700 | -1.56278600 |

59

RR-Me_hs_D1_TS1_R, E(SCF) = -2487.50340249,
E(ZPE) = -2487.058405, E(G) = -2487.126814
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.19261300 | -2.24634800 | -2.13504900 |
| H | -0.51345300 | -3.26980600 | -1.92892000 |
| H | -0.46343400 | -2.01389200 | -3.16794000 |
| C | 1.29670800 | -2.12214000 | -1.91184400 |
| H | 1.83826300 | -2.79699500 | -2.57955100 |
| H | 1.64168700 | -1.10036400 | -2.10161900 |
| N | 1.56540300 | -2.43320000 | -0.48683700 |
| N | -0.89338400 | -1.33956900 | -1.19595700 |
| C | 2.97937700 | -2.26409400 | -0.00189500 |
| H | 2.97743400 | -2.81432600 | 0.94608700 |
| C | -2.33163100 | -1.60228600 | -0.95743300 |
| C | 3.26207100 | -0.82421600 | 0.33556900 |
| C | 2.53507400 | -0.25186700 | 1.40801500 |
| C | 4.20946000 | -0.06177500 | -0.32781300 |
| C | 2.82489600 | 1.06517500 | 1.79227600 |
| C | 4.46784500 | 1.24517000 | 0.05550300 |
| H | 4.77427300 | -0.47767600 | -1.15400700 |
| C | 3.77851200 | 1.80522200 | 1.12221000 |
| H | 3.98440400 | 2.82778700 | 1.42271400 |
| C | -2.96521400 | -0.41672400 | -0.27108600 |
| C | -2.37548800 | 0.26950000 | 0.81489200 |
| C | -4.24148800 | -0.05117900 | -0.69060700 |
| C | -3.11717900 | 1.30659800 | 1.41588200 |
| C | -4.95135700 | 0.95936000 | -0.07736000 |
| H | -4.69876300 | -0.57961300 | -1.52213200 |
| C | -4.37739900 | 1.64640800 | 0.98633100 |
| H | -4.92202200 | 2.44821800 | 1.47468300 |
| O | 1.58521200 | -0.93885600 | 2.02497200 |
| O | -1.17098000 | 0.04227600 | 1.31689000 |
| S | 5.67052500 | 2.24349600 | -0.82977600 |
| S | -6.58594600 | 1.42410400 | -0.65100400 |
| O | -6.46022300 | 2.82361600 | -1.14977600 |
| O | -7.47829400 | 1.32527100 | 0.53927800 |
| O | -6.93602400 | 0.45271000 | -1.72402100 |
| O | 6.28605000 | 1.34339100 | -1.84365800 |
| O | 6.64176500 | 2.71661600 | 0.19705400 |
| O | 4.89729200 | 3.36401900 | -1.43847300 |
| H | 0.05434100 | -4.05470700 | 2.16602000 |
| H | 0.55877500 | -3.53370400 | 2.35747500 |
| H | 1.30060500 | -3.40555800 | -0.32020600 |
| H | -0.79636300 | -0.37931400 | -1.54178900 |
| H | -2.80585100 | -1.71281400 | -1.94198700 |
| Pd | 0.20245500 | -1.25272500 | 0.52230200 |
| H | 2.26159000 | 1.49204600 | 2.61594200 |
| H | -2.65214500 | 1.83465600 | 2.24229600 |
| H | 0.62093400 | -0.29125100 | 3.47596000 |
| O | -0.16078800 | 0.06633500 | 3.93462400 |
| H | -0.75008800 | 0.19733400 | 3.17362700 |
| H | -0.16200000 | 1.36410000 | 0.11838000 |
| O | 0.17912800 | 1.67946700 | -0.73457700 |
| H | 1.13286800 | 1.56471600 | -0.65702500 |
| C | -2.54740800 | -2.87711200 | -0.16153900 |
| H | -2.06802200 | -3.74689300 | -0.61570900 |
| H | -2.16875500 | -2.76300400 | 0.85785000 |
| H | -3.61850000 | -3.07884700 | -0.10629600 |
| C | 3.97040100 | -2.92292700 | -0.93646700 |
| H | 4.96240300 | -2.92181700 | -0.48302200 |
| H | 3.68677000 | -3.96114600 | -1.12141000 |
| H | 4.04221200 | -2.41332500 | -1.89924600 |

59

RR-Me_hs_D1_TS1, E(SCF) = -2487.48285477,
E(ZPE) = -2487.038245, E(G) = -2487.104791
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.10110400 | -1.40940500 | -2.42863100 |
| H | -0.15484000 | -2.43227400 | -2.71285800 |
| H | -0.04431200 | -0.76816200 | -3.30251400 |
| C | 1.51668300 | -1.33983700 | -1.92215300 |
| H | 2.22422700 | -1.67151700 | -2.68627200 |
| H | 1.77744400 | -0.31635000 | -1.64129000 |
| N | 1.61386900 | -2.17645900 | -0.70026400 |
| N | -0.79601200 | -0.98961700 | -1.33047100 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.93077800 | -2.09008000 | 0.03577900 |
| H | 2.74239500 | -2.64925600 | 0.95833400 |
| C | -2.24601200 | -1.22496800 | -1.54044800 |
| C | 3.26350600 | -0.67499500 | 0.41083300 |
| C | 2.49750200 | -0.05497100 | 1.43673400 |
| C | 4.29377700 | 0.02588900 | -0.20187800 |
| C | 2.86168000 | 1.26259100 | 1.81106400 |
| C | 4.61103400 | 1.31901500 | 0.17317800 |
| H | 4.87940300 | -0.43483500 | -0.98980800 |
| C | 3.88626600 | 1.93637200 | 1.18876500 |
| H | 4.13576200 | 2.94938500 | 1.49061200 |
| C | -3.03408600 | -0.48678700 | -0.49190900 |
| C | -2.76605700 | -0.61793500 | 0.88881900 |
| C | -4.10390200 | 0.29712900 | -0.90782300 |
| C | -3.62090700 | 0.04660800 | 1.07994600 |
| C | -4.92757100 | 0.93929800 | -0.00562100 |
| H | -4.30700200 | 0.40390800 | -1.96911300 |
| C | -4.68134200 | 0.80734200 | 1.35544600 |
| H | -5.32172900 | 1.30704500 | 2.07546200 |
| O | 1.49156900 | -0.64929800 | 1.99424300 |
| O | -1.78358000 | -1.33426300 | 1.40593400 |
| S | 5.92343100 | 2.22626200 | -0.63956000 |
| S | -6.29638700 | 1.95735300 | -1.56747400 |
| O | -6.00990800 | 3.33237900 | -0.06022500 |
| O | -7.51841800 | 1.37149600 | 0.06088700 |
| O | -6.29822200 | 1.86748400 | -2.04700900 |
| O | 6.54328000 | 1.28245500 | -1.61245800 |
| O | 6.86503000 | 2.65007800 | 0.43803600 |
| O | 5.26888900 | 3.39230200 | -1.30303600 |
| H | 0.08301200 | -3.29515900 | 1.91538900 |
| H | 0.59056800 | -2.77042500 | 2.15291900 |
| H | 1.49425000 | -3.15307500 | -0.97591300 |
| H | -0.65333200 | 0.01154000 | -1.13282000 |
| H | -2.48985500 | -0.77940200 | -2.51442300 |
| Pd | -0.07921700 | -1.77931600 | 0.41327400 |
| H | 2.28695300 | 1.73469500 | 2.60361600 |
| H | -3.42013700 | -0.05943100 | 2.85076500 |
| H | 0.31025400 | -0.15475800 | 3.25100300 |
| O | -0.56630800 | -0.07953500 | 3.67757300 |
| H | -1.12725900 | -0.54189800 | 3.03314300 |
| H | 0.19225900 | 0.84372300 | 1.04632600 |
| O | -0.08402800 | 1.40807200 | 0.30475300 |
| H | 0.69778000 | 1.93955700 | 1.12091900 |
| C | -2.58844500 | -2.70174300 | -1.58125200 |
| H | -2.04571200 | -3.23683000 | -2.36216400 |
| H | -2.38092000 | -3.17893500 | -0.62028700 |
| H | -3.65430600 | -2.80486600 | -1.79120100 |
| C | 4.00039100 | -2.82362000 | -0.74977400 |
| H | 4.93429200 | -2.83135200 | -0.18615400 |
| H | 3.70390500 | -3.86087600 | -0.91967400 |
| H | 4.20039300 | -2.36600000 | -1.72059900 |

59

RR-Me_hs_D1_TS2_P, E(SCF) = -2487.52147094,
E(ZPE) = -2487.071870, E(G) = -2487.139040
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.27763100 | -1.34494600 | -2.49751200 |
| H | 0.02198800 | -2.35145800 | -2.83764300 |
| H | 0.18642300 | -0.67129300 | -3.35747100 |
| C | 1.68663000 | -1.32380800 | -1.96363700 |
| H | 2.40011700 | -1.57950900 | -2.75116200 |
| H | 1.92326200 | -0.31968500 | -1.60454700 |
| N | 1.80961400 | -2.25417000 | -0.80745200 |
| N | -0.63258800 | -0.96439900 | -1.41106500 |
| C | 3.11342400 | -2.13737800 | -0.05857600 |
| H | 3.01187700 | -2.84502600 | 0.76834000 |
| C | -2.07446900 | -1.10390500 | -1.68515100 |
| C | 3.30501800 | -0.75552700 | 0.52028700 |
| C | 2.83763300 | -0.42391100 | 1.79760500 |
| C | 3.97816800 | 0.23502200 | -0.19421000 |
| C | 3.05945200 | 0.84483700 | 2.32933600 |
| C | 4.17494000 | 1.49832900 | 0.32454100 |
| H | 4.37121300 | 0.02576100 | -1.18277200 |
| C | 3.71471400 | 1.80880600 | 1.59660500 |
| H | 3.87494200 | 2.79839200 | 2.00971000 |
| C | -2.87103000 | -0.54250000 | -0.53351000 |
| C | -2.67956600 | -0.94118600 | 0.81150800 |

H -0.91546900 -0.53956600 2.53745200
H -0.07763400 1.00810600 1.16682200
O 0.10778100 1.34954700 0.26701300
H 1.04541000 1.57262900 0.29755100
C -2.47677800 -2.62569700 -1.87017000
H -1.96194000 -3.06435400 -2.72619900
H -2.25756700 -3.22464700 -0.98296800
H -3.54870500 -2.68246900 -2.06516700
C 4.21222900 -2.68434500 -0.87395900
H 5.13514600 -2.68307400 -0.29216000
H 4.00472400 -3.71399200 -1.17447800
H 4.39020300 -2.10074300 -1.77840800

59

RR-Me_hs_Hbond-reor_TS1_P, E(SCF) = -
2487.49335938, E(ZPE) = -2487.046057, E(G)
= -2487.111914 a.u.

C 0.28513800 -1.29180000 -2.47824900
H 0.04159900 -2.28676500 -2.85542300
H 0.15844700 -0.57778200 -3.29742700
C 1.68734000 -1.25945800 -1.93748200
H 2.41146300 -1.51249900 -2.71557400
H 1.92374900 -0.26035300 -1.56490700
N 1.78160900 -2.20049700 -0.79215300
C 3.07694200 -2.12274700 -0.00784000
H 2.91591100 -2.79610500 0.83804300
C 3.29237500 -0.74216400 0.54410800
C 2.70303300 -0.39678200 1.79820200
C 4.03724700 0.19844900 -0.14863600
C 2.88755300 0.93672900 2.24205400
C 4.19146900 1.49663300 0.31260200
H 4.50068800 -0.06969600 -1.09418800
C 3.61439400 1.86040200 1.52163100
H 3.73428700 2.87582100 1.88355400
O 2.01735900 -1.23399100 2.50760800
S 5.16364600 2.65133500 -0.64954100
O 4.59551300 2.61788300 -2.02965500
O 6.56924700 2.14999800 -0.61032300
O 5.00376100 3.97650700 0.01222200
H 0.46723400 -3.03728000 1.60363400
H 0.94622700 -2.36014600 1.80656600
H 1.71951000 -3.15176500 -1.16066200
H 2.43993500 1.21380600 3.19198500
H 0.51814200 -0.31878600 2.92824000
O -0.35259200 0.13344600 2.87284500
H -0.94078400 -0.56937600 2.54820800
H -0.10703200 1.00095100 1.20545200
O 0.08906100 1.35128600 0.31098200
H 1.02786000 1.56831000 0.35488600
N -0.63484800 -0.96744500 -1.36915100
C -2.08099800 -1.11852400 -1.66582500
C -2.89464600 -0.52475500 -0.54843300
C -2.70780600 -0.90342200 0.79744300
C -3.91026900 0.36798100 -0.87129500
C -3.57989700 -0.36265700 1.76123700
C -4.75480400 0.88428700 0.09107200
H -4.05041200 0.66550800 -1.90607300
C -4.58784000 0.50835800 1.41815700
H -5.24623200 0.90717600 2.18334200
O -1.77758900 -1.73960800 1.23213600
S -6.06670000 2.03057400 -0.33850500
O -5.79228300 3.27256600 0.43905000
O -7.33510100 1.36875900 0.08130000
O -5.97278700 2.23044100 -1.81099600
H -0.45621800 -0.00090900 -1.04616100
H -2.27546400 -0.52781000 -2.57082500
Pd -0.00328700 -2.00701200 0.27401500
H -3.43411700 -0.65971300 2.79479900
C -2.45847400 -2.56400600 -1.93500700
H -2.25177200 -3.18861100 -1.06251200
H -3.52828500 -2.61188000 -2.14348300
H -1.93562700 -2.98079900 -2.79701600
C 4.21509600 -2.67724300 -0.84233000
H 5.13247100 -2.68065200 -0.25184800
H 4.00368700 -3.70628100 -1.14205000
H 4.40564700 -2.09784400 -1.74721100

59

RR-Me_hs_Hbond-reor_TS1_R, E(SCF) = -
2487.50793161, E(ZPE) = -2487.062379, E(G)
= -2487.131251 a.u.

C -0.29840600 -2.39852100 -1.90531700
H -0.57767300 -3.42104500 -1.63811700
H -0.60908100 -2.22894900 -2.94001100
C 1.19444100 -2.21800900 -1.74353700
H 1.73646400 -2.91751400 -2.38509300
H 1.49930000 -1.19969300 -2.00422500
N 1.50733600 -2.43525600 -0.31105700
C 2.92648900 -2.25222500 0.13871500
H 2.94032700 -2.77441400 1.10336400
C 3.24124500 -0.81045900 0.44215000
C 2.54663300 -0.19154800 1.52257700
C 4.24017300 -0.11303500 -0.20867300
C 2.96874400 1.08307900 1.93366100
C 4.60278400 1.17038700 0.18520600
H 4.77472000 -0.57313400 -1.94010100
C 3.97805800 1.75928000 1.26887600
H 4.28351300 2.74999700 1.58654400
O 1.54446500 -0.78401100 2.13386300
S 5.88829600 -2.02425700 -0.72913900
O 5.37289300 2.15978100 -2.12237000
O 7.09388600 1.14939900 -0.65636200
O 6.07679700 3.33474600 -0.04795600
H 0.17064900 -4.33527600 -2.21642600
H 0.48907700 -3.66144800 2.30393200
H 1.24222200 -3.39406400 -0.08005800
H 2.46985200 1.52978100 2.78870600
H 1.11944800 2.09726000 0.92634800
O 0.18509200 2.22378700 0.71292200
H -0.26973300 1.49336300 1.18188100
H -0.13574500 1.66770800 -0.99308100
O -0.40837900 1.24310200 -1.83341700
H 0.29064500 1.43628100 -2.46256900
N -0.98774500 -1.45720900 -0.99654700
C -2.40940300 -1.73021300 -0.69637600
C -0.51179600 -0.51179600 -0.06006900
C -2.43052700 0.21846900 0.99160000
C -4.30042200 -0.14108000 -0.50258300
C -3.15366000 1.30168000 1.53308700
C -4.99250500 0.91422200 0.05600300
H -4.76529500 -0.69978600 -1.30969400
C -4.40587300 1.64494900 1.08239700
H -4.93438800 2.48300700 1.52574900
O -1.24232600 -0.01597400 1.52118000
S -6.62099400 1.37514700 -0.53465000
O -6.49057600 2.76820200 -1.05080100
O -7.52295300 1.29431200 0.65046700
O -6.96825300 0.39086800 -1.59718500
H -0.91079400 -0.51245300 -1.41139000
H -2.91511600 -1.89953500 -1.65715200
Pd 0.16036700 -1.23014400 0.67464100
H -2.67938700 1.86317800 2.33167500
C -2.58874100 -2.96434000 0.17047500
H -2.19877100 -2.79372100 1.17703600
H -3.65477900 -3.18455000 0.25211100
H -2.09792000 -3.84703000 -0.24600800
C 3.89464200 -2.95040100 -0.79217800
H 4.89404900 -2.95575700 -0.35572700
H 3.58999100 -3.98784600 -0.94557200
H 3.95717700 -2.46729200 -1.76940700

59

RR-Me_hs_Hbond-reor_TS1, E(SCF) = -
2487.48710244, E(ZPE) = -2487.041793, E(G)
= -2487.106998 a.u.

C 0.13815900 -1.42962100 -2.34616500
H -0.13307300 -2.45080800 -2.62057500
H 0.00186400 -0.79527700 -3.22662800
C 1.55454900 -1.38087200 -1.84532100
H 2.25171900 -1.73605700 -2.60841300
H 1.83547800 -0.35963000 -1.57719000
N 1.63796200 -2.20453700 -0.61388600
C 2.96643000 -2.14523900 0.10058900
H 2.78925900 -2.71371700 1.01903300

| | | | |
|----|-------------|-------------|-------------|
| C | 3.29862500 | -0.73535800 | 0.48754100 |
| C | 2.57411200 | -0.15936700 | 1.57461400 |
| C | 4.26173300 | 0.00400400 | -0.17522900 |
| C | 2.91072900 | 1.16792700 | 1.93360700 |
| C | 4.54986400 | 1.31245900 | 0.18889100 |
| H | 4.80597200 | -0.43680600 | -1.00565500 |
| C | 3.87353300 | 1.88660300 | 1.25579500 |
| H | 4.10876200 | 2.90470700 | 1.54637600 |
| O | 1.64541200 | -0.81414000 | 2.19266500 |
| S | 5.81989200 | 2.20779400 | -0.69883200 |
| O | 5.43166000 | 2.16356200 | -2.13966000 |
| O | 7.10050200 | 1.48424700 | -0.44195800 |
| O | 5.81622800 | 3.58968200 | -0.14094100 |
| H | 0.10340400 | -3.30544800 | 1.97249900 |
| H | 0.61685000 | -2.79085900 | 2.21954900 |
| H | 1.48541400 | -3.18055300 | -0.87593500 |
| H | 2.38740800 | 1.61675700 | 2.77263000 |
| H | 0.43795400 | 0.35581200 | 2.62177500 |
| O | -0.36015800 | 0.93226900 | 2.26187400 |
| H | -1.05536200 | 0.27502200 | 2.48198400 |
| H | -0.12503800 | 1.46217400 | 0.84465300 |
| O | 0.02292600 | 1.62316100 | -0.11234500 |
| H | 0.95884000 | 1.84225500 | -0.17206500 |
| N | -0.75057200 | -0.98043900 | -1.25286900 |
| C | -2.19883800 | -1.21304800 | -1.47047300 |
| C | -3.00825700 | -0.48473400 | -0.43219700 |
| C | -2.75767900 | -0.61264000 | 0.95120100 |
| C | -4.10179900 | 0.25968800 | -0.86063400 |
| C | -3.65158600 | 0.01644400 | 1.84111300 |
| C | -4.96074200 | 0.87077600 | 0.03037400 |
| H | -4.29218800 | 0.36239100 | -1.92467000 |
| C | -4.73419800 | 0.73761700 | 1.39479100 |
| H | -5.40181100 | 1.21078500 | 2.10781000 |
| O | -1.74734800 | -1.27293700 | 1.48943600 |
| S | -6.38245900 | 1.80301700 | -0.54417500 |
| O | -6.28821700 | 3.13787800 | 0.11191300 |
| O | -7.57918600 | 1.03441200 | -0.09538200 |
| O | -6.25701600 | 1.87055400 | -2.02632500 |
| H | -0.58935400 | 0.02620000 | -1.07896000 |
| H | -2.43401000 | -0.76777300 | -2.44685700 |
| Pd | -0.04069800 | -1.74282100 | 0.50439200 |
| H | -3.46040800 | -0.08997600 | 2.90421300 |
| C | -2.54666900 | -2.68963300 | -1.51292800 |
| H | -2.33546600 | -3.16878400 | -0.55353200 |
| H | -3.61438800 | -2.78790600 | -1.71551200 |
| H | -2.01239700 | -3.22712800 | -2.29766700 |
| C | 4.02374000 | -2.87005800 | -0.70916800 |
| H | 4.96122000 | -2.89320000 | -0.15172400 |
| H | 3.71997300 | -3.90230000 | -0.89640900 |
| H | 4.22220500 | -2.39746100 | -1.67294100 |

59

RR-Me_D1_TS1_P, E(SCF) = -2487.47941640,
E(ZPE) = -2487.032375, E(G) = -2487.098424
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.63464500 | 3.24556100 | -0.54680100 |
| H | -0.39454900 | 3.35084600 | -1.60631600 |
| H | -1.34736900 | 4.03089300 | -0.27646200 |
| C | 0.60511200 | 3.31635000 | 0.29485000 |
| H | 1.11953100 | 4.27290400 | 0.17076600 |
| H | 0.33317800 | 3.20551300 | 1.34447600 |
| N | 1.50034900 | 2.18767400 | -0.07335700 |
| N | -1.23586800 | 1.91371500 | -0.32395800 |
| C | 2.73125000 | 2.04760100 | 0.82634100 |
| H | 3.49136800 | 2.66328900 | 0.33132500 |
| C | -2.47197300 | 1.64190300 | -1.09752000 |
| C | 3.24684500 | 0.63930800 | 0.84456100 |
| C | 2.56357500 | -0.38450900 | 1.56952600 |
| C | 4.41193600 | 0.34886600 | 0.14868300 |
| C | 3.16019000 | -1.67390200 | 1.54304300 |
| C | 4.95211000 | -0.92471800 | 0.13267500 |
| H | 4.91769700 | 1.13760400 | -0.40145600 |
| C | 4.31204400 | -1.93862000 | 0.83938700 |
| H | 4.72850100 | -2.94185900 | 0.83896200 |
| C | -3.06761400 | 0.32080700 | -0.69635800 |
| C | -2.32306100 | -0.87946900 | -0.72946100 |
| C | -4.42513100 | 0.27278700 | -0.39864100 |

| | | | |
|----|-------------|-------------|-------------|
| C | -3.00024400 | -2.08205600 | -0.47543100 |
| C | -5.06901100 | -0.92215200 | -0.14977700 |
| H | -4.99792400 | 1.19444600 | -0.37196700 |
| C | -4.34724000 | -2.10877600 | -0.19808500 |
| H | -4.84363400 | -3.05514400 | -0.00796200 |
| O | 1.44183700 | -0.19200200 | 2.17488900 |
| O | -1.02957600 | -0.95510700 | -1.00222400 |
| S | 6.43786200 | -1.29575900 | -0.79121900 |
| S | -6.82396100 | -0.97546600 | 0.22319600 |
| O | -6.93585300 | -1.61550800 | 1.56491300 |
| O | -7.43850100 | -1.80387800 | -0.85317300 |
| O | -7.29125300 | 0.43809900 | 0.21030300 |
| O | 6.92837600 | 0.00521700 | -1.32877800 |
| O | 6.03449000 | -2.24979200 | -1.86698600 |
| O | 7.38663400 | -1.91726100 | -0.17897200 |
| H | 0.34972300 | -1.58339000 | 1.86238300 |
| H | 1.48670800 | -0.52807500 | -1.36275800 |
| H | 1.64787600 | -0.64647700 | -0.58037700 |
| O | -0.26342700 | -2.26107000 | -2.54866700 |
| H | -0.48683800 | -1.99488900 | 0.64910200 |
| H | -0.01319000 | 0.76265000 | 2.34941200 |
| O | -0.85747600 | 1.26205800 | 2.43692600 |
| H | -1.42305900 | 0.71919900 | 2.99123200 |
| H | 1.87400900 | 2.39616700 | -0.99972900 |
| H | -1.42438000 | 1.79405300 | 0.68658600 |
| H | -3.18358200 | 2.42705900 | -0.80910200 |
| Pd | 0.25669700 | -0.55027900 | -0.55736900 |
| H | 2.65865900 | -2.46483500 | 2.09206000 |
| H | -2.42346000 | -3.00034300 | -0.50809200 |
| C | -2.24310100 | 1.72341000 | -2.59592600 |
| H | -3.17970800 | 1.48379800 | -3.10125800 |
| H | -1.94147600 | 2.72024100 | -2.91952800 |
| H | -1.48871700 | 1.00206500 | -2.91848800 |
| C | 2.54350500 | 2.61730000 | 2.22158400 |
| H | 3.47642700 | 2.44922000 | 2.76303200 |
| H | 2.36423600 | 3.69278800 | 2.21148000 |
| H | 1.74885200 | 2.11617600 | 2.77164600 |

59

RR-Me_D1_TS1_R, E(SCF) = -2487.51232071,
E(ZPE) = -2487.066866, E(G) = -2487.134861
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.59783000 | -3.10444400 | 0.10581400 |
| H | 0.28488600 | -3.26452800 | -0.92806900 |
| H | 1.22556500 | -3.94788000 | 0.40468700 |
| C | -0.61189100 | -2.96403500 | 0.99577700 |
| H | -1.23790200 | -3.86025700 | 0.96933500 |
| H | -0.30682500 | -2.79163700 | 2.02958400 |
| N | -1.37025300 | -1.78027000 | 0.52746200 |
| N | 1.36333500 | -1.83588800 | 0.16903200 |
| C | -2.53264400 | -1.35679300 | 1.35472200 |
| H | -3.18196200 | -2.23596500 | 1.46075100 |
| C | 2.43716300 | -1.66452400 | -0.84810400 |
| C | -3.30305700 | -0.31157100 | 0.58982400 |
| C | -2.70020000 | 0.87999000 | 0.12803300 |
| C | -4.65405000 | -0.53079800 | 0.34654400 |
| C | -3.51406200 | 1.81477400 | -0.53648200 |
| C | -5.43142500 | 0.39918500 | -0.31520600 |
| H | -5.11388200 | -1.45367200 | 0.68581400 |
| C | -4.85389200 | 1.58491100 | -0.75205500 |
| H | -5.45515400 | 2.32201000 | -1.27472900 |
| C | 3.29618600 | -0.48819300 | -0.46365500 |
| C | 2.74953400 | 0.78907700 | -0.19735900 |
| C | 4.67606200 | -0.65794700 | -0.44518400 |
| C | 3.64642000 | 1.84306200 | 0.06772600 |
| C | 5.53362900 | 0.39309800 | -0.18880300 |
| H | 5.09448700 | -1.63951700 | -0.64585700 |
| C | 5.00832200 | 1.65506000 | 0.06623900 |
| H | 5.67284100 | 2.48834500 | 0.27202500 |
| O | -1.41885400 | 1.17557800 | 0.28492200 |
| O | 1.46340600 | 1.07381800 | -0.20105900 |
| S | -7.17446900 | 0.10256800 | -0.62547100 |
| S | 7.31152000 | 0.16147700 | -0.16382200 |
| O | 7.74927600 | 0.51570900 | 1.21727700 |
| O | 7.85797200 | 1.09809400 | -1.18729700 |
| O | 7.54739100 | -1.27011900 | -0.49929700 |
| O | -7.46283300 | -1.25690400 | -0.09104000 |

O -7.34295900 0.19728300 -2.10368200
O -7.90445200 1.18166500 0.09905000
H -0.67297000 2.87803400 -0.37625800
H -1.88921200 -1.00104900 -2.76344700
H -2.09531600 -0.48540200 -2.25881300
O 0.11219500 3.44533200 -0.45501100
H 0.80677300 2.75853200 -0.44720900
H -0.81738200 2.15148200 1.85846300
O -0.36305900 2.85230700 2.35364800
H -0.00657500 3.38221800 1.62502700
H -1.73793100 -1.99724000 -0.40176300
H 1.81483200 -1.78793700 1.08451400
H 3.06016300 -2.56767700 -0.80158400
Pd 0.00971000 -0.29995700 0.19015100
H -3.04982900 2.73006600 -0.88917400
H 3.22232500 2.82021000 0.27743700
C 1.88090000 -1.52901600 -2.25358500
H 2.71797200 -1.49432700 -2.95287500
H 1.24850900 -1.397144200 -2.54019200
H 1.30648100 -0.60665600 -2.36309100
C -2.11210600 -0.90126200 2.73847100
H -1.66456000 -1.70977000 3.31867900
H -1.40027600 -1.07450900 2.68882000
H -2.99710700 -0.56061300 3.27781700

59

RR-Me_Dl_TS1-trigo_P, E(SCF) = -
2487.47730568, E(ZPE) = -2487.030278, E(G)
= -2487.098099 a.u.

C -0.47716800 3.17299100 0.20571800
H -0.18402200 3.47174900 -0.80147000
H -1.06273600 3.98324900 0.65048100
C 0.72904900 2.84197400 1.04198700
H 1.41353100 3.68947900 1.11514400
H 0.40799900 2.580921600 2.05309400
N 1.43481700 1.65530600 0.47464600
N -1.28995000 1.93701200 0.10815100
C 2.31898400 0.96889900 1.49740000
H 2.97754100 1.77295700 1.85473200
C -2.55063100 2.01834300 -0.68724300
C 3.21749000 -0.05986600 0.86063100
C 2.79219400 -1.39336900 0.58410100
C 4.53256700 0.31176300 0.59599300
C 3.76775000 -2.27806100 0.05986800
C 5.45317800 -0.57593300 0.07391000
H 4.85598800 1.32662500 0.81319700
C 5.06064400 -1.88513600 -0.19049900
H 5.77736600 -2.59234200 -0.59770600
C -3.27291200 0.70080700 -0.59227900
C -2.66382900 -0.50548800 -1.00155200
C -4.58461500 0.68113900 -0.13737700
C -3.42206300 -1.68733800 -0.93895300
C -5.31456100 -0.49126400 -0.08973600
H -5.05504200 1.60514200 0.18450100
C -4.72751900 -1.68104500 -0.49802600
H -5.29178600 -2.60730300 -0.45973600
O 1.56749600 -1.78849000 0.72978900
O -1.42424500 -0.58835500 -1.46186600
S 7.13651100 -0.07744300 -0.27170800
S -7.01466600 -0.50115400 0.49096200
O -7.04139100 -1.43964300 1.64799700
O -7.82901500 -0.99090700 -0.65712300
O -7.32474200 0.90423600 0.87043000
O 8.01141500 -0.97767100 0.53532700
O 7.23929800 1.35149900 0.13911400
O 7.33235200 -0.27379400 -1.73847400
H 0.60902300 -2.86606900 -0.46679500
O -0.02648800 -3.16946500 -1.14298100
H -0.54503000 -2.37602800 -1.35308800
H -0.08894800 -1.77192100 1.48882300
O -0.99880300 -1.79460300 1.84469500
H -1.56483800 -1.80647500 1.06610700
H 2.05968500 1.98504000 -0.26238800
H -1.55576100 1.64853900 1.05350200
H -3.17250900 2.77660800 -0.19440700
Pd 0.01864700 0.51239000 -0.56000800
H 1.13516900 -0.84199400 -0.83695900

H 3.44700200 -3.29326300 -0.15468000
H -2.95091700 -2.61226600 -1.25561400
H 1.19717800 -0.37872300 -1.52363500
C -2.29820500 2.45228900 -2.11751900
H -1.89026500 3.46209200 -2.17545000
H -1.62305100 1.76460000 -2.63018700
H -3.25091900 2.45223700 -2.64872000
C 1.52041000 0.46363300 2.68671700
H 1.25141600 1.27127000 3.36874200
H 0.61530800 -0.06007900 2.38133100
H 2.13567200 -0.23942000 3.24981700

59

RR-Me_Dl_TS1-trigo, E(SCF) = -
2487.47649824, E(ZPE) = -2487.032979, E(G)
= -2487.099703 a.u.

C -0.52198800 3.22652100 0.06156500
H -0.24749600 3.48206900 -0.96250800
H -1.13133500 4.03877200 0.46993100
C 0.69869200 2.97759000 0.90219900
H 1.35906800 3.84712300 0.92399900
H 0.39184100 2.77053700 1.92760400
N 1.43177800 1.78317400 0.39041300
N -1.29502700 1.96228000 0.03380000
C 2.35530800 1.18822600 1.43092400
H 3.04055900 2.00883000 1.68415300
C -2.55472800 1.97699200 -0.76609900
C 3.19791700 0.08935800 0.84816200
C 2.65647400 -1.20254100 0.59204100
C 4.53955500 0.34515400 0.59764500
C 3.55168400 -2.17935700 0.08915100
C 5.38580000 -0.63207900 0.10574300
H 4.94193700 1.33382200 0.79882100
C 4.87851900 -1.90291000 -0.14857600
H 5.53380500 -2.67689900 -0.53623500
C -3.24779300 0.65075300 -0.61367200
C -2.60774700 -0.55479800 -0.97333900
C -4.55712100 0.61748200 -0.15499000
C -3.33446400 -1.75278500 -0.85988300
C -5.25691700 -0.57077700 -0.05798800
H -5.05063800 1.54158000 0.13000600
C -4.64029200 -1.76067800 -0.41837700
H -5.18076100 -2.69867600 -0.34112700
O 1.40073100 -1.47039200 0.74646500
O -1.36662800 -0.61899000 -1.42873700
S 7.10826100 -0.28677500 -0.23675700
S -6.96061500 -0.59729500 0.51192700
O -6.98368600 -1.52623300 1.67640800
O -7.76000800 -1.10680800 -0.63825400
O -7.29132400 0.80736500 0.87608700
O 7.89682000 -1.28155200 0.54811400
O 7.34715500 1.11759000 0.20191900
O 7.28211700 -0.46912800 -1.70836600
H 0.59616100 -2.70503500 -0.32442600
O 0.03544100 -3.12158000 -1.01016600
H -0.50854100 -2.37778100 -1.31541400
H -0.20859400 -1.46009800 1.57048300
O -1.11496800 -1.48456500 1.93422500
H -1.67307900 -1.69550600 1.17787300
H 2.03395100 2.09322100 -0.37356200
H -1.55182600 1.71335400 0.99252300
H -3.19436800 2.74335100 -0.30886600
Pd 0.05342500 0.53376700 -0.56764400
H 1.28669600 -0.71865300 -1.30125300
H 3.14917700 -3.16765500 -0.11319100
H -2.83972400 -2.67785300 -1.13724500
H 1.29127600 -0.15129900 -1.85157200
C -2.30762200 2.35149500 -2.21425300
H -1.93906200 3.37260800 -2.31900400
H -1.60049900 1.66674900 -2.68643500
H -3.25473000 2.28826000 -2.75168900
C 1.61297400 0.79627300 2.69829000
H 1.39875800 1.65888400 3.33040000
H 0.68095900 0.27336400 2.48496900
H 2.24463500 0.12218000 3.27838100

59

RR-Me_D1_TS1, E(SCF) = -2487.47663289,
E(ZPE) = -2487.031389, E(G) = -2487.098705
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.61751900 | 3.20632600 | -0.16405900 |
| H | -0.33656900 | 3.42152700 | -1.19630300 |
| H | -1.28153400 | 4.00299600 | 0.18635800 |
| C | 0.59193000 | 3.07451700 | 0.71507900 |
| H | 1.17591000 | 3.99804200 | 0.75658600 |
| H | 0.26389800 | 2.83509600 | 1.72723600 |
| N | 1.42821100 | 1.94712500 | 0.22922300 |
| N | -1.31106400 | 1.90294800 | -0.12337000 |
| C | 2.57611100 | 1.62172700 | 1.16384700 |
| H | 3.29140400 | 2.44165300 | 1.01429800 |
| C | -2.53724300 | 1.78401300 | -0.95228400 |
| C | 3.26908200 | 0.34775800 | 0.77719400 |
| C | 2.61518000 | -0.90907900 | 0.94663700 |
| C | 4.57506600 | 0.39718900 | 0.32706800 |
| C | 3.37282900 | -2.06427400 | 0.65868300 |
| C | 5.28836700 | -0.75971000 | 0.03971700 |
| H | 5.05542000 | 1.36519700 | 0.20145500 |
| C | 4.67857800 | -1.99167500 | 0.21301700 |
| H | 5.23699200 | -2.89413000 | -0.01103200 |
| C | -3.21422600 | 0.47182100 | -0.66727300 |
| C | -2.53318200 | -0.75642200 | -0.80513700 |
| C | -4.56167300 | 0.47357800 | -0.32945700 |
| C | -3.26522300 | -1.94223300 | -0.61166800 |
| C | -5.26087000 | -0.70306500 | -0.14487100 |
| H | -5.08352600 | 1.41890700 | -0.21805700 |
| C | -4.60434600 | -1.91799500 | -0.29360100 |
| H | -5.14510200 | -2.84863900 | -0.15367200 |
| O | 1.36576300 | -0.99079300 | 1.28563100 |
| O | -1.25671300 | -0.86523600 | -1.13396800 |
| S | 6.97341800 | -0.62430400 | -0.54762900 |
| S | -7.00253500 | -0.69294100 | 0.29106700 |
| O | -7.69063800 | -1.46573500 | -0.78180100 |
| O | -7.40819300 | 0.73897100 | 0.33073600 |
| O | -7.09344500 | -1.36264700 | 1.61997000 |
| O | 6.91221100 | 0.18113300 | -1.80282900 |
| O | 7.44399600 | -2.01928700 | -0.77792800 |
| O | 7.73524400 | 0.07478700 | 0.52903500 |
| H | 0.49915300 | -2.45665500 | 0.73611500 |
| H | 1.44389300 | -0.38936500 | -1.74834100 |
| H | 1.44854500 | -0.93271400 | -1.19911600 |
| O | -0.07177400 | -3.08333800 | 0.24418100 |
| H | -0.53563300 | -2.48711800 | -0.36523100 |
| H | -0.16918700 | -0.28991100 | 2.05463900 |
| O | -1.00856300 | 0.13506300 | 2.32409200 |
| H | -1.66460500 | -0.56753700 | 2.29193200 |
| H | 1.86484300 | 2.24721700 | -0.64392600 |
| H | -1.54791700 | 1.67188300 | 0.85085600 |
| H | -3.20987900 | 2.58499700 | -0.61632100 |
| Pd | 0.11266400 | 0.46968900 | -0.48116400 |
| H | 2.88954300 | -3.02853300 | 0.78372600 |
| H | -2.74484400 | -2.88704200 | -0.72443100 |
| C | -2.24888100 | 1.97827900 | -2.42835100 |
| H | -3.17966200 | 1.85189300 | -2.98310300 |
| H | -1.86661000 | 2.97571600 | -2.65015200 |
| H | -1.53222000 | 1.23631200 | -2.78673400 |
| C | 2.18194700 | 1.62922500 | 2.63160900 |
| H | 1.35552100 | 0.95149900 | 2.84028500 |
| H | 3.04510000 | 1.28753800 | 3.20496000 |
| H | 1.93171100 | 2.62766000 | 2.99167600 |

59

RR-Me_D1_TS2_P, E(SCF) = -2487.50953629,
E(ZPE) = -2487.060735, E(G) = -2487.130761
a.u.

| | | | |
|---|-------------|-------------|------------|
| C | 0.37489200 | -2.70402800 | 0.94694700 |
| H | 0.04072400 | -3.16034900 | 0.01275500 |
| H | 0.83838100 | -3.48853300 | 1.55536800 |
| C | -0.79903000 | -2.09661100 | 1.66947400 |
| H | -1.52867200 | -2.86059300 | 1.95251300 |
| H | -0.45429500 | -1.61188200 | 2.58537700 |
| N | -1.45263700 | -1.05712400 | 0.82382400 |
| N | 1.32346200 | -1.62495600 | 0.63258900 |
| C | -2.45416400 | -0.26836500 | 1.61660400 |
| H | -3.00317200 | -1.01247500 | 2.20979100 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.46019700 | -1.96798500 | -0.25200500 |
| C | -3.49467900 | 0.35539200 | 0.71478600 |
| C | -3.43011300 | 1.64350900 | 0.17302200 |
| C | -4.64234300 | -0.39676900 | 0.46262000 |
| C | -4.51139200 | 2.16594000 | -0.53055200 |
| C | -5.69832800 | 0.11161000 | -0.26429400 |
| H | -4.72040300 | -1.40313900 | 0.86404700 |
| C | -5.64360300 | 1.41108000 | -0.74744800 |
| H | -6.47773700 | 1.82230000 | -1.30557400 |
| C | 3.37460900 | -0.77346700 | -0.37875700 |
| C | 2.93368700 | 0.49420300 | -0.83115000 |
| C | 4.72553000 | -0.96413700 | -0.10847700 |
| C | 3.90649700 | 1.50013500 | -1.00407500 |
| C | 5.65794700 | 0.03975700 | -0.28253100 |
| H | 5.06311800 | -1.93544200 | 0.82453900 |
| C | 5.23837700 | 1.28365700 | -0.73755200 |
| H | 5.95986500 | 2.08191700 | -0.88156500 |
| O | -2.34713700 | 2.45560400 | 0.31939600 |
| O | 1.68715200 | 0.80652000 | -1.13661200 |
| S | -7.17609600 | -0.87489800 | -0.55999800 |
| S | 7.39021600 | -0.22398500 | 0.09560800 |
| O | 8.13909800 | 0.12829700 | -1.14499500 |
| O | 7.51966600 | -1.66130900 | 0.46506400 |
| O | 7.70670300 | 0.69636100 | 1.22642200 |
| O | -6.87842600 | -2.22619300 | -0.01472100 |
| O | -7.36738800 | -0.86487700 | -2.03620400 |
| O | -8.27233800 | -0.17583000 | 0.16607100 |
| H | 0.36372200 | 3.64102500 | -1.55377800 |
| H | -0.85399200 | 0.93442600 | -0.94931100 |
| H | -1.54167300 | 1.93671700 | 0.10850600 |
| O | 0.94790100 | 3.42869100 | -0.82180600 |
| H | 1.21303800 | 2.49237900 | -0.96900200 |
| H | -1.15021800 | 3.64216000 | 1.53818300 |
| O | -0.24146100 | 3.92781300 | 1.68798100 |
| H | 0.19550200 | 3.76552200 | 0.83049500 |
| H | -1.97773300 | -1.54233000 | 0.09535600 |
| H | 1.71301400 | -1.27090600 | 1.50564800 |
| C | 3.03382600 | -2.77025400 | 0.23380100 |
| Pd | 0.09226500 | -0.09226500 | -0.20765800 |
| H | -4.42649700 | 3.17365900 | -0.92031800 |
| H | 3.56535700 | 2.46881000 | -1.35497500 |
| C | 2.00340000 | -2.47469300 | -1.60934600 |
| H | 2.88562900 | -2.66314100 | -2.22333600 |
| H | 1.44911700 | -3.41169500 | -1.53779900 |
| H | 1.38198400 | -1.73621600 | -2.12130900 |
| C | -1.77830800 | 0.67244600 | 2.59814800 |
| H | -2.50683600 | 1.38610700 | 2.98635000 |
| H | -1.37198200 | 0.12453000 | 3.44898200 |
| H | -0.96289300 | 1.23442700 | 2.13962900 |

59

RR-Me_D1_TS2, E(SCF) = -2487.47882708,
E(ZPE) = -2487.032184, E(G) = -2487.100210
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.44700000 | -3.04103000 | 0.42780500 |
| H | 0.15317900 | -3.40140000 | -0.55891800 |
| H | 0.99667600 | -3.83875900 | 0.93642000 |
| C | -0.75755700 | -2.61335200 | 1.22151000 |
| H | -1.45942600 | -3.43783300 | 1.36514400 |
| H | -0.44005300 | -2.27249400 | 2.20832300 |
| N | -1.43615200 | -1.47321600 | 0.54210900 |
| N | 1.30498500 | -1.84704500 | 0.25357400 |
| C | -2.36632600 | -0.73241600 | 1.47681400 |
| H | -2.98335000 | -1.52501400 | 1.92192500 |
| C | 2.54125700 | -2.01966300 | -0.56170300 |
| C | -3.32505600 | 0.16661000 | 0.73417500 |
| C | -3.00556400 | 1.49563700 | 0.33442900 |
| C | -4.60431800 | -0.32451600 | 0.50166600 |
| C | -4.03771200 | 2.26072200 | -0.24620100 |
| C | -5.58732800 | 0.44276700 | -0.09924000 |
| H | -4.84254200 | -1.34217800 | 0.80237200 |
| C | -5.30192100 | 1.75414300 | -0.45399900 |
| H | -6.07124400 | 2.36411100 | -0.91484800 |
| C | 3.33606400 | -0.74124300 | -0.52524800 |
| C | 2.78739400 | 0.48908900 | -0.94910400 |
| C | 4.66466100 | -0.79235000 | -0.12121400 |
| C | 3.62708100 | 1.61638800 | -0.96781600 |

| | | | |
|----|-------------|-------------|-------------|
| C | 5.47006500 | 0.32888800 | -0.14445000 |
| H | 5.08710100 | -1.73528300 | 0.21210800 |
| C | 4.94439900 | 1.53977400 | -0.57634100 |
| H | 5.57047800 | 2.42597300 | -0.60012000 |
| O | -1.79987000 | 1.98415600 | 0.43608200 |
| O | 1.53931200 | 0.64457600 | -1.36548500 |
| S | -7.23751400 | -0.22803300 | -0.29808600 |
| S | 7.18039300 | 0.25509700 | 0.39614700 |
| O | 7.26896300 | 1.15253600 | 1.58322400 |
| O | 7.98989900 | 0.75188200 | -0.75254800 |
| O | 7.44593100 | -1.17260900 | 0.72416100 |
| O | -7.53515900 | -0.16009400 | -1.75616700 |
| O | -8.14075900 | 0.64097900 | 0.51305700 |
| O | -7.17847400 | -1.62407100 | 0.22223100 |
| H | -0.48533000 | 3.52374400 | -0.60380900 |
| H | -1.03603900 | 0.57891400 | -1.37716800 |
| H | -1.09699800 | 1.02497600 | -0.63784400 |
| O | 0.41206000 | 3.25595100 | -0.89838800 |
| H | 0.81394800 | 2.40678800 | -1.15873200 |
| H | -0.41543400 | 2.39107800 | 1.64441500 |
| O | 0.47513200 | 2.66169900 | 1.93184800 |
| H | 0.83607800 | 3.01726100 | 1.10624400 |
| H | -2.01960900 | -1.85216000 | -0.20488800 |
| H | 1.60238000 | -1.52621700 | 1.17784600 |
| H | 3.13412400 | -2.79669900 | -0.06184100 |
| Pd | 0.04577400 | -0.38962100 | -0.46498500 |
| H | -3.79320500 | 3.27501500 | -0.54547100 |
| H | 3.20716000 | 2.55861700 | -1.30349000 |
| C | 2.23712000 | -2.47730800 | -1.97541400 |
| H | 3.17962500 | -2.56424500 | -2.51784700 |
| H | 1.75353600 | -3.45494600 | -2.00637000 |
| H | 1.60797100 | -1.75615700 | -2.50095200 |
| C | -1.59540300 | -0.06261100 | 2.60260600 |
| H | -2.21757200 | 0.70916600 | 3.05723100 |
| H | -1.33129400 | -0.77283200 | 3.38725100 |
| H | -0.68308200 | 0.41473900 | 2.24417700 |

59

RR-Me_D2_TS1_P, E(SCF) = -2487.50832890,
E(ZPE) = -2487.060014, E(G) = -2487.128411
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.41499400 | 1.97779700 | 1.22741100 |
| H | 0.13010500 | 1.44142100 | 2.13572700 |
| H | 0.78482100 | 2.96561300 | 1.52201500 |
| C | -0.78282300 | 2.10134000 | 0.32055600 |
| H | -1.56681800 | 2.69772100 | 0.79801300 |
| H | -0.51060000 | 2.59605100 | -0.61724000 |
| N | -1.30651700 | 0.74853500 | -0.00606400 |
| N | 1.44481600 | 1.19991400 | 0.52421400 |
| C | -2.49354700 | 0.84393600 | -0.91517800 |
| C | 2.60116300 | 0.73249300 | 1.32049500 |
| H | 3.05043400 | 1.60917000 | 1.80940800 |
| C | -3.67272700 | 0.01768500 | -0.45238600 |
| C | -3.62832900 | -1.32875200 | -0.07670200 |
| C | -4.91720700 | 0.64875200 | -0.44853500 |
| C | -4.79590800 | -1.99030100 | 0.30241300 |
| C | -6.07103000 | -0.01105400 | -0.08368200 |
| H | -4.98038100 | 1.69341500 | -0.73610800 |
| C | -6.01039100 | -1.34341300 | 0.30060400 |
| H | -4.71635600 | -3.03037600 | 0.59707300 |
| H | -6.91100300 | -1.87029500 | 0.59659700 |
| C | 3.63553900 | 0.15075700 | 0.38797300 |
| C | 3.34449800 | -0.89670100 | -0.52668700 |
| C | 4.93738200 | 0.61807200 | 0.48838900 |
| C | 4.41388300 | -1.42181000 | -1.27412700 |
| C | 5.97156000 | 0.08239100 | -0.26217400 |
| H | 5.14997600 | 1.42195000 | 1.18906400 |
| C | 5.70331700 | -0.94975000 | -1.14628300 |
| H | 4.18710900 | -2.22555800 | -1.96665200 |
| H | 6.50958800 | -1.37378800 | -1.73403300 |
| O | -2.49665700 | -2.07222200 | 0.01190900 |
| O | 2.15577500 | -1.43846800 | -0.71510200 |
| S | -7.65764000 | 0.83833200 | -0.05779600 |
| S | 7.61981300 | 0.77030000 | -0.10248500 |
| O | 7.53970900 | 2.15953800 | -0.64162600 |
| O | 8.51168800 | -0.11141700 | -0.90575800 |
| O | 7.93790400 | 0.74893700 | 1.35440000 |

| | | | |
|----|-------------|-------------|-------------|
| O | -8.54648700 | 0.04880500 | -0.95447200 |
| O | -7.39340800 | 2.21474900 | -0.55567000 |
| O | -8.10024700 | 0.80277500 | 1.36397800 |
| H | -2.83051800 | 1.88495900 | -0.85007400 |
| H | 1.81542100 | 1.77526100 | -0.23206400 |
| H | -1.60198100 | 0.33682800 | 0.88967400 |
| H | -1.91081400 | -1.58588200 | 1.96436000 |
| O | -1.64320200 | -0.80850000 | 2.47473700 |
| H | -2.29650800 | -0.72950900 | 3.17507000 |
| H | 0.43474500 | -3.32508900 | 1.03370700 |
| O | 1.27356600 | -3.66293500 | 0.70921000 |
| H | 1.63165700 | -2.92160600 | 0.18163000 |
| Pd | 0.41091900 | -0.39125700 | -0.46254300 |
| H | -1.71874400 | -1.68097900 | -0.44211700 |
| H | -0.33432900 | -1.53920000 | -1.25899900 |
| C | 2.19855800 | -0.25707000 | 2.40051200 |
| H | 1.45514200 | 0.15164800 | 3.08822100 |
| H | 1.79907600 | -1.17748800 | 1.96771400 |
| C | 3.08458100 | -2.51262200 | 0.98468400 |
| C | -2.13150300 | 0.58842400 | -2.36487800 |
| H | -1.89111400 | -0.46193500 | -2.54158300 |
| H | -2.97596600 | 0.86420600 | -3.00034400 |
| H | -1.26637900 | 1.18871200 | -2.65850500 |

59

RR-Me_D2_TS1_R, E(SCF) = -2487.50961144,
E(ZPE) = -2487.065047, E(G) = -2487.134367
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.78106600 | 3.10492200 | 0.18520100 |
| H | 0.58934400 | 3.20289800 | 1.25518000 |
| H | 1.39194000 | 3.95452400 | -0.13341000 |
| C | -0.52281700 | 3.04455000 | -0.56971800 |
| H | -1.11831500 | 3.94692000 | -0.40972800 |
| H | -0.32915900 | 2.95858200 | -1.64003300 |
| N | -1.26948800 | 1.84300400 | -0.12597200 |
| N | 1.50177600 | 1.82705400 | -0.03884500 |
| C | -2.36669800 | 1.40918000 | -1.02365200 |
| C | 2.73488800 | 1.62207200 | 0.77198900 |
| H | 3.40099800 | 2.46726900 | 0.55279300 |
| C | -3.21308800 | 0.33527100 | -0.38046100 |
| C | -2.69116900 | -0.75435200 | 0.35172400 |
| C | -4.58055200 | 0.38061800 | -0.63988300 |
| C | -3.59143400 | 3.95452400 | -0.17455200 |
| C | -5.44106200 | -0.61000100 | -0.21590300 |
| H | -4.98561600 | 1.21689900 | -1.20240100 |
| C | -4.93615600 | -1.69029000 | 0.49906200 |
| H | -3.18226000 | -2.58805100 | 1.33551600 |
| H | -5.60027300 | -2.47926300 | 0.83766400 |
| C | 3.42710800 | 0.36206400 | 0.32184500 |
| C | 2.76752000 | -0.89443300 | 0.31540900 |
| C | 4.77080700 | 0.42550800 | -0.01128500 |
| C | 3.52791300 | -2.03009800 | -0.01025800 |
| C | 5.49684800 | -0.70973700 | -0.33499600 |
| H | 5.26770600 | 1.39271200 | -0.00869400 |
| C | 4.86822900 | -1.94470300 | -0.32452200 |
| H | 3.02003900 | -2.98949000 | -0.01138300 |
| H | 5.43453800 | -2.83440800 | -0.57524100 |
| O | -1.42722800 | -0.91590800 | 0.70297400 |
| O | 1.49847100 | -1.06601100 | 0.61660300 |
| S | -7.19991800 | -0.52175600 | -0.55526500 |
| S | 7.23538200 | -0.54869300 | -0.74365000 |
| O | 7.29980300 | 0.39085200 | -1.90005100 |
| O | 7.70679700 | -1.92035000 | -1.08137500 |
| O | 7.89324600 | 0.00846100 | 0.47365400 |
| O | -7.53895800 | -1.78063700 | -1.27849300 |
| O | -7.39818200 | 0.69851000 | -1.38563300 |
| O | -7.86791400 | -0.43727500 | 0.77541100 |
| H | -3.00865200 | 2.28625400 | -1.18243800 |
| H | 1.77897200 | 1.78241400 | -1.02091900 |
| H | -1.66237900 | 2.01517800 | 0.80914800 |
| H | -1.61161200 | 0.39447500 | 2.40858900 |
| O | -1.76737600 | 1.29978900 | 2.71910100 |
| H | -2.59565200 | 1.25848400 | 3.20485700 |
| H | -0.74213200 | -2.57392500 | 1.32761800 |
| O | -0.02381000 | -3.18552400 | 1.56200600 |
| H | 0.73646100 | -2.64905100 | 1.27745900 |
| Pd | 0.09542900 | 0.36595100 | 0.24065100 |

H -0.97285500 -2.43839800 -1.14020600
H -1.05552900 -2.77222400 -1.80811300
C 2.44050700 1.61348900 2.26180600
H 2.05728500 2.57152300 2.61654500
H 1.72284200 0.83061200 2.51934800
H 3.37070800 1.41527100 2.79646700
C -1.85128800 0.93628900 -2.37347000
H -1.22751500 0.04596700 -2.25844500
H -2.70642200 0.67418400 -2.99856100
H -1.27817700 1.69844700 -2.90343000

59

RR-Me_D2_TS1, E(SCF) = -2487.47639044,
E(ZPE) = -2487.031857, E(G) = -2487.100536
a.u.

C 0.73011100 2.68728700 0.81852600
H 0.49721500 2.46064600 1.86043500
H 1.31553300 3.60907300 0.78212600
C -0.54297900 2.79543000 0.02210400
H -1.18859100 3.58676500 0.41558300
H -0.33043200 3.02091700 -1.02545200
N -1.22424800 1.48416800 0.11050800
N 1.51825400 1.56056200 0.26443100
C -2.51303300 1.41256100 -0.61732300
C 2.66692100 1.09025000 1.09191300
H 3.26069000 1.98471500 1.32279700
C -3.44164300 0.32223000 -0.11060400
C -3.05656900 -0.82798100 0.63432900
C -4.78222500 0.49267400 -0.45171600
C -4.08051600 -1.75804400 0.94671700
C -5.75399900 -0.42737600 -0.11865100
H -5.08379800 1.38358000 -0.99642400
C -5.39120100 -1.57288100 0.58478500
H -3.78218400 -2.63830500 1.50765500
H -6.14274600 -2.30934200 0.85256000
C 3.52672600 0.16419800 0.27362600
C 2.99328400 -0.98450100 -0.36049500
C 4.89039000 0.40371100 0.20993100
C 3.88153900 -1.83965600 -1.03000300
C 5.74906600 -0.46138000 -0.44790700
H 5.29316600 1.28755800 0.69825100
C 5.23823800 -1.59111600 -1.06562200
H 3.46533700 -2.71583000 -1.51500700
H 5.91028100 -2.26672700 -1.58216500
O -1.84143500 -1.05710500 1.04594100
O 1.71520300 -1.31743700 -0.34352100
S -7.46416800 -0.18454300 -0.59083000
S 7.50514200 -0.09000200 -0.48433700
O 7.62798100 1.22934300 -1.16798400
O 8.14161800 -1.20154500 -1.24277900
O 7.93825700 -0.03227500 0.94109400
O -7.78282700 -1.27430500 -1.55993100
O -7.54003600 1.17217000 -1.20326500
O -8.26013900 -0.30007300 0.66606100
H -3.01292000 2.37178300 -0.41251000
H 1.89780300 1.85043200 -0.63925700
H -1.40955800 1.32013800 1.11031900
H -1.45108100 -0.07820700 2.45389800
O -1.24093600 0.74308700 2.95362200
H -1.97060800 0.86748400 3.56518400
H -0.65621100 -2.41745800 1.37821500
O 0.13851200 -2.97789100 1.46286500
H 0.79168000 -2.54285100 0.89306500
Pd 0.22890800 0.04832200 -0.23388000
H -0.98717900 -1.42823100 -0.82395100
H -0.63131300 -1.27421300 -1.49949900
C 2.21212400 0.45521800 2.39138200
H 1.60871100 1.12920200 3.00037900
H 1.63023700 -0.45080800 2.20520800
H 3.09710500 0.18239100 2.96839300
C -2.29123100 1.32850300 -2.11867900
H -1.85982600 0.36604600 -2.39835300
H -3.24714100 1.42765700 -2.63384700
H -1.63713000 2.12388400 -2.48174000

59

RR-Me_D2_TS2_P, E(SCF) = -2487.50841775,
E(ZPE) = -2487.060191, E(G) = -2487.128847
a.u.

C -0.43664000 -1.86671200 1.45792900
H -0.16524400 -1.25789800 2.32393000
H -0.80774000 -2.82865600 1.82804800
C 0.77284400 -2.06334400 0.57928900
H 1.55057700 -2.61833400 1.11351500
H 0.51012900 -2.63598100 -0.31580800
N 1.30473200 -0.74380400 0.14245400
N -1.45836300 -1.15310600 0.67902500
C 2.48107700 -0.92403300 -0.76787800
C -2.63632300 -0.63695700 1.41166600
H -3.09893500 -1.48036700 1.94448600
C 3.66908800 -0.06139600 -0.40349500
C 3.63416000 1.30915300 -0.12824700
C 4.91617100 -0.68840300 -0.39920500
C 4.81104800 1.99632500 0.16808600
C 6.07910900 -0.00302600 -0.12143400
H 4.97394600 -1.75071900 -0.61490300
C 6.02704200 1.35281300 0.17094600
H 6.93517900 1.89957200 0.40051900
C -3.64657600 -0.12413400 0.41453900
C -3.33550600 0.85226300 -0.56315100
C -4.95192600 -0.59388900 0.51393600
C -4.38613200 1.31011600 -1.38441100
C -5.96213500 -0.12778100 -0.40425200
H -5.19090700 -1.34489200 1.26097800
C -5.67205200 0.83915400 -1.25958200
H -6.45543400 1.21362400 -1.91119700
O 2.50512500 -2.05967600 -0.06417800
O -2.14645500 1.39114200 -0.75786300
S 7.67422200 -0.83666000 -0.13436600
S -7.63216500 -0.76618800 -0.17294000
O -7.62405800 -1.71517800 0.97514300
O -7.91867700 -1.43371500 -1.47611500
O -8.50701500 0.41984300 0.05712900
O 8.45504200 -0.17530000 -1.21648500
O 7.38585400 -2.26944200 -0.41028100
O 8.25593700 -0.60322100 1.21653100
H 2.81805500 -1.95528700 -0.61087600
H -1.80892900 -1.78619200 -0.03987200
H 1.61603900 -0.26721400 0.99949300
H 1.97822100 1.73245800 1.90965400
O 1.69476100 1.01148000 2.49000400
H 2.34011000 0.98995500 3.20155300
H -0.42983100 3.34530600 0.89984600
O -1.26262300 3.68101800 0.55769600
H -1.62972500 2.92029400 0.06524200
Pd -0.40850400 0.36389300 -0.40476600
H 1.71856600 1.64033500 -0.47734300
H 0.34393800 1.44740100 -1.28084900
H -4.14178100 2.05927900 -2.12992000
H 4.73717400 3.05463100 0.39042300
C -2.26090300 0.41824100 2.43717400
H -3.17084600 0.75923300 2.93433400
H -1.59294000 0.02985100 3.20813600
H -1.78667700 1.28241000 1.96528500
C 2.10086800 -0.80031800 -2.23013900
H 1.24060200 -1.43293500 -2.46327900
H 1.84528600 0.22883900 -2.48963300
H 2.94246000 -1.11871700 -2.84923500

59

RR-Me_D2_TS2_TS_V2, E(SCF) = -
2487.47892914, E(ZPE) = -2487.034579, E(G) =
-2487.104213 a.u.

C -0.64407000 -2.08941800 1.42249300
H -0.38492100 -1.55515900 2.33877500
H -1.11296100 -3.03839400 1.69649700
C 0.58918100 -2.29502400 0.58656700
H 1.32465600 -2.90733700 1.11629100
H 0.34392400 -2.80345500 -0.35087800
N 1.16630000 -0.96898800 0.26154000
N -1.58193600 -1.25139500 0.64392200
C 2.33937100 -1.09082100 -0.66382600
C -2.78174300 -0.75198000 1.37112200

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | -3.26838000 | -1.63374700 | 1.80911600 | O | -1.39789700 | -1.35636100 | -0.22480800 |
| C | 3.51189200 | -0.21361500 | -0.29203400 | C | 1.39965400 | -1.35319800 | 0.20905100 |
| C | 3.40476000 | 1.15130200 | 0.06751800 | S | -7.22849700 | -0.53257500 | 0.25155100 |
| C | 4.77396600 | -0.78972600 | -0.40628600 | S | 7.23577100 | -0.53922300 | -0.22396900 |
| C | 4.60326500 | 1.86178900 | 0.29464900 | O | 7.56604400 | -0.81646800 | -1.65200200 |
| C | 5.93042300 | -0.06943200 | -0.18314000 | O | 7.84084700 | -1.54327900 | 0.69941100 |
| H | 4.85800500 | -1.83687900 | -0.68362800 | O | 7.52736000 | 0.86591300 | 0.17681100 |
| C | 5.83912300 | 1.27158700 | 0.17185600 | O | -7.56938100 | 0.72316400 | -0.46632700 |
| H | 6.74041900 | 1.84818500 | 0.35552300 | O | -7.46294000 | -0.44526400 | 1.72277700 |
| C | -3.73992500 | -0.13744700 | 0.38655300 | O | -7.87249300 | -1.74152400 | -0.34782700 |
| C | -3.33848300 | 0.88290600 | -0.50740300 | H | -1.85428500 | 1.69803200 | 0.72335500 |
| C | -5.07225900 | -0.53248400 | 0.42420900 | H | -1.90008400 | 0.82873100 | -2.04295400 |
| C | -4.33230700 | 1.46660900 | -1.31997300 | H | 1.84461000 | 1.70873300 | -0.73077900 |
| C | -6.02545300 | 0.05573000 | -0.38274100 | Pd | -0.00136200 | 0.08987800 | -0.00647300 |
| H | -5.37660600 | -1.31880200 | 1.10859000 | C | 0.59222600 | 2.81238400 | 0.45871000 |
| C | -5.64725900 | 1.07107600 | -1.25467700 | C | -0.60484500 | 2.81273900 | -0.45896100 |
| H | -6.38821800 | 1.54135500 | -1.89365500 | H | -1.19970500 | 3.71794900 | -0.31627600 |
| O | 2.25493100 | 1.76262600 | 0.24788900 | H | -0.28385000 | 2.77612000 | -1.50442800 |
| O | -2.11632600 | 1.35290600 | -0.62267500 | H | O.27156200 | 2.76859300 | 1.50401300 |
| S | 7.54629500 | -0.82843800 | -0.35035600 | H | 1.18357500 | 3.72069500 | 0.32115400 |
| S | -7.74458700 | -0.44919500 | -0.31456300 | C | 3.23720300 | 2.43439100 | 1.62190800 |
| O | -8.50007100 | 0.73946800 | 0.17668000 | H | 4.00845000 | 2.13739100 | 2.33286000 |
| O | -7.79957700 | -1.60181500 | 0.62699000 | H | 3.71983600 | 2.93892800 | 0.78014200 |
| O | -8.11754000 | -0.81807100 | -1.71056400 | H | 2.59476900 | 3.15320400 | 2.13056100 |
| O | 8.24126100 | -0.07714600 | -1.43566100 | C | -3.24650300 | 2.43148100 | -1.62661400 |
| O | 7.30023600 | -2.25564800 | -0.69858800 | H | -4.01380400 | 2.13677300 | -2.34271200 |
| O | 8.21664000 | -0.65931600 | 0.97129300 | H | 3.73437900 | -2.92753500 | -2.78280800 |
| H | 2.68828100 | -2.12476200 | -0.54704700 | H | -2.60525600 | 3.15681600 | -2.12743200 |
| H | -1.92216900 | -1.80399100 | -0.14565000 | | | | |
| H | 1.47634700 | -0.54887500 | 1.14885800 | | | | |
| H | 1.78156700 | 1.29273600 | 1.95035300 | 51 | | | |
| O | 1.53625800 | 0.67645300 | 2.67051000 | RR-Me-eq-axMe, E(SCF) = -2333.45270739, | | | |
| H | 2.28751200 | 0.66956100 | 3.26868800 | E(ZPE) = -2333.072459, E(G) = -2333.132688 | | | |
| H | 2.25346600 | 3.54337400 | 0.37165400 | a.u. | | | |
| O | 2.23235100 | 4.52146800 | 0.44121800 | N | -1.40607200 | 1.67897200 | -0.15375700 |
| H | 2.65461200 | 4.82843700 | -0.36358200 | N | 1.37198600 | 1.66676800 | 0.11443400 |
| Pd | -0.47079800 | 0.24747400 | -0.22896600 | C | -2.51964000 | 1.39408900 | -1.11532500 |
| H | 0.96168400 | 1.47405800 | -0.53751300 | C | 2.46848100 | 1.26274300 | 1.03198400 |
| H | 0.31368400 | 1.49839600 | -1.11640200 | C | -3.29375100 | 0.20088900 | -0.60371300 |
| H | -4.02178800 | 2.25009800 | -2.00272300 | C | -2.63974200 | -1.04896700 | -0.43660400 |
| H | 4.51748900 | 2.90597300 | 0.57872800 | C | -4.65427500 | 0.28865000 | -0.33043300 |
| C | -2.41849500 | 0.20669500 | 2.48950400 | C | -3.42082400 | -2.15745400 | -0.04940000 |
| H | -1.77099300 | -0.24771700 | 3.24110800 | C | -5.39254200 | -0.81184600 | 0.06308500 |
| H | -1.93111400 | 1.10299500 | 2.09893600 | H | -5.17907700 | 1.23025500 | -0.44087200 |
| H | -3.33833600 | 0.51169100 | 2.99107600 | C | -4.76776900 | -2.04580900 | 0.19921300 |
| C | 1.93196800 | -0.92070600 | -2.11599200 | H | -2.91344300 | -3.11031300 | 0.05733700 |
| H | 1.05365400 | -1.52375700 | -2.36214900 | H | -5.34190500 | -2.91697700 | 0.49904400 |
| H | 1.71342500 | 0.12250100 | -2.35003500 | C | 3.30295500 | 0.19309500 | 0.37289900 |
| H | 2.75655900 | -1.24311500 | -2.75514300 | C | 2.73818200 | -0.96964500 | -0.21288900 |
| | | | | C | 4.68618000 | 0.32759100 | 0.43268000 |
| | | | | C | 3.63618600 | -1.94431900 | -0.70499500 |
| | | | | C | 5.53739000 | -0.64358500 | -0.05403700 |
| | | | | H | 5.11310100 | 1.21936100 | 0.88228400 |
| | | | | C | 4.99894600 | -1.79229600 | -0.62538800 |
| | | | | H | 3.20392500 | -2.83310900 | -1.15259100 |
| | | | | H | 5.65642200 | -2.56414600 | -1.01381400 |
| | | | | O | -1.36391200 | -1.25076100 | -0.65225500 |
| | | | | O | 1.45963300 | -1.23076500 | -0.32610800 |
| | | | | S | -7.13641300 | -0.65756800 | 0.44577700 |
| | | | | S | 7.31666900 | -0.45723500 | 0.03512700 |
| | | | | O | 7.80670200 | -0.49636000 | -1.37373100 |
| | | | | O | 7.80950700 | -1.61644800 | 0.83467400 |
| | | | | O | 7.56460000 | 0.85333800 | 0.69891100 |
| | | | | O | -7.53855500 | 0.70687900 | 0.00221100 |
| | | | | O | -7.25274700 | -0.84203800 | 1.92261800 |
| | | | | O | -7.82251400 | -1.74266200 | -0.31303500 |
| | | | | H | -1.80425000 | 1.69748600 | 0.78763400 |
| | | | | H | -2.01253000 | 1.11605500 | -2.04893300 |
| | | | | H | 1.79915400 | 1.83446100 | -0.79808400 |
| | | | | H | 3.10688800 | 2.14489500 | 1.17526000 |
| | | | | Pd | 0.00794700 | 0.17920000 | -0.22628900 |
| | | | | C | 0.60348900 | 2.87747500 | 0.48433000 |
| | | | | C | -0.63737400 | 2.92848400 | -0.37304600 |
| | | | | H | -1.23433900 | 3.81210300 | -0.13467100 |
| | | | | H | -0.37265000 | 2.97065600 | -1.43388900 |
| | | | | H | 0.32511900 | 2.80284300 | 1.53719100 |
| | | | | H | 1.21303700 | 3.77654900 | 0.36040000 |
| | | | | C | 1.94574300 | 0.81842400 | 2.38569300 |

H 2.79817200 0.57698100 3.02289200
H 1.36728900 1.59436000 2.89029700
H 1.32438700 -0.07502400 2.29117900
C -3.36193300 2.62635600 -1.37668000
H -4.17507700 2.38634500 -2.06208000
H -3.79499200 3.02462600 -0.45471900
H -2.77025100 3.41335300 -1.84430900

62

RR-Me_ID1_TS1_R_V2-type_H2-out_REF, E(SCF) = -2563.95783800, E(ZPE) = -2563.486880, E(G) = -2563.557348 a.u.

C -0.58107800 2.89903000 -0.89336100
H -0.27738700 2.79693000 -1.93803000
H -1.22873000 3.77656800 -0.81416900
C 0.63045800 3.02485300 -0.00423200
H 1.23351300 3.90105300 -0.25742700
H 0.31611100 3.10995100 1.03725000
N 1.42742700 1.78154900 -0.14580900
N -1.30717700 1.67689000 -0.48755300
C 2.57116600 1.62400600 0.79531200
H 3.21579700 2.50147000 0.65252500
C -2.40580400 1.23932300 -1.38285400
C 3.37201600 0.40526300 0.41203200
C 2.79389600 -0.88068500 0.29960600
C 4.74307300 0.55349000 0.23561900
C 3.65180600 -1.96462500 0.03360600
C 5.56342100 -0.52571600 -0.02822400
H 5.18662700 1.54113400 0.31663100
C 5.00829100 -1.79556600 -0.12580300
H 5.64190700 -2.65245500 -0.33138100
C -3.24421500 0.21157600 -0.66915800
C -2.68101700 -0.93904600 -0.07589900
C -4.62191100 0.39053600 -0.63260000
C -3.55211100 -1.86049300 0.53289900
C -5.45879400 -0.53103600 -0.03394600
H -5.05585600 1.27807900 -1.08304100
C -4.91501200 -1.66787200 0.54986700
H -5.56138500 -2.39699200 -1.02785200
O 1.50514200 -1.13790100 0.44084800
O -1.38502600 -1.21736400 -0.04797100
S 7.32624300 -0.31152300 -0.28543300
S -7.23776500 -0.29405700 -0.01937700
O -7.65060100 -0.38785300 1.41002800
O -7.80080300 -1.39990800 -0.84628000
O -7.47775700 1.05252200 -0.60786800
O 7.61239100 1.12328800 -0.00867100
O 7.57886600 -0.69164600 -1.70516100
O 7.99304100 -1.23610400 0.67535600
H 0.32640800 -1.29902400 2.45613600
O -0.62422500 -1.27224400 2.62798500
H -0.98429800 -1.48215900 1.74397000
H -2.57855300 1.40086600 2.83319400
O -1.71717000 1.42145700 2.40840900
H -1.32437300 0.54441000 2.58291700
H 1.81998000 1.76675300 -1.08946200
H -1.68677300 1.81035300 0.46328200
H -3.03764800 2.11931200 -1.56372500
Pd 0.08067800 0.23332300 -0.10688600
O 0.31911900 -3.06478300 -1.26760000
H -0.52160400 -2.63579100 -1.04267100
H 0.92263300 -2.54956400 -0.70497500
H 3.20806800 -2.95232700 -0.04034300
H -3.11268700 -2.74196300 0.98938100
C 2.12280200 1.59328000 2.24416000
H 1.40461000 0.79051500 2.42247300
H 2.99672700 1.41705100 2.87271300
H 1.67528300 2.53630500 2.56157600
C -1.88855400 0.72827000 -2.71572600
H -2.74031500 0.50166400 -3.35918600
H -1.26837600 1.46295200 -3.23335900
H -1.30622000 -0.18688600 -2.58340300
H 1.58119100 -0.24227500 -2.45484000
H 1.71233000 0.08819200 -3.11700300

60

RR-Me_ID1_TS1_R_V2-type_REF, E(SCF) = -2562.78110792, E(ZPE) = -2562.326145, E(G) = -2562.395595 a.u.

C 0.54437500 3.06653300 0.45084000
H 0.22049500 3.11026700 1.49237400
H 1.17599700 3.93640300 0.25294100
C -0.64977100 3.02476000 -0.46943600
H -1.28011000 3.91019400 -0.35507200
H -0.32328000 2.97279600 -1.51008700
N -1.41839200 1.79471600 -0.15791100
N 1.30747000 1.81129300 0.25355500
C -2.50890300 1.43468000 -1.10624700
H -3.13539100 2.32938000 -1.21786500
C 2.41046900 1.54015800 1.21700600
C -3.35563800 0.35563800 -0.48479100
C -2.80420400 -0.85912200 -0.01991000
C -4.73078600 0.54868200 -0.41945500
C -3.68660800 -1.83603600 0.47559500
C -5.57677200 -0.42369800 -0.47498000
H -5.15547600 1.48385400 -0.77120600
C -5.04595300 -1.62808000 0.52066400
H -5.70194200 -2.40017800 0.91002200
C 3.24312600 0.40717700 0.67789300
C 2.67837200 -0.84779500 0.35670700
C 4.61064700 0.59943600 0.52172000
C 3.54134500 -1.86060600 -0.10125500
C 5.43836400 -0.41034200 0.07121100
H 5.04394000 1.56549800 0.76060700
C 4.89576200 -1.65051000 -0.23888300
H 5.53575400 -2.45080000 -0.59656600
O -1.51212300 -1.15089300 -0.03516000
O 1.39087800 -1.13389700 0.46462700
S -7.34783200 -0.14992100 0.17246400
S 7.20392100 -0.14726200 -0.12680600
O 7.49746800 -0.44466400 -1.55722600
O 7.86205600 -1.11045100 0.80111000
O 7.45061800 1.27488000 0.23682400
O -7.58910900 1.19360000 -0.42232000
O -7.68871200 -0.21457900 1.62250200
O -7.97356600 -1.25555600 -0.60730500
H -0.58592300 -2.23407300 -1.41735000
O 0.29980000 -2.55670900 -1.65093300
H 0.78968100 -2.30593000 -0.84442700
H 2.59347000 -0.48989100 -2.23264800
O 1.84623900 -0.43236600 -2.83818200
H 1.25026500 -1.14467500 -2.53948300
H -1.85654500 1.92319400 0.75646100
H 1.72895100 1.84216900 -0.67801700
H 3.03997700 2.43965200 1.23671900
Pd -0.06134500 0.29312700 0.13396600
O -0.34886000 -2.60187000 2.10639200
H 0.50200900 -2.25491900 1.79777300
H -0.94455200 -2.22319800 1.43732100
H -3.26022200 -2.77166400 0.82296100
H 3.10683900 -2.82557200 -0.34292300
C -1.97853800 -1.03965500 -2.47145900
H -1.37983300 0.12812500 -2.41605200
H -2.82770700 0.84980100 -3.12980400
H -1.37579600 1.82504900 -2.93071600
C 1.89471800 1.27572200 2.61883900
H 2.74998900 1.12162700 3.27866900
H 1.32259900 2.11647900 3.01457600
H 1.27015800 0.37943600 2.65257500

60

RR-Me_ID2_TS1_N-trigo-square_P, E(SCF) = -2562.75768544, E(ZPE) = -2562.303054, E(G) = -2562.373808 a.u.

C 0.52811300 2.29560000 1.12489700
H 0.25603700 1.85445700 2.08541400
H 0.99259300 3.26746700 1.31027700
C -0.69845300 2.41364600 2.60517000
H -1.44814400 3.04821600 0.74321800
H -0.45783000 2.85575300 -0.71093400
N -1.23797800 1.05197800 0.04136500
C -2.49103700 1.06778200 -0.77407700
C -3.58029600 0.13316300 -0.27905200

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -3.38135600 | -1.16370700 | 0.26034000 | O | -7.56076400 | 1.31210500 | -1.10165900 |
| C | -4.88143100 | 0.61120900 | -0.41909900 | H | -2.97940100 | 2.26162600 | -0.78973700 |
| C | -4.52739000 | -1.89296700 | 0.64372500 | H | -1.48535900 | 1.26996300 | 0.95024900 |
| C | -5.98457000 | -0.13541500 | -0.05676100 | O | -0.46670800 | -1.77795800 | -1.65322200 |
| H | -5.04118100 | 1.60426800 | -0.83099500 | H | -1.08585700 | -1.98721000 | -0.92124600 |
| C | -5.80145100 | -1.39969300 | 0.49169100 | H | -1.52608100 | -0.41606400 | 2.14635600 |
| H | -4.36263100 | -2.87918300 | 1.06589400 | O | -1.58684200 | 0.37908800 | 2.71249500 |
| H | -6.65988300 | -1.99301200 | 0.79089400 | H | -0.91741900 | 0.27062300 | 3.39211100 |
| O | -2.19407300 | -1.69216300 | 0.44584400 | H | 0.34079000 | -2.28110700 | -1.48092600 |
| S | -7.64270800 | 0.52739600 | -0.21391500 | H | -0.62469700 | -2.47329700 | 1.36992100 |
| O | -8.12286400 | 0.77161400 | 1.17816100 | O | 0.21200900 | -2.88314900 | 1.65110500 |
| O | -8.43916800 | -0.52504500 | -0.90861500 | H | 0.88438000 | -2.42412700 | 1.12254000 |
| O | -7.51646500 | 1.78142100 | -1.00827100 | Pd | 0.27371400 | 0.03537800 | -0.24436700 |
| H | -2.89875000 | 2.07876000 | -0.64122900 | N | 1.48913500 | 1.60965900 | 0.24321600 |
| H | -1.45242000 | 0.70750500 | 0.97193800 | C | 2.63677200 | 1.22694500 | 1.12381300 |
| O | -0.57251900 | -1.66167500 | -1.44071000 | H | 3.20163700 | 2.15046300 | 1.29868100 |
| H | -1.31616300 | -1.82044800 | -0.75437300 | C | 3.54151600 | 0.27818900 | 0.37094300 |
| H | -1.74216200 | -0.98500100 | 2.06369400 | C | 3.06683900 | -0.92780200 | -0.19006000 |
| O | -1.60694100 | -0.25446000 | 2.70155000 | C | 4.90041100 | 0.56641900 | 0.34338100 |
| H | -0.89931400 | -0.54317900 | 3.28336500 | C | 4.00071200 | -1.79931400 | -0.77697200 |
| H | -0.00416200 | -2.44048700 | -1.47720900 | C | 5.80016600 | -0.30679200 | -0.26352300 |
| H | -0.57541200 | -2.70797400 | 1.09011900 | H | 5.27063300 | 1.49398300 | 0.74021900 |
| O | 0.28602100 | -0.12650800 | 1.23744900 | C | 5.34380500 | -1.50212500 | -0.80552700 |
| H | 0.92689800 | -2.56890300 | 0.77040600 | H | 3.62559900 | -2.72266200 | -1.20453300 |
| Pd | 0.43411900 | -0.13107800 | -0.41690300 | H | 6.04522100 | -2.19323900 | -1.26225200 |
| N | 1.48141200 | 1.38807900 | 0.44812600 | O | 1.79811100 | -1.30005500 | -0.18408600 |
| C | 2.65023100 | 0.94086900 | 1.26098900 | S | 7.55251600 | 0.07578500 | -0.32932800 |
| H | 3.13719400 | 1.85570400 | 1.62340200 | O | 8.23325200 | -1.01428100 | 0.42593500 |
| C | 3.63742300 | 0.21646600 | 0.38278000 | O | 7.70599900 | 1.41195700 | 0.30890000 |
| C | 3.26941900 | -0.89235900 | -0.41174000 | O | 7.91359100 | 0.07481400 | -1.77571300 |
| C | 4.97135900 | 0.60564500 | 0.43100800 | H | 1.88131400 | 1.88135500 | -0.66075700 |
| C | 4.28267900 | -1.57008600 | -1.11228100 | C | 2.18369600 | 0.66028400 | 2.44546800 |
| C | 5.95002200 | -0.07694900 | -0.26383600 | H | 3.06865500 | 0.41602400 | 3.03491300 |
| H | 5.25708200 | 1.46031100 | 1.03660400 | H | 1.59225400 | 1.37221200 | 3.02374200 |
| C | 5.59915000 | -1.17809100 | -1.03573300 | H | 1.60225200 | -0.25456600 | 2.30676900 |
| H | 3.99019900 | -2.42101200 | -1.71772900 | C | -2.14611000 | 1.02798100 | -2.31426800 |
| H | 6.36157200 | -1.72101500 | -1.58524000 | H | -1.46121900 | 1.77897200 | -2.71588700 |
| O | 2.03461500 | -1.34908700 | -0.52777100 | H | -1.69655000 | 0.04159000 | -2.44365300 |
| S | 7.66864300 | 0.43773000 | -0.19885900 | H | -3.06675700 | 1.06933000 | -2.89907800 |
| O | 8.42580000 | -0.74228800 | 0.30775300 | | | | |
| O | 7.71559300 | 1.60201500 | 0.72784200 | | | | |
| O | 8.04025300 | 0.79054900 | -1.59916600 | 60 | | | |
| H | 1.86207900 | 1.88223400 | -0.36214800 | RR-Me_ID2_TS1_P, E(SCF) = -2562.75973046, | | | |
| C | 2.23219800 | 0.11127400 | 2.45979600 | E(ZPE) = -2562.304527, E(G) = -2562.374501 | | | |
| H | 3.13004700 | -0.18103900 | 3.00620600 | a.u. | | | |
| H | 1.59611100 | 0.66778300 | 3.15013000 | C | 0.94083100 | 2.71358100 | -1.40238800 |
| H | 1.70934300 | -0.79698500 | 2.15265800 | H | 0.73365500 | 3.35044700 | -0.54137500 |
| C | -2.18922700 | 0.90515400 | -2.25264500 | H | 1.61411600 | 3.23904900 | -2.08617600 |
| H | -1.41396100 | 1.60685400 | -2.57349600 | C | -0.35373300 | 2.33837900 | -2.06716900 |
| H | -1.85706800 | -0.10697300 | -2.48302700 | H | -0.91447000 | 3.23130100 | -2.36226800 |
| H | -3.09286500 | 1.11585500 | -2.82798100 | H | -0.16171400 | 1.75224500 | -2.96881800 |
| | | | | N | -1.16262100 | 1.52783500 | -1.12626300 |
| | | | | N | 1.57310600 | 1.46264100 | -0.91943300 |
| | | | | C | -2.29479000 | 0.82634100 | -1.81167800 |
| | | | | C | 2.82036700 | 1.63802600 | -0.11815700 |
| | | | | H | 3.52474800 | 2.17716000 | -0.76531700 |
| | | | | C | -3.40499700 | 0.52270200 | -0.83148500 |
| | | | | C | -3.81990500 | 1.51614800 | 0.10038900 |
| | | | | C | -4.06516700 | -0.69796900 | -0.86086100 |
| | | | | C | -4.88816600 | 1.18901100 | 0.96768100 |
| | | | | C | -5.11414300 | -0.98274900 | -0.00460900 |
| | | | | H | -3.76786400 | -1.46933900 | -1.56102800 |
| | | | | C | -5.52679500 | -0.02797900 | 0.91733400 |
| | | | | H | -5.19231400 | 1.94491800 | 1.68589800 |
| | | | | H | -6.34638500 | -0.24524200 | 1.59589700 |
| | | | | C | 3.42138900 | 0.29359400 | 0.19473100 |
| | | | | C | 2.69111300 | -0.69766100 | 0.89189900 |
| | | | | C | 4.75100100 | 0.05936600 | -0.13270400 |
| | | | | C | 3.36395400 | -1.88051000 | 1.25180100 |
| | | | | C | 5.38880700 | -1.11206500 | 0.22854900 |
| | | | | H | 5.31225900 | 0.81757800 | -0.67053800 |
| | | | | C | 4.68565400 | -2.08551700 | 0.92850200 |
| | | | | H | 2.80102500 | -2.63377500 | 1.79221100 |
| | | | | H | 5.17856800 | -3.00842800 | 1.21749300 |
| | | | | O | -3.22012200 | 2.66763100 | 0.20961000 |
| | | | | O | 1.43022200 | -0.57166500 | 1.24400900 |
| | | | | S | -5.95624700 | -2.56064200 | -0.06780100 |
| | | | | S | 7.08818400 | -1.42373000 | -0.25122500 |

H -3.23434800 0.85405500 -2.86255300
H -1.67058200 1.65778400 -2.92767100
H -1.78029600 -0.03646300 -2.39073300

62

RR-Me_ID2_TS2-square, E(SCF) = -
2563.92044064, E(ZPE) = -2563.450709, E(G)
= -2563.521393 a.u.

C -0.08212700 -0.69385900 1.71097000
H 0.03324100 0.17887400 2.35610100
H -0.25590400 -1.57853300 2.33007700
C 1.13407100 -0.84418300 0.84035900
H 2.03513600 -0.99491300 1.44112700
H 1.02382800 -1.70554500 0.17674900
N 1.25755100 0.37865700 0.01506100
N -1.24146200 -0.45926700 0.81811600
C 2.32324900 0.32107300 -1.04117500
H 2.25871000 1.30826100 -1.51482300
C -2.53349800 -0.12981200 1.48454900
H -2.74204800 -0.96412500 2.16770100
C 3.67507300 0.21620600 -0.38049600
C 4.05410000 1.27938000 0.48948000
C 4.52306000 -0.86290600 -0.57412100
C 5.31510200 1.17741100 1.11998100
C 5.75532300 -0.92797600 0.05559200
H 4.24190900 -1.67380100 -1.23686200
C 6.14326900 0.09794600 0.91216500
H 5.61169900 1.98399700 1.78322500
H 7.10734500 0.04853200 1.40985800
C -3.63348500 -0.08905600 0.45879700
C -3.56453900 0.77426100 -0.65906600
C -4.77259700 -0.85776700 0.66211000
C -4.68023200 0.83307000 -1.51545800
C -5.85390100 -0.78461500 -0.19411200
H -4.82392700 -1.52446300 1.51714300
C -5.80607200 0.07664100 -1.28427700
H -4.62438000 1.50016000 -2.36857400
H -6.65279700 0.14235500 -1.96028300
O 3.26925000 2.29083600 0.69928000
O -2.53393800 1.54434100 -0.93594500
S 6.83912600 -2.33320700 -0.17751900
S -7.32041000 -1.78325800 0.07336400
O -7.46892000 -2.62313200 -1.14974400
O -8.44547300 -0.81871400 0.23687800
O -7.05640900 -2.58425600 1.30039300
O 8.16837400 -1.77342400 -0.56175500
O 6.22571800 -3.15946800 -1.25614700
O 6.88924800 -3.04445900 1.13474300
H -1.39548500 -1.29904000 0.25673800
H 1.54793400 1.14774500 0.63377200
O -0.09336400 3.39867900 -0.22371100
H 0.71772700 3.76889000 -0.64762800
H 1.96831500 2.58235800 1.94029700
O 1.06528700 2.58810100 2.31353500
H 0.52945200 2.96591000 1.59775800
H -0.83539200 3.96070200 -0.46444400
H 2.80599400 3.41293900 -0.47655900
O 2.36056700 4.07831800 -1.06120900
H 2.67146700 3.90387800 -1.95259900
H -0.14409500 2.13329600 -2.37458400
H -0.26154200 1.45133700 -2.68970600
Pd -0.65408700 0.97852300 -0.52731800
C -2.45089300 1.15123000 2.29217000
H -1.71963900 1.08978300 3.09887800
H -2.20278500 2.00361100 1.65496800
H -3.42693400 1.33479100 2.74365000
C 2.01380200 -0.72902400 -2.08106500
H 2.09750800 -1.74684500 -1.69542500
H 1.00059700 -0.60105200 -2.46812100
H 2.70906900 -0.63616500 -2.91654600

62

RR-Me_ID2_TS2-square_P, E(SCF) = -
2563.92841915, E(ZPE) = -2563.458174, E(G)
= -2563.529875 a.u.

C -0.11734500 -0.44651200 1.72641000
H -0.02304100 0.48365500 2.29124500

H -0.29466500 -1.27337500 2.41933100
C 1.12247100 -0.65683700 0.90355400
H 2.00670000 -0.72108100 1.54357100
H 1.05612900 -1.58213100 0.32469800
N 1.24651400 0.48574200 -0.03362000
N -1.26121600 -0.31194400 0.79145000
C 2.35243100 0.35685800 -1.04153800
H 2.37080200 1.34459200 -1.51970300
C -2.56020800 0.09082100 1.40466900
H -2.75494200 -0.63686500 2.20338400
C 3.66764000 0.16948600 -0.32968900
C 4.06670800 1.19084400 0.58024100
C 4.46956000 -0.94461000 -0.52367700
C 5.30580700 1.01754400 1.23924100
C 5.67740000 -1.08278900 0.13971200
H 4.16615000 -1.72792600 -1.20914900
C 6.09164900 -0.09145700 1.02451900
H 5.61944200 1.79320800 1.93088400
H 7.03892300 -0.19642900 1.45452400
C -3.65427700 -0.04000100 0.38127700
C -3.57971700 0.62478400 -0.86396300
C -4.78804800 -0.77724500 0.69972000
C -4.68486100 0.52000200 -1.73984100
C -5.85973700 -0.86400700 -0.16710600
H -4.83922300 -1.29333200 1.65356800
C -5.80483500 -0.20123500 -1.38821300
H -4.62430000 0.09211900 -2.68498900
H -6.64059100 -0.26500400 -2.07804000
O 3.31977800 2.22721600 0.80330800
O -2.56125200 1.35874500 -1.26163700
S 6.73667800 -2.49757300 -0.14358900
S -7.32510700 -1.80865600 0.25732600
O -7.50619900 -2.79446800 -0.84630300
O -8.44132100 -0.82174100 0.32377200
O -7.03699200 -2.44954900 1.57028500
O 8.00038700 -1.95901600 -0.72892700
O 6.00149800 -3.39034400 -1.08416000
O 6.96271500 -3.12403100 1.19234200
H -1.41120000 -1.21232300 0.33068800
H 1.50638800 1.30777300 0.52807900
O 0.20206100 4.00030400 -0.14957900
H 1.09893900 4.22679500 -0.48541300
H 1.94552800 2.58695800 1.97494300
O 1.01340200 2.66395200 2.25423000
H 0.60594900 3.17884200 1.53540600
H -0.31582700 4.80802200 -0.18819500
H 3.10089100 3.48715200 -0.30096100
O 2.80715600 4.25133500 -0.85808900
H 3.08176100 4.04579900 -1.75456100
H -0.12676600 2.42460900 -1.57764300
H -0.14221400 1.84865700 -2.16102400
Pd -0.66531100 0.94836300 -0.70505300
C -2.49768800 1.47932700 2.01329800
H -1.72023400 1.56963000 2.77316200
H -2.32462400 2.23904600 1.24709200
H -3.45691000 1.68793000 2.48950400
C 2.01405200 -0.67601600 -2.09013500
H 1.96398900 -1.68848600 -1.68370400
H 1.04919800 -0.45005000 -2.55011300
H 2.76997700 -0.67226300 -2.87655700

60

RR-Me_ID2_TS2-square_R noH2, E(SCF) = -
2562.76167028, E(ZPE) = -2562.306321, E(G)
= -2562.376136 a.u.

C -0.09661200 -0.80307300 1.83225400
H -0.00652000 0.00366600 2.56196600
H -0.28331200 -1.73775400 2.36893900
C 1.14094400 -0.87931700 0.98138000
H 2.03276700 -1.06416300 1.58464800
H 1.04623300 -1.69868100 0.26601600
N 1.26641400 0.38964500 0.22603900
N -1.23310200 -0.49004400 0.93110000
C 2.24063600 0.34079900 -0.92036400
H 2.13682400 1.32631200 -1.38314200
C -2.55418600 -0.27611000 1.59371700
H -2.77009500 -1.20141500 2.14414400

O -7.12195500 -2.08774900 1.87726400
O -7.52423500 -2.85607800 -0.45106300
O -8.46555800 -0.69687300 0.31451700
O 7.22570600 -2.81818900 1.15455000
O 8.39630200 -1.34280900 -0.45202500
O 6.61605500 -2.88096900 -1.25296700
H -1.43129500 -1.32780800 0.29803900
H 1.51348800 1.14649600 0.43640800
O -0.69712700 3.90871800 -1.63061400
H -0.03666700 3.97783000 -0.91175300
H 1.91338300 2.21375500 2.35436900
O 1.03622500 2.41117300 2.73567400
H 0.71751700 3.08722400 2.12059600
H -1.52956100 3.69611900 -1.19763600
H 2.04865800 3.39185400 0.33575600
O 1.28870300 4.01710400 0.30270100
H 1.66264300 4.89253000 0.43085500
H -0.19674600 2.04324500 -2.04980300
H -0.01460200 1.33260000 -2.42607700
Pd -0.61358700 0.70989800 -0.87903000
C -2.35783400 1.50161200 1.83266600
H -3.29751700 1.79022400 2.30611800
H -1.56216800 1.60899800 2.57104300
H -2.16518500 2.19520800 1.01009500
C 2.24289000 -0.85890200 -2.10318700
H 2.30411100 -1.85432600 -1.65773100
H 1.26877400 -0.76327400 -2.58705600
H 3.00815600 -0.79428300 -2.87746600

60

RR-Me_ID2_TS2_trigo-square_R_nOH2, E(SCF) =
-2562.76833525, E(ZPE) = -2562.312718, E(G)
= -2562.382390 a.u.

C -0.05003000 -0.94380900 1.50383300
H 0.06214300 -0.21442700 2.30667000
H -0.22177300 -1.93069500 1.94184100
C 1.17467300 -0.92118900 0.62943800
H 2.07351800 -1.16106000 1.20538200
H 1.08292300 -1.65265400 -0.17727000
N 1.28156400 0.43214300 0.03729700
N -1.20888500 -0.54535600 0.66762700
C 2.37991500 0.60176800 -0.97130600
H 2.30981500 1.65610900 -1.25619000
C -2.48081700 -0.27920100 1.39850100
H -2.68169400 -1.17612200 1.99893600
C 3.71975700 0.40427800 -0.31337200
C 4.13045500 1.38290700 0.63755300
C 4.53104700 -0.68723500 -0.58563500
C 5.39344200 1.19518700 1.24737400
C 5.75605600 -0.84591400 0.03985800
H 4.21809400 -1.43815900 -1.30299400
C 6.18466800 0.10737100 0.95901200
H 5.71948100 1.94130800 1.96532200
H 7.14716900 -0.01091900 1.44835700
C -3.61137200 -0.12264700 0.41538800
C -3.56214900 0.811102300 -0.64724000
C -4.77086600 -0.86103300 0.62338500
C -4.71829500 0.96449900 -1.43875500
C -5.89003300 -0.69288400 -0.16773800
H -4.80755300 -1.58008800 1.43602700
C -5.85907700 0.23343000 -1.20447800
H -4.67692700 1.68447900 -2.24887000
H -6.73345300 0.37538900 -1.83188300
O 3.38498000 2.39743400 0.94837900
O -2.52243500 1.55998600 -0.93944100
S 6.81048300 -2.24700300 -0.31885400
S -7.37148200 -1.66676900 0.10077000
O -7.12238900 -2.46643000 1.33221700
O -7.53256100 -2.51182400 -1.11798900
O -8.48271000 -0.68514100 0.25774000
O 7.05492400 -2.92707400 0.98775600
O 8.06709000 -1.68783200 -0.90032400
O 6.06004600 -3.10085500 -1.28341300
H -1.39859500 -1.30215300 0.00715200
H 1.48235900 1.07439200 0.81340100
O -0.07150100 2.62973600 -1.72480800
H 0.54545900 3.23945400 -1.23187900

H 2.23345500 2.18998300 2.25390600
O 1.43401800 1.86898800 2.72901300
H 0.82793500 2.61449100 2.73434300
H -0.88099600 3.11843200 -1.91705100
H 2.35362000 3.40660200 0.11782600
O 1.65541800 3.99623900 -0.27238200
H 2.11487300 4.75264100 -0.64382600
Pd -0.63475700 1.01532300 -0.49642100
C -2.36612200 0.91229900 2.33150700
H -3.31175700 1.02197800 2.86482100
H -1.57911400 0.78980500 3.07767400
H -2.17977100 1.83380600 1.77542600
C 2.11144300 -0.22794000 -2.20506800
H 2.13185400 -1.30210000 -2.01195500
H 1.13234900 0.02219400 -2.61973200
H 2.86741200 -0.01629200 -2.96274100

62

RR-Me_ID2_TS2_trigo-square_R, E(SCF) = -
2563.94250140, E(ZPE) = -2563.471482, E(G)
= -2563.541972 a.u.

C -0.03999600 -0.89150400 1.54649900
H 0.08132600 -0.14433600 2.33177300
H -0.21271400 -1.86772300 2.00722400
C 1.17605100 -0.89369600 0.65962000
H 2.07893700 -1.13505600 1.22844200
H 1.06679900 -1.36528100 -0.13667200
N 1.28924100 0.44991600 0.04737800
N -1.20213500 -0.50778500 0.70818500
C 2.38606800 0.59957900 -0.96648800
H 2.32144400 1.65023700 -1.26582400
C -2.47297800 -0.22526000 1.43467200
H -2.67293700 -1.10866200 2.05497700
C 3.72561500 0.40363600 -0.30784400
C 4.14582100 1.39581800 0.62475000
C 4.52779900 -0.69874300 -0.56278600
C 5.40802700 1.20806800 1.23632000
C 5.75276500 -0.85608100 0.06303800
H 4.20717000 -1.45930000 -1.26653800
C 6.19017700 0.10933100 0.96531300
H 5.74126800 1.96378900 1.94081100
H 7.15266700 -0.00802200 1.45490800
C -3.60170800 -0.09455100 0.44526500
C -3.55166700 0.81221000 -0.64039600
C -4.75803000 -0.83511300 0.66395900
C -4.70128200 0.93457200 -1.44630800
C -5.87188000 -0.69553200 -0.13966200
H -4.79584600 -1.53360200 1.49420900
C -5.83915500 0.20240800 -1.20088900
H -4.65774000 1.63176200 -2.27596600
H -6.70929400 0.32020900 -1.83907000
O 3.40959700 2.42217800 0.91830500
O -2.51515500 1.56227300 -0.94361500
S 6.79948600 -2.26715000 -0.27866000
S -7.35204600 -1.66636000 0.14743700
O -7.09385000 -2.45809600 1.38202000
O -7.52319300 -2.51830200 -1.06491000
O -8.46056200 -0.68215800 0.30706800
O 7.04389400 -2.93100600 1.03618200
O 8.05706600 -1.72077000 -0.86999000
O 6.04336400 -3.13029000 -1.23038800
H -1.39518800 -1.28135600 0.06806400
H 1.49420600 1.10287000 0.81354700
O -0.05895400 2.61696800 -1.74859100
H 0.56314300 3.23299400 -1.26995400
H 2.25729200 2.24353300 2.22545400
O 1.45608100 1.93299200 2.70489800
H 0.85518500 2.68271500 2.70377800
H -0.86474100 3.10709100 -1.95225200
H 2.38001700 3.42004300 0.06839700
O 1.68355900 4.00389600 -0.33335100
H 2.14635100 4.74645800 -0.72786700
H -1.42165200 -0.94085800 -2.30167600
H -1.34430800 -1.61368800 -2.62711000
Pd -0.62642500 1.02968700 -0.48989900
C -2.35818600 0.98633800 2.34081000
H -3.30292700 1.10618800 2.87349900

H -1.56946500 0.88000700 3.08775200
 H -2.17415300 1.89636800 1.76561100
 C 2.11002700 -0.24511300 -2.18836600
 H 2.11004100 -1.31647100 -1.97784100
 H 1.13804400 0.01518700 -2.61320500
 H 2.87425200 -0.05915900 -2.94452900

62

RR-Me_ID2_TS2_trigo-square, E(SCF) = -
 2563.91756800, E(ZPE) = -2563.447679, E(G)
 = -2563.519095 a.u.

C -0.12461600 -0.37370700 1.73911700
 H -0.01594600 0.60804400 2.20607400
 H -0.31975300 -1.12222700 2.51178900
 C 1.11040800 -0.69389400 0.94156200
 H 1.99570300 -0.72295400 1.58407500
 H 1.01490000 -1.66613800 0.45050200
 N 1.25354200 0.35499900 -0.09192900
 N -1.26380900 -0.31241300 0.79269200
 C 2.39687200 0.16312500 -1.04215400
 H 2.36374300 1.07877100 -1.65075300
 C -2.54878500 0.20590600 1.34120200
 H -2.76300700 -0.40271100 2.23016700
 C 3.71148100 0.14983100 -0.29386100
 C 3.98207000 1.21627000 0.61126900
 C 4.65525500 -0.85014100 -0.48017100
 C 5.23008000 1.20577000 1.27423600
 C 5.87194100 -0.82672400 0.18104800
 H 4.46940400 -1.67018500 -1.16495600
 C 6.15298800 0.20627200 1.06836700
 H 5.43636100 2.01787100 1.96431900
 H 7.10443600 0.22676400 1.59173200
 C -3.65135500 -0.03011100 0.34528000
 C -3.56097900 0.44084400 -0.98519600
 C -4.81333400 -0.66114400 0.77220400
 C -4.67789000 0.25699800 -1.82387100
 C -5.89608700 -0.82644500 -0.06870400
 H -4.87985300 -1.02642600 1.79256500
 C -5.82505800 -0.35421100 -1.37448500
 H -4.60449900 0.62099300 -2.84284300
 H -6.67154900 -0.47917200 -2.04232900
 O 3.11149500 2.15181700 0.83591000
 O -2.51564000 1.06028300 -1.48878900
 S 7.07164200 -2.13644900 -0.05347800
 S -7.39346700 -1.64049000 0.48905600
 O -7.15525300 -2.01395700 1.91073900
 O -7.57149200 -2.82344600 -0.40150200
 O -8.48490900 -0.63843500 0.32297000
 O 7.15160300 -2.86571200 1.24621700
 O 8.35910600 -1.46249600 -0.39769100
 O 6.54947300 -2.98516000 -1.16097900
 H -1.44535100 -1.25549600 0.44280300
 H 1.50247600 1.22873400 0.39885200
 O -0.21664600 3.19004400 -1.53698100
 H 0.48020500 3.63894900 -1.01005600
 H 1.83687000 2.47501800 2.09911400
 O 0.94433400 2.74325200 2.39188600
 H 0.74980400 3.46791500 1.78393500
 H -1.05200000 3.57883300 -1.26213800
 H 2.44218900 3.55855500 0.17013300
 O 1.77093700 4.25781000 -0.01310400
 H 2.24782500 5.05192900 -0.26272400
 H -0.14713800 1.41818900 -2.82185200
 H -0.06605400 0.66569800 -2.93514900
 Pd -0.63789700 0.70991400 -0.86923000
 C -2.44977900 1.66007100 1.75990500
 H -3.39608600 1.94947700 2.21973100
 H -1.65395300 1.83583300 2.48489500
 H -2.28032400 2.30798500 0.89659700
 C 2.16355200 -1.02920400 -1.94094900
 H 2.26467600 -1.97706600 -1.40775300
 H 1.16273700 -0.99701000 -2.37520300
 H 2.88384400 -1.03113400 -2.75973300

62

RR-Me_ID2_TS3-square_P, E(SCF) = -
 2563.95704707, E(ZPE) = -2563.483487, E(G)
 = -2563.556630 a.u.

C 0.01847400 -0.73149900 1.49479400
 H 0.10761500 0.06783600 2.23331400
 H -0.05358800 -1.68308600 2.03253800
 C 1.23462200 -0.71084900 0.60078300
 H 2.13716600 -0.91198200 1.18686200
 H 1.15657100 -1.48357200 -0.16926200
 N 1.32506900 0.61484800 -0.06058500
 N -1.17500800 -0.47995200 0.67325000
 C 2.43967100 0.75057300 -1.05285800
 H 2.43201300 1.81394800 -1.30809700
 C -2.43750000 -0.18642700 1.38644300
 H -2.64889600 -1.02669600 2.06095600
 C 3.76698300 0.40718300 -0.41366400
 C 4.40135200 1.30746900 0.45131200
 C 4.35696400 -0.84084300 -0.60072500
 C 5.55996900 0.93550200 1.12944200
 C 5.51128200 -1.20110400 0.06400600
 H 3.90521900 -1.56162100 -1.27270600
 C 6.11174200 -0.31306100 0.94530900
 H 6.01719600 1.65766300 1.79589300
 H 7.01606400 -0.59502600 1.47381100
 C -3.56752000 -0.11623100 0.38699100
 C -3.55309800 0.75096000 -0.73957600
 C -4.69764600 -0.88611200 -0.64062900
 C -4.72178800 0.78774600 -1.53532500
 C -5.82250700 -0.83010600 -0.15889700
 H -4.70252800 -1.54918400 1.50066600
 C -5.82988200 0.02458300 -1.25596500
 H -4.71218400 1.45211700 -2.39333300
 H -6.70648400 0.08196500 -1.89410400
 O 3.92958500 2.55049800 0.72195500
 O -2.56934800 1.53930200 -1.09650800
 S 6.25029000 -2.82443000 -0.17860700
 S -7.26299100 -1.83731800 0.18188100
 O -7.45124400 -2.70597600 -1.01722600
 O -8.39728400 -0.88575200 0.36844100
 O -6.94930500 -2.61339000 1.41467800
 O 7.63839300 -2.56258700 -0.65068000
 O 5.40487200 -3.51066400 -1.19229200
 O 6.21510700 -3.48216400 1.15761000
 H -1.34245700 -1.29771000 0.08816500
 H 1.48237800 1.29417700 0.69681500
 O 0.07271600 4.15410100 0.46030100
 H 1.64049600 4.35045800 -0.45305000
 H 2.41277300 2.69362200 2.05447600
 O 1.49304200 2.46920700 2.25800500
 H 0.96303800 3.16559800 1.83351500
 H -0.58551200 4.84573600 0.57510900
 H 3.43982300 2.98275700 -0.01517900
 O 2.52753500 4.22645300 -0.84336100
 H 2.40589200 4.26716900 -1.79520900
 H -0.34775500 3.45503900 -0.07910800
 H -0.15168100 2.27596000 -1.61968100
 Pd -0.61967300 1.11002600 -0.66051900
 C -2.34436200 1.07781000 2.22468300
 H -1.59752200 0.99967800 3.01711700
 H -2.10627000 1.94631800 1.60543800
 H -3.31084200 1.25144600 2.70136400
 C 2.13097200 -0.01497800 -2.31992900
 H 1.99644600 -1.08482300 -2.14903600
 H 1.20986600 0.37124400 -2.75986800
 H 2.94200000 0.10756000 -3.03967300

62

RR-Me_ID2_TS3_trigo-square_P, E(SCF) = -
 2563.95780047, E(ZPE) = -2563.483320, E(G)
 = -2563.555662 a.u.

C -0.01415100 -0.57357300 1.55907400
 H 0.05843500 0.26719600 2.25142400
 H -0.08571900 -1.49133100 2.15297400
 C 1.21482200 -0.60082900 0.68360400
 H 2.10959000 -0.74983300 1.29654600
 H 1.15702200 -1.42719200 -0.03001000
 N 1.30850900 0.67424400 -0.07362200

Pd 0.21136500 0.46144500 -0.62646700
 H 2.90203800 -2.92050700 1.40080800
 H -2.73952400 -2.86884400 -1.07427600
 C -2.20434100 2.31025000 -1.96224600
 H -3.17154200 2.41533000 -2.45634900
 H -1.72512000 3.29235900 -1.95986200
 H -1.59201200 1.62276400 -2.55112900
 C 1.89913900 2.03392400 2.39255000
 H 1.03862100 1.40559700 2.60646200
 H 2.65288200 1.82222900 3.15330500
 H 1.62280000 3.08458200 2.49813900
 H -1.21716500 3.83675800 0.31375400

59
 RR-Me_EI_D1_TS1_R, E(SCF) = -2487.50198035,
 E(ZPE) = -2487.056710, E(G) = -2487.125343
 a.u.

C -0.65927700 3.11590600 0.58939400
 H -0.38850200 3.24040100 1.63851800
 C 0.57997000 3.13427600 -0.27834700
 H 0.31612000 3.32432400 -1.31892100
 H 1.24598300 3.94230600 0.03776400
 N 1.31087500 1.83215900 -0.25868100
 N -1.40190600 1.82294400 0.50418800
 C 2.53467900 1.72437800 0.57400200
 H 3.15975100 2.59262600 0.32558900
 C -2.57716300 1.73536500 -0.39621000
 C 3.30653300 0.48808100 0.17071800
 C 2.71954900 -0.77033600 -0.09507000
 C 4.69327400 0.61040800 0.11573800
 C 3.57828400 -1.84018800 -0.42017600
 C 5.51247900 -0.45683300 -0.18409700
 H 5.14759500 1.57585000 0.31876100
 C 4.94393600 -1.69541800 -0.45891800
 H 5.57515800 -2.54257300 -0.70739200
 C -3.36147400 0.47919000 -0.08530000
 C -2.78583900 -0.77666800 0.22403700
 C -4.74810000 0.58272500 -0.17664400
 C -3.66328800 -1.86533400 0.42044400
 C -5.58125800 -0.49749000 0.01822600
 H -5.19152300 1.54703000 -0.40805600
 C -5.02634200 -1.73758400 0.31738400
 H -5.66798500 -2.59776800 0.47936800
 O 1.42605600 -1.05039400 -0.05863600
 O -1.49957700 -1.04049200 0.35709500
 S 7.29582600 -0.27324700 -0.25788000
 S -7.36221600 -0.33846100 -0.11786100
 O -7.75998200 -1.18739100 -1.27777500
 O -7.63274400 1.10922200 -0.33817600
 O -7.91509800 -0.84594200 1.17033400
 O 7.84434100 -1.27927300 0.69550100
 O 7.58443500 1.13081100 0.14466900
 O 7.67586500 -0.56491300 -1.66993300
 H 0.55327400 -2.57593700 -0.95582100
 H 1.00554500 -0.10599300 -3.11486700
 H 1.19297600 -0.60833700 -2.58983300
 O -0.23299600 -3.14618700 -0.95285500
 H -0.87476500 -2.54863600 -0.52421000
 H 1.19407900 -2.42041800 1.35313200
 O 0.94191300 -3.28951100 1.70335800
 H 0.45349900 -3.65016700 0.94858300
 H 1.61001800 1.64772100 -1.21574200
 H -1.75373400 1.62399600 1.43961200
 H -3.22126300 2.59100700 -0.15188400
 Pd -0.04011000 0.35484000 0.13906800
 H 3.11803300 -2.80144600 -0.62870400
 H -3.21399600 -2.82332600 0.66284200
 C -2.19333300 -1.82938200 -1.85936600
 H -3.09915000 1.77119000 -2.46496400
 H -1.70108800 2.77500800 -2.09643500
 H -1.53585100 1.00292200 -2.14631500
 C 2.22620700 1.76659600 2.05653400
 H 1.60639200 0.91598700 2.35477300
 H 3.16412000 1.71990200 2.61253000
 H 1.71889700 2.69091200 2.34255600
 H -1.31980100 3.94619700 0.32236400

59
 RR-Me_EI_D1_TS1, E(SCF) = -2487.47613519,
 E(ZPE) = -2487.031210, E(G) = -2487.097454
 a.u.

C -0.55917000 2.96412700 0.60161000
 H -0.38230300 2.97213600 1.67699200
 C 0.73561500 3.08506600 -0.16928400
 H 0.52466600 3.35134200 -1.20665200
 H 1.36829800 3.87228000 0.25411100
 N 1.48265200 1.79354700 -0.21586100
 N -1.26826200 1.69187100 0.28106200
 C 2.49931200 1.56469300 0.86944000
 H 3.18167800 2.42303100 0.79707900
 C -2.53905300 1.79678700 -0.47617500
 C 3.30959600 0.33373500 0.569315800
 C 2.72535100 -0.96253300 0.55393700
 C 4.66810100 0.48052800 0.31552000
 C 3.58572000 -2.05592700 0.30409900
 C 5.48322800 -0.61002000 0.07241200
 H 5.10976200 1.47290500 0.31483700
 C 4.93183900 -1.88647700 0.07210400
 H 5.56442000 -2.74787100 -0.12003800
 C -3.28877200 0.48978800 -0.39973000
 C -2.68821200 -0.76639400 -0.64278300
 C -4.65056000 0.54547300 -0.11751500
 C -3.50691600 -1.91160300 -0.58162400
 C -5.43472400 -0.58885200 -0.07817500
 H -5.11511200 1.50801300 0.07497500
 C -4.85237100 -1.82847100 -0.31287700
 H -5.45657200 -2.72924900 -0.27616400
 O 1.45015800 -1.15814800 0.72634500
 O -1.41836600 -0.96303300 -0.94060500
 S 7.23445400 -0.40883900 -0.24381800
 S -7.18902200 -0.49946800 0.28681200
 O -7.88092400 -1.04702600 -0.91502600
 O -7.48770500 0.93934100 0.52628800
 O -7.39522200 -1.34846700 1.49495800
 O 7.93831900 -1.15746700 0.83798300
 O 7.49775300 1.05692300 -0.20003500
 O 7.47958200 -1.00335400 -1.59023500
 H 0.64854600 -2.69977400 0.20915700
 H 1.11419700 -0.46894500 -2.28622700
 H 1.32463000 -0.98719800 -1.76627900
 O 0.00378200 -3.30365700 -0.21029500
 H -0.62022400 -2.66710800 -0.59548200
 H -0.03043400 -0.90875600 1.83615000
 O -0.85906100 -0.64984700 2.28547600
 H -1.48318600 -1.34748300 2.06441900
 H 2.02844900 1.80831600 -1.07704400
 H -1.46796600 1.19806800 1.15806300
 H -3.14650600 2.54776200 0.04742500
 Pd 0.05422600 0.34455800 -0.54410700
 H 3.14386400 -3.04785200 0.29353000
 H -3.03931200 -2.87425600 -0.76053300
 C -2.31092200 2.27314800 -1.89527500
 H -3.27676700 2.39624800 -2.38811700
 H -1.79841400 3.23811600 -1.92326600
 H -1.72229900 1.54744200 -2.46288700
 C 1.90264400 1.57223100 2.26145500
 H 1.12230000 0.82199100 2.37975400
 H 2.69721200 1.34445100 2.97383100
 H 1.50447900 2.55220900 2.53008600
 H -1.20624200 3.81548400 0.37628200

59
 RR-Me_EI_D1_TS2_P, E(SCF) = -2487.50769484,
 E(ZPE) = -2487.059178, E(G) = -2487.128350
 a.u.

C 0.44217400 -2.71662100 0.96244800
 H 0.26872500 -2.60705000 2.03252200
 C -0.87309100 -2.79419900 0.20814800
 H -0.70048400 -3.19781700 -0.79234600
 H -1.56340900 -3.47050200 0.72489100
 N -1.51927200 -1.46397300 0.00629400
 N 1.27844600 -1.58235500 0.51072200
 C -2.38878300 -1.00276500 1.13920800
 H -2.97823200 -1.88393100 1.42584000

H -1.64356400 1.45728700 1.38672000
H 1.64351600 1.45711600 -1.38669300
H 3.21304700 2.38565600 0.10683100
Pd -0.00001700 0.17328000 0.00008300
H -3.10004500 -3.02545600 0.68573700
H 3.10004000 -3.02555400 -0.68547500
C 2.26964000 1.68296000 1.88254700
H 3.20917200 1.62343000 2.43451000
H 1.80915200 2.64372500 2.12412400
H 1.61622700 0.87838700 2.23196600
C -2.26957200 1.68275900 -1.88256800
H -1.61633200 0.87799700 -2.23187700
H -3.20911300 1.62335300 -2.43452600
H -1.80887900 2.64339300 -2.12426200
H 1.27700800 3.76266900 -0.18384300

51

RR-Me, E(SCF) = -2333.45509067, E(ZPE) = -
2333.075857, E(G) = -2333.136568 a.u.

N -1.37819100 1.67181300 -0.14976400
N 1.37260600 1.67523100 0.14505500
C -2.50270500 1.34743600 -1.06819300
H -3.15288000 2.23227700 -1.10085800
C 2.50026200 1.35317800 1.06051800
C -3.30138800 0.21004300 -0.48558900
C -2.70238300 -1.02109500 -0.10978600
C -4.67999300 0.35917900 -0.39243900
C -3.56485400 -2.05185500 0.32394700
C -5.49801400 -0.66809800 0.03673600
H -5.13246900 1.30391400 -0.67975400
C -4.92731400 -1.88383500 0.39778900
H -3.10780800 -2.99486300 0.60503000
H -5.55883600 -2.69943200 0.73584600
C 3.29942900 0.21778000 0.47496200
C 2.70254700 -1.01530300 0.10433400
C 4.67703900 0.37260400 0.37032100
C 3.56594200 -2.04359900 -0.33506200
C 5.49460000 -0.64863400 -0.07156500
H 5.12862500 1.32006300 0.64874500
C 4.92681400 -1.87042000 -0.41865300
H 3.11024000 -2.98800900 -0.61359200
H 5.55734600 -2.68279000 -0.76732300
O -1.42004400 -1.28566700 -0.15385500
O 1.42102800 -1.28317700 0.15414500
S -7.26378600 -0.42952000 0.21906500
S 7.26772500 -0.43223600 -0.20431000
O 7.61014500 -0.71989300 -1.62755300
O 7.87422100 -1.42315800 0.73196100
O 7.54421600 0.97893500 0.18517800
O -7.59195400 0.82083400 -0.52175400
O -7.51472500 -0.31331100 1.68600700
O -7.90424900 -1.64138300 -0.36821200
H -1.77884100 1.75474400 0.78624500
H 1.77088300 1.75955700 -0.79185300
H 3.14866900 2.23937100 1.09154500
Pd -0.00097500 0.15905700 -0.00107900
C 0.61416900 2.91606500 0.43146000
C -0.62270100 2.91502800 -0.43413100
H -1.24339000 3.79576700 -0.24862400
H -0.34337600 2.91452700 -1.48935400
H 0.33505400 2.91337300 1.48673500
H 1.23255200 3.79866700 0.24698900
C -2.02109300 1.04623800 -2.47517500
H -2.89101800 0.83989300 -3.10086100
H -1.48581300 1.88465400 -2.92403500
H -1.37203500 0.16738300 -2.48843600
C 2.02269100 1.05078600 2.46859500
H 2.89437100 0.84478000 3.09192800
H 1.48784600 1.88848100 2.91934100
H 1.37440400 0.17139800 2.48306500

59

RR-NMe_hs_D1_TS1_P, E(SCF) = -
2487.46390593, E(ZPE) = -2487.018781, E(G)
= -2487.085125 a.u.

C 0.29449600 -1.06582100 -2.68473300
H -0.14268200 -1.98458100 -3.08244000

H 0.24178200 -0.30504500 -3.47113600
H 1.71358500 -1.28206800 -2.23136700
C 2.33730200 -1.65758700 -3.04914400
H 2.15505400 -0.34595000 -1.89107300
N 1.74552000 -2.24339000 -1.09371800
N -0.53582300 -0.63900000 -1.52433000
C 2.98816800 -2.06941300 -0.25719200
H 2.94142100 -2.85528800 0.50097300
C -1.98343700 -0.82821300 -1.81243400
H -2.11215200 -1.88992900 -2.04877200
C 3.18147500 -0.73365200 0.37475800
C 2.53414400 -0.40425700 1.60222900
C 4.08347300 0.15707000 -0.19984000
C 2.87270800 0.85145600 2.17703000
C 4.36436700 1.38132700 0.37328100
H 4.58830400 -0.11426600 -1.12362900
C 3.75341600 1.72006000 1.57911100
H 3.98327000 2.67136200 2.05021300
C -2.87697200 -0.39666800 -0.69609200
C -2.71589700 -0.89459800 0.61605800
C -3.91173800 0.49158000 -0.96354200
C -3.64065500 -0.49358000 1.59741200
C -4.80865800 0.87223300 0.01426200
H -4.02891400 0.88907100 -1.96693100
C -4.66894900 0.37116500 1.30378300
H -5.36832100 0.66739300 2.07927500
O 1.67481600 -1.18012000 -2.17424400
O -1.76403700 -1.73048600 0.97893300
S 5.52634800 2.51776700 -0.37467800
S -6.14379800 2.01486100 -0.34522800
O -5.92245800 3.19384200 0.54009200
O -7.40111600 1.28606800 -0.01224800
O -6.02561400 2.34323100 -1.79282000
O 6.00733800 1.85673300 -1.62083000
O 6.61116600 2.72300900 0.62944600
O 4.76539700 3.77371100 -0.64173700
H 0.31546300 -3.28229700 1.10859200
H 0.76532000 -2.65783100 1.42449900
H 3.83350700 -2.29583100 -0.92020100
H -2.22413800 -0.25276700 -2.71533400
Pd -0.01770300 -1.94167200 -0.02075900
H 2.41622300 1.10174800 3.13043200
H -3.50891700 -0.88007900 2.60271100
H 0.24580400 -1.58069900 3.38046200
O -0.64132800 -1.87538600 3.64447700
H -1.14797500 -1.82547300 2.81610700
O 0.18405100 0.20280400 2.16683100
H -0.32271400 1.03178700 2.11482000
H 0.35702300 1.69585900 1.96495800
C 1.72951700 -3.62978600 -1.60718100
H 1.72346800 -4.32919100 -0.77256600
H 0.84269600 -3.79949000 -2.21580000
H 2.62319000 -3.80466200 -2.21527300
C -0.25695000 0.76676500 -1.16330400
H 0.80848100 0.90131500 -0.97554400
H -0.57063200 1.41544700 -1.98860200
H -0.79712600 1.02686000 -0.25414000

59

RR-NMe_hs_D1_TS1_R, E(SCF) = -
2487.48629441, E(ZPE) = -2487.042245, E(G)
= -2487.110814 a.u.

C -0.26429400 -2.63323100 -1.82621800
H -0.75237900 -3.51843800 -1.41522700
H -0.47585000 -2.62109500 -2.90023200
C 1.22435200 -2.66825400 -1.57104900
H 1.66807500 -3.57569800 -1.99752400
H 1.72476400 -1.80886000 -2.02544400
N 1.49045700 -2.61247600 -0.10999800
N -0.86788400 -1.43359500 -1.17949600
C 2.92550700 -2.30096100 0.18209300
H 3.15294000 -2.80523700 1.12487300
C -2.28783800 -1.66408500 -0.82936900
H -2.30148300 -2.52131400 -0.14644200
C 3.24479200 -0.85112900 0.33823400
C 2.58861500 -0.12640600 1.36053100
C 4.24687500 -0.24917300 -0.40316400

O 6.25209800 -3.47349600 1.12154600
H -2.24337000 0.45189600 1.86729400
H 1.94483700 0.02054100 -1.71695000
O 0.07231100 4.56383400 0.13436000
H 1.65645500 4.36287500 -0.70799800
H 4.62310300 3.22791300 1.77240900
O 4.79571400 3.38456300 2.71393700
H 3.94361800 3.63695100 3.07620400
H 0.01744800 4.67454900 1.08765700
H 3.60024900 2.95830200 -0.50839000
O 2.48826000 4.12802200 -1.16853000
H 2.28714700 4.15553700 -2.10715100
H -0.34544700 3.70562200 -0.05568800
H -0.17188700 2.34545900 -1.26780000
Pd -0.66912100 1.05745900 -0.51721600
C 1.61140400 1.48974700 1.28928500
H 2.55261200 1.18634500 1.76217400
H 1.70459800 2.50724900 0.91332600
O 0.81995600 1.47403400 2.03697700
C -1.52506900 -1.88460200 -0.41839500
H -1.85297500 -2.76863100 0.14510900
H -2.29735400 -1.61984100 -1.13923700
H -0.61415700 -2.12746600 -0.96461400

62

RR-NMe_ID2_TS3, E(SCF) = -2563.88629314,
E(ZPE) = -2563.419007, E(G) = -2563.490927
a.u.

C -0.16730300 -1.11239300 1.37918100
H -0.24200600 -0.46907400 2.25806500
H -0.26859600 -2.14753100 1.72499700
C 1.14392400 -0.91160500 0.66847500
H 1.98350200 -1.14790900 1.33012400
H 1.21424800 -1.57579500 -0.19482800
N 1.25873900 0.48738400 0.17052300
N -1.28794900 -0.77167300 0.46771600
C 2.29139100 0.59013500 -0.92333300
H 2.22455600 1.61044900 -1.30359700
C -2.51027500 -0.43741300 1.23692000
H -2.74817800 -1.28323300 1.89595800
C 3.69369100 0.28802000 -0.50662700
C 4.53921700 1.34802400 -0.06590400
C 4.18387900 -1.01081300 -0.58149700
C 5.84989500 0.98407600 0.34388700
C 5.46963900 -1.32557100 -0.18551600
H 3.55127600 -1.80630900 -0.96512100
C 6.30097200 -0.31226400 0.28966200
H 6.49944500 1.77996300 0.69663500
H 7.31240600 -0.54967700 0.60708600
C -3.69484800 -0.13149900 0.37517600
C -3.63472300 0.82085800 -0.67359600
C -4.89091000 -0.78092200 0.63967700
C -4.82252200 1.08346200 -1.38204300
C -6.04508400 -0.50578200 -0.07464500
H -4.91978500 -1.52099700 1.43526700
C -6.00533800 0.43920700 -1.08854200
H -4.77479000 1.81452100 -2.18190400
H -6.90660000 0.65642300 -1.65084400
O 4.16025700 2.57860400 -0.02000300
O -2.56070000 1.48398300 -1.03014200
S 6.08035900 -3.00455900 -0.25915200
S -7.56248000 -1.36098700 0.34900900
O -8.57161000 -0.92802700 -0.65720600
O -7.90278900 -0.92891100 1.73592800
O -7.25143500 -2.81764800 0.27309800
O 7.32772600 -2.96084700 -1.07763900
O 4.99962900 -3.81248900 -0.89322700
O 6.35287500 -3.41181900 1.15183300
H -2.24513900 0.41531700 1.87309500
H 1.95268400 -0.08772500 -1.71123600
O -0.05645300 4.15301600 -0.32958300
H 0.92963900 4.37151400 -0.36541200
H 4.38722300 3.26127100 1.57988400
O 4.44360200 3.59530200 2.50250800
H 3.54195300 3.83541100 2.72596200
H -0.35081000 4.17869000 0.58890200
H 3.09291100 3.76365800 -0.42514800

O 2.49758900 4.55434600 -0.50733300
H 2.80410100 5.05486600 -1.26673500
H -0.19124500 2.99655000 -0.81350200
H -0.14564900 2.23245200 -1.45890800
Pd -0.67134600 0.97151100 -0.51371900
C 1.58030400 1.39588000 1.29012700
H 2.48658100 1.06067100 1.80476000
H 1.75816400 2.39581900 0.90208900
H 0.75352000 1.42560600 1.99863000
C -1.54423500 -1.87292600 -0.47597100
H -1.89080800 -2.75647400 0.07284200
H -2.30983600 -1.57508100 -1.18991500
H -0.63399900 -2.11906700 -1.01992200

59

RR-NMe_EI_D1_TS1_P, E(SCF) = -
2487.46092414, E(ZPE) = -2487.015411, E(G)
= -2487.082997 a.u.

C 0.41984300 -1.53348000 2.32261000
H -0.16498700 -0.93491600 3.02289300
C -0.47565700 -2.29818000 1.39487400
H 0.11000200 -2.94015500 0.73334900
H -1.15401700 -2.94787600 1.95917100
N -1.26827400 -1.37417200 0.53229400
N 1.28884700 -0.58986400 1.56210500
C -2.40686100 -0.76872300 1.31762800
H -2.90567900 -1.620632500 1.82262400
C 2.46830300 -1.26200400 0.97285700
H 2.10351400 -2.10661100 0.37876500
C -3.40644700 -0.00871400 0.51155300
C -3.12765200 1.32347500 0.09695100
C -4.62962000 -0.59576700 0.20783200
C -4.14008500 1.98792500 -0.64089700
C -5.59570400 0.08168900 -0.51049400
H -4.83503100 -1.61023100 0.53835000
C -5.33930800 1.38504700 -0.93485600
H -6.09407800 1.92308200 -1.50121300
C 3.36036300 -0.37350600 0.14658100
C 2.92596700 0.76111200 -0.57103300
C 4.70108400 -0.74442700 0.07284600
C 3.87102800 1.45930500 -1.34627300
C 5.60889800 -0.04645300 -0.69405600
H 5.04570300 -1.60852800 0.63238700
C 5.18790600 1.07272400 -1.40423900
H 5.89404500 1.63407900 -2.00745200
O -2.00062900 1.89327100 0.36420500
O 1.69789200 1.25437600 -0.54448600
S -7.17769900 -0.66598400 -0.88334200
S 7.33758800 -0.52865200 -0.75410800
O 8.09531300 0.61624900 -0.17272400
O 7.64897600 -0.74166900 -2.19603800
O 7.44725700 -1.77197500 0.05721000
O -7.31720600 -0.62374600 -2.36892900
O -8.20528900 0.17542000 -0.20158400
O -7.11981800 -2.05543900 -0.34669300
H -0.63670700 3.11160300 0.09651200
H -0.55127800 0.37386100 -1.67012000
H -0.94849100 0.88514900 -1.17062700
O 0.21846000 3.56186700 0.22995400
H 0.87404300 2.90270600 -0.05178000
H -1.95627500 -0.13213600 2.08271800
H 3.05476500 -1.68016700 1.80155500
Pd 0.17042300 0.04108000 -0.04893800
H -3.93739600 3.00372500 -0.96565300
H 3.52220800 2.32931700 -1.89126700
C -1.78175100 -2.14767400 -0.61379000
H -2.41538900 -2.96640200 -0.25303700
H -2.37158300 -1.50541000 -1.26284700
H -0.94163700 -2.55814400 -1.17326900
C 1.70678100 0.50928000 2.45786300
H 2.22508700 0.07970000 3.32200600
H 2.38106500 1.17960600 1.93116000
H 0.82531400 1.06589000 2.78206500
H -1.40452400 2.20867800 2.04746600
O -0.85901600 2.58626700 2.76742300
H -0.23519200 3.11451800 2.24724700
H 1.04480300 -2.20899800 2.91613100

| | | | |
|---|-------------|------------|------------|
| H | -2.04188300 | 0.53623900 | 2.39962200 |
| H | -0.50453300 | 1.33520800 | 2.77758900 |
| H | -1.06601500 | 3.75005600 | 0.68439600 |

51

RR-NMe, E(SCF) = -2333.43656325, E(ZPE) = -2333.057750, E(G) = -2333.117098 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.70820900 | 2.98814500 | -0.25764700 |
| H | -0.72574500 | 3.00755200 | -1.34920800 |
| H | -1.25507200 | 3.87027300 | 0.09307700 |
| C | 0.70825300 | 2.98813700 | 0.25766200 |
| H | 1.25515600 | 3.87022300 | -0.09310600 |
| H | 0.72577800 | 3.00757800 | 1.34922300 |
| N | 1.40525300 | 1.75017100 | -0.18449200 |
| N | -1.40525000 | 1.75022300 | 0.18457800 |
| C | 2.53463800 | 1.42877700 | 0.72112900 |
| H | 2.09557300 | 1.30648500 | 1.71830300 |
| C | -2.53455300 | 1.42872000 | -0.72108200 |
| H | -3.20602700 | 2.29718900 | -0.75865000 |
| C | 3.31594400 | 0.21816900 | 0.31154100 |
| C | 2.69458100 | -1.00822700 | -0.03418000 |
| C | 4.70398200 | 0.30527000 | 0.32121400 |
| C | 3.53964900 | -2.10422600 | -0.32001600 |
| C | 5.50472700 | -0.78231800 | 0.03558800 |
| H | 5.17631000 | 1.25114700 | 0.56894300 |
| C | 4.90885000 | -1.99777600 | -0.28697800 |
| H | 3.06293300 | -3.04369600 | -0.57890900 |
| H | 5.52622900 | -2.86105500 | -0.51570600 |
| C | -3.31588800 | 0.21816200 | -0.31140100 |
| C | -2.69457200 | -1.00816900 | 0.03464100 |
| C | -4.70392700 | 0.30522900 | -0.32138200 |
| C | -3.53968800 | -2.10411200 | 0.32055700 |
| C | -5.50472000 | -0.78229800 | -0.03564900 |
| H | -5.17623000 | 1.25104800 | -0.56937800 |
| C | -4.90888400 | -1.99768800 | 0.28725700 |
| H | -3.06301500 | -3.04352300 | 0.57973900 |
| H | -5.52628400 | -2.86092300 | 0.51610000 |
| O | 1.40533200 | -1.20878800 | -0.11320000 |
| O | -1.40534500 | -1.20870800 | 0.11399400 |
| S | 7.29104600 | -0.65405800 | 0.04595600 |
| S | -7.29104400 | -0.65407700 | -0.04650000 |
| O | -7.60529200 | 0.74139700 | -0.46341200 |
| O | -7.73444100 | -0.95742800 | 1.34582000 |
| O | -7.77014500 | -1.67450800 | -1.02363700 |
| O | 7.60536400 | 0.74141900 | 0.46278700 |
| O | 7.73404100 | -0.95737000 | -1.34649900 |
| O | 7.77044500 | -1.67449200 | 1.02293500 |
| H | -2.09541700 | 1.30634200 | -1.71821500 |
| H | 3.20610900 | 2.29725100 | 0.75857300 |
| Pd | 0.00000100 | 0.25056300 | 0.00020200 |
| C | -1.87064600 | 1.89158200 | 1.57610100 |
| H | -1.03466500 | 2.15097900 | 2.22349100 |
| H | -2.63290600 | 2.67746900 | 1.63163200 |
| H | -2.30071900 | 0.95223800 | 1.91779500 |
| C | 1.87052700 | 1.89140300 | -1.57607200 |
| H | 2.63277400 | 2.67729300 | -1.63175600 |
| H | 2.30058600 | 0.95203100 | -1.91770800 |
| H | 1.03448900 | 2.15072600 | -2.22342300 |

47

RR_no2W_D2_TS1_P, E(SCF) = -2256.00769361, E(ZPE) = -2255.668911, E(G) = -2255.729857 a.u.

| | | | |
|---|-------------|------------|-------------|
| C | 0.83579300 | 3.26625100 | -0.70705200 |
| H | 0.71283400 | 3.73150600 | 0.27446800 |
| H | 1.53916300 | 3.86883300 | -1.28786300 |
| C | -0.48684700 | 3.11180800 | -1.40274600 |
| H | -0.97359200 | 4.07771700 | -1.56390000 |
| H | -0.34680600 | 2.64148000 | -2.38161800 |
| N | -1.34704200 | 2.22754500 | -0.59178100 |
| N | 1.37928400 | 1.90632300 | -0.48875700 |
| C | -2.53852600 | 1.75782600 | -1.33909000 |
| H | -2.20518700 | 1.11159800 | -2.15593500 |
| C | 2.57555000 | 1.85476500 | 0.38244500 |
| H | 3.31181600 | 2.57534500 | 0.01136600 |
| C | -3.50252000 | 1.05948500 | -0.44189500 |
| C | -3.84468300 | 1.69206800 | 0.79792800 |

| | | | |
|----|-------------|-------------|-------------|
| C | -4.05727100 | -0.15721100 | -0.80663900 |
| C | -4.77989500 | 0.99160100 | 1.61232900 |
| C | -4.96876900 | -0.80052900 | 0.01362300 |
| H | -3.77426900 | -0.61808600 | -1.74875300 |
| C | -5.32341700 | -0.21092200 | 1.22806600 |
| H | -5.05542000 | 1.44411300 | 2.56038000 |
| H | -6.03344700 | -0.71545300 | 1.87783700 |
| C | 3.16730700 | 0.48441100 | 0.40847100 |
| C | 2.38601200 | -0.62178200 | 0.80882600 |
| C | 4.50131400 | 0.30104800 | 0.06695000 |
| C | 3.01065100 | -1.88210700 | 0.86950000 |
| C | 5.09224200 | -0.94518100 | 0.13567300 |
| H | 5.09807700 | 1.15108800 | -0.24829400 |
| C | 4.33872900 | -2.03936700 | 0.54686900 |
| H | 2.40978700 | -2.72849400 | 1.37413900 |
| H | 4.79848600 | -3.02108600 | 0.60471600 |
| O | -3.31289900 | 2.79863600 | 1.15509400 |
| O | 1.12227300 | -0.53836500 | 1.16400100 |
| S | -5.69556400 | -2.36548200 | -0.46807900 |
| S | 6.81636100 | -1.18171600 | -0.29999900 |
| O | 6.82123500 | -2.14074900 | -1.44183900 |
| O | 7.46820100 | -1.74585300 | 0.91639500 |
| O | 7.33650600 | -0.16422900 | -0.66802800 |
| O | -5.31762600 | -3.33719900 | 0.62531200 |
| O | -5.12056800 | -2.72075200 | -1.77447600 |
| O | -7.17211800 | -2.14486300 | -0.49586900 |
| H | 2.24997600 | 2.18741800 | 1.37410300 |
| H | -2.99691000 | 2.65347700 | -1.78589500 |
| H | 1.61680000 | 1.48979300 | -1.39171000 |
| H | -1.76478600 | 2.73997000 | 0.21290300 |
| Pd | -0.14746300 | 0.77412700 | 0.28607900 |
| H | -1.28782500 | -0.14888900 | 1.29878300 |
| H | -1.70787100 | -0.08574200 | 0.60262400 |

47

RR_no2W_D2_TS1_R, E(SCF) = -2256.03571260, E(ZPE) = -2255.696906, E(G) = -2255.757467 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.66993600 | 3.04417800 | -0.35191300 |
| H | -0.49109000 | 3.05837700 | -1.43091800 |
| H | -1.27021300 | 3.92173400 | -0.09678200 |
| C | 0.63518300 | 3.02192100 | 0.40384700 |
| H | 1.23192600 | 3.91699700 | 0.20970300 |
| H | 0.45156000 | 2.96445500 | 1.48068200 |
| N | 1.37505000 | 1.79952100 | 0.01585000 |
| N | -1.40053500 | 1.79553700 | -0.03988400 |
| C | 2.47669000 | 1.43303300 | 0.92540300 |
| H | 2.01204400 | 1.19433300 | 1.88890100 |
| C | -2.52663200 | 1.49099800 | -0.94404200 |
| H | -3.17805400 | 2.36854100 | -1.02395000 |
| C | 3.28878000 | 0.29187900 | 0.39366600 |
| C | 2.69632400 | -0.92047500 | -0.04453900 |
| C | 4.67382000 | 0.42035700 | 0.38596200 |
| C | 3.56834900 | -1.96042300 | -0.43873300 |
| C | 5.50035300 | -0.61188900 | -0.00941500 |
| H | 5.12259500 | 1.35394900 | 0.71103500 |
| C | 4.93435900 | -1.81507400 | -0.42013800 |
| H | 3.11523800 | -2.89100000 | -0.76370400 |
| H | 5.57267600 | -2.63662000 | -0.73071900 |
| C | -3.32080900 | 0.31770700 | -0.46024700 |
| C | -2.70822000 | -0.92348200 | -0.15158600 |
| C | -4.70209400 | 0.44562000 | -0.36309600 |
| C | -3.55705000 | -1.99041100 | 0.21781000 |
| C | -5.50648400 | -0.61495500 | 0.00274800 |
| H | -5.16673600 | 1.40011800 | -0.59075400 |
| C | -4.92157400 | -1.84409200 | 0.29131100 |
| H | -3.08877700 | -2.94177700 | 0.44714800 |
| H | -5.54351300 | -2.68565000 | 0.58106800 |
| O | 1.41146100 | -1.16121900 | -0.10057700 |
| O | -1.42253700 | -1.16357300 | -0.20490700 |
| S | 7.28147800 | -0.42248200 | -0.02686700 |
| S | -7.28462800 | -0.43776100 | 0.12537200 |
| O | -7.63023300 | -0.72985400 | 1.54709400 |
| O | -7.86177700 | -1.44436300 | -0.81231000 |
| O | -7.59034800 | 0.96598400 | -0.26889400 |
| O | 7.82099500 | -1.53669900 | 0.80534100 |
| O | 7.56013900 | 0.92235900 | 0.55072900 |

O 7.69525600 -0.53604100 -1.45624800
H -2.08737500 1.31373300 -1.93267700
H 3.12566300 2.30220300 1.08080600
H -1.75759600 1.84818300 0.91510600
H 1.75589100 1.92376600 -0.92308000
Pd -0.00941000 0.28748300 -0.08408700
H 0.95861100 -1.29431800 2.42828600
H 0.86882500 -0.98487500 3.10597200

47

RR_no2W_D2_TS1, E(SCF) = -2255.99300938,
E(ZPE) = -2255.654464, E(G) = -2255.713286
a.u.

C 0.83190800 3.12553400 -0.20563800
H 0.74137500 3.41336700 0.84538500
H 1.44446100 3.87538400 -0.71314800
C -0.52395800 2.98595100 -0.84340400
H -1.08231000 3.92588000 -0.81224600
H -0.42651100 2.68774100 -1.89198100
N -1.25808200 1.91674700 -0.14061000
N 1.49164800 1.80211700 -0.24477500
C -2.51317200 1.54041100 -0.80450200
H -2.24847100 1.07406400 -1.76080600
C 2.69892700 1.68549800 0.60157000
H 3.37712500 2.51384800 0.36932500
C -3.41596800 0.64504300 0.00195000
C -3.11985500 0.22917800 1.33575800
C -4.59395600 0.24629300 -0.61370200
C -4.09534800 -0.59947000 1.95866800
C -5.51989900 -0.55174000 0.03136800
H -4.80023700 0.57073900 -1.63046400
C -5.25968900 -0.97447800 1.33400400
H -3.88351200 -0.92735700 2.97205700
H -5.97870000 -1.60362600 1.85082900
C 3.39762800 0.38231000 0.38647000
C 2.71796600 -0.84273200 0.58353700
C 4.74035700 0.37625300 0.03043900
C 3.45591100 -2.03362600 0.43503800
C 5.44104500 -0.80568900 -0.11108300
H 5.25684900 1.31734700 -0.13068400
C 4.79073000 -2.01642400 0.10294500
H 2.93451600 -2.97145300 0.59287300
H 5.33511100 -2.94946800 -0.00496200
O -2.03362400 0.54676100 1.95094000
O 1.45394300 -0.93425700 0.92584400
S -7.02255600 -1.07765000 -0.78175000
S 7.18036000 -0.80740300 -0.54956100
O 7.29081600 -1.64595900 -1.77749800
O 7.89320000 -1.41097200 0.61326000
O 7.54886900 0.61680200 -0.78107800
O -6.94557400 -2.56603100 -0.87827900
O -7.03139100 -0.41399500 -2.11715900
O -8.14931000 -0.63269500 0.09143700
H 2.36121900 1.80802700 1.63644700
H -3.04612900 2.47018900 -1.05283400
H 1.74339600 1.57677500 -1.20873900
H -1.48025900 2.17706100 0.82516700
Pd 0.07509400 0.40825500 0.30807100
H -1.20306900 -1.17305800 0.56732200
H -1.07017300 -1.26749300 -0.18636300

53

RR-PhCl_hs_D1_TS1_P, E(SCF) = -
3328.08034959, E(ZPE) = -3327.708655, E(G)
= -3327.776838 a.u.

C -0.22969100 1.09352800 -2.79358600
H 0.06870100 2.05333000 -3.22512900
H -0.15854200 0.33194700 -3.57485400
C -1.61126600 1.16067000 -2.20744700
H -2.36727700 1.41166300 -2.95694500
H -1.88156000 0.19844300 -1.76586800
N -1.60220200 2.16816500 -1.11905500
N 0.70682200 0.78153200 -1.69238100
C -2.87486400 2.21817400 -0.32952700
H -2.67975400 2.87273000 0.52264200
C 2.12614400 0.92418800 -2.05677800
H 2.29218400 1.98437900 -2.27922200

C -3.40433400 0.89274600 0.10726700
C -2.67118700 0.12486800 1.06025800
C -4.60942500 0.44218900 -0.39970000
C -3.28704700 -1.09331100 1.44613000
C -5.16278000 -0.76084900 0.01458200
H -5.13658600 1.05005000 -1.13111300
C -4.49023400 -1.53629300 0.84556400
H -4.91407300 -2.47720600 1.27550800
C 3.05236100 0.43188200 -0.98992600
C 2.95961700 0.92296100 0.33624200
C 4.05255500 -0.46017200 -1.33582800
C 3.97647300 0.51376500 1.22086100
C 5.01064600 -0.86456300 -0.42115400
H 4.09392700 -0.83867100 -2.35319400
C 4.97940400 -0.36262800 0.86522900
H 5.73340400 -0.65425700 1.58624300
O -1.53159900 0.50595700 1.50307400
O 2.03051100 1.73962800 0.76883500
S -6.70835800 -1.31986300 -0.70188600
S 6.28691100 -2.02206700 -0.93395100
O 7.03085700 -1.34012900 -2.02969500
O 5.56034300 -3.23343600 -1.40592100
O 7.11851100 -2.26826200 0.27465300
O -7.09601100 -2.53665000 0.06384400
O -6.41566400 -1.60530800 -2.13661900
O -7.67005400 -0.19270700 -0.53630400
H -0.06635600 3.29739600 1.09635700
H -0.41703600 2.65459400 1.43822600
H -1.49159900 3.08837500 -1.54656300
H -3.62290100 2.71010400 -0.95972400
H 0.52252500 -0.16825300 -1.32312700
H 2.30754400 0.36394100 -2.98021800
Pd 0.21141000 1.95836400 -0.10921500
H -0.18354200 0.30078700 2.67559000
O 0.68498300 0.35247800 3.11608400
H 1.23805400 0.84207500 2.48985200
H -0.46995800 -0.81526500 0.68494600
O 0.00902900 -1.36702500 0.03306800
H -0.46420600 -2.20215200 -0.00181900
Cl 3.97878700 1.17209200 2.85163200
Cl -2.43658000 -2.08886000 2.63251400

53

RR-PhCl_hs_D1_TS1_R, E(SCF) = -
3328.09439542, E(ZPE) = -3327.723841, E(G)
= -3327.793097 a.u.

C 0.19133000 -3.10246800 1.84000800
H 0.48845500 -4.03910500 1.35809800
H 0.52971500 -3.13597800 2.87890500
C -1.30554700 -2.91276400 1.74666300
H -1.84292800 -3.71512800 2.25966800
H -1.61125500 -1.96104600 2.19151800
N -1.66231800 -2.87525800 0.30888100
N 0.84452000 -1.99474700 1.11141900
C -3.07215200 -2.52029500 -0.00487200
H -3.30170400 -3.01617600 -0.95183200
C 2.26986100 -2.18222400 0.79396900
H 2.32673700 -2.97358000 0.03819500
C -3.28621200 -1.04716800 -0.14393200
C -2.56929400 -0.36865700 -1.16657400
C -4.16389800 -0.36773400 0.67462900
C -2.81709100 1.00620800 -1.29551000
C -4.38056900 0.99471500 0.50551600
H -4.69173200 -0.90586000 1.45735100
C -3.70684600 1.68405600 -0.48303700
H -3.86495500 2.74851500 -0.60852200
C 2.89037800 -0.89952300 0.32382900
C 2.30229400 -0.13386300 -0.71902500
C 4.06538500 -0.47447200 0.92071900
C 2.98899100 1.04191000 -1.08380800
C 4.70928100 0.68444900 0.51857700
H 4.49200500 -1.06853600 1.72398600
C 4.16645100 1.44950600 -0.49643800
H 4.65229600 2.36373000 -0.81494800
O -1.70176500 -1.00390400 -1.92254700
O 1.20038700 -0.44513200 -1.34759100
S -5.50777500 1.84823600 1.61673600

| | | | |
|----|-------------|-------------|-------------|
| S | 6.24312200 | 1.16797300 | 1.31998800 |
| O | 7.23065200 | 0.10625400 | 0.97610100 |
| O | 5.93865600 | 1.211109500 | 2.77738800 |
| O | 6.59418600 | 2.49845800 | 0.75354100 |
| O | -5.51413600 | 3.26916700 | 1.17741400 |
| O | -4.93832000 | 1.65651000 | 2.97984300 |
| O | -6.82564500 | 1.17506500 | 1.44898500 |
| H | -0.26385400 | -4.33910500 | -2.86577300 |
| H | -0.76586200 | -3.82003400 | -2.66680400 |
| H | -1.47378500 | -3.79697500 | -0.08403500 |
| H | -3.73065000 | -2.93672400 | 0.76342100 |
| H | 0.71929400 | -1.11637700 | 1.63310100 |
| H | 2.80119200 | -2.53539200 | 1.68440400 |
| Pd | -0.27243200 | -1.61569500 | -0.54990000 |
| H | -0.65870000 | -0.64561500 | -3.48311800 |
| O | 0.17877400 | -0.62254500 | -3.97545500 |
| H | 0.79893500 | -0.44718800 | -3.25035700 |
| H | -0.06045300 | 1.07626500 | 0.66260900 |
| O | -0.05630700 | 0.82338000 | 1.59327600 |
| H | -0.97040300 | 0.93476800 | 1.87297700 |
| Cl | 2.29203700 | 2.03763000 | -2.35643900 |
| Cl | -1.91718200 | 1.90503700 | -2.50856300 |

53

RR-PhCl_hs_D1_TS1, E(SCF) = -3328.07438944,
E(ZPE) = -3327.703850, E(G) = -3327.771544
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.11725800 | -3.04077800 | -0.97070500 |
| H | 0.23693500 | -3.45327800 | -1.91987200 |
| H | -0.00310800 | -3.81076800 | -0.20304400 |
| C | -1.54165400 | -2.57132700 | -1.08419200 |
| H | -2.22085300 | -3.38481400 | -1.35480200 |
| H | -1.88381900 | -2.14335300 | -0.13828700 |
| N | -1.58487600 | -1.49590200 | -2.10278700 |
| N | 0.72610900 | -1.86896700 | -0.65377100 |
| C | -2.90857400 | -0.82731800 | -2.22842500 |
| H | -2.80500900 | -0.10944100 | -3.04649700 |
| C | 2.16408400 | -2.08592000 | -0.86140900 |
| H | 2.30408500 | -2.24735800 | -1.93598600 |
| C | -3.36854400 | -0.16112300 | -0.97621900 |
| C | -2.66123700 | 0.98594800 | -0.51331000 |
| C | -4.47892000 | -0.63778500 | -0.30488600 |
| C | -3.20677800 | 1.60052600 | 0.63993900 |
| C | -4.96295100 | -0.00083800 | 0.82821700 |
| H | -4.98641300 | -1.52246900 | -0.68151900 |
| C | -4.31903300 | 1.12937800 | 1.30221000 |
| H | -4.69045700 | 1.63766500 | 2.18428400 |
| C | 3.00918700 | -0.95809700 | -0.35486000 |
| C | 2.73334000 | 0.39679700 | -0.68135100 |
| C | 4.13057500 | -1.28456800 | 0.39008700 |
| C | 3.69989800 | 1.33351400 | -0.25726200 |
| C | 5.03632200 | -0.32430100 | 0.80431900 |
| H | 4.30903900 | -2.32660800 | 0.63960200 |
| C | 4.82103400 | 0.99789200 | 0.46936400 |
| H | 5.52730400 | 1.76114500 | 0.77346700 |
| O | -1.60022900 | 1.41962800 | -1.09967600 |
| O | 1.68832600 | 0.81891400 | -1.34622800 |
| S | -6.38214100 | -0.68206300 | 1.68802000 |
| S | 6.46338300 | -0.80961400 | 1.78240000 |
| O | 7.16528700 | -1.85119800 | 0.98170600 |
| O | 5.91348700 | -1.34648800 | 3.05886400 |
| O | 7.26572000 | 0.42989100 | 1.96528800 |
| O | -6.71653500 | 0.29491900 | 2.76038100 |
| O | -5.93806800 | -2.00252300 | 2.22008100 |
| O | -7.45549400 | -0.81746100 | 0.66289500 |
| H | -0.05610400 | 0.80904200 | -3.66311700 |
| H | -0.49730200 | 1.25510000 | -3.22947100 |
| H | -1.36504700 | -1.90704900 | -3.01116400 |
| H | -3.63810600 | -1.58489000 | -2.53493900 |
| H | 0.54653600 | -1.53787000 | 0.30410300 |
| H | 2.45840100 | -3.00956100 | -0.35054700 |
| Pd | 0.02555200 | -0.27597200 | -1.73171500 |
| H | -0.54542900 | 2.87394700 | -1.09781600 |
| O | 0.25972100 | 3.40635900 | -1.23651200 |
| O | 0.95619100 | 2.73285700 | -1.25204100 |
| H | -0.35260700 | 0.83180400 | 0.65235900 |
| O | -0.02712400 | 0.22486300 | 1.33722200 |

| | | | |
|----|-------------|------------|-------------|
| H | -0.71387400 | 0.23107100 | 2.01068400 |
| Cl | 3.47613000 | 3.02308600 | -0.69183200 |
| Cl | -2.39742100 | 3.04122100 | 1.25897400 |

53

RR-PhCl_hs_D1_TS2_Hbond-reordered, E(SCF)
= -3328.08556437, E(ZPE) = -3327.713085,
E(G) = -3327.779897 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.18862700 | 0.35777700 | -3.21157100 |
| H | -0.15397600 | -0.30002000 | -4.01601800 |
| H | 0.08481800 | 1.39161200 | -3.55271900 |
| C | 1.60673700 | 0.04935100 | -2.81851100 |
| H | 2.30249700 | 0.18447000 | -3.65130700 |
| H | 1.91807600 | 0.70918300 | -2.00488500 |
| N | 1.66282200 | -1.34233000 | -2.31860400 |
| N | -0.66530900 | 0.11280100 | -2.03313600 |
| C | 2.97820200 | -1.72044400 | -1.71407100 |
| H | 2.91712500 | -2.78460600 | -1.47840500 |
| C | -2.10750900 | 0.12237600 | -2.32155200 |
| H | -2.30527500 | -0.73017300 | -2.98127600 |
| C | 3.33945600 | -0.92372500 | -0.50494900 |
| C | 2.84856500 | -1.31240000 | 0.77573500 |
| C | 4.19280700 | 0.15848100 | -0.64170400 |
| C | 3.31055400 | -0.52143600 | 1.85879200 |
| C | 4.58659000 | 0.91520100 | 0.44919500 |
| H | 4.56567000 | 0.41518000 | -1.63070800 |
| C | 4.14455500 | 0.56460600 | 1.71284400 |
| H | 4.46169500 | 1.13654900 | 2.57702300 |
| C | -2.93703700 | 0.06079200 | -1.07794300 |
| C | -2.75519100 | -0.98487500 | -0.13751800 |
| C | -3.92688300 | -1.00853600 | -0.88719200 |
| C | -3.66804200 | -1.01713900 | 0.93580300 |
| C | -4.78696900 | 0.94881100 | 0.19659400 |
| H | -4.03928100 | 1.80770800 | -1.61422900 |
| C | -4.66179500 | -0.07763100 | 1.11194100 |
| H | -5.33589400 | -0.14068800 | 1.95810400 |
| O | 2.05826700 | -2.31715100 | 0.95973200 |
| O | -1.83070700 | -1.91111700 | -0.21868700 |
| S | 5.68394100 | 2.31368400 | 0.20752300 |
| S | -6.06346600 | 2.20107000 | 0.38107600 |
| O | -6.92375200 | 2.07511300 | -0.82876400 |
| O | -5.34328800 | 3.50346400 | 0.43628100 |
| O | -6.77580000 | 1.86851300 | 1.64397900 |
| O | 5.90485100 | 2.89450600 | 1.55990800 |
| O | 4.96595000 | 3.23670500 | -0.71721700 |
| O | 6.92584200 | 1.75694500 | -0.40034200 |
| H | 0.43812600 | -3.18950600 | -0.58893100 |
| H | 1.01004400 | -2.74042300 | -0.08674800 |
| H | 1.51819600 | -1.97017700 | -3.11417000 |
| H | 3.74089800 | -1.58919200 | -2.48975000 |
| H | -0.44039600 | 0.77857400 | -1.27589700 |
| H | -2.35491800 | 1.03218400 | -2.87933000 |
| Pd | -0.05501300 | -1.65446100 | -1.20004900 |
| H | 0.58581700 | -1.58860200 | 1.91874200 |
| O | -0.25290600 | -1.11162800 | 2.07592800 |
| H | -0.88585700 | -1.57180400 | -1.49951000 |
| H | 0.00597400 | 0.48252000 | 1.13359400 |
| O | 0.12820800 | 1.25751800 | 0.54527100 |
| H | 1.03177600 | 1.54816600 | 0.69890600 |
| Cl | -3.53950900 | -2.33020700 | 2.10075200 |
| Cl | 2.80927200 | -0.97352600 | 3.48873500 |

53

RR-PhCl_hs_D1_TS2_P-Hbond-reordered,
E(SCF) = -3328.11196394, E(ZPE) = -
3327.736247, E(G) = -3327.803464 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.19434900 | 0.93806600 | -3.01231200 |
| H | -0.15789200 | 0.42647700 | -3.91461100 |
| H | 0.14655600 | 2.01541600 | -3.20402900 |
| C | 1.60472500 | 0.51957600 | -2.68480800 |
| H | 2.30791200 | 0.81030500 | -3.47171100 |
| H | 1.92237500 | 0.99791400 | -1.75473600 |
| N | 1.65078600 | -0.95056200 | -2.46989000 |
| N | -0.67721400 | 0.54282600 | -1.89967200 |
| C | 2.97346500 | -1.42366100 | -1.97639800 |
| H | 2.92549100 | -2.51325900 | -1.93680700 |
| C | -2.10687400 | 0.56643100 | -2.21171400 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | -2.26917900 | -0.16572000 | -3.01377800 | O | -0.18604100 | -1.28789300 | 0.41627900 |
| C | 3.38261300 | -0.84355100 | -0.65559000 | H | -1.08516200 | -1.60847100 | 0.53200000 |
| C | 2.95694800 | -1.38898300 | 0.56554800 | N | 0.64098300 | 0.05163000 | -2.00987600 |
| C | 4.25226300 | 0.23826200 | -0.63741600 | C | 2.08371000 | 0.03517000 | -2.30525700 |
| C | 3.44104700 | -0.83345100 | 1.75030500 | H | 2.29191300 | 0.91895700 | -2.91896500 |
| C | 4.70302000 | 0.78478100 | 0.55030500 | C | 2.92410000 | 0.01037400 | -1.06838200 |
| H | 4.59506500 | 0.65338000 | -1.58120900 | C | 2.75177900 | 0.98657400 | -0.05739400 |
| C | 4.29892100 | 0.24697400 | 1.75597500 | C | 3.91415700 | -0.94971900 | -0.95203600 |
| H | 4.65526400 | 0.66432400 | 2.68977800 | C | 3.66170900 | 0.93565100 | 1.01686500 |
| C | -2.96064500 | 0.25111100 | -1.01884300 | C | 4.78016400 | -0.96772200 | 0.12854800 |
| C | -2.78718200 | -0.94523400 | -0.26893400 | H | 4.02099800 | -1.69542800 | -1.73460400 |
| C | -3.97647500 | 1.13414700 | -0.69394200 | C | 4.65566300 | -0.01399000 | 1.11986500 |
| C | -3.73180200 | -1.16385500 | 0.75800300 | H | 5.32846600 | -0.01563500 | 1.96901100 |
| C | -4.86864000 | 0.88071500 | 0.33534200 | O | 1.83238000 | 1.92207400 | -0.06897800 |
| H | -4.08262100 | 2.04506100 | -1.27546000 | S | 6.05509200 | -2.23300500 | -0.21815300 |
| C | -4.74683600 | -0.28445700 | 1.06674500 | O | 5.33023200 | -3.53392800 | 0.20656000 |
| H | -5.43917800 | -0.50394800 | 1.87023800 | O | 6.78776300 | -1.97902200 | 1.48736500 |
| O | 2.14342500 | -2.45622500 | 0.66771200 | O | 6.89733800 | -2.03776800 | -0.99503800 |
| O | -1.85599400 | -1.84154000 | -0.46575300 | H | 0.40194900 | -0.65272300 | -1.29536100 |
| S | 5.79734500 | 2.21808500 | 0.50365000 | H | 2.30793900 | -0.84685500 | -2.91413600 |
| S | -6.17306300 | 2.06416600 | 0.68496900 | Pd | 0.07488300 | 1.77973900 | -1.09260800 |
| O | -6.97580300 | 2.16222600 | -0.56708600 | Cl | 3.52252600 | 2.14944700 | 2.28341900 |
| O | -5.48280600 | 3.34212100 | 1.01800500 | Cl | -2.84224000 | 0.67925600 | 3.56583400 |
| O | -6.94068400 | 1.49782800 | 1.82743900 | | | | |
| O | 6.15854900 | 2.49029500 | 1.91894200 | 53 | | | |
| O | 4.98861200 | 3.30071600 | -0.11932000 | RR-PhCl_hs_Hbond-reor_TS1_R, E(SCF) = - | | | |
| O | 6.95343600 | 1.80406400 | -0.33551100 | 3328.09888614, E(ZPE) = -3327.729066, E(G) | | | |
| H | 0.36221000 | -2.96497300 | -1.23718400 | = -3327.799091 a.u. | | | |
| H | 1.57542400 | -2.56779800 | -0.12936600 | C | 0.37451700 | -3.52822700 | 0.75527600 |
| H | 1.50668000 | -1.40084100 | -3.37350800 | H | 0.69000300 | -4.23592400 | -0.01864200 |
| H | 3.72998900 | -1.15853800 | -2.72280500 | H | 0.73753200 | -3.89926900 | -1.71802400 |
| H | -0.47309600 | 1.09250700 | -1.05539600 | C | -1.12873300 | -3.37461700 | 0.74792400 |
| H | -2.39799900 | 1.54650100 | -2.60957500 | H | -1.63249100 | -4.31845500 | 0.97400700 |
| Pd | -0.08887900 | -1.45705800 | -1.45029500 | H | -1.44883000 | -2.62798400 | 1.48131200 |
| H | 0.50966800 | -1.76715200 | 1.82162200 | N | -1.51553900 | -2.88041400 | -0.59432600 |
| O | -0.32318000 | -1.27985600 | 1.89747000 | C | -2.94419200 | -2.50984900 | -0.76618600 |
| H | -0.87819700 | -1.65955900 | 1.19011400 | H | -3.19350900 | -2.75736900 | -1.80166200 |
| H | -0.05857400 | 0.44780200 | 1.25517300 | C | -3.25070900 | -1.06325900 | -0.52812800 |
| O | 0.03941300 | 1.32903100 | 0.84123600 | C | -2.60250700 | -0.09513900 | -1.34183600 |
| H | 0.92806100 | 1.61644900 | 1.06637500 | C | -4.21637300 | -0.68684500 | 0.38774000 |
| Cl | -3.61218600 | -2.65422200 | 1.69198700 | C | -3.07508000 | 1.22938200 | -1.22539000 |
| Cl | 2.93358800 | -1.52829600 | 3.27688400 | C | -4.61217700 | 0.63652400 | 0.50203500 |
| | | | | H | -4.69099000 | -1.43565900 | 1.01384300 |
| 53 | | | | C | -4.04935600 | 1.59883300 | -0.32066900 |
| RR-PhCl_hs_Hbond-reor_TS1_P, E(SCF) = - | | | | H | -4.36323700 | 2.63538100 | -0.25810200 |
| 3328.08588713, E(ZPE) = -3327.712614, E(G) | | | | O | -1.62440800 | -0.40584800 | -2.14749300 |
| = -3327.779569 a.u. | | | | S | -5.82049100 | 1.14038700 | 1.13501100 |
| C | -0.21341900 | -0.10602700 | -3.20464400 | O | -6.35871500 | -0.12230400 | 2.30892400 |
| H | 0.14078100 | 0.59676600 | -3.96444700 | O | -6.84229600 | 1.93529400 | 0.99944500 |
| H | -0.11986400 | -1.11798300 | -3.60821100 | O | -5.06528300 | 1.95819300 | 2.72568100 |
| C | -1.62591800 | 0.19589200 | -2.79335200 | H | 1.22183400 | -3.71536800 | -3.17849900 |
| H | -2.32338700 | 0.12478500 | -3.63240600 | H | 0.72302100 | -3.19364000 | -2.97364200 |
| H | -1.94863800 | -0.50723600 | -2.02237300 | H | -1.29691100 | -3.60996600 | -1.27165100 |
| N | -1.66491200 | 1.55697100 | -2.20285500 | H | -3.55955200 | -3.13976400 | -0.11658100 |
| C | -2.97411200 | 1.88787600 | -1.55111800 | O | -1.31980300 | 1.74542000 | 0.38137500 |
| H | -2.89762700 | 2.92539000 | -1.22155700 | H | -0.38525200 | 1.69778800 | 0.61622300 |
| C | -3.34408000 | 0.98729800 | -0.42138000 | H | 0.05465200 | 1.34515500 | -0.18188200 |
| C | -2.85310900 | 1.26524700 | 0.89057300 | H | -0.02071200 | 0.45324900 | 1.87308500 |
| C | -4.19676400 | -0.08166100 | -0.66187300 | O | 0.30445900 | -0.27855700 | 2.43785300 |
| C | -3.33095600 | 0.37149400 | 1.89678100 | H | -0.37035800 | -0.41604900 | 3.10653400 |
| C | -4.59559600 | -0.93286300 | 0.35023900 | N | 0.97057600 | -2.21245400 | 0.44450100 |
| H | -4.56723100 | -0.25716900 | -1.66812500 | C | 2.38046800 | -2.23607300 | 0.03957500 |
| C | -4.15480800 | -0.69734900 | 1.64727600 | H | 2.43258700 | -2.75913900 | -0.92266400 |
| H | -4.46932600 | -1.34066000 | 2.46265700 | C | 2.97455600 | -0.85781200 | -0.04508700 |
| O | -2.05706600 | 2.23121900 | 1.15550900 | C | 2.31856400 | 0.21925600 | -0.70217400 |
| S | -5.63251500 | -2.35611900 | 0.02166400 | C | 4.23305100 | -0.66952700 | 0.50368800 |
| O | -6.05507300 | -2.23385900 | -1.40121300 | C | 3.03892100 | 1.43183700 | -0.76782100 |
| O | -6.77171300 | -2.26861500 | 0.97952500 | C | 4.90150000 | 0.53880400 | 0.40761400 |
| O | -4.77463600 | -3.55094800 | 0.27214100 | H | 4.71330200 | -1.50241400 | 1.00951400 |
| H | -0.29177000 | 3.39953100 | -0.49725500 | C | 4.29523900 | 1.60352800 | -0.23137800 |
| H | -0.80367300 | 2.93869400 | -0.02146000 | H | 4.80500700 | 2.55614500 | -0.31344300 |
| H | -1.53274800 | 2.23099000 | -2.95795000 | O | 1.12906000 | 0.17409200 | -1.24593500 |
| H | -3.73751700 | 1.83763000 | -2.33558100 | S | 6.51826900 | 0.72583700 | 1.16913300 |
| H | -0.62525100 | 1.42793000 | 1.97272400 | O | 6.28077700 | 0.68617900 | 2.63966500 |
| O | 0.20040300 | 0.91999800 | 2.12623700 | O | 7.03623800 | 2.03834900 | 0.69647400 |
| H | 0.86561500 | 1.411395200 | 1.62047200 | O | 7.32584900 | -0.43109200 | 0.69167400 |
| H | -0.08250100 | -0.56578700 | 1.07317900 | H | 0.84483100 | -1.59022100 | 1.26188700 |

H 2.95652000 -2.82759900 0.76014300
Pd -0.20698000 -1.34094200 -0.97167500
Cl 2.28494100 2.79567400 -1.58821300
Cl -2.36382900 2.45901100 -2.26676400

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RR-PhCl_hs_Hbond-reor_TS1, E(SCF) = -
3328.07777394, E(ZPE) = -3327.707708, E(G)
= -3327.775875 a.u.

C -0.01513500 3.16468100 0.39270700
H 0.33506100 3.74725800 1.25010800
H 0.13078900 3.76754200 -0.50734600
C -1.45254500 2.76070700 0.57054300
H -2.11381600 3.62555300 0.67583200
H -1.79706000 2.16898700 -0.28131200
N -1.52620400 1.90055400 1.77395400
C -2.86970500 1.31758100 2.02908100
H -2.79305600 0.80134600 2.98999500
C -3.35144700 0.39423900 0.96500100
C -2.74514100 -0.89126300 0.85651300
C -4.41746200 0.76735900 0.16153400
C -3.39541900 -1.77059000 -0.05646900
C -4.96374700 -0.11058700 -0.75558600
H -4.84409900 1.76135500 0.26033800
C -4.45499600 -1.39943900 -0.84797000
H -4.89578800 -2.11678800 -1.53268700
O -1.71368100 -1.22986800 1.54242900
S -6.34618600 0.35424400 -1.79676900
O -6.63947300 1.77784400 -1.47335900
O -7.46108900 -0.56741600 -1.43441300
O -5.88608000 0.15690200 -3.20152100
H -0.02450300 -0.07267500 3.72305000
H -0.53935800 -0.56834400 3.45397300
H -1.28543500 2.47167400 2.58565600
H -3.57395900 2.14851000 2.14753800
H -0.56857800 -2.09781900 0.37784700
O 0.22097300 -2.22641800 -0.18914200
H 0.92622900 -1.93543600 0.41081500
H 0.10706400 -0.76602900 -1.27572100
O 0.11677200 0.08914900 -1.75944900
H -0.73377000 0.14620600 -2.20232600
N 0.79981000 1.93350000 0.32097700
C 2.23753000 2.16552800 0.52687000
H 2.35823600 2.51369400 1.55884000
C 3.07516100 0.95663100 0.24830000
C 2.77409000 -0.30263900 0.82651100
C 4.20164600 1.10768800 -0.54267900
C 3.70541500 -1.33297800 0.58372500
C 5.07889500 0.06066000 -0.76769800
H 4.40604000 2.07740000 -0.98769200
C 4.83191900 -1.17085800 -0.19347500
H 5.51307000 -1.99761300 -0.35534100
O 1.71838700 -0.56621000 1.55639000
S 6.52080800 0.32542400 -1.80812300
O 5.98623100 0.73579400 -3.13642000
O 7.23927400 -0.97660100 -1.840527400
O 7.29887400 1.40993300 -1.14695300
H 0.63020800 1.43977600 -0.57525900
H 2.55819400 2.98056500 -0.13192600
Pd 0.04546400 0.58596000 1.65648700
Cl 3.41433600 -2.90542600 1.32004500
Cl -2.83032800 -3.44090300 -0.14879800

53

RR-PhCl_D1_TS1_P, E(SCF) = -3328.08001797,
E(ZPE) = -3327.707417, E(G) = -3327.775511
a.u.

C 0.58668200 -3.67498000 -0.01994900
H 0.40869700 -3.90120000 -1.07451500
H 1.27453400 -4.42630600 0.37890900
C -0.69076200 -3.62671300 0.76468200
H -1.24394900 -4.56646400 0.71015700
H -0.46678200 -3.43201600 1.81667500
N -1.52947800 -2.49655700 0.27836100
N 1.19754600 -2.33062100 0.05703000
C -2.55883900 -2.12759800 1.30583100
H -3.27650000 -2.95332400 1.35290800

C 2.40369900 -2.18736300 -0.77641300
H 2.08997300 -2.37321900 -1.80985500
C -3.23341900 -0.83429100 1.02407900
C -2.66484000 0.34973600 1.60171100
C -4.33129300 -0.78579400 0.18729200
C -3.32867300 1.55088200 1.22447800
C -4.92299000 0.42231000 -0.15132900
H -4.72862000 -1.71209300 -0.22237900
C -4.41386100 1.59760700 0.37822500
H -4.86900800 2.54758300 0.12260600
C 3.06494800 -0.85338600 -0.64271800
C 2.33670400 0.33272900 -0.90091700
C 4.41852300 -0.79545500 -0.36021100
C 3.07438500 1.53135700 -0.89887800
C 5.10186400 0.40948600 -0.328315200
H 4.95696000 -1.71707300 -0.15848000
C 4.42603600 1.58141200 -0.63348500
H 4.95240900 2.52829400 -0.63831900
O -1.63695300 0.96821200 2.32636500
O 1.05271300 0.37335800 -1.16274100
S -6.37077500 0.43844400 -1.20735800
S 6.86711900 0.42194300 -0.01029400
O 7.27136900 1.85326500 -0.02891400
O 7.48952200 -0.37883300 -1.10115300
O 7.02088200 -0.21651000 1.32606300
O -6.62765100 1.87009400 -1.52677700
O -7.46745800 -0.18451500 -0.41074100
O -6.01305700 -0.37352000 -2.40562700
H -0.27265800 1.43949700 1.87208300
H -1.48623700 -0.09096900 -1.39732200
H -1.56195700 0.23257300 -0.65641600
O 0.61634100 1.75548900 1.60151700
H 0.62544900 1.65446500 0.63972100
H -0.07742000 -0.72901200 2.58236700
O 0.88203200 -0.92103600 2.58240500
H 1.22742600 -0.05140600 2.31734000
H -2.02607100 -2.79977400 -0.56071000
H -2.03569700 -2.07305200 2.26158600
H 1.37718300 -2.06660900 1.04038200
H 3.11196600 -2.97539700 -0.50070000
Pd -0.25673000 -1.00718300 -0.47142500
Cl 2.22806800 3.02871200 -1.26367800
Cl -2.70448100 3.06890100 1.87577100

53

RR-PhCl_D1_TS1_R_REF, E(SCF) = -
3328.10428402, E(ZPE) = -3327.733404, E(G)
= -3327.802098 a.u.

C -0.64331500 -3.47709800 0.37084700
H -0.43902000 -3.44785200 1.44473400
H -1.25082300 -4.36137900 0.16357700
C 0.64070800 -3.47877800 -0.41496100
H 1.25243300 -4.35742400 -0.19634000
H 0.43754600 -3.46347600 -1.48930000
N 1.37556100 -2.23522600 -0.08483500
N -1.38560700 -2.24135000 0.02698100
C 2.47247200 -1.90978100 -1.01684900
H 3.09188900 -2.79966400 -1.16927900
C -2.47933200 -1.91162800 0.96071900
H -2.00731500 -1.65987900 -1.91670500
C 3.32434200 -0.79248500 -0.50216200
C 2.75420700 0.44016800 -0.10721300
C 4.70040100 -0.97689300 -0.46020700
C 3.66791100 1.44417600 0.28372900
C 5.55262000 0.03222000 -0.06176500
H 5.12084900 -1.93293600 -0.75372900
C 5.02965100 1.26171200 0.30723600
H 5.67821600 2.07193900 0.62272200
C -3.33743900 -0.79751500 0.44928800
C -2.77433900 0.43485000 0.04219200
C -4.71414900 -0.97960400 0.43968700
C -3.69615600 1.44323900 -0.31826400
C -5.57453300 0.03342900 0.06938700
H -5.12877100 -1.93413100 0.74628700
C -5.05831400 1.26287000 -0.30934500
H -5.71377900 2.07740500 -0.59825500
O 1.46989000 0.70412900 -0.09199800

| | | | |
|----|-------------|-------------|-------------|
| O | -1.49106200 | 0.69912100 | 0.00381500 |
| S | 7.33442700 | -0.20479700 | -0.02713100 |
| S | -7.35480100 | -0.21396900 | 0.04221800 |
| O | -7.75244800 | -0.11968200 | -1.39046200 |
| O | -7.92385900 | 0.88788200 | 0.86648700 |
| O | -7.58317500 | -1.56354800 | 0.62492000 |
| O | 7.55766600 | -1.63474100 | -0.37071800 |
| O | 7.75741300 | 0.14073600 | 1.35840100 |
| O | 7.88277400 | 0.73646800 | -1.04294400 |
| H | 1.76048800 | -2.31445200 | 0.85844200 |
| H | 2.00457600 | -1.66378600 | -1.97616200 |
| H | -1.77404100 | -2.33648400 | -0.91278700 |
| H | -3.09635900 | -2.80179200 | 1.12141500 |
| Pd | -0.00964600 | -0.73151700 | -0.03951600 |
| H | 0.67751200 | 2.16503700 | 1.30978800 |
| H | 1.83814300 | -0.25471100 | 3.06573300 |
| H | 1.71286400 | 0.07387700 | 2.40278400 |
| O | -0.14919500 | 2.45838200 | 1.71930500 |
| H | -0.80381700 | 1.96075500 | 1.20208700 |
| H | 0.76444600 | 1.95137300 | -1.30020300 |
| O | 0.09726100 | 2.43751900 | -1.81191000 |
| H | -0.71971800 | 2.15312200 | -1.37711900 |
| Cl | 3.02422700 | 3.00875000 | 0.76628600 |
| Cl | -3.06398200 | 3.01578900 | -0.79057200 |

53

RR-PhCl_D1_TS1_R, E(SCF) = -3328.10207127,
E(ZPE) = -3327.730501, E(G) = -3327.800120
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.64428500 | -3.44476200 | -0.31804800 |
| H | 0.39318900 | -3.44755800 | -1.38244200 |
| H | 1.25969100 | -4.32353900 | -0.11060400 |
| C | -0.60289400 | -3.41686900 | 0.52532100 |
| H | -1.22420200 | -4.30164100 | 0.36770700 |
| H | -0.35067900 | -3.36183900 | 1.58794600 |
| N | -1.34960000 | -2.18485600 | 0.18123500 |
| N | 1.40018100 | -2.20062900 | -0.04321100 |
| C | -2.41036400 | -1.81509100 | 1.13969500 |
| H | -3.01080500 | -2.69954200 | 1.37670500 |
| C | 2.46850300 | -1.89837900 | -1.01697500 |
| H | 1.97209100 | -1.64690500 | -1.96033100 |
| C | -3.29063500 | -0.75132500 | 0.56558500 |
| C | -2.73793900 | 0.46285700 | 0.07931300 |
| C | -4.65565200 | -0.97528700 | 0.51989400 |
| C | -3.66769800 | 1.38900100 | -0.43556100 |
| C | -5.52813900 | -0.02700800 | 0.01471400 |
| H | -5.04742900 | -1.91802600 | 0.89077400 |
| C | -5.02841800 | 1.16761300 | -0.46394100 |
| H | -5.69724100 | 1.91571500 | -0.87266200 |
| C | 3.34754200 | -0.79387800 | -0.52211400 |
| C | 2.79005500 | 0.44751300 | -0.11680400 |
| C | 4.71610300 | -0.99622800 | -0.48569200 |
| C | 3.71432700 | 1.42627900 | 0.30252200 |
| C | 5.58440800 | 0.00219500 | -0.07809800 |
| H | 5.11534800 | -1.95807900 | -0.79473700 |
| C | 5.07764000 | 1.22483700 | 0.31905800 |
| H | 5.74564800 | 2.01155800 | 0.64933800 |
| O | -1.45830000 | 0.75492000 | 0.10035100 |
| O | 1.51215800 | 0.72479400 | -0.13519000 |
| S | -7.29594600 | -0.35479400 | 0.01635400 |
| S | 7.35327400 | -0.31380300 | -0.06855000 |
| O | 7.98383300 | 0.93721900 | 0.43186500 |
| O | 7.71268000 | -0.62844200 | -1.47978700 |
| O | 7.54923800 | -1.47627400 | 0.84208300 |
| O | -7.91266600 | 0.76052600 | -0.75056500 |
| O | -7.69855000 | -0.37376700 | 1.45057700 |
| O | -7.45786900 | -1.68178300 | -0.63940200 |
| H | -0.64839200 | 2.47181500 | -0.88070000 |
| H | -1.52860200 | -0.17976800 | -2.96793200 |
| H | -1.50622100 | 0.34282600 | -2.42986400 |
| O | 0.16653100 | 2.99578400 | -0.91536800 |
| H | 0.83699700 | 2.33256500 | -0.66710400 |
| H | -0.98590600 | 2.03003000 | 1.51161200 |
| O | -0.62895700 | 2.84926800 | 1.88905100 |
| H | -0.20506400 | 3.23803600 | 1.10869300 |
| H | -1.77155000 | -2.29944600 | -0.74257800 |
| H | -1.90896100 | -1.49569200 | 2.05919600 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.81837900 | -2.26630500 | 0.88641100 |
| H | 3.06920000 | -2.79809900 | -1.18617100 |
| Pd | 0.02968700 | -0.68396600 | 0.02493100 |
| Cl | 3.09689900 | 2.98509300 | 0.83604400 |
| Cl | -3.07536400 | 2.91368600 | -1.08564800 |

53

RR-PhCl_D1_TS1, E(SCF) = -3328.07428313,
E(ZPE) = -3327.703486, E(G) = -3327.771060
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.61471800 | -3.55420000 | -0.14006000 |
| H | 0.45442400 | -3.72489400 | -1.20789900 |
| H | 1.24855200 | -4.35915200 | 0.24375900 |
| C | -0.68296900 | -3.47171200 | 0.60816700 |
| H | -1.26443200 | -4.39256700 | 0.52364700 |
| H | -0.48590900 | -3.29539900 | 1.66969800 |
| N | -1.46642800 | -2.31047800 | 0.11078000 |
| N | 1.29319200 | -2.25050500 | 0.00588700 |
| C | -2.58567100 | -1.99898200 | -1.05047200 |
| H | -3.23705400 | -2.87844900 | 1.09278500 |
| C | 2.49146800 | -2.10631700 | -0.83485700 |
| H | 2.15126300 | -2.17771400 | -1.87371900 |
| C | -3.36686600 | -0.78585000 | -0.78779100 |
| C | -2.72345800 | 0.47136200 | 0.87136000 |
| C | -4.66824400 | -0.86988300 | 0.23672400 |
| C | -3.50072400 | 1.60321400 | 0.54445300 |
| C | -5.39192800 | 0.27843700 | -0.05812400 |
| H | -5.13144000 | -1.84564600 | 0.11490100 |
| C | -4.80227400 | 1.52111400 | 0.09526200 |
| H | -5.36124700 | 2.41751000 | -0.14746300 |
| C | 3.23646400 | -0.83307500 | -0.59015900 |
| C | 2.57989300 | 0.42086200 | -0.68279100 |
| C | 4.60135700 | -0.89340100 | -0.36766600 |
| C | 3.41045700 | 1.55752900 | -0.61079700 |
| C | 5.37149500 | 0.25331700 | -0.27132600 |
| H | 5.07941600 | -1.86551000 | -0.28735900 |
| C | 4.77151800 | 1.49017000 | -0.40622500 |
| H | 5.36477600 | 2.39500000 | -0.35252600 |
| O | -1.49668500 | 0.53280200 | 1.25407500 |
| O | 1.29368200 | 0.57988000 | -0.85778000 |
| S | -7.08235200 | 0.12907600 | -0.63988400 |
| S | 7.13785000 | 0.11070800 | 0.03033400 |
| O | 7.66319800 | 1.50229000 | 0.01471400 |
| O | 7.66727300 | -0.73051400 | -1.07890300 |
| O | 7.26497800 | -0.55091000 | 1.35893400 |
| O | -7.55178000 | 1.51971300 | -0.88891400 |
| O | -7.83077400 | -0.55394700 | 0.45370400 |
| O | -7.01458300 | -0.69567600 | -1.87972000 |
| H | -0.22304300 | 1.74048700 | 1.62216800 |
| H | -1.37871400 | 0.14510400 | -1.78147300 |
| H | -1.38276300 | 0.68950500 | -1.24258100 |
| O | 0.69732800 | 2.06275400 | 1.71168400 |
| H | 1.01516800 | 2.00584200 | 0.79958200 |
| H | -0.16256200 | -0.52330600 | 2.34618500 |
| O | 0.76518600 | -0.69531500 | 2.58309100 |
| H | 1.14544500 | 0.18436300 | 2.41531800 |
| H | -1.87613900 | -2.55733500 | -0.79166900 |
| H | -2.12625200 | -1.87414800 | 2.03520300 |
| H | 1.51409600 | -2.06540500 | 0.99382100 |
| H | 3.15656700 | -2.95632900 | -0.64647600 |
| Pd | -0.10332900 | -0.80103800 | -0.36468100 |
| Cl | 2.67113800 | 3.14242900 | -0.81784400 |
| Cl | -2.74268500 | 3.18769000 | 0.70167300 |

53

RR-PhCl_D1_TS2_P, E(SCF) = -3328.10813527,
E(ZPE) = -3327.733754, E(G) = -3327.803678
a.u.

| | | | |
|---|-------------|-------------|------------|
| C | 0.56967800 | -3.16602900 | 1.11131500 |
| H | 0.31131700 | -3.59817400 | 0.13898200 |
| H | 1.12238400 | -3.92799400 | 1.67121100 |
| C | -0.68047800 | -2.76441000 | 1.85068500 |
| H | -1.29807800 | -3.63645700 | 2.08835000 |
| H | -0.41954000 | -2.27144400 | 2.79235600 |
| N | -1.46006300 | -1.78396000 | 1.04960900 |
| N | 1.38527800 | -1.96816400 | 0.86207100 |
| C | -2.58026100 | -1.23905000 | 1.85884600 |

| | | | | | | | |
|----|-------------|-------------|--------------|--|-------------|-------------|-------------|
| H | -3.16337100 | -2.08605900 | 2.24065600 | O | -1.63246900 | 0.33125800 | 2.33480100 |
| C | 2.38616100 | -2.13076400 | -0.19848000 | O | 1.07077900 | 0.35460200 | -1.18536500 |
| H | 1.82973800 | -2.35312300 | -1.11784400 | S | -6.39484900 | 0.45780700 | -1.18863000 |
| C | -3.47572500 | -0.34195900 | 1.06813200 | S | 6.87080500 | 0.45875900 | 0.03336400 |
| C | -3.42330400 | 1.05360800 | 1.18339100 | O | 7.52175600 | 0.99457600 | -1.19441600 |
| C | -4.37595800 | -0.92345000 | 0.18252600 | O | 7.27596400 | -0.93677600 | 0.35076500 |
| C | -4.30204900 | 1.80705700 | 0.39214700 | O | 6.98927000 | 1.38472900 | 1.19328400 |
| C | -5.21575100 | -0.15666800 | -0.59728800 | O | -6.65581600 | -0.94846000 | -1.60306400 |
| H | -4.42652100 | -2.00539400 | 0.10304200 | O | -6.02394800 | 1.34315700 | -2.32968700 |
| C | -5.18380700 | 1.22474800 | -0.48855700 | O | -7.49223800 | 1.03507400 | -0.36019800 |
| H | -5.83989300 | 1.84675400 | -1.08706900 | H | -0.27440300 | 1.43464200 | 1.80829900 |
| C | 3.24687800 | -0.91465500 | -0.37777400 | H | -1.38127400 | 0.08192700 | -1.37368300 |
| C | 2.69308400 | 0.36612400 | -0.63963700 | H | -1.75364900 | 0.01571200 | -0.65879900 |
| C | 4.62507500 | -1.08629200 | -0.34754500 | O | 0.60842200 | 1.75766100 | 1.52804300 |
| C | 3.63052800 | 1.39506300 | -0.90648400 | H | 0.62812400 | 1.60372500 | 0.57303900 |
| C | 5.49777600 | -0.04519500 | -0.59477800 | H | -0.06679300 | -0.71741600 | 2.56303800 |
| H | 5.03197300 | -2.07054100 | -0.13987200 | O | 0.89281400 | -0.90742500 | 2.56501200 |
| C | 4.99170700 | 1.21398600 | -0.87944300 | H | 1.23692200 | -0.04042300 | 2.29079400 |
| H | 5.65363000 | 2.40792900 | -1.108705400 | H | -2.00861700 | -2.81862300 | -0.56590600 |
| O | -2.61239900 | 1.72448100 | 2.00057500 | H | -2.02015700 | -2.06960800 | 2.25096400 |
| O | 1.42218800 | 0.66106200 | -0.67018800 | H | 1.38668400 | -2.06832700 | 1.02917900 |
| S | -6.40458000 | -0.91913900 | -1.71502300 | H | 3.12146300 | -2.99241800 | -0.49974100 |
| S | 7.27682900 | -0.27622300 | -0.52437800 | Pd | -0.24708900 | -1.02366100 | -0.48842800 |
| O | 7.80378600 | 0.23959200 | -1.81923200 | Cl | 2.25915100 | 3.00371800 | -1.32184700 |
| O | 7.49054500 | -1.73831300 | -0.34585300 | Cl | -2.75637900 | 3.05920300 | 1.90770200 |
| O | 7.74529500 | 0.52864400 | 0.63970700 | | | | |
| O | -6.07602600 | -2.36923100 | -1.71642400 | 53 | | | |
| O | -6.19030300 | -0.26281900 | -3.03322900 | RR-PhCl_D1_TS2, E(SCF) = -3328.07394215, | | | |
| O | -7.74234700 | -0.61878500 | -1.13421400 | E(ZPE) = -3327.703314, E(G) = -3327.773233 | | | |
| H | 1.07786500 | 3.13083500 | 1.55658000 | a.u. | | | |
| H | -1.15899000 | 0.44675500 | -0.40396800 | C | 0.59048100 | -3.34070400 | 0.25869800 |
| H | -1.90105400 | 1.19044500 | 2.42590100 | H | 0.36691400 | -3.57491200 | -0.78576800 |
| O | 1.26793600 | 2.19692400 | 1.67602000 | H | 1.14135600 | -4.18325500 | 0.68515200 |
| H | 1.25186600 | 1.80788300 | 0.77858500 | H | -0.66618400 | -3.05890800 | 1.03136300 |
| H | -0.33946000 | 0.96976900 | 4.16954200 | C | -1.32716400 | -3.92865300 | 1.06123000 |
| O | -0.42126900 | 0.70981400 | 3.24829800 | H | -0.42150800 | -2.78944300 | 2.06355800 |
| H | 0.23952900 | 1.24284500 | 2.75373900 | N | -1.37380300 | -1.89465600 | 0.43367700 |
| H | -1.86762800 | -2.27720800 | 0.25401000 | N | 1.41355700 | -2.11433600 | 0.27457700 |
| H | -2.13271400 | -0.74172300 | 2.71897500 | C | -2.43267400 | -1.40299500 | 1.36526200 |
| H | 1.84284000 | -1.67341100 | 1.72283600 | H | -2.95415400 | -2.28696600 | 1.74895700 |
| H | 3.02801900 | -2.99696800 | 0.00510500 | C | 2.53362700 | -2.12315900 | -0.68552700 |
| Pd | -0.06191300 | -0.50768700 | 0.16466200 | H | 2.08583100 | -2.16804500 | -1.68454100 |
| Cl | 3.00679100 | 2.99608100 | -1.29840000 | C | -3.42985900 | -0.46968600 | 0.75599300 |
| Cl | -4.26249400 | 3.55544300 | 0.52335900 | C | -3.15302500 | 0.91653700 | 0.69720300 |
| | | | | C | -4.65614300 | -0.96468600 | 0.33001100 |
| | | | | C | -4.18363100 | 1.74018800 | 0.19583000 |
| | | | | C | -5.63059000 | -0.12008700 | -0.16390900 |
| | | | | H | -4.86105400 | -2.02924700 | 0.38724500 |
| | | | | C | -5.39732500 | 1.24718400 | -0.22250000 |
| | | | | H | -6.15567600 | 1.92176600 | -0.60572200 |
| | | | | C | 3.42203100 | -0.93061500 | -0.52787200 |
| | | | | C | 2.90004600 | 0.38212600 | -0.61434700 |
| | | | | C | 4.78298400 | -1.13971600 | -0.35302300 |
| | | | | C | 3.85317600 | 1.42512700 | -0.58242400 |
| | | | | C | 5.67344000 | -0.08660900 | -0.29914500 |
| | | | | H | 5.16201800 | -2.15309000 | -0.27457000 |
| | | | | C | 5.20167300 | 1.21091000 | -0.42169100 |
| | | | | H | 5.88221800 | 2.05534900 | -0.39713300 |
| | | | | O | -1.98773800 | 1.38970700 | 1.03879300 |
| | | | | O | 1.63214700 | 0.67754000 | -0.75800000 |
| | | | | S | -7.22600500 | -0.75178200 | -0.70097700 |
| | | | | S | 7.42967900 | -0.36184300 | -0.03423200 |
| | | | | O | 8.12222400 | 0.38397100 | -1.12126800 |
| | | | | O | 7.62265300 | -1.83480900 | -0.11614100 |
| | | | | O | 7.72374100 | 0.19395700 | 1.31659800 |
| | | | | O | -7.12041500 | -2.23360500 | -0.62005500 |
| | | | | O | -7.41040800 | -0.25048600 | -2.09137100 |
| | | | | O | -8.22390200 | -0.18190300 | 0.24709100 |
| | | | | H | -0.59014200 | 2.71980800 | 0.67510900 |
| | | | | H | -0.90712600 | 0.59565600 | -0.84183000 |
| | | | | H | -1.14378600 | 0.82152000 | -0.00551800 |
| | | | | O | 0.33931600 | 2.99866700 | 0.70745600 |
| | | | | H | 0.81073100 | 2.40853100 | 0.09611100 |
| | | | | H | -0.76775900 | 1.09059000 | 2.52170600 |
| | | | | O | 0.09241200 | 1.19518300 | 2.96050500 |
| | | | | H | 0.51058500 | 1.84723400 | 2.37640400 |
| | | | | H | -1.82988700 | -2.19614700 | -0.42847200 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|--|--|--|
| 53 | | | | | | | |
| RR-PhCl_D1_TS2_R, E(SCF) = -3328.08003006, | | | | | | | |
| E(ZPE) = -3327.707188, E(G) = -3327.775172 | | | | | | | |
| a.u. | | | | | | | |
| C | 0.60056200 | -3.68786800 | -0.01682600 | | | | |
| H | 0.42205500 | -3.92340400 | -1.06921800 | | | | |
| H | 1.29142100 | -4.43345200 | 0.38770400 | | | | |
| C | -0.67601400 | -3.63584300 | 0.76842300 | | | | |
| H | -1.22875000 | -4.57626600 | 0.72159900 | | | | |
| H | -0.45185500 | -3.43220500 | 1.81874000 | | | | |
| N | -1.51406400 | -2.51015700 | 0.27265600 | | | | |
| N | 1.20735100 | -2.34115000 | 0.04829100 | | | | |
| C | -2.54369000 | -2.13087000 | 1.29569000 | | | | |
| H | -3.26147700 | -2.95614000 | 1.34982300 | | | | |
| C | 2.41546600 | -2.20493000 | -0.78299700 | | | | |
| H | 2.10418200 | -2.39723200 | -1.81604500 | | | | |
| C | -3.22215400 | -0.84073700 | 1.00945900 | | | | |
| C | -2.66885100 | 0.34368000 | 1.59461600 | | | | |
| C | -4.33851100 | -0.80256900 | 0.18754800 | | | | |
| C | -3.36151300 | 1.54161700 | 1.24170600 | | | | |
| C | -4.95324300 | 0.39427200 | -0.12565100 | | | | |
| H | -4.73565600 | -1.72474600 | -0.22753400 | | | | |
| C | -4.45399800 | 1.57705800 | 0.41145700 | | | | |
| H | -4.92494200 | 2.52723100 | 0.17993600 | | | | |
| C | 3.07742500 | -0.87181300 | -0.65279500 | | | | |
| C | 2.35424800 | 0.30993400 | -0.92274900 | | | | |
| C | 4.43132800 | -0.81319000 | -0.35280100 | | | | |
| C | 3.09770200 | 1.50984900 | -0.92965600 | | | | |
| C | 5.11465500 | 0.38319600 | -0.34570400 | | | | |
| H | 4.97044300 | -1.73217100 | -0.13472400 | | | | |
| C | 4.44268800 | 1.55740600 | -0.64881100 | | | | |
| H | 4.96409200 | 2.50851200 | -0.66053800 | | | | |

H -1.91449900 -0.93407400 2.20479400
H 1.78043000 -1.96085600 1.21528800
H 3.12008700 -3.03702500 -0.54557100
Pd 0.12503500 -0.56631500 -0.17680800
Cl 3.28643700 3.07821600 -0.77127200
Cl -3.87729000 3.46869300 0.08773900

53

RR-PhCl_D2_TS1_P, E(SCF) = -3328.07509429,
E(ZPE) = -3327.704094, E(G) = -3327.775319
a.u.

C -0.79611700 -3.15559500 -1.09620700
H -0.56108000 -3.63117600 -0.13959100
H -1.47534300 -3.80426200 -1.65438200
C 0.46086100 -2.85215600 -1.85872000
H 1.03412500 -3.75858400 -2.07411800
H 0.23302600 -2.34264900 -2.80022400
N 1.28003000 -1.93910900 -1.03016100
N -1.45228800 -1.86013500 -0.79872700
C 2.47046000 -1.43734300 -1.75944500
H 2.11756200 -0.85487000 -2.61377300
C -2.56658800 -1.94191100 0.17378400
H -3.24260800 -2.74580700 -0.13351600
C 3.35520600 -0.61686400 -0.88312300
C 3.82671600 -1.20498200 0.32622400
C 3.64525700 0.69483700 -1.21617400
C 4.57749300 -0.33139100 1.15652500
C 4.39518800 1.49574000 -0.37121300
H 3.26332000 1.11393000 -2.14234400
C 4.86166600 0.97372300 0.82824500
H 5.43868000 1.59032200 1.50942700
C -3.31676900 -0.65198200 0.25354600
C -2.63066000 0.53918000 0.58572700
C -4.68519100 -0.64039300 0.02619000
C -3.42109400 1.70391800 0.69701200
C -5.41860400 0.52343100 0.14650200
H -5.19492400 -1.56096800 -0.23813900
C -4.77992800 1.70615200 0.48883700
H -5.33995500 2.62988500 0.58715300
O 3.55552200 -2.41790900 0.64637900
O -1.34792400 0.60747700 0.82323900
S 4.82314000 3.17719200 -0.82409100
S -7.19040000 0.54860900 -0.15493900
O -7.80119600 1.08571400 1.09248800
O -7.57238800 -0.86130300 -0.43591600
O -7.38501400 1.45397200 -1.32159800
O 6.26861600 3.15023500 -1.19243200
O 4.56353800 4.00588800 0.38700500
O 3.94100000 3.52504400 -1.97239000
H -2.12041100 -2.22615900 1.13339700
H 2.99599700 -2.32211000 -2.14446500
H -1.80610500 -1.45542100 -1.66862100
H 1.63146500 -2.47245700 -0.22270400
H 3.28780100 -3.90208500 -0.29361400
O 2.91549400 -4.68824600 -0.74438400
H 3.58435900 -4.95576600 -1.37812500
H 2.15430500 -2.86501300 1.68503200
O 1.24439500 -3.15658200 1.90005400
H 0.82822400 -2.39008300 2.30417200
Pd -0.00597100 -0.57968300 -0.12071000
H 1.18732200 0.31379000 0.85164800
H 1.27030200 0.65573300 0.11560100
Cl 5.16464300 -0.96606500 2.69347500
Cl -2.62659500 3.21139300 1.12362600

53

RR-PhCl_D2_TS1_R, E(SCF) = -3328.09858829,
E(ZPE) = -3327.729637, E(G) = -3327.800133
a.u.

C -0.83675800 -3.45829900 0.74507300
H -0.69345100 -3.38629900 1.82692000
H -1.44591600 -4.34252600 0.53699300
C 0.48793400 -3.51811900 0.02645800
H 1.07070300 -4.39401600 0.32035900
H 0.32357200 -3.57373600 -1.05378200
N 1.24298400 -2.27061900 0.29578300
N -1.52883700 -2.22470700 0.30373000

C 2.22481700 -1.94264500 -0.74824200
H 1.65469000 -1.77559800 -1.67052000
C -2.75564300 -1.88542000 1.05481400
H -3.43010500 -2.74800400 1.05855800
C 3.09473600 -0.75871200 -0.42922300
C 2.63184700 0.39243300 0.25315700
C 4.40503900 -0.81076200 -0.89310100
C 3.57909300 1.42855800 0.42965700
C 5.28468000 0.23577600 -0.71676000
H 4.75016800 -1.69835000 -1.41337900
C 4.86859500 1.37021500 -0.03740800
H 5.54490400 2.20153400 0.12909900
C -3.44321400 -0.70133500 0.44953600
C -2.75305000 0.52986000 0.33868200
C -4.75951100 -0.81094500 0.02707400
C -3.48909400 1.61364300 -0.18680400
C -5.43841300 0.27699800 -0.48768800
H -5.27496500 -1.76235500 0.10897100
C -4.79850200 1.50331100 -0.51704000
H -5.31676500 2.36722100 -0.99404900
O 1.43315400 0.55656100 0.75885600
O -1.51577000 0.70587400 0.71468400
S 6.97678800 0.14753000 -1.31720100
S -7.14251300 0.13573900 -1.04056600
O -7.91658700 1.10301900 -0.21308600
O -7.52799800 -1.28132400 -0.80076100
O -7.12972000 0.50442200 -2.48410700
O 7.83916400 0.19164400 -0.10296900
O 7.15491600 1.34359900 -2.18688100
H 7.07618800 -1.13828300 -2.05893600
H -2.44614000 -1.69377400 2.08763000
H 2.86647400 -2.81364200 -0.92336900
H -1.76956600 -2.31270100 -0.68487300
H 1.69891400 -2.30754400 1.21765500
H 1.80267900 -0.43311300 2.54312100
O 1.99073500 -1.29121600 2.95492100
H 2.82807800 -1.17581700 3.41162700
H 0.71446500 1.88984500 2.07919100
O -0.06638500 2.17637800 2.57703000
H -0.78050500 1.80669800 2.03094200
Pd -0.11197100 -0.75988700 0.47201800
H 0.39838800 1.01297400 -1.78575300
H 0.09872000 0.72394800 -2.40988800
Cl 3.07184100 2.86426800 1.31106300
Cl -2.67819300 3.16821300 -0.32708800

53

RR-PhCl_D2_TS1, E(SCF) = -3328.06604264,
E(ZPE) = -3327.697576, E(G) = -3327.769264
a.u.

C -0.83454700 -3.26557800 0.46347000
H -0.65564700 -3.19325500 1.53946500
H -1.45059300 -4.14535100 0.26491200
C 0.47542300 -3.30750700 -0.27877400
H 1.07074000 -4.17875100 0.01097400
H 0.32263000 -3.34404800 -1.36130200
N 1.19468700 -2.05838000 0.05162100
N -1.54772600 -2.03423800 0.05285400
C 2.48227800 -1.92092100 -0.63588200
H 2.26706300 -1.82477400 -1.70605500
C -2.64498100 -1.61488700 0.95301300
H -3.27807700 -2.48181400 1.16777200
C 3.38284200 -0.79514100 -0.18207600
C 3.04134600 0.16713400 0.81054300
C 4.61907500 -0.74857700 -0.81358000
C 4.03511300 1.15451700 1.05422900
C 5.54970100 0.22944300 -0.52631700
H 4.85980600 -1.49477200 -1.56573900
C 5.25605700 1.19369100 0.42850900
H 5.97081900 1.97396100 0.66529600
C -3.47237900 -0.53171900 0.33554200
C -2.86912700 0.67210800 -0.09606800
C -4.84290700 -0.71421900 0.21424900
C -3.73705900 1.65684900 -0.61357600
C -5.65436700 0.27644600 -0.30163400
H -5.29241500 -1.64611900 0.54027400
C -5.09652300 1.47684300 -0.71474800

H -5.71811200 2.26747500 -1.12129000
O 1.91161800 0.18415200 1.43249300
O -1.58616500 0.92291300 -0.01964200
S 7.17057400 0.21565100 -1.29449300
S -7.42869500 0.03561200 -0.47145300
O -8.05835600 1.14859400 0.29150000
O -7.71001900 -1.30636400 0.10523700
O -7.70433000 0.11657400 -1.93283700
O 8.09417800 -0.38543600 -0.28911000
O 7.49543200 1.64050600 -1.58376900
O 7.03301800 -0.16588900 -2.52196200
H -2.17560700 -1.30149600 1.89260100
H 3.02044000 -2.87178200 -0.51596000
H -1.92476000 -2.15948000 -0.88855400
H 1.34116800 -2.05257400 1.07023400
H 1.35447900 -0.95807000 2.65564100
O 0.92903500 -1.79006900 2.95420600
H 1.45619600 -2.11046600 3.68963000
H 0.72322900 1.46652500 2.03635000
O -0.08389900 1.96420100 2.26627900
H -0.70353000 1.74942900 1.55319600
Pd -0.16722500 -0.52767100 -0.12193900
H 1.03917300 1.01567400 -0.53272800
H 0.91318600 0.71274100 -1.23782700
Cl 3.65780200 2.39894000 2.24550600
Cl -3.04311800 3.18186000 -1.14106300

53
RR-PhCl_D2_TS2_P, E(SCF) = -3328.09533901,
E(ZPE) = -3327.723288, E(G) = -3327.796546
a.u.
C -0.21092900 -2.31702700 0.65001800
H 0.07580000 -1.95047000 1.64067200
H -0.47182000 -3.37577300 0.74683200
C 0.92043800 -2.12606800 -0.32828300
H 1.79744800 -2.72103800 -0.04986000
H 0.60701600 -2.43533500 -1.32952700
N 1.27909500 -0.68578100 -0.38413300
N -1.35464200 -1.51427200 0.18806500
C 2.28850800 -0.38227400 -1.44461300
H 1.89146900 0.39829900 -2.09521600
C -2.41862200 -1.30721600 1.18032900
H -2.75322500 -2.26600700 1.59416100
C 3.60441900 0.26072600 -0.84854600
C 3.75717900 1.25759400 -0.23837400
C 4.66670600 -0.88762600 -0.85106600
C 4.99303000 1.57244500 0.33284900
C 5.87810800 -0.55481900 -0.27861500
H 4.54764600 -1.85880000 -1.31995600
C 6.04424300 0.68276300 0.32093800
H 6.98881100 0.95770500 0.77684500
C -3.58781200 -0.58922500 0.57612400
C -3.43117800 0.70670800 0.01110900
C -4.83215600 -1.19335300 0.60372900
C -4.61083100 1.31568300 -0.46451000
C -5.96061300 -0.55731000 0.11024300
H -4.92528400 -2.18677100 1.03408300
C -5.84976900 0.71281000 -0.42229500
H -6.72563400 1.22141400 -0.80780800
O 2.78680700 2.18168100 -0.16639400
O -2.29768800 1.34948000 -0.05838300
S 7.25366300 -1.72012400 -0.25881600
S -7.54628200 -1.39727200 0.17553100
O -7.80742300 -1.65977600 1.61909400
O -7.36973500 -2.65322000 -0.60707000
O -8.52751400 -0.46016800 -0.43590200
O 8.41408200 -0.96695500 -0.80581100
O 6.82741200 -2.85734600 -1.11541000
O 7.43090300 -2.09304700 1.17123900
H -1.97592000 -0.73028200 2.00099300
H 2.41868000 -1.26971900 -2.06594700
H -1.75633300 -1.94364600 -0.64434100
H 1.69487400 -0.45685200 0.53077100
H 2.12693800 0.91465600 2.50645200
O 2.21562000 -0.02051500 2.29769500
H 3.12045500 -0.24419900 2.53619600
H -0.48358400 3.67421200 0.51908400

O -1.41317700 3.91561200 0.53933900
H -1.86267600 3.08264400 0.29982500
Pd -0.49682000 0.38753100 -0.30958300
H 1.90997800 1.84898900 -0.43957300
H 0.18860900 1.77586300 -0.65082500
Cl 5.19626400 3.13110600 1.10493600
Cl -4.48611200 2.93280900 -1.15190200

53
RR-PhCl_D2_TS2_R, E(SCF) = -3328.06980033,
E(ZPE) = -3327.698432, E(G) = -3327.769008
a.u.
C -0.37225000 -2.65301500 0.63787600
H -0.03871100 -2.29475700 1.61574600
H -0.80870800 -3.64632100 0.76334500
C 0.77611000 -2.65366600 -0.33896800
H 1.58020200 -3.31781600 -0.00826000
H 0.45077400 -2.97692600 -1.33127500
N 1.26045800 -1.25936700 -1.43203800
N -1.39408100 -1.69869000 0.14398300
C 2.41040400 -1.03218000 -1.35894300
H 2.03740200 -0.48612700 -2.22845000
C -2.38734200 -1.26511300 -1.25181100
H -2.78298700 -2.14667200 1.66622900
C 3.54782800 -0.31575800 -0.69139300
C 3.31686200 0.93118900 -0.04338300
C 4.81544600 -0.87658300 -0.72536700
C 4.45415800 1.51249700 0.57314500
C 5.89561600 -0.24825200 -0.13313200
H 4.97202300 -1.82700800 -1.22586500
C 5.71019000 0.95703300 0.52991100
H 6.54249300 1.45432500 1.01710500
C -3.51258800 -0.50658800 0.51848000
C -3.25721900 0.64895600 -0.25675800
C -4.81496200 -0.93859800 0.72826400
C -4.38896500 1.32878200 -0.75620600
C -5.89208100 -0.24481300 0.21438800
H -4.99655300 -1.83175900 1.31655600
C -5.67712400 0.90399900 -0.53156500
H -6.51064500 1.46308300 -0.94284700
O 2.14849500 1.47332100 0.03107600
O -2.06295500 1.12448400 -0.50760800
S 7.54027300 -0.96284900 -0.19326300
S -7.57782000 -0.81973100 0.46153100
O -7.47168400 -2.01709900 1.33761100
O -8.09572400 -1.13270400 -0.89970000
O -8.30016200 0.31549800 1.09962800
O 8.39887200 0.04974000 -0.87172200
O 7.40663800 -2.22758100 -0.96725300
O 7.94249500 -1.18627700 1.22511500
H -1.84085100 -0.66578000 1.88887400
H 2.75599300 -2.00441800 -1.72026500
H -1.88944100 -2.11860300 -0.64519300
H 1.54529400 -0.97882400 0.51846800
H 1.62040600 0.69555500 1.72979700
O 1.43566200 -0.09509900 2.26928700
H 2.15843900 -0.14720300 2.90048700
H 0.70808800 2.56922100 0.76155300
O -0.14010500 2.92222500 1.07436400
H -0.81773000 2.41287300 0.60605800
Pd -0.42398500 -0.07262700 -0.63999400
H 0.81691800 1.23634900 -1.02172300
H 0.21069100 1.25291600 -1.60280000
Cl -4.13034500 2.78731400 -1.70018500
Cl 4.21796800 3.02603900 1.44553300

53
RR-PhCl_D2_TS2_TS, E(SCF) = -3328.06937299,
E(ZPE) = -3327.699582, E(G) = -3327.769948
a.u.
C -0.40464900 -2.72438100 0.57768000
H -0.08380400 -2.38024200 1.56544700
H -0.84220700 -3.71961000 0.68439800
C 0.76361700 -2.71753800 -0.37633100
H 1.55086900 -3.40112700 -0.04443700
H 0.45465700 -3.01400700 -1.38227400
N 1.27041400 -1.32894300 -0.43055000

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| N | -1.41479600 | -1.76056100 | 0.08111200 | C | -4.74008000 | 1.66264000 | 0.69507700 |
| C | 2.43194900 | -1.10467800 | -1.34029000 | H | -5.26944400 | 2.57946000 | 0.93319700 |
| H | 2.06393600 | -0.60697100 | -2.24041900 | O | 3.56875300 | -2.41124000 | 0.68708200 |
| C | -2.41000500 | -1.32764600 | 1.08392500 | O | -1.36110200 | 0.39285200 | 0.96941400 |
| H | -2.83098800 | -2.20817000 | 1.58045100 | S | 4.85902500 | 3.12218600 | -1.03213900 |
| C | 3.54122400 | -0.33420900 | -0.68020500 | S | -7.15253100 | 0.73916900 | -0.24760900 |
| C | 3.29187400 | 0.91470100 | -0.05365000 | O | -7.82136700 | 1.00578300 | 1.05811000 |
| C | 4.82328700 | -0.86595500 | -0.69877800 | O | -7.55365700 | -0.55999600 | -0.85422900 |
| C | 4.40688300 | 1.53267800 | 0.55813600 | O | -7.27638100 | 1.88703800 | -1.19088600 |
| C | 5.88633400 | -0.20676700 | -0.11206500 | O | 5.63547600 | 2.93811400 | -2.28800000 |
| H | 5.00306700 | -1.82175300 | -1.18072400 | O | 5.64971900 | 3.73568800 | 0.06621200 |
| C | 5.67489100 | 1.00363000 | 0.53131500 | O | 3.54423400 | 3.78094900 | -1.25620000 |
| H | 6.49345300 | 1.52536200 | 1.01554100 | H | -2.25048400 | -2.42512400 | 0.74465000 |
| C | -3.51461600 | -0.53029400 | 0.45974800 | H | 3.09114100 | -2.39444600 | -2.13069300 |
| C | -3.23435300 | 0.63686800 | -0.29834100 | H | -1.87579700 | -1.33367300 | -1.93360000 |
| C | -4.82379100 | -0.92620800 | 0.67322200 | H | 1.55696900 | -2.70355600 | -0.45992600 |
| C | -4.35131800 | 1.35125800 | -0.77333100 | H | 1.16206900 | -1.44399700 | 2.00278000 |
| C | -5.89077300 | -0.19251600 | 0.18185700 | H | 2.96201700 | -4.27511700 | 0.04700100 |
| H | -5.01577200 | -1.82175300 | 1.24866800 | O | 2.07611200 | -4.64724700 | -0.05002400 |
| C | -5.65273300 | 0.95940300 | -0.54311100 | H | 2.17591000 | -5.41151200 | -0.62290400 |
| H | -6.48044200 | 1.54062000 | -0.93182200 | H | 3.05548700 | -2.40067300 | 1.53192100 |
| O | 2.11118200 | 1.45595400 | 0.02500700 | O | 1.68554100 | -2.04391000 | 2.56676500 |
| O | -2.03204700 | 1.08874300 | -0.55031600 | H | 1.10284200 | -2.78624200 | -2.75349800 |
| S | 7.54638000 | -0.89150800 | -0.15218000 | Pd | 0.00440100 | -0.70930300 | -0.09467200 |
| S | -7.56875600 | -0.75665200 | 0.49357700 | H | 1.16254200 | 0.02943400 | 0.65707600 |
| O | -7.71545800 | -0.78206100 | 1.97551700 | Cl | -2.57986900 | 2.93572900 | 1.69697800 |
| O | -7.65315300 | -2.11183900 | -0.11118300 | Cl | 5.16774600 | -0.88224700 | 2.68540500 |
| O | -8.45800600 | 0.23592500 | -0.16741400 | | | | |
| O | 8.38472100 | 0.12522000 | -0.84802100 | 53 | | | |
| O | 7.43804700 | -2.17313000 | -0.90078200 | RR-PhCl_D2_TS2W_R, E(SCF) = -3328.07520683, | | | |
| O | 7.94358900 | -1.07683300 | 1.27222600 | E(ZPE) = -3327.704132, E(G) = -3327.773729 | | | |
| H | -1.86081500 | -0.75210400 | 1.83827100 | a.u. | | | |
| H | 2.81617400 | -2.07946300 | -1.65302700 | C | -0.75566700 | -3.25708400 | -1.41999700 |
| H | -1.90493900 | -2.16938200 | -0.71618900 | H | -0.58736900 | -3.86264900 | -0.52485600 |
| H | 1.54738900 | -1.07216500 | 0.52892600 | H | -1.42824200 | -3.80428600 | -2.08549800 |
| H | 1.58148200 | 0.63499200 | 1.75870700 | C | 0.54219000 | -2.91062000 | -2.09006700 |
| O | 1.42028300 | -0.18025000 | 2.26469900 | H | 1.08446800 | -3.80665800 | -2.40643100 |
| H | 2.12230200 | -0.21737600 | 2.91997300 | H | O.36222600 | -2.29194200 | -2.97376900 |
| H | 0.64099000 | 2.55834400 | 0.81666200 | N | 1.36866600 | -2.12884200 | -1.13843100 |
| O | -0.22816300 | 2.84835400 | 1.13090900 | N | -1.37917800 | -1.98512000 | -0.98683000 |
| H | -0.86695200 | 2.33923700 | 0.60845800 | C | 2.56373500 | -1.55682700 | -1.81932800 |
| Pd | -0.40054700 | -0.12448600 | -0.65331400 | H | 2.20926900 | -1.06591700 | -2.72817200 |
| H | 0.99463000 | 1.16459800 | -0.87069900 | C | -2.56623600 | -2.15156300 | -0.11744100 |
| H | 0.33647200 | 1.18953000 | -1.47042200 | H | -3.26654300 | -2.83719000 | -0.60470100 |
| Cl | 4.13271600 | 3.05080100 | 1.40608300 | C | 3.33642300 | -0.58893900 | -0.99141100 |
| Cl | -4.06451200 | 2.82088000 | -1.69450400 | C | 4.02366500 | -1.06202500 | 0.16709300 |
| | | | | C | 3.34126000 | 0.74951900 | -1.33735100 |
| | | | | C | 4.68782700 | -0.05228800 | 0.91182100 |
| | | | | C | 4.00900300 | 1.69095900 | -0.56718600 |
| | | | | H | 2.79817000 | 1.07080600 | -2.22291000 |
| | | | | C | 4.68514000 | 1.28195900 | 0.57003200 |
| | | | | H | 5.20409700 | 2.00836600 | 1.18440500 |
| | | | | C | -3.23786800 | -0.84518900 | 0.15395900 |
| | | | | C | -2.50563200 | 0.19906900 | 0.76436900 |
| | | | | C | -4.58039400 | -0.68316300 | -0.15473100 |
| | | | | C | -3.22657400 | 1.37682500 | 1.05941100 |
| | | | | C | -5.24411100 | 0.48880600 | 0.14971000 |
| | | | | H | -5.12714300 | -1.49023400 | -0.63097400 |
| | | | | C | -4.56185700 | 1.52600100 | 0.76821600 |
| | | | | H | -5.06888700 | 2.45280700 | 1.01565400 |
| | | | | O | 4.00036900 | -2.28888000 | 0.53269500 |
| | | | | O | -1.24467300 | 0.11392900 | 1.09350900 |
| | | | | S | 3.97490300 | 3.41523000 | -1.05651100 |
| | | | | S | -6.98563700 | 0.70366300 | -0.24003900 |
| | | | | O | -7.66085900 | 0.95519200 | 1.06371100 |
| | | | | O | -7.41276100 | -0.56616800 | -0.88694400 |
| | | | | O | -7.05092800 | 1.87915100 | -1.15229800 |
| | | | | O | 4.60442300 | 3.47160100 | -2.40756100 |
| | | | | O | 4.75217600 | 4.15011600 | -0.02072800 |
| | | | | O | 2.53484600 | 3.80271400 | -1.08976700 |
| | | | | H | -2.21076300 | -2.62898000 | 0.80189600 |
| | | | | H | 3.18764900 | -2.41035400 | -2.11873500 |
| | | | | H | -1.64842600 | -1.44311100 | -1.81056900 |
| | | | | H | 1.71126900 | -2.81452800 | -0.45157900 |
| | | | | H | 1.34053300 | -0.45066900 | 1.16640400 |
| | | | | H | 3.24952000 | -3.81993800 | 0.21053200 |
| | | | | O | 2.51810900 | -4.47201700 | 0.14731900 |

| | | | | | | | |
|---|-------------|-------------|-------------|--|--|--|--|
| 53 | | | | | | | |
| RR-PhCl_D2_TS2W_P, E(SCF) = -3328.09943674, | | | | | | | |
| E(ZPE) = -3327.727681, E(G) = -3327.799741 | | | | | | | |
| a.u. | | | | | | | |
| C | -0.87767200 | -3.07160400 | -1.50735100 | | | | |
| H | -0.71282400 | -3.66905400 | -0.60433300 | | | | |
| H | -1.49115700 | -3.66543700 | -2.19346900 | | | | |
| C | 0.44420000 | -2.71378100 | -2.13574900 | | | | |
| H | 0.96814600 | -3.60695100 | -2.49169500 | | | | |
| H | 0.28740400 | -2.05041200 | -2.99187700 | | | | |
| N | 1.28412700 | -1.99237200 | -1.14584800 | | | | |
| N | -1.54849600 | -1.82706700 | -1.10763500 | | | | |
| C | 2.53079700 | -1.51433200 | -1.78522600 | | | | |
| H | 2.24755000 | -0.94040900 | -2.67019000 | | | | |
| C | -2.66885700 | -1.99103100 | -0.17196500 | | | | |
| H | -3.40234300 | -2.70563200 | -0.56577700 | | | | |
| C | 3.38597100 | -0.65875500 | -0.90580100 | | | | |
| C | 3.85239700 | -1.13784400 | 0.32256400 | | | | |
| C | 3.70584200 | 0.63024100 | -1.29430600 | | | | |
| C | 4.59933100 | -0.29250300 | 1.13610600 | | | | |
| C | 4.46428100 | -1.29251800 | -0.47443900 | | | | |
| H | 3.34177700 | 1.00691300 | -2.24545600 | | | | |
| C | 4.90751500 | 1.00019200 | 0.75149400 | | | | |
| H | 5.49300300 | 1.64504900 | 1.39514500 | | | | |
| C | -3.34632100 | -0.68310700 | 0.10512100 | | | | |
| C | -2.62442600 | 0.40314200 | 0.67339600 | | | | |
| C | -4.70108000 | -0.56540400 | -0.16980000 | | | | |
| C | -3.39623600 | 1.55814300 | 0.96030900 | | | | |
| C | -5.40268900 | 0.59001900 | 0.11693400 | | | | |
| H | -5.23093500 | -1.40313800 | -0.61196600 | | | | |

H 2.79927400 -5.13331700 -0.48903300
H 2.85046900 -2.19163700 1.94315200
O 2.08429300 -1.96630200 2.51183800
H 1.50492400 -2.73136700 2.45660200
Pd 0.08587500 -0.92385800 -0.02178100
H 1.34084400 0.15722100 0.60987800
Cl -2.37540500 2.69917700 1.84247300
Cl 5.54742500 -0.54510800 2.37314500

53

RR-PhCl_D2_TS2W, E(SCF) = -3328.06540669,
E(ZPE) = -3327.696350, E(G) = -3327.765488
a.u.

C -0.89922400 -3.10537700 -1.52465400
H -0.78555500 -3.73908400 -0.63985500
H -1.52985000 -3.63535900 -2.24428200
C 0.44045000 -2.76091600 -2.11034700
H 0.97378000 -3.65550500 -2.44563700
H 0.31563700 -2.09890300 -2.97236400
N 1.24672500 -2.04047300 -1.09288700
N -1.53404600 -1.84397800 -1.09232100
C 2.48366600 -1.50432700 -1.71690200
H 2.17946700 -0.93778400 -2.59986600
C -2.74577400 -2.02553300 -0.26915800
H -3.44950000 -2.67951100 -0.79536500
C 3.33803400 -0.63909200 -0.84961300
C 3.84609200 -1.14715800 0.37819000
C 3.65770000 0.63552300 -1.27847400
C 4.67660900 -0.26192100 1.10195900
C 4.48460500 1.46119700 -0.53022400
H 3.24984000 0.99814200 -2.21853100
C 4.99903100 1.00758500 0.67025600
H 5.64041200 1.64772800 1.26435200
C -3.40753800 -0.72192200 0.04619800
C -2.68553000 0.29313300 0.72119800
C -4.74506700 -0.54338500 -0.27684700
C -3.41916300 1.45624400 1.05220000
C -5.41810500 0.61284200 0.06628900
H -5.28187900 -1.32906400 -0.79844100
C -4.74798700 1.62107900 0.74330300
H -5.25898800 2.53690600 1.02136400
O 3.51290500 -2.31321500 0.83021200
O -1.43589400 0.20347700 1.07707800
S 4.88355100 3.10031900 -1.14303100
S -7.15664800 0.83573700 -0.32427400
O -7.85385900 0.94472000 0.98833500
O -7.55599800 -0.37005500 -1.09935400
O -7.23559300 2.09518200 -1.11621400
O 5.62501300 2.88892900 -2.41936000
O 5.71471600 3.73966400 -0.08626700
O 3.57661000 3.78529900 -1.35445200
H -2.42605600 -2.54611100 0.64077800
H 3.05547500 -2.37588700 -2.06789400
H -1.77325800 -1.28726500 -1.91363100
H 1.54842800 -2.75467100 -0.41992300
H 1.22490900 -0.73473400 1.53234900
H 3.01467000 -3.89014700 0.21843800
O 2.37910500 -4.58265900 -0.05882200
H 2.80483900 -5.05769300 -0.77600700
H 2.46485400 -1.96132000 1.98116700
O 1.72311800 -1.47452000 2.47368000
H 1.06312400 -2.12479400 2.74434000
Pd -0.06731200 -0.83815300 -0.00367300
H 1.10887400 -0.01644800 0.84472400
Cl -2.58312100 2.74838200 1.90437700
Cl 5.32372100 -0.81847700 2.64666000

56

RR-PhCl_ID1_TS1_H2-out_R, E(SCF) = -
3404.54123968, E(ZPE) = -3404.144989, E(G)
= -3404.217716 a.u.

C 0.61349500 -3.50215700 -0.11433400
H 0.37624100 -3.54060000 -1.18123700
H 1.22505400 -4.37420600 0.12821700
C -0.64616000 -3.44772300 0.70789100
H -1.26914800 -4.33305700 0.55932400
H -0.41409800 -3.36600600 1.77307900

N -1.37820000 -2.22180300 0.31453200
N 1.37222200 -2.25073600 0.12542000
C -2.50692000 -1.86354300 1.19592000
H -3.13552400 -2.74602000 1.35279300
C 2.40492400 -1.96517100 -0.88807000
H 1.87372100 -1.74243900 -1.82022600
C -3.32758300 -0.76777600 -0.59060800
C -2.72975600 0.45318500 0.20414700
C -4.68595400 -0.97761400 0.39651700
C -3.59833800 1.42609900 -0.33265400
C -5.49523900 0.00106000 -0.14474800
H -5.12737400 -1.92668900 0.68099600
C -4.94557100 1.21934900 -0.51159900
H -5.56186000 2.00188800 -0.94097100
C 3.30388200 -0.84283700 -0.47309600
C 2.78719000 0.40944100 -0.06355900
C 4.67547500 -1.04688800 -0.55585700
C 3.74755400 1.41381500 0.19209900
C 5.57455300 -0.03882800 -0.27806900
H 5.05332100 -2.01745100 -0.85949400
C 5.10335200 1.20983600 0.09272700
H 5.78901100 2.02260200 0.30679000
O -1.44990500 0.72414100 0.32944000
O 1.50963700 0.69260500 0.06629800
S -7.25103700 -0.28149000 -0.41826900
S 7.34891500 -0.31295500 -0.37110700
C 7.85995400 -0.10377300 -0.12333800
O 7.86102900 0.70562600 -1.32895600
O 7.51541600 -1.71015200 -0.85297500
O -7.52858900 -1.63943600 0.12098700
O -7.44251000 -0.18239700 -1.89172500
O -7.95026500 0.80282600 0.32431100
H -0.71495100 2.41673400 0.87759500
H -2.64633700 -0.76496400 -2.90679300
H -2.45208800 -0.25725100 -2.39061000
O 0.02460800 2.88162300 1.30326500
H 0.78620400 2.38022000 0.96629700
H -1.21094600 0.66412900 2.58026800
O -0.78382700 0.19256000 3.33148900
H -0.36105800 1.85012500 2.89031200
H -1.73964500 -2.34567800 -0.63356100
H -2.07852700 -1.59266200 2.16648700
H 1.81628600 -2.30039000 1.04368000
H 3.00329700 -2.86638200 -1.05698800
Pd 0.01536400 -0.72654200 0.20470400
O 0.15197600 1.96097900 -2.07397000
H 0.76076800 1.59448200 -1.41118000
H -0.70332100 1.87828000 -1.63285700
Cl -2.90962500 2.96651700 -0.83181900
Cl 3.18670900 3.01741600 0.64419900

54

RR-PhCl_ID2_TS1_N-trigo-square, E(SCF) = -
3403.34022948, E(ZPE) = -3402.960852, E(G)
= -3403.031943 a.u.

C -0.50792800 -3.03917600 0.59153000
H -0.20554100 -2.79629600 1.61411300
H -1.01732600 -4.00564500 0.60275400
C 0.68921400 -3.03817200 -0.32644600
H 1.42472400 -3.79012800 -0.02688700
H 0.39389200 -3.24154300 -1.35963700
N 1.27514600 -1.68267000 -0.27019000
C 2.41312800 -1.43472400 -1.18561300
H 1.99951900 -1.04984900 -2.12419200
C 3.43816200 -0.51399700 -0.58909500
C 3.04985200 0.71406800 0.01879200
C 4.77082200 -0.88399200 -0.63378000
C 4.09882500 1.47771400 0.57508600
C 5.76528600 -0.07853300 -0.10086300
H 5.04336800 -1.82960600 -1.09478200
C 5.42574600 1.11185500 0.51570300
H 6.19377700 1.73878500 0.95287900
O 1.81285500 1.09773100 0.10079600
S 7.47613700 -0.61613300 -0.19225800
O 7.77936600 -0.75844900 -1.64463100
O 7.53174800 -1.91985000 0.52822300
O 8.27337900 0.45196900 0.47019300

H 2.88918700 -2.39331500 -1.41632900
H 1.57187800 -1.50328500 0.69958900
O 0.30296500 1.29286300 -2.03590500
H 0.99441400 1.59821500 -1.41486000
H 1.44296100 0.35003400 1.83366400
O 1.49239600 -0.40590800 2.44709500
H 0.70099500 -0.34407200 2.98882100
H -0.46319900 1.86497800 -1.89471900
H 0.68853300 2.38757500 0.88423200
O -0.13645700 2.81117100 1.17809700
H -0.83470500 2.27282000 0.77321600
Pd -0.28869700 -0.36563600 -0.41568700
N -1.42814000 -1.97182400 0.13612200
C -2.47186600 -1.57409900 1.10477000
H -2.98027200 -2.47287900 1.46919300
C -3.47784600 -0.64231900 0.49799100
C -3.07088400 0.57143600 -0.11246900
C -4.82378500 -0.95454500 0.58511700
C -4.09294000 1.42184500 -0.56916600
C -5.79801100 -0.08880400 0.11503500
H -5.12129400 -1.89300100 1.04397200
C -5.43159400 1.11372100 -0.45983800
H -6.18761100 1.79737100 -0.82718100
O -1.82362800 0.94186200 -0.25064500
S -7.52987800 -0.55256900 0.25814300
O -8.29898100 0.56936400 -0.34364000
O -7.77958800 -0.72161400 1.71664600
O -7.66477300 -1.83000300 -0.49584800
H -1.95071500 -1.11811100 1.95353300
H -1.88169100 -2.27189400 -0.72920600
Cl -3.62102800 2.94458800 -1.31056600
Cl 3.66447600 2.97264900 1.40198600

54
RR-PhCl_ID2_TS1_P, E(SCF) = -3403.35420484,
E(ZPE) = -3402.973838, E(G) = -3403.047296
a.u.
C -0.91113000 -3.23477600 -1.03459700
H -0.73619300 -3.72188100 -0.07160100
H -1.55215400 -3.88395600 -1.63756300
C 0.37990900 -2.91806500 -1.73222600
H 0.98224000 -3.81229900 -1.91731000
H 0.17259400 -2.43780200 -2.69398100
N 1.15607200 -1.95543200 -0.91131900
N -1.58683900 -1.94628700 -0.76260300
C 2.18806100 -1.28690000 -1.74108100
H 1.67236400 -0.63631300 -2.45158400
C -2.78441700 -2.06023100 0.09910800
H -3.45885900 -2.80915200 -0.32828900
C 3.18952000 -0.51520700 -0.94742100
C 3.86447800 -1.16927800 0.12231100
C 3.47424600 0.79223600 -1.28239900
C 4.84299900 -0.38985900 0.78018500
C 4.44104100 1.51418900 -0.59547900
H 2.93105900 1.26368800 -2.09753500
C 5.13138100 0.91621100 0.44325900
H 5.88949100 1.47037300 0.98405900
C -3.49763500 -0.75410200 0.23616900
C -2.81464800 0.36360300 0.78224200
C -4.82699700 -0.65822000 -0.13144500
C -3.58071100 1.53212300 0.95761300
C -5.53892600 0.51645800 0.05290900
H -5.32331800 -1.52652300 -0.55531700
C -4.91093500 1.61784000 0.60363300
H -5.46029000 2.53971200 0.75435300
O 3.56168200 -2.37217300 0.48831100
O -1.56049500 0.33349800 1.14323000
S 4.76176000 3.21668400 -1.05812400
S -7.25348100 0.60354900 -0.47854200
O -7.92970900 -0.56681800 0.14672300
O -7.21659900 0.51373500 -1.96561500
O -7.76446700 1.91011600 0.01655000
O 5.86661400 3.68245600 -0.17488200
O 3.48337200 3.94983300 -0.82780300
O 5.14211900 3.18490900 -2.49974200
H -2.43388700 -2.43627400 1.06584600
H 2.68966800 -2.07523300 -2.32144800

H -1.85929700 -1.51540100 -1.64808700
H 1.68537400 -2.46830500 -0.19367900
O 1.17519800 0.39816000 1.22751700
H 1.59155000 -0.24744600 1.86058100
H 3.44026800 -3.83014100 -0.51059900
O 3.18560700 -4.62686600 -1.02168800
H 3.74614800 -4.61091900 -1.80011700
H 0.60598700 0.97681800 1.75323500
H 2.76240800 -2.04782100 2.02460100
O 2.21362900 -1.58248900 2.69930500
H 1.53816700 -2.20963300 2.97039500
Pd -0.19551600 -0.75437400 0.12060800
Cl 5.73463100 -1.13745000 2.10869100
Cl -2.80167400 2.94433200 1.65826300

54
RR-PhCl_ID2_TS1_R, E(SCF) = -3403.36302132,
E(ZPE) = -3402.984062, E(G) = -3403.057494
a.u.
C -0.83870400 -3.52311000 0.49126600
H -0.69462800 -3.52652900 1.57543200
H -1.45283600 -4.38761000 0.22464200
C 0.48447700 -3.53558000 -0.22675200
H 1.06685200 -4.43000900 0.00646000
H 0.32571700 -3.51103900 -1.30892300
N 1.23585500 -2.31256500 0.13977400
N -1.52967200 -2.26605700 0.13771600
C 2.24654300 -1.93522300 -0.85918600
H 1.69969600 -1.67637700 -1.77366400
C -2.72376700 -1.97085400 0.95739300
H -3.37905100 -2.84820200 0.96375000
C 3.14437400 -0.81489600 -0.42346900
C 2.68349400 0.30406200 0.31879600
C 4.46951100 -0.88848800 -0.82354200
C 3.66228700 1.27230700 0.63113900
C 5.38146600 0.10638200 -0.52355900
H 4.79839900 -1.75747200 -1.38664400
C 4.97404000 1.19777900 0.21780100
H 5.68060500 1.97558200 0.48137600
C -3.46777700 -0.78738400 0.42776000
C -2.80652200 0.46002600 0.27617400
C -4.80864200 -0.91724200 0.11447700
C -3.60724200 1.52425900 -0.18402900
C -5.55382000 0.16215700 -0.33112300
H -5.28752800 -1.88499000 0.23427400
C -4.94746700 1.39423800 -0.47997300
H -5.52056900 2.24459500 -0.82996000
O 1.45919000 0.46919200 0.76503100
O -1.54630800 0.65808100 0.56027200
S 7.07825400 -0.03827000 -1.09814400
S -7.29291500 -0.06516800 -0.72265400
O -7.92184500 -0.57803000 0.52630400
O -7.32922100 -1.06095600 -1.83043400
O -7.79479300 1.27667800 -1.12381400
O 7.79479100 1.13648800 -0.53300300
O 7.00223600 -0.01970800 -2.58575400
O 7.57325800 -1.33939400 -0.56836500
H -2.36958000 -1.80993900 1.98110300
H 2.86265400 -2.81108600 -1.09202500
H -1.80793600 -2.29420000 -0.84419200
H 1.66884600 -2.41036300 1.06863400
O 0.46868700 3.36118500 -1.24260100
H 0.32784500 3.25456000 -0.28235800
H 1.79982300 -0.63771700 2.50515700
O 1.97509700 -1.52419600 2.85757200
H 2.83027100 -1.46032200 3.29085800
H -0.34128600 3.01098600 -1.62377000
H 0.70321600 2.13669000 1.47276900
O -0.04326600 2.75954200 1.49524400
H -0.78524900 2.18392400 1.23148300
Pd -0.11175100 -0.80275600 0.35607000
Cl 3.19066400 -2.65043100 1.61926000
Cl -2.85828300 3.10424000 -0.39254900

54

RR-PhCl_ID2_TS1_trigo-square_P, E(SCF) = -
3403.35911780, E(ZPE) = -3402.977384, E(G)
= -3403.047337 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.17841700 | -2.14045500 | 1.04911000 |
| H | 0.07055400 | -1.59811300 | 1.96618000 |
| H | -0.47358700 | -3.15792100 | 1.31697100 |
| C | 0.98121800 | -2.12265800 | 0.08899600 |
| H | 1.86734800 | -2.60635400 | 0.51190100 |
| H | 0.71972300 | -2.64266400 | -0.83651700 |
| N | 1.26734500 | -0.71012100 | -0.24519300 |
| C | 2.28410700 | -0.52741500 | -1.32585700 |
| H | 1.90253000 | 0.22478200 | -2.01982500 |
| C | 3.61077600 | -0.12780300 | -0.77140600 |
| C | 3.71912600 | 1.16997050 | -0.19363700 |
| C | 4.68649100 | -0.98486100 | -0.80654800 |
| C | 4.99330400 | 1.47422300 | 0.35148200 |
| C | 5.91437000 | -0.63638700 | -0.28157900 |
| H | 4.57137600 | -1.97977500 | -1.25935000 |
| C | 6.06208500 | 0.61069300 | 0.31133900 |
| H | 7.01391500 | 0.90817300 | 0.73896400 |
| O | 2.73205500 | 1.99279200 | -0.13961200 |
| S | 7.31188200 | -1.75971800 | -0.30404400 |
| O | 8.44822100 | -0.98486100 | -0.87939200 |
| O | 6.89771400 | -2.90920900 | -1.15524400 |
| O | 7.55419000 | -2.14679500 | 1.11610000 |
| H | 2.35885400 | -1.46603600 | -1.87809600 |
| H | 1.60054200 | -0.24730700 | 0.61314600 |
| O | 0.36510300 | 2.00806100 | -1.17456100 |
| H | 1.30934200 | 2.06266600 | -0.81569200 |
| H | 1.96056200 | 1.63557500 | 1.52997600 |
| O | 1.52170300 | 1.07681000 | 2.19822700 |
| H | 0.61903300 | 1.43955100 | 2.26241600 |
| H | -0.11132900 | 2.80075000 | -0.90368300 |
| H | -1.33262700 | 3.04278100 | 2.54918600 |
| O | -1.14545900 | 2.14513700 | 2.26437000 |
| H | -1.62173600 | 2.02597000 | 1.42217700 |
| Pd | -0.52880600 | 0.28179200 | -0.39075700 |
| N | -1.30543000 | -1.42277200 | 0.40504700 |
| C | -2.42983200 | -1.11607300 | 1.31910500 |
| H | -2.74461000 | -2.03835200 | 1.81767700 |
| C | -3.58962800 | -0.51208900 | 0.59086500 |
| C | -3.42076800 | 0.69864000 | -0.12581800 |
| C | -4.83115100 | -1.11862900 | 0.65762600 |
| C | -4.56989900 | 1.23631800 | -0.72911800 |
| C | -5.93820900 | -0.55297000 | 0.04495300 |
| H | -4.93963800 | -2.04840000 | 1.20855500 |
| C | -5.80913000 | 0.63482500 | -0.64829200 |
| H | -6.67118400 | 1.08084600 | -1.13030700 |
| O | -2.27094400 | 1.32641700 | -0.21662800 |
| S | -7.53453400 | -1.37063300 | 0.18085700 |
| O | -8.47579500 | -0.55471800 | -0.63193800 |
| O | -7.86098700 | -1.37025900 | 1.63401200 |
| O | -7.32684700 | -2.74313800 | -0.35802100 |
| H | -2.03011300 | -0.43876400 | 2.08167200 |
| H | -1.65794000 | -1.98311400 | -0.37335100 |
| Cl | -4.41751800 | 2.74592900 | -1.61509900 |
| Cl | 5.20133100 | 3.04791500 | 1.11974600 |

54

RR-PhCl_ID2_TS1_trigo-square_R, E(SCF) = -
3403.36892548, E(ZPE) = -3402.988235, E(G)
= -3403.059825 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.66361200 | -3.47903200 | 0.27293600 |
| H | -0.42819200 | -3.45713600 | 1.34075400 |
| H | -1.28271200 | -4.35790300 | 0.07862800 |
| C | 0.59807700 | -3.48324500 | -0.54956200 |
| H | 1.20903600 | -4.36837600 | -0.35627400 |
| H | 0.36693200 | -3.45360800 | -1.61781100 |
| N | 1.34795400 | -2.24868900 | -0.22097200 |
| C | 2.44929800 | -1.92430200 | -1.14797500 |
| H | 1.98714700 | -1.67324100 | -2.10858900 |
| C | 3.29803500 | -0.80897200 | -0.62264000 |
| C | 2.72552200 | 0.43457000 | -0.26338800 |
| C | 4.67005300 | -1.00326900 | -0.53490200 |
| C | 3.63639900 | 1.44363700 | 0.11935300 |
| C | 5.51853300 | 0.00958600 | -0.13599400 |
| H | 5.09158700 | -1.96690500 | -0.80079200 |

| | | | |
|----|-------------|-------------|-------------|
| C | 4.99545700 | 1.25092000 | 0.18967900 |
| H | 5.64249800 | 2.06550500 | 0.49699400 |
| O | 1.44244400 | 0.70246500 | -0.28859300 |
| S | 7.28869700 | -0.26341800 | 0.02518600 |
| O | 7.93665200 | 0.83666800 | -0.74057200 |
| O | 7.54160800 | -1.61131300 | -0.55077600 |
| O | 7.57061400 | -0.18729300 | -1.48585100 |
| H | 3.06852100 | -2.81436100 | -1.29956000 |
| H | 1.73329800 | -2.34084900 | 0.72106100 |
| O | 0.02546900 | 2.33936800 | -2.06578900 |
| H | 0.70755700 | 1.85836500 | -1.56917600 |
| H | 1.58509600 | 0.09701700 | 2.42799700 |
| O | 0.97892500 | 0.46350400 | 3.07794100 |
| H | 0.54614800 | 1.19729700 | 2.60015100 |
| H | -0.78051500 | 2.06591400 | -1.64863100 |
| H | 0.65177200 | 2.48211800 | 0.90925600 |
| O | -0.12809000 | 2.53013300 | 1.48249100 |
| H | -0.77735400 | 1.99721300 | 0.98620200 |
| Pd | -0.02579300 | -0.02579300 | -0.15948200 |
| N | -1.40678900 | -2.23612000 | -0.04253700 |
| C | -2.46347400 | -1.89021500 | 0.92820500 |
| H | -3.07607500 | -2.77567900 | 1.12729300 |
| C | -3.33617900 | -0.87935900 | -0.42496600 |
| C | -2.78271000 | 0.44556000 | -0.01637800 |
| C | -4.70868900 | -0.96646900 | 0.44003900 |
| C | -3.70875900 | 1.44156300 | -0.38213100 |
| C | -5.57900600 | 0.03921200 | 0.05858300 |
| H | -5.10905600 | -1.92041300 | 0.77106000 |
| C | -5.07413200 | 1.25877200 | -0.35088300 |
| H | -5.74439900 | 2.05604700 | -0.64955300 |
| O | -1.49774900 | 0.70540300 | -0.08093600 |
| S | -7.35111000 | -0.26072500 | 0.09347600 |
| O | -7.98198100 | 1.00513200 | -0.36674200 |
| O | -7.67371800 | -0.59929900 | 1.50753900 |
| O | -7.58047600 | -1.40358000 | -0.83359700 |
| H | -1.95563300 | -1.62160400 | 1.86159000 |
| H | -1.82919800 | -2.32750300 | -0.96785000 |
| Cl | -3.08758700 | 3.00280300 | -0.90532700 |
| Cl | 2.99770600 | 3.03631600 | 0.51364500 |

54

RR-PhCl_ID2_TS1_trigo-square, E(SCF) = -
3403.33846827, E(ZPE) = -3402.959197, E(G)
= -3403.028914 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.50014200 | -3.04590500 | 0.70508800 |
| H | -0.19505200 | -2.76182200 | 1.71704500 |
| H | -1.01317300 | -4.00905200 | 0.75942600 |
| C | 0.69462300 | -3.09123100 | -0.21569700 |
| H | 1.42510400 | -3.83767100 | 0.10771600 |
| H | 0.39480300 | -3.32597400 | -1.24048300 |
| N | 1.29262400 | -1.73730600 | -0.21343400 |
| C | 2.42650600 | -1.51578500 | -1.14548900 |
| H | 2.00139500 | -1.14403900 | -2.08347500 |
| C | 3.45213400 | -0.58568300 | -0.56482000 |
| C | 3.06494300 | 0.65785300 | 0.00453400 |
| C | 4.78694800 | -0.96563400 | -0.59234300 |
| C | 4.11872100 | 1.44128100 | 0.53593900 |
| C | 5.77847900 | -0.15072000 | -0.08129900 |
| H | 5.06561800 | -1.92096700 | -1.02523400 |
| C | 5.43934600 | 1.06539900 | 0.49529400 |
| H | 6.20263900 | 1.71285100 | 0.91368600 |
| O | 1.83167500 | 1.05615600 | 0.06218200 |
| S | 7.50532600 | -0.64313500 | -0.11278200 |
| O | 8.19328900 | 0.35192600 | -0.98298900 |
| O | 7.52562300 | -2.02223600 | -0.67215300 |
| O | 7.97140600 | -0.57772300 | 1.30143100 |
| H | 2.89651900 | -2.48080800 | -1.35918400 |
| H | 1.63067900 | -1.55079600 | -0.73324000 |
| O | 0.43282900 | 1.04396500 | -2.14743600 |
| H | 1.09858000 | 1.41915900 | -1.53680400 |
| H | 1.27873000 | 0.76305400 | 1.89075900 |
| O | 0.78349000 | 0.78051800 | 2.72772600 |
| H | 0.17033800 | 1.50849700 | 2.55360500 |
| H | -0.28843800 | 1.68288800 | -2.19761500 |
| H | 0.66138600 | 2.49719400 | 0.59897600 |
| O | -0.17963800 | 2.88696300 | 0.89426600 |
| H | -0.85859000 | 2.33500600 | 0.47053700 |

Pd -0.26786800 -0.42319900 -0.41478600
N -1.41662100 -1.99467100 0.20710400
C -2.45933000 -1.55396000 1.15688100
H -2.97103700 -2.43536000 1.55732400
C -3.46282100 -0.64800600 0.50762700
C -3.05482400 0.52310700 -0.18073300
C -4.81026700 -0.94021700 0.63507200
C -4.07755700 1.35168000 -0.67590800
C -5.78452500 -0.09516300 0.12969200
H -5.10827200 -1.84470500 1.15749400
C -5.41681000 1.06414100 -0.52718100
H -6.17275700 1.73065200 -0.92513100
O -1.80840900 0.87848400 -0.36115400
S -7.51753300 -0.53660300 0.31967600
O -8.28759400 0.59375000 -0.26482800
O -7.73134800 -0.69985600 1.78438600
O -7.68824600 -1.81363400 -0.42810600
H -1.94001000 -1.06335400 1.98721100
H -1.87162800 -2.32907800 -0.64483300
Cl -3.60601700 2.82124700 -1.51794200
Cl 3.69197200 2.98038300 1.27991200

54

RR-PhCl_ID2_TS1, E(SCF) = -3403.34025683,
E(ZPE) = -3402.960182, E(G) = -3403.030874
a.u.

C -0.72826300 -3.24351700 0.42228700
H -0.51206800 -3.12438500 1.48764900
H -1.29809200 -4.16475800 0.28228500
C 0.55739900 -3.24065800 -0.36884900
H 1.21276100 -4.06393000 -0.06792800
H 0.36706400 -3.33000700 -1.44225900
N 1.20367400 -1.93837400 -0.11163100
N -1.52808200 -2.06979000 -0.00112800
C 2.45083200 -1.69502100 -0.84824500
H 2.16956400 -1.38645800 -1.86166800
C -2.58814600 -1.66049100 0.94119500
H -3.17808500 -2.54001000 1.22081000
C 3.38234300 -0.68710400 -0.22123600
C 2.94635500 0.39920200 0.60275100
C 4.72070100 -0.82433200 -0.54865100
C 3.97657100 1.29041500 1.00103300
C 5.68167500 0.07774700 -0.12153200
H 5.02623400 -1.66518900 -1.16703500
C 5.30300600 1.15374500 0.66047200
H 6.04174300 1.86849500 1.00352400
C -3.49955600 -0.62601000 0.36038100
C -2.99248900 0.58542600 -0.19226100
C -4.86700600 -0.82879400 0.43035900
C -3.95008200 1.54020000 -0.58789900
C -5.77100400 0.13133100 0.00738600
H -5.23788300 -1.76337100 0.84185200
C -5.30862400 1.33241100 -0.49752200
H -6.00712300 2.09491800 -0.82112500
O 1.72649500 0.57124600 0.98677800
O -1.72538500 0.86561100 -0.33301400
S 7.39258600 -0.16103400 -0.60112700
S -7.53250200 -0.21116600 0.10216600
O -7.81072600 -0.50993700 1.53471800
O -7.75846200 -1.39063200 -0.77969200
O -8.20945100 1.02167100 -0.38272200
O 8.15995000 0.92188800 0.07377700
O 7.42152400 -0.05487800 -2.08855600
O 7.76513300 -1.52443400 -0.12603300
H -2.07938200 -1.30192400 1.84257600
H 2.98436500 -2.64861200 -0.94528500
H -1.95416700 -2.26843300 -0.90793200
H 1.37923600 -1.87938500 0.90205200
O 0.87350900 1.01556600 -1.67340200
H 0.76545500 1.83159100 -1.13634000
H 1.29840000 -0.51047200 2.32508300
O 1.07198100 -1.36940100 2.74442900
H 1.71894200 -1.50137000 3.44117200
H 0.30883300 1.14014300 -2.44360300
O 0.81371400 2.15186200 0.81193500
H 0.25039900 2.79918400 0.33708900
H -0.61873300 2.36600500 0.28661400

Pd -0.24385700 -0.51951400 -0.36552500
Cl 3.51138700 2.66666600 2.00663300
Cl -3.36290700 3.07324800 -1.22137000

56

RR-PhCl_ID2_TS2_P, E(SCF) = -3404.51550166,
E(ZPE) = -3404.119385, E(G) = -3404.193975
a.u.

C -0.08183700 0.16480500 -1.95673600
H -0.05981000 -0.79891400 -2.47307400
H -0.19176000 0.95718700 -2.70139400
C 1.15359000 0.34312500 -1.11927900
H 2.05485300 0.34016500 -1.73876600
H 1.12499900 1.29167200 -0.57329000
N 1.20090300 -0.75957800 -0.12944300
N -1.24443500 0.15535400 -1.03975400
C 2.22057200 -0.57842000 0.94220800
H 2.31009500 -1.55360100 1.43176600
C -2.51702500 -0.28256900 -1.65293300
H -2.67196800 0.27050200 -2.58424900
C 3.54703300 -0.08649400 0.45751000
C 4.33236700 -0.94001200 -0.36797800
C 3.98295700 1.17964300 0.81360400
C 5.58251500 -0.39456000 -0.76953300
C 5.20972300 1.65812700 0.39065500
H 3.35717400 1.80966800 1.43884100
C 6.01466200 0.85926400 -0.41212200
H 6.97900900 1.21928200 -0.75589700
C -3.66818400 -0.05125400 -0.72829400
C -3.65456200 -0.61374100 0.57449300
C -4.74715000 0.69867700 -1.16045600
C -4.79892500 -0.37758700 1.36177500
C -5.85109200 0.90377400 -0.34939400
H -4.72827700 1.12611500 -2.15888700
C -5.87896900 0.35668600 0.91975600
H -6.73727100 0.51366100 1.56209700
O 3.93356800 -2.10321200 -0.72663100
O -2.68158000 -1.34409200 1.04986200
S 5.78865300 3.29079900 0.84936600
S -7.23552400 1.86686700 -0.97151300
O -8.19667800 1.97101900 0.15918300
O -7.77112500 1.09575700 -2.12835800
O -6.66083000 3.17930700 -1.37875400
O 6.00748000 4.02330900 -0.43124000
O 7.05870100 3.08131500 1.60290900
O 4.70923200 3.88785800 1.68372600
H -2.39384500 -1.34110800 -1.90933500
H 1.80619500 0.12824900 1.66579700
H -1.37381500 1.09274700 -0.65280500
H 1.40970500 -1.61954900 -0.65752800
O 0.25846900 -4.24590400 1.10910000
H 1.19035400 -4.31070600 0.81017300
H 2.65867500 -2.56059600 -1.87150500
O 1.75807300 -2.81590300 -2.16598100
H 1.66018300 -3.70805500 -1.81560900
H -0.26979600 -4.58232700 0.38076200
H 3.33507700 -3.50829800 0.03457400
O 2.84636100 -4.34366500 0.22017700
H 3.47645200 -4.95191800 0.61161900
H -0.23380000 -2.45864400 1.55951000
H -0.32531200 -1.80194100 2.06098900
Pd -0.74426900 -1.05139300 0.53475700
Cl 6.62138200 -1.39095100 -1.79050600
Cl -4.84805800 -1.05609100 2.98253600

54

RR-PhCl_ID2_TS2_R_noH2, E(SCF) = -
3403.35965861, E(ZPE) = -3402.978011, E(G)
= -3403.049231 a.u.

C 0.05821200 1.03031200 1.64567600
H -0.01131700 0.26205900 2.42086900
H 0.18926700 2.00284300 2.12716100
C -1.16035900 0.99291200 0.76547100
H -2.07195500 1.17996700 1.34004800
H -1.09839800 1.74984700 -0.02316900
N -1.21656900 -0.33806300 0.11769500
N 1.23400200 0.70805800 0.80280800

C -2.22057900 -0.41866800 -0.97241800
H -2.13312900 -1.41653000 -1.40818400
C 2.46402700 0.40977900 1.56903900
H 2.63734400 1.21707900 2.28799000
C -3.61601700 -0.16944000 -0.49584700
C -4.21049000 -1.14626700 0.35314100
C -4.29150700 0.98313000 -0.86019300
C -5.53430300 -0.84510600 0.77103200
C -5.58109800 1.22396000 -0.41912100
H -3.80759300 1.71504500 -1.50044200
C -6.20641600 0.29614400 0.40457600
H -7.21626200 0.46850200 0.76294300
C 3.66208000 0.25766600 0.68512600
C 3.65885600 -0.68826900 -0.37502000
C 4.79373700 1.00851900 0.95068400
C 4.86615800 -0.81907200 -1.09043500
C 5.95718000 0.84607800 0.21636900
H 4.77101600 1.73112100 1.76132400
C 5.99463000 -0.07999000 -0.80916000
H 6.89952700 -0.21376500 -1.39003500
O -3.59073700 -2.20962900 0.71867100
O 2.63646200 -1.43180700 -0.69151400
S -6.47897300 2.69408300 -0.91454700
S 7.40454500 1.82726500 0.62802300
O 8.44154500 1.45573900 -0.37233000
O 7.76846500 1.44204200 2.02065900
C 6.97143100 3.24902700 0.52619200
O -6.97743900 3.31544900 0.34597000
O -7.59229900 2.22413700 -1.78963800
O -5.49478100 3.54779700 -1.63626400
H 2.25722200 -0.50290500 2.13828100
H -1.93079400 0.30721900 -1.73627000
H 1.41978200 1.49014100 0.17223500
H -1.46524900 -1.01574100 0.85099300
O 0.22427600 -2.55120700 -1.51760600
H -0.43282000 -3.12844000 -1.03958500
H -2.47819000 -2.14859600 2.12535900
O -1.63388700 -1.97044600 2.59099200
H -1.09757500 -2.74796500 2.40707900
H 1.03578300 -3.05823200 -1.64188900
H -2.41877200 -3.22889100 0.07709200
O -1.63235600 -3.79795200 -0.11956600
H -1.97417600 -4.64836800 -0.40482600
Pd 0.72353500 -0.88252800 -0.34590600
Cl -6.34391600 -2.00607000 1.82445700
Cl 4.92876200 -1.98363300 -2.40754300

56
RR-PhCl_ID2_TS2_R, E(SCF) = -3404.53337075,
E(ZPE) = -3404.137075, E(G) = -3404.211292
a.u.

C -0.05618000 0.91331100 -1.75454300
H 0.01624800 0.11169800 -2.49508000
H -0.18531300 1.86422200 -2.27793400
C 1.15755600 0.91556800 -0.86649100
H 2.07201200 1.08609300 -1.44119800
H 1.08435400 1.70185300 -0.10735300
N 1.21680700 -0.38804300 -0.16564200
N -1.23298300 0.62909500 -0.90024100
C 2.19735300 -0.41051900 0.94886100
H 2.11603800 -1.39297300 1.41958900
C -2.47425400 0.32341500 -1.64485300
H -2.64842200 1.11311400 -2.38286800
C 3.59899800 -0.15403800 0.49530900
C 4.23009900 -1.15097700 -0.30210000
C 4.24478600 1.02432600 0.82993700
C 5.56044900 -0.84455500 -0.69484000
C 5.54108600 1.27054400 0.41271600
H 3.73196300 1.77159000 1.42862800
C 6.20318900 0.32220300 -0.35722600
H 7.21954200 0.49819500 -0.69503200
C -3.65938300 0.20881200 -0.73796300
C -3.65246400 -0.72242100 0.33515700
C -4.78107900 0.97882900 -0.98990700
C -4.84498900 -0.81875600 1.07924100
C -5.93155600 0.84837300 -0.22899000
H -4.76229000 1.68949200 -1.81114400

C -5.96477600 -0.06147000 0.81100000
H -6.85962200 -0.16914400 1.41244900
O 3.63541600 -2.23596200 -0.64512500
O -2.63824700 -1.48477200 0.63514500
S 6.39520700 2.78347500 0.85286100
S -7.36710900 1.85512200 -0.62099700
O -8.40156400 1.49084400 0.38458300
O -7.74771500 1.48783200 -2.01390700
O -6.91110000 3.26901500 -0.51002700
O 6.84500900 3.38916300 -0.43355000
O 7.54248700 2.37611900 1.71482200
O 5.39592800 3.62057400 1.57331100
H -2.28526500 -0.60708600 -2.19067800
H 1.87754800 0.33840600 1.67802600
H -1.40570200 1.43208600 -0.29154800
H 1.48789700 -1.09199500 -0.86587500
O -0.22515500 -2.56863000 1.50846000
H 0.45258800 -3.14966400 1.06481700
H 2.55281900 -2.24472600 -2.17483200
O 1.71717000 -2.09783000 -2.56769300
H 1.19475700 -2.88408900 -2.38145800
H -1.03053300 -3.08492000 1.63398100
H 2.46478900 -3.25480100 0.00530700
O 1.68788000 -3.83166200 0.20611300
H 2.03869400 -4.66512400 0.52789800
H -0.72096500 1.02078600 2.35381200
H -0.60648400 1.75432300 2.46573300
Pd -0.72518000 -0.93460400 0.29179600
Cl 6.41827700 -2.03275600 -1.67728100
Cl -4.90058800 -1.96276600 2.41410800

56
RR-PhCl_ID2_TS2-square_P, E(SCF) = -
3404.52013284, E(ZPE) = -3404.123381, E(G)
= -3404.197116 a.u.

C -0.07975700 0.66857600 -1.84274900
H -0.02578400 -0.17797300 -2.53272800
H -0.19838000 1.58472700 -2.42671400
C 1.13624000 0.71522900 -0.96143200
H 2.04798800 0.84130100 -1.55077600
H 1.07535600 1.55027400 -0.25602600
N 1.19288800 -0.54350300 -0.18164100
N -1.25745600 0.45749200 -0.96991000
C 2.17490900 -0.50754400 0.93642400
H 2.19385200 -1.51665200 1.35657000
C -2.50829600 0.12905700 -1.68917000
H -2.66440000 0.86904500 -2.48058200
C 3.54030200 -0.07894000 0.50184800
C 4.31058200 -0.98584400 -0.28977100
C 4.01789100 1.17395800 0.83538100
C 5.57834500 -0.49230600 -0.68989200
C 5.27000300 1.59853300 0.41619900
H 3.40087200 1.83671100 1.43788200
C 6.05196700 0.75751800 -0.35809700
H 7.02932900 1.08638200 -0.69267600
C -3.68300000 0.11827000 -0.76502100
C -3.67713100 -0.72518200 0.37082300
C -4.78353400 0.91322300 -1.05036200
C -4.85130100 -0.71838200 1.15569700
C -5.91017100 0.88718100 -0.25289200
H -4.76856000 1.56088700 -1.92051800
C -5.94565900 0.05882300 0.85887300
H -6.82171500 0.02638800 1.49778400
O 3.87856400 -2.15021900 -0.60814300
O -2.68790900 -1.51029900 0.70215800
S 5.84348400 3.23684400 0.86029300
S -7.34179400 1.91061600 -0.62011500
O -7.53376500 2.77442300 2.57820700
O -8.47116100 0.96135900 -0.82519800
O -6.98856800 2.67696000 -1.84520900
O 7.21353200 3.35792000 0.28903600
O 5.82495600 3.29042100 2.35046900
O 4.87215200 4.19037100 0.25046700
H -1.41263700 1.29562400 -0.40567200
H 1.45253600 -1.29937400 -0.83665600
O 0.70329300 -4.12066600 0.00423700
H 1.56162800 -4.26109100 0.46680000

H 2.59994800 -2.54632300 -1.80237700
O 1.70082800 -2.62698300 -2.18242300
H 1.26593100 -3.27951700 -1.60517100
H 0.24728200 -4.96594700 0.00629300
H 3.54458900 -3.39643100 0.49646400
O 3.20712800 -4.16263300 1.02200500
H 3.39216300 -3.95808100 1.94124500
H -0.18576500 -2.61928600 1.00732000
H -0.36989900 -2.14035100 1.65407000
Pd -0.75385500 -1.04148900 0.32892500
H 1.77771900 0.17328600 1.69355600
H -2.34647900 -0.84359400 -2.16604700
Cl -4.90722400 -1.75795000 2.57181800
Cl 6.59580800 -1.54717300 -1.67385200

54

RR-PhCl_ID2_TS2-square_R_noH2, E(SCF) = -
3403.35618516, E(ZPE) = -3402.974750, E(G)
= -3403.045658 a.u.

C 0.12191500 1.35169100 1.74386300
H 0.08617500 0.69894500 2.62016100
H 0.27407900 2.37909600 2.08616900
C -1.12275400 1.22056900 0.91188200
H -2.01727100 1.48978500 1.47850200
H -1.06285500 1.89063400 0.04891300
N -1.21315300 -0.16626200 0.39397400
N 1.26472400 0.90769800 0.90984500
C -2.08645400 -0.27700400 -0.80679900
H -1.90467900 -1.26019800 -1.24169100
C 2.53909500 0.78655500 1.65395300
H 2.74999800 1.74042000 2.14834500
C -3.53792500 -0.09160700 -0.49743800
C -4.26298800 -1.20783700 0.02592900
C -4.15183500 1.12827400 -0.71241100
C -5.62523100 -0.94409400 0.31705600
C -5.49180400 1.32288000 -0.41114800
H -3.57488900 1.95019200 -1.13017200
C -6.23154700 0.27529100 0.11141900
H -7.27875100 0.41810500 0.35238500
C 3.68477600 0.41301400 0.76850100
C 3.63340400 -0.78395500 0.01335800
C 4.81671100 1.21416500 0.74555700
C 4.79809300 -1.10991200 -0.71571700
C 5.93078800 0.85775200 0.01110400
H 4.83958300 2.13162300 1.32467000
C 5.92286800 -0.31913000 -0.72211700
H 6.78959900 -0.61580300 -1.30323600
O -3.72293400 -2.35791900 0.21291100
O 2.60439200 -1.58409300 -0.01350500
S -6.24041000 2.92410700 -0.71054200
S 7.40201200 1.88908300 -0.01472800
O 7.60612900 2.26592700 -1.44170900
O 8.50225000 1.03321000 0.51094000
O 7.09474800 3.05240800 0.86031500
O -7.64986800 2.81153200 -0.24335200
O -6.13082000 3.16090800 -2.17905400
O -5.44039100 3.90400700 0.07949500
H 1.39454600 1.56109300 0.13534300
H -1.56843300 -0.79411100 1.13058500
O 0.18848400 -2.88683400 -0.30254600
H -0.60257800 -3.16480400 -0.84333100
H -2.51791800 -2.60699500 1.46645500
O -1.73791100 -2.53151400 2.05963100
H -1.02502300 -2.98456000 1.59339500
H 0.97108000 -3.33835800 -0.63923900
H -2.77376400 -3.21078100 -0.88569100
O -2.06383300 -3.69355400 -1.38213800
H -2.29261100 -3.64591500 -2.31319000
Pd 0.71280600 -0.89370700 0.15699100
H -1.73521700 0.47054800 -1.52194500
H 2.36746700 0.03636400 2.43323700
Cl 4.80112300 -2.59593600 -1.65550100
Cl -6.59399700 -2.26573300 0.97352900

56

RR-PhCl_ID2_TS2-square_R, E(SCF) = -
3404.52967669, E(ZPE) = -3404.132644, E(G)
= -3404.204727 a.u.

C -0.13303100 1.17541600 -2.09291000
H -0.09789800 0.46642100 -2.92381300
C -0.28270700 2.17937400 -2.50059600
C 1.11049200 1.10015600 -1.24733400
H 2.01056900 1.30767100 -1.82979400
H 1.05537000 1.84773500 -0.45026300
N 1.18667500 -0.23459500 -0.59898300
N -1.27055600 0.78874900 -1.22605500
C 1.96109200 -0.21253200 0.67276900
H 1.76084700 -1.15620100 1.18116200
C -2.58111000 0.68784900 -1.91024800
H -2.79493400 1.63933400 -2.40784600
C 3.43090900 -0.02647100 0.47197500
C 4.21721100 -1.17974600 0.16088400
C 4.00535700 1.22442500 0.60040200
C 5.60027100 -0.92110200 -0.101597400
C 5.36711400 1.41316100 0.41609800
H 3.37746100 2.07444800 0.85796600
C 6.16869600 0.32752500 0.10480800
H 7.23422200 0.46508100 -0.03904400
C -3.67403300 0.35708100 -0.94351800
C -3.60855800 -0.85652200 -0.21671900
C -4.74470400 1.22203300 -0.77960800
C -4.69646500 -1.13429600 0.63670200
C -5.78700300 0.91064500 0.07319600
H -4.77681000 2.15272500 -1.33613300
C -5.76395300 -0.27935600 0.78478400
H -6.57331300 -1.05366600 1.45963800
O 3.71100500 -2.35520600 0.05568200
O -2.62395200 -1.70591100 -0.33050200
S 6.06925400 3.05036500 0.61815100
S -7.17375300 2.03136700 0.30297800
O -7.15687300 2.40127100 1.74596100
O -8.38624500 1.25172200 -0.07144700
O -6.91545700 3.18471000 -0.60038400
O 7.51946600 2.91490200 0.30738400
O 5.81114600 3.43465600 2.03606900
O 5.34523400 3.92973500 -0.34466800
H -1.35682800 1.46213600 -0.46216700
H 1.61112000 -0.91866100 -1.24324700
O -0.21837700 -2.95586000 0.18411200
H 0.50050300 -3.14874400 0.84855000
H 2.64451400 -2.73451100 -1.28528600
O 1.93128600 -2.73158300 -1.96173700
H 1.17854200 -3.15502600 -1.53101900
H -1.03435000 -3.37767200 0.48050300
H 2.65390600 -3.10205600 1.14135100
O 1.90324800 -3.53955300 1.61946900
H 2.01972700 -3.34784600 2.55300900
H -1.14381700 -1.31772500 2.65835800
H -1.25277700 -0.58319300 2.55418600
Pd -0.73316800 -0.99380000 -0.41890800
H 1.53883800 0.58787400 1.28548800
H -2.46953100 -0.08144200 -2.68090800
Cl -4.67066700 -2.63296000 1.55538700
Cl 6.64623800 -2.28914100 -0.40447400

56

RR-PhCl_ID2_TS2-square, E(SCF) = -
3404.51199027, E(ZPE) = -3404.116898, E(G)
= -3404.190065 a.u.

C 0.07483700 1.24581800 1.53800000
H -0.03714500 0.52984400 2.35692500
H 0.22500500 2.24094700 1.96448100
C -1.11775400 1.19297700 0.62398500
H -2.03898800 1.45569200 1.15132200
H -0.99979200 1.88601900 -0.21510600
N -1.20279700 -0.17898600 0.07559000
N 1.26247300 0.83852900 0.75190300
C -2.21691800 -0.33361000 -0.99672700
H -2.10081600 -1.34771700 -1.38605800
C 2.46491000 0.53680200 1.55953200
H 2.64880700 1.37350300 2.24144800
C -3.61252800 -0.11214300 -0.50909700

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -4.20913500 | -1.13798700 | 0.28826300 | O | -2.65567500 | -1.25306000 | 1.09547900 |
| C | -4.29002200 | 1.05172200 | -0.81757100 | S | 6.13595200 | 3.06232500 | 0.76642400 |
| C | -5.53199200 | -0.85769900 | 0.71577300 | S | -7.28280000 | 1.79280800 | -1.00784700 |
| C | -5.58529600 | 1.26722600 | -0.36921500 | O | -8.25255400 | 1.89174800 | 0.11593600 |
| H | -3.79957500 | 1.80761100 | -1.42685700 | O | -7.79163300 | 0.98696300 | -2.15304200 |
| C | -6.20779800 | 0.30123500 | 0.40423300 | O | -6.74084700 | 3.11235500 | -1.43636000 |
| H | -7.22030800 | 0.45994500 | 0.75715200 | O | 6.51881400 | 3.70638700 | -0.52342800 |
| C | 3.67109100 | 0.31255500 | 0.70400000 | O | 7.32380400 | 2.74098500 | 1.60956100 |
| C | 3.65264300 | -0.67989600 | -0.30551200 | O | 5.08593000 | 3.81709700 | 1.50542900 |
| C | 4.81774400 | 1.05721200 | 0.94031800 | H | -2.34943200 | -1.28328800 | -1.86859000 |
| C | 4.86140800 | -0.87346400 | -1.01002800 | H | 1.86223400 | 0.32714200 | 1.65090800 |
| C | 5.97820100 | 0.83157000 | 0.22613500 | H | -1.38455200 | 1.18191300 | -0.63050200 |
| H | 4.81376300 | 1.82017200 | 1.71145700 | H | 1.40583100 | -1.50089500 | -0.60041600 |
| C | 6.00000100 | -0.14606700 | -0.75741600 | O | -0.24962800 | -3.46468300 | 0.96812900 |
| H | 6.90144900 | -0.34001700 | -1.32861200 | H | 0.65560400 | -3.76643700 | 0.73736900 |
| O | -3.58835600 | -2.21870200 | 0.58887300 | H | 2.50397700 | -2.49678700 | -1.93254600 |
| O | 2.61841600 | -1.42256000 | -0.58871200 | O | 1.59067300 | -2.68251200 | -2.23402700 |
| S | -6.43073100 | 2.78546000 | -0.80761500 | H | 1.40565400 | -3.54088100 | -1.83548200 |
| S | 7.45597200 | 1.81419400 | 0.51429600 | H | -0.84101700 | -3.91424100 | -0.35896800 |
| O | 7.63273600 | 2.64290500 | -0.71137300 | H | 2.93174500 | -3.44503800 | 0.07316200 |
| O | 8.55987700 | 0.83314100 | 0.70386000 | O | 2.29402600 | -4.17560800 | 0.25433800 |
| O | 7.17211600 | 2.62265900 | 1.73024200 | H | 2.77502600 | -4.85783800 | 0.72703200 |
| O | -7.77952000 | 2.69905900 | -0.18178000 | H | -0.35335700 | -1.80308700 | 2.46979800 |
| O | -6.47976300 | 2.81198200 | -2.29792600 | H | -0.25413300 | -1.05362600 | 2.60715300 |
| O | -5.60075400 | 3.89324800 | -0.25203000 | Pd | -0.73194800 | -0.92711500 | 0.59203100 |
| H | 1.49096200 | 1.57197500 | 0.07839700 | Cl | 6.48548500 | -1.72597200 | -1.79468100 |
| H | -1.44002800 | -0.81108300 | 0.85724900 | Cl | -4.85382000 | -1.01696500 | 3.00202000 |
| O | 0.07865200 | -3.21137200 | 0.29613500 | | | | |
| H | -0.65891700 | -3.64356600 | -0.19624300 | | | | |
| H | -2.35033800 | -2.23809200 | 1.89129700 | 56 | | | |
| O | -1.50655400 | -2.05554500 | 2.35474500 | RR-PhCl_ID2_TS3_P, E(SCF) = -3404.54169428, | | | |
| H | -0.85331100 | -2.59114600 | 1.87463300 | E(ZPE) = -3404.142349, E(G) = -3404.215478 | | | |
| H | 0.84044900 | -3.79576100 | 0.25241300 | a.u. | | | |
| O | -2.80983200 | -3.36717600 | -0.39532800 | C | -0.02720500 | 0.56216500 | -1.79413800 |
| O | -2.22026500 | -4.04248200 | -0.81200900 | H | 0.00914700 | -0.31611500 | -2.44620000 |
| H | -2.41176100 | -4.02788000 | -1.75234400 | H | -0.05196300 | 1.45196600 | -2.43207500 |
| H | 0.26175500 | -2.18032800 | -1.94839800 | C | 1.18492300 | 0.58281200 | -0.89694600 |
| H | 0.35876800 | -1.50761200 | -2.30085000 | H | 2.09921600 | 0.69900600 | -1.48616100 |
| Pd | 0.71870300 | -0.79890200 | -0.35242300 | H | 1.12679300 | 1.42149600 | -0.19489300 |
| H | -1.95759400 | 0.36942100 | -1.79253400 | N | 1.23547500 | 0.67161600 | -0.10289400 |
| H | 2.21738500 | -0.34131000 | 2.16589400 | N | -1.22823100 | 0.45096000 | -0.95496500 |
| Cl | 4.90597500 | -2.11032500 | -2.25768000 | C | 2.21677000 | -0.62121700 | 1.00973000 |
| Cl | -6.35014700 | -2.07446100 | 1.69906400 | H | 2.21687100 | -1.61092400 | 1.46772200 |

| | | | | | | | |
|--|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 56 | | | | | | | |
| RR-PhCl_ID2_TS2, E(SCF) = -3404.50919990, | | | | | | | |
| E(ZPE) = -3404.113821, E(G) = -3404.187107 | | | | | | | |
| a.u. | | | | | | | |
| C | -0.07066600 | 0.26104100 | -1.91984900 | C | 5.23641700 | 1.57762400 | 0.43877800 |
| H | -0.03085200 | -0.70685300 | -2.42752200 | H | 3.36199500 | 1.75556700 | 1.45582200 |
| H | -0.18806400 | 1.04889600 | -2.66846600 | C | 6.06071500 | 0.76819700 | -0.31616600 |
| C | 1.15980200 | 0.45615500 | -1.07864600 | H | 7.01507400 | 1.13825500 | -0.67085000 |
| H | 2.06435400 | 0.44954000 | -1.69371600 | C | -3.63890100 | 0.07933400 | -0.73393700 |
| H | 1.12493200 | 1.40866800 | -0.53966300 | C | -3.66021000 | -0.71436800 | 0.44611700 |
| N | 1.20200500 | -0.63703000 | -0.07993900 | C | -4.72785800 | 0.86925500 | -1.07350800 |
| N | -1.23676300 | 0.24377300 | -1.00783000 | C | -4.86350100 | -0.65411100 | -1.19446400 |
| C | 2.22572100 | -0.45688000 | 0.98096500 | C | -5.87425700 | 0.89741400 | -0.30286900 |
| H | 2.24213800 | -1.39903200 | 1.53898700 | H | -4.68756400 | 1.47450600 | -1.97355600 |
| C | -2.49777400 | -0.22713900 | -1.61983400 | C | -5.94182600 | 0.12217900 | 0.84535300 |
| H | -2.65979800 | 0.31784000 | -2.55578700 | H | -6.83063400 | 0.12673200 | 1.46759000 |
| C | 3.58443800 | -0.09712600 | 0.46867000 | O | 4.11847200 | -2.29064000 | -0.48763100 |
| C | 4.27348600 | -1.03640600 | -0.34905800 | O | -2.70107500 | -1.48886700 | 0.85203600 |
| C | 4.13820100 | 1.13225300 | 0.78524500 | S | 5.72191500 | 3.26922500 | 0.83191600 |
| C | 5.56092600 | -0.61692900 | -0.78056400 | S | -7.27179000 | 1.93465900 | -0.73751600 |
| C | 5.39631200 | 1.48816600 | 0.33292000 | O | -8.44228500 | 1.01808000 | -0.84797300 |
| H | 3.58084700 | 1.83298100 | 1.39959100 | O | -6.91304300 | 2.58194200 | -2.02948900 |
| C | 6.11341300 | 0.59951800 | -0.45864900 | O | -7.41874000 | 2.90776800 | 0.38248200 |
| H | 7.10103200 | 0.85975000 | -0.82550900 | O | 4.68376200 | 4.12967200 | 0.20265300 |
| C | -3.66214900 | -0.01445200 | -0.70661600 | O | 7.07322500 | 3.44412300 | 0.23861400 |
| C | -3.64755600 | -0.56280800 | 0.60282600 | O | 5.71184800 | 3.34569600 | 2.31758200 |
| C | -4.75734600 | 0.70024000 | -1.15727400 | H | -2.27991100 | -0.95028800 | -2.05582100 |
| C | -4.80730200 | -0.35341200 | 1.37511600 | H | 1.82599800 | 0.07654400 | 1.75335100 |
| C | -5.87638500 | 0.87951000 | -0.36069000 | H | -1.39031800 | 1.33184300 | -0.47010900 |
| H | -4.73980300 | 1.11954500 | -2.15912600 | H | 1.49772900 | -1.41359100 | -0.76382700 |
| C | -5.90364000 | 0.34301700 | 0.91301700 | O | 0.11339600 | -4.35067900 | -0.22845600 |
| H | -6.77415000 | 0.48032600 | 1.54339400 | H | 1.73368200 | -4.18937500 | 0.48607900 |
| O | 3.76071900 | -2.16376900 | -0.67896100 | H | 3.00863000 | -2.35905500 | -2.11542700 |

O 2.16538900 -2.05746700 -2.48534500
H 1.87205100 -2.75531000 -3.07599300
H 0.06430600 -4.29286800 -1.18707200
H 3.53082100 -2.77216300 0.14894900
O 2.61688900 -3.98922200 0.86375900
H 2.55167500 -4.13563700 1.81015100
H -0.29740000 -3.52747700 0.09608100
H -0.30213100 -2.23221500 1.45803200
Pd -0.72864800 -1.10152300 0.45005300
Cl 6.70736500 -1.55196200 -1.54755200
Cl -4.96894200 -1.62840300 2.65994800

56

RR-PhCl_ID2_TS3_R, E(SCF) = -3404.51594930,
E(ZPE) = -3404.119490, E(G) = -3404.193613
a.u.

C -0.05851000 0.33734100 -1.93233800
H -0.02706300 -0.58366300 -2.52096700
H -0.16218300 1.18442700 -2.61512400
C 1.16760300 0.45460900 -1.07177700
H 2.07562400 0.49889900 -1.67914700
H 1.13019100 1.36038800 -0.45772800
N 1.20888600 -0.71544000 -0.16169200
N -1.22893700 0.25746700 -1.02898200
C 2.21107400 -0.59205400 0.93356800
H 2.27835600 -1.58367700 1.39108100
C -2.49899900 -0.11716600 -1.68741700
H -2.64946800 0.52863500 -2.55816600
C 3.55138800 -0.10854700 0.47658300
C 4.34115100 -0.96500500 -0.34864500
C 3.99157100 1.15032700 0.83821000
C 5.59063300 -0.42408300 -0.74255400
C 5.22621400 1.62584000 0.42106800
H 3.35852900 1.77637000 1.46276700
C 6.02842900 0.83034800 -0.37948300
H 6.99302200 1.19725100 -0.71133400
C -3.65952900 0.01519100 -0.75403800
C -3.65960900 -0.67769800 0.47985600
C -4.74372400 0.79641900 -1.12692800
C -4.82961600 -0.55158400 1.26204000
C -5.86396600 0.89467200 -0.32585000
H -4.72141900 1.33428500 -2.06898500
C -5.90956100 0.20723500 0.87789200
H -6.78131600 0.27024400 1.52049600
O 3.93774100 -2.12968800 -0.70455200
O -2.68244900 -1.43092400 0.90654900
S 5.74983400 3.27053900 0.90340400
S -7.27260300 1.90237200 -0.80685700
O -8.42582600 0.96407100 -0.90119000
O -6.90436600 2.51179700 -2.11318900
O -7.43990700 2.90349200 0.28323700
O 4.74609800 4.20755500 0.32128000
O 7.11254300 3.44928900 0.32996900
O 5.73695400 3.28616600 2.39445500
H -2.37178900 -1.14286000 -2.04962800
H 1.79642700 0.09788300 1.67287400
H -1.35511100 1.15959000 -0.56483500
H 1.43615400 -1.53538700 -0.74283700
O 0.32771000 -4.24819900 0.65173600
H 1.30985200 -4.27049800 0.67009100
H 2.74828100 -2.44012100 -1.94428700
O 1.87255400 -2.45936500 -2.39039400
H 1.69477700 -3.38231700 -2.58434900
H 0.08534400 -4.29674800 -0.27663100
H 3.43358900 -3.41949800 0.27622000
O 3.06452200 -4.21343100 0.73263400
H 3.47390300 -4.23428500 1.60035100
H -0.22974700 -2.55542700 1.36091400
H -0.34803200 -1.95011700 1.91676300
Pd -0.74281400 -1.07436800 0.44642000
Cl 6.63264300 -1.42057300 -1.76149400
Cl -4.90121500 -1.41086200 2.79394500

56

RR-PhCl_ID2_TS3-square_P, E(SCF) = -
3404.54565638, E(ZPE) = -3404.146475, E(G)
= -3404.219908 a.u.

C -0.03676400 0.82226400 -1.69289600
H 0.01479900 -0.01276500 -2.39893800
H -0.07594500 1.74926900 -2.27484300
C 1.16993400 0.80687200 -0.78730200
H 2.08737400 0.97644400 -1.35959800
H 1.09142400 1.60149100 -0.03740300
N 1.23399300 -0.49151900 -0.07047200
N -1.24266200 0.63975300 -0.87256700
C 2.21904300 -0.50082500 1.03798100
H 2.16339700 -1.48845100 1.49661400
C -2.45475600 0.26608200 -1.61280500
H -2.65302000 0.98330600 -2.41889700
C 3.61340600 -0.15308500 0.60151800
C 4.39947900 -1.07111200 -0.11352300
C 4.11798800 1.11287800 0.85524600
C 5.64450200 -0.65466900 -0.58445800
C 5.36617200 1.49510800 0.39579800
H 3.51351600 1.81872000 1.41792100
C 6.13239200 0.61415400 -0.34033700
H 7.10637600 0.91103100 -0.70956300
C -3.64870500 0.18870200 -0.70919900
C -3.66463400 -0.69474800 0.40614000
C -4.75870900 0.96547600 -1.00944800
C -4.88191500 -0.73061700 1.13294500
C -5.91875700 0.89693600 -0.26222200
H -4.72412300 1.63683800 -1.86148600
C -5.97981400 0.03416600 0.82215200
H -6.87942600 -0.03847700 1.42408800
O 4.00124300 -2.32149700 -0.40889000
O -2.68870700 -1.46881700 0.77074100
S 5.96249300 3.15952400 0.75051400
S -7.34870100 1.90865400 -0.65032500
O -7.56510100 2.78055800 0.53971700
O -8.47481200 0.95586500 -0.86547100
O -6.98841300 -2.67379700 -1.87547000
O 7.31921300 3.23611900 0.14875000
O 5.96522600 3.26616400 2.23441100
O 4.97806300 4.07215700 0.10858600
H -1.42562600 1.48669700 -0.33741600
H 1.50262100 -1.19563200 -0.77235700
O 0.22124800 -4.01631400 -0.72682300
H 1.60725500 -4.12462400 0.45862500
H 2.72729700 -2.52111500 -2.02473900
O 1.82937800 -2.31313600 -2.31788800
H 1.27868900 -3.03884100 -1.97631200
H -0.37148800 -4.74274100 -0.94124700
H 3.40298000 -2.74471400 0.25451200
O 2.41598200 -3.94886200 0.97797000
H 2.14854200 -3.95876200 1.90041600
H -0.31987400 -3.33797500 -0.27916300
H -0.26567700 -2.20680300 1.32521800
Pd -0.72374000 -0.99917700 0.42766900
H 1.87523100 0.21678000 1.78623800
H -2.24783000 -0.70344700 -2.08304100
Cl -4.98186700 -1.81937800 2.51560800
Cl 6.62632700 -1.77746500 -1.50300500

56

RR-PhCl_ID2_TS3-square, E(SCF) = -
3404.50890728, E(ZPE) = -3404.114507, E(G)
= -3404.186750 a.u.

C -0.09353800 1.02875000 -1.64144800
H -0.01052400 0.26531000 -2.42122200
H -0.20452300 2.00273700 -2.12640500
C 1.11159200 0.98684200 -0.74134600
H 2.02701800 1.21887000 -1.29261700
H 1.01467000 1.71690900 0.06916400
N 1.19525900 -0.36164700 -0.13292600
N -1.28168100 0.70566000 -0.82570100
C 2.21481800 -0.45843900 0.94467900
H 2.17567100 -1.48422800 1.31716300
C -2.49680900 0.39596000 -1.60253300
H -2.67728800 1.19155400 -2.33372300
C 3.59607100 -0.10851300 0.48887100
C 4.30828000 -1.05780000 -0.30536100
C 4.15547300 1.10953400 0.82611100
C 5.60489700 -0.64722800 -0.70152700

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|--------------|
| C | 5.43149000 | 1.45676400 | 0.40702300 | O | -8.43354800 | 0.98306200 | -0.92725900 |
| H | 3.58370700 | 1.80637000 | 1.43487600 | O | -6.91962000 | 2.66691100 | -1.95320900 |
| C | 6.15964200 | 0.56853100 | -0.36624700 | O | -7.52392600 | 2.82790200 | 0.45318300 |
| H | 7.15777600 | 0.82937100 | -0.69825100 | O | 4.93902900 | 4.15210700 | 0.31270200 |
| C | -3.69385700 | 0.24578000 | -0.71696600 | O | 7.27266700 | 3.29807900 | 0.33959600 |
| C | -3.68773900 | -0.69444600 | 0.34517800 | O | 5.88180800 | 3.20934400 | 2.39864200 |
| C | -4.82284100 | 1.05870500 | -0.97970800 | H | -2.34169300 | -0.94929000 | -2.10464900 |
| C | -4.89780900 | -0.80683300 | 1.07086200 | H | 1.81116400 | 0.16679600 | 1.68829600 |
| C | -5.98052300 | 0.86206600 | -0.24102900 | H | -1.37789000 | 1.28312800 | -0.48794500 |
| H | -4.80561900 | 1.72726200 | -1.79240900 | H | 1.45811300 | -1.39908700 | -0.77541700 |
| C | -6.01703600 | -0.05874500 | 0.79577100 | O | 0.18417200 | -4.07450800 | 0.63572800 |
| H | -6.91479700 | -0.19062500 | 1.39009100 | H | 1.19132000 | -4.14432000 | 0.62264000 |
| O | 3.80857200 | -2.19610400 | -0.63291200 | H | 2.73657500 | -2.36679500 | -1.97490500 |
| O | -2.68344600 | -1.45905300 | 0.66240100 | O | 1.88189200 | -2.31470800 | -2.45616400 |
| S | 6.10344400 | 3.40537800 | 0.85783300 | H | 1.63083900 | -3.22173700 | -2.64500900 |
| S | -7.43632200 | 1.85987600 | -0.57334600 | H | -0.13886000 | -4.19846100 | -0.26495300 |
| O | -7.63220200 | 2.70584200 | 0.63816500 | H | 3.23164000 | -3.38979300 | 0.23099300 |
| O | -8.55110900 | 0.89266700 | -0.77704900 | O | 2.77854700 | -4.17361700 | 0.64018700 |
| O | -7.11700200 | 2.65139300 | -1.79235100 | H | 3.19844300 | -4.32374900 | 1.49023600 |
| O | 7.48181300 | 3.09523900 | 0.29491000 | H | -0.14847800 | -2.90554300 | 1.04404900 |
| O | 6.07905200 | 3.10706100 | 2.34768800 | H | -0.31949400 | -2.11118800 | 1.61698200 |
| O | 5.19520400 | 4.06793100 | 0.24416300 | Pd | -0.74311300 | -1.04820200 | 0.40329000 |
| H | -1.48195400 | 1.48515600 | -0.19802300 | Cl | 6.59841000 | -1.56110700 | -1.71995000 |
| H | 1.43789100 | -1.02429600 | -0.88482800 | Cl | -4.93506500 | -1.60951400 | 2.65899800 |
| O | 0.41963400 | -3.86310100 | 0.04112700 | | | | |
| H | 1.35057600 | -4.07769800 | 0.40215200 | | | | |
| H | 2.51957300 | -3.42334200 | -1.82424400 | 53 | | | |
| O | 1.65111400 | -2.32907900 | -2.27916300 | RR-PhCl EI D1 TS1 P, E(SCF) = - | | | |
| H | 1.10958300 | -3.01846000 | -1.87627900 | 3328.07997595, E(ZPE) = -3327.707257, E(G) | | | |
| H | -0.15147900 | -4.63401600 | 0.14552100 | = -3327.775174 a.u. | | | |
| H | 3.30917200 | -3.42375800 | 0.34305500 | C | 0.44239900 | -3.13597100 | 1.08465600 |
| O | 2.84197400 | -4.18984000 | 0.77435100 | H | 1.15707200 | -3.95788000 | 1.16485600 |
| H | 3.08050700 | -4.18263500 | 1.70432500 | H | 0.04276000 | -2.95398900 | 2.08426100 |
| H | -0.03682800 | -2.87836900 | 0.64682700 | C | -0.65488700 | -3.46802700 | 0.11164200 |
| H | -0.29484500 | -2.17511300 | 1.34549100 | H | -0.23884600 | -3.73504300 | -0.86194300 |
| Pd | -0.74404200 | -0.93286100 | 0.33598200 | H | -1.26213300 | -4.30655000 | 0.46565300 |
| H | 1.89222000 | 0.20320200 | 1.75275100 | N | -1.50333300 | -2.26059700 | -0.08370400 |
| H | -2.28308600 | -0.52288800 | -2.16071800 | N | 1.13984400 | -1.89261200 | 0.65948000 |
| Cl | -4.96539600 | -1.96694900 | 2.39266900 | C | -2.45393000 | -2.00848500 | 1.04441100 |
| Cl | 6.55704200 | -1.76523100 | -1.68089700 | H | -3.06727000 | -2.91015700 | 1.14984100 |
| | | | | C | 2.38384100 | -2.10258000 | -0.10065300 |
| | | | | H | 2.11580700 | -2.55951200 | -1.06064400 |
| 56 | | | | C | -3.30262100 | -0.81102000 | 0.79462800 |
| RR-PhCl ID2 TS3, E(SCF) = -3404.50888348, | | | | C | -2.81938000 | 0.46381200 | 1.22239400 |
| E(ZPE) = -3404.114536, E(G) = -3404.187243 | | | | C | -4.51214000 | -0.94822300 | 0.13275400 |
| a.u. | | | | C | -3.67865700 | 1.55340000 | 0.89836900 |
| C | -0.05734200 | 0.53485100 | -1.87094500 | C | -5.30640100 | 0.15004500 | -0.14395500 |
| H | -0.01850600 | -0.35302800 | -2.50845700 | H | -4.85255200 | -1.93528900 | -0.16848400 |
| H | -0.14121300 | 1.41676200 | -2.51229200 | C | -4.87481800 | 1.41500100 | 0.23852300 |
| C | 1.16423000 | 0.59933100 | -0.99540000 | H | -5.48085800 | 2.28989200 | 0.02728400 |
| H | 2.07456700 | 0.68261600 | -1.59562200 | C | 3.18390700 | -0.84494700 | -0.27810700 |
| H | 1.12085500 | 1.46853400 | -0.33058300 | C | 2.59578900 | 0.39743900 | 0.60225800 |
| N | 1.20977200 | -0.61940700 | -0.15158600 | C | 4.56521100 | -0.94627000 | -0.15212700 |
| N | -1.23765300 | 0.40693000 | -0.99265300 | C | 3.48241800 | 1.48180200 | -0.79224500 |
| C | 2.20609400 | -0.53668800 | 0.95099100 | C | 5.39405700 | 0.13637600 | -0.35487800 |
| H | 2.23341300 | -1.52706300 | 1.41320200 | H | 5.00908000 | -1.90225600 | 0.10525200 |
| C | -2.49114900 | 0.05153100 | -1.68377600 | C | 4.84572700 | 1.36914700 | -0.67425100 |
| H | -2.65693500 | 0.74147000 | -2.51818000 | H | 5.47638700 | 2.23691100 | -0.83308300 |
| C | 3.56830300 | -0.11007600 | 0.50156500 | O | -1.70374100 | 0.61202200 | 1.82123600 |
| C | 4.32698800 | -1.00386000 | -0.31242300 | O | 1.31195200 | 0.62975400 | -0.74472600 |
| C | 4.05901200 | 1.13214400 | 0.85497400 | S | -6.83903500 | -0.01514400 | -1.05574000 |
| C | 5.59601100 | -0.51672100 | -0.71005100 | S | 7.17759400 | -0.00144200 | -0.17012900 |
| C | 5.31273100 | 1.55436600 | 0.43707100 | O | 7.52778500 | 0.85439200 | 0.99747500 |
| H | 3.45125100 | 1.78791200 | 1.47412200 | O | 7.74993300 | 0.51056500 | -1.44571300 |
| C | 6.08359400 | 0.72252000 | -0.35660100 | O | 7.44957000 | -1.44558600 | 0.05921200 |
| H | 7.06253400 | 1.04832500 | -0.68938700 | O | -7.15982300 | -1.46952900 | -1.05246000 |
| C | -3.66230000 | 0.09659800 | -0.75309100 | O | -6.56352900 | 0.51336700 | -2.42382500 |
| C | -3.66833300 | -0.69063200 | 0.42572800 | O | -7.84516100 | 0.80776600 | -0.32555900 |
| C | -4.75354000 | 0.88845100 | -1.08077800 | H | -0.43349800 | 1.91651600 | 1.55860000 |
| C | -4.85452500 | -0.63573100 | 1.19499800 | H | -1.03688900 | 0.04203200 | -1.78527700 |
| C | -5.88612600 | 0.91518900 | -0.29102300 | H | -1.36742300 | 0.37151200 | -1.12004800 |
| H | -4.72586000 | 1.49486800 | -1.98032300 | O | 0.45902800 | 2.30640100 | 1.45405500 |
| C | -5.93857400 | 0.13801100 | 0.85657100 | H | 0.76141300 | 1.94688200 | 0.60427100 |
| H | -6.81884400 | 0.14331500 | 1.49070100 | H | -0.24093500 | -0.12101600 | 2.63717600 |
| O | 3.88194400 | -2.15820900 | -0.66055200 | O | 0.70949100 | -0.17813600 | 2.86631600 |
| O | -2.69271600 | -1.46188500 | 0.81202900 | H | 1.00785100 | 0.70160700 | 2.57783400 |
| S | 5.90112100 | 3.18028700 | 0.90789000 | H | -2.06503700 | -2.39346400 | -0.239385000 |
| S | -7.30386400 | 1.93199300 | -0.71757300 | H | -1.86721800 | -1.88359900 | 1.95552700 |

H 1.30911000 -1.31372400 1.50152800
H 2.99673900 -2.83117900 0.43957700
Pd -0.13016000 -0.74676200 -0.45530700
Cl 2.79509600 3.04486800 -1.20946400
Cl -3.15249700 3.16984400 1.37345000

53

RR-PhCl_EI_D1_TS1_R, E(SCF) = -
3328.08971371, E(ZPE) = -3327.718613, E(G)
= -3327.789073 a.u.

C 0.58290800 -3.34736200 0.72438900
H 1.24853600 -4.21461900 0.69257000
H 0.10370600 -3.33120100 1.70488500
C -0.45374900 -3.43120500 -0.36659600
H 0.02235700 -3.57232500 -1.33851200
H -1.12210500 -4.28001600 -0.19809600
N -1.23171600 -2.16534700 -0.45163800
N 1.36337800 -2.08517100 0.61698200
C -2.40981400 -2.02874900 0.42175000
H -3.03347300 -2.92307900 0.33448200
C 2.52717200 -2.07179800 -0.28422200
H 2.16075400 -2.18486900 -1.31008200
C -3.23102000 -0.82092100 0.04641400
C -2.66779000 0.41483400 -0.36704800
C -4.61222600 -0.95825300 0.13897900
C -3.59598500 1.43868400 -0.67963700
C -5.47217100 0.07854700 -0.15210900
H -5.03183800 -1.90955500 0.44971000
C -4.95662100 1.29510100 -0.57321200
H -5.61147300 2.12199300 -0.82583200
C 3.34180000 -0.81423000 -0.12034900
C 2.77944400 0.46388300 0.16151700
C 4.71330200 -0.94647900 -0.27905800
C 3.70395000 1.52876500 0.25632700
C 5.57296100 0.13193400 -0.18494500
H 5.12335600 -1.93177600 -0.48336400
C 5.06199700 1.38631000 0.08988800
H 5.72315500 2.24043400 0.17530100
O -1.39437100 0.68642900 -0.50904100
O 1.51253700 0.72929200 0.35333500
S -7.25448400 -0.12436900 -0.04636900
S 7.33866100 -0.11815500 -0.40277800
O 7.74679400 -1.07406000 0.66470900
O 7.95601300 1.22721700 -0.25260500
O 7.49980300 -0.68885800 -1.76929700
O -7.47482600 -1.49853900 0.47954900
O -7.76376000 0.06101700 -1.43441700
O -7.72568700 0.94239800 0.88009800
H -0.85807500 2.18946600 0.53710400
H -1.71116700 -0.39679900 -3.47471000
H -1.68353200 0.12534700 -2.93694100
O -0.32646400 2.60124500 1.24134300
H 0.55502200 2.23670700 1.04500400
H -0.63130300 -0.11842400 2.83073200
O -1.02800900 0.67493100 3.20189400
H -0.80104300 1.37744200 2.56131100
H -1.54271100 -2.04707500 -1.41491400
H -2.05705800 -1.97728500 1.45775000
H 1.68712700 -1.83332000 1.54955600
H 3.16075300 -2.93882500 -0.06752400
Pd 0.05938900 -0.65465600 -0.00749500
Cl 3.07095500 3.13353200 0.60905600
Cl -2.95463300 2.97829500 -1.24151200

53

RR-PhCl_EI_D1_TS1, E(SCF) = -3328.07025631,
E(ZPE) = -3327.699453, E(G) = -3327.766865
a.u.

C 0.43730700 -3.11292000 1.22401900
H 1.08729300 -3.98644300 1.32194700
H -0.06638200 -2.96596800 2.18160100
C -0.56045400 -3.30470400 0.11453500
H -0.05122600 -3.50124000 -0.83102000
H -1.22002800 -4.15209000 0.32340900
N -1.35468000 -2.05957900 -0.06780000
N 1.24910600 -1.89289000 0.96853900
C -2.49168400 -1.89907300 0.88549600

H -3.05869800 -2.83591500 0.89905500
C 2.48535300 -2.09540200 0.20982800
H 2.21151600 -2.54686700 -0.74998400
C -3.38168500 -0.76957200 0.48045900
C -2.88612900 0.55909000 0.57266400
C -4.65950100 -1.02598400 0.00876900
C -3.77641300 1.57319200 0.14415900
C -5.49602300 0.00523900 -0.37898700
H -5.01916700 -2.04817600 -0.05258600
C -5.04640100 1.31739900 -0.31528100
H -5.68585000 2.13671500 -0.62693900
C 3.29861600 -0.84428400 0.00393200
C 2.76876900 0.46761300 -0.00836700
C 4.65665000 -1.04383000 -0.22747500
C 3.69486200 1.50921400 -0.25747200
C 5.51803500 0.00153400 -0.47534200
H 5.05426100 -2.05349600 -0.21145100
C 5.03180200 1.30087200 -0.48268000
H 5.69106300 2.14291000 -0.62637400
O -1.69569300 0.81714400 0.99912000
O 1.52007600 0.80497200 0.21184400
S -7.15034900 -0.31548100 -0.99854200
S 7.26954600 -0.27520100 -0.76976000
O 7.97883200 0.46775900 0.30876700
O 7.53975400 0.28663800 -2.12249600
O 7.46497900 -1.74792000 -0.69465700
O -7.34953400 -1.78604500 -0.88186100
O -7.15654200 0.16469000 -2.40982600
O -8.06951800 0.47088900 -0.12841700
H -0.65719200 2.28018700 1.51959900
H -0.57443400 0.41630500 -1.87974800
H -1.00462700 0.85388500 -1.42818800
O 0.17780800 2.69296900 1.80974300
H 0.82425200 2.28889800 1.20748200
H -0.70861900 0.13920600 2.58260400
O 0.07794300 0.06289400 3.15045200
H 0.47200500 0.93794300 3.01263400
H -1.75259400 -2.07091700 -1.00625800
H -2.06868400 -1.75071600 1.88254900
H 1.44248300 -1.42769000 1.85972000
H 3.10244600 -2.82918600 0.74226300
Pd 0.02952000 -0.52945900 0.04524300
Cl 3.08621500 3.15848800 -0.27044000
Cl -3.20429200 3.23823600 0.20528000

53

RR-PhCl_EI_D1_TS2_P, E(SCF) = -
3328.10790329, E(ZPE) = -3327.732759, E(G)
= -3327.801172 a.u.

C 0.46535900 -3.06164900 1.17039500
H 1.12149100 -3.93757800 1.21940700
H 0.10777500 -2.87804000 2.18618300
C -0.69743500 -3.35387800 0.24746300
H -0.33648700 -3.64819100 -0.74036300
H -1.30728700 -4.17343700 0.64389600
N -1.52892700 -2.13566000 0.05553000
N 1.20253500 -1.86497900 0.73884200
C -2.37686800 -1.82047800 1.23332200
H -2.96983800 -2.70830600 1.48415700
C 2.35555500 -2.09833600 -0.13419800
H 1.97850500 -2.48166500 -1.09191500
C -3.28676500 -0.67048500 0.93593700
C -2.98963200 0.64401700 1.32284000
C -4.42691000 -0.91241400 0.18363900
C -3.84879100 1.66504400 0.91267600
C -5.26806300 0.11528000 -0.20181300
H -4.66249300 -1.93488700 -0.10049000
C -4.97493000 1.41686600 0.15609600
H -5.62612900 2.22745700 -0.14780900
C 3.18090700 -0.85624400 -0.33516100
C 2.62307900 0.39180100 -0.72480100
C 4.55450400 -0.97626500 -0.15824300
C 3.55395500 1.44190600 -0.92938200
C 5.41929200 0.07827700 -0.37101300
H 4.96682000 -1.93232300 0.14777900
C 4.91001600 1.30792800 -0.75911700
H 5.56510300 2.15442600 -0.93439000

O -1.93424400 1.00210500 2.06578100
O 1.35827400 0.64948700 -0.91842100
S -6.72991400 -0.25933900 -1.18809500
S 7.18586800 -0.09187400 -0.09985700
O 7.42371000 -1.54190700 0.13718700
O 7.49816000 0.75207500 1.08890500
O 7.83614400 0.41346900 -1.34152600
O -7.44274300 1.03457500 -1.34982200
O -7.49268800 -1.26101300 -0.39535000
O -6.20993300 -0.81256900 -2.46804300
H -0.34534300 2.24818000 1.31483800
H -1.16417900 0.10468400 -1.37378000
H -1.30556000 0.28387000 2.28484300
O 0.62154400 2.22213600 1.29788200
H 0.83881700 1.81734000 0.43405300
H 0.65298600 0.05168000 3.80490000
O 0.46891700 -0.05738200 2.86809200
H 0.72763800 0.78615600 2.43681600
H -2.14881600 -2.29458000 -0.73571000
H -1.71858700 -1.63054000 2.08306100
H 1.46863800 -1.32629700 1.56293300
H 3.00119000 -2.88031800 0.28565800
Pd -0.15127700 -0.66879100 -0.46197800
Cl 2.92739300 3.00464600 -1.44961400
Cl -3.46108600 3.31680200 1.35339100

53

RR-PhCl_EI_D1_TS2 R, E(SCF) = -
3328.08006127, E(ZPE) = -3327.707126, E(G)
= -3327.774588 a.u.

C 0.43273700 -3.11906500 1.10247500
H 1.14441500 -3.94259400 1.19247100
H 0.02960600 -2.92778700 2.09897000
C -0.66109800 -3.45518000 0.12703700
H -0.24126200 -3.73056300 -0.84254200
H -1.27253600 -4.28917200 0.48435700
N -1.50519500 -2.24688700 -0.08121700
N 1.13604900 -1.88154400 0.67041400
C -2.46231600 -1.98696500 1.03854600
H -3.07931400 -2.88602300 1.14480100
C 2.38053200 -2.10135700 -0.08581600
H 2.11271200 -2.56348900 -1.04337200
C -3.30571100 -0.78804100 0.77662700
C -2.82239900 0.48977900 1.20596300
C -4.50419700 -0.92246500 0.10128000
C -3.67296200 1.57754600 0.86759200
C -5.28978100 0.18101500 -0.19782300
H -4.83355300 -1.91384200 -0.20271400
C -4.86606200 1.44102700 0.19541300
H -5.46967200 2.31180400 -0.03298900
C 3.18580000 -0.84798700 -0.26986500
C 2.60306700 0.39586600 -0.59807000
C 4.56675900 -0.95530200 -0.14519200
C 3.49452100 1.47551700 -0.79230300
C 5.40044700 0.12264800 -0.35285800
H 5.00627000 -1.91252100 0.11503600
C 4.85743800 1.35700100 -0.67539100
H 5.49186000 2.22137000 -0.83776700
O -1.71059000 0.63282000 1.81339500
O 1.32020900 0.63387200 -0.74057100
S -6.85734800 -0.04665000 -1.03470500
S 7.18350100 -0.02329400 -0.16916200
O 7.44891900 -1.46869400 0.06009200
O 7.53830400 0.83098200 0.99822100
O 7.75728700 0.48597700 -1.44520800
O -7.35400700 1.32107000 -1.35254200
O -7.73809200 -0.77438100 -0.07499100
O -6.55786400 -0.85725500 -2.24998600
H -0.43487200 1.93372000 1.54752900
H -1.02863500 0.05196600 -1.78749700
H -1.35896200 0.38449700 -1.12375800
O 0.45822800 2.32307100 1.44588300
H 0.76700900 1.95701700 0.60127000
H -0.24909500 -0.09899100 2.63484700
O 0.70047900 -0.15696900 2.86714300
H 1.00039400 0.72294900 2.58100500
H -2.06104300 -2.38344100 -0.92463900

H -1.88243400 -1.85842600 1.95339000
H 1.30557300 -1.29798700 1.50909100
H 2.98944900 -2.82883400 0.46040300
Pd -0.12711900 -0.73708400 -0.45311400
Cl 2.81378000 3.04035400 -1.21355900
Cl -3.14592700 3.19647900 1.33683400

53

RR-PhCl_EI_D1_TS2, E(SCF) = -3328.07041465,
E(ZPE) = -3327.699246, E(G) = -3327.767951
a.u.

C 0.41379700 -2.97443700 0.84558000
H 1.01924200 -3.88300900 0.89229800
H -0.01669900 -2.81754900 1.83655800
C -0.66786100 -3.10690300 -0.19367700
H -0.23445200 -3.32126900 -1.17269300
H -1.35526200 -3.92012400 0.05911200
N -1.40811300 -1.82092900 -0.31345700
N 1.26700500 -1.79711700 0.54346600
C -2.37100500 -1.58060800 0.80248200
H -2.85815000 -2.53580400 1.02713700
C 2.49192500 -2.06316100 -0.22796000
H 2.18578700 -2.37455100 -1.23349700
C -3.41892000 -0.55982900 0.47867000
C -3.10988900 0.82464300 0.49449500
C -4.70975900 -0.98680300 0.21283500
C -4.17632600 1.70554300 0.23814000
C -5.72690200 -0.08031700 -0.03861100
H -4.92974800 -2.05085600 0.21198100
C -5.46140300 1.27632400 -0.02100500
H -6.25369900 1.98926800 -0.21574300
C 3.41305000 -0.87562700 -0.26027000
C 2.95807400 0.45110200 -0.46342500
C 4.77157500 -1.12849500 -0.10796100
C 3.96126400 1.44817600 -0.50747700
C 5.71331700 -0.12264100 -0.16686000
H 5.10847000 -2.14757900 0.05284600
C 5.30091300 1.18651500 -0.36104700
H 6.01909600 1.99799700 -0.40436900
O -1.89114600 1.24985800 0.70594100
O 1.71434100 0.82901700 -0.62174000
S -7.38690900 -0.69005300 -0.36779900
S 7.45814700 -0.46813800 0.08769900
O 7.59084400 -1.94816700 0.00926200
O 7.78449700 0.07720700 1.43569100
O 8.17337700 0.24617200 -1.00564300
O -8.21477200 0.51594700 -0.63786400
O -7.79711400 -1.42090700 0.86350000
O -7.25487800 -1.58953300 -1.54768300
H -0.46150200 2.59645700 0.90003800
H -0.82809200 0.72393000 -1.31581300
H -1.16601000 0.92227700 -0.47428900
O 0.46723000 2.84307000 1.03461300
H 0.95568500 2.34731800 0.35442500
H -0.62724100 0.51651900 2.13441400
O 0.22357200 0.39949900 2.59035500
H 0.67781500 1.21151200 2.31429500
H -1.94351300 -1.84088800 -1.17950400
H -1.79902900 -1.29135900 1.68622800
H 1.49877400 -1.31866600 1.41694500
H 3.02383100 -2.90730500 0.22317600
Pd 0.12434100 -0.42186300 -0.48091700
Cl 3.45797100 3.11291900 -0.77284500
Cl -3.84301400 3.43228800 0.23903700

45

RR-PhCl_EI, E(SCF) = -3174.03353803, E(ZPE)
= -3173.728532, E(G) = -3173.790964 a.u.

C -0.54358800 -3.32132800 -0.56146900
H -1.21067000 -4.17958200 -0.43935000
H -0.09157100 -3.39121400 -1.55277500
C -0.52442100 -3.32552700 0.50499400
H 0.07281500 -3.40111000 1.49604600
H 1.18940700 -4.18451500 0.37724200
N 1.29999500 -2.05675600 0.48908500
N -1.31589900 -2.05074100 -0.53866000
C 2.45607100 -1.95982200 -0.41846300

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|----|-------------|-------------|-------------|
| H | 3.09331300 | -2.84220800 | -0.29331400 |
| C | -2.46232700 | -1.95038500 | 0.38007500 |
| H | -2.07404300 | -1.96751800 | 1.40405700 |
| C | 3.26920300 | -0.72299300 | -0.13255700 |
| C | 2.69372900 | 0.53036600 | 0.22389100 |
| C | 4.64913000 | -0.85016000 | -0.24529800 |
| C | 3.62052600 | 1.58485900 | 0.43651000 |
| C | 5.50358500 | 0.21246400 | -0.04021600 |
| H | 5.07367200 | -1.81446000 | -0.50611200 |
| C | 4.97981700 | 1.44798000 | 0.31263600 |
| H | 5.62851100 | 2.29881400 | 0.49067800 |
| C | -3.27366200 | -0.70911300 | 0.10656500 |
| C | -2.69663800 | 0.54352600 | -0.26564000 |
| C | -4.64806600 | -0.82519600 | 0.24811500 |
| C | -3.61982600 | 1.59863000 | -0.46603400 |
| C | -5.50265800 | 0.24449200 | 0.05259500 |
| H | -5.06570000 | -1.79049400 | 0.52184400 |
| C | -4.98073600 | 1.47147800 | -0.31414100 |
| H | -5.63686000 | 2.31713900 | -0.48224900 |
| O | 1.42901900 | 0.79371400 | 0.38111400 |
| O | -1.43256000 | 0.79538400 | -0.44695600 |
| S | 7.28414100 | 0.01557700 | -0.14837800 |
| S | -7.27207000 | 0.01321500 | 0.24520500 |
| O | -7.66528500 | -0.99389100 | -0.78115200 |
| O | -7.88171400 | 1.35131600 | 0.01463800 |
| O | -7.46745400 | -0.48817200 | 1.63478400 |
| O | 7.50985700 | -1.35144200 | -0.69219100 |
| O | 7.79705600 | 0.18244900 | 1.24166000 |
| O | 7.75649500 | 1.09506700 | -1.06024000 |
| H | 1.63374000 | -1.87731200 | 1.43429500 |
| H | 2.07705200 | -1.97445500 | -1.44608000 |
| H | -1.65707800 | -1.87015100 | -1.48098900 |
| H | -3.10442000 | -2.82998600 | 0.26009800 |
| Pd | -0.00356800 | -0.57947700 | -0.02932500 |
| Cl | -2.97627000 | 3.16794600 | -0.94073300 |
| Cl | 2.97491500 | 3.15933500 | 0.88783600 |

45

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|---|-------------|-------------|-------------|
| RR-PhCl, E(SCF) = -3174.04543462, E(ZPE) = -3173.740537, E(G) = -3173.803252 a.u. | | | |
| C | -0.63750900 | -3.35282100 | 0.40342500 |
| H | -0.41584800 | -3.32822400 | 1.47409400 |
| H | -1.24542100 | -4.23859300 | 0.20233300 |
| C | 0.63733900 | -3.35276600 | -0.40359900 |
| H | 1.24520600 | -4.23860400 | -0.20266600 |
| H | 0.41570600 | -3.32795000 | -1.47426900 |
| N | 1.38333100 | -2.11611200 | -0.07573200 |
| N | -1.38344600 | -2.11607400 | 0.07581300 |
| C | 2.47128800 | -1.77223900 | -1.01168700 |
| H | 3.10904700 | -2.64881600 | -1.16898600 |
| C | -2.47144800 | -1.77234800 | 1.01177500 |
| H | -1.99473600 | -1.53319000 | 1.96880900 |
| C | 3.30154500 | -0.63629800 | -0.49716100 |
| C | 2.69877100 | 0.59618200 | -0.11422700 |
| C | 4.67578600 | -0.79309200 | -0.44292100 |
| C | 3.59597300 | 1.61668000 | 0.27416000 |
| C | 5.51067600 | 0.23883000 | -0.04732000 |
| H | 5.10864300 | -1.74743500 | -0.73002400 |
| C | 4.96331700 | 1.45739300 | 0.30982700 |
| H | 5.60492500 | 2.27318400 | 0.62151700 |
| C | -3.30164400 | -0.63635300 | 0.49727400 |
| C | -2.69876000 | 0.59614000 | 0.11456700 |
| C | -4.67586800 | -0.79313800 | 0.44268600 |
| C | -3.59581800 | 1.61658300 | -0.27424000 |
| C | -5.51064500 | 0.23881200 | 0.04689200 |
| H | -5.10880200 | -1.74748000 | 0.72967200 |
| C | -4.96317300 | 1.45733400 | -0.31018600 |
| H | -5.60468000 | 2.27313200 | -0.62206600 |
| O | 1.42258700 | 0.83830900 | -0.12286000 |
| O | -1.42257200 | 0.83832700 | 0.12388900 |
| S | 7.28559100 | -0.02535800 | -0.00505700 |
| S | -7.28560600 | -0.02521800 | 0.00469100 |
| O | -7.87366900 | 1.25124000 | -0.48509700 |
| O | -7.68128500 | -0.35286100 | 1.40393200 |
| O | -7.50322000 | -1.16664800 | -0.92840200 |
| O | 7.87374800 | 1.25123300 | 0.48429800 |
| O | 7.68119500 | -0.35356000 | -1.40419600 |

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|----|-------------|-------------|-------------|
| O | 7.50303600 | -1.16647900 | 0.92846300 |
| H | 1.77856700 | -2.20642500 | 0.86145800 |
| H | 1.99453100 | -1.53297000 | -1.96867300 |
| H | -1.77861300 | -2.20613700 | -0.86143100 |
| H | -3.10921000 | -2.64874800 | 1.16892600 |
| Pd | -0.00001800 | -0.60902400 | 0.00024300 |
| Cl | -2.92171600 | 3.17457200 | -0.74376300 |
| Cl | 2.92201200 | 3.17471200 | 0.74374000 |

59

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|---|-------------|-------------|-------------|
| RR-PhMe_hs_D1_TS1_P, E(SCF) = -2487.49144547, E(ZPE) = -2487.046126, E(G) = -2487.117226 a.u. | | | |
| C | 0.14260800 | -0.89230600 | -2.74302700 |
| H | -0.15593600 | -1.82937100 | -3.22271000 |
| H | 0.04689500 | -0.08928900 | -3.47914000 |
| C | 1.53877200 | -0.98103700 | -2.19487300 |
| H | 2.27610600 | -1.18545900 | -2.97695100 |
| H | 1.81890600 | -0.04410500 | -1.70737000 |
| N | 1.56409000 | -2.04593100 | -1.16443800 |
| N | -0.77416800 | -0.65555500 | -1.60804200 |
| C | 2.86206700 | -2.12866900 | -0.41938000 |
| H | 2.70288600 | -2.85540400 | -0.38107300 |
| C | -2.19833400 | -0.80647500 | -1.94784500 |
| H | -2.34488100 | -1.85672300 | -2.22628100 |
| C | 3.38364900 | -0.83577200 | 0.11240900 |
| C | 2.70086400 | -0.17219500 | 1.16258900 |
| C | 4.56916200 | -0.31846300 | -0.39542500 |
| C | 3.29796100 | 1.00309200 | 1.70942900 |
| C | 5.12000600 | 0.83350800 | 0.12976600 |
| H | 5.07911800 | -0.82740400 | -1.20878000 |
| C | 4.47923000 | 1.48156100 | 1.18444600 |
| H | 4.92292500 | 2.38024500 | 1.60761000 |
| C | -3.11114100 | -0.39187000 | -0.83778200 |
| C | -2.98341600 | -0.91380200 | -0.46522400 |
| C | -4.15717900 | 0.47447900 | -1.13750100 |
| C | -3.98333400 | -0.60611000 | 1.42326700 |
| C | -5.10414100 | 0.79777900 | -0.19083100 |
| H | -4.24448500 | 0.88929000 | -2.13650500 |
| C | -5.01561100 | 0.24310100 | 1.07979000 |
| H | -5.77558100 | 0.47329200 | 1.82193300 |
| O | 1.56257800 | -0.59989900 | 1.60133100 |
| O | -2.00601000 | -1.71472200 | 0.85657300 |
| S | 6.63968000 | 1.51493300 | -0.52196400 |
| S | -6.44328000 | 1.92969200 | -0.56718800 |
| O | -6.23953500 | 3.11328200 | 0.31722300 |
| O | -7.70165100 | 1.19612200 | -0.24772600 |
| O | -6.31143900 | 2.25735300 | -2.01407600 |
| O | 6.29775900 | 2.87053500 | -1.04703300 |
| O | 7.08975200 | 0.57947300 | -1.59238400 |
| O | 7.59376100 | 1.58411000 | 0.62438100 |
| H | 0.12044500 | -3.27644400 | 1.05121900 |
| H | 0.48825500 | -2.64036200 | 1.39162600 |
| H | 1.44686500 | -2.94122100 | -1.64022600 |
| H | 3.59766900 | -2.55377100 | -1.11128800 |
| H | -0.59552300 | 0.27301500 | -1.18692000 |
| H | -2.41001500 | -0.20192200 | -2.83671100 |
| Pd | -0.22387600 | -1.90001600 | -0.09668800 |
| H | 0.24938400 | -0.43530200 | 2.79293600 |
| O | -0.63921800 | -0.51982200 | 3.19139500 |
| H | -1.15684700 | -0.94013200 | 2.48654000 |
| H | 0.51360600 | 0.74680400 | 0.81867600 |
| O | 0.03180300 | 1.37467300 | 0.23870500 |
| H | 0.64206000 | 2.10087500 | 0.08289800 |
| C | -3.91914800 | -1.21883600 | 2.78527300 |
| H | -3.73739900 | -2.29471500 | 2.72681400 |
| H | -3.10907700 | -0.79588900 | 3.38625300 |
| H | -4.85335700 | -1.05441300 | 3.32461200 |
| C | 2.61328200 | 1.67770000 | 2.85338000 |
| H | 1.60450700 | 2.01246900 | 2.58739700 |
| H | 2.48729900 | 0.99367900 | 3.69901500 |
| H | 3.17848100 | 2.54643000 | 3.19512800 |

59

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|---|
| RR-PhMe_hs_D1_TS1_R, E(SCF) = -2487.51101267, E(ZPE) = -2487.066181, E(G) = -2487.133551 a.u. |
|---|

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|----|-------------|-------------|--------------|---------------------------------------|-------------|-------------|-------------|
| C | 0.35878200 | 3.02198000 | -1.79496500 | C | 2.80116000 | -0.87773200 | 1.38654400 |
| H | 0.66982200 | 3.92139500 | -1.25355000 | C | 4.20269400 | -0.09930400 | -0.45888900 |
| H | 0.72191600 | 3.10540500 | -2.82226700 | C | 3.20278200 | 0.28754700 | 2.11502200 |
| C | -1.14312400 | 2.86905400 | -1.73882800 | C | 4.56048000 | 1.02647800 | 0.25185200 |
| H | -1.64846500 | 3.70418900 | -2.23204900 | H | 4.61076000 | -0.24822900 | -1.45495700 |
| H | -1.46417500 | 1.94073700 | -2.22151400 | C | 4.05728700 | 1.20385400 | 1.53921100 |
| N | -1.52807000 | 2.78709700 | -0.311063100 | H | 4.35238100 | 2.08160300 | 2.10973300 |
| N | 0.97132900 | 1.85991700 | -1.11197900 | C | -2.92705900 | -0.34857600 | -0.89263800 |
| C | -2.95943500 | 2.48716600 | -0.03648200 | C | -2.79797500 | -1.02261200 | 0.33771100 |
| H | -3.20442400 | 3.02800200 | 0.88177900 | C | -3.91817100 | 0.61360600 | -1.05407200 |
| C | 2.37842200 | 2.02324500 | -0.70506500 | C | -3.73469500 | -0.75329900 | -1.36787300 |
| H | 2.38837000 | 2.78098300 | 0.08692900 | C | -4.80469600 | 0.89313600 | -0.03706000 |
| C | -3.26206900 | 1.03444000 | 0.15501200 | H | -4.00557900 | 1.14548700 | -1.99598900 |
| C | -2.61289300 | 0.33376200 | 1.19589900 | C | -4.71461000 | 0.19680200 | 1.16147600 |
| C | -4.22872500 | 0.40318700 | -0.61159800 | H | -5.42505800 | 0.40332600 | 1.04765700 |
| C | -3.00867000 | -0.99066500 | 1.48680800 | O | 1.99350100 | -1.73682300 | 1.92251800 |
| C | -4.58825100 | -0.90509000 | -0.34249500 | O | -1.86514500 | -1.92520300 | 0.59809700 |
| H | -4.72115700 | 0.93685000 | -1.41851800 | S | 5.68118500 | 2.24266000 | -0.42997200 |
| C | -3.98518800 | -1.57324800 | -0.77331900 | S | -6.09645900 | 2.12135000 | -2.44368200 |
| H | -4.27886200 | -2.61160000 | 0.92036700 | O | -5.87141100 | 2.73917000 | -1.57708200 |
| C | 2.97857100 | 0.72263200 | -0.25850200 | O | -5.92442600 | 3.08379500 | 0.88447400 |
| C | 2.34959600 | -0.12986200 | 0.67399600 | O | -7.38520800 | 1.37531900 | -0.15487700 |
| C | 4.22511500 | 0.73581100 | -0.77331000 | O | 4.93317400 | -0.34330400 | -0.44368200 |
| C | 3.01886900 | -1.31336000 | 1.07773300 | O | 6.03164700 | 1.76278100 | -1.79702000 |
| C | 4.86687800 | -0.77600900 | -0.37598900 | O | 6.85764500 | 2.28691600 | 0.48762300 |
| H | 4.70490100 | 1.02467300 | -1.49867100 | H | 0.34044200 | -3.31884500 | 0.74020100 |
| C | 4.25900000 | -1.61226200 | 0.55246500 | H | 0.86884000 | -2.72113400 | -2.03717200 |
| H | 4.75987700 | -2.52420300 | 0.86654200 | H | 1.56040400 | -2.99118700 | -1.99710300 |
| O | -1.63729300 | 0.89728700 | 1.88964600 | H | 3.75683200 | -2.43018500 | -1.48182500 |
| O | 1.16091800 | 0.08868300 | 1.21675900 | H | -0.39368100 | 0.24153600 | -1.27331700 |
| S | -5.81706500 | -1.74904800 | -1.34327700 | H | -2.28122600 | -0.00773400 | -2.89166300 |
| S | 6.48420400 | -1.20920900 | -1.02041300 | Pd | -0.07779400 | -2.02788300 | -0.37247200 |
| O | 6.34943900 | -2.58917600 | -1.56809900 | H | 0.52156700 | -0.87906000 | 2.44114400 |
| O | 7.41528500 | -1.15046300 | 0.14358000 | O | -0.32862100 | -0.38368000 | 2.47873200 |
| O | 6.79796100 | -0.19569000 | -2.06541300 | H | -0.95261200 | -0.98232700 | 2.03464500 |
| O | -5.09665100 | -2.86817200 | -2.01565300 | H | 0.04303800 | 0.78908700 | 1.06316200 |
| O | -6.33464200 | -0.73280800 | -2.30031500 | O | 0.32314500 | 1.28509600 | 0.26520200 |
| O | -6.85478000 | -2.23435300 | -0.38959400 | H | 1.28611900 | 1.28515500 | 0.32573600 |
| H | 0.90030600 | 3.96525600 | 1.85711100 | C | -3.66195000 | -1.51477700 | 2.65204600 |
| H | 0.60170700 | 3.64603700 | 2.46621500 | H | -3.69449900 | -2.59351000 | 2.47790100 |
| H | -1.30456400 | 3.67985200 | 0.12793700 | H | -2.73418100 | -1.31641600 | 3.19721400 |
| H | -3.57294600 | 2.90395200 | -0.84107600 | H | -4.49426700 | -1.24757100 | 3.30471900 |
| H | 0.90152800 | 1.04229500 | -1.72111200 | C | 2.70857800 | 0.47776400 | 0.51278500 |
| H | 2.95805400 | 2.41994000 | -1.54557300 | H | 1.63645200 | 0.69504600 | 3.54498800 |
| Pd | -0.20982600 | 1.42979000 | 0.49947200 | H | 2.85937900 | -0.42571400 | 4.10991400 |
| H | -0.58701200 | 0.57370300 | 3.43106100 | H | 3.22911500 | 1.30455300 | 3.99941900 |
| O | 0.27658300 | 0.48256000 | 3.86820300 | | | | |
| H | 0.83413900 | 0.28207900 | 3.09843000 | 59 | | | |
| H | 0.05899300 | -1.23909100 | 0.28426700 | RR-PhMe_hs_D1_TS2_P-Hbond-reoredered, | | | |
| O | -0.39846300 | -1.81504300 | -0.35288400 | E(SCF) = -2487.52772712, E(ZPE) = - | | | |
| H | -1.33425300 | -1.63976600 | -0.19278700 | 2487.077893, E(G) = -2487.144869 a.u. | | | |
| C | 2.36745900 | -2.21927300 | 2.07221700 | C | 0.23126300 | -0.69927700 | -2.95053600 |
| H | 2.19860500 | -1.71669200 | 3.02933200 | H | -0.12397700 | -1.58008000 | -3.49633600 |
| H | 1.38717200 | -2.56077800 | 1.72610300 | H | 0.19483900 | 0.15209500 | -3.63949000 |
| H | 2.98755700 | -3.09721500 | 2.25843600 | C | 1.63579100 | -0.91174500 | -2.44917300 |
| C | -2.34835500 | -1.71831600 | 2.61148900 | H | 2.34524600 | -1.05126800 | -3.27085700 |
| H | -1.26016900 | -1.73149200 | 2.49174900 | H | 1.95096900 | -0.03490800 | -1.87840900 |
| H | -2.54233000 | -1.23131200 | 3.57188700 | N | 1.67549400 | -2.07975800 | -1.52969400 |
| H | -2.70236500 | -2.74826700 | 2.67372400 | N | -0.64642600 | -0.50115600 | -1.79163700 |
| | | | | C | 2.98476200 | -2.21287500 | -0.82890100 |
| | | | | H | 2.94137700 | -3.13916100 | -0.25283400 |
| | | | | C | -2.07658000 | -0.57876400 | -2.09169700 |
| | | | | H | -2.25923800 | -1.58883100 | -2.48220700 |
| | | | | C | 3.34597500 | -1.04069200 | 0.03273300 |
| | | | | C | 2.90587600 | -0.90215000 | 1.35118700 |
| | | | | C | 4.19906300 | -0.06787900 | -0.48666000 |
| | | | | C | 3.32631400 | 0.17429800 | 2.14859900 |
| | | | | C | 4.59603700 | 1.00802500 | 0.27520500 |
| | | | | H | 4.56742500 | -0.16371900 | -1.50301400 |
| | | | | C | 4.16179600 | 1.12272300 | 1.58816700 |
| | | | | H | 4.48943700 | 1.96303800 | 2.19324800 |
| | | | | C | -2.93982400 | -0.30532800 | -0.89602100 |
| | | | | C | -2.82492400 | -1.04462400 | 0.30368000 |
| | | | | C | -3.93356400 | 0.66131300 | -1.01619400 |
| | | | | C | -3.78580200 | -0.82590700 | 1.32838500 |
| | | | | C | -4.83746700 | 0.89040600 | -0.00100500 |
| | | | | H | -4.00885900 | 1.24003500 | -1.93147700 |

| | | | |
|----|-------------|-------------|-------------|
| C | -4.76337200 | 0.13321300 | 1.16144900 |
| H | -5.48636600 | 0.29598500 | 1.95684800 |
| O | 2.10382200 | -1.81165800 | 1.96274100 |
| O | -1.89953600 | -1.95315200 | 0.55004300 |
| S | 5.69563300 | 2.26587400 | -0.39509400 |
| S | -6.12346300 | 2.12838300 | -0.15893800 |
| O | -5.90791800 | 2.78738800 | -1.47767000 |
| O | -5.94228400 | 3.05964400 | 0.99263800 |
| O | -7.41767200 | 1.38876700 | -0.08543900 |
| O | 4.93022600 | 3.54103900 | -0.31897400 |
| O | 5.99568400 | 1.84286400 | -1.78911900 |
| O | 6.89156400 | 2.26084200 | 0.49166900 |
| H | 0.34382600 | -3.26439700 | 0.49260800 |
| H | 1.58783400 | -2.33939200 | 1.31565600 |
| H | 1.56633400 | -2.92280800 | -2.09247000 |
| H | 3.76393600 | -2.34009700 | -1.58886900 |
| H | -0.41305700 | 0.37046800 | -1.30156200 |
| H | -2.33823300 | 0.12488700 | -2.89236700 |
| Pd | -0.09879700 | -2.05389600 | -0.43939200 |
| H | 0.40944400 | -0.89159100 | 2.55849300 |
| O | -0.42079400 | -0.41047200 | 2.42389400 |
| H | -0.95898600 | -1.03603400 | 1.89926400 |
| O | 0.04238200 | 0.80463900 | 1.07246700 |
| O | 0.28823400 | 1.37501000 | 0.31634100 |
| H | 1.23183900 | 1.53097600 | 0.42272700 |
| C | -3.73095600 | -1.65316600 | 2.57232200 |
| H | -3.78928000 | -2.72085700 | 2.34335400 |
| H | -2.79639000 | -1.50680200 | 3.12168000 |
| H | -4.55653700 | -1.40040300 | 3.23963200 |
| C | 2.87862800 | 0.28007700 | 3.57033400 |
| H | 1.80634100 | 0.48289800 | 3.64467600 |
| H | 3.06501300 | -0.64626000 | 4.11806800 |
| H | 3.40245400 | 1.09097600 | 4.07680000 |

59

RR-PhMe_hs_D1_TS2 R-Hbond-reordered,

E(SCF) = -2487.49773320, E(ZPE) = -

2487.050320, E(G) = -2487.116701 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.25687200 | -0.80652700 | -2.93379400 |
| H | -0.09028900 | -1.69216000 | -3.47419700 |
| H | 0.17732900 | 0.05253700 | -3.60580600 |
| C | 1.66221200 | -0.98535300 | -2.43258900 |
| H | 2.37008500 | -1.15867700 | -3.24796600 |
| H | 1.98372600 | -0.09238400 | -1.89221800 |
| N | 1.68668900 | -2.11873200 | -1.47610300 |
| N | -0.61977000 | -0.62378800 | -1.75852000 |
| C | 2.98150600 | -2.24314900 | -0.72921700 |
| H | 2.88668000 | -3.13197500 | -0.10273200 |
| C | -2.05785800 | -0.67545000 | -2.07026100 |
| H | -2.25959300 | -1.68601700 | -2.44449700 |
| C | 3.33191200 | -1.04310900 | 0.08242300 |
| C | 2.80285500 | -0.88629700 | 1.39316800 |
| C | 4.20254000 | -0.09954900 | -0.45281200 |
| C | 3.19963800 | 0.28266600 | 2.12104400 |
| C | 4.55492100 | 1.02812100 | 0.25787000 |
| H | 4.61100400 | -0.24606200 | -1.44913300 |
| C | 4.04963100 | 1.20298500 | 1.54511200 |
| H | 4.33945500 | 2.08290800 | 2.11511600 |
| C | -2.92045800 | -0.33776000 | -0.89588000 |
| C | -2.79669500 | -1.02451800 | 0.32773900 |
| C | -3.91098900 | 0.62595200 | -1.05152400 |
| C | -3.73429600 | -0.76289000 | 1.35886400 |
| C | -4.80092600 | 0.89536000 | -0.03477700 |
| H | -3.99539600 | 1.16664800 | -1.98865700 |
| C | -4.71351500 | 0.18914200 | 1.15815500 |
| H | -5.42575100 | 0.38920000 | 1.95439100 |
| O | 1.99918100 | -1.74892700 | 1.92375700 |
| O | -1.86735100 | -1.93303900 | 0.58029200 |
| S | 5.66841600 | 2.24987100 | -0.42451500 |
| S | -6.09339800 | 2.12415200 | -0.23146100 |
| O | -5.87001000 | 2.74846700 | -1.56474800 |
| O | -5.92053700 | 3.08115500 | 0.89850400 |
| O | -7.38147600 | 1.37682200 | -0.14752200 |
| O | 4.91341500 | 3.53764300 | -0.43940700 |
| O | 6.02170500 | 1.77136800 | -1.79150500 |
| O | 6.84525300 | 2.30243100 | 0.49234300 |
| H | 0.30489100 | -3.36955600 | 0.69321000 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.82246400 | -2.77951800 | 0.99973500 |
| H | 1.56864500 | -2.98133300 | -2.00884800 |
| H | 3.76026300 | -2.43376600 | -1.47658000 |
| H | -0.38131400 | 0.25104200 | -1.26124400 |
| H | -2.26468600 | 0.02330700 | -2.88807200 |
| Pd | -0.07893900 | -2.03104300 | -0.38633700 |
| H | 0.52743700 | -0.90682800 | 2.43575800 |
| O | -0.32401600 | -0.41202400 | 2.47787900 |
| H | -0.94836100 | -1.00636800 | 2.02910600 |
| H | 0.04747100 | 0.77271200 | 1.07602200 |
| O | 0.32882300 | 1.27561800 | 0.28258800 |
| H | 1.29177700 | 1.27600600 | 0.34568700 |
| C | -3.66338700 | -1.53391700 | 2.63740300 |
| H | -3.69944400 | -2.61133700 | 2.45588300 |
| H | -2.73459500 | -1.34200400 | 3.18315200 |
| H | -4.49434300 | -1.26865200 | 3.29251400 |
| C | 2.70465200 | 0.47152700 | 3.51874800 |
| H | 1.62955000 | 0.67340300 | 3.55230300 |
| H | 2.86957500 | -0.42698800 | 4.11985000 |
| H | 3.21428500 | 1.30759500 | 4.00120100 |

59

RR-PhMe_hs_Hbond-reor_TS1_P, E(SCF) = -

2487.49773412, E(ZPE) = -2487.050315, E(G)

= -2487.116699 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.25712900 | -0.80563800 | -2.93447300 |
| H | -0.09028900 | -1.69120500 | -3.47485300 |
| H | 0.17750700 | 0.05355500 | -3.60629600 |
| C | 1.66255800 | -0.98474000 | -2.43347000 |
| H | 2.37025600 | -1.15799000 | -3.24901500 |
| H | 1.98428000 | -0.09179600 | -1.89310900 |
| N | 1.68693400 | -2.11819400 | -1.47719900 |
| C | 2.98188500 | -2.24303500 | -0.73039500 |
| H | 2.88704500 | -3.13231700 | -0.10457000 |
| C | 3.33207600 | -1.04344200 | 0.08191900 |
| C | 2.80321100 | -0.88758200 | 1.39290600 |
| C | 4.20220400 | -0.09922800 | -0.45295700 |
| C | 3.19957600 | 0.28129400 | 2.12119200 |
| C | 4.55402400 | 1.02830200 | 0.25815100 |
| H | 4.61061100 | -0.24502600 | -1.44940800 |
| C | 4.04899600 | 1.20230400 | 1.54556200 |
| H | 4.33846200 | 2.08209100 | 2.11599000 |
| O | 2.00012400 | -1.75082100 | 1.92319600 |
| S | 5.66731400 | 2.25067700 | -0.42363400 |
| O | 6.02015100 | 1.77332700 | -1.79114700 |
| O | 6.84451600 | 2.30258300 | 0.49282500 |
| O | 4.91223700 | 3.53840600 | -0.43719500 |
| H | 0.30604200 | -3.37001400 | 0.69101000 |
| H | 0.82302900 | -2.77984800 | 0.99833700 |
| H | 1.56875000 | -2.98065800 | -2.01010100 |
| H | 3.76055100 | -2.43315800 | -1.47790700 |
| H | 0.52707900 | -0.90933300 | -2.43616800 |
| O | -0.32327600 | -0.41292900 | 2.47869900 |
| H | -0.94915200 | -1.00620100 | 2.03056600 |
| H | 0.04824100 | 0.77266600 | 1.07620800 |
| O | 0.33001800 | 1.27568700 | 0.28307100 |
| H | 1.29300600 | 1.27445500 | 0.34581600 |
| N | -0.61917200 | -0.62287200 | -1.75885100 |
| C | -2.05738800 | -0.67414900 | -2.07025500 |
| H | -2.25928500 | -1.68450900 | -2.44491200 |
| C | -2.91986300 | -0.33698500 | -0.89562500 |
| C | -2.79618200 | -1.02435500 | 0.32773700 |
| C | -3.91067200 | 0.62646600 | -1.05105500 |
| C | -3.73432100 | -0.76355300 | 1.35861200 |
| C | -4.80100000 | 0.89510800 | -0.03445500 |
| H | -3.99489500 | 1.16766100 | -1.98791700 |
| C | -4.71379300 | 0.18828000 | 1.15808800 |
| H | -5.42634800 | 0.38762400 | 1.95423100 |
| O | -1.86650200 | -1.93235300 | 0.58029500 |
| S | -6.09384000 | 2.12358700 | -0.23087800 |
| O | -5.92149600 | 3.08024200 | 0.89944700 |
| O | -7.38172700 | 1.37586700 | -0.14745400 |
| O | -5.87042000 | 2.74850800 | -1.56391700 |
| H | -0.38034800 | 0.25199300 | -1.26186200 |
| H | -2.26429300 | 0.02502400 | -2.88771300 |
| Pd | -0.07845300 | -2.03051000 | -0.38709300 |
| C | -3.66357200 | -1.53503300 | 2.63691800 |

| | | | |
|---|-------------|-------------|------------|
| H | -3.69873500 | -2.61240300 | 2.45511600 |
| H | -2.73525100 | -1.34266600 | 3.18332000 |
| H | -4.49511700 | -1.27054200 | 3.29164500 |
| C | 2.70438700 | 0.46938200 | 3.51891400 |
| H | 1.62979400 | 0.67404500 | 3.55209100 |
| H | 2.86642100 | -0.43059400 | 4.11858000 |
| H | 3.21593200 | 1.30336300 | 4.00297000 |

59

RR-PhMe_hs_Hbond-reor_TS1_R, E(SCF) = -2487.51294670, E(ZPE) = -2487.068637, E(G) = -2487.136652 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.33652800 | 3.14373300 | -1.45612200 |
| H | 0.66836700 | 4.01595600 | -0.88347800 |
| H | 0.67902900 | 3.26886900 | -2.48728000 |
| C | -1.16636500 | 3.00654900 | -1.38155100 |
| H | -1.67312600 | 3.87053700 | -1.82101900 |
| H | -1.50069300 | 2.10634700 | -1.90710900 |
| N | -1.52773500 | 2.85270000 | 0.04626000 |
| C | -2.95157600 | 2.52747300 | 0.32524700 |
| H | -3.18092900 | 3.00351000 | 1.28278400 |
| C | -3.24611900 | 1.06356600 | 0.42588600 |
| C | -2.59453600 | 0.30631100 | 1.42938000 |
| C | -4.21001100 | 0.47680000 | -0.37799900 |
| C | -3.01496000 | -1.02671400 | 1.65828400 |
| C | -4.57736300 | -0.84265100 | -0.18116400 |
| H | -4.69525200 | 1.05688800 | -1.15648200 |
| C | -3.99004700 | -1.57658300 | 0.84251400 |
| H | -4.29689800 | -2.60650600 | 1.00729500 |
| O | -1.61042700 | 0.81235000 | 2.14163100 |
| S | -5.80134200 | -1.63009900 | -1.23021500 |
| O | -6.28313000 | -0.57572000 | -2.16512200 |
| O | -6.86755700 | -2.12683100 | -0.31362400 |
| O | -5.09012300 | -2.74197900 | -1.92491000 |
| H | 2.17840200 | 2.83669700 | 2.93867800 |
| H | 1.67127900 | 2.33654800 | 2.70156200 |
| H | -1.30115600 | 3.72308900 | 0.52461300 |
| H | -3.58272600 | 2.99398600 | -0.43770300 |
| H | -1.39919800 | -1.75288500 | 0.10563800 |
| O | -0.47207300 | -1.83640000 | -0.15752900 |
| H | 0.01540100 | -1.27703000 | 0.48194500 |
| H | -0.10045600 | -0.96850300 | -1.70028300 |
| O | 0.25398200 | -0.38619400 | -2.40389600 |
| H | -0.41711700 | -0.36199500 | -3.08996100 |
| N | 0.93759500 | 1.93988900 | -0.84722400 |
| C | 2.35275700 | 2.05672100 | -0.47977300 |
| H | 2.41493600 | 2.80734100 | 0.31753100 |
| C | 2.94870800 | 0.74115200 | -0.06066900 |
| C | 2.30654400 | -0.16618000 | 0.81342000 |
| C | 4.21938400 | 0.43985000 | -0.54484100 |
| C | 2.99610500 | -1.34987600 | 1.19131800 |
| C | 4.87910200 | -0.70968100 | -0.17053700 |
| H | 4.70912400 | 1.12950300 | -1.22476500 |
| C | 4.25818300 | -1.60127800 | 0.69607900 |
| H | 4.77200700 | -2.51158700 | 0.99412300 |
| O | 1.09967200 | -0.01127100 | 1.32648600 |
| S | 6.50239900 | -1.10238400 | -0.82214500 |
| O | 6.32060800 | -2.31697800 | -1.66952200 |
| O | 7.36851100 | -1.36541700 | 0.36351900 |
| O | 6.93519400 | 0.08884900 | -1.60475000 |
| H | 0.80358200 | 1.14439700 | -1.49388100 |
| H | 2.91946300 | 2.44699600 | -1.33329600 |
| Pd | -0.21492500 | 1.43574100 | 0.75718300 |
| C | 2.33636200 | -2.30502000 | 2.13279300 |
| H | 2.08944900 | -1.82358700 | 3.08342600 |
| H | 1.39386300 | -2.68786300 | 1.72900800 |
| H | 2.98730800 | -3.15612100 | 2.33849000 |
| C | -2.37853400 | -1.81032500 | 2.76057200 |
| H | -1.29026600 | -1.85354200 | 2.64658000 |
| H | -2.56235800 | -1.34810800 | 3.73450100 |
| H | -2.76366300 | -2.83087700 | 2.78791300 |

59

RR-PhMe_hs_Hbond-reor_TS1, E(SCF) = -2487.48905156, E(ZPE) = -2487.044055, E(G) = -2487.111888 a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.03809300 | -1.66947300 | -2.57051900 |
|---|------------|-------------|-------------|

| | | | |
|----|-------------|-------------|--------------|
| H | -0.30957000 | -2.69522000 | -2.72771500 |
| H | -0.10932800 | -1.11590600 | -3.50208000 |
| C | 1.47453600 | -1.65019000 | -2.12722300 |
| H | 2.14070700 | -2.09801800 | -2.87042700 |
| H | 1.80721900 | -0.62530300 | -1.94345500 |
| N | 1.55554900 | -2.38372400 | -0.84438600 |
| C | 2.89676700 | -2.34499200 | -2.120217800 |
| H | 2.83136500 | -3.01611200 | 0.65876100 |
| C | 3.34223700 | -0.98695600 | 0.21357200 |
| C | 2.74263300 | -0.38212200 | 1.35022600 |
| C | 4.37279100 | -0.35931500 | -0.47302300 |
| C | 3.32953400 | 0.82928500 | 1.83141900 |
| C | 4.87381400 | 0.85038700 | -0.03598900 |
| H | 4.80159200 | -0.82733200 | -1.35493300 |
| C | 4.36020100 | 1.41743700 | 1.41764600 |
| H | 4.78953500 | 2.34459300 | 1.50119200 |
| O | 1.71982000 | -0.91782500 | 1.94087300 |
| S | 6.19120500 | 1.68539600 | -0.91115600 |
| O | 6.52683200 | 0.82253300 | -2.07963000 |
| O | 7.32183700 | 1.81544000 | 0.05556900 |
| O | 5.64518000 | 3.01571800 | -1.31415600 |
| H | 0.06721200 | -3.36033300 | 1.81270300 |
| H | 0.58185800 | -2.85253300 | -2.06223100 |
| H | 1.33503800 | -3.36348900 | -1.02791100 |
| H | 3.61479600 | -2.77248000 | -0.91182100 |
| O | 0.56895100 | 0.40790800 | 2.17887200 |
| H | -0.18964700 | 1.02753000 | 1.06847700 |
| H | -0.91843700 | 0.39120100 | 1.98119500 |
| H | -0.00996700 | 1.46247200 | 0.30391700 |
| O | -0.00112500 | 1.57508000 | -0.67191200 |
| H | 0.87211000 | -1.91526400 | -0.88367700 |
| N | -0.77612300 | -1.07788700 | -1.48889800 |
| C | -2.21837100 | -1.32754400 | -1.62805800 |
| H | -2.35661600 | -2.41232700 | -1.55080700 |
| C | -3.05096100 | -2.89661800 | -0.62648300 |
| C | -2.78036100 | -0.63270300 | 0.75645700 |
| C | -4.17185200 | 0.09366900 | -1.08837500 |
| C | -3.70312700 | -0.03118800 | 1.65201300 |
| C | -5.04873400 | 0.69710500 | -0.21399900 |
| H | -4.37003800 | 0.14167000 | -2.15416600 |
| C | -4.81194700 | 0.62041700 | 1.15273500 |
| H | -5.51142100 | 1.07910900 | 1.84674500 |
| O | -1.71959000 | -1.20678800 | 1.29848500 |
| S | -6.49305300 | 1.58121300 | -0.80599000 |
| O | -6.33099200 | 2.98786900 | -0.33812100 |
| O | -7.66745000 | 0.90864000 | -0.17917700 |
| O | -6.47439500 | 1.45599000 | -2.28975500 |
| H | -0.58154000 | -0.06333800 | -1.41549000 |
| H | -2.52721700 | -1.03235300 | -2.63770600 |
| Pd | -0.04349600 | -1.75603800 | 0.29351100 |
| C | -3.46883700 | -0.12920300 | 3.12532000 |
| H | -3.36802600 | -1.17007000 | 3.44403600 |
| H | -2.54929000 | 0.37767200 | 3.43359600 |
| H | -4.29601400 | 0.32014600 | 3.67655100 |
| C | 2.84022000 | 1.43633400 | 3.10840100 |
| H | 1.88921100 | 1.96273500 | 2.98501100 |
| H | 2.67371800 | 0.66980100 | 3.86993900 |
| H | 3.56495700 | 2.15489400 | 3.49598600 |

59

RR-PhMe_D1_TS1_P, E(SCF) = -2487.49219568, E(ZPE) = -2487.045736, E(G) = -2487.110355 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.56003700 | 3.52545700 | -0.24045100 |
| H | -0.38510800 | 3.67968000 | -1.30842500 |
| H | -1.24899300 | 4.30093100 | 0.10757600 |
| C | 0.72036600 | 3.53644400 | 0.54206800 |
| H | 1.27376100 | 4.46867300 | 0.41223100 |
| H | 0.49781700 | 3.42553900 | 1.60637100 |
| N | 1.55492000 | 2.36932600 | 0.14700500 |
| N | -1.16828000 | 2.18939600 | -0.07216700 |
| C | 2.55620500 | 2.04769300 | 1.21927500 |
| H | 3.27906400 | 2.87063600 | 1.23822000 |
| C | -2.37881000 | 1.99463700 | -0.88739300 |
| H | -2.06971900 | 2.12854100 | -1.93074600 |
| C | 3.22432500 | 0.73626700 | 1.02980400 |
| C | 2.65450900 | -0.40961800 | 1.65918300 |

| | | | | | | | |
|--|-------------|-------------|--------------|--|-------------|---------------|-------------|
| C | 4.34695500 | 0.63500200 | 0.21885400 | H | 5.71653700 | -2.22342400 | -0.68241000 |
| C | 3.29116000 | -1.66733000 | 1.40468000 | O | -1.47965000 | -0.87336500 | -0.01640600 |
| C | 4.93212400 | -0.59116100 | -0.01985800 | O | 1.50214600 | -0.86932000 | -0.05360700 |
| H | 4.76476000 | 1.52606200 | -0.24204300 | S | -7.33194300 | 0.02952700 | -0.01277200 |
| C | 4.39471700 | -1.73022100 | 0.58112700 | S | 7.35392100 | 0.03431900 | 0.01734400 |
| H | 4.85854000 | -2.69659300 | 0.39528100 | O | 7.77310800 | -0.06727200 | -1.41061300 |
| C | -3.03889100 | 0.66951000 | -0.68498600 | O | 7.91591800 | -1.06601700 | 0.85178400 |
| C | -2.33330700 | -0.53324100 | -0.87239600 | O | 7.59274000 | 1.38538800 | 0.59670200 |
| C | -4.40302500 | 0.63753800 | -0.41453800 | O | -7.56919900 | 1.44323000 | -0.41640100 |
| C | -3.04868400 | -1.75680200 | -0.86581100 | O | -7.77070800 | -0.26000100 | 1.38267900 |
| C | -5.08588300 | -0.55829000 | -0.36834400 | O | -7.87552700 | -0.95485400 | -0.99230500 |
| H | -4.94126800 | 1.56580900 | -0.25350800 | H | -1.75638200 | 2.15235800 | 0.88092900 |
| C | -4.40546900 | -1.74520500 | -0.61251700 | H | -2.00676500 | 1.47488500 | -1.94553800 |
| H | -4.94742200 | -2.68730400 | -0.60173000 | H | 1.77571000 | 2.15809200 | -0.93256800 |
| O | 1.60215300 | -0.34169200 | -2.39599600 | H | 3.10382300 | 2.62228600 | 1.10244100 |
| O | -1.02810000 | -0.60470600 | -1.08150100 | Pd | 0.01086300 | 0.55693600 | -0.03166800 |
| S | 6.39068100 | -0.74199000 | -1.04408800 | H | -0.62702800 | -2.12532500 | 1.24901500 |
| S | -6.84559600 | -0.61205100 | -0.02307000 | H | -1.82800900 | 0.18632300 | 3.11323600 |
| O | -6.99833800 | -1.49616700 | -0.141761800 | H | -0.14110800 | -2.0.14110800 | 2.44480000 |
| O | -7.48307600 | -1.18797300 | -1.24200200 | O | 0.12292700 | -2.51897100 | 1.72405000 |
| O | -7.25833900 | 0.79460000 | 0.23858200 | H | 0.85973200 | -2.07717400 | 1.27198000 |
| O | 6.66161200 | 0.62065000 | -1.58469700 | H | -0.81939500 | -2.03695100 | -1.38022100 |
| O | 6.05200700 | -1.73124900 | -2.10973200 | O | -0.07823200 | -2.44816900 | -2.85330900 |
| O | 7.48109100 | -1.23529300 | -0.15068700 | H | 0.66981200 | -2.06615000 | -1.36546300 |
| H | 0.23716700 | -1.38858400 | 1.94959600 | C | -3.09727200 | -2.94458200 | 0.83859200 |
| H | 1.48952300 | -0.22697600 | -1.33116600 | H | -2.36704200 | -3.34647500 | 0.13057100 |
| H | 1.67996500 | -0.34169200 | -0.55009400 | H | -2.58060900 | -2.78407800 | 1.79871800 |
| O | -0.63216200 | -1.74574500 | 1.65857300 | H | -3.88980500 | -3.68238400 | 0.97030300 |
| H | -0.66328400 | -1.53819300 | 0.71200900 | C | 3.13329100 | -2.94921900 | -0.86943000 |
| H | 0.09431600 | 0.75545300 | 2.56414300 | H | 2.39075900 | -3.34475900 | -0.17099900 |
| O | -0.85829800 | 0.98867800 | 2.56761000 | H | 2.63348900 | -2.85809000 | -1.83910000 |
| H | -1.24725900 | 0.12248700 | 2.36380400 | H | 3.92871700 | -3.68763500 | -0.97855200 |
| H | 2.07322700 | 2.60842700 | -0.69948000 | | | | |
| H | 2.00756600 | 2.05056600 | 2.16243400 | 59 | | | |
| H | -1.34288000 | 1.99107700 | 0.92800500 | RR-PhMe_D1_TS1_R, E(SCF) = -2487.51540577, | | | |
| H | -3.08720900 | 2.79579000 | -0.65099300 | E(ZPE) = -2487.069152, E(G) = -2487.137256 | | | |
| Pd | 0.28206000 | 0.83496800 | -0.51517500 | a.u. | | | |
| C | 2.73239100 | -2.89564400 | 2.04477000 | C | 0.62426800 | -3.28326500 | -0.13579900 |
| H | 2.67536500 | -2.78814500 | 3.13216600 | H | 0.35159700 | -3.34885700 | -1.19308400 |
| H | 1.71179600 | -3.09861900 | 1.70464100 | H | 1.24264100 | -4.15033200 | 0.10981800 |
| H | 3.34443400 | -3.77027600 | 1.81711700 | C | -0.60682100 | -3.20262200 | 0.72743800 |
| C | -2.32670200 | -3.03440200 | -1.14744500 | H | -1.23212600 | -4.09410300 | 0.63493000 |
| H | -1.80757800 | -2.99345500 | -2.10869100 | H | -0.33464900 | -3.08563700 | 1.78017800 |
| H | -1.56554800 | -3.25033400 | -0.39201400 | N | -1.35603000 | -1.99208800 | 0.32225600 |
| H | -3.02369400 | -3.87331000 | -1.17017500 | N | 1.38646200 | -2.02757900 | 0.04911400 |
| | | | | C | -2.41847600 | -1.57301300 | 1.25948800 |
| 59 | | | | H | -3.01776700 | -2.44519700 | 1.54219500 |
| RR-PhMe_D1_TS1_R_REF, E(SCF) = - | | | | C | 2.43454200 | -1.78237000 | -0.96221200 |
| 2487.51820385, E(ZPE) = -2487.072287, E(G) | | | | H | 1.91654000 | -1.57426000 | -1.90498300 |
| = -2487.141645 a.u. | | | | C | -3.29263000 | -0.54495900 | 0.61804000 |
| C | 0.65468300 | 3.30341600 | 0.35694200 | C | -2.74937400 | 0.64922700 | 0.09876800 |
| H | 0.46582900 | 3.27929700 | 1.43392800 | C | -4.65628900 | -0.79651100 | 0.52043700 |
| H | 1.25949200 | 4.18687600 | 0.13765500 | C | -3.63194000 | 1.58567700 | -0.49673400 |
| C | -0.64132300 | 3.30336300 | -0.40885800 | C | -5.50348600 | 0.12076200 | -0.06235100 |
| H | -1.24737600 | 4.18534500 | -0.18698600 | H | -5.06277400 | -1.72456700 | 0.90910500 |
| H | -0.45332100 | 3.28207200 | -1.48597300 | C | -4.98320500 | 1.30630000 | -0.56274700 |
| N | -1.37471500 | 2.06403400 | -0.06250300 | H | -5.64762100 | 2.02871100 | -1.02947700 |
| N | 1.39112900 | 2.06612400 | 0.00883100 | C | 3.33003100 | -0.66491900 | -0.53271300 |
| C | -2.47491400 | 1.72938500 | -0.98808400 | C | 2.80592600 | 0.59392700 | -0.16505100 |
| H | -3.09218900 | 2.61964000 | -1.14967100 | C | 4.70260800 | -0.88589800 | -0.50682000 |
| C | 2.48794900 | 1.73150600 | 0.93808900 | C | 3.71467300 | 1.61437600 | 0.22018100 |
| H | 2.01606800 | 1.47704500 | 1.89386200 | C | 5.57487100 | 0.11609700 | -0.14149800 |
| C | -3.32751700 | 0.61942600 | -0.46052600 | H | 5.09654600 | -1.85881700 | -0.78240700 |
| C | -2.77735000 | -0.60742100 | -0.03690300 | C | 5.07072200 | 1.35974300 | 0.21935800 |
| C | -4.70623800 | 0.80692600 | -0.43505400 | H | 5.75410300 | 2.14953900 | 0.52056100 |
| C | -3.65772900 | -1.63790800 | 0.37983700 | O | -1.45905000 | 0.94705400 | 0.15109400 |
| C | -5.55271400 | -0.19918900 | -0.02577800 | O | 1.51929200 | 0.88750800 | -0.17788600 |
| H | -5.12522600 | -1.75686800 | -0.75052700 | S | -7.26291700 | -0.19933700 | -0.20814100 |
| C | -5.02002900 | -1.41907300 | 0.37221000 | S | 7.34758600 | -0.15137300 | -0.12756700 |
| H | -5.68390700 | -2.21753100 | 0.69335700 | O | 7.80297200 | 0.18324100 | 1.25261600 |
| C | 3.34473900 | 0.62188800 | 0.41658500 | O | 7.90871000 | 0.78030100 | -1.14834500 |
| C | 2.79916000 | -0.60384400 | -0.01702300 | O | 7.55230300 | -1.58503400 | -1.47545200 |
| C | 4.72383600 | 0.80670600 | 0.41572000 | O | -7.48737100 | -1.54304200 | 0.39312600 |
| C | 3.68547700 | -1.63785900 | -0.41299700 | O | -7.56341400 | -0.15721400 | -1.66798200 |
| C | 5.57598200 | -0.20282500 | 0.02709000 | O | -7.94179100 | 0.89597900 | 0.54185200 |
| H | 5.13847800 | 1.75523100 | 0.74103000 | H | -0.65597700 | 2.59335100 | -0.54475300 |
| C | 5.04781800 | -1.42159600 | -0.38037900 | H | -2.35581600 | -0.15815100 | -2.44991200 |

```
H -1.68693400 -0.25079400 -2.77715700
O 0.11199900 3.18818300 -0.57430100
H 0.83056900 2.53387700 -0.47859400
H -0.95277100 1.98128300 1.73651700
O -0.59471900 2.75575600 2.20049100
H -0.20833800 3.24440700 1.45718300
H -1.78341500 -2.15947600 -0.59061700
H -1.91728300 -1.20452900 2.16099700
H 1.82733300 -2.04085100 0.97041700
H 3.02325800 -2.69566300 -1.10031600
Pd 0.02383500 -0.49799600 0.07229800
C -3.09751700 2.86028000 -1.06068900
H -2.61141200 3.47061200 -0.29337600
H -2.35368700 2.67337700 -1.84224300
H -3.89901000 3.45569500 -1.49963700
C 3.19308700 2.95422600 0.62387700
H 2.78634700 3.50593400 -0.22953800
H 2.38310300 2.86376800 1.35264800
H 3.98603000 3.56333000 1.06006400
```

59

RR-PhMe_D1_TS1, E(SCF) = -2487.48658472,
E(ZPE) = -2487.040541, E(G) = -2487.106325
a.u.

```
C -0.60979800 3.41725800 -0.20366500
H -0.45479900 3.56005600 -1.27643400
H -1.24317400 4.23157900 0.16142600
C 0.69266000 3.35721800 0.53991700
H 1.27110700 4.27731500 0.42877200
H 0.50030300 3.20820300 1.60652900
N 1.47536700 2.18519400 0.07079600
N -1.28460900 2.11685200 -0.01933000
C 2.59854400 1.89270500 1.01538900
H 3.25703800 2.76823400 1.02457800
C -2.48857100 1.94738700 -0.84671900
H -2.15481200 2.01883900 -1.88823300
C 3.36375100 0.65977900 0.69184100
C 2.72583200 -0.58326900 0.91906200
C 4.66826100 0.71620200 0.22478600
C 3.45197000 -1.77207800 0.64100300
C 5.36474800 -0.44962600 -0.03266100
H 5.14890300 1.67605300 0.06259100
C 4.74852700 -1.68158000 0.17598500
H 5.29838500 -2.59471000 -0.04070800
C -3.22038200 0.66673100 -0.59738400
C -2.57752900 -0.58500700 -0.68169900
C -4.59538800 0.72432800 -0.39286100
C -3.36895400 -1.76277500 -0.65951500
C -5.35066800 -0.42534200 -0.31954700
H -5.08747700 1.68810900 -0.31061300
C -4.73259100 -1.66004100 -0.47154600
H -5.33080000 -2.56717500 -0.44989500
O 1.49072000 -0.62500700 1.31352600
O -1.27197900 -0.74486000 -0.81193700
S 7.05245800 -0.41192300 -0.62932000
S -7.11758000 -0.35751500 -0.01752400
O -7.32729900 -0.99365400 1.31510100
O -7.75131800 -1.13368200 -1.12148700
O -7.48391100 1.08588400 -0.03460800
O 7.40660300 1.02724300 -0.78764900
O 7.05127800 -1.15358600 -1.92481100
O 7.87607300 -1.09935600 0.40891400
H 0.19806100 -1.79645700 1.73520600
H 1.39694700 -0.28537200 -1.74631700
H 1.41009900 -0.82384600 -1.20049700
O -0.74339800 -2.06725200 1.74017000
H -1.00380200 -1.80119400 0.84348300
H 0.21316800 0.46239700 2.33851600
O -0.68352300 0.69313400 2.64578400
H -1.12268400 -0.16647100 2.54042700
H 1.88424800 2.40988800 -0.83769200
H 2.13945300 1.80893800 2.00489700
H -1.49624600 1.96269200 0.97507900
H -3.16298300 2.79093400 -0.66008700
Pd 0.11292000 0.66092200 -0.36580100
C 2.76778100 -3.08496400 0.83223300
H 2.41785900 -3.21005700 1.86173500
```

```
H 1.87720900 -3.16335300 0.19744200
H 3.43150400 -3.91698300 0.59131400
C -2.72517500 -3.09475400 -0.87881000
H -2.18125900 -3.11930900 -1.82712900
H -2.00036400 -3.34372400 -0.09884800
H -3.47762800 -3.88426400 -0.89830000
```

59

RR-PhMe_D1_TS2_P, E(SCF) = -2487.51997218,
E(ZPE) = -2487.070899, E(G) = -2487.139499
a.u.

```
C 0.61403600 -3.33426000 0.16828000
H 0.34308900 -3.49570300 -0.87998800
H 1.14101000 -4.22958300 0.51515000
C -0.61792600 -3.08757700 1.00145400
H -1.27326600 -3.96300600 1.02102000
H -0.32724200 -2.86866700 2.03360100
N -1.36352500 -1.89995600 0.49976000
N 1.46136900 -2.13644600 0.23248500
C -2.36235400 -1.45817700 1.51154200
H -2.91626300 -2.34267000 1.84712600
C 2.51796100 -2.05789600 -0.78749700
H 2.01251300 -2.03999900 -1.76075600
C -3.33209400 -0.44338900 0.99658000
C -3.09382200 0.92726700 1.10571700
C -4.53045700 -0.87256000 0.43431100
C -4.04024500 1.86566500 0.68297400
C -5.46955000 0.04223800 0.00772000
H -4.73814600 -1.93447600 0.34931600
C -5.22629500 1.40159700 0.13900800
H -5.97020300 2.11790400 -0.19779300
C 3.36670100 -0.84042100 -0.58505500
C 2.81837100 0.46104800 -0.64677900
C 4.72484200 -1.01070700 -0.34313500
C 3.68735700 1.56893500 -0.47703700
C 5.56029000 0.07409500 -0.17897600
H 5.13937700 -2.01249300 -0.29338100
C 5.03236200 1.35729900 -0.24702300
H 5.68626200 2.21511500 -0.11223800
O -1.94561800 1.40455200 1.66844400
O 1.54223800 0.70654300 -0.88520000
S -7.04061300 -0.50518700 -0.68360000
S 7.31073000 -0.13932900 0.14000900
O 8.01898400 0.60592500 -0.94088800
O 7.56458700 -1.60655000 0.09531800
O 7.55823700 0.45175900 1.48754700
O -6.96527600 -1.98961000 -0.73888100
O -7.12901000 0.12857800 -2.02824300
O -8.08102800 -0.00450000 0.25707900
H -0.80424900 2.50175600 -1.81564600
H -1.00350500 0.51753800 -0.60073100
H -1.18793400 0.90126300 1.30768400
O 0.01116200 2.91251000 -1.51479500
H 0.61560100 2.15828000 -1.33625400
H -0.90316700 3.15374100 1.50413400
O -0.23728600 3.76712800 1.16813200
H -0.16997700 3.53542900 0.22257900
H -1.87653800 -2.17400400 -0.33862400
H -1.80343600 -1.07956800 2.37044700
H 1.88147800 -2.05825000 1.15683700
H 3.14835200 -2.95544300 -0.76261600
Pd 0.06973100 -0.53708600 -0.17821900
C 3.12703400 2.95165300 -0.53542600
H 2.69628200 3.17311100 -1.51631400
H 2.32063000 3.08645100 0.19267200
H 3.90074300 3.69382700 -0.33260200
C -3.74786300 3.32633200 0.78760900
H -3.54878900 3.62799300 1.81927500
H -2.85780100 3.59012000 0.20782400
H -4.58523700 3.91682700 0.41537700
```

59

RR-PhMe_D1_TS2_R, E(SCF) = -2487.49216463,
E(ZPE) = -2487.045458, E(G) = -2487.112251
a.u.

```
C 0.56185700 -3.51635200 -0.21987000
H 0.38269100 -3.67370400 -1.28668000
```

| | | | | | | | |
|--|-------------|--------------|-------------|----|--------------|-------------|-------------|
| H | 1.25058100 | -4.29192000 | 0.12827800 | C | -4.17998500 | 1.97799100 | 0.07576800 |
| C | -0.71587700 | -3.52170700 | 0.56686700 | C | -5.62041100 | 0.04577400 | -0.10250700 |
| H | -1.27013600 | -4.45452800 | 0.44492800 | H | -4.83292200 | -1.80921800 | 0.59591700 |
| H | -0.49039500 | -3.40372100 | 1.62982500 | C | -5.38393900 | 1.40684700 | -0.28037100 |
| N | -1.55088100 | -2.35720500 | 0.16618000 | H | -6.16183600 | 2.03308000 | -0.71047000 |
| N | 1.17351900 | -2.18078400 | -0.05891800 | C | 3.38475300 | -0.80178300 | -0.55363200 |
| C | -2.55686000 | -2.05353900 | 1.23386500 | C | 2.89026700 | 0.51805000 | -0.61400300 |
| H | -3.27406000 | -2.86321300 | 1.25610000 | C | 4.74582800 | -1.02987300 | -0.38322700 |
| C | 2.37681300 | -1.98856100 | -0.88568600 | C | 3.81361800 | 1.59042000 | -0.52702600 |
| H | 2.05648500 | -2.11818800 | -1.92617700 | C | 5.63504100 | 0.01902300 | -0.30116300 |
| C | -3.23343400 | -0.73010200 | 1.03292900 | H | 5.11728700 | -2.04777800 | -0.32832100 |
| C | -2.67541300 | 0.42405200 | 1.65788900 | C | 5.15899900 | 1.32215600 | -0.37360200 |
| C | -4.35070000 | -0.64196300 | 0.21319200 | H | 5.85627700 | 2.15319800 | -0.30676500 |
| C | -3.31927600 | 1.67547000 | 1.39046700 | O | -1.99151900 | 1.68705000 | 0.92510600 |
| C | -4.94267200 | 0.57484300 | -0.03954000 | O | 1.61359700 | 0.82179400 | -0.78481000 |
| H | -4.75942500 | -1.53876000 | -0.24478400 | S | -7.20159200 | -0.63785900 | -0.59837000 |
| C | -4.41755700 | 1.72522400 | 0.55893200 | S | 7.38844600 | -0.26831300 | -0.05568900 |
| H | -4.88659400 | 2.68714900 | 0.36342700 | O | 8.08133100 | 0.48163300 | -1.14200100 |
| C | 3.04453300 | -0.66687200 | -0.68470900 | C | -0.758022300 | -1.74220800 | -0.15102800 |
| C | 2.34139600 | 0.54054400 | -0.85122700 | O | 7.70552900 | 0.27322200 | 1.29756000 |
| C | 4.41335200 | -0.64315100 | -0.43823500 | O | -7.17320800 | -2.07535800 | -0.20780500 |
| C | 3.06180100 | 1.76108100 | -0.83989600 | O | -7.29040500 | -0.44079700 | -2.07514800 |
| C | 5.10318400 | 0.54884100 | -0.39540800 | O | -8.23713500 | 0.13459600 | 0.13745000 |
| H | 4.95102400 | -1.57540100 | -0.29955500 | H | -0.74191500 | 2.94794900 | 0.24462500 |
| C | 4.42246000 | 1.74158500 | -0.60804900 | H | -0.93741800 | 0.69396100 | -0.96551700 |
| H | 4.96768300 | 2.68169500 | -0.59767000 | H | -1.12205900 | 0.97359800 | -0.16089800 |
| O | -1.62661300 | 0.36173200 | 2.40084100 | O | 0.14295900 | 3.30397300 | 0.04718900 |
| O | 1.03483300 | 0.61949700 | -1.04909000 | H | 0.63799200 | 2.56139600 | -0.33839100 |
| S | -6.39546800 | 0.71100300 | -1.07302000 | H | -0.66429200 | 1.64118100 | 2.24620800 |
| S | 6.86300200 | 0.58987800 | -0.04856300 | O | 0.19255000 | 1.86839500 | 2.65153700 |
| O | 7.47727000 | 1.37963000 | -1.15372800 | H | 0.54972800 | 2.48816800 | 2.00010100 |
| O | 7.31190600 | -0.82975000 | -0.02657200 | H | -1.89765400 | -2.00425400 | -0.32363900 |
| O | 7.00169700 | 1.26367800 | 1.27470900 | H | -1.81514400 | -0.56257200 | 2.21435100 |
| O | -6.65234500 | -0.65733900 | -1.60606600 | H | 1.77702100 | -1.77222100 | 1.21775300 |
| O | -6.05763000 | 1.69563300 | -2.14318600 | H | 3.05239900 | -2.90550400 | -0.56426000 |
| O | -7.49551600 | 1.20178700 | -0.19010900 | Pd | 0.10731500 | -0.40409600 | -0.18816300 |
| H | -0.26195100 | 1.41807600 | 1.95475400 | C | 3.31827800 | 2.99696800 | -0.58969800 |
| H | -1.48174700 | 0.24305700 | -1.30325800 | H | 2.73778600 | 3.18126800 | -1.49823300 |
| H | -1.67021800 | 0.35642600 | -0.52104800 | H | 2.65723200 | 3.22438300 | 0.25196700 |
| O | 0.60770900 | 1.77683400 | 1.66688900 | H | 4.15004700 | 3.70222700 | -0.56669700 |
| H | 0.64776900 | 1.56075100 | 0.72237400 | C | -3.91027500 | 3.43209200 | -0.13065900 |
| H | -0.10994800 | -0.72647800 | 2.57624100 | H | -3.62486200 | 3.92223400 | 0.80450500 |
| O | 0.84390900 | -0.95331300 | 2.57852300 | H | -3.07679000 | 3.58639200 | -0.82361700 |
| H | 1.22631000 | -0.08533500 | 2.36979700 | H | -4.78670500 | 3.94198100 | -0.53392400 |
| H | -2.06551300 | -2.59892200 | -0.68185600 | | | | |
| H | -2.01083100 | -2.02849700 | 2.17853100 | | | | |
| H | 1.35750300 | -1.938234600 | 0.93878500 | | | | |
| H | 3.08418600 | -2.79341000 | -0.65902900 | | | | |
| Pd | -0.27662800 | -0.82264500 | -0.49230300 | | | | |
| C | 2.34239400 | 3.04458300 | -1.10074100 | | | | |
| H | 1.81291500 | 3.01514500 | -2.05680900 | | | | |
| H | 1.59057900 | 3.25672000 | -0.33509500 | | | | |
| H | 3.04300500 | 3.88044600 | -1.12321600 | | | | |
| C | -2.77304300 | 2.91218900 | 2.02509700 | | | | |
| H | -2.72236900 | 2.81305500 | 3.11357900 | | | | |
| H | -1.75168700 | 3.11968500 | 1.69006700 | | | | |
| H | -3.38948200 | 3.78097200 | 1.78706200 | | | | |
| 59 | | | | | | | |
| RR-PhMe_D1_TS2, E(SCF) = -2487.48772115, | | | | | | | |
| E(ZPE) = -2487.041819, E(G) = -2487.110016 | | | | | | | |
| a.u. | | | | | | | |
| C | 0.54450200 | -3.16329600 | 0.32925900 | C | 0.81631100 | 3.04025600 | -1.11906300 |
| H | 0.29657400 | -3.42415100 | -0.70326200 | H | 0.59273300 | 3.56005000 | -0.18204900 |
| H | 1.09566600 | -3.99924800 | 0.76823500 | H | 1.51898900 | 3.64955500 | -1.69273900 |
| C | -0.69209700 | -2.84064300 | 1.11957300 | C | -0.44606600 | 2.75189500 | -1.87817900 |
| H | -1.36594800 | -3.69804500 | 1.18888000 | H | -0.98066800 | 3.67220100 | -2.12707800 |
| H | -0.42137800 | -2.54556600 | 2.13780700 | H | -0.23146200 | 2.20270400 | -2.80018400 |
| N | -1.39199300 | -1.68260400 | 0.50253800 | N | -1.29349900 | 1.89787800 | -1.02134400 |
| N | 1.38259900 | -1.94658800 | 0.29207600 | N | 1.42991100 | 1.73760400 | -0.77427700 |
| C | -2.38937700 | -1.09632700 | 1.45283100 | C | -2.52436400 | 1.43673500 | -1.70967000 |
| H | -2.89275200 | -1.93825600 | 1.94201700 | H | -2.22375900 | 0.82291200 | -2.56232200 |
| C | 2.47932800 | -1.98212100 | -0.69804800 | C | 2.54492200 | 1.81611900 | 0.19914700 |
| H | 2.00457400 | -2.02680000 | -1.68466500 | H | 3.23794600 | 2.59945000 | -0.12435400 |
| C | -3.40792700 | -0.21136800 | 0.81121500 | C | -3.41315000 | 0.67720100 | -0.78450600 |
| C | -3.15619100 | 1.16800700 | 0.63307700 | C | -3.79646100 | 1.28192700 | 0.44198700 |
| C | -4.63752800 | -0.75178300 | 0.44388300 | C | -3.80681900 | -0.61791800 | -1.09865000 |
| | | | | C | -4.55530100 | 0.49328700 | 1.35616200 |
| | | | | C | -4.56371000 | -1.35422900 | -0.21042300 |
| | | | | H | -3.50080300 | -1.06252900 | -2.04051900 |
| | | | | C | -4.92071200 | -0.79181300 | 0.10526900 |
| | | | | H | -5.50026900 | -1.38087700 | 1.72243900 |
| | | | | C | 3.25974900 | 0.50924900 | 0.29600900 |
| | | | | C | 2.55271100 | -0.65653500 | 0.65230800 |
| | | | | C | 4.62391700 | 0.44863900 | 0.04079500 |
| | | | | C | 3.26170500 | -1.87699900 | 0.77526300 |
| | | | | C | 5.30622500 | -0.74369700 | 0.16199300 |
| | | | | H | 5.16309400 | 1.34598200 | -0.24508900 |
| | | | | C | 4.62042400 | -1.89528900 | -0.53241400 |
| | | | | H | 5.16053200 | -2.83403700 | 0.62609600 |

| | | | |
|----|-------------|-------------|-------------|
| O | -3.43471200 | 2.48697000 | 0.74608700 |
| O | 1.26278200 | -0.66495500 | 0.92234300 |
| S | -5.05895100 | -3.03471700 | -0.57854700 |
| S | 7.06613600 | -0.84308900 | -0.17176600 |
| O | 7.50111600 | 0.54108700 | -0.50693100 |
| O | 7.21100100 | -1.79146500 | -1.31328200 |
| O | 7.68970400 | -1.36278900 | 1.07878600 |
| O | -4.41066300 | -3.89381100 | 0.45622400 |
| O | -4.56859400 | -3.32194400 | -1.95643500 |
| O | -6.54775900 | -3.06236900 | -0.47597500 |
| H | 2.10134100 | 2.12872900 | 1.15125100 |
| H | -3.02094000 | 2.33730900 | -2.09821600 |
| H | 1.77779900 | 1.29805900 | -1.62951300 |
| H | -1.62961500 | 2.46633500 | -0.23126200 |
| H | -2.99642200 | 3.99871200 | -0.03709100 |
| O | -2.47546200 | 4.75791200 | -0.37361500 |
| H | -3.00761400 | 5.14498100 | -1.07183700 |
| H | -2.12923800 | 2.63772400 | 1.93224700 |
| O | -1.29862900 | 2.74318600 | 2.44528900 |
| H | -0.94573500 | 1.85238100 | 2.52166100 |
| Pd | -0.05179200 | 0.50676200 | -0.07980400 |
| H | -1.64675900 | -0.26889000 | 0.40308800 |
| H | -1.07707000 | -0.79294600 | 0.63809800 |
| C | -4.92900200 | 1.09328000 | 2.67086700 |
| H | -4.04180100 | 1.41495900 | 3.22576400 |
| H | -5.54693500 | 1.98673100 | 2.54120900 |
| H | -5.48028700 | 0.38096700 | 3.28711100 |
| C | 2.52350800 | -3.11425900 | 1.16639600 |
| H | 2.04795800 | -3.00505700 | 2.14492200 |
| H | 1.72158700 | -3.33949100 | 0.45778600 |
| H | 3.19638800 | -3.97209900 | 1.20727400 |

59

RR-PhMe_D2_TS1_R, E(SCF) = -2487.51325158,
E(ZPE) = -2487.068552, E(G) = -2487.138118
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.85698800 | 3.36340600 | 0.46032400 |
| H | 0.72961200 | 3.40810000 | 1.54559600 |
| H | 1.46972000 | 4.21554800 | 0.15173100 |
| C | -0.47877900 | 3.35991700 | -0.24112700 |
| H | -1.05118000 | 4.26585700 | -0.02890000 |
| H | -0.32975100 | 3.30595100 | -1.32380000 |
| N | -1.23800100 | 2.15177400 | 0.16040200 |
| N | 1.53082400 | 2.08427300 | 0.14256000 |
| C | -2.22680200 | 1.72658200 | -0.84088300 |
| H | -1.65857900 | 1.48150700 | -1.74715800 |
| C | 2.76841400 | 1.81275500 | 0.90322400 |
| H | 3.44963300 | 2.66518300 | 0.80797500 |
| C | -3.08895400 | 0.57056400 | -0.41826500 |
| C | -2.64339000 | -0.51560000 | 0.36460800 |
| C | -4.39654100 | 0.57408900 | -0.90091200 |
| C | -3.54714000 | -1.57732100 | 0.63141800 |
| C | -5.26053000 | -0.46600300 | -0.64554800 |
| H | -4.74477800 | 1.41202400 | -1.49649900 |
| C | -4.82895900 | -1.53785500 | 0.12602200 |
| H | -5.50858200 | -2.35864600 | 0.33937500 |
| C | 3.43137500 | 0.56594600 | 0.40855800 |
| C | 2.74045900 | -0.66853400 | 0.43833000 |
| C | 4.73557600 | 0.61764800 | -0.05594700 |
| C | 3.41279300 | -1.83661000 | 0.01665800 |
| C | 5.38519800 | -0.53231200 | -0.47053800 |
| H | 5.25429300 | 1.57234700 | -0.08095200 |
| C | 4.72048800 | -1.74791900 | -0.42977800 |
| H | 5.23808900 | -2.64391900 | -0.75825000 |
| O | -1.44399200 | -0.61347400 | 0.91864200 |
| O | 1.50349000 | -0.78619900 | 0.87594900 |
| S | -6.94601600 | -0.44612900 | -1.25849300 |
| S | 7.06372000 | -0.41120000 | -1.09210200 |
| O | 6.98359400 | 0.41467100 | -2.33215300 |
| O | 7.50914800 | -1.80788100 | -1.35519300 |
| O | 7.85257800 | 0.25874000 | -0.01808400 |
| O | -7.09883000 | -1.68693400 | -2.07148800 |
| O | -7.07802400 | 0.79878600 | -2.06530300 |
| O | -7.82152300 | -0.45074100 | -0.05080700 |
| H | 2.47495700 | 1.73158600 | 1.95539600 |
| H | -2.87205200 | 2.57696300 | -1.09095700 |
| H | 1.75608800 | 2.06419400 | -0.85331600 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.69144400 | 2.28969600 | 1.07225100 |
| H | -1.83524000 | 0.53071700 | 2.51625100 |
| O | -2.02669800 | 1.39461700 | 2.91867400 |
| H | -2.88488100 | 1.29352200 | 3.33829700 |
| H | -0.69366000 | -1.71808700 | 2.32061600 |
| O | 0.04660500 | -2.01438000 | 2.87365500 |
| H | 0.79613400 | -1.71193800 | 2.33225200 |
| Pd | 0.10698800 | 0.65313600 | 0.48660400 |
| H | 0.05485700 | -1.15590100 | -1.76304700 |
| H | 0.14450200 | -0.84218200 | -2.43915800 |
| C | -3.09459900 | -2.71676600 | 1.48360900 |
| H | -2.16942600 | -3.15985800 | 1.10470500 |
| H | -2.88830200 | -2.39025800 | 2.50888400 |
| H | -3.85730200 | -3.49517100 | 1.52955800 |
| C | 2.69247400 | -3.14954000 | 0.06495100 |
| H | 2.41217700 | -3.41110700 | 1.08851600 |
| H | 1.75967100 | -3.10454900 | -0.50567500 |
| H | 3.31179900 | -3.94675700 | -0.33806400 |

59

RR-PhMe_D2_TS1, E(SCF) = -2487.47896644,
E(ZPE) = -2487.035403, E(G) = -2487.105110
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.80762500 | 3.05008100 | 0.50533700 |
| H | 0.60595600 | 2.94776600 | 1.57510800 |
| H | 1.41246100 | 3.94469700 | 0.34140200 |
| C | -0.48924500 | 3.08806700 | -0.26210800 |
| H | -1.10092300 | 3.94692300 | 0.03135900 |
| H | -0.31587400 | 3.14711100 | -1.34081700 |
| N | -1.19610900 | 1.82450900 | 0.03152900 |
| N | 1.54861100 | 1.84108000 | 0.07984800 |
| C | -2.46303700 | 1.65979500 | -0.69125000 |
| H | -2.21035600 | 1.46449600 | -1.74041400 |
| C | 2.65331000 | 1.42609700 | 0.97437000 |
| H | 3.27038900 | 2.30090400 | 1.20495800 |
| C | -3.40576500 | 0.60384300 | -0.16061900 |
| C | -3.08562400 | -0.36756900 | 0.82346400 |
| C | -4.67886300 | 0.62316100 | -0.72645500 |
| C | -4.09675600 | -1.31063000 | -1.17809800 |
| C | -5.64100500 | -0.29395600 | -0.36608000 |
| H | -4.92135600 | 1.37423200 | -1.47326200 |
| C | -5.34192000 | -1.25852500 | 0.59353200 |
| H | -6.09780300 | -1.98485400 | 0.88199600 |
| C | 3.49480000 | 0.36872900 | 0.33266200 |
| C | 2.91911400 | -0.83980700 | -0.11925700 |
| C | 4.85887300 | 0.57507300 | 0.19509400 |
| C | 3.75373800 | -1.82952800 | -0.68134000 |
| C | 5.66958700 | -0.39785000 | -0.36142800 |
| H | 5.29258900 | 1.51173600 | 0.53398500 |
| C | 5.11359500 | -1.59416600 | -0.78602300 |
| H | 5.75704200 | -2.35187300 | -1.22168200 |
| O | -1.91920700 | -0.44584600 | 1.39728600 |
| O | 1.62965400 | -1.11102000 | -0.02147000 |
| S | -7.28547800 | -0.24205600 | -1.07074400 |
| S | 7.43631700 | -0.10080400 | -0.48401700 |
| O | 7.58368000 | 1.21576600 | -1.16770100 |
| O | 7.99001700 | -1.23387500 | -1.27527700 |
| O | 7.94109300 | -0.07035400 | 0.91928900 |
| O | -7.54597400 | -1.60696600 | -1.61563000 |
| O | -7.25659000 | 0.80728000 | -2.12899200 |
| O | -8.20741200 | 0.09775400 | 0.05363200 |
| H | 2.18756500 | 1.08780000 | 1.90709900 |
| H | -2.98086000 | 2.62895700 | -0.67948600 |
| H | 1.92874200 | 1.99175300 | -0.85673600 |
| H | -1.36939400 | 1.79980200 | 1.04454000 |
| H | -1.34116700 | 0.66772800 | 2.59338400 |
| O | -0.94299900 | 1.49720600 | 2.94354100 |
| H | -1.49287700 | 1.76280400 | 3.68392000 |
| H | -0.74430800 | -1.73498400 | 1.91850400 |
| O | 0.04203400 | -2.27805100 | 2.12293300 |
| H | 0.69339900 | -2.00850900 | 1.45674700 |
| Pd | 0.19938800 | 0.31507600 | -0.14136800 |
| H | -1.08331300 | -1.12745900 | -0.49185600 |
| H | -0.75839100 | -1.02218500 | -1.19653200 |
| C | -3.75995800 | -2.34989300 | 2.19622200 |
| H | -2.93891300 | -2.98984300 | 1.85698700 |
| H | -3.42242100 | -1.89657700 | 3.13307200 |

H -4.62153700 -2.98504200 2.40974500
 C 3.14843700 -3.11348300 -1.14430900
 H 2.66400300 -3.64742500 -0.32147500
 H 2.37250400 -2.93819700 -1.89476000
 H 3.90624300 -3.76836600 -1.57668300

59

RR-PhMe_D2_TS2_P, E(SCF) = -2487.51194580,
 E(ZPE) = -2487.064677, E(G) = -2487.135354
 a.u.

C -0.21876500 -2.13695400 0.80313500
 H 0.04162200 -1.65124200 1.74896000
 H -0.49193400 -3.17428800 1.02089000
 C 0.95012000 -2.06983800 -0.14856100
 H 1.81011800 -2.63157800 0.23259900
 H 0.67536900 -2.48994600 -1.12018900
 N 1.31752400 -0.64589100 -0.34745000
 N -1.34145500 -1.38943900 0.21317000
 C 2.41108100 -0.28806400 -1.34732000
 H 2.05193100 0.23149200 -2.12030100
 C -2.39957800 -0.99887200 1.15777900
 H -2.74571600 -1.86930800 1.72850400
 C 3.67056700 0.05071000 -0.71169400
 C 3.71976500 1.30124000 -0.09225500
 C 4.81718600 -0.73681400 -0.72220800
 C 4.89310900 1.76245200 0.51899000
 C 5.98193100 -0.28806400 -0.13732000
 H 4.79851900 -1.71050400 -1.20032000
 C 6.01387400 0.95249600 0.48330100
 H 6.93154100 1.29949500 0.94952800
 C -3.56115800 -0.36876400 0.45085100
 C -3.40833000 0.79697300 -0.33282800
 C -4.82319600 -0.93003100 0.61578800
 C -4.56627600 1.39021200 -0.89969000
 C -5.93907600 -0.35510900 0.04473500
 H -4.93597400 -1.82924100 1.21287600
 C -5.80187000 0.80838600 -0.70387700
 H -6.68121500 1.26934100 -1.14703400
 O 2.64987100 2.13440300 -0.01112600
 O -2.25861500 1.40475300 -0.55074000
 S 7.46740400 -1.30350300 -0.14054900
 S -7.56883900 -1.06918100 0.25889900
 O -7.38251900 -2.29157500 1.09000800
 O -8.06931700 -1.37221400 -1.11383400
 O -8.38896300 -0.02405200 0.93858800
 O 8.52505500 -0.46249600 -0.76690400
 O 7.13104700 -2.51351900 -0.93798700
 O 7.74897400 -1.60463900 1.29103000
 H -1.93687000 -0.30288400 1.87060200
 H 2.60776900 -1.40484500 -1.83942900
 H -1.75427900 -1.93277800 -0.54328700
 H 1.63851300 -0.30893800 0.57081600
 H 1.91785400 1.44197800 1.98743800
 O 1.64647100 0.57442300 2.31553000
 H 2.28563000 0.35402900 2.99907400
 H -0.43062400 3.31215100 1.10244700
 O -1.35096300 3.22286400 1.36351400
 H -1.72073700 2.61873700 0.68977700
 Pd -0.46449700 0.40868500 -0.55972300
 H 1.85774400 1.81685700 -0.48917000
 H 0.23206400 1.72977200 -1.09670800
 C 4.90918800 3.09473800 1.19335200
 H 4.64684800 3.89751400 0.49975900
 H 4.18088800 3.13780200 2.00868100
 H 5.89501600 3.30610600 1.60803700
 C -4.41760100 2.64681300 -1.69264100
 H -3.97038300 3.44521200 -1.09278000
 H -3.75529000 2.50250000 -2.55082800
 H -5.38522300 2.99436400 -2.05854400

59

RR-PhMe_D2_TS2W_P, E(SCF) = -2487.51478177,
 E(ZPE) = -2487.067708, E(G) = -2487.137989
 a.u.

C -0.84438300 -3.01622500 -1.44651500
 H -0.70799600 -3.62452700 -0.54593700
 H -1.46046700 -3.59057800 -2.14712100

C 0.49565700 -2.68503600 -2.05130600
 H 1.00376700 -3.58802800 -2.40602900
 H 0.36608200 -2.01415200 -2.90638500
 N 1.33673700 -1.98658000 -1.04730600
 N -1.49169100 -1.75989100 -1.04700900
 C 2.59660000 -1.51735300 -1.67077300
 H 2.32614200 -0.93527900 -2.55481400
 C -2.63900200 -1.90311500 -0.13986300
 H -3.38487700 -2.58728900 -0.56437800
 C 3.44663800 -0.67527900 -0.77482900
 C 3.90891700 -1.15434100 0.44691200
 C 3.75422600 0.62913300 -1.14250200
 C 4.64550200 -0.34683600 1.31903400
 C 4.48847500 1.43539000 -0.29656300
 H 3.40216400 1.02862100 -2.06870000
 C 4.92211100 0.95406600 0.92902500
 H 5.49283300 1.59817600 1.59171800
 C -3.27818100 -0.57932600 0.14932700
 C -2.54826500 0.47493200 0.75288700
 C -4.62652700 -0.41149800 -0.14619500
 C -3.24430400 1.67509200 1.07141100
 C -5.28396300 0.76246300 0.15748700
 H -5.17855400 -1.22062100 -0.61835000
 C -4.58414300 1.79688800 0.77017000
 H -5.09928200 2.72330600 1.01338700
 O 3.62880400 -2.44780100 0.79450800
 O -1.28107500 0.41568600 1.07832900
 S 4.87958700 3.13378300 -0.75244800
 S -7.01991900 0.98114300 -0.21861200
 O -7.70088500 1.23265300 1.08611300
 O -7.46718000 -0.28356300 -0.86867500
 O -7.10241200 2.16065000 -1.12970200
 O 4.29164200 3.33945600 -2.10327800
 O 6.36675400 3.21729600 -0.74080600
 O 4.24988100 3.98241800 0.29712300
 H -2.25369900 -2.36924200 0.77596100
 H 3.14910000 -2.40194100 -2.01781200
 H -1.78573700 -1.24712900 -1.87636300
 H 1.59575700 -2.70674000 -0.36564400
 H 1.22788100 -1.44100100 2.11174900
 H 2.99441200 -4.22237300 0.13559800
 O 2.14709700 -4.67264100 0.01186300
 H 2.31167200 -5.35803800 -0.64032700
 H 3.10120200 -2.44304900 1.62694200
 O 1.74558400 -2.03385800 2.68949800
 H 1.14418000 -2.74591700 2.92677800
 Pd 0.06610700 -0.69449000 -0.01395200
 H 1.22730600 0.00489100 0.80132400
 C 5.11405000 -0.88531600 2.63164300
 H 4.27292900 -1.14238900 3.28222300
 H 5.70227200 -1.79697100 2.49917000
 H 5.72937500 -0.15225000 3.15348700
 C -2.49648700 2.78778700 1.72925900
 H -2.08718700 2.47948000 2.69562800
 H -1.64248300 3.10713600 1.12498400
 H -3.14491100 3.65035700 1.89284800

59

RR-PhMe_D2_TS2W_R, E(SCF) = -2487.48738770,
 E(ZPE) = -2487.042710, E(G) = -2487.112435
 a.u.

C -0.72185200 -3.18055800 -1.35942900
 H -0.56620900 -3.80017600 -0.47139400
 H -1.39730900 -3.71104800 -2.03574600
 C 0.58518300 -2.84223300 -2.01743100
 H 1.11551200 -3.74077600 -2.34663700
 H 0.41732400 -2.20832000 -2.89295900
 N 1.41647500 -2.08439200 -1.05237100
 N -1.33075100 -1.90677900 -0.91339400
 C 2.61919900 -1.50684500 -1.71661500
 H 2.26861400 -0.98412600 -2.60964100
 C -2.53243500 -2.06077400 -0.60679200
 H -3.23991600 -2.72629200 -0.56602000
 C 3.40267100 -0.57653500 -0.85712900
 C 4.07450200 -1.07239500 0.28935500
 C 3.41966800 0.77847500 -1.16406100
 C 4.77751400 -0.12844700 1.09883700

| | | | | | | | |
|--|-------------|--------------|-------------|--|--------------|-------------|-------------|
| C | 4.09069700 | 1.67663400 | -0.35854800 | O | 1.34995400 | -0.20898700 | 1.19911200 |
| H | 2.88823300 | 1.14247700 | -2.03864900 | S | -4.82430500 | -3.17753400 | -0.80106900 |
| C | 4.76750600 | 1.20966000 | 0.76725800 | S | 7.01011800 | -1.05536700 | -0.26656500 |
| H | 5.29712800 | 1.91644300 | 1.40223200 | O | 7.72400900 | -1.16085400 | 1.03953500 |
| C | -3.17589300 | -0.74193900 | 0.21534600 | O | 7.45130000 | 0.11658300 | -1.07352400 |
| C | -2.43979500 | 0.28262300 | 0.84383300 | O | 7.04520100 | -2.33492300 | -1.03229400 |
| C | -4.50981100 | -0.453966900 | -0.11740900 | O | -4.20331400 | -3.37318800 | -2.14155200 |
| C | -3.09039600 | 1.50233600 | 1.15450100 | O | -6.30883200 | -3.32671000 | -0.82234900 |
| C | -5.13414800 | 0.65161800 | 0.18636900 | O | -4.19073800 | -4.01914200 | 0.25707400 |
| H | -5.07240500 | -1.32631100 | -0.60956600 | H | 2.40664900 | 2.50347600 | 0.66471500 |
| C | -4.42097100 | 1.66062600 | 0.82418200 | H | -3.11852700 | 2.34310300 | -1.98878400 |
| H | -4.91558800 | 2.59920100 | 1.06144700 | H | 1.68137700 | 1.19195100 | -1.84171300 |
| O | 4.02574500 | -2.31743800 | 0.63368100 | H | -1.60774100 | 2.75517900 | -0.35258400 |
| O | -1.17802600 | 0.15497700 | 1.20089100 | H | -1.30874200 | 0.84536900 | 1.62922400 |
| S | 4.11743300 | 3.422404600 | -0.73843500 | H | -3.08171300 | 3.88501400 | 0.25330000 |
| S | -6.85753000 | 0.92767700 | -0.22768600 | O | -2.42737200 | 4.57600700 | 0.00851700 |
| O | -7.55571500 | 1.17271300 | 1.06733400 | H | -2.81080500 | 5.05309400 | -0.73084100 |
| O | -7.31997700 | -0.31182100 | -0.91181100 | H | -2.58421500 | 2.09704900 | 1.95653800 |
| O | -6.87693400 | 0.21158800 | -1.11595400 | O | -1.822006300 | 1.67285200 | 2.149514000 |
| O | 3.25327900 | 3.60173100 | -1.94037500 | H | -1.16934300 | 2.35809800 | 2.69081800 |
| O | 5.54551600 | 3.77716400 | -0.99697500 | Pd | -0.00285800 | 0.83260200 | 0.10842600 |
| O | 3.58074400 | 4.12189700 | 0.46770200 | H | -1.18497700 | 0.07198700 | 1.01028000 |
| H | -2.19668000 | -2.55763200 | 0.85597100 | C | -5.40649900 | 0.87997200 | 0.48231400 |
| H | 3.22893700 | -2.36073400 | -2.04460900 | H | -4.64107600 | 1.16454100 | 3.21066700 |
| H | -1.58174300 | -1.34789200 | -1.73156700 | H | -5.98447200 | 1.78593400 | 2.27780700 |
| H | 1.75666400 | -2.78121100 | -0.37719600 | H | -6.06680200 | 0.15033700 | 2.95429000 |
| H | 1.39133600 | -0.42887200 | 1.27607500 | C | 2.50316100 | -2.59122800 | 1.94258100 |
| H | 3.30056500 | -3.80988800 | 0.21314700 | H | 2.15617200 | -2.21391500 | 2.90881100 |
| O | 2.60173800 | -4.49670300 | 0.11122200 | H | 1.60808800 | -2.90450100 | 1.39767200 |
| H | 2.90378200 | -5.08650300 | -0.58308500 | H | 3.12344800 | -3.47056500 | 2.12320300 |
| H | 2.83606300 | -2.26747400 | 1.97486400 | | | | |
| O | 2.08726800 | -2.06273500 | 2.57791700 | 62 | | | |
| H | 1.47497400 | -2.79591000 | 2.47121500 | RR-PhMe_ID1_TS1_H2-out_R, E(SCF) = - | | | |
| Pd | 0.14125700 | -0.87908400 | 0.07917700 | 2563.95482284, E(ZPE) = -2563.484949, E(G) | | | |
| H | 1.41870500 | 0.16579200 | 0.71786200 | = -2563.557754 a.u. | | | |
| C | 5.50310500 | -0.62553300 | 2.30554900 | C | -0.64473200 | 3.30775200 | -0.01539900 |
| H | 4.82241800 | -1.10181500 | 3.01801900 | H | -0.38042500 | 3.38809100 | -1.07374800 |
| H | 6.24321300 | -1.38587800 | 2.03876300 | H | -1.26550800 | 4.16832100 | 0.24453000 |
| H | 6.01681500 | 0.18925900 | 2.81924700 | C | 0.59536800 | 3.22418100 | 0.83443000 |
| C | -2.32155900 | 2.58421400 | 1.83748900 | H | 1.21719300 | 4.11798200 | 0.74102700 |
| H | -1.95164100 | 2.25635600 | 2.81295000 | H | 0.33784800 | 3.09511200 | 1.88916700 |
| H | -1.44090200 | 2.87401300 | 1.25728900 | N | 1.34166000 | 2.01966600 | 0.40498300 |
| H | -2.94250500 | 3.46855900 | 1.98726700 | N | -1.40260900 | 2.04582700 | 0.15749900 |
| | | | | C | 2.44426800 | 1.61063300 | 1.29769300 |
| 59 | | | | H | 3.05269200 | 2.48683800 | 1.54585300 |
| RR-PhMe_D2_TS2W, E(SCF) = -2487.47709469, | | | | C | -2.40763600 | 1.78051700 | -0.89314000 |
| E(ZPE) = -2487.033902, E(G) = -2487.101798 | | | | H | -1.84994400 | 1.55755900 | -1.81003000 |
| a.u. | | | | C | 3.29764400 | 0.57488300 | 0.63742600 |
| C | 0.85488100 | 3.03859300 | -1.48230400 | C | 2.74789700 | -0.63028300 | 0.15712500 |
| H | 0.76680200 | 3.69337900 | -0.60984000 | C | 4.65637600 | 0.82756500 | 0.48475600 |
| H | 1.48724600 | 3.53983200 | -2.22111000 | C | 3.61583200 | -1.60072500 | -0.39920100 |
| C | -0.50022200 | 2.71311000 | -2.04369100 | C | 5.48728900 | -0.10509600 | -0.09708600 |
| H | -1.01823500 | 3.61339700 | -2.38842200 | H | 5.07189400 | 1.76789500 | 0.83168200 |
| H | -0.39923000 | 2.03590700 | -2.89725400 | C | 4.96167200 | -1.31716900 | -0.52375200 |
| N | -1.30931100 | 2.02364500 | -1.00831100 | H | 5.61776600 | -2.06037800 | -0.96871800 |
| N | 1.46823700 | 1.77370700 | -1.03074900 | C | -3.32013100 | 0.66858200 | -0.48495600 |
| C | -2.55033900 | 1.47651500 | -1.61923100 | C | -2.82217100 | -0.58731500 | -0.07875200 |
| H | -2.24527100 | 0.89126600 | -2.49006200 | C | -4.69138400 | 0.89779500 | -0.52121800 |
| C | 2.69871100 | 1.94511400 | -0.23246500 | C | -3.75038200 | -1.59178300 | 0.29337000 |
| H | 3.41066600 | 2.56386600 | -0.79021400 | C | -5.58428800 | -0.09280700 | -0.17825000 |
| C | -3.40298900 | 0.63114300 | -0.73278800 | H | -5.06653100 | 1.86787300 | -0.83032500 |
| C | -3.95259700 | 1.16074000 | 0.45630200 | C | -5.10453700 | -1.33019600 | 0.22912200 |
| C | -3.67711100 | -0.67670300 | -1.11281300 | H | -5.80554400 | -2.11061100 | 0.51314300 |
| C | -4.80349600 | 0.32835300 | 1.23184900 | O | 1.45140100 | -0.92059300 | 0.21627800 |
| C | -4.49962900 | -1.47649200 | -0.34469800 | O | -1.52936800 | -0.89117000 | -0.04656800 |
| H | -3.24591800 | -1.08015700 | -2.02435600 | S | 7.23673300 | 0.22453500 | -0.33038200 |
| C | -5.05693900 | -0.96628800 | 0.82316400 | S | -7.35534100 | 0.18848700 | -0.23897500 |
| H | -5.70705300 | -1.59529700 | 1.42662800 | O | -7.85292900 | -0.02728400 | -1.15008700 |
| C | 3.32653400 | 0.63227700 | 0.10967800 | O | -7.89267800 | -0.82072000 | -1.19591100 |
| C | 2.59968300 | -0.34927100 | 0.81814600 | O | -7.53285500 | 1.58969300 | -0.71012200 |
| C | 4.65588600 | 0.40552000 | -0.22854000 | O | 7.47912400 | 1.57709800 | 0.24263000 |
| C | 3.26083800 | -1.55007500 | 1.18693000 | O | 7.46374700 | 0.16449700 | -1.80252000 |
| C | 5.28810400 | -0.76474300 | 0.13538500 | O | 7.95629800 | -0.85715700 | 0.40018300 |
| H | 5.21041600 | 1.16126100 | -0.77574000 | H | 0.68039000 | -2.70100600 | 0.21724500 |
| C | 4.58454200 | -1.73255900 | 0.84456100 | H | 3.05345300 | 0.94669400 | -2.83479200 |
| H | 5.08146700 | -2.65645900 | 1.12982200 | H | 2.87523000 | 0.43648500 | -2.31440700 |
| O | -3.65106500 | 2.36314100 | 0.87519300 | O | -0.08226300 | -3.25209700 | 0.45669000 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.80284100 | -2.60944100 | 0.32787200 |
| H | 1.10649900 | -1.36618800 | 2.18603900 |
| O | 0.76762000 | -1.95852900 | 2.87319200 |
| H | 0.34817400 | -2.64317500 | 2.32729900 |
| H | 1.73009400 | 2.18761600 | -0.52536900 |
| H | 1.98400300 | 1.25360100 | 2.22589400 |
| H | -1.87476500 | 2.06055200 | 1.06291600 |
| H | -2.99152200 | 2.68960700 | -1.07168500 |
| Pd | -0.03804900 | 0.52349100 | 0.20326000 |
| O | 0.00367500 | -1.37715900 | -2.43693300 |
| H | -0.73123200 | -1.33441400 | -1.80315000 |
| H | 0.75989200 | -1.20806400 | -1.85842700 |
| C | 3.07339600 | -2.92048400 | -0.84113600 |
| H | 2.65463700 | -3.48025400 | 0.00183200 |
| H | 2.27564500 | -2.81650500 | -1.58306200 |
| H | 3.86017600 | -3.53319300 | -1.28254000 |
| C | -3.26169500 | -2.92756800 | 0.74672500 |
| H | -2.72877500 | -3.45664400 | -0.04927900 |
| H | -2.56985200 | -2.83790600 | 1.59016100 |
| H | -4.09490900 | -3.55737300 | 1.06065300 |

60

RR-PhMe_ID2_TS1_P, E(SCF) = -2562.77138663,
E(ZPE) = -2562.316075, E(G) = -2562.386428
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.05037400 | 1.01985700 | -1.54696800 |
| H | 0.01133600 | 0.28374700 | -2.35336900 |
| H | -0.18704100 | 2.01031400 | -1.98920000 |
| C | 1.17791900 | 0.94958400 | -0.68157300 |
| H | 2.08311600 | 1.16448800 | -1.25724200 |
| H | 1.12047700 | 1.67208800 | 0.13906900 |
| N | 1.24548800 | -0.40723100 | -0.09240200 |
| N | -1.21754200 | 0.66146800 | -0.70853500 |
| C | 2.27582600 | -0.53393300 | 0.97125800 |
| H | 2.16834800 | -1.53502900 | 1.39409900 |
| C | -2.45480800 | 0.38322800 | -1.47192100 |
| H | -2.64000400 | 1.21543000 | -2.15926700 |
| C | 3.66127000 | -0.31712700 | 0.45528900 |
| C | 4.21794200 | -1.29201900 | -0.41138900 |
| C | 4.37329800 | 0.82524300 | 0.79447500 |
| C | 5.52058300 | -1.04648200 | -0.93374500 |
| C | 5.64470200 | 1.03293400 | 0.29626700 |
| H | 3.93385400 | 1.56329100 | 1.45985200 |
| C | 6.20231200 | 0.09648600 | -0.57200500 |
| H | 7.19876200 | 0.26799900 | -0.97311300 |
| C | -3.64122000 | 0.19231100 | -0.58042000 |
| C | -3.63199600 | -0.76945300 | 0.45321300 |
| C | -4.78882200 | 0.93993800 | -0.82155900 |
| C | -4.81641000 | -0.97198900 | 1.20724300 |
| C | -5.93504600 | 0.73608600 | -0.08290000 |
| H | -4.79177800 | 1.68275700 | -1.61252700 |
| C | -5.93868400 | -0.22056800 | 0.92695700 |
| H | -6.84092900 | -0.38269400 | 1.51114600 |
| O | 3.56737000 | -2.36357100 | -0.74425700 |
| O | -2.59262700 | -1.51713500 | 0.74947100 |
| S | 6.58561600 | 2.49180500 | 0.72714500 |
| S | -7.41220400 | 1.70841900 | -0.37811800 |
| O | -7.13682900 | 2.51997300 | -1.59645000 |
| O | -7.60573800 | 2.54395500 | 0.84304400 |
| O | -8.51797200 | 0.72663300 | -0.57099600 |
| O | 7.86033500 | 2.00210000 | 1.33104800 |
| O | 5.74726500 | 3.25904400 | 1.69236600 |
| O | 6.82116600 | 3.23238900 | -0.54846700 |
| H | -2.24433300 | -0.50584400 | -2.07687800 |
| H | 2.02437800 | 0.18773200 | 1.75292900 |
| H | -1.40324300 | 1.41944000 | -0.04920200 |
| H | 1.49346900 | -1.04359000 | -0.86108600 |
| O | -0.19127900 | -2.65577300 | 1.52227900 |
| H | 0.44648000 | -3.23842600 | 1.02066600 |
| O | 2.61981600 | -2.06332100 | -2.17522400 |
| O | 1.87084100 | -1.73385900 | -2.72325900 |
| H | 2.26379600 | -1.12308700 | -3.35177300 |
| H | -1.01225700 | -3.14630800 | 1.65095500 |
| H | 2.39542700 | -3.34326900 | -0.10006200 |
| O | 1.65628600 | -3.94842200 | 0.17556700 |
| H | 1.39092100 | -4.41674800 | -0.61953100 |
| Pd | -0.69164900 | -0.96271200 | 0.38611100 |

| | | | |
|---|-------------|-------------|-------------|
| C | -4.81800400 | -1.99912600 | 2.29075000 |
| H | -4.58054400 | -2.99267200 | 1.90010100 |
| H | -4.06139900 | -1.77965900 | 3.04954100 |
| H | -5.79182100 | -2.04701500 | 2.78053900 |
| C | 6.10937800 | -2.04527300 | -1.87421300 |
| H | 6.20635700 | -3.02919900 | -1.40539900 |
| H | 5.46858700 | -2.18930400 | -2.75031900 |
| H | 7.09615200 | -1.73046000 | -2.21898000 |

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RR-PhMe_ID2_TS1_R, E(SCF) = -2562.77665973,
E(ZPE) = -2562.322022, E(G) = -2562.393591
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.85462200 | -3.41891000 | 0.39772200 |
| H | -0.70469100 | -3.47017800 | 1.47996600 |
| H | -1.47017100 | -4.27144500 | 0.09690000 |
| C | 0.46496300 | -3.39967700 | -0.32810500 |
| H | 1.04863600 | -4.30330800 | -0.13753900 |
| H | 0.29845700 | -3.33044900 | -1.40723700 |
| N | 1.21911900 | -2.19308700 | 0.08297600 |
| N | -1.54533100 | -2.14227700 | 0.10460300 |
| C | 2.21504300 | -1.76472600 | -0.91070300 |
| H | 1.65228200 | -1.46774900 | -1.80425900 |
| C | -2.75008800 | -1.89212100 | 0.92404400 |
| H | -3.40761800 | -2.76703700 | 0.87661200 |
| C | 3.11537400 | -0.66460200 | -0.43171300 |
| C | 2.68569500 | 0.41087000 | 0.37419400 |
| C | 4.43816100 | -0.71792200 | -0.86457200 |
| C | 3.64050900 | 1.39166000 | 0.75526700 |
| C | 5.34360500 | 0.26023600 | -0.52411200 |
| H | 4.76568600 | -1.54609200 | -1.48505300 |
| C | 4.93861300 | 1.30441500 | 0.29638500 |
| H | 5.65544800 | 2.06541900 | 0.59285100 |
| C | -3.47757800 | -0.67928200 | 0.44285400 |
| C | -2.82384300 | 0.56959300 | 0.38506700 |
| C | -4.81051600 | -0.78853200 | 0.06540400 |
| C | -3.56345800 | 1.70388000 | -0.03333800 |
| C | -5.51978500 | 0.32087400 | -0.34375600 |
| H | -5.30613100 | -1.75466600 | -0.10193500 |
| C | -4.88937700 | 1.55866200 | -0.38942600 |
| H | -5.44657300 | 2.43267200 | -0.71715800 |
| O | 1.45554600 | 0.55221100 | 0.85186400 |
| O | -1.56195900 | 0.73963600 | 0.73009200 |
| S | 7.05086300 | 0.17949900 | -1.06798600 |
| S | -7.22990700 | 0.18712500 | -0.86573500 |
| O | -7.61787400 | -1.23422500 | -0.64597600 |
| O | -7.24858900 | 0.57847700 | -2.30514700 |
| O | -7.99755300 | 1.13908300 | -0.01191700 |
| O | 7.32433600 | 1.47910300 | -1.74587000 |
| O | 7.13615600 | -0.98744600 | -1.98920000 |
| O | 7.86677800 | 0.00430100 | 0.16869800 |
| H | -2.40527600 | -1.78710000 | 1.95851600 |
| H | 2.82976100 | -2.62733400 | -1.19338100 |
| H | -1.81663100 | -2.12657300 | -0.87984900 |
| H | 1.66831700 | -2.33660400 | 0.99684300 |
| O | 0.67158300 | 3.61592200 | -0.80646800 |
| H | 0.38880700 | 3.38637400 | 0.10021700 |
| H | 1.80713300 | -0.62278700 | 2.47388700 |
| O | 2.01258700 | -1.49535800 | 2.84853700 |
| H | 2.89918300 | -1.41053300 | 3.20912400 |
| H | 0.23765800 | 4.45150600 | -0.99292800 |
| H | 0.68302900 | 2.03514200 | 1.66487700 |
| O | -0.02262200 | 2.69640500 | 1.78924200 |
| H | -0.79590300 | 2.17366000 | 1.50037400 |
| Pd | -0.12675900 | -0.69500400 | 0.39975600 |
| C | -2.89340500 | 3.03686000 | -0.09139400 |
| H | -2.59987600 | 3.38703900 | 0.90346200 |
| H | -1.97720400 | 2.99789500 | -0.68075900 |
| H | -3.55723800 | 3.78680000 | -0.52405000 |
| C | 3.23858400 | 2.50799100 | 1.66329800 |
| H | 2.51484600 | 3.17787300 | 1.18971400 |
| H | 2.77551200 | 2.13168300 | 2.58121800 |
| H | 4.10731200 | 3.10369900 | 1.94687000 |

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RR-PhMe_ID2_TS1_trigo-square_P, E(SCF) = -
2562.77166612, E(ZPE) = -2562.315471, E(G)
= -2562.383873 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.15834000 | -2.03148600 | 1.01944100 |
| H | 0.08580200 | -1.48695700 | 1.93667900 |
| H | -0.45715900 | -3.04751200 | 1.28909000 |
| C | 1.01023900 | -2.01807800 | 0.06960900 |
| H | 1.89173700 | -2.50261600 | 0.50178900 |
| H | 0.75661200 | -2.53940200 | -0.85742100 |
| N | 1.30107300 | -0.60727800 | -0.26325900 |
| C | 2.34661900 | -0.42329700 | -1.31784800 |
| H | 1.96509300 | 0.30368200 | -2.03862300 |
| C | 3.64640000 | 0.01777400 | -0.73282500 |
| C | 3.72293500 | 1.31237700 | -0.15755800 |
| C | 4.74684900 | -0.18355100 | -0.73199300 |
| C | 4.95685700 | 1.70133300 | 0.43585800 |
| C | 5.94327300 | -0.42234000 | -0.17384500 |
| H | 4.67380700 | -1.81553700 | -1.17969800 |
| C | 6.03237400 | 0.83755700 | 0.41368900 |
| H | 6.97102300 | 1.15054300 | 0.86536700 |
| O | 2.70551200 | 2.12033500 | -0.13203700 |
| S | 7.37015300 | -1.50167700 | -0.15133000 |
| O | 6.99737500 | -2.70120800 | -0.95425900 |
| O | 7.62841500 | -1.82691100 | 1.28327500 |
| O | 8.49074300 | -0.72405200 | -0.75812900 |
| H | 2.45827100 | -1.37238100 | -1.84639600 |
| H | 1.61563000 | -0.14300600 | 0.59969600 |
| O | 0.40673700 | 2.09202300 | -1.24813400 |
| H | 1.34649200 | 2.14855700 | -0.85333200 |
| H | 1.91124800 | 1.75875500 | 1.48926000 |
| O | 1.47409800 | 1.23627300 | 2.19039800 |
| H | 0.56833000 | 1.59394500 | 2.22718000 |
| H | -0.08037200 | 2.88339100 | -0.99352800 |
| H | -1.38882100 | 3.22553900 | 2.37794400 |
| O | -1.20139000 | 2.31000700 | 2.15825000 |
| H | -1.63852400 | 2.14456400 | 1.30078600 |
| Pd | -0.49697400 | 0.38100600 | -0.44785600 |
| N | -1.27917900 | -1.31329800 | 0.36685600 |
| C | -2.40334000 | -0.98650600 | 1.27507600 |
| H | -2.72292200 | -1.90000300 | 1.78743400 |
| C | -3.55789100 | -0.38833100 | 0.53498500 |
| C | -3.39887500 | 0.79830300 | -0.20747800 |
| C | -4.80677400 | -0.99316400 | 0.61649300 |
| C | -4.52570000 | 1.37120400 | -0.84084300 |
| C | -5.90103200 | -0.43124200 | -0.00724200 |
| H | -4.92771600 | -1.91017900 | 1.18341200 |
| C | -5.75375400 | 0.74932900 | -0.72528700 |
| H | -6.61785100 | 1.19076100 | -1.21531100 |
| O | -2.23719500 | 1.42559500 | -0.31781500 |
| S | -7.52247500 | -1.19419100 | 0.09749500 |
| O | -7.93125600 | -1.47943100 | -1.30812600 |
| O | -8.40510600 | -0.18466000 | 0.74985700 |
| O | -7.34647900 | -2.42740300 | 0.91329500 |
| H | -1.99707300 | -0.30173700 | 2.02810500 |
| H | -1.63652300 | -1.87915400 | -0.40515800 |
| C | -4.36343000 | 2.63856500 | -1.61319100 |
| H | -3.99097700 | 3.44766500 | -0.97891700 |
| H | -3.63649400 | 2.52210400 | -2.42172200 |
| H | -5.31309600 | 2.95421600 | -2.04756900 |
| C | 5.04447300 | 3.04518900 | 1.08003700 |
| H | 4.81867500 | 3.84578100 | 0.36947500 |
| H | 4.31367000 | 3.14306700 | 1.88978400 |
| H | 6.03892400 | 3.22118600 | 1.49418100 |

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RR-PhMe_ID2_TS1_trigo-square_R, E(SCF) = -
2562.78119220, E(ZPE) = -2562.327595, E(G)
= -2562.399436 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.71683000 | -3.28657300 | 0.30947000 |
| H | -0.54739600 | -3.25608000 | 1.39001400 |
| H | -1.31325700 | -4.17410900 | 0.08293500 |
| C | 0.59378900 | -3.28296100 | -0.43036400 |
| H | 1.20031100 | -4.15964800 | -0.18866200 |
| H | 0.42425900 | -3.27680300 | -1.51116000 |
| N | 1.31313500 | -2.03830100 | -0.08451300 |
| C | 2.39872100 | -1.69833200 | -1.01951800 |
| H | 1.92064100 | -1.44975700 | -1.97440600 |

| | | | |
|----|-------------|-------------|-------------|
| C | 3.26508700 | -0.58459400 | -0.51806900 |
| C | 2.73900100 | 0.60453200 | 0.02292600 |
| C | 4.64380200 | -0.73926300 | -0.63051600 |
| C | 3.63558800 | 1.62212600 | 0.43472500 |
| C | 5.50749200 | 0.25948700 | -0.24018600 |
| H | 5.04922200 | -1.66079100 | -1.03540200 |
| C | 4.99552700 | 1.43619000 | 0.29045300 |
| H | 5.67386400 | 2.22304800 | 0.60981000 |
| O | 1.44285300 | 0.84537000 | 0.18832400 |
| S | 7.28511900 | 0.06273300 | -0.38678600 |
| C | 4.50457200 | -1.30000300 | -0.94568300 |
| O | 7.82779300 | 0.22093800 | 0.99310500 |
| O | 7.74126500 | 1.14795200 | -1.30222200 |
| H | 3.01694000 | -2.58702400 | -1.18864800 |
| H | 1.67513400 | -2.08416600 | 0.29045300 |
| O | 0.08954800 | 2.58293000 | -1.57540700 |
| H | 0.81994600 | 2.13852900 | -1.11800400 |
| H | 1.52003900 | -0.17439200 | 2.30539700 |
| O | 1.82233000 | -1.02225000 | -0.94568300 |
| H | 1.22887600 | -1.20716400 | 3.39069100 |
| H | -0.66926000 | 2.16479700 | -1.13498700 |
| O | 0.59680300 | 2.03010400 | 1.47329100 |
| H | -0.14791600 | 2.33355900 | 2.01746400 |
| H | -0.89060000 | 1.94760700 | 1.52454500 |
| Pd | -0.07308200 | -0.54448200 | -0.01255800 |
| N | -1.45343500 | -2.05360800 | -0.05616200 |
| C | -2.57992800 | -1.74211200 | 0.84574900 |
| H | -3.20562400 | -2.63414800 | 0.95839700 |
| C | -3.41235900 | -0.60754800 | 0.34038200 |
| C | -2.84632500 | 0.64198600 | 0.01425100 |
| C | -4.78868500 | -0.79142200 | -0.25125500 |
| C | -3.71178300 | 1.70294300 | -0.35364400 |
| C | -5.61984400 | 0.24185000 | -0.12085100 |
| H | -5.21865500 | -1.75856800 | 0.49019600 |
| C | -5.07339900 | 1.48559900 | -0.41186200 |
| H | -5.72659500 | 2.30654900 | -0.69638500 |
| O | -1.54834000 | 0.89970700 | 0.06027400 |
| S | -7.39471200 | 0.01313100 | -0.24040800 |
| O | -7.74886100 | 0.31330500 | -1.65762100 |
| O | -7.99729300 | 0.98944000 | 0.71227000 |
| O | -7.65480800 | -1.40400200 | 0.13610600 |
| H | -2.13732900 | -1.52447500 | 1.82490700 |
| H | -1.80724900 | -2.14003500 | -1.00989900 |
| C | -3.13892900 | -3.04395400 | -0.67886800 |
| H | -2.42914100 | 3.37731300 | 0.08343700 |
| H | -2.59508200 | 3.02987600 | -1.62876500 |
| H | -3.92832900 | 3.79192100 | -0.76434800 |
| C | 3.09679100 | 2.87412600 | 1.04658400 |
| H | 2.34593500 | 3.35449900 | 0.41241500 |
| H | 2.61313900 | 2.67047900 | 2.00833600 |
| H | 3.89735400 | 3.59263000 | 1.22695600 |

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RR-PhMe_ID2_TS1_trigo-square, E(SCF) = -
2562.75410741, E(ZPE) = -2562.299866, E(G)
= -2562.368900 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.53203400 | -2.93705200 | 0.55082300 |
| H | -0.25494200 | -2.70869300 | 1.58399800 |
| H | -1.04406500 | -3.90221900 | 0.53786300 |
| C | 0.68978600 | -2.92938200 | -0.33460900 |
| H | 1.41398600 | -3.68813500 | -0.02383600 |
| H | 0.42161100 | -3.12072400 | -1.37763800 |
| N | 1.27772400 | -1.57748100 | -0.24834100 |
| C | 2.44254500 | -1.32607400 | -1.12854400 |
| H | 2.05121300 | -0.95735700 | -2.08359400 |
| C | 3.44566400 | -0.39093900 | -0.51620700 |
| C | 3.05944600 | 0.82419600 | 0.09694900 |
| C | 4.79064000 | -0.74348500 | -0.56704200 |
| C | 4.06768900 | 1.64632400 | 0.66588500 |
| C | 5.76162200 | 0.07915400 | -0.03518300 |
| H | 5.08731200 | -1.67985800 | -1.02924700 |
| C | 5.39166600 | 1.26992100 | 0.58216700 |
| H | 6.15570700 | 1.91050400 | 1.01581400 |
| O | 1.80537200 | 1.19695600 | 0.18969400 |
| S | 7.49621700 | -0.36700100 | -0.10036900 |
| O | 7.56150900 | -1.69064300 | -0.78181400 |
| O | 7.96133200 | -0.41972400 | 1.31652200 |

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|----|-------------|-------------|-------------|
| O | 8.17195000 | 0.71598100 | -0.87329000 |
| H | 2.93250300 | -2.28366000 | -1.33607400 |
| H | 1.54921900 | -1.40882900 | 0.72969500 |
| O | 0.40471200 | 1.41593100 | -1.99941900 |
| H | 1.06244100 | 1.67814900 | -1.31834800 |
| H | 1.40616400 | 0.41491400 | 1.84068200 |
| O | 1.42087700 | -0.31512900 | 2.49020000 |
| H | 0.60341100 | -0.22717000 | 2.98758300 |
| H | -0.36254500 | 1.98862900 | -1.86954800 |
| H | 0.65487900 | 2.44788300 | 0.92692000 |
| O | -0.17477500 | 2.87613300 | 1.20429600 |
| H | -0.86268300 | 2.34160200 | 0.77511800 |
| Pd | -0.28214700 | -0.25605600 | -0.43246600 |
| N | -1.43783300 | -1.86159800 | 0.08727900 |
| C | -2.49363700 | -1.46265300 | 1.04243900 |
| H | -3.01545900 | -2.36085900 | 1.39010000 |
| C | -3.48203500 | -0.51545500 | 0.43189100 |
| C | -3.07745500 | 0.69081900 | -0.17690500 |
| C | -4.83771200 | -0.81431500 | 0.52622800 |
| C | -4.06240300 | 1.59345700 | -0.64457100 |
| C | -5.79106400 | 0.06632900 | 0.06179500 |
| H | -5.15543500 | -1.74638300 | 0.98209800 |
| C | -5.39658800 | 1.26931800 | -0.51289500 |
| H | -6.14911300 | 1.96501100 | -0.87512300 |
| O | -1.81654300 | 1.05359800 | -0.32324300 |
| S | -7.54108900 | -0.31108900 | 0.17977100 |
| O | -8.05262600 | -0.31159100 | -1.22106300 |
| O | -8.13867100 | 0.78152000 | 0.99982400 |
| O | -7.63311400 | -1.64606400 | 0.83353100 |
| H | -1.97875400 | -1.02356900 | 1.90433700 |
| H | -1.88148200 | -2.15271600 | -0.78590800 |
| C | -3.62574200 | 2.87771600 | -1.26921000 |
| H | -3.00905000 | 3.46819700 | -0.58492300 |
| H | -3.01299300 | 2.69880600 | -2.15825900 |
| H | -4.48563900 | 3.48138500 | -1.56285200 |
| C | 3.65195500 | 2.90342200 | 1.35628000 |
| H | 3.09529100 | 3.56650100 | 0.68692100 |
| H | 2.98447200 | 2.68901000 | 2.19861900 |
| H | 4.51716900 | 3.44758000 | 1.73840200 |

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RR-PhMe_ID2_TS1, E(SCF) = -2562.75174153,
E(ZPE) = -2562.297844, E(G) = -2562.367096
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67968000 | 3.05609500 | 0.33404300 |
| H | 0.43622600 | 2.95256200 | 1.39521800 |
| H | 1.23805400 | 3.98442900 | 0.19308400 |
| C | -0.58382900 | 3.01619600 | -0.49278300 |
| H | -1.25977500 | 3.83581000 | -0.22955500 |
| H | -0.36251700 | 3.08570900 | -1.56175800 |
| N | -1.21469500 | 1.70998900 | -0.22504400 |
| N | 1.50917900 | 1.88904700 | -0.04560500 |
| C | -2.44418000 | 1.41631200 | -0.97853700 |
| H | -2.13562200 | 1.01958000 | -1.95259900 |
| C | 2.55659600 | 1.50737300 | 0.92442800 |
| H | 3.12374700 | 2.40070600 | 1.20851400 |
| C | -3.39388900 | 0.48099100 | -0.27492500 |
| C | -2.98530600 | -0.55751600 | 0.60628100 |
| C | -4.74438500 | 0.65352400 | -0.56433600 |
| C | -4.00326800 | -1.38805300 | 1.16467200 |
| C | -5.70961000 | -0.16892200 | -0.02281800 |
| H | -5.05168500 | 1.45305800 | -1.23220800 |
| C | -5.32825400 | -1.18747000 | 0.84539300 |
| H | -6.08654800 | -1.83088300 | 1.28536900 |
| C | 3.49504400 | 0.48280400 | 0.36096800 |
| C | 3.03520400 | -0.73121800 | -0.19440500 |
| C | 4.86257600 | 0.72750300 | 0.43925800 |
| C | 3.98489000 | -1.69241800 | -0.62368200 |
| C | 5.77850300 | -0.20901900 | 0.01073800 |
| H | 5.21935600 | 1.66464200 | 0.85406000 |
| C | 5.33165100 | -1.41715800 | -0.51298800 |
| H | 6.05301500 | -2.15736900 | -0.84960500 |
| O | -1.74489000 | -0.76349900 | 0.94735800 |
| O | 1.76375300 | -1.04966600 | -0.32764100 |
| S | -7.44413700 | 0.06029900 | -0.39746100 |
| S | 7.54137300 | 0.10753900 | 0.10111300 |
| O | 7.68919500 | 1.45178400 | 0.72544300 |

| | | | |
|----|-------------|-------------|-------------|
| O | 8.03843000 | 0.06222800 | -1.30471900 |
| O | 8.11112900 | -0.98823400 | 0.93708200 |
| O | -7.90396700 | -1.21071100 | -1.03228000 |
| O | -7.52344300 | 1.22753500 | -1.32139300 |
| O | -8.12501000 | 0.31083300 | 0.90788300 |
| H | 2.03316600 | 1.14866000 | 1.81770100 |
| H | -2.96408100 | 2.36273000 | -1.17183600 |
| H | 1.95442300 | 2.07772400 | -0.94534300 |
| H | -1.41225700 | 1.66780100 | 0.78382300 |
| O | -0.79971400 | -1.28726400 | -1.67771500 |
| O | -0.73179000 | -2.06000300 | -1.07438400 |
| H | -1.32455900 | 0.33323700 | 2.24226000 |
| O | -1.12326300 | 1.18928200 | 2.68610600 |
| H | -1.81226700 | 1.30895400 | 3.34374700 |
| H | -0.17293400 | -1.47280000 | -2.39150700 |
| H | -0.81061500 | -2.26551300 | 0.85811800 |
| O | -0.21736700 | -2.94308300 | 0.46177000 |
| H | 0.64037200 | -2.49030000 | 0.39066800 |
| Pd | 0.26565100 | 0.30866500 | -0.41461000 |
| C | 3.49559200 | -2.98722600 | -1.18425700 |
| H | 2.92829500 | -3.55676600 | -0.44138600 |
| H | 2.81866300 | -2.82564100 | -2.02811100 |
| H | 4.32825300 | -3.60653800 | -1.52103800 |
| C | -3.59046500 | -2.47229600 | 2.10555500 |
| H | -2.94183000 | -3.20613900 | 1.61636000 |
| H | -3.01624500 | -2.07073100 | 2.94622100 |
| H | -4.45949500 | -3.00082200 | 2.50157600 |

62

RR-PhMe_ID2_TS2_P, E(SCF) = -2563.92773785,
E(ZPE) = -2563.457425, E(G) = -2563.530781
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.09727500 | 0.25041400 | 1.89039200 |
| H | 0.07647900 | -0.68474600 | 2.45720900 |
| H | 0.22415500 | 1.08105200 | 2.58955400 |
| C | -1.15448300 | 0.38735900 | 1.07005900 |
| H | -2.04277300 | 0.42691800 | 1.70639000 |
| H | -1.13250000 | 1.30130800 | 0.46704500 |
| N | -1.22607800 | -0.77056500 | 0.14807600 |
| N | 1.24108000 | 0.18666300 | 0.95298700 |
| C | -2.27964700 | -0.64985600 | -0.89862400 |
| H | -2.34471800 | -1.63792600 | -1.36532400 |
| C | 2.52789100 | -0.21882300 | 1.56140100 |
| H | 2.70569400 | 0.39208500 | 2.45245200 |
| C | -3.60573900 | -0.19792200 | -0.37680800 |
| C | -4.34003200 | -1.05064600 | 0.48604800 |
| C | -4.09296600 | 1.05577300 | -0.72225100 |
| C | -5.59708400 | -0.58104600 | 0.96815200 |
| C | -5.31313200 | 1.49228400 | -0.24605600 |
| H | -3.51379700 | 1.70026500 | -1.37719000 |
| C | -6.05260500 | 0.66710700 | 0.59967100 |
| H | -7.01326400 | 1.01290800 | 0.97530600 |
| C | 3.65678600 | -0.05209600 | 0.59643200 |
| C | 3.62184500 | -0.68230900 | -0.66509700 |
| C | 4.75568700 | 0.71649400 | 0.96160600 |
| C | 4.73564600 | -0.53701700 | -1.53071200 |
| C | 5.83289500 | 0.85369500 | 0.11212100 |
| H | 4.77314400 | 1.21030600 | 1.92784700 |
| C | 5.81550800 | 0.22071000 | -1.12621400 |
| H | 6.66275500 | 0.33137600 | -1.79805600 |
| O | -3.89302700 | -2.21517700 | 0.83468200 |
| O | 2.62497900 | -1.43517300 | -1.08228200 |
| S | -5.95885900 | 3.10282400 | -0.68035500 |
| S | 7.26806800 | 1.82131300 | 0.58344200 |
| O | 8.40434900 | 0.85760800 | 0.65978900 |
| O | 6.93763400 | 2.43283900 | 1.90072300 |
| O | 7.45482500 | 2.83083100 | -0.49787000 |
| O | -7.27487100 | 2.86177800 | -1.34376400 |
| O | -4.95731900 | 3.72318800 | -1.59437600 |
| O | -6.11020100 | 3.85224500 | 0.60250400 |
| H | 2.40286200 | -1.25718300 | 1.88753900 |
| H | -1.90871100 | 0.05549700 | -1.64732900 |
| H | 1.36463400 | 1.10025900 | 0.51122100 |
| H | -1.42311600 | -1.59656400 | 0.72945600 |
| O | -0.34988300 | -4.29072500 | -0.76883900 |
| H | -1.33136100 | -4.30767900 | -0.71972500 |
| H | -2.65423100 | -2.49366500 | 1.99461400 |

| | | | |
|----|-------------|-------------|-------------|
| O | -1.76976300 | -2.52468900 | 2.42979300 |
| H | -1.58631600 | -3.45375700 | 2.58513900 |
| H | -0.04484400 | -4.37100000 | 0.13848200 |
| H | -3.42668100 | -3.46459100 | -0.17641600 |
| O | -3.08463100 | -4.25119300 | -0.67330100 |
| H | -3.53766000 | -4.24678700 | -1.51923200 |
| H | 0.17007000 | -2.55827100 | -1.47529100 |
| H | 0.26092800 | -1.94265200 | -2.02378300 |
| Pd | 0.70643900 | -1.10212800 | -0.54480100 |
| C | 4.71303300 | -1.21196900 | -2.86189100 |
| H | 4.63483700 | -2.29788400 | -2.75914500 |
| H | 3.84817500 | -0.89661600 | -3.45217500 |
| H | 5.61814600 | -0.98732200 | -3.42837700 |
| C | -6.38897100 | -1.46603500 | 1.87297800 |
| H | -6.61919900 | -2.42242000 | 1.39373300 |
| H | -5.83083900 | -1.71001300 | 2.78210500 |
| H | -7.32860700 | -0.99286600 | 2.16427000 |

60

RR-PhMe_ID2_TS2_R_noH2, E(SCF) = -
 2562.77133526, E(ZPE) = -2562.316539, E(G)
 = -2562.389154 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.04416100 | 0.72364100 | 1.80677100 |
| H | -0.00477400 | -0.08145100 | 2.54484700 |
| H | 0.17141400 | 1.67265100 | 2.33497900 |
| C | -1.18324800 | 0.72315200 | 0.93723900 |
| H | -2.09165300 | 0.87572300 | 1.52582100 |
| H | -1.12633700 | 1.52640400 | 0.19498300 |
| N | -1.24188500 | -0.56600500 | 0.20872400 |
| N | 1.20782400 | 0.45798700 | 0.93085200 |
| C | -2.19463000 | -0.54156700 | -0.93392900 |
| H | -2.11198600 | -1.51038500 | -1.43132400 |
| C | 2.47843500 | 0.19538300 | 1.64403000 |
| H | 2.65623300 | 1.00545300 | 2.35926500 |
| C | -3.60122400 | -0.27008000 | -0.50925600 |
| C | -4.30145300 | -1.27807000 | 0.20144000 |
| C | -4.19168700 | 0.95924700 | -0.76961700 |
| C | -5.62778000 | -0.98222400 | 0.63258500 |
| C | -5.48001200 | 1.22405000 | -0.34892900 |
| H | -3.64026100 | 1.72461300 | -1.30862200 |
| C | -6.18444900 | 0.24817600 | 0.35338200 |
| H | -7.19564900 | 0.46161500 | 0.69273900 |
| C | 3.63204600 | 0.08868100 | 0.69781700 |
| C | 3.62381000 | -0.86849100 | -0.33996000 |
| C | 4.73541200 | 0.91649400 | 0.87074300 |
| C | 4.77228400 | -0.99605100 | -1.16084600 |
| C | 5.84292900 | 0.79447000 | 0.05782200 |
| H | 4.73482100 | 1.65894900 | 1.66189300 |
| C | 5.85328100 | -0.16537600 | -0.94891000 |
| H | 6.72617500 | -0.26173600 | -1.58957900 |
| O | -3.76168000 | -2.42523700 | 0.47366300 |
| O | 2.61261500 | -1.67629600 | -0.57309000 |
| S | -6.25286500 | 2.80591400 | -0.65974700 |
| S | 7.25661300 | 1.88198200 | 0.24326800 |
| O | 8.43965100 | 0.99122100 | 0.42192600 |
| O | 6.97726500 | 2.72474800 | 1.43919900 |
| O | 7.33304200 | 2.67411600 | -1.01884600 |
| O | -7.47332100 | 2.52526500 | -1.47328300 |
| O | -5.24627100 | 3.62552600 | -1.39373900 |
| O | -6.59290100 | 3.37304400 | 0.67937100 |
| H | 2.32452900 | -0.72698200 | 2.21441200 |
| H | -1.83802700 | 0.22279200 | -1.62967200 |
| H | 1.34647400 | 1.25663000 | 0.30864200 |
| H | -1.55107900 | -1.27504700 | 0.88840300 |
| O | 0.22044300 | -2.75320000 | -1.46506500 |
| H | -0.52048500 | -3.30876100 | -1.09158300 |
| H | -2.87626600 | -2.34576200 | 1.97232400 |
| O | -2.17998300 | -2.05146100 | 2.60367400 |
| H | -1.77176200 | -2.85489400 | 2.93441800 |
| H | 1.01255800 | -3.30062600 | -1.52136000 |
| H | -2.58036200 | -3.39293300 | -0.15047000 |
| O | -1.82980200 | -3.99929600 | -0.39328100 |
| H | -2.22060100 | -4.73752200 | -0.86586300 |
| Pd | 0.70405800 | -1.11936500 | -0.24074300 |
| C | 4.78010600 | -2.02314900 | -2.24430300 |
| H | 4.67332500 | -3.03377000 | -1.83978500 |
| H | 3.94454000 | -1.87902600 | -2.93491200 |

| | | | |
|---|-------------|-------------|-------------|
| H | 5.70985800 | -1.98150900 | -2.81379100 |
| C | -6.37619300 | -2.02071900 | 1.40078800 |
| H | -6.47394200 | -2.94912700 | 0.83031200 |
| H | -5.85162700 | -2.28532900 | 2.32482900 |
| H | -7.37655300 | -1.67222100 | 1.66442900 |

62

RR-PhMe_ID2_TS2_R, E(SCF) = -2563.94561611,
 E(ZPE) = -2563.475495, E(G) = -2563.548213
 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.02991800 | 0.69613800 | 1.83241600 |
| H | -0.02825600 | -0.11156000 | 2.56695600 |
| H | 0.15868500 | 1.64231300 | 2.36525600 |
| C | -1.19128600 | 0.70622100 | 0.95421100 |
| H | -2.10280700 | 0.86268300 | 1.53694600 |
| H | -1.12403600 | 1.51184300 | 0.21527800 |
| N | -1.25355500 | -0.57972200 | 0.22014100 |
| N | 1.19827100 | 0.42744900 | 0.96377600 |
| C | -2.20014200 | -0.54488800 | -0.92745100 |
| H | -2.11950300 | -1.51131200 | -1.42980300 |
| C | 2.46340400 | 0.15376100 | 1.68406400 |
| H | 2.63811500 | 0.95572800 | 2.40903300 |
| C | -3.60721100 | -0.26867100 | -0.50748900 |
| C | -4.31627800 | -1.27795700 | 0.19261200 |
| C | -4.18878000 | 0.96666000 | -0.75929700 |
| C | -5.64199100 | -0.97693100 | 0.62212400 |
| C | -5.47658400 | 1.23652400 | -0.34028000 |
| H | -3.63049400 | 1.73294700 | -1.28987700 |
| C | -6.18944100 | 0.25963000 | 0.35212400 |
| H | -7.20015700 | 0.47696900 | 0.69047700 |
| C | 3.61932500 | 0.05734200 | 0.73987200 |
| C | 3.60982900 | -0.88753700 | -0.30823000 |
| C | 4.71730800 | 0.89236800 | 0.91242200 |
| C | 4.74350100 | -0.98514100 | -1.15215800 |
| C | 5.81617300 | 0.79120900 | 0.08496900 |
| H | 4.71888700 | 1.62455300 | 1.71305500 |
| C | 5.82024800 | -0.14842500 | -0.94049400 |
| H | 6.68296300 | -0.22130700 | -1.59785000 |
| O | -3.78474300 | -2.43063500 | 0.45753800 |
| O | 2.60271800 | -1.70240800 | -0.53864200 |
| S | -6.23581800 | 2.82795500 | -0.63600000 |
| S | 7.22740400 | 1.88161400 | 0.27575900 |
| O | 8.41178300 | 0.99205600 | 0.45124100 |
| O | 6.94526600 | 2.71809000 | 1.47531900 |
| O | 7.30252700 | 2.67885900 | -0.98295000 |
| O | -7.46326500 | 2.56525200 | -1.44500000 |
| O | -5.22491400 | 3.64285000 | -1.36930600 |
| O | -6.56323300 | 3.38866300 | 0.70895600 |
| H | 2.30386700 | -0.77486200 | 2.24240600 |
| H | -1.83625700 | 0.22161700 | -1.61717400 |
| H | 1.34632100 | 1.22839800 | 0.34569000 |
| H | -1.56998000 | -1.29003700 | 0.89545000 |
| O | 0.20833200 | -2.76251300 | -1.46012300 |
| H | -0.53967300 | -3.31642600 | -1.09781400 |
| O | -2.90543600 | -2.36518100 | 1.96094500 |
| O | -2.21112900 | -2.07589800 | 2.59678600 |
| H | -1.80872000 | -2.88193900 | 2.92828300 |
| H | 0.99692100 | -3.31494100 | -1.51670000 |
| H | -2.60523500 | -3.39845200 | -0.16956300 |
| O | -1.85603900 | -4.00569600 | -0.41456800 |
| H | -2.24763400 | -4.73846600 | -0.89493700 |
| H | 2.04888000 | 0.35456300 | -2.25527500 |
| H | 2.13810300 | 1.02131600 | -2.58887100 |
| Pd | 0.69202000 | -1.14171100 | -0.22208100 |
| C | 4.73286400 | -1.97553200 | -2.26887300 |
| H | 4.62422200 | -2.99918900 | -1.89990000 |
| H | 3.88808400 | -1.79931900 | -2.94185200 |
| H | 5.65448100 | -1.91814800 | -2.85000100 |
| C | -6.39949600 | -2.01689500 | 1.37937100 |
| H | -6.50174100 | -2.93977400 | 0.80077500 |
| H | -5.87925300 | -2.29275900 | 2.30254500 |
| H | -7.39824900 | -1.66399100 | 1.64319900 |

62

RR-PhMe_ID2_TS3-square_P, E(SCF) = -
 2563.96126589, E(ZPE) = -2563.487425, E(G)
 = -2563.560235 a.u.

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -0.04266600 | -0.74437900 | 1.65077100 | C | -2.52750900 | -0.07049300 | 1.58999600 |
| H | -0.00863100 | 0.09128900 | 2.35731900 | H | -2.70562500 | -0.81098100 | 2.37676100 |
| H | -0.09267500 | -1.67103100 | 2.23272300 | C | 3.59530500 | 0.17706700 | -0.41733100 |
| C | 1.18353900 | -0.72618500 | 0.77196300 | C | 4.35074100 | 1.09261400 | 0.36162700 |
| H | 2.08971000 | -0.89232000 | 1.36300000 | C | 4.09203700 | -1.08594700 | -0.71373800 |
| H | 1.12328900 | -1.52195300 | 0.02151900 | C | 5.63672900 | 0.66914000 | 0.81370700 |
| N | 1.25843200 | 0.57108500 | 0.05564200 | C | 5.33705000 | -1.47646200 | -0.26415900 |
| N | -1.23019000 | -0.56477500 | 0.80434900 | H | 3.49884700 | -1.77624400 | -1.30674900 |
| C | 2.27859900 | 0.58481100 | -1.02285700 | C | 6.09716900 | -0.59131500 | 0.49991700 |
| H | 2.22203900 | 1.56917200 | -1.48908400 | H | 7.07845600 | -0.90004300 | 0.85394200 |
| C | -2.46049600 | -0.19184800 | 1.51569100 | C | -3.67698900 | -0.05199300 | 0.63585300 |
| H | -2.67431700 | -0.90890400 | 2.31853600 | C | -3.64781100 | 0.78113800 | -0.50176900 |
| C | 3.66180700 | 0.25756900 | -0.54062800 | C | -4.79009600 | -0.84412900 | 0.89156900 |
| C | 4.42943600 | 1.18058900 | 0.17391900 | C | -4.77914300 | 0.81006800 | -1.35555000 |
| C | 4.18010500 | -1.01725500 | -0.75385200 | C | -5.88523600 | -0.80951300 | -0.85008500 |
| C | 5.67641400 | 0.82522000 | 0.70869900 | H | -4.80515000 | -1.49105700 | 1.76246600 |
| C | 5.41205100 | -1.37159500 | -0.24882100 | C | -5.87264500 | 0.02220700 | -1.05904700 |
| H | 3.60376800 | -1.74670600 | -1.31384100 | H | -6.73637300 | 0.04767300 | -1.71861900 |
| C | 6.14932000 | -0.45541300 | 0.48779600 | C | 3.90453600 | 2.27064000 | 0.63559900 |
| H | 7.11757000 | -0.73940300 | 0.88985700 | O | -2.63807300 | 1.57016900 | -0.80569400 |
| C | -3.63108700 | -0.11774600 | 0.58328900 | S | 5.99139500 | -3.10069200 | -0.62854000 |
| C | -3.63571400 | 0.75608600 | -0.53292400 | S | -7.33046000 | -1.82290100 | 0.37491500 |
| C | -4.74788300 | -0.89946200 | 0.85800300 | O | -7.50222300 | -2.68042800 | -0.83316600 |
| C | -4.81668500 | 0.82409900 | -1.32425700 | O | -8.46442200 | -0.87179400 | 0.55828500 |
| C | -5.88169700 | -0.82910000 | 0.07587800 | O | -7.02370500 | -2.60565900 | 1.60411000 |
| H | -4.73450000 | -1.57020200 | 1.71134900 | O | 7.26574600 | -2.88267500 | -1.37644500 |
| C | -5.90595500 | 0.03899900 | -1.01074600 | O | 4.95565700 | -3.79447400 | -1.44670000 |
| H | -6.79795100 | 0.09977700 | -1.62957100 | O | 6.22449800 | -3.76276500 | 0.68989900 |
| O | 4.01384900 | 2.44672200 | 0.43207100 | H | -1.41300700 | -1.23899000 | 0.32652700 |
| O | -2.64351300 | 1.53980400 | -0.87639500 | H | 1.44647300 | 1.33913200 | 0.85931100 |
| S | 6.09152100 | -3.01277900 | -0.53597900 | O | 0.70648300 | 4.19070000 | -0.00523600 |
| S | -7.31875500 | -1.83865200 | 0.42288400 | H | 1.57285700 | 4.32888000 | -0.45394000 |
| O | -7.51566700 | -2.70524300 | -0.77679200 | H | 2.59559200 | 2.60943200 | 1.78450100 |
| O | -8.45393600 | -0.88995400 | 0.62089400 | O | 1.69841600 | 2.68469400 | 2.17899700 |
| O | -6.99628100 | -2.61851100 | 1.65133900 | H | 1.25306200 | 3.33346300 | 1.60606400 |
| O | 7.32695100 | -2.79805900 | -1.34081400 | H | 0.25416600 | 5.03781800 | -0.01286800 |
| O | 5.03893900 | -3.76656000 | -1.26921300 | H | 3.55481500 | 3.47404400 | -0.45216400 |
| O | 6.37920800 | -3.56924700 | 0.81545100 | O | 3.22167800 | 4.23576500 | -0.99404400 |
| H | -1.40107300 | -1.41253800 | 0.26651500 | H | 3.40645500 | 4.01362200 | -1.90916500 |
| H | 1.50925500 | 1.27455100 | 0.76388600 | H | -0.14132900 | 2.67284400 | -1.04430800 |
| O | 0.21641000 | 4.07054000 | 0.71744500 | H | -0.29635600 | 2.19292700 | -1.69746300 |
| H | 1.60887800 | 4.21767300 | -0.46642100 | Pd | -0.72138100 | 1.09579000 | -0.38270600 |
| H | 2.73502500 | 2.59748800 | 1.97483800 | H | 1.87837800 | -0.10294700 | -1.67034600 |
| O | 1.85264300 | 2.39809700 | 2.32159700 | H | -2.36761200 | 0.90000500 | 2.07278800 |
| H | 1.28319500 | 3.10558600 | 1.97314000 | C | 6.45346700 | 1.61879300 | 1.62618500 |
| H | -0.39539700 | 4.77946900 | 0.93684300 | H | 6.64335400 | 2.54850500 | 1.08121400 |
| H | 3.42186800 | 2.84369300 | -0.24821500 | H | 5.93501300 | 1.90814000 | 2.54541900 |
| O | 2.41523100 | 4.05922100 | -0.99418400 | H | 7.41447900 | 1.17873300 | 1.89919500 |
| H | 2.13021200 | 4.04229300 | -1.91130100 | C | -4.76269400 | 1.69665900 | -2.55689400 |
| H | -0.30499700 | 3.38672100 | 0.25379600 | H | -4.64408700 | 2.74751800 | -2.27871500 |
| H | -0.21968400 | 2.28457600 | -1.37731300 | H | -3.92407900 | 1.45671100 | -3.21644100 |
| Pd | -0.69201200 | 1.07290600 | -0.48869600 | H | -5.68795600 | 1.59650600 | -3.12617700 |
| H | 1.96411000 | -0.14145100 | -1.77604200 | | | | |
| H | -2.26255900 | 0.77793400 | 1.99020100 | 60 | | | |
| C | 6.46690500 | 1.82307700 | 1.48966600 | RR-PhMe_ID2_TS2-square_R_noH2, E(SCF) = - | | | |
| H | 6.67556200 | 2.71751200 | 0.89755100 | 2562.76778688, E(ZPE) = -2562.312478, E(G) | | | |
| H | 5.92396400 | 2.15686800 | 2.37787100 | = -2562.384572 a.u. | | | |
| H | 7.41642600 | 1.39536900 | 1.81295200 | C | 0.12592100 | 1.25187000 | 1.74576800 |
| C | -4.84717300 | 1.75352900 | -2.49282500 | H | 0.10214500 | 0.59376600 | 2.61860300 |
| H | -4.71404000 | 2.79410400 | -2.18273500 | H | 0.28453700 | 2.27691300 | 2.09283300 |
| H | -4.03623800 | 1.53862200 | -3.19441800 | C | -1.13262900 | 1.12803700 | 0.93239200 |
| H | -5.79580100 | 1.67642400 | -3.02713400 | H | -2.01870800 | 1.39234700 | 1.51461900 |
| | | | | H | -1.08609900 | 1.80686900 | 0.07531100 |
| 62 | | | | N | -1.23244200 | -0.25231300 | 0.40126200 |
| RR-PhMe_ID2_TS2-square_P, E(SCF) = - | | | | N | 1.25540900 | 0.81161000 | 0.89270000 |
| 2563.93176680, E(ZPE) = -2563.461169, E(G) | | | | C | -2.12627200 | -0.34851100 | -0.78760100 |
| = -2563.536080 a.u. | | | | H | -1.93079900 | -1.31724700 | -1.24855700 |
| C | -0.10503400 | -0.63418800 | 1.79506400 | C | 2.54415100 | 0.68415200 | 1.62136100 |
| H | -0.06107500 | 0.20465900 | 2.49550400 | H | 2.76608700 | 1.63595500 | 2.10672200 |
| H | -0.24236300 | -1.55596600 | 2.36622300 | C | -3.57520700 | -0.20329900 | -0.45279600 |
| C | 1.13050400 | -0.67689400 | 0.94024200 | C | -4.27884400 | -1.33620500 | 0.03774200 |
| H | 2.02888700 | -0.82142500 | 1.54565800 | C | -4.22037000 | 1.01589800 | -0.62396400 |
| H | 1.07682400 | -1.49981900 | 0.21974000 | C | -5.65966700 | -1.16903700 | 0.35365400 |
| N | 1.21214600 | 0.59323200 | 0.18406000 | C | -5.55699100 | 1.15545800 | -0.30944000 |
| N | -1.26175300 | -0.40594000 | 0.89922400 | H | -3.67530700 | 1.87086000 | -1.01441300 |
| C | 2.23823300 | 0.58017300 | -0.85959500 | C | -6.26429000 | 0.05693700 | 0.17681600 |
| H | 2.24996600 | 1.59202300 | -1.31022600 | H | -7.31810800 | 0.16814300 | 0.42298800 |

| | | | |
|----|-------------|-------------|-------------|
| C | 3.66855000 | 0.31017900 | 0.70097900 |
| C | 3.60925700 | -0.87680800 | -0.06023100 |
| C | 4.80338400 | 1.11084000 | 0.65253800 |
| C | 4.73227800 | -1.24448200 | -0.84238400 |
| C | 5.88991800 | 0.74689800 | -0.11488700 |
| H | 4.84514300 | 2.02572000 | 1.23482400 |
| C | 5.84647500 | -0.43041200 | -0.85343400 |
| H | 6.70385200 | -0.71642800 | -1.45754700 |
| O | -3.70833900 | -2.48969600 | 0.19592300 |
| O | 2.57025700 | -1.68334600 | -0.05890700 |
| S | -6.40942600 | 2.70944400 | -0.54819500 |
| S | 7.36545900 | 1.76391600 | -0.17602900 |
| O | 7.53666400 | 2.15487800 | -1.60554700 |
| O | 8.47918000 | 0.89838700 | 0.30930100 |
| O | 7.10339000 | 2.92724800 | 0.71649100 |
| O | -7.44159800 | 2.46510000 | -1.59996000 |
| O | -5.37346400 | 3.69282800 | -0.97610800 |
| O | -7.02435100 | 3.05475200 | 0.76787800 |
| H | 1.37473600 | 1.46892400 | 0.11990600 |
| H | -1.58452600 | -0.88453500 | 1.13453000 |
| O | 0.15859000 | -2.97498100 | -0.33967300 |
| H | -0.62800200 | -3.24276300 | -0.89378900 |
| H | -2.50742200 | -2.92763600 | 1.42361600 |
| O | -1.73386800 | -2.66598000 | 2.03226400 |
| H | -1.00783000 | -3.07381100 | 1.54456900 |
| H | 0.94563500 | -3.41890600 | -0.67635900 |
| H | -2.77875000 | -3.28088700 | -0.92313100 |
| O | -2.08286400 | -3.75280600 | -1.45790700 |
| H | -2.31067200 | -3.62683600 | -2.38187100 |
| Pd | 0.69087100 | -0.98451600 | 0.13442000 |
| H | -1.79722000 | 0.42235300 | -1.48897600 |
| H | 2.38223700 | -0.06829400 | 2.39202000 |
| C | -6.42070900 | -2.34508000 | 0.86914400 |
| H | -6.38273000 | -3.18268600 | 0.16651600 |
| H | -5.99636300 | -2.71640900 | 1.80703600 |
| H | -7.46769700 | -2.09077700 | 1.04519300 |
| C | 4.68120500 | -2.50728300 | -1.63713600 |
| H | 4.55009100 | -3.38126000 | -0.99286700 |
| H | 3.83470900 | -2.50684600 | -2.32957000 |
| H | 5.59796000 | -2.64289000 | -2.21286000 |

62

RR-PhMe_ID2_TS2-square_R, E(SCF) = -
2563.94144265, E(ZPE) = -2563.470047, E(G)
= -2563.541273 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.12660900 | -1.15665500 | 1.95490600 |
| H | -0.10257300 | -0.47087600 | 2.80573100 |
| H | -0.28338600 | -2.17071500 | 2.33412600 |
| C | 1.12977400 | -1.05962300 | 1.13209500 |
| H | 2.02033300 | -1.29149200 | 1.72072400 |
| H | 1.08407300 | -1.77891300 | 0.30868500 |
| N | 1.22075400 | 0.29483000 | 0.53283700 |
| N | -1.25447700 | -0.74519400 | 1.08655500 |
| C | 2.04824700 | 0.32111700 | -0.70706600 |
| H | 1.83921900 | 1.26945800 | -1.20273400 |
| C | -2.56164700 | -0.63218300 | 1.77597100 |
| H | -2.78403100 | -1.58480800 | 2.26844900 |
| C | 3.51263200 | 0.17212300 | -0.45398500 |
| C | 4.27013400 | 1.32782200 | -0.12275300 |
| C | 4.12118800 | -1.07304600 | -0.55928800 |
| C | 5.66798700 | 1.15456600 | 0.10645800 |
| C | 5.47405200 | -1.21771700 | -0.32920800 |
| H | 3.53219500 | -1.94430000 | -0.83228900 |
| C | 6.23507000 | -0.09736900 | 0.00063000 |
| H | 7.30240000 | -0.21206600 | 0.17678500 |
| C | -3.65839400 | -0.27826400 | 0.82350500 |
| C | -3.59420800 | 0.92319600 | 0.08592200 |
| C | -4.75504200 | -1.12011300 | 0.68767900 |
| C | -4.67785900 | 1.26885400 | -0.75731500 |
| C | -5.80294700 | -0.77952700 | -0.14267300 |
| H | -4.79747500 | -2.04848600 | 1.24783500 |
| C | -5.75751000 | 0.41405700 | -0.85474300 |
| H | -6.58475500 | 0.67953100 | -1.50829000 |
| O | 3.73298500 | 2.50402000 | -0.03001300 |
| O | -2.58036600 | 1.75871200 | 0.16841000 |
| S | 6.27944300 | -2.80558200 | -0.49961600 |
| S | -7.21600700 | -1.86515700 | -0.34557300 |

| | | | |
|----|-------------|-------------|-------------|
| O | -7.22986600 | -2.25287300 | -1.78595800 |
| O | -8.41162500 | -1.05864300 | 0.03386600 |
| O | -6.98280800 | -3.02142800 | 0.56380900 |
| O | 7.23657400 | -2.66995400 | -1.63826000 |
| O | 5.19801200 | -3.79489700 | -0.77346800 |
| O | 6.98210300 | -3.05988800 | 0.79322700 |
| H | -1.35051700 | -1.40980100 | 0.31651700 |
| H | 1.62090200 | 0.95620400 | 1.21439500 |
| O | -0.16719800 | 3.03336300 | -0.20161000 |
| H | 0.55221200 | 3.24738900 | -0.86032600 |
| H | 2.63732500 | 2.79603900 | 1.28296200 |
| O | 1.91531800 | 2.77964600 | 1.95404700 |
| H | 1.15443300 | 3.16965900 | 1.50538400 |
| H | -0.98181300 | 3.46883200 | -0.48131600 |
| H | 2.69690100 | 3.22651500 | -1.10832600 |
| O | 1.95682700 | 3.67117600 | -1.60540300 |
| H | 2.08971900 | 3.47258100 | -2.53522800 |
| H | -0.63503500 | 1.57495600 | -3.02056700 |
| H | -0.71585700 | 0.91236300 | -2.67870300 |
| Pd | -0.69992200 | 1.04735300 | 0.31212100 |
| H | 1.66830900 | -0.47619300 | -1.35135300 |
| H | -2.43140000 | 0.12800900 | 2.55354400 |
| C | 6.48883100 | 2.35238300 | 2.45429200 |
| H | 6.42597200 | 3.11904800 | -0.32364000 |
| H | 6.13592100 | 2.82510600 | 1.37585000 |
| H | 7.53881500 | 2.08494700 | 0.58792000 |
| C | -4.61837400 | 2.54579600 | -1.52853700 |
| H | -4.54486500 | 3.41189400 | -0.86481800 |
| H | -3.73558800 | 2.57803700 | -2.17432300 |
| H | -5.50555600 | 2.66685900 | -2.15176800 |

62

RR-PhMe_ID2_TS2-square, E(SCF) = -
2563.92376176, E(ZPE) = -2563.454728, E(G)
= -2563.526804 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.07342300 | -1.15041000 | 1.50650300 |
| H | 0.02037500 | -0.43417100 | 2.32768300 |
| H | -0.22604700 | -2.14634200 | 1.93081900 |
| C | 1.13664200 | -1.09179900 | 0.61537400 |
| H | 2.04878200 | -1.35260200 | 1.15943900 |
| H | 1.03632200 | -1.78503300 | -0.22602900 |
| N | 1.22802200 | 0.27945400 | 0.06880300 |
| N | -1.24811300 | -0.74847600 | 0.69981200 |
| C | 2.27112100 | 0.43834100 | -0.97749800 |
| H | 2.15200900 | 1.44995800 | -1.37312800 |
| C | -2.46953200 | -0.45463800 | 1.48245500 |
| H | -2.66505900 | -1.29565700 | 2.15628400 |
| C | 3.65312300 | 0.23247800 | -0.44945800 |
| C | 4.22966900 | 1.25254100 | 0.35382400 |
| C | 4.34555800 | -0.93985900 | -0.72322600 |
| C | 5.54638500 | 1.02873100 | 0.85522000 |
| C | 5.61756600 | -1.13658000 | -0.22409400 |
| H | 3.88722500 | -1.71163700 | -1.33555400 |
| C | 6.20578500 | -0.14527500 | 0.56061700 |
| H | 7.20894900 | -0.30071200 | 0.95170300 |
| C | -3.65536900 | -0.22943200 | 0.60003000 |
| C | -3.62923200 | 0.75930900 | -0.40662200 |
| C | -4.80716700 | -0.97982500 | 0.80663800 |
| C | -4.80106400 | 0.98888300 | -1.17083400 |
| C | -5.94305500 | -0.74782800 | 0.05984400 |
| H | -4.82263900 | -1.74624700 | 1.57457400 |
| C | -5.93070900 | 0.23650700 | -0.92249300 |
| H | -6.82546900 | 0.41933400 | -1.51190700 |
| O | 3.59484400 | 2.34542700 | 0.63227500 |
| O | -2.58203300 | 1.51335500 | -0.66091300 |
| S | 6.54091700 | -2.62196700 | -0.59801600 |
| S | -7.42584300 | -1.72801600 | 0.30331200 |
| O | -7.58319400 | -2.54742200 | -0.93347300 |
| O | -8.53811100 | -0.75105000 | 0.47926200 |
| O | -7.17907500 | -2.55418800 | 1.51760900 |
| O | 7.70478200 | -2.19683700 | -1.43261000 |
| O | 5.60466200 | -3.52032100 | -1.33293300 |
| O | 6.97331200 | -3.18770000 | 0.71436500 |
| H | -1.46043400 | -1.48152600 | 0.02072100 |
| H | 1.44993700 | 0.91062600 | 0.85492200 |
| O | -0.06347900 | 3.31343800 | 0.27099200 |
| H | 0.68491500 | 3.73776200 | -0.21234700 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.34204200 | 2.34470800 | 1.87768100 |
| O | 1.50066400 | 2.17338900 | 2.35581100 |
| H | 0.84281700 | 2.69312700 | 1.86535800 |
| H | -0.82480400 | 3.89554700 | 0.19943900 |
| H | 2.83069700 | 3.45142100 | -0.36931600 |
| O | 2.25416200 | 4.12854500 | -0.81004000 |
| H | 2.45402300 | 4.08748800 | -1.74779200 |
| H | -0.20680400 | 2.27159100 | -1.97939400 |
| H | -0.30429000 | 1.59882600 | -2.33236000 |
| Pd | -0.69172300 | 0.89342600 | -0.39453700 |
| H | 2.03702000 | -0.27046500 | -1.77659400 |
| H | -2.23479400 | 0.42062900 | 2.09856800 |
| C | 6.17585100 | 2.08705200 | 1.69881100 |
| H | 6.21653100 | 3.04448600 | 1.17110900 |
| H | 5.59723100 | 2.26841800 | 2.60992000 |
| H | 7.19108900 | 1.80959600 | 1.98882900 |
| C | -4.78549600 | 2.04847900 | -2.22233200 |
| H | -4.55872900 | 3.03012000 | -1.79698700 |
| H | -4.01415500 | 1.85381800 | -2.97296300 |
| H | -5.75021700 | 2.10910300 | -2.72830800 |

62

RR-PhMe_ID2_TS2, E(SCF) = -2563.92148438,
E(ZPE) = -2563.453005, E(G) = -2563.525867
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.04724300 | 0.41909800 | 1.86612600 |
| H | 0.01972300 | -0.47616200 | 2.49334000 |
| H | 0.16123900 | 1.29495100 | 2.51083400 |
| C | -1.18869600 | 0.50257600 | 1.01569400 |
| H | -2.09079000 | 0.56923100 | 1.62968900 |
| H | -1.15722300 | 1.38571100 | 0.36870300 |
| N | -1.23803200 | -0.69695400 | 0.14835000 |
| N | 1.20576900 | 0.29481200 | 0.95521500 |
| C | -2.23955500 | -0.58983700 | -0.94702200 |
| H | -2.23677900 | -1.56011000 | -1.45089500 |
| C | 2.48815900 | -0.03856800 | 1.61279600 |
| H | 2.65643400 | 0.66969800 | 2.43134800 |
| C | -3.60870900 | -0.22356100 | -0.46994000 |
| C | -4.34812300 | -1.16574900 | 0.28965200 |
| C | -4.12709900 | 1.03603000 | -0.74038700 |
| C | -5.64187500 | -0.77752500 | 0.74717000 |
| C | -5.38209900 | 1.39294900 | -0.28891200 |
| H | -3.54447100 | 1.75159400 | -1.31359300 |
| C | -6.12720200 | 0.47935400 | 0.45504700 |
| H | -7.11437700 | 0.76246600 | 0.81382300 |
| C | 3.62900300 | 0.01917000 | 0.64936200 |
| C | 3.61437000 | -0.76924300 | -0.52077500 |
| C | 4.71881200 | 0.83576000 | 0.92553500 |
| C | 4.74070100 | -0.73590800 | -1.38118700 |
| C | 5.80775500 | 0.86475500 | 0.08007700 |
| H | 4.72149200 | 1.45235400 | 1.81852100 |
| C | 5.81279000 | 0.07212500 | -1.06222100 |
| H | 6.67223400 | 0.09598700 | -1.72743500 |
| O | -3.87469500 | -2.33771300 | 0.57323800 |
| O | 2.61953600 | -1.56587100 | -0.84511800 |
| S | -6.06446200 | 3.01226200 | -0.62184300 |
| S | 7.22557200 | 1.90658800 | 0.42852200 |
| O | 8.38104200 | 0.97997900 | 0.60435400 |
| O | 6.89057900 | 2.66002300 | 1.66873300 |
| O | 7.38583700 | 2.78894200 | -0.76305400 |
| O | -7.31437900 | 2.78869200 | -1.40827100 |
| O | -5.02448000 | 3.75301200 | -1.39201200 |
| O | -6.34556600 | 3.62785700 | 0.70954000 |
| H | 2.36019100 | -1.03473500 | 2.05026200 |
| H | -1.86376300 | 0.15997100 | -1.64934700 |
| H | 1.32200500 | 1.16685700 | 0.43567100 |
| H | -1.48407000 | -1.49168800 | 0.75522900 |
| O | 0.18440100 | -3.66847100 | -0.32885500 |
| H | -0.76829300 | -3.88166700 | -0.45687700 |
| H | -2.78924000 | -2.46925400 | 1.91377100 |
| O | -1.97796100 | -2.35769500 | 2.46270700 |
| H | -1.68288100 | -3.24536000 | -2.67789000 |
| H | 0.40241800 | -3.95466900 | 0.56159000 |
| H | -3.03273100 | -3.44932100 | -0.33731800 |
| O | -2.46026200 | -4.15332500 | -0.73835800 |
| H | -2.77011800 | -4.27475300 | -1.63824500 |
| H | 0.31577900 | -2.28876300 | -2.13970900 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.23135300 | -1.59232300 | -2.44803900 |
| Pd | 0.70292100 | -1.13168800 | -0.42976500 |
| C | 4.73881900 | -1.57907700 | -2.61337800 |
| H | 4.63847900 | -2.64098000 | -2.37240900 |
| H | 3.89467300 | -1.33065100 | -3.26295100 |
| H | 5.66089400 | -1.44216800 | -3.18021100 |
| C | -6.43501400 | -1.75385300 | 1.55125500 |
| H | -6.60275500 | -2.68378500 | 0.99967000 |
| H | -5.90797300 | -2.03639500 | 2.46806500 |
| H | -7.40584100 | -1.33940500 | 1.82942200 |

62

RR-PhMe_ID2_TS3_P, E(SCF) = -2563.96233868,
E(ZPE) = -2563.488333, E(G) = -2563.560497
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.05704300 | 0.65668700 | 1.66857300 |
| H | 0.03071600 | -0.20031900 | 2.34972000 |
| H | 0.10456400 | 1.56434100 | 2.27996800 |
| C | -1.17442200 | 0.66064500 | 0.79680700 |
| H | -2.07735400 | 0.80117200 | 1.39940200 |
| H | -1.12457400 | 1.48037400 | 0.07217700 |
| N | -1.24786600 | -0.61284200 | 0.03737100 |
| N | 1.24158400 | 0.50827600 | 0.81322400 |
| C | -2.26781100 | -0.59143100 | -1.04199900 |
| H | -2.22551300 | -1.56769900 | -1.52609400 |
| C | 2.47301300 | 0.10799600 | 1.50692800 |
| H | 2.68865200 | 0.79163800 | 2.33802700 |
| C | -3.64609500 | -0.25189300 | -0.55502100 |
| C | -4.41256400 | -1.16462200 | 0.17236200 |
| C | -4.15717400 | 1.02515300 | -0.77018900 |
| C | -5.65078800 | -0.80024700 | 0.71825700 |
| C | -5.38254300 | 1.38909700 | -0.25526200 |
| H | -3.58019500 | 1.74871000 | -1.33707400 |
| C | -6.11815900 | 0.48249200 | 0.49409700 |
| H | -7.07994300 | 0.77553100 | 0.90498100 |
| C | 3.64167700 | 0.07361900 | 0.57000700 |
| C | 3.64633600 | -0.75360200 | -0.58121300 |
| C | 4.75563900 | 0.84848200 | 0.87396700 |
| C | 4.82654600 | -0.78402900 | -1.37674400 |
| C | 5.88744500 | 0.81625800 | 0.08677800 |
| H | 4.74070000 | 1.48491900 | 1.75328100 |
| C | 5.91314100 | -0.00774700 | -1.03349200 |
| H | 6.80363700 | -0.03689900 | -1.65678500 |
| O | -3.99243600 | -2.43064200 | 0.43858000 |
| O | 2.65603200 | -1.52512200 | -0.95539200 |
| S | -6.05457600 | 3.03369400 | -0.54452900 |
| S | 7.32435000 | 1.81022500 | 0.47649700 |
| O | 8.44808400 | 0.85050200 | 0.68733100 |
| O | 6.98177700 | 2.57789700 | 1.70730700 |
| O | 7.55329500 | 2.68911100 | -0.70826000 |
| O | -4.99875000 | 3.78073600 | -1.27961400 |
| O | -6.33826800 | 3.59281400 | 0.80645300 |
| O | -7.29127000 | 2.82268200 | -1.34805000 |
| H | 2.27684800 | -0.88056700 | 1.94196800 |
| H | -1.94050000 | 0.14442500 | -1.77997700 |
| H | 1.41166900 | 1.37457400 | 0.30577200 |
| H | -1.50060800 | -1.33403400 | 0.72041400 |
| O | -0.35754600 | -4.07900800 | 0.75626300 |
| H | -1.66723100 | -4.17689300 | -0.48258400 |
| H | -2.87376200 | -2.51570700 | -2.00838100 |
| O | -1.96706200 | -2.39685200 | 2.33877900 |
| H | -2.03066700 | -2.17037200 | 3.26999700 |
| H | -0.79553800 | -3.59912400 | 1.48226400 |
| H | -3.44481800 | -2.85108300 | -0.26755900 |
| O | -2.46572100 | -4.05508700 | -1.04092300 |
| H | -2.15452500 | -4.02122100 | -1.94885100 |
| H | 0.19739900 | -3.40430500 | 0.32944500 |
| H | 0.23596900 | -2.27969900 | -1.45057800 |
| Pd | 0.70357400 | -1.09109400 | -0.53319700 |
| C | 4.85855800 | -1.66422900 | -2.58286800 |
| H | 4.72144300 | -2.71639500 | -2.31687500 |
| H | 4.05092200 | -1.41785500 | -3.27795300 |
| H | 5.80904600 | -1.56726000 | -3.11064100 |
| C | -6.43632000 | -1.78725600 | 1.51774900 |
| H | -6.65480000 | -2.68686200 | 0.93724700 |
| H | -5.88422200 | -2.11376800 | 2.40328800 |
| H | -7.38032400 | -1.35274400 | 1.84784300 |

62
RR-PhMe_ID2_TS3-square P, E(SCF) = -
2563.96126589, E(ZPE) = -2563.487425, E(G)
= -2563.560235 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.04266600 | -0.74437900 | 1.65077100 |
| H | -0.00863100 | 0.09128900 | 2.35731900 |
| H | -0.09267500 | -1.67103100 | 2.23272300 |
| C | 1.18353900 | -0.72618500 | 0.77196300 |
| H | 2.08971000 | -0.89232000 | 1.36300000 |
| H | 1.12328900 | -1.52195300 | 0.02151900 |
| N | 1.25843200 | 0.57108500 | 0.05564200 |
| N | -1.23019000 | -0.56477500 | 0.80434900 |
| C | 2.27859900 | 0.58481100 | -1.02285700 |
| H | 2.22203900 | 1.56917200 | -1.48908400 |
| C | -2.46049600 | -0.19184800 | 1.51569100 |
| H | -2.67431700 | -0.90890400 | 2.31853600 |
| C | 3.66180700 | 0.25756900 | -0.54062800 |
| C | 4.42943600 | 1.18058900 | 0.17391900 |
| C | 4.18010500 | -1.01725500 | -0.75385200 |
| C | 5.67641400 | 0.82522000 | 0.70869900 |
| C | 5.41205100 | -1.37159500 | -0.24882100 |
| H | 3.60376800 | -1.74670600 | -1.31384100 |
| C | 6.14932000 | -0.45541300 | 0.48779600 |
| H | 7.11757000 | -0.73940300 | 0.88985700 |
| C | -3.63108700 | -0.11774600 | 0.58328900 |
| C | -3.63571400 | 0.75608600 | -0.53292400 |
| C | -4.74788300 | -0.89946200 | 0.85800300 |
| C | -4.81668500 | 0.82409900 | -1.32425700 |
| C | -5.88169700 | -0.82910000 | 0.07587800 |
| H | -4.73450000 | -1.57020200 | 1.71134900 |
| C | -5.90595500 | 0.03899900 | -1.01074600 |
| H | -6.79795100 | 0.09977700 | -1.62957100 |
| O | 4.01384900 | 2.44672200 | 0.43207100 |
| O | -2.64351300 | 1.53980400 | -0.87639500 |
| S | 6.09152100 | -3.01277900 | -0.53597900 |
| S | -7.31875500 | -1.83865200 | 0.42288400 |
| O | -7.51566700 | -2.70524300 | -0.77679200 |
| O | -8.45393600 | -0.88995400 | 0.62089400 |
| O | -6.99628100 | -2.61851100 | 1.65133900 |
| O | 7.32695100 | -2.79805900 | -1.34081400 |
| O | 5.03893900 | -3.76656000 | -1.26921300 |
| O | 6.37920800 | -3.56924700 | 0.81545100 |
| H | -1.40107300 | -1.41253800 | 0.26651500 |
| H | 1.50925500 | 1.27455100 | 0.76388600 |
| O | 0.21641000 | 4.07054000 | 0.71744500 |
| H | 1.60887800 | 4.21767300 | -0.46642100 |
| H | 2.73502500 | 2.59748800 | 1.97483800 |
| O | 1.85264300 | 2.39809700 | 2.32159700 |
| H | 1.28319500 | 3.10558600 | 1.97314000 |
| H | -0.39539700 | 4.77946900 | 0.93684300 |
| H | 3.42186800 | 2.84369300 | -0.24821500 |
| O | 2.41523100 | 4.05922100 | -0.99418400 |
| H | 2.13021200 | 4.04229300 | -1.91130100 |
| H | -0.30499700 | 3.38672100 | 0.25379600 |
| H | -0.21968400 | 2.28457600 | -1.37731300 |
| Pd | -0.69201200 | 1.07290600 | -0.48869600 |
| H | 1.96411000 | -0.14145100 | -1.77604200 |
| H | -2.26255900 | 0.77793400 | 1.99020100 |
| C | 6.46690500 | 1.82307700 | 1.48966600 |
| H | 6.67556200 | 2.71751200 | 0.89755100 |
| H | 5.92396400 | 2.15686800 | 2.37787100 |
| H | 7.41642600 | 1.39536900 | 1.81295200 |
| C | -4.84717300 | 1.75352900 | -2.49282500 |
| H | -4.71404000 | 2.79410400 | -2.18273500 |
| H | -4.03623800 | 1.53862200 | -3.19441800 |
| H | -5.79580100 | 1.67642400 | -3.02713400 |

62
RR-PhMe_ID2_TS3-square, E(SCF) = -
2563.91985396, E(ZPE) = -2563.451390, E(G)
= -2563.523017 a.u.

| | | | |
|---|-------------|-------------|------------|
| C | -0.09591100 | -0.93200000 | 1.61619900 |
| H | -0.02784900 | -0.16787200 | 2.39698700 |
| H | -0.21435500 | -1.90585400 | 2.10020400 |
| C | 1.12572100 | -0.88868100 | 0.73829500 |
| H | 2.03170800 | -1.12214100 | 1.30451300 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.04249300 | -1.61827800 | -0.07439600 |
| N | 1.22054800 | 0.45948100 | 0.13286300 |
| N | -1.26845400 | -0.61051700 | 0.77898100 |
| C | 2.26690300 | 0.55685800 | -0.92131300 |
| H | 2.22687500 | 1.58093600 | -1.29890200 |
| C | -2.50326900 | -0.30900900 | 1.52856100 |
| H | -2.69734800 | -1.10932800 | 2.25165000 |
| C | 3.63795300 | 0.21753000 | -0.43175000 |
| C | 4.34724000 | 1.16365700 | 0.35184900 |
| C | 4.19836800 | -1.01818900 | -0.73099500 |
| C | 5.65046100 | 0.80366100 | 0.80471500 |
| C | 5.45908400 | -1.35029000 | -0.27856900 |
| H | 3.64267500 | -1.73336000 | -1.33075900 |
| C | 6.17337100 | -0.43272400 | 0.48969500 |
| H | 7.16775900 | -0.64882600 | 0.84489900 |
| C | -3.67556100 | -0.15960800 | 0.61150200 |
| C | -3.65808500 | 0.77933000 | -0.44477300 |
| C | -4.80814000 | -0.93423000 | 0.83632700 |
| C | 4.82624500 | 0.92303600 | -1.24030400 |
| C | -5.93602700 | -0.78536700 | 0.05714800 |
| H | -4.81305400 | -1.65753200 | 1.64526200 |
| C | -5.93450400 | 0.14527800 | -0.97685100 |
| H | -6.82111800 | 0.26306700 | -1.59482300 |
| O | 3.84496300 | 2.32135700 | 0.65644200 |
| O | -2.64199100 | 1.56279900 | -0.72490000 |
| S | 6.18014100 | -2.94986400 | -0.62733300 |
| S | -7.39376100 | -1.79098500 | 0.33254200 |
| O | -7.55009400 | -2.63541600 | -0.88809600 |
| O | -8.52672300 | -0.83590900 | 0.50440600 |
| O | -7.12001300 | -2.59233900 | 1.55829300 |
| O | 7.49209100 | -2.68343000 | -1.28845400 |
| O | 5.21661400 | -3.65604700 | -1.51961600 |
| O | 6.34750200 | -3.62890600 | 0.69249800 |
| H | -1.45327900 | -1.38802900 | 0.14420300 |
| H | 1.45350200 | 1.11899600 | 0.89031900 |
| O | 0.46072300 | 3.96062900 | -0.05903400 |
| H | 1.39965600 | 4.16627000 | -0.41485300 |
| H | 2.54827100 | 2.49098600 | 1.80162500 |
| O | 1.68426600 | 4.34660400 | 2.27321700 |
| H | 1.13693500 | 3.11734400 | 1.86393900 |
| H | -0.10439200 | 4.73482300 | -0.17101900 |
| H | 3.34122300 | 3.50081400 | -0.32754600 |
| O | 2.88014400 | 4.26749700 | -0.77691200 |
| H | 3.11815000 | 4.24108600 | -1.70659900 |
| H | 0.00570100 | 2.98486200 | -0.66297900 |
| H | -0.25183100 | 2.27749400 | -1.36911800 |
| Pd | -0.71367800 | 1.03331100 | -0.36951300 |
| H | 1.96426600 | -0.11033500 | -1.73317600 |
| H | -2.30359000 | 0.60743400 | 2.09644800 |
| C | 6.42087400 | 1.78890100 | 1.62032100 |
| H | 6.56389800 | 2.72948300 | 1.08000100 |
| H | 5.89154700 | 2.04665100 | 2.54266800 |
| H | 7.40305900 | 1.39535100 | 1.88884100 |
| C | -4.82677200 | 1.92050900 | -2.35123500 |
| H | -4.67996900 | 2.93790100 | -1.97736900 |
| H | -4.01113800 | 1.73251000 | -3.05497800 |
| H | -5.76997800 | 1.89233000 | -2.89938100 |

62
RR-PhMe_ID2_TS3, E(SCF) = -2563.91978274,
E(ZPE) = -2563.451447, E(G) = -2563.523121
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.08001300 | -0.44996200 | 1.82598500 |
| H | -0.05760100 | 0.44070800 | 2.46052000 |
| H | -0.17990500 | -1.32898000 | 2.46932700 |
| C | 1.16435000 | -0.51624400 | 0.98320000 |
| H | 2.05849900 | -0.60116100 | 1.60711800 |
| H | 1.13714500 | -1.38555600 | 0.31732500 |
| N | 1.23281900 | 0.70187600 | 0.14108700 |
| N | -1.23761200 | -0.32567200 | 0.91863600 |
| C | 2.26982900 | 0.62340200 | -0.92574400 |
| H | 2.29923800 | 1.61243000 | -1.39138200 |
| C | -2.50638100 | 0.04724400 | 1.57283900 |
| H | -2.69429400 | -0.62650100 | 2.41632000 |
| C | 3.61751000 | 0.21224000 | -0.42537700 |
| C | 4.34446900 | 1.09555400 | 0.41129500 |
| C | 4.12901500 | -1.03633800 | -0.75348600 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|--------------|
| C | 5.61223100 | 0.66001400 | 0.89448100 | H | 5.00217600 | -1.74689000 | 0.03768900 |
| C | 5.36196000 | -1.43949700 | -0.28043100 | C | 4.82002000 | 1.53679200 | -0.69553600 |
| H | 3.55773700 | -1.70450700 | -1.39133600 | H | 5.46452500 | 2.39740400 | -0.85298100 |
| C | 6.08994600 | -0.58620900 | 0.54667500 | O | -1.69683900 | 0.74298200 | 1.84212300 |
| H | 7.05919300 | -0.90625600 | 0.92285400 | O | 1.30402900 | 0.81638700 | -0.72442700 |
| C | -3.65136200 | -0.01293600 | 0.61234800 | S | -6.86079700 | 0.19423900 | -0.96483500 |
| C | -3.63370200 | 0.73453700 | -0.58663900 | S | 7.16195400 | 0.15895200 | -0.24309500 |
| C | -4.75558300 | -0.79486700 | 0.93025900 | O | 7.54010400 | 1.01086400 | 0.92100600 |
| C | -4.77598800 | 0.68593600 | -1.42933500 | O | 7.72166100 | 0.67199200 | -1.52598200 |
| C | -5.85853700 | -0.83463200 | 0.10363400 | O | 7.44390500 | -1.28613300 | -0.02093200 |
| H | -4.75835900 | -1.37304900 | 1.84873500 | O | -7.07931300 | -1.25994600 | -1.21211900 |
| C | -5.85823500 | -0.09155100 | -1.07181200 | O | -6.70140000 | 0.97580300 | -2.22795600 |
| H | -6.72541000 | -0.12127100 | -1.72680500 | O | -7.89614000 | 0.79008500 | -0.06885500 |
| O | 3.88066500 | 2.26155100 | 0.74214200 | H | -0.44177200 | 2.00311000 | 1.61821900 |
| O | -2.63954700 | 1.50710300 | -0.96278700 | H | -1.04570400 | 0.25035100 | -1.76862700 |
| S | 6.03348100 | -3.04734500 | -0.68647300 | H | -1.37324500 | 0.56809700 | -1.09535000 |
| S | -7.27060900 | -1.86694500 | 0.49336700 | O | 0.44211600 | 2.41522100 | 1.50017700 |
| O | -8.46544000 | -0.97748000 | 0.41671900 | H | 0.75180800 | 2.02091200 | 0.66707700 |
| O | -7.02903400 | -2.39905400 | 1.86381900 | H | -0.26634600 | -0.01785600 | 2.62923500 |
| O | -7.29673500 | -2.93689300 | -0.54690600 | O | 0.67706600 | -0.10093200 | 2.88853400 |
| O | 5.04676800 | -3.69488000 | -1.59774300 | H | 1.00102900 | 0.78063600 | 2.63999000 |
| O | 6.18643300 | -3.77577800 | 0.60827200 | H | -2.07902100 | -2.19864900 | -0.95853100 |
| O | 7.35028400 | -2.79725800 | -1.34471900 | H | -1.85533100 | -1.75287800 | -1.92820400 |
| H | -2.35997100 | 1.05461500 | 1.97993300 | H | 1.30790900 | -1.18646100 | 1.48119300 |
| H | 1.90514600 | -0.08654000 | -1.67306800 | H | 2.99178500 | -2.67338800 | 0.37847100 |
| H | -1.37272200 | -1.20677900 | 0.42133200 | Pd | -0.13421500 | -0.56570500 | -0.46015900 |
| H | 1.46236100 | 4.147978100 | 0.77355900 | C | -3.19135400 | 3.08573200 | 1.43058300 |
| O | 0.22955300 | 4.13425100 | -0.67982700 | H | -2.94789200 | 3.09046600 | 2.49732500 |
| H | 1.23891800 | 4.20375000 | -0.64298000 | H | -2.27536000 | 3.38179600 | 0.90808900 |
| H | 2.70842100 | 2.43676700 | 1.99740400 | H | -3.94727500 | 3.85103700 | 1.24496200 |
| O | 1.85266000 | 2.38865100 | 2.48392400 | C | 2.85677400 | 3.02169100 | -1.13864600 |
| H | 1.60075500 | 3.29754500 | 2.66192000 | H | 2.21412600 | 2.95845400 | -2.02061600 |
| H | -0.11212500 | 4.24494500 | 0.21591700 | H | 2.23165800 | 3.40475600 | -0.32649700 |
| H | 3.25477700 | 3.45210300 | -0.17265400 | H | 3.63821400 | 3.75741700 | -1.33370600 |
| O | 2.81373700 | 4.23568000 | -0.60738800 | | | | |
| H | 3.25917800 | 4.37632400 | -1.44584600 | 59 | | | |
| H | -0.09206000 | 2.97719200 | -1.10189700 | RR-PhMe_EI_D1_TS1_R, E(SCF) = - | | | |
| H | -0.25221000 | 2.17658600 | -1.68465200 | 2487.50244943, E(ZPE) = -2487.057016, E(G) | | | |
| Pd | -0.70683800 | 1.11564000 | -0.48105400 | = -2487.127333 a.u. | | | |
| C | -4.77696800 | 1.48238600 | -2.69234000 | C | 0.57386800 | -3.15298800 | 1.00885800 |
| H | -4.65546600 | 2.55090200 | -2.49316300 | H | 1.22803100 | -4.02978400 | 1.02146400 |
| H | -3.94592500 | 1.19640400 | -3.34339800 | H | 0.09024800 | -3.08151600 | 1.98470200 |
| H | -5.70896600 | 1.34039500 | -3.24193400 | C | -0.45862200 | -3.27041300 | -0.08157600 |
| C | 6.39159400 | 1.57592500 | 1.77929300 | H | 0.01897400 | -3.45750200 | -1.04512100 |
| H | 6.60005100 | 2.52865800 | 1.28313400 | H | -1.13787600 | -4.10361500 | 0.11837500 |
| H | 5.83409100 | 1.82361300 | 2.68795300 | N | -1.22025000 | -2.00035600 | -0.21798600 |
| H | 7.34210700 | 1.12649000 | 2.07277800 | N | 1.37174500 | -1.91020500 | 0.83998800 |
| | | | | C | -2.42287500 | -1.83156400 | 0.61903400 |
| 59 | | | | H | -3.02977700 | -2.74260200 | 0.57211100 |
| RR-PhMe_EI_D1_TS1_P, E(SCF) = - | | | | C | 2.51143000 | -1.95625100 | -0.08743400 |
| 2487.49195511, E(ZPE) = -2487.045278, E(G) | | | | H | 2.11719300 | -2.12456700 | -1.09573900 |
| = -2487.111983 a.u. | | | | C | -3.24437900 | -0.66814700 | -0.13555800 |
| C | 0.43719600 | -2.99476000 | 1.01852000 | C | -2.69031000 | 0.57656300 | -0.24763400 |
| H | 1.15123500 | -3.81929200 | 1.07565700 | C | -4.62382000 | -0.85426500 | 0.07912200 |
| H | 0.03775200 | -2.83957500 | 2.02255900 | C | -3.57416000 | 1.60218800 | -0.67973900 |
| C | -0.66278700 | -3.30011400 | 0.03946500 | C | -5.46846800 | 0.15117300 | -0.33167900 |
| H | -0.24923800 | -3.54234700 | -0.94176800 | H | -5.04524100 | -1.81341900 | 0.36200300 |
| H | -1.26876300 | -4.14815600 | 0.37349900 | C | -4.93377400 | 1.37719500 | -0.70826300 |
| N | -1.50989100 | -2.08810800 | -0.12030100 | H | -5.59317700 | 2.17399400 | -1.04220400 |
| N | 1.13526700 | -1.74196000 | 0.62527600 | C | 3.34191700 | -0.70223300 | -0.101385700 |
| C | -2.45231000 | -1.85994700 | 1.02108900 | C | 2.83207500 | 0.59052500 | 0.25977100 |
| H | -3.06171400 | -2.76638200 | 1.11262200 | C | 4.70329600 | -0.87017700 | -0.26000100 |
| C | 2.37559200 | -1.93502300 | -0.14523500 | C | 3.75087200 | 1.67826800 | 0.27600600 |
| H | 2.09974700 | -2.37769500 | -1.11018000 | C | 5.57485600 | 0.19338100 | -0.25400000 |
| C | -3.30283900 | -0.65887500 | 0.80577600 | H | 5.09010200 | -1.86478400 | -0.45861900 |
| C | -2.83081100 | 0.60799200 | 1.24857800 | C | 5.08746800 | 1.46583000 | 0.01847800 |
| C | -4.51904300 | -0.78216500 | 0.14566100 | H | 5.76911600 | 2.31213800 | 0.03679100 |
| C | -3.66322800 | 1.74076800 | 0.98612700 | O | -1.40215700 | 0.87661200 | -0.23247700 |
| C | -5.30488700 | 0.32647700 | -0.09579100 | O | 1.57053800 | 0.88462200 | 0.52787300 |
| H | -4.86125300 | -1.76024500 | -0.18234600 | S | -7.24545600 | -0.08643400 | -0.37631100 |
| C | -4.86321000 | 1.57997600 | 0.32882600 | S | 7.32328900 | -0.03244500 | -0.57859400 |
| H | -5.48136100 | 2.45440600 | 0.13796500 | O | 8.03398500 | 0.48490000 | 0.62642600 |
| C | 3.17344200 | -0.67453900 | -0.30778000 | O | 7.62032700 | 0.77331200 | -1.79837100 |
| C | 2.60133900 | 0.57767400 | -0.60361800 | O | 7.52023100 | -1.49434800 | -0.78603600 |
| C | 4.55811000 | -0.78548200 | -0.19916700 | O | -7.47986900 | -1.51590700 | -0.03045500 |
| C | 3.45459500 | 1.69396700 | -0.80348500 | O | -7.66961400 | 0.25457400 | -1.76466600 |
| C | 5.37982500 | 0.30021000 | -0.39792000 | O | -7.80668600 | 0.85621600 | 0.63414800 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.67612800 | 2.52455400 | 0.19322200 |
| H | -1.02204100 | -0.21687700 | -3.18561000 |
| H | -1.43323700 | 0.21807400 | -2.73429000 |
| O | -0.08704400 | 3.09587600 | 0.72017800 |
| H | 0.70678600 | 2.53227500 | 0.76115400 |
| H | -1.61939300 | 1.01007400 | 2.15037500 |
| O | -1.48703400 | 1.73654900 | 2.77074100 |
| H | -0.98187000 | 2.36966200 | 2.22887500 |
| H | -1.50955100 | -1.90566200 | -1.19075100 |
| H | -2.09459900 | -1.71533600 | 1.65828200 |
| H | 1.72194600 | -1.62759300 | 1.75389000 |
| H | 3.14026200 | -2.81903100 | 0.16105500 |
| Pd | 0.07641200 | -0.47729800 | 0.20776400 |
| C | -3.01355000 | 2.92866400 | -1.07614200 |
| H | -2.61108800 | 3.46655700 | -0.21114500 |
| H | -2.19383700 | 2.82213700 | -1.79208300 |
| H | -3.78439300 | 3.55723200 | -1.52394600 |
| C | 3.25071700 | 3.05443700 | 0.56998000 |
| H | 2.50511100 | 3.37839700 | -0.16194100 |
| H | 2.77269600 | 3.10966100 | 1.55303000 |
| H | 4.07032600 | 3.77406900 | 0.55565400 |

59

RR-PhMe_EI_D1_TS1, E(SCF) = -2487.48355521,
E(ZPE) = -2487.039055, E(G) = -2487.106827
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.43200800 | -2.93694000 | 1.27076700 |
| H | 1.08062100 | -3.80979400 | 1.38526000 |
| H | -0.09150400 | -2.78618700 | 2.21689500 |
| C | -0.54230800 | -3.13483800 | 0.14057000 |
| H | -0.01154500 | -3.33276100 | -0.79286300 |
| H | -1.20175500 | -3.98528800 | 0.33834400 |
| N | -1.33796700 | -1.89505900 | -0.06127400 |
| N | 1.24672300 | -1.71781200 | 1.02860500 |
| C | -2.49295900 | -1.74022700 | 0.87226500 |
| H | -3.05970500 | -2.67791800 | 0.86772300 |
| C | 2.49630200 | -1.92408900 | 0.29527700 |
| H | 2.24260200 | -2.41744600 | -0.64983100 |
| C | -3.37417400 | -0.60586000 | 0.46628100 |
| C | -2.89892100 | 0.72225700 | 0.59133500 |
| C | -4.64360800 | -0.85638900 | -0.03792900 |
| C | -3.75000300 | 1.78306800 | 0.18002700 |
| C | -5.46524200 | 0.18676600 | -0.41767200 |
| H | -5.00246700 | -1.87719900 | -0.12719100 |
| C | -5.00753500 | 1.49757000 | -0.31136600 |
| H | -5.65268900 | 2.31622200 | -0.62159300 |
| C | 3.29385300 | -0.67078000 | 0.04694100 |
| C | 2.77636000 | 0.64109000 | 0.04350700 |
| C | 4.64434600 | -0.87123700 | -0.23628100 |
| C | 3.65317400 | 1.72046800 | -0.24776700 |
| C | 5.48273700 | 0.17967500 | -0.52470300 |
| H | 5.04612300 | -1.87975100 | -0.23025700 |
| C | 4.98096900 | 1.47649000 | -0.52007600 |
| H | 5.64000500 | 2.31206700 | -0.73981600 |
| O | -1.70800900 | 0.97238900 | 1.05411900 |
| O | 1.52449100 | 0.97300000 | 0.31914000 |
| S | -7.10436700 | -0.11595100 | -1.07320400 |
| S | 7.22171300 | -0.08648100 | -0.87582200 |
| O | 7.96740200 | 0.64397600 | 0.18916300 |
| O | 7.45547300 | 0.49304800 | -2.22971300 |
| O | 7.43356000 | -1.55957200 | -0.82754700 |
| O | -7.31876700 | -1.58842200 | -0.99035400 |
| O | -7.09068100 | 0.38789700 | -2.47828600 |
| O | -8.04445300 | 0.65604400 | -0.20914000 |
| H | -0.68395500 | 2.38508600 | 1.62792200 |
| H | -0.54805600 | 0.58068100 | -1.82034400 |
| H | -0.98183600 | 1.01238500 | -1.36408900 |
| O | 0.15256500 | 2.80455700 | 1.90750900 |
| H | 0.79649000 | 2.34785900 | 1.33869700 |
| H | -0.77397900 | 0.25072200 | 2.57965800 |
| O | -0.03191800 | 0.10869500 | 3.19791100 |
| H | 0.40753100 | 0.96955200 | 3.14302200 |
| H | -1.72021900 | -1.91016100 | -1.00585900 |
| H | -2.08515900 | -1.60217300 | 1.87723000 |
| H | 1.41719500 | -1.24746600 | 1.92156300 |
| H | 3.11688000 | -2.62959100 | 0.86213400 |
| Pd | 0.04027700 | -0.35449000 | 0.08232800 |

| | | | |
|---|-------------|------------|-------------|
| C | -3.24867600 | 3.18467500 | 0.29463600 |
| H | -3.00191600 | 3.43688000 | 1.33091000 |
| H | -2.32806400 | 3.32706100 | -0.28133300 |
| H | -3.99059100 | 3.90018200 | -0.06371400 |
| C | 3.11148600 | 3.11204000 | -0.23257400 |
| H | 2.21038500 | 3.19521200 | -0.84599700 |
| H | 2.82690600 | 3.41973100 | 0.77867300 |
| H | 3.85295800 | 3.82229100 | -0.60099600 |

59

RR-PhMe_EI_D1_TS2_P, E(SCF) = -
2487.51628803, E(ZPE) = -2487.068354, E(G)
= -2487.138860 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.42072400 | -2.43345100 | 1.54407300 |
| H | 0.98948800 | -3.33638300 | 1.79345500 |
| H | -0.03416200 | -2.06951600 | 2.46853800 |
| C | -0.65223700 | -2.77160200 | 0.53463600 |
| H | -0.21078200 | -3.18471100 | -0.37474800 |
| H | -1.33431100 | -3.52385700 | 0.94533200 |
| N | -1.41021100 | -1.55441400 | 0.13945000 |
| N | 1.30140800 | -1.36819300 | 1.03596900 |
| C | -2.39134800 | -1.12172300 | 1.17340300 |
| H | -2.01948100 | -2.01948100 | 1.58878600 |
| C | 2.41342400 | -1.81095700 | 0.18244400 |
| H | 1.97989400 | -2.25492300 | -0.72323800 |
| C | -3.45619400 | -0.22877400 | 0.61597300 |
| C | -3.31957200 | 1.15842000 | 0.57331200 |
| C | -4.64460200 | -0.79722000 | 0.16355000 |
| C | -4.36431600 | 1.98191300 | 0.13998600 |
| C | -5.67302000 | 0.00171100 | -0.28743500 |
| H | -4.77411300 | -1.87461300 | 0.18495300 |
| C | -5.53672700 | 1.38234500 | -0.28604500 |
| H | -6.35585300 | 2.00557600 | -0.63295900 |
| C | 3.35779200 | -0.69125400 | -0.16256200 |
| C | 2.94696200 | 0.59311800 | -0.59167500 |
| C | 4.71921000 | -0.97879300 | -0.07978200 |
| C | 3.94654800 | 1.54034000 | -0.94670900 |
| C | 5.67691300 | -0.05246200 | -0.42654100 |
| H | 5.03682600 | -1.95905400 | 0.26141000 |
| C | 5.28079300 | 1.20763900 | -0.85786300 |
| H | 6.03079200 | 1.94479400 | -1.13240500 |
| O | -2.18216800 | 1.77821800 | 1.00416700 |
| O | 1.69905100 | 1.01962000 | -0.68973800 |
| S | -7.22543200 | -0.71999300 | -0.84776800 |
| S | 7.42509000 | -0.42753600 | -0.30466400 |
| O | 7.98893700 | -0.20654100 | -1.66804100 |
| O | 7.51565400 | -1.84714800 | -1.37875000 |
| O | 7.98149600 | 0.52881400 | 0.69627300 |
| O | -7.03018700 | -2.19353300 | -0.79762200 |
| O | -7.43124000 | -0.20069900 | -2.22797800 |
| O | -8.25718600 | -0.23140700 | 0.10882700 |
| H | 1.24229800 | 3.31410900 | 1.58281200 |
| H | -0.80414100 | 0.57783500 | -1.35082500 |
| H | -1.40239400 | 1.32559200 | 0.62160600 |
| O | 1.37870100 | 2.37174500 | 1.70784100 |
| H | 1.44467500 | 1.99245900 | 0.80649800 |
| H | -1.35586700 | 1.47000300 | 2.89573100 |
| O | -0.56910200 | 1.18882700 | 3.37890500 |
| H | 0.15654400 | 1.56681600 | 2.84786600 |
| H | -1.93336600 | -1.76998800 | -0.70670000 |
| H | -1.83959300 | -0.63317400 | 1.97972100 |
| H | 1.68017700 | -0.83730300 | 1.81513900 |
| H | 2.97660600 | -2.60860200 | 0.68319900 |
| Pd | 0.08865600 | -0.18112600 | -0.31166500 |
| C | 3.52375600 | 2.89439600 | -1.41510300 |
| H | 2.86445700 | 2.82886500 | -2.28479900 |
| H | 2.96170700 | 3.43129600 | -0.64504500 |
| H | 4.39123000 | 3.49944300 | -1.68356000 |
| C | -4.19435900 | 3.46542100 | 0.12934000 |
| H | -3.99586800 | 3.85239100 | 1.13189500 |
| H | -3.34530900 | 3.76036200 | -0.49223900 |
| H | -5.08972000 | 3.95468300 | -0.25496100 |

59

RR-PhMe_EI_D1_TS2_R, E(SCF) = -
2487.49194339, E(ZPE) = -2487.045208, E(G)
= -2487.114394 a.u.

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 0.43855300 | -3.00240800 | 1.01040800 | C | -3.15750400 | 0.99394900 | 0.50757900 |
| H | 1.15367200 | -3.82634500 | 1.06198400 | C | -4.71191300 | -0.84044400 | 0.18487800 |
| H | 0.04371200 | -2.85019700 | 2.01670900 | C | -4.18496100 | 1.90051400 | 0.15015100 |
| C | -0.66580700 | -3.30635800 | 0.03592000 | C | -5.70403800 | 0.05087000 | -0.16500600 |
| H | -0.25669800 | -3.54688100 | -0.94759100 | H | -4.93455500 | -1.90285600 | 0.20084800 |
| H | -1.27027700 | -4.15496400 | 0.37121000 | C | -5.43571000 | 1.41593000 | -0.17620300 |
| N | -1.51359200 | -2.09412300 | -0.11826100 | H | -6.22199800 | 2.11369800 | -0.45260500 |
| N | 1.13357700 | -1.74783400 | 0.61729400 | C | 3.40019600 | -0.70828500 | -0.13956300 |
| C | -2.45143500 | -1.86665200 | 1.02711200 | C | 2.95717500 | 0.61821700 | -0.33325200 |
| H | -3.06249300 | -2.77194300 | 1.11880800 | C | 4.76803200 | -0.97559400 | -0.12174400 |
| C | 2.37112500 | -1.93658800 | -0.15909400 | C | 3.92659200 | 1.64245400 | -0.50537800 |
| H | 2.09164700 | -2.37342800 | -1.12565800 | C | 5.69816400 | 0.02212300 | -0.30207400 |
| C | -3.29904100 | -0.66292300 | 0.81540500 | H | 5.11256500 | -1.99325200 | 0.03272800 |
| C | -2.82567400 | 0.60109500 | 1.26492000 | C | 5.26820500 | 1.33103000 | -0.48789900 |
| C | -4.51209000 | -0.78075600 | 0.14844700 | H | 5.99809300 | 2.12426200 | -0.62425100 |
| C | -3.65189200 | 1.73762000 | 0.99818600 | O | -1.95165100 | 1.44605700 | 0.78158700 |
| C | -5.29263200 | 0.33103700 | -0.09545900 | O | 1.69590000 | 1.01177700 | -0.37102000 |
| H | -4.85549100 | -1.75698400 | -0.18388000 | S | -7.34444200 | -0.51936700 | -0.61354100 |
| C | -4.84840500 | 1.85221300 | 0.33327200 | S | 7.45589900 | -0.32975900 | -0.27280200 |
| H | -5.46162900 | 2.45937100 | 0.13900100 | O | 7.99099800 | 0.15831300 | -1.57657500 |
| C | 3.16747000 | -0.67455400 | -0.31635700 | O | 7.57987600 | -1.80507700 | -0.10862100 |
| C | 2.59313400 | 0.57762700 | -0.60798100 | O | 8.00731200 | 0.43277300 | 0.88466300 |
| C | 4.55217200 | -0.78312600 | -0.20624900 | O | -7.30717300 | -2.10489800 | -0.51260100 |
| C | 3.44426100 | 1.69641000 | -0.80273700 | O | -7.57717400 | -0.03659500 | -2.00551500 |
| C | 5.37185400 | 0.30505600 | -0.39983400 | O | -8.27979800 | 0.10699800 | 0.36472300 |
| H | 4.99799000 | -1.74443000 | 0.02770400 | H | -0.59476400 | 2.82583500 | 0.86005200 |
| C | 4.80991000 | 1.54150500 | -0.69382600 | H | -0.80460200 | 0.84574700 | -1.19767800 |
| H | 5.45291600 | 2.40395000 | -0.84732700 | H | -1.16029100 | 1.06927800 | -0.38843000 |
| O | -1.69556500 | 0.73073500 | 1.86697600 | O | 0.32003600 | 3.13930200 | 0.95481600 |
| S | 1.29538000 | 0.81378400 | -0.72946800 | H | 0.84726900 | 2.52441800 | 0.41394400 |
| S | -6.84491000 | 0.20630800 | -0.97210300 | H | -0.78288700 | 0.86838900 | 2.19531500 |
| S | 7.15410300 | 0.16682600 | -0.24363600 | O | 0.01534700 | 0.77863700 | 2.74926200 |
| O | 7.71397500 | 0.68157500 | -1.52576600 | H | 0.51198800 | 1.56244500 | 2.47504100 |
| O | 7.43833800 | -1.27792300 | -0.02212900 | H | -1.88549900 | -1.74444800 | -0.99167500 |
| O | 7.52986900 | 1.01869400 | 0.92124000 | H | -1.88030900 | -1.06153700 | -1.84757800 |
| O | -7.06618600 | -1.24624000 | -1.22628200 | H | 1.54070100 | -1.07990800 | 1.64472200 |
| O | -6.67794600 | 0.99266700 | -2.23124200 | H | 3.03247900 | -2.70090600 | 0.50991200 |
| O | -7.88266000 | 0.80115200 | -0.07821700 | Pd | 0.12917700 | -0.25522200 | -0.27326300 |
| H | -0.44031300 | 1.98596700 | 1.63125300 | C | 3.46596700 | 3.05023400 | -0.69712800 |
| H | -1.05727700 | 0.24743600 | -1.76467800 | H | 2.75021800 | 3.12964000 | -1.51993500 |
| H | -1.38330600 | 0.56354700 | -1.08984500 | H | 2.95597000 | 3.43016500 | 0.19335800 |
| O | 0.44031200 | 2.40301200 | 1.50578200 | H | 4.30984900 | 3.70883300 | -0.90711300 |
| H | 0.74538100 | 2.01172700 | 0.66959000 | C | -3.87558000 | 3.36088200 | 0.12147000 |
| H | -0.25853500 | -0.03208700 | 2.63551400 | H | -3.55699800 | 3.72126500 | 1.10395300 |
| O | 0.68613800 | -0.11740800 | 2.88982100 | H | -3.05057900 | 3.57670500 | -0.56441700 |
| H | 1.01036000 | 0.76461400 | 2.64368300 | H | -4.74461700 | 3.94146200 | -0.19188100 |
| H | -2.08611300 | -2.20326800 | -0.95437600 | | | | |
| H | -1.85130100 | -1.76221000 | 1.93240500 | 51 | | | |
| H | 1.30934900 | -1.19483200 | 1.47422200 | RR-PhMe_EI, E(SCF) = -2333.44652499, E(ZPE) | | | |
| H | 2.98944200 | -2.67778900 | 0.35801200 | = -2333.067391, E(G) = -2333.128900 a.u. | | | |
| Pd | -0.14052100 | -0.57034200 | -0.46126200 | C | -0.53351300 | -3.15755700 | -0.53502000 |
| C | 2.84418500 | 3.02419300 | -1.13364100 | H | -1.20034700 | -4.01693500 | -0.41703900 |
| H | 2.20217700 | 2.96281800 | -2.01620200 | H | -0.07275900 | -3.22944500 | -1.52229300 |
| H | 2.21791000 | 3.40332600 | -0.32053200 | C | 0.52659400 | -3.16093200 | 0.54011500 |
| H | 3.62439700 | 3.76202800 | -1.32563000 | H | 0.06584000 | -3.23665100 | 1.52709100 |
| C | -3.17874700 | 3.08049800 | 1.44782700 | H | 1.19182100 | -4.02095200 | -0.41804600 |
| H | -2.98861300 | 3.09833800 | 2.52547900 | N | 1.30211100 | -1.89377100 | 0.52980600 |
| H | -2.23298200 | 3.35253200 | 0.96730000 | N | -1.30657100 | -1.88905800 | -0.51922500 |
| H | -3.91181400 | 3.85526300 | 1.21586500 | C | 2.46144800 | -1.79534100 | -0.37270400 |
| | | | | H | 3.10116700 | -2.67586700 | -0.24268900 |
| | | | | C | -2.46321400 | -1.79004000 | 0.38664300 |
| | | | | H | -2.08410000 | -1.81415600 | 1.41452400 |
| | | | | C | 3.26635500 | -0.55363200 | -0.08815300 |
| | | | | C | 2.70058100 | 0.70121200 | 0.26027600 |
| | | | | C | 4.65015100 | -0.67734000 | -0.19679600 |
| | | | | C | 3.58728300 | 1.79683800 | 0.47306300 |
| | | | | C | 5.49100200 | 0.39247900 | 0.01031100 |
| | | | | H | 5.08081900 | -1.44808500 | -0.44636300 |
| | | | | C | 4.94743100 | 1.62942900 | 0.34329200 |
| | | | | H | 5.60351200 | 2.47915700 | 0.51393200 |
| | | | | C | -3.26609300 | -0.54622600 | 0.10562400 |
| | | | | C | -2.69861600 | 0.70759000 | -0.24413900 |
| | | | | C | -4.64962600 | -0.66704100 | 0.21778000 |
| | | | | C | -3.58361000 | 1.80520600 | -0.45379700 |
| | | | | C | -5.48840700 | 0.40620500 | 0.01971200 |
| | | | | H | -5.08179000 | -1.63024500 | -0.47126100 |
| | | | | C | -4.94401600 | 1.64033900 | -0.32177000 |

| | | | | | | | |
|---|-------------|-------------|-------------|--|--|--|--|
| 59 | | | | | | | |
| RR-PhMe_EI_D1 TS2, E(SCF) = -2487.48432426, | | | | | | | |
| E(ZPE) = -2487.038914, E(G) = -2487.107051 | | | | | | | |
| a.u. | | | | | | | |
| C | 0.41712100 | -2.73617400 | 1.16121500 | | | | |
| H | 1.02100200 | -3.63830700 | 1.28838200 | | | | |
| H | -0.03720700 | -2.50444800 | 2.12662900 | | | | |
| C | -0.64318900 | -2.94315300 | 0.11177400 | | | | |
| H | -0.19221200 | -3.22198600 | -0.84274600 | | | | |
| H | -1.32882500 | -3.74356400 | 0.40746700 | | | | |
| N | -1.38932600 | -1.67501400 | -0.10527300 | | | | |
| N | 1.27783500 | -1.58276200 | 0.79614000 | | | | |
| C | -2.40915900 | -1.38874900 | 0.95021200 | | | | |
| H | -2.90431400 | -2.33662600 | 1.18976900 | | | | |
| C | 2.48505800 | -1.89254900 | 0.01266200 | | | | |
| H | 2.15567100 | -2.27965000 | -0.95867400 | | | | |
| C | -3.43954700 | -0.38840400 | 0.52504600 | | | | |

| | | | |
|----|-------------|-------------|-------------|
| H | -5.59886500 | 2.49212600 | -0.48652200 |
| O | 1.42442700 | 0.96265500 | 0.42297900 |
| O | -1.42208600 | 0.96666000 | -0.40774600 |
| S | 7.26665700 | 0.22779600 | -0.15176400 |
| S | -7.26688900 | 0.22500000 | 0.12043300 |
| O | -7.78140800 | 0.40895600 | -1.26904400 |
| O | -7.74075500 | 1.29891100 | 1.04114100 |
| O | -7.51571700 | -1.14516000 | 0.65097200 |
| O | 7.53180800 | -1.21989500 | -0.38466900 |
| O | 7.84517100 | 0.72484900 | 1.13045800 |
| O | 7.65725800 | 1.08090300 | -1.31260000 |
| H | 1.63328600 | -1.71430800 | 1.47566200 |
| H | 2.08479800 | -1.81705600 | -1.40156900 |
| H | -1.63972900 | -1.70623000 | -1.46375400 |
| H | -3.10520400 | -2.66896500 | 0.25681000 |
| Pd | -0.00021400 | -0.41158800 | 0.00629800 |
| C | 3.00556000 | 3.12204200 | 0.84019800 |
| H | 2.30869500 | 3.47774300 | 0.07588100 |
| H | 2.43227800 | 3.06027600 | 1.76980800 |
| H | 3.79005600 | 3.87009600 | 0.96668400 |
| C | -2.99973200 | 3.13026600 | -0.81807500 |
| H | -2.30285000 | 3.48337400 | -0.05251300 |
| H | -2.42589100 | 3.07202400 | -1.74737900 |
| H | -3.78302600 | 3.87978900 | -0.94331700 |

51
RR-PhMe, E(SCF) = -2333.45827969, E(ZPE) = -2333.078835, E(G) = -2333.139516 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.64016900 | -3.20314200 | 0.39966000 |
| H | -0.42346100 | -3.17915700 | 1.47154000 |
| H | -1.24583300 | -4.09021300 | 0.19597700 |
| C | 0.63978700 | -3.20306200 | -0.39998700 |
| H | 1.24543500 | -4.09022100 | -0.19666200 |
| H | 0.42299300 | -3.17865400 | -1.47183800 |
| N | 1.38457200 | -1.96759900 | -0.06999600 |
| N | -1.38482400 | -1.96754200 | 0.07005100 |
| C | 2.47705700 | -1.62252000 | -1.00066000 |
| H | 3.11918300 | -2.49756000 | -1.15098700 |
| C | -2.47707100 | -1.62231300 | 1.00100400 |
| H | -2.00141600 | -1.39206100 | 1.96144000 |
| C | 3.29753100 | -0.48047800 | -0.48566900 |
| C | 2.70482800 | 0.74870900 | -0.10802100 |
| C | 4.67897700 | -0.63388200 | -0.42663800 |
| C | 3.56113100 | 1.81425800 | 0.28682500 |
| C | 5.49522400 | 0.40402800 | -0.03218400 |
| H | 5.12678900 | -1.58260500 | -0.70495800 |
| C | 4.92603700 | 1.62513500 | 0.31606300 |
| H | 5.56653900 | 2.44692100 | 0.62713500 |
| C | -3.29759000 | -0.48033200 | 0.48600100 |
| C | -2.70484100 | 0.74889100 | 0.10845500 |
| C | -4.67897900 | -0.63377600 | 0.42674200 |
| C | -3.56098700 | 1.81430200 | -0.28676100 |
| C | -5.49515300 | 0.40406400 | 0.03179100 |
| H | -5.12682900 | -1.58251000 | 0.70494400 |
| C | -4.92593000 | 1.62512800 | -0.31639800 |
| H | -5.56635000 | 2.44685500 | -0.62778900 |
| O | 1.41745500 | 0.99043500 | -0.11796200 |
| O | -1.41742600 | 0.99057000 | 0.11863600 |
| S | 7.27411400 | 0.21358600 | 0.04430700 |
| S | -7.27405600 | 0.21359200 | -0.04464400 |
| O | -7.65919900 | 0.49777100 | -1.45819100 |
| O | -7.83746200 | 1.21888500 | 0.90344800 |
| O | -7.56055000 | -1.19094600 | 0.36241100 |
| O | 7.56071000 | -1.19069600 | -0.36355400 |
| O | 7.65919700 | 0.49685400 | 1.45807100 |
| O | 7.83760300 | 1.21941200 | -0.90316700 |
| H | 1.77744300 | -2.05689300 | 0.86810100 |
| H | 2.00164000 | -1.39239400 | -1.96124800 |
| H | -1.77791400 | -2.05650800 | -0.86797900 |
| H | -3.11917000 | -2.49732300 | 1.15163000 |
| Pd | -0.00004200 | -0.45632300 | 0.00015100 |
| C | 2.95410100 | 3.12453300 | 0.66694900 |
| H | 2.38216300 | 3.55659200 | -0.15923300 |
| H | 2.25294700 | 3.01424800 | 1.49895100 |
| H | 3.72440500 | 3.84006600 | 0.95957300 |
| C | -2.95388500 | 3.12450800 | -0.66694300 |
| H | -2.38200400 | 3.55661600 | 0.15924500 |

| | | | |
|---|-------------|------------|-------------|
| H | -2.25271800 | 3.01412200 | -1.49892900 |
| H | -3.72409800 | 3.84009000 | -0.95974400 |

61
RR-PhOMe_hs_D1_TS1_P, E(SCF) = -2637.93422837, E(ZPE) = -2637.474540, E(G) = -2637.542936 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.49453100 | -1.20762900 | -3.16090400 |
| H | 0.13505700 | -2.16792900 | -3.54609000 |
| H | 0.39893000 | -0.47134400 | -3.96721900 |
| C | 1.92755100 | -1.31173000 | -2.71012800 |
| H | 2.60367000 | -1.54357600 | -3.53844700 |
| H | 2.22888400 | -0.35068800 | -2.28656100 |
| N | 2.05565700 | -2.33886000 | -1.63961400 |
| N | -0.32403600 | -0.84870100 | -1.99701900 |
| C | 3.36862200 | -2.26926800 | -0.93015600 |
| H | 3.46350300 | -3.18687500 | -0.34811300 |
| C | -1.76466300 | -1.00064900 | -2.20949700 |
| H | -1.93896600 | -2.05889700 | -2.44643500 |
| C | 3.48748500 | -1.05523800 | -0.06127800 |
| C | 3.07423400 | -1.06933400 | 1.26889900 |
| C | 3.95665100 | 0.13643500 | -0.61221900 |
| C | 3.14099800 | 0.10821400 | 2.03634600 |
| C | 3.96595600 | 1.29153500 | 0.13354400 |
| H | 4.29556000 | 0.16283900 | -1.64234500 |
| C | 3.56399000 | 1.29073500 | 1.46161500 |
| H | 3.56518400 | 2.21915200 | 2.01897500 |
| C | -2.57881900 | -0.57851100 | -1.02202900 |
| C | -2.35889500 | -1.12313100 | 0.25947700 |
| C | -3.61346200 | 0.33116900 | -1.22637400 |
| C | -3.25474200 | -0.73836300 | 1.29792900 |
| C | -4.45447600 | 0.69717800 | -0.19796700 |
| H | -3.76263300 | 0.74569400 | -2.21945600 |
| C | -4.27546300 | 0.16360400 | 1.07222500 |
| H | -4.94863900 | 0.46357100 | 1.86514600 |
| O | 2.60469200 | -2.17515400 | 1.88899300 |
| O | -1.40642500 | -1.96914000 | 0.58820700 |
| S | 4.18465900 | 2.86918900 | -0.69220800 |
| S | -5.75403800 | 1.89629400 | -0.50576900 |
| O | -6.56137900 | 1.34979600 | -1.63475800 |
| O | -5.06453500 | 3.16840100 | -0.86888800 |
| O | -6.52858400 | 2.00026300 | 0.76279900 |
| O | 2.77643500 | 3.25357700 | -1.04031600 |
| O | 5.02130800 | 2.61617900 | -1.89133700 |
| O | 4.80100400 | 3.79480600 | 0.29079600 |
| H | 0.75954600 | -3.37265600 | 0.50530600 |
| H | 1.94588300 | -2.63097600 | 1.31630400 |
| H | 2.00752800 | -3.25609100 | -2.08040800 |
| H | 4.16538500 | -2.26473300 | -1.68212200 |
| H | -0.09206900 | 0.09881600 | -1.66633300 |
| H | -2.08323500 | -0.42221300 | -3.08627400 |
| Pd | 0.31120900 | -2.22338500 | -0.49871300 |
| H | 0.74667400 | -0.20259600 | 2.56249100 |
| O | 0.02784200 | 0.11868700 | 2.00150100 |
| H | -0.41680700 | -0.68722600 | 1.67641100 |
| H | 0.54281200 | 1.13741800 | 0.39580600 |
| O | 0.53560600 | 1.52098300 | -0.49922800 |
| H | 1.34586500 | 2.05429200 | -0.59700400 |
| O | -3.01228100 | -1.31947100 | 2.50161500 |
| O | 2.67662400 | -0.00046700 | 3.30557000 |
| C | 2.64364500 | 1.17413800 | 4.09617500 |
| H | 1.98239400 | 1.92876200 | 3.65654400 |
| H | 2.25468300 | 0.87827000 | 5.06755800 |
| H | 3.64390700 | 1.59820900 | 4.22143600 |
| C | -3.82784200 | -0.94412400 | 3.58603100 |
| H | -3.47379100 | -1.50278600 | 4.45044300 |
| H | -3.75078600 | 0.12822100 | 3.79765100 |
| H | -4.87971800 | -1.19362800 | 3.40782200 |

61
RR-PhOMe_hs_D1_TS1_R, E(SCF) = -2637.91294745, E(ZPE) = -2637.459465, E(G) = -2637.532119 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.32202500 | -3.67603900 | 0.29819100 |
| H | 0.66527200 | -4.23210700 | -0.57956700 |
| H | 0.63841500 | -4.22569600 | -1.18760000 |
| C | -1.17718600 | -3.50040700 | 0.24712700 |

| | | | | | | | |
|--|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -1.68986200 | -4.46662900 | 0.25183500 | C | -3.01875800 | 1.60574100 | -0.60371800 |
| H | -1.54009100 | -2.91489400 | 1.09690500 | C | -4.82882200 | 0.58308600 | 0.60039200 |
| N | -1.48684400 | -2.74550100 | -0.98790200 | H | -4.99832500 | -1.53592300 | 0.45483200 |
| N | 0.96239600 | -2.33945400 | 0.25066300 | C | -4.11347100 | 1.72327800 | 0.22216900 |
| C | -2.91287600 | -2.38992000 | -1.19562900 | H | -4.43390500 | 2.69374800 | 0.58455600 |
| H | -3.06286900 | -2.39566200 | -2.27872200 | C | 2.96861600 | -1.12369400 | 0.33112600 |
| C | 2.36781500 | -2.33713500 | -0.19332400 | C | 2.70300100 | -0.36413300 | -0.81937600 |
| H | 2.36146300 | -2.64888100 | -1.24424100 | C | 4.03264800 | -0.78330700 | 1.16834400 |
| C | -3.30589500 | -1.05240900 | -0.65502800 | C | 3.57093600 | 0.72997600 | -1.10049800 |
| C | -2.64361700 | 0.08990200 | -1.13889000 | C | 4.85045800 | 0.28051600 | 0.87309300 |
| C | -4.36668800 | -0.93459600 | 0.23669200 | H | 4.22249700 | -1.36573100 | -0.81937600 |
| C | -3.16202400 | 1.35973100 | -0.77012000 | C | 4.62274900 | 1.04466900 | -0.27046000 |
| C | -4.80889100 | 0.31071500 | 0.62750800 | H | 5.27078800 | 1.88505200 | -0.49213200 |
| H | -4.85897400 | -1.82264200 | 0.61876100 | O | -1.51333200 | 0.24156600 | -1.81574500 |
| C | -4.21471500 | 1.46328600 | 0.11944500 | O | 1.72745700 | -0.67459000 | -1.67545900 |
| H | -4.59011200 | 2.43461600 | 0.42103900 | S | -6.24048200 | 0.77825300 | 1.68417200 |
| C | 3.02303000 | -0.99942200 | -0.00786500 | S | 6.22586000 | 0.71686100 | 1.93927000 |
| C | 2.40939300 | 0.20565600 | -0.38619100 | O | 7.45362500 | 0.55066300 | 1.10883000 |
| C | 4.31797100 | -0.93459600 | 0.23669200 | O | 6.17000500 | -0.22593400 | -1.09812800 |
| C | 3.15867200 | 1.40852900 | -0.23045300 | O | 5.99926400 | 2.13612900 | 2.33624700 |
| C | 5.01459600 | 0.18842300 | 0.66014000 | O | -7.18807600 | 1.68478100 | 0.97133600 |
| H | 4.78457900 | -1.91780700 | 0.81947200 | O | -5.71592400 | 1.39166200 | 2.93987300 |
| C | 4.43546900 | 1.39918200 | 0.28226500 | O | -6.79457500 | -0.58836300 | -1.89592500 |
| H | 4.99298300 | 2.32078500 | 0.40145300 | H | -0.13136100 | -1.99829100 | -3.33633100 |
| O | -1.58354500 | 0.02322100 | -1.92240000 | H | -0.48138900 | -1.31959800 | -3.28522800 |
| O | 1.19879800 | 0.34270600 | -0.89004600 | H | -1.47357800 | -3.55585900 | -1.06479500 |
| S | -6.14310300 | 0.48528400 | 1.81696100 | H | -3.70883800 | -2.87307700 | -2.91330100 |
| S | 6.69273700 | 0.19958100 | 1.29771300 | H | 0.52222500 | -1.12818800 | 1.15564300 |
| O | 7.54843500 | 0.67411800 | 0.17210500 | H | 2.42142200 | -2.67049300 | 1.68449700 |
| O | 6.98976800 | -1.20170100 | 1.70335900 | Pd | 0.02708600 | -1.55628700 | -1.20972700 |
| O | 6.68835400 | 1.15110500 | 2.44528000 | H | -0.35744400 | 1.38766700 | -2.58625800 |
| O | -7.17441500 | 1.33223000 | 1.15271800 | O | 0.43930300 | 1.77482000 | -2.99820500 |
| O | -5.54002800 | 1.15415400 | 3.00519300 | H | 1.15935900 | 1.21855200 | -2.66298900 |
| O | -6.61883900 | -0.89565400 | 2.10445200 | H | -0.33662600 | 0.88188900 | -0.15473200 |
| H | 2.12002500 | -1.14011500 | -3.61405600 | O | -0.00106900 | 0.91187600 | 0.75857000 |
| H | 1.88874600 | -0.64633900 | -3.12477100 | H | -0.68703800 | 1.37430100 | 1.24917900 |
| H | -1.18919700 | -3.31083800 | -1.78223000 | O | 3.26513400 | 1.40534700 | -2.23551000 |
| H | -3.54420500 | -3.17502400 | -0.76818200 | O | -2.25433700 | 2.65023800 | -1.01968800 |
| H | 0.91256300 | -1.91309100 | 1.17727900 | C | -2.55373200 | 3.92549600 | -0.50359700 |
| H | 2.92733800 | -3.09247000 | 0.36936200 | H | -2.48197000 | 3.94246000 | 0.59031300 |
| Pd | -0.19053100 | -1.15026000 | -0.95367000 | H | -1.81824100 | 4.61164300 | -0.91931300 |
| H | -0.62957300 | 1.68167300 | -2.52693000 | H | -3.55601100 | 4.25735700 | -0.79659700 |
| O | 0.17021700 | 2.17447000 | -2.77844700 | C | 3.97532600 | 2.58972200 | -2.51652200 |
| H | 0.81820400 | 1.81074000 | -2.15433000 | H | 3.53128800 | 3.00894100 | -3.41756500 |
| H | 0.16313800 | 1.43155900 | 0.27508200 | H | 3.88433900 | 3.31423600 | -1.70036100 |
| O | -0.36733700 | 1.77473800 | 1.01746000 | H | 5.03648100 | 2.39011300 | -2.69958400 |
| H | -1.26039100 | 1.46750500 | 0.82471300 | | | | |
| O | 2.50262700 | 2.52359400 | -0.63561900 | | | | |
| O | -2.53918500 | 2.41188700 | -1.35100900 | | | | |
| C | -2.88893400 | 3.71059500 | -0.93011800 | | | | |
| H | -2.72937700 | 4.83936300 | 0.14642500 | | | | |
| H | -2.23771200 | 3.39468300 | -1.47094200 | | | | |
| H | -3.93195200 | 3.94551800 | -1.16731000 | | | | |
| C | 3.17160200 | 3.76020000 | -0.53295500 | | | | |
| H | 2.48632900 | 4.51385400 | -0.91586300 | | | | |
| H | 3.42050800 | 3.99701500 | 0.50683700 | | | | |
| H | 4.08887300 | 3.77217200 | -1.13127700 | | | | |
| 61 | | | | | | | |
| RR-PhOMe_hs_D1_TS1, E(SCF) = - | | | | | | | |
| 2637.89090930, E(ZPE) = -2637.437791, E(G) | | | | | | | |
| = -2637.509416 a.u. | | | | | | | |
| C | -0.16862900 | -3.08501000 | 1.20852600 | C | -3.12133200 | -3.16594000 | 0.54248200 |
| H | 0.15656800 | -4.03104700 | 0.76546400 | H | 0.23438100 | -3.99444000 | -0.07753000 |
| H | -0.05523600 | -3.16128500 | 2.29347400 | H | -0.01229700 | -3.45833700 | 1.59053700 |
| C | -1.58688900 | -2.76320500 | 0.81755400 | C | -1.54551800 | -2.81824800 | 0.20506800 |
| H | -2.29189500 | -3.52472100 | 1.16347200 | H | -2.22254000 | -3.66308300 | 0.36303400 |
| H | -1.89261100 | -1.80161900 | 1.23909900 | H | -1.89703500 | -1.98387500 | 0.81697900 |
| N | -1.63730700 | -2.63428500 | -0.65761500 | N | -1.58042400 | -2.37884700 | -1.20802000 |
| N | 0.69996300 | -2.01834900 | 0.67060000 | C | -2.90705500 | -1.86668600 | -1.65140800 |
| C | -2.94099100 | -2.14046200 | -1.18559300 | H | -2.80318700 | -1.65812400 | -2.71977200 |
| H | -2.83933200 | -2.14864100 | -2.27441100 | C | -3.36966400 | -0.66416200 | -0.90551000 |
| C | 2.14196200 | -2.32114700 | 0.68395700 | C | -2.72383600 | 0.57031300 | -1.13869300 |
| H | 2.29279400 | -3.15430500 | -0.01164900 | C | -4.43922200 | -0.76989700 | -0.01660700 |
| C | -3.32850800 | -0.79220200 | -0.68190800 | C | -3.27569900 | 1.70987100 | -0.46310200 |
| C | -2.57421200 | 0.33077600 | -1.10796200 | C | -4.91463800 | 0.34015400 | 0.64042200 |
| C | -4.43574500 | -0.65711700 | 0.15534100 | H | -4.90604300 | -1.73497300 | 0.15644700 |
| | | | | C | -4.33055400 | 1.59019200 | 0.41199100 |
| | | | | H | -4.72569200 | 2.45956400 | 0.92563600 |
| | | | | O | -1.70094400 | 0.69500000 | -1.91735300 |
| | | | | S | -6.29061800 | 0.23002800 | 1.77855300 |
| | | | | O | -6.64690700 | -1.21471900 | 1.86084100 |
| | | | | O | -7.38392400 | 1.06180200 | 1.19331800 |
| | | | | O | -5.80263700 | 0.78203300 | 3.07706500 |
| | | | | H | -0.05846900 | -1.01765200 | -3.67375300 |
| | | | | H | -0.57660400 | -0.49828900 | -3.45511100 |
| | | | | H | -1.34978500 | -3.18138500 | -1.79560100 |
| | | | | H | -3.63191600 | -2.68040900 | -1.53388000 |

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | -0.58384500 | 1.84640200 | -1.16563800 | O | -7.26583900 | 1.29481400 | -0.27106700 |
| O | 0.22361200 | 2.17124700 | -0.70036900 | H | -0.02952400 | 1.59100600 | 1.70638700 |
| H | 0.92610600 | 1.68159500 | -1.15909900 | H | -1.57318500 | -0.29671400 | -1.46171800 |
| H | 0.07509500 | 1.13694200 | 0.79739100 | H | -1.63087500 | 0.03468300 | -0.71906500 |
| O | 0.03839900 | 0.48812800 | 1.53613000 | O | 0.87025900 | 1.91958400 | 1.48376500 |
| H | -0.82886100 | 0.60364600 | 1.93303200 | H | 0.88028400 | 2.02805300 | 0.52322900 |
| N | 0.72404900 | -1.99003700 | 0.24762900 | O | 0.13665400 | -0.57889000 | 2.40251900 |
| C | 2.16223700 | -2.29484800 | 0.17133300 | O | 1.08665100 | -0.82574900 | 2.36111900 |
| H | 2.29652600 | -2.96539300 | -0.68520300 | H | 1.46211600 | 0.01515600 | 2.04968000 |
| C | 3.01763000 | -1.07006500 | 0.06564100 | H | -2.11375300 | -2.93250400 | -0.27301300 |
| C | 2.74059300 | -0.05421900 | -0.86164200 | H | -1.76997800 | -1.90815600 | -1.43561700 |
| C | 4.14704300 | -0.98582300 | 0.88202200 | H | 1.42249900 | -2.09363200 | 0.92213400 |
| C | 3.65187300 | 1.04005700 | -0.93978600 | H | 3.07097300 | -3.15509400 | -0.63438800 |
| C | 5.01339000 | 0.07457300 | 0.77957900 | Pd | -0.30788000 | -1.17731600 | -0.56536300 |
| H | 4.35245600 | -1.77261300 | 1.59963900 | O | 2.00569200 | 2.43334200 | -1.18520400 |
| C | 4.76606800 | 1.09846700 | -0.13264100 | O | -2.40566500 | 2.77990800 | 1.48370600 |
| H | 5.45511800 | 1.93223000 | -0.19638600 | C | 2.53144400 | 3.72807100 | -0.97129600 |
| O | 1.71017400 | -0.01874500 | -1.68043900 | H | 2.88684800 | 3.84780900 | 0.05817700 |
| S | 6.46542900 | 0.19140400 | 1.82828700 | H | 3.35177000 | 3.94559300 | -1.66193000 |
| O | 6.26487100 | 1.40696600 | 2.66843400 | H | 1.71706500 | 4.42619400 | -1.15260500 |
| O | 7.62429900 | 0.32933900 | 0.90030500 | C | -2.94642800 | 4.00984200 | 1.06532400 |
| O | 6.50294300 | -1.06596200 | 2.62444800 | H | -2.29280500 | 4.78804700 | 1.45521100 |
| H | 0.54580900 | -1.22842900 | 0.92771400 | H | -2.98053700 | 4.08695000 | -0.40272300 |
| H | 2.44794000 | -2.85379600 | 1.07034700 | H | -3.95708100 | 4.16187700 | 1.46103500 |
| Pd | 0.03268400 | -1.12614400 | -1.46606500 | | | | |
| O | 3.32121300 | 1.98197400 | -1.85758800 | | | | |
| O | -2.66568800 | 2.88531500 | -0.76720600 | 61 | | | |
| C | 4.16023700 | 3.10914500 | -1.97375700 | RR-PhOMe_D1_TS1_R REF, E(SCF) = - | | | |
| H | 3.72441600 | 3.74234700 | -2.74369500 | 2637.92443397, E(ZPE) = -2637.469600, E(G) | | | |
| H | 4.21242500 | 3.67072000 | -1.03497600 | = -2637.540707 a.u. | | | |
| H | 5.17425800 | 2.82628400 | -2.27584300 | C | -0.62664600 | -3.58591800 | 0.41113400 |
| C | -3.10172700 | 4.04465300 | -0.10113200 | H | -0.37246300 | -3.55344900 | 1.47446100 |
| H | -2.97963900 | 3.95680000 | 0.98456400 | H | -1.23614900 | -4.47586400 | 0.23452700 |
| H | -2.48432400 | 4.86499200 | -0.46262200 | C | 0.62417700 | -3.58810400 | -0.43585600 |
| H | -4.15236000 | 4.26691000 | -0.32015700 | H | 1.23864900 | -4.47213100 | -0.24728300 |
| | | | | H | 0.37024200 | -3.57127600 | -1.49956500 |
| | | | | N | 1.37737400 | -2.34790900 | -0.14021800 |
| | | | | N | -1.38728900 | -2.35412700 | 0.09893300 |
| | | | | C | 2.45276200 | -2.00736400 | -1.09537900 |
| | | | | H | 3.09727500 | -2.88004400 | -1.24554700 |
| | | | | C | -2.46654300 | -2.01073800 | 1.04842100 |
| | | | | H | -1.97931100 | -1.78429500 | 2.00330700 |
| | | | | C | 3.27545200 | -0.85552500 | -0.60038600 |
| | | | | C | 2.67585100 | 0.36149400 | -0.23925400 |
| | | | | C | 4.66186900 | -1.00025000 | -0.52426700 |
| | | | | C | 3.52401900 | 1.42122800 | 0.18532700 |
| | | | | C | 5.45794200 | 0.04386000 | -0.11797900 |
| | | | | H | 5.12177800 | -1.94442100 | -0.79531500 |
| | | | | C | 4.89051600 | 1.26657100 | 0.24054400 |
| | | | | H | 5.52957400 | 2.07795300 | 0.56957200 |
| | | | | C | -3.29283800 | -0.86322600 | 0.54931000 |
| | | | | C | -2.69752200 | 0.35476500 | 0.18399800 |
| | | | | C | -4.67983700 | -1.00895800 | 0.48634300 |
| | | | | C | -3.55141000 | 1.41773600 | -0.22101800 |
| | | | | C | -5.48083100 | 0.03643200 | 0.09328500 |
| | | | | H | -5.13617600 | -1.95435800 | 0.75919700 |
| | | | | C | -4.91806900 | 1.26255200 | -0.26158000 |
| | | | | H | -5.56147300 | 2.07641000 | -0.57577400 |
| | | | | O | 1.38538900 | 0.60902700 | -0.26416200 |
| | | | | O | -1.40765700 | 0.60459700 | 0.20043100 |
| | | | | S | 7.24236400 | -0.13076200 | -0.10277700 |
| | | | | S | -7.26551200 | -0.13926100 | 0.01671800 |
| | | | | O | -7.64159200 | 0.14544900 | -1.39788700 |
| | | | | O | -7.81330600 | 0.87479300 | 0.96265100 |
| | | | | O | -7.56121000 | -1.53925900 | 0.42759500 |
| | | | | O | 7.54140000 | -1.53096800 | -0.43531100 |
| | | | | O | 7.60772700 | 0.15541500 | 1.38920600 |
| | | | | O | 7.79607600 | 0.88271400 | -0.97081200 |
| | | | | H | 1.78962500 | -2.42366400 | 0.79177000 |
| | | | | H | 1.96245700 | -1.78744500 | -2.05011000 |
| | | | | H | -1.79728200 | -2.44598400 | -0.83200200 |
| | | | | H | -3.10857100 | -2.88470400 | 1.20202100 |
| | | | | Pd | -0.00972400 | -0.84532800 | -0.02767400 |
| | | | | H | 0.94672400 | 2.34803400 | 1.21304800 |
| | | | | H | 1.91816300 | -0.35654800 | 2.98682300 |
| | | | | H | 1.79097200 | -0.02429000 | 2.32599500 |
| | | | | O | 0.10718900 | 2.52782000 | 1.66369700 |
| | | | | H | -0.51176500 | 1.94195800 | 1.19483000 |

| | | | |
|---|-------------|------------|-------------|
| H | 0.47395700 | 1.93599600 | -1.26672900 |
| O | -0.15489600 | 2.50549200 | -1.74208700 |
| H | -0.98519400 | 2.33997100 | -1.26935800 |
| O | 2.86274000 | 2.55800000 | 0.52730500 |
| O | -2.89551100 | 2.56061000 | -0.55356900 |
| C | 3.62173500 | 3.65421200 | 0.99117400 |
| H | 4.18590300 | 3.39818900 | 1.89396100 |
| H | 4.31624900 | 4.01141200 | 0.22409700 |
| H | 2.91000300 | 4.44348500 | 1.22528200 |
| C | -3.66191200 | 3.66498500 | -0.98378300 |
| H | -4.23790800 | 3.42763000 | -1.88422700 |
| H | -4.34659700 | 4.00471600 | -0.20007800 |
| H | -2.95467500 | 4.46039400 | -1.21060900 |

61

RR-PhOMe_D1_TS1_R, E(SCF) = -2637.92142147,
E(ZPE) = -2637.466855, E(G) = -2637.538529
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.60945700 | -3.58491400 | -0.22484200 |
| H | 0.33828100 | -3.59614500 | -1.28461400 |
| H | 1.22213200 | -4.46714400 | -0.02319500 |
| C | -0.62795400 | -3.55072500 | 0.63914900 |
| H | -1.24839200 | -4.43875000 | 0.49287000 |
| H | -0.36041200 | -3.49208200 | 1.69789500 |
| N | -1.37700300 | -2.32069800 | 0.29927100 |
| N | 1.37732800 | -2.34254900 | 0.02208900 |
| C | -2.47293300 | -1.95664000 | 1.22188300 |
| H | -3.11040000 | -2.83018700 | 1.39515300 |
| C | 2.41731800 | -2.03362700 | -0.98037700 |
| H | 1.89073800 | -1.82422600 | -1.91858000 |
| C | -3.29104900 | -0.83939500 | 0.65067100 |
| C | -2.68377100 | 0.36920100 | 0.27659100 |
| C | -4.66696500 | -1.01087400 | 0.49540500 |
| C | -3.51742000 | 1.39981500 | -0.23792200 |
| C | -5.44864900 | 0.00351000 | -0.00487500 |
| H | -5.12991500 | -1.95022200 | 0.77754300 |
| C | -4.87565100 | 1.21907900 | -0.37678600 |
| H | -5.50307500 | 2.00730000 | -0.77676700 |
| C | 3.27622200 | -0.88631900 | -0.54300500 |
| C | 2.71142400 | 0.34677900 | -0.17540700 |
| C | 4.66258600 | -1.05366300 | -0.54306800 |
| C | 3.60183200 | 1.40659600 | 0.16348600 |
| C | 5.49668000 | -0.01363300 | -0.21200000 |
| H | 5.08899300 | -2.01224400 | -0.81821300 |
| C | 4.96688700 | 1.22744900 | 0.14203300 |
| H | 5.63630000 | 2.03806300 | 0.40620200 |
| O | -1.39854500 | 0.63183700 | 0.38143100 |
| O | 1.42507800 | 0.61085600 | -0.14234100 |
| S | -7.21470900 | -0.21909200 | -0.24044500 |
| S | 7.27960600 | -0.21339600 | -0.21653200 |
| O | 7.72652500 | 0.08071900 | 1.17584200 |
| O | 7.79763700 | 0.78273800 | -1.19809700 |
| O | 7.53876000 | -1.62150100 | -0.62542600 |
| O | -7.53313300 | -1.57503500 | 0.28518100 |
| O | -7.44290200 | -0.09471100 | -1.70881500 |
| O | -7.87069300 | 0.87563100 | 0.53000000 |
| H | -0.82483700 | 2.57094800 | -0.62150800 |
| H | -1.27460800 | -0.11596600 | -2.78019300 |
| H | -1.45515700 | 0.38850200 | -2.25506100 |
| O | 0.04316200 | 3.00439300 | -0.66947800 |
| H | 0.66638900 | 2.27044800 | -0.50582000 |
| H | -0.85847500 | 1.86303900 | 1.74693900 |
| O | -0.46974400 | 2.65894200 | 2.14816800 |
| H | -0.11360600 | 3.09355200 | 1.35722300 |
| H | -1.77404200 | -2.42520600 | -0.63685400 |
| H | -2.00503300 | -1.68851500 | 2.17516300 |
| H | 1.82337700 | -2.40514200 | 0.93860000 |
| H | 3.04229800 | -2.91870000 | -1.14135600 |
| Pd | 0.01183200 | -0.82123000 | 0.14621400 |
| O | 2.98652600 | 2.56715700 | 0.49565000 |
| O | -2.85482800 | 2.53629800 | -0.57364700 |
| C | 3.79537100 | 3.66829100 | 0.83810700 |
| H | 4.41542600 | 3.45528800 | 1.71571500 |
| H | 4.44565600 | 3.96518800 | 0.00804000 |
| H | 3.11878500 | 4.48848000 | 1.07105000 |
| C | -3.59839400 | 3.61757600 | -1.09284100 |
| H | -2.88314200 | 4.41433300 | -1.28885300 |

| | | | |
|---|-------------|------------|-------------|
| H | -4.10137400 | 3.34747400 | -2.02696400 |
| H | -4.34349700 | 3.97142600 | -0.37312900 |

61

RR-PhOMe_D1_TS1, E(SCF) = -2637.89074346,
E(ZPE) = -2637.436111, E(G) = -2637.506968
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.63119300 | -3.64901000 | -0.12362600 |
| H | 0.43225700 | -3.86734900 | -1.17624700 |
| H | 1.27115400 | -4.44223200 | 0.27510300 |
| C | -0.64108500 | -3.52240800 | 0.66486600 |
| H | -1.22891300 | -4.44318200 | 0.64305800 |
| H | -0.40507300 | -3.30476300 | 1.71100400 |
| N | -1.43834600 | -2.37746500 | 0.15250500 |
| N | 1.32086200 | -2.34543500 | -0.06206600 |
| C | -2.48954100 | -1.98779400 | 1.14290400 |
| H | -3.13932500 | -2.85629500 | 1.29607500 |
| C | 2.50996200 | -2.23577600 | -0.92942000 |
| H | 2.15260200 | -2.33510800 | -2.33506300 |
| C | -3.28819900 | -0.79658600 | 0.74856300 |
| C | -2.64762200 | 0.45737600 | 0.81302700 |
| C | -4.62434500 | -0.90992100 | 0.37438400 |
| C | -3.42147200 | 0.45292900 | 1.45420200 |
| C | -5.34519100 | 0.21559600 | 0.04341800 |
| H | -5.10186300 | -1.88380700 | 0.34025800 |
| C | -4.74399000 | 1.47701800 | 0.08525900 |
| H | -5.32657100 | 2.34867200 | -0.19171900 |
| C | 3.24069900 | -0.95163400 | -0.70309800 |
| C | 2.56548000 | 0.27202400 | -0.83543400 |
| C | 4.59646300 | -0.98002400 | -0.38132800 |
| C | 3.31878400 | 1.46442000 | -0.65113900 |
| C | 5.29940400 | 0.18962000 | -0.21098700 |
| H | 5.10653900 | -1.93087600 | -0.27206000 |
| C | 4.66075800 | 1.42098400 | -0.34527100 |
| H | 5.22699900 | 2.33390200 | -0.20243000 |
| O | -1.39607000 | 0.56094900 | 1.12014300 |
| O | 1.29433700 | 0.39665300 | -1.13999600 |
| S | -7.07351800 | 0.10532900 | -0.41487400 |
| S | 7.04609300 | 0.17272300 | 0.20630000 |
| O | 7.15418300 | 0.84474000 | 1.53275500 |
| O | 7.72625900 | 0.94074900 | -0.87525200 |
| O | 7.44617500 | -1.26045500 | 0.24449500 |
| O | -7.39051700 | -1.34844100 | -0.49229000 |
| O | -7.19840900 | 0.79660600 | -1.73136900 |
| O | -7.83369500 | 0.80647300 | 0.66161300 |
| H | -0.15744200 | 1.83630300 | 1.20684800 |
| H | -1.39298000 | -0.04588000 | -1.86281900 |
| H | -1.39306900 | 0.50074200 | -1.32212100 |
| O | 0.71168300 | 2.26840600 | 1.34922300 |
| H | 1.12265000 | 2.27922000 | 0.47184000 |
| H | -0.04180800 | -0.32259000 | 2.15404400 |
| O | 0.88804900 | -0.44341400 | 2.42261900 |
| H | 1.24366600 | 0.42649600 | 2.17442800 |
| H | -1.90923700 | -2.66641600 | -0.70607200 |
| H | -1.95713400 | -1.79667900 | 2.07951100 |
| H | 1.57309800 | -2.11531200 | 0.90705900 |
| H | 3.17703500 | -3.08013300 | -0.72286400 |
| Pd | -0.08590400 | -0.91273500 | -0.48598000 |
| O | 2.60315200 | 2.61077800 | -0.80435800 |
| O | -2.73918800 | 2.77555300 | 0.49816200 |
| C | 3.23388500 | 3.83247000 | -0.47883200 |
| H | 3.58197300 | 3.83511700 | 0.55982400 |
| H | 4.07909200 | 4.03733700 | -1.14282000 |
| H | 2.48361300 | 4.61009800 | -0.60744600 |
| C | -3.43703100 | 3.94894900 | 0.15341100 |
| H | -2.73075200 | 4.77157400 | 0.24819200 |
| H | -3.80595000 | 3.91203600 | -0.87772300 |
| H | -4.28438200 | 4.12663600 | 0.82496800 |

61

RR-PhOMe_D1_TS2_P, E(SCF) = -2637.92490627,
E(ZPE) = -2637.465819, E(G) = -2637.536285
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.58282500 | -3.51544600 | 0.28533800 |
| H | 0.30549600 | -3.75689300 | -0.74605400 |
| H | 1.16327600 | -4.35859000 | 0.67749600 |
| C | -0.64632700 | -3.28503200 | 1.12707800 |

| | | | | | | | |
|--|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -1.25542600 | -4.19007400 | 1.20625300 | C | -3.98003500 | 1.76592100 | 0.30515200 |
| H | -0.34441000 | -2.99753000 | 2.13875200 | C | -5.55998900 | -0.02885100 | 0.07119100 |
| N | -1.45672400 | -2.16002300 | 0.58429600 | H | -4.86366500 | -1.99286900 | 0.51291400 |
| N | 1.36100200 | -2.27280000 | 0.25953800 | C | -5.25425900 | 1.33119900 | 0.00635300 |
| C | -2.43051500 | -1.69865300 | 1.60853700 | H | -6.02589600 | 2.03184000 | -0.29154400 |
| H | -3.05002400 | -2.55446500 | 1.90361200 | C | 3.41344700 | -1.01788400 | -0.69384600 |
| C | 2.42564900 | -2.12516800 | -0.74764300 | C | 2.83377900 | 0.24868400 | -0.86398500 |
| H | 1.93668500 | -2.33451700 | -1.72397500 | C | 4.75103400 | -1.13750500 | -0.31862200 |
| C | -3.30283100 | -0.59485900 | 1.11054000 | C | 3.66425800 | 1.38854900 | -0.68128300 |
| C | -3.03971300 | 0.73647300 | 1.40636900 | C | 5.52737400 | -0.01701100 | -0.13589800 |
| C | -4.37879500 | -0.91433400 | 0.28019100 | H | 5.18884100 | -2.11974400 | -0.17678600 |
| C | -3.85548700 | 1.74941000 | 0.85879800 | C | 4.98559500 | 1.25457900 | -0.31547500 |
| C | -5.16407300 | 0.07696700 | -0.25546000 | H | 5.61093400 | 2.12742600 | -0.16679200 |
| H | -4.59787400 | -1.95343600 | 0.05567200 | O | -1.74203200 | 1.25701600 | 0.91270400 |
| C | -4.90858100 | 1.41532600 | 0.03080100 | O | 1.58410200 | 0.46161900 | -1.21783000 |
| H | -5.53942700 | 2.18290900 | -0.40072400 | S | -7.23564400 | -0.54485000 | -0.31013500 |
| C | 3.20430600 | -0.94649800 | -0.66887900 | S | 7.24781600 | -0.15024400 | 0.36030100 |
| C | 2.57817900 | 0.30352000 | -0.84225100 | O | 8.03272300 | 0.52924800 | -0.70985900 |
| C | 4.58098000 | -1.02150200 | -0.44983500 | O | 7.53580300 | -1.04227200 | 0.45900100 |
| C | 3.41741200 | 1.45955500 | -0.83304200 | O | 7.34836700 | 0.55429100 | 1.67047900 |
| C | 5.35828500 | 0.11173900 | -0.42709400 | O | -7.24193500 | -2.03098100 | -0.21867400 |
| H | 5.04964000 | -1.99012800 | -0.30983700 | O | -7.51237900 | -0.04459900 | -1.68756500 |
| C | 4.77439600 | 1.36739800 | -0.61565700 | O | -8.10551600 | 0.10474700 | 0.71267700 |
| H | 5.39778600 | 2.24972600 | -0.60119900 | H | -0.30488200 | 2.50850300 | 0.57748500 |
| O | -2.03279200 | 1.16239600 | 2.19325000 | H | -0.95089200 | 0.44056900 | -1.13772000 |
| O | 1.29637400 | 0.49829400 | -1.04815700 | H | -1.06849000 | 0.70090900 | -0.29158200 |
| S | -6.58085400 | -0.32739000 | -1.28858400 | O | 0.61125700 | 2.83224200 | 0.60557700 |
| S | 7.11757600 | 0.02462200 | -0.09545200 | H | 1.07594500 | 2.39655400 | -0.12767300 |
| O | 7.78168100 | 0.78479500 | -1.19375600 | H | -0.38607500 | 0.70570900 | 2.16659700 |
| O | 7.46958000 | -1.42271300 | -0.09475800 | O | 0.50757300 | 0.69327000 | 2.55300600 |
| O | 7.31708900 | 0.66855900 | 1.23609200 | H | 0.92084100 | 1.41460600 | 2.05266200 |
| O | -6.50923900 | -1.79475900 | -1.52224200 | H | -1.90506100 | -2.30998100 | -0.60289700 |
| O | -6.41400600 | 0.47526900 | -2.53193200 | H | -1.70292300 | -1.10583700 | 2.05091600 |
| O | -7.77693900 | 0.08172600 | -0.49960100 | H | 1.72397700 | -2.09083000 | 0.93163400 |
| H | -0.37882600 | 2.11272700 | 1.23752100 | H | 3.19665100 | -3.14122400 | -0.72303100 |
| H | -1.24428500 | 0.21417400 | -0.70471500 | Pd | 0.10959000 | -0.72795400 | -0.50488400 |
| H | -1.40816700 | 0.45497500 | 2.45804200 | O | -3.58454900 | 3.06116000 | 0.25658800 |
| O | 0.58859700 | 2.12119700 | 1.20449500 | O | 3.04195100 | 2.57357400 | -0.89825200 |
| H | 0.80905400 | 1.76630300 | 0.32038400 | C | 3.72945400 | 3.75757300 | -0.55832700 |
| H | 0.64568500 | -0.05955800 | 3.70881500 | H | 4.03763000 | 3.75230100 | 0.49256400 |
| O | 0.30548100 | -0.16068700 | 2.81553100 | H | 4.61084800 | 3.90673300 | -1.19003500 |
| H | 0.66553000 | 0.59398900 | 2.30478100 | H | 3.03114900 | 4.57623700 | -0.72129500 |
| H | -1.99066100 | -2.50495300 | -0.21356500 | C | -4.54024000 | 4.02336300 | -0.12583300 |
| H | -1.84674200 | -1.41351900 | 2.48588000 | H | -4.03844800 | 4.98861900 | -0.09971000 |
| H | 1.74878500 | -2.08253200 | 1.18273500 | H | -4.91210300 | 3.84156100 | -1.14016800 |
| H | 3.11047600 | -3.07512400 | -0.63199800 | H | -5.39091800 | 4.04439000 | 0.56407400 |
| Pd | -0.11889500 | -0.77853900 | -0.25995500 | | | | |
| O | -3.50977700 | 3.01178800 | 1.19391800 | 61 | | | |
| O | 2.76524200 | 2.63030700 | -1.04964400 | RR-PhOMe_D2_TS1_P, E(SCF) = -2637.88848936, | | | |
| C | 3.51010400 | 3.82212900 | -0.96669700 | E(ZPE) = -2637.433951, E(G) = -2637.507629 | | | |
| H | 3.96951200 | 3.94234500 | 0.02087000 | a.u. | | | |
| H | 4.29492700 | 3.86468100 | -1.72982700 | C | -0.77985100 | -3.23081600 | -1.04814500 |
| H | 2.81014800 | 4.63847700 | -1.13448000 | H | -0.50361900 | -3.68487800 | -0.09117900 |
| C | -4.28937800 | 4.06662000 | 0.67133600 | H | -1.47178500 | -3.89987600 | -1.56531500 |
| H | -3.85800700 | 4.98870600 | 1.05465500 | C | 0.44697100 | -2.93321800 | -1.86185500 |
| H | -4.25898600 | 4.08409600 | -0.42277500 | H | 1.00861800 | -3.84416000 | -2.08504200 |
| H | -5.33145000 | 3.99440500 | 0.99918700 | H | 0.18328200 | -2.43930900 | -2.80238500 |
| | | | | N | 1.28845500 | -2.00799600 | -1.07530100 |
| 61 | | | | N | -1.43634500 | -1.93584700 | -0.75559500 |
| RR-PhOMe_D1_TS2, E(SCF) = -2637.89115818, | | | | C | 2.47621900 | -1.52939600 | -1.82386700 |
| E(ZPE) = -2637.435973, E(G) = -2637.507550 | | | | H | 2.12423500 | -0.95747800 | -2.68584800 |
| a.u. | | | | C | -2.52833100 | -1.99836100 | 0.24444700 |
| C | 0.59903500 | -3.48986300 | -0.06869400 | H | -3.20922500 | -2.81051600 | -0.02916500 |
| H | 0.36144000 | -3.69658700 | -1.11579500 | C | 3.36493000 | -0.70396900 | -0.95558800 |
| H | 1.15906600 | -4.34152100 | 0.32830700 | C | 3.78657100 | -1.25248100 | 0.27501900 |
| C | -0.64404000 | -3.23211800 | 0.73833400 | C | 3.68241200 | 0.60111000 | -1.32132600 |
| H | -1.30805800 | -4.09971400 | 0.75127900 | C | 4.53366600 | -0.38653300 | 1.13715500 |
| H | -0.36959700 | -3.01053900 | 1.77472300 | C | 4.41430200 | 1.39927500 | -0.47227800 |
| N | -1.36211000 | -2.03704600 | 0.21668200 | H | 3.33694100 | 1.00156200 | -2.26919800 |
| N | 1.41134000 | -2.25893200 | -0.02719200 | C | 4.83426000 | 0.90677000 | 0.76646600 |
| C | -2.31481400 | -1.51977900 | 1.24596000 | H | 5.39645900 | 1.55735400 | 1.42673700 |
| H | -2.84875900 | -2.38715500 | 1.65104900 | C | -3.27438300 | -0.70528600 | 0.30131600 |
| C | 2.59249800 | -2.24848200 | -0.91558600 | C | -2.58358900 | 0.48293500 | 0.58549400 |
| H | 2.21133200 | -2.31354500 | -1.94045700 | C | -4.64948500 | -0.69316100 | 0.07461800 |
| C | -3.30756300 | -0.51796000 | 0.75143700 | C | -3.33723900 | 1.68846700 | 0.65939000 |
| C | -2.96431800 | 0.84367500 | 0.68838000 | C | -5.35456300 | 0.48412400 | 0.15671000 |
| C | -4.60393500 | -0.94109700 | 0.44807900 | H | -5.16940200 | -1.61624200 | -0.15745200 |

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -4.70104900 | 1.67943900 | 0.45191200 | O | 7.07701000 | 1.46978100 | -2.07614300 |
| H | -5.27575600 | 2.59663900 | 0.50707900 | H | -2.43053300 | -1.94408000 | 2.01017500 |
| O | 3.48067500 | -2.45539400 | 0.63845900 | H | 2.87576100 | -2.83164500 | -1.05466100 |
| O | -1.29247300 | 0.54767800 | 0.82741800 | H | -1.79561600 | -2.30006800 | -0.81641200 |
| S | 4.81625500 | 3.08972400 | -0.90604800 | H | 1.67552600 | -2.52493900 | 1.08885000 |
| S | -7.12574000 | 0.52602500 | -0.13516400 | H | 1.84617100 | -0.77663400 | 2.50773500 |
| O | -7.53203200 | -0.87949800 | -0.40879100 | O | 2.04439700 | -1.64350800 | 2.90217100 |
| O | -7.32094400 | 1.42874100 | -1.30545000 | H | 2.91825200 | -1.55168400 | 3.29001400 |
| O | -7.72899100 | 1.07545300 | 1.11227900 | H | 0.83919800 | 2.30075700 | 1.10095000 |
| O | 4.24723700 | 3.31574500 | -2.26449000 | O | 0.11881300 | 2.94718700 | 1.02514800 |
| O | 6.30557300 | 3.18413500 | -0.87786100 | H | -0.65138600 | 2.38210300 | 0.84476600 |
| O | 4.18066800 | 3.94691800 | 0.13779200 | Pd | -0.11077700 | -0.88014600 | 0.48434500 |
| H | -2.05956100 | -2.25762700 | 1.20017300 | H | -0.28116600 | 1.19712200 | -1.54845700 |
| H | 2.99184700 | -2.42489400 | -2.19944400 | H | 0.02958500 | 0.91846900 | -2.17315100 |
| H | -1.81556100 | -1.55094400 | -1.62394300 | O | -2.72149700 | 2.72190700 | 0.02969500 |
| H | 1.67185200 | -2.52523900 | -0.27048600 | O | 3.02830900 | 2.32960900 | 1.37480900 |
| H | 3.12355900 | -4.01315200 | -0.10090100 | C | -3.34033400 | 3.91201400 | -0.40052500 |
| O | 2.65862800 | -4.81841500 | -0.41187000 | H | -3.66055600 | 3.84404500 | -1.44587200 |
| H | 3.19989800 | -5.16283300 | -1.12361800 | H | -4.20682700 | 4.16341100 | 0.22066100 |
| H | 2.16504700 | -2.67088100 | 1.80750200 | H | -2.59390800 | 4.69873400 | -0.30678000 |
| O | 1.31049600 | -2.85741200 | 2.25392500 | C | 3.81665000 | 3.48026100 | 1.57749500 |
| H | 0.95552200 | -1.99392700 | 2.48105900 | H | 4.09912300 | 3.94499700 | 0.62694200 |
| Pd | 0.02438200 | -0.62085700 | -0.16400300 | H | 3.20515300 | 4.17645100 | 2.14844100 |
| H | 1.38800400 | 0.22953900 | 0.61333500 | H | 4.72443200 | 3.25176000 | 2.14594200 |
| H | 1.13664600 | 0.75613100 | 0.04389300 | | | | |
| O | -2.61621800 | 2.79743000 | 0.94402800 | | | | |
| O | 4.89925700 | -0.94590500 | 2.31973700 | 61 | | | |
| C | -3.30753000 | 4.02241100 | 1.04050200 | RR-PhOMe_D2_TS1, E(SCF) = -2637.88056831, | | | |
| H | -3.80724500 | 4.27908900 | 0.10017200 | E(ZPE) = -2637.427538, E(G) = -2637.499513 | | | |
| H | -4.05160800 | 4.00192300 | 1.84377400 | a.u. | | | |
| H | -2.56213800 | 4.78241000 | 1.26517100 | C | -0.84613900 | -3.31056900 | 0.41173300 |
| C | 5.62786400 | -0.14817600 | 3.22203700 | H | -0.64502600 | -3.26653400 | 1.48538100 |
| H | 5.05752700 | 0.73397800 | 3.53459300 | H | -1.46605600 | -4.18553900 | 0.20300700 |
| H | 5.82982000 | -0.76653500 | 4.09463100 | C | 0.44964700 | -3.33498800 | -0.35876200 |
| H | 6.58000800 | 0.18309000 | 2.79221400 | H | 1.04702500 | -4.21656700 | -0.10599600 |
| | | | | H | 0.27189300 | -3.34241800 | -1.43826500 |
| | | | | N | 1.17960800 | -2.09808000 | -0.01260600 |
| | | | | N | -1.56577900 | -2.06939000 | 0.04804400 |
| | | | | C | 2.45391400 | -1.93600600 | -0.72109200 |
| | | | | H | 2.21612800 | -1.78353700 | -1.78046200 |
| | | | | C | -2.65596800 | -1.67408700 | 0.96874400 |
| | | | | H | -3.29185800 | -2.54460800 | 1.16049300 |
| | | | | C | 3.36944100 | -0.84079600 | -0.22595400 |
| | | | | C | 3.06113000 | 0.06009400 | 0.81561100 |
| | | | | C | 4.60112900 | -0.76703900 | -0.88388700 |
| | | | | C | 4.05498000 | 1.04429800 | 1.13202600 |
| | | | | C | 5.53079000 | 0.18455200 | -0.54663800 |
| | | | | H | 4.82597400 | -1.46860200 | -1.68175700 |
| | | | | C | 5.26233400 | 1.09851700 | 0.47623800 |
| | | | | H | 6.00424800 | 1.84651600 | 0.73003100 |
| | | | | C | -3.48011200 | -0.56957000 | 0.38530100 |
| | | | | C | -2.87798100 | 0.63521000 | -0.00888700 |
| | | | | C | -4.85588000 | -0.75099000 | 0.24356300 |
| | | | | C | -3.71668000 | 1.66378500 | -0.52282100 |
| | | | | C | -5.64342100 | 0.25643200 | -0.26026600 |
| | | | | H | -5.31132300 | -1.69010900 | 0.53745600 |
| | | | | C | -5.07745700 | 1.47223400 | -0.63972000 |
| | | | | H | -5.71305200 | 2.25515800 | -1.03658100 |
| | | | | O | 1.93672100 | 0.06674700 | 1.46461100 |
| | | | | O | -1.58923000 | 0.88852200 | 0.08664600 |
| | | | | S | 7.11976600 | 0.26411200 | -1.37078500 |
| | | | | S | -7.41908900 | 0.04533100 | -0.43424500 |
| | | | | O | -7.70892800 | -1.35872700 | -0.03420800 |
| | | | | O | -7.72029000 | 0.31779700 | -1.86840300 |
| | | | | O | -8.03605300 | 1.05126600 | 0.47706600 |
| | | | | O | 7.06558200 | -0.72620000 | -2.48267700 |
| | | | | O | 8.13834900 | -0.08360500 | -0.33617700 |
| | | | | O | 7.26494600 | 1.66910900 | -1.85194300 |
| | | | | H | -2.17733200 | -1.39308100 | -1.91385700 |
| | | | | H | 2.98728900 | -2.89587800 | -0.66405000 |
| | | | | H | -1.95324900 | -2.16704700 | -0.89236900 |
| | | | | H | 1.34861600 | -2.11594000 | 1.00114800 |
| | | | | H | 1.38148500 | -1.09403000 | 2.62088800 |
| | | | | O | 0.93982100 | -1.91793000 | 2.92848900 |
| | | | | H | 1.48470200 | -2.26302600 | 3.63919300 |
| | | | | H | 0.87270000 | 1.44658600 | 1.98276600 |
| | | | | O | 0.12347800 | 2.04732900 | 2.17100600 |
| | | | | H | -0.55837400 | 1.78126100 | 1.53580900 |

61
RR-PhOMe_D2_TS1_R, E(SCF) = -2637.91673115,
E(ZPE) = -2637.463399, E(G) = -2637.536277
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.86567100 | -3.59218000 | 0.48444000 |
| H | -0.72801400 | -3.63580400 | 1.56860300 |
| H | -1.48262500 | -4.44395700 | 0.18361000 |
| C | 0.46407000 | -3.59256600 | -0.22758000 |
| H | 1.03470200 | -4.50119300 | -0.02125400 |
| H | 0.30748400 | -3.53522300 | -1.30898600 |
| N | 1.22878200 | -2.38845400 | 0.17296400 |
| N | -1.54192400 | -2.31270700 | 0.17258500 |
| C | 2.22918400 | -1.97728200 | -0.82190200 |
| H | 1.67350000 | -1.74056100 | -1.73833600 |
| C | -2.75617300 | -2.03368000 | 0.96799700 |
| H | -3.43984700 | -2.88689500 | 0.90157500 |
| C | 3.08877300 | -0.81729700 | -0.40562600 |
| C | 2.62848300 | 0.26129600 | 0.36609100 |
| C | 4.39828400 | -0.81279400 | -0.89765000 |
| C | 3.53964300 | 1.33074800 | 0.61386800 |
| C | 5.24874200 | 0.23482500 | -0.64978800 |
| H | 4.75114900 | -1.65044200 | -1.48987700 |
| C | 4.82122900 | 1.31982200 | 0.11392500 |
| H | 5.50218900 | 2.13844000 | 0.31089000 |
| C | -3.43626800 | -0.79421100 | 0.47905300 |
| C | -2.73953800 | 0.42622000 | 0.45339800 |
| C | -4.76532200 | -0.86121600 | 0.06117100 |
| C | -3.45036600 | 1.57921400 | 0.01299300 |
| C | -5.42434400 | 0.26927000 | -0.36046300 |
| H | -5.28945800 | -1.81068400 | 0.07795500 |
| C | -4.76542800 | 1.49870400 | -0.38884300 |
| H | -5.29561000 | 2.38043600 | -0.73074100 |
| O | 1.44007600 | 0.37078100 | 0.93074800 |
| O | -1.49424900 | 0.58327500 | 0.83457300 |
| S | 6.93474200 | 0.22674700 | -1.26517500 |
| S | -7.12776300 | 0.19500800 | -0.91844600 |
| O | -7.56170900 | -1.21756600 | -0.73364800 |
| O | -7.10797000 | 0.61432600 | -2.34985800 |
| O | -7.88191800 | 1.15352700 | -0.05998500 |
| O | 7.07410300 | -1.01608200 | -2.07294300 |
| O | 7.80959500 | 0.23625800 | -0.05728200 |

| | | | |
|----|-------------|-------------|-------------|
| Pd | -0.18721900 | -0.55556500 | -0.11123800 |
| H | 1.10249500 | 0.87905700 | -0.44476000 |
| H | 0.78475600 | 0.77111900 | -1.15216500 |
| O | -3.07389400 | 2.80326000 | -0.86718900 |
| O | 3.68783300 | 1.89483000 | 2.12517700 |
| C | -3.84851300 | 3.86812100 | -1.37115100 |
| H | -4.36702600 | 3.58909100 | -2.29470000 |
| H | -4.58729200 | 4.21064100 | -0.63868500 |
| H | -3.15671100 | 4.68045100 | -1.58403600 |
| C | 4.59986600 | 2.90093800 | 2.49511500 |
| H | 4.83145900 | 3.56674400 | 1.65610300 |
| H | 4.12368600 | 3.47875000 | 3.28514400 |
| H | 5.53608800 | 2.47871900 | 2.87781800 |

61

RR-PhOMe_D2_TS2_P, E(SCF) = -2637.91238566,
E(ZPE) = -2637.456032, E(G) = -2637.530477
a.u.

| | | | |
|----|-------------|--------------|-------------|
| C | -0.22693500 | -2.20854300 | 0.91467000 |
| H | 0.06320000 | -1.71156700 | 1.84612400 |
| H | -0.49330900 | -3.24259900 | 1.15602400 |
| C | 0.90772400 | -2.15757100 | -0.07822300 |
| H | 1.77832400 | -2.72041700 | 0.27569200 |
| H | 0.59280100 | -2.58711000 | -1.03345000 |
| N | 1.27580600 | -0.73867700 | -0.31343700 |
| N | -1.36564400 | -1.46819300 | 0.34830100 |
| C | 2.31062200 | -0.516941800 | -1.38045800 |
| H | 1.92314400 | 0.12199400 | -2.13076400 |
| C | -2.41253100 | -1.08288200 | 1.30817500 |
| H | -2.74453400 | -1.95396700 | 1.88593800 |
| C | 3.61937300 | -0.10236800 | -0.82290900 |
| C | 3.72691400 | 1.15103300 | -0.23294400 |
| C | 4.73849200 | -0.93419200 | -0.87090300 |
| C | 4.94878300 | 1.56372800 | 0.33263300 |
| C | 5.93564300 | -0.51604400 | -0.33906700 |
| H | 4.66616900 | -1.91328900 | -1.33143400 |
| C | 6.04824000 | 0.72858100 | 0.27025400 |
| H | 6.99797600 | 1.03154500 | 0.69412100 |
| C | -3.58548400 | -0.47055900 | 0.60414900 |
| C | -3.43318000 | 0.69036800 | -0.17485100 |
| C | -4.83941200 | -1.06444700 | 0.75249100 |
| C | -4.60490300 | 1.23622100 | -0.77762500 |
| C | -5.95077800 | -0.51814600 | 0.15601000 |
| H | -4.94108900 | -1.96205500 | 1.35274900 |
| C | -5.83680300 | 0.63957800 | -0.61198100 |
| H | -6.72257000 | 1.05742600 | -1.07606400 |
| O | 2.70061300 | 2.02825900 | -0.11232300 |
| O | -2.29930300 | 1.33163900 | -0.36074500 |
| S | 7.38321600 | -1.58738700 | -0.37230500 |
| S | -7.57353400 | -1.25614100 | 0.35690900 |
| O | -8.05981100 | -1.56017700 | -1.02020000 |
| O | -8.40917600 | -0.22253400 | 1.03458600 |
| O | -7.37557200 | -2.47775600 | 1.18520800 |
| O | 7.65951600 | -1.92379500 | 1.05222200 |
| O | 8.46720500 | -0.77442900 | -0.98954200 |
| O | 6.99558300 | -2.76818600 | -1.18877000 |
| H | -1.94849300 | -0.37842600 | 2.01074300 |
| H | 2.45152200 | -1.52831300 | -1.88247200 |
| H | -1.78801400 | -2.01446600 | -0.40097000 |
| H | 1.65600900 | -0.39257500 | 0.57757700 |
| H | 2.24850700 | 1.40249900 | 1.92718300 |
| O | 1.93232900 | 0.56892200 | 2.30080900 |
| H | 2.61140500 | 0.30035600 | 2.92582800 |
| H | -0.35384500 | 2.84477100 | 1.45661600 |
| O | -1.28440500 | 2.96635900 | 1.66436900 |
| H | -1.73132600 | 2.45339200 | 0.96303400 |
| Pd | -0.50402700 | 0.33155300 | -0.44237400 |
| H | 1.86956800 | 1.71836000 | -0.52357100 |
| H | 0.18507400 | 1.65290000 | -0.98617900 |
| O | -4.39990300 | 2.36255000 | -1.50453100 |
| O | 4.93427300 | 2.77988700 | 0.91755400 |
| C | -5.51763200 | 2.95992100 | -2.11886300 |
| H | -5.99049800 | 2.28664000 | -2.84233300 |
| H | -6.26683100 | 3.26989800 | -1.38213500 |
| H | -5.15082200 | 3.84062600 | -2.64252300 |
| C | 6.13071600 | 3.23882500 | 1.51295200 |
| H | 5.91139700 | 4.22041900 | 1.92677000 |

| | | | |
|---|------------|------------|------------|
| H | 6.45729000 | 2.57451900 | 2.31920900 |
| H | 6.93425500 | 3.33213100 | 0.77565900 |

61

RR-PhOMe_D2_TS2_R, E(SCF) = -2637.88389784,
E(ZPE) = -2637.428785, E(G) = -2637.501866
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.39992200 | -2.66640000 | 0.72214300 |
| H | -0.05935000 | -2.29566200 | 1.69328100 |
| H | -0.84062800 | -3.65575400 | 0.86509800 |
| C | 0.74650800 | -2.68899000 | -0.25752300 |
| H | 1.54261300 | -3.36142900 | 0.07632300 |
| H | 0.41351800 | -3.01745300 | -1.24586100 |
| N | 1.24808800 | -1.30256900 | -0.36583200 |
| N | -1.41602300 | -1.71305000 | 0.21832100 |
| C | 2.38509200 | -1.09632300 | -1.31149700 |
| H | 1.99522200 | -0.58734900 | -2.19651100 |
| C | -2.40516900 | -1.25739900 | 1.22083500 |
| H | -2.81002500 | -2.12810700 | -1.74708600 |
| C | 3.52854400 | -0.35054100 | -0.68532700 |
| C | 3.31902000 | 0.88951400 | -0.04494500 |
| C | 4.80701900 | -0.90343600 | -0.76784700 |
| C | 4.46196400 | 1.51947500 | 0.53783400 |
| C | 5.88900800 | -0.25444500 | -0.22202300 |
| H | 4.95441100 | -1.85542600 | -1.26720300 |
| C | 5.71789300 | 0.96164900 | 0.44041900 |
| H | 6.57967500 | 1.45178000 | 0.87902600 |
| C | -3.52093600 | -0.49827900 | 0.57189400 |
| C | -3.25571000 | 0.63560500 | -0.21286500 |
| C | -4.83222000 | -0.93097400 | 0.77022400 |
| C | -4.36569200 | 1.33471600 | -0.76617200 |
| C | -5.88527900 | -0.23990100 | 0.22132100 |
| H | -5.02612800 | -1.81395400 | 1.36913400 |
| C | -5.65591200 | 0.89842400 | -0.54891100 |
| H | -6.49876200 | 1.42842700 | -0.97701600 |
| O | 2.14522600 | 1.44203100 | 0.08111200 |
| O | -2.05197400 | 1.11525400 | -0.45252600 |
| S | 7.53837200 | -0.94756300 | -0.32935600 |
| S | -7.57729800 | -0.79697100 | 0.44616000 |
| O | -8.08483400 | -1.10866500 | -0.92090000 |
| O | -8.30218300 | 0.34517400 | 1.07272900 |
| O | -7.50343000 | -1.99491200 | 1.32659400 |
| O | 7.97947300 | -1.18598900 | 1.07652700 |
| O | 8.37271100 | 0.08351000 | -1.01303200 |
| O | 7.41077100 | -2.20579600 | -1.11652700 |
| H | -1.85154800 | -0.65412600 | 1.94980000 |
| H | 2.73619700 | -2.07778800 | -1.64264100 |
| H | -1.91706600 | -2.13861300 | -0.56384200 |
| H | 1.55001300 | -1.01896100 | 0.57781600 |
| H | 1.65800400 | 0.66531800 | 1.73788400 |
| O | 1.45523600 | -0.09699900 | 2.31487400 |
| H | 2.18751200 | -0.14979700 | 2.93451800 |
| H | 0.66713400 | 2.54462200 | 0.80790400 |
| O | -0.18521000 | 2.89702800 | 1.10774900 |
| H | -0.85576800 | 2.37477000 | 0.64070500 |
| Pd | -0.42650800 | -0.09722800 | -0.57569300 |
| H | 0.88153400 | 1.18776400 | -0.90721600 |
| H | 0.25742400 | 1.21729600 | -1.49089700 |
| O | -4.04519600 | 2.42778400 | -1.49755300 |
| O | 4.19414000 | 2.68631900 | 1.17801700 |
| C | -5.10093600 | 3.16859200 | -2.06654000 |
| H | -5.67883800 | 2.56780600 | -2.77705200 |
| H | -5.77804800 | 3.55963900 | -1.29959600 |
| H | -4.64434100 | 4.00226900 | -2.59609800 |
| C | 5.27259000 | 3.36679100 | 1.77509800 |
| H | 4.86031400 | 4.26369400 | 2.23368900 |
| H | 5.75582100 | 2.75993100 | 2.54889800 |
| H | 6.02586600 | 3.65924000 | 1.03513200 |

61

RR-PhOMe_D2_TS2, E(SCF) = -2637.87943053,
E(ZPE) = -2637.424145, E(G) = -2637.495620
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.40069000 | -2.71673600 | 0.60687500 |
| H | -0.07268200 | -2.39713900 | 1.60030400 |
| H | -0.84241000 | -3.71222500 | 0.69113400 |
| C | 0.75861200 | -2.68649700 | -0.35681400 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|--------------|-------------|
| H | 1.55149800 | -3.37466300 | -0.04840000 | C | 4.64668300 | -0.34451900 | 1.11414400 |
| H | 0.44017300 | -2.96155800 | -1.36595400 | C | 4.50514900 | 1.33713400 | -0.58300300 |
| N | 1.25848200 | -1.29566300 | -0.38394400 | H | 3.36941400 | 0.86878000 | -2.32580400 |
| N | -1.41200100 | -1.73827100 | 0.14038200 | C | 4.96130300 | 0.92558400 | 0.66297900 |
| C | 2.40746700 | -1.03823700 | -1.30214200 | H | 5.56408000 | 1.59748600 | 1.26189600 |
| H | 2.03127000 | -0.47124100 | -2.15711800 | C | -3.35165700 | -0.71918100 | 0.17569000 |
| C | -2.41472600 | -1.33874500 | 1.15372900 | C | -2.63851900 | 0.40540100 | 0.64083200 |
| H | -2.82574800 | -2.23822000 | 1.62385500 | C | -4.71676300 | -0.63301500 | -0.09849800 |
| C | 3.54825800 | -0.33902400 | -0.62057500 | C | -3.38811000 | 1.60552200 | 0.85279000 |
| C | 3.33751900 | 0.87368300 | 0.08705300 | C | -5.40392800 | 0.54093800 | 0.09818500 |
| C | 4.82041500 | -0.88932000 | -0.72323800 | H | -5.24654800 | -1.50580500 | -0.46563200 |
| C | 4.48102500 | 1.45567800 | 0.70173500 | C | -4.73695900 | 1.66795300 | 0.58038200 |
| C | 5.91055100 | -0.27958100 | -0.13543200 | H | -5.29152100 | 2.58713000 | 0.72976500 |
| H | 4.96478800 | -1.81485500 | -1.27129500 | O | 3.56207900 | -2.44450300 | 0.75972500 |
| C | 5.73444700 | 0.89563900 | 0.58499600 | O | -1.36462100 | 0.43806600 | 0.92829600 |
| H | 6.57973200 | 1.36810300 | 1.07747000 | S | 4.93360000 | 2.99663300 | -1.14128800 |
| C | -3.52254000 | -0.54198400 | 0.53743700 | S | -7.15856300 | 0.65896400 | -0.24107400 |
| C | -3.24868700 | 0.63208000 | -0.18255400 | O | -7.55916900 | -0.65301000 | -0.82268900 |
| C | -4.83678400 | -0.97844100 | -0.72323800 | O | -7.31868600 | 1.79117200 | -1.19965700 |
| C | -4.35299100 | 1.36827700 | -0.69772700 | O | -7.81650700 | 0.93645800 | 1.07002500 |
| C | -5.88427200 | -0.25180100 | 0.19330000 | O | 4.32479300 | 3.91870600 | -0.14309000 |
| H | -5.03735800 | -1.89214900 | 1.25439200 | O | 4.34734100 | 3.13289800 | -2.50088600 |
| C | -5.64608400 | 0.92572300 | -0.51105200 | O | 6.42197700 | 3.04575500 | -1.13507900 |
| H | -6.48452400 | 1.48429300 | -0.91136700 | H | -2.22166800 | -2.40553000 | 0.91354700 |
| O | 2.16310600 | 1.41499800 | 0.22539100 | H | 3.04397000 | -2.53223200 | -2.07648300 |
| O | -2.04236900 | 1.11894700 | -0.39273800 | H | -1.92040800 | -1.47966100 | -1.83608200 |
| S | 7.56026300 | -0.95722300 | -0.31390700 | H | 1.54039900 | -2.73011500 | -0.34601900 |
| S | -7.57885100 | -0.81879300 | 0.37137900 | H | 1.21927800 | -1.26988100 | 2.03604900 |
| O | -8.06209800 | -1.08744400 | -1.01367600 | H | 2.92022600 | -4.25531200 | 0.22134400 |
| O | -8.31699800 | 0.30095400 | 1.02219600 | O | 2.06071300 | -4.69132600 | 0.14147000 |
| O | -7.51685400 | -2.04471400 | 1.21316600 | H | 2.20759800 | -5.45837600 | -0.41711900 |
| O | 8.12774800 | -1.03040400 | 1.06339600 | H | 3.08329400 | -2.36345800 | 1.61788300 |
| O | 8.30565400 | 0.00267800 | -1.18008400 | O | 1.73433400 | -1.82302200 | 2.65304000 |
| O | 7.39218600 | -2.29552600 | -0.94629300 | H | 1.12018900 | -2.49937300 | 2.95361600 |
| H | -1.86965900 | -0.77846400 | 1.92249500 | Pd | -0.00878300 | -0.722086900 | -0.08960400 |
| H | 2.75601800 | -1.99903600 | -1.69104900 | H | 1.15838800 | 0.09256700 | 0.56907400 |
| H | -1.90094200 | -2.12205800 | -0.67066200 | O | -2.66015100 | 2.65058300 | 1.32400900 |
| H | 1.54539700 | -1.06084300 | 0.57736500 | O | 5.03692500 | -0.86221300 | 2.29773200 |
| H | 1.62124800 | 0.55774000 | 1.81361200 | C | -3.33223400 | 3.86496600 | 1.55669300 |
| O | 1.40567800 | -0.22736300 | 2.35467900 | H | -3.76642400 | 4.27190600 | 0.63633700 |
| H | 2.11794900 | -0.29909400 | 2.99529800 | H | -4.12807400 | 3.75176800 | 2.30164200 |
| H | 0.66954000 | 2.49385000 | 0.96337100 | H | -2.58980800 | 4.56478600 | 1.93599000 |
| O | -0.18778600 | 2.83866700 | 1.25791300 | C | 5.81016800 | -0.04405100 | 3.15207500 |
| H | -0.85106200 | 2.33402900 | 0.76207000 | H | 5.26166400 | 0.85605200 | 3.44683300 |
| Pd | -0.41526600 | -0.08416800 | -0.55375400 | H | 6.02500900 | -0.63789800 | 4.03743900 |
| H | 0.87682800 | 1.21771600 | -0.81596400 | H | 6.75265300 | 0.24798500 | 2.67842700 |
| H | 0.26941800 | 1.27809700 | -1.40504400 | | | | |
| O | -4.02390900 | 2.50042800 | -1.36267900 | 61 | | | |
| O | 4.27663700 | 2.57817800 | 1.46216700 | RR-PhOMe_D2_TS2W_R, E(SCF) = - | | | |
| C | -5.07409100 | 3.28548500 | -1.88063000 | 2637.88845837, E(ZPE) = -2637.434557, E(G) | | | |
| H | -5.66170000 | 2.73501500 | -2.62320400 | = -2637.507998 a.u. | | | |
| H | -5.74322800 | 3.63662600 | -1.08782900 | C | -0.88203900 | -3.27354100 | -1.06509000 |
| H | -4.61084900 | 4.14479100 | -2.36128600 | H | -0.68138200 | -3.75814000 | -0.10480300 |
| C | 4.95174100 | 3.73632400 | 1.01367300 | H | -1.54733000 | -3.91988600 | -1.64350400 |
| H | 4.63904500 | 4.56225000 | 1.65176200 | C | 0.39654700 | -2.97889200 | -1.79604900 |
| H | 6.033972100 | 3.63318600 | 1.08612200 | H | 0.966663600 | -3.89031000 | -1.99674000 |
| H | 4.68887600 | 3.96595700 | -0.02524700 | H | 0.18524000 | -2.48277600 | -2.74874000 |
| | | | | N | 1.20655100 | -2.05378500 | -0.97382600 |
| 61 | | | | N | -1.53843900 | -1.97714300 | -0.77989500 |
| RR-PhOMe_D2_TS2W_P, E(SCF) = - | | | | C | 2.35046700 | -1.50203100 | -1.73842200 |
| 2637.91673726, E(ZPE) = -2637.460142, E(G) | | | | H | 1.94791100 | -0.90973400 | -2.56400800 |
| = -2637.534005 a.u. | | | | C | -2.70150100 | -2.06318500 | 0.13420200 |
| C | -0.89461700 | -3.18078700 | -1.33423000 | H | -3.38792600 | -2.82961000 | -0.23993900 |
| H | -0.70628200 | -3.72545700 | -0.40276300 | C | 3.27554100 | -0.68308800 | -0.90040900 |
| H | -1.51668300 | -3.81692900 | -1.97331300 | C | 3.74047500 | -1.21126100 | 0.32221900 |
| C | 0.41156800 | -2.84686500 | -2.00813900 | C | 3.65918300 | 0.58177400 | -1.33975100 |
| H | 0.93598400 | -3.75354600 | -2.32729300 | C | 4.62157700 | -0.38035400 | 1.08412100 |
| H | 0.23226000 | -2.23058300 | -2.89479700 | C | 4.51004400 | 1.35131800 | -0.58055400 |
| N | 1.26211200 | -2.06693600 | -1.07543200 | H | 3.28287400 | 0.97073100 | -2.28076400 |
| N | -1.56774700 | -1.92234200 | -0.98916300 | C | 4.99499300 | 0.86887500 | 0.63705300 |
| C | 2.50457900 | -1.63108800 | -1.75101400 | H | 5.66195300 | 1.49227700 | 1.22160200 |
| H | 2.21274400 | -1.08423600 | -2.65049800 | C | -3.40861400 | -0.75169500 | 0.23760300 |
| C | -2.66587700 | -2.03698200 | -0.01975600 | C | -2.70524300 | 0.38083300 | 0.67592000 |
| H | -3.39705600 | -2.78533400 | -0.35081300 | C | -4.76222700 | -0.67124700 | -0.08343100 |
| C | 3.38787100 | -0.76059500 | -0.91449600 | C | -3.42675500 | 1.60194400 | 0.80410600 |
| C | 3.86055700 | -1.19171400 | 0.31430600 | C | -5.43505000 | 0.52054400 | 0.04783500 |
| C | 3.72878400 | 0.51333200 | -1.36638700 | H | -5.29165400 | -1.55185500 | -0.43045500 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -4.77040100 | 1.66072500 | 0.49716200 | O | 6.60985100 | 2.67609300 | -1.63276400 |
| H | -5.31866300 | 2.59106400 | 0.58926400 | H | -2.45534000 | -2.50940700 | 0.94789500 |
| O | 3.35436600 | -2.36395700 | 0.77624000 | H | 2.85992900 | -2.31305400 | -2.13467100 |
| O | -1.43492900 | 0.37420600 | 1.01237400 | H | -1.86479400 | -1.49958600 | -1.72791300 |
| S | 5.04325700 | 2.96714700 | -1.13698800 | H | 1.60532300 | -2.62537200 | -0.19739700 |
| S | -7.18833800 | 0.63763800 | -0.32116700 | H | 1.18411100 | -0.55203300 | 1.57449700 |
| O | -7.57701100 | -0.67999200 | -0.89471100 | H | 3.22361300 | -3.85888200 | 0.09984000 |
| O | -7.32667500 | 1.76076000 | -1.29125500 | O | 2.89197800 | -4.68417200 | -0.31411500 |
| O | -7.85733000 | 0.92676100 | 0.98013500 | H | 3.44912500 | -4.82220200 | -1.08313200 |
| O | 4.66067800 | 3.92716600 | -0.05994800 | H | 2.40309600 | -1.79342700 | 2.03805900 |
| O | 4.32864200 | 3.22083400 | -2.41970300 | O | 1.72291500 | -1.22406200 | 2.54676100 |
| O | 6.52386900 | 2.87729100 | -1.30676200 | H | 1.05433100 | -1.81257500 | 2.91738100 |
| H | -2.31038800 | -2.40256400 | 1.09941500 | Pd | -0.15213100 | -0.81775900 | 0.10259800 |
| H | 2.87463300 | -2.36420000 | -2.17740200 | H | 1.02242300 | 0.10950500 | 0.84166300 |
| H | -1.84609400 | -1.55522800 | -1.65860400 | O | -2.77015700 | 2.51133700 | 1.53371400 |
| H | 1.64250600 | -2.57294000 | -0.19749200 | O | 5.09421000 | -0.86177400 | 2.26956900 |
| H | 1.15601800 | -0.07594500 | 1.08030600 | C | -3.41458600 | 3.74331500 | 1.76066500 |
| H | 3.21086400 | -3.92277000 | -0.02256400 | H | -3.77418400 | 4.18952300 | 0.82691800 |
| O | 2.87854800 | -4.75034100 | -0.43280900 | H | -4.25921800 | 3.63685300 | 1.900419000 |
| H | 3.46359200 | -4.91609900 | -1.17499600 | H | -2.67423800 | 4.40414400 | 2.20721500 |
| H | 2.31741100 | -1.88691900 | 2.16182000 | C | 6.00561900 | -0.10741800 | 3.03293600 |
| O | 1.67314600 | -1.43679700 | 2.75238700 | H | 5.58087700 | 0.85660300 | 3.33423500 |
| H | 0.89059300 | -1.99455300 | 2.73288100 | H | 6.22596900 | -0.69247200 | 3.92427200 |
| Pd | -0.09298200 | -0.74635200 | -0.00156700 | H | 6.93789100 | 0.07382000 | 2.48642400 |
| H | 1.16575600 | 0.43429400 | 0.43414500 | | | | |
| O | -2.69602900 | 2.65353300 | 1.24245000 | 64 | | | |
| O | 5.04371500 | -0.92771800 | 2.25398200 | RR-PhOMe_ID1_TS1_H2-out_R, E(SCF) = - | | | |
| C | -3.35776600 | 3.88574000 | 1.41757000 | 2714.36390998, E(ZPE) = -2713.884296, E(G) | | | |
| H | -3.76512700 | 4.26419300 | 0.47374900 | = -2713.959176 a.u. | | | |
| H | -4.16974900 | 3.80594400 | 2.14835400 | C | 0.57127700 | -3.59658300 | -0.20477700 |
| H | -2.61372600 | 4.58764000 | 1.78867200 | H | 0.27822100 | -3.61029500 | -1.25862000 |
| C | 5.91408100 | -0.16464500 | 3.05442400 | H | 1.18474000 | -4.48026000 | -0.01335200 |
| H | 5.44953100 | 0.77364000 | 3.37823200 | C | -0.64846000 | -3.55551400 | 0.68517100 |
| H | 6.14326600 | -0.76734900 | 3.93133100 | H | -1.27520100 | -4.44115400 | 0.55225000 |
| H | 6.84713800 | 0.06836600 | 2.52874200 | H | -0.36044900 | -3.49482400 | 1.73834700 |
| | | | | N | -1.39719100 | -2.32266800 | 0.35364400 |
| 61 | | | | N | 1.35044600 | -2.35633800 | 0.02239100 |
| RR-PhOMe_D2_TS2W, E(SCF) = -2637.87864656, | | | | C | -2.49510700 | -1.95208700 | 1.27394500 |
| E(ZPE) = -2637.425690, E(G) = -2637.496930 | | | | H | -3.14483600 | -2.81812900 | 1.43717000 |
| a.u. | | | | C | 2.36300400 | -2.04363200 | -1.00630700 |
| C | -0.93323800 | -3.24446000 | -1.17414900 | H | 1.81223500 | -1.82724000 | -1.92848000 |
| H | -0.78082900 | -3.77890000 | -0.23132200 | C | -3.29122100 | -0.82268800 | 0.69289800 |
| H | -1.56042300 | -3.86725200 | -1.81928800 | C | -2.66461300 | 0.38746800 | 0.36263100 |
| C | 0.38186300 | -2.92290900 | -1.82743800 | C | -4.65156400 | -0.99621800 | 0.44231300 |
| H | 0.94666700 | -3.82894700 | -2.06498000 | C | -3.45490100 | 1.41790100 | -0.20691600 |
| H | 0.21030300 | -2.37346000 | -2.75865000 | C | -5.39660500 | 0.02148500 | -0.10779200 |
| N | 1.17984300 | -2.04993200 | -0.93399100 | H | -5.13227600 | -1.93734100 | 0.68602500 |
| N | -1.60102200 | -1.96643300 | -0.85947500 | C | -4.80113100 | 1.23713200 | -0.43784200 |
| C | 2.32521800 | -1.46763100 | -1.67496500 | H | -5.40001700 | 2.02368400 | -0.88208300 |
| H | 1.91795700 | -0.86299800 | -2.48911800 | C | 3.23858500 | -0.89993500 | -0.58834600 |
| C | -2.79952700 | -2.09199300 | -0.00522800 | C | 2.69647400 | 0.32865200 | -0.17871000 |
| H | -3.49394400 | -2.81134400 | -0.45316400 | C | 4.62370900 | -1.06516700 | -0.65015600 |
| C | 3.26484000 | -0.64898000 | -0.84936900 | C | 3.59923600 | 1.38375500 | 0.12886300 |
| C | 3.75111900 | -1.15111600 | 0.37006500 | C | 5.47222600 | -0.02957800 | -0.34150100 |
| C | 3.68437900 | 0.58825600 | -1.33384900 | H | 5.03902100 | -2.01875800 | -0.95760100 |
| C | 4.67382300 | -0.33633100 | 1.08982200 | C | 4.96183400 | 1.20747300 | 0.05102800 |
| C | 4.58158700 | 1.34707900 | -0.61817000 | H | 5.64312700 | 2.01457900 | 0.29424400 |
| H | 3.29788400 | 0.96617500 | -2.27509600 | O | -1.38192600 | 0.63364800 | 0.55768700 |
| C | 5.08451400 | 0.88531400 | 0.59737100 | O | 1.41291900 | 0.60121000 | -0.06900600 |
| H | 5.78445900 | 1.50289200 | 1.14818200 | S | -7.14808200 | -0.19369600 | -0.44794100 |
| C | -3.47994400 | -0.77343700 | 0.17772500 | S | 7.25380000 | -0.24273600 | -0.40241700 |
| C | -2.77891000 | 0.29946600 | 0.75468200 | O | 7.73399700 | -0.05740200 | 0.99733900 |
| C | -4.81466100 | -0.63375600 | -0.20026000 | O | 7.75801100 | 0.81916500 | -1.31905200 |
| C | -3.49289700 | 1.51687000 | 0.96255900 | O | 7.48653000 | -1.61881900 | -0.92031000 |
| C | -5.47589500 | 0.55323300 | 0.00752700 | O | -7.49854400 | -1.55290000 | 0.04629800 |
| H | -5.34039400 | -1.46766500 | -0.65266600 | O | -7.29049000 | -0.05452400 | -1.92536000 |
| C | -4.81630600 | 1.63270200 | 0.59491400 | O | -7.84054300 | 0.89664100 | 0.29520200 |
| H | -5.35472600 | 2.56078600 | 0.74810800 | H | -0.47838600 | 2.29961400 | 0.97952600 |
| O | 3.33137400 | -2.28276600 | 0.87827200 | H | -2.71691000 | -0.79317700 | -2.78867000 |
| O | -1.52958500 | 0.24485200 | 1.14898800 | H | -2.52465400 | -0.28653400 | -2.26998100 |
| S | 5.18380100 | 2.90974200 | -1.25776100 | O | 0.21167000 | 2.85143800 | 1.38709500 |
| S | -7.19857900 | 0.74872600 | -0.45180000 | H | 1.02625400 | 2.49567700 | 0.99231400 |
| O | -7.60511600 | -0.53438500 | -1.08916900 | H | -0.93163000 | 0.55784700 | 2.56652700 |
| O | -7.24399200 | 1.90602900 | -1.39152500 | O | -0.47683600 | 0.90735500 | 3.34684000 |
| O | -7.93132300 | 1.02403700 | 0.81822800 | H | -0.06074400 | 1.69870700 | 2.96491500 |
| O | 5.04839800 | 3.89307400 | -0.14448100 | H | -1.79532100 | -2.42535200 | -0.58206300 |
| O | 4.32580500 | 3.23616500 | -2.43082300 | H | -2.03167700 | -1.69694300 | 2.23285900 |

| | | | |
|--|-------------|-------------|-------------|
| H | 1.82023100 | -2.42214400 | 0.92684200 |
| H | 2.98134300 | -2.92894000 | -1.18936900 |
| Pd | 0.00112700 | -0.83088000 | 0.20143200 |
| O | -0.17747700 | 2.11069100 | -1.91121400 |
| H | 0.44988100 | 1.63342800 | -1.34192800 |
| H | -0.98640900 | 2.13593100 | -1.37867700 |
| O | 2.99439400 | 2.54338600 | 0.49629400 |
| O | -2.76452000 | 2.54850300 | -0.51144400 |
| C | 3.81062300 | 3.63809000 | 0.85306800 |
| H | 4.45137700 | 3.39675900 | 1.70730600 |
| H | 4.43663200 | 3.95921600 | 0.01449300 |
| H | 3.13655800 | 4.44729400 | 1.12753200 |
| C | -3.47441800 | 3.62381200 | -1.09289300 |
| H | -3.92271200 | 3.33647600 | -2.04924200 |
| H | -4.25821400 | 3.98928400 | -0.42253000 |
| H | -2.74742700 | 4.41572800 | -1.26117100 |
| 62 | | | |
| RR-PhOMe_ID2_TS1_P, E(SCF) = - | | | |
| 2713.16708850, E(ZPE) = -2712.702612, E(G) | | | |
| = -2712.776854 a.u. | | | |
| C | -0.89538000 | -3.35520600 | -0.91453900 |
| H | -0.72222100 | -3.80140200 | 0.06841000 |
| H | -1.53478500 | -4.03006100 | -1.49082600 |
| C | 0.39777700 | -3.07006100 | -1.62253600 |
| H | 1.00023000 | -3.97142200 | -1.76725400 |
| H | 0.19098800 | -2.63775300 | -2.60702000 |
| N | 1.17289300 | -2.06692500 | -0.85206900 |
| N | -1.57221300 | -2.05770600 | -0.69700000 |
| C | 2.19491100 | -1.43181100 | -1.72185400 |
| H | 1.66910000 | -0.82902300 | -2.46688200 |
| C | -2.77505700 | -2.13964500 | 0.16344400 |
| H | -3.45104100 | -2.89698700 | -0.24705300 |
| C | 3.18329700 | -0.60456300 | -0.96933300 |
| C | 3.85197700 | -1.17974900 | 0.12738200 |
| C | 3.44382200 | 0.70194600 | -1.37172100 |
| C | 4.80575600 | -0.36070200 | 0.80490800 |
| C | 4.37052500 | 1.46390000 | -0.69690500 |
| H | 2.131046800 | 1.13129000 | -2.21397100 |
| C | 5.05574200 | 0.93244500 | 0.39766100 |
| H | 5.77757900 | 1.54910000 | 0.92143800 |
| C | -3.48179800 | -0.82671600 | 0.26254400 |
| C | -2.80125200 | 0.29184600 | 0.76918100 |
| C | -4.81965300 | -0.73459700 | -0.11749000 |
| C | -3.53301200 | 1.50399000 | 0.91625400 |
| C | -5.50179300 | 0.45020100 | 0.02761100 |
| H | -5.33177500 | -1.60392600 | -0.51545900 |
| C | -4.85998200 | 1.57429300 | 0.54651500 |
| H | -5.41523900 | 2.49914400 | 0.65162500 |
| O | 3.58483200 | -2.38151800 | 0.55445700 |
| O | -1.54266300 | 0.27241100 | 1.14312200 |
| S | 4.72269000 | 3.14839600 | -1.18949000 |
| S | -7.21613400 | 0.60041500 | -0.48125300 |
| O | -7.22182500 | 1.57758800 | -1.60830100 |
| O | -7.95254900 | 1.10845400 | 0.71151900 |
| O | -7.64595000 | -0.76414800 | -0.89381500 |
| O | 3.82804600 | 3.43989100 | -2.34508900 |
| O | 6.16981100 | 3.18173900 | -1.55634500 |
| O | 4.42805200 | 3.99955400 | 0.00103300 |
| H | -2.42733000 | -2.49331900 | 1.13999800 |
| H | 2.70202500 | -2.25002800 | -2.25535500 |
| H | -1.84226500 | -1.66174400 | -1.59937100 |
| H | 1.71839100 | -2.53814600 | -0.11645900 |
| O | 1.17385100 | 0.35784100 | 1.23348000 |
| H | 1.61267000 | -0.26767000 | 1.87217300 |
| H | 3.52121900 | -3.81078300 | -0.44833500 |
| O | 3.32228700 | -4.61835300 | -0.97279100 |
| H | 3.91579900 | -4.57823000 | -1.72536100 |
| H | 0.58252200 | 0.91771200 | 1.75544500 |
| O | 2.83706300 | -2.00820000 | 2.07089600 |
| O | 2.28365500 | -1.54833000 | 2.75126500 |
| H | 1.63342000 | -2.19216400 | 3.04322300 |
| Pd | -0.18151900 | -0.83327500 | 0.14445100 |
| O | 5.41543500 | -0.95857400 | 1.86307900 |
| O | -2.82543600 | 2.53864700 | 1.43000800 |
| C | 6.32594700 | -0.18943300 | 2.61044300 |
| H | 7.18079500 | 0.13183600 | 2.00419600 |

| | | | |
|--|-------------|-------------|-------------|
| H | 5.84822100 | 0.69806200 | 3.04118500 |
| H | 6.68490100 | -0.82541400 | 3.41770500 |
| C | -3.49432800 | 3.76616100 | 1.60807200 |
| H | -3.86275900 | 4.16775300 | 0.65774800 |
| H | -4.33612700 | 3.66937500 | 2.30225100 |
| H | -2.76696300 | 4.45868100 | 2.02689300 |
| 62 | | | |
| RR-PhOMe_ID2_TS1_R, E(SCF) = - | | | |
| 2713.18387190, E(ZPE) = -2712.719570, E(G) | | | |
| = -2712.793272 a.u. | | | |
| C | -0.85934300 | -3.69311100 | 0.40504800 |
| H | -0.73806100 | -3.74249300 | 1.49101200 |
| H | -1.47294200 | -4.54256100 | 0.09163100 |
| C | 0.48224500 | -3.69455700 | -0.28482100 |
| H | 1.04403100 | -4.60798000 | -0.07440400 |
| H | 0.34546200 | -3.62821100 | -1.36828600 |
| N | 1.24528300 | -2.49754300 | 0.13997700 |
| N | -1.53124600 | -2.41086400 | 0.09126000 |
| C | 2.29056200 | -2.10333200 | -0.81452500 |
| H | 1.77991900 | -1.89613200 | -1.76293100 |
| C | -2.73869700 | -2.12795700 | 0.89595400 |
| H | -3.42756200 | -2.97693000 | 0.83023500 |
| C | 3.12356000 | -0.92316700 | -0.39664400 |
| C | 2.63422600 | 0.15774600 | 0.35150300 |
| C | 4.43875500 | -0.89628300 | -0.87200800 |
| C | 3.51009800 | 1.25800500 | 0.58052200 |
| C | 5.26062800 | 0.17699200 | -0.63480700 |
| H | 4.81876000 | -1.73512000 | -1.44555000 |
| C | 4.79875500 | 1.26853200 | 0.09986900 |
| H | 5.45513000 | 2.11115700 | 0.28343400 |
| C | -3.42069900 | -0.88167700 | 0.42515700 |
| C | -2.72628700 | 0.34014600 | 0.39901700 |
| C | -4.75738600 | -0.94476900 | 0.03303800 |
| C | -3.44393000 | 1.49348600 | -0.02235300 |
| C | -5.42512300 | 0.18883900 | -0.36579500 |
| H | -5.28044200 | -1.89477700 | 0.04934400 |
| C | -4.76779700 | 1.41783400 | -0.39378000 |
| H | -5.30398300 | 2.30112500 | -0.72129600 |
| O | 1.44144800 | 0.24747900 | 0.90897400 |
| O | -1.47033300 | 0.48952300 | 0.75486200 |
| S | 6.95689200 | 0.19137700 | -1.22245900 |
| S | -7.14449500 | 0.12379200 | -0.87693500 |
| O | -7.17138400 | 0.63066100 | -2.27901300 |
| O | -7.88285100 | 1.01689400 | 0.06151200 |
| O | -7.55335300 | -1.30364000 | -0.76703900 |
| O | 7.12357200 | -1.04645800 | -2.03265400 |
| O | 7.81124000 | 0.20583800 | 0.00004400 |
| O | 7.09728600 | 1.43933800 | -2.02582200 |
| H | -2.40496000 | -2.04726400 | 1.93630100 |
| H | 2.95260400 | -2.95907800 | -0.99211800 |
| H | -1.78863600 | -2.39822800 | -0.89651800 |
| H | 1.65546200 | -2.63750400 | 1.07280700 |
| O | 0.00870900 | 3.24510200 | -0.82633400 |
| H | 0.25172900 | 3.18024500 | 0.11390000 |
| H | 1.82655900 | -0.90940900 | 2.49262200 |
| O | 1.99861000 | -1.78390500 | 2.88159200 |
| H | 2.86149900 | -1.71276200 | 3.29725500 |
| H | -0.86730400 | 2.83345100 | -0.81493900 |
| H | 0.89710000 | 1.99113300 | 1.76896000 |
| O | 0.09032100 | 2.51049100 | 1.93231400 |
| H | -0.60726800 | 1.91130400 | 1.60541800 |
| Pd | -0.09696300 | -0.98604100 | 0.41782200 |
| O | 2.95609500 | 2.26185000 | 1.30621900 |
| O | -2.71471800 | 2.64187700 | -0.03032900 |
| C | 3.71857500 | 3.42867100 | 1.51924700 |
| H | 4.61806200 | 3.21886400 | 2.10731500 |
| H | 4.01147800 | 3.89294900 | 0.57181200 |
| H | 3.08163000 | 4.11576600 | 2.07330100 |
| C | -3.37405400 | 3.84474900 | -0.36924400 |
| H | -3.76008200 | 3.81744600 | -1.39344200 |
| H | -4.19817200 | 4.05427000 | 0.31959400 |
| H | -2.62797700 | 4.63349900 | -0.29052400 |

62

RR-PhOMe_ID2_TS1, E(SCF) = -2713.15310784,
 E(ZPE) = -2712.689535, E(G) = -2712.762712
 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.76176100 | -3.34753600 | 0.36341100 |
| H | -0.55612600 | -3.24485800 | 1.43265400 |
| H | -1.34559700 | -4.25685700 | 0.20469000 |
| C | 0.53689100 | -3.35838800 | -0.40640400 |
| H | 1.17061300 | -4.19800600 | -0.10221200 |
| H | 0.36512900 | -3.43305400 | -1.48413500 |
| N | 1.19922500 | -2.07153600 | -0.12051100 |
| N | -1.53610000 | -2.15426100 | -0.05070900 |
| C | 2.48692000 | -1.86124400 | -0.78990500 |
| H | 2.27294000 | -1.63805900 | -1.84197800 |
| C | -2.58708000 | -1.73354400 | 0.89815600 |
| H | -3.19689500 | -2.60420100 | 1.16343400 |
| C | 3.36992900 | -0.79522400 | -0.18593400 |
| C | 2.92114300 | 0.23821400 | 0.66718600 |
| C | 4.70722100 | -0.84727500 | -0.58836300 |
| C | 3.89805400 | 1.21254000 | 1.05990300 |
| C | 5.61207200 | 0.10611100 | -0.19118500 |
| H | 5.04013200 | -1.65002700 | -1.23983100 |
| C | 5.20773900 | 1.14926100 | 0.64486600 |
| H | 5.93077300 | 1.89519900 | 0.95436100 |
| C | -3.47498800 | -0.66303800 | 0.33798300 |
| C | -2.95268400 | 0.52428900 | -0.20254600 |
| C | -4.85707200 | -0.84437300 | 0.42707000 |
| C | -3.87474000 | 1.53689000 | -0.59731600 |
| C | -5.72355700 | 0.14160300 | 0.02387800 |
| H | -5.25433000 | -1.76888000 | 0.83184200 |
| C | -5.23402700 | 1.34313300 | -0.48689500 |
| H | -5.93173900 | 2.11220400 | -0.79714400 |
| O | 1.70640300 | 0.35994400 | 1.11209200 |
| O | -1.67561400 | 0.79096400 | -0.35412700 |
| S | 7.32704700 | 0.02986800 | -0.69952900 |
| S | -7.50097200 | -0.07956200 | 0.13725000 |
| O | -8.01927600 | 0.06287000 | -1.25399400 |
| O | -7.98939500 | 1.00554300 | 1.03615400 |
| O | -7.71339100 | -1.44127700 | 0.70063700 |
| O | 7.43700600 | -1.12842000 | -1.63056800 |
| O | 8.12493300 | -0.15529500 | 0.54915200 |
| O | 7.62002700 | 1.33522900 | -1.36181600 |
| H | -2.06672200 | -1.40540200 | 1.80515300 |
| H | 3.03415000 | -2.81375000 | -0.78240900 |
| H | -1.96788100 | -2.33397800 | -0.95860800 |
| H | 1.33619900 | -2.02279600 | 0.89862000 |
| O | 0.94653300 | 0.94518900 | -1.55783500 |
| H | 0.85948400 | 1.72319600 | -0.96085000 |
| H | 1.28759800 | -0.75662500 | 2.36018700 |
| O | 1.03333100 | -1.61567300 | 2.77323800 |
| H | 1.69628900 | -1.79241600 | 3.44432100 |
| H | 0.38893700 | 1.14456000 | -2.31742300 |
| H | 0.86861100 | 1.93843900 | 0.97542900 |
| O | 0.32517400 | 2.62609000 | 0.52697400 |
| H | -0.54459900 | 2.20499000 | 0.41415000 |
| Pd | -0.22648500 | -0.62160800 | -0.39522500 |
| O | 3.40449200 | 2.18889100 | 1.86850400 |
| O | -3.30011700 | 2.66894700 | -1.07250600 |
| C | 4.29514800 | 3.18550500 | 2.30704500 |
| H | 5.11807000 | 2.76246700 | 2.89440600 |
| H | 4.71715200 | 3.75144200 | 1.46871900 |
| H | 3.72144000 | 3.86246300 | 2.93759900 |
| C | -4.15226100 | 3.72852600 | -1.44348800 |
| H | -4.81549100 | 3.44398600 | -2.26749400 |
| H | -4.76171300 | 4.06900300 | -0.59938100 |
| H | -3.51034900 | 4.54390000 | -1.77077600 |

64

RR-PhOMe_ID2_TS2_P, E(SCF) = -
 2714.33407522, E(ZPE) = -2713.853412, E(G)
 = -2713.930201 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.06604900 | 0.57762100 | -1.86222300 |
| H | -0.00422900 | -0.27285900 | -2.54755600 |
| H | -0.16814400 | 1.49098500 | -2.45394300 |
| C | 1.13604700 | 0.62018900 | -0.96109100 |
| H | 2.05859800 | 0.74371300 | -1.53448000 |
| H | 1.06732400 | 1.45438100 | -0.25549900 |
| N | 1.17448200 | -0.63907900 | -0.18232400 |

| | | | |
|----|-------------|-------------|-------------|
| N | -1.25878500 | 0.37624500 | -1.01010800 |
| C | 2.14893000 | -0.61460500 | 0.94538600 |
| H | 2.17141000 | -1.63309600 | 1.34241400 |
| C | -2.50331500 | 0.05851600 | -1.74633200 |
| H | -2.64166400 | 0.79836000 | -2.54153100 |
| C | 3.51128300 | -0.15367800 | 0.53548900 |
| C | 4.30885700 | -1.01045700 | -0.25352900 |
| C | 3.95117400 | 1.11863700 | 0.89957100 |
| C | 5.58801400 | -0.50531700 | -0.65499400 |
| C | 5.18671200 | 1.56772200 | 0.49787800 |
| H | 3.31878100 | 1.75986200 | 1.50594800 |
| C | 6.00705800 | 0.75446600 | -0.28975200 |
| H | 6.97607700 | 1.13001900 | -0.59906600 |
| C | -3.68508100 | 0.06706900 | -0.83194200 |
| C | -3.69967800 | -0.76552100 | 0.29862300 |
| C | -4.76823600 | 0.89538700 | -1.12224200 |
| C | -4.86496800 | -0.74580400 | 1.11858900 |
| C | -5.87994600 | 0.89322400 | -0.31491600 |
| H | -4.73986800 | 1.54072200 | -1.99338900 |
| C | -5.93274200 | 0.06976500 | 0.80846900 |
| H | -6.81657200 | 0.08723400 | 1.43531700 |
| O | 3.92425000 | -2.19503000 | -0.60310900 |
| O | -2.72868700 | -1.58569100 | 0.63117900 |
| S | 5.77492200 | 3.19741200 | 0.94773000 |
| S | -7.28897500 | 1.94618700 | -0.67337000 |
| O | -6.93519600 | 2.70488200 | -1.90433000 |
| O | -7.45654200 | 2.82075200 | 0.52862300 |
| O | -8.44522000 | 1.02484900 | -0.86719700 |
| O | 7.04640100 | 2.98824900 | 1.70163500 |
| O | 4.70359600 | 3.81195100 | 1.78148300 |
| O | 5.99803200 | 3.92613000 | -0.33602900 |
| H | -2.34415900 | -0.91731700 | -2.21794600 |
| H | 1.73335500 | 0.04486800 | 1.71168800 |
| H | -1.41762800 | 1.21606400 | -0.44948700 |
| H | 1.44004000 | -1.38965700 | -0.83450900 |
| O | 0.78716300 | -4.12060200 | 0.07842000 |
| H | 1.64645400 | -4.22395900 | 0.53482000 |
| H | 2.76595400 | -2.56156600 | -1.74988900 |
| O | 1.86117300 | -2.72100100 | -2.12313700 |
| H | 1.92622200 | -2.71542700 | -3.08005900 |
| H | 1.03084900 | -3.78679000 | -0.80228500 |
| H | 3.66881300 | -3.41933300 | 0.54634600 |
| O | 3.37382700 | -4.17200000 | 1.11672800 |
| H | 3.55851400 | -3.90331400 | 2.01942100 |
| H | -0.17687200 | -2.69850400 | 0.98014600 |
| H | -0.45579600 | -2.24203100 | 1.61659600 |
| Pd | -0.78734200 | -1.12649100 | 0.30110100 |
| O | 6.32166700 | -1.36186400 | -1.41309800 |
| O | -4.82688100 | -1.57702600 | 2.18686800 |
| C | -5.95050800 | -1.59963700 | 3.03763200 |
| H | -5.73248200 | -2.32140100 | 3.82203500 |
| H | -6.13098000 | -0.61985200 | 3.49331700 |
| H | -6.85400900 | -1.91362700 | 2.50386200 |
| C | 7.58053300 | -0.92269500 | -1.86264000 |
| H | 8.00191800 | -1.73318600 | -2.45466900 |
| H | 7.49738900 | -0.02854300 | -2.49093100 |
| H | 8.25623500 | -0.70302100 | -1.02821800 |

62

RR-PhOMe_ID2_TS2_R_noH2, E(SCF) = -
 2713.17263391, E(ZPE) = -2712.708554, E(G)
 = -2712.783897 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.04632500 | 0.92457800 | 1.77062900 |
| H | -0.02116600 | 0.13855200 | 2.52749200 |
| H | 0.16442000 | 1.88732100 | 2.27532500 |
| C | -1.16609500 | 0.89702000 | 0.88113500 |
| H | -2.08370600 | 1.05885100 | 1.45350800 |
| H | -1.10467700 | 1.67810300 | 0.11602800 |
| N | -1.20659700 | -0.41354100 | 0.19171500 |
| N | 1.22899100 | 0.63296100 | 0.92805100 |
| C | -2.16218500 | -0.44343500 | -0.94485900 |
| H | -2.06367900 | -1.42672800 | -1.41042800 |
| C | 2.47179700 | 0.36410500 | 1.68613700 |
| H | 2.63540200 | 1.18140200 | 2.39643400 |
| C | -3.57560200 | -0.18829900 | -0.53001800 |
| C | -4.22755400 | -1.17019200 | -0.24677800 |
| C | -4.21446700 | 0.99461200 | -0.89574500 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -5.58184300 | -0.89323300 | 0.62070500 | H | -4.73742600 | 1.74237500 | -1.84835100 |
| C | -5.51610300 | 1.22710700 | -0.51519200 | C | -5.92339600 | -0.05977800 | 0.75698500 |
| H | -3.68674900 | 1.73801600 | -1.48548100 | H | -6.81636800 | -0.13839000 | 1.36572900 |
| C | -6.20373800 | 0.27762300 | 0.24676600 | O | 3.68869400 | -2.28995700 | -0.54373600 |
| H | -7.22873700 | 0.47846500 | 0.53740800 | O | -2.65745500 | -1.56967300 | 0.47283500 |
| C | 3.66097200 | 0.22879800 | 0.78820400 | S | 6.29063200 | 2.80645500 | 0.92745900 |
| C | 3.66745800 | -0.72817600 | -0.24102800 | S | -7.32608400 | 1.30759300 | -0.55425000 |
| C | 4.77919800 | 1.03114500 | 1.01767400 | O | -6.93137800 | 2.90485300 | -1.58698300 |
| C | 4.86185900 | -0.86996300 | -1.00547500 | O | -7.65635100 | 2.52845800 | 0.76047600 |
| C | 5.91386200 | 0.88140500 | 0.25717500 | O | -8.39255300 | 0.97591200 | -1.02337800 |
| H | 4.75806200 | 1.77429000 | 1.80708000 | O | 7.45897400 | 2.44023200 | 1.78184900 |
| C | 5.96127400 | -0.07796700 | -0.75439900 | O | 5.28147300 | 3.63046200 | 1.65143600 |
| H | 6.86424500 | -0.18033700 | -1.34472500 | O | 6.71538700 | 3.41760300 | -0.36695200 |
| O | -3.64710700 | -2.26387200 | 0.62174400 | H | -2.30492400 | -0.63879800 | -2.31273000 |
| O | 2.65945200 | -1.51574400 | -0.52981000 | H | 1.77498900 | 0.32637600 | 1.65697600 |
| S | -6.37075600 | 2.72606900 | -0.99006600 | H | -1.37556400 | 1.36364700 | -0.40202800 |
| S | 7.37164900 | 1.88354100 | 0.55720800 | H | 1.52815000 | -1.17491800 | -0.90362500 |
| O | 6.98181000 | 2.88437000 | 1.58842300 | O | -0.27978200 | -2.65207400 | 1.40723600 |
| O | 7.71729400 | 2.50429000 | -0.75467900 | H | 0.46601400 | -3.20660400 | -1.04277100 |
| O | 8.42502300 | 0.93969000 | 1.03160100 | H | 2.78038000 | -2.21990600 | -2.03619800 |
| O | -7.50806600 | 2.30166400 | -1.85988400 | O | 2.05593600 | -1.96322600 | -2.65147700 |
| O | -5.37276300 | 3.56338500 | -1.71429400 | H | 1.62001500 | -2.78400900 | -2.89245300 |
| O | -6.84286800 | 3.35577800 | 0.27863700 | H | -1.07288500 | -3.19930600 | -1.45033400 |
| H | 2.28526700 | -0.54751200 | 2.26418800 | H | 2.53239300 | -3.28543200 | 0.10318100 |
| H | -1.82482500 | 0.30337100 | -1.66852700 | O | 1.78867700 | -3.89417200 | 0.35761700 |
| H | 1.39589500 | 1.42034300 | 0.29860800 | H | 2.18747000 | -4.62230200 | 0.83913100 |
| H | -1.50128800 | -1.10637600 | 0.89247200 | H | -1.04645700 | 1.09429600 | 2.09423100 |
| O | 0.28024400 | -2.62597400 | -1.41986400 | H | -1.15837200 | 1.79734300 | 2.21326100 |
| H | -0.44336000 | -3.18263300 | -1.01677900 | Pd | -0.74152300 | -1.01559700 | 0.17830600 |
| H | -2.71106400 | -2.12442300 | 2.09291400 | O | 6.22361700 | -1.87795200 | -1.24247700 |
| O | -1.97939400 | -1.83699900 | 2.68540400 | O | -4.78335600 | -1.81562000 | 1.96448400 |
| H | -1.52405400 | -2.64278600 | 2.94069600 | C | -5.92428700 | -1.98856700 | 2.77337200 |
| H | 1.08216200 | -3.16000800 | -1.46801300 | H | -5.69153300 | -2.79031300 | 3.47129300 |
| H | -2.48482500 | -3.26031300 | -0.01586500 | H | -6.16054400 | -1.08078400 | 3.33929400 |
| O | -1.73667100 | -3.86483900 | -0.26715600 | H | -6.80001100 | -2.27434100 | -2.18040500 |
| H | -2.13469000 | -4.61914700 | -0.70724700 | C | 7.55603200 | -1.66049100 | -1.63803100 |
| Pd | 0.74502400 | -0.96091700 | -0.22884600 | H | 7.87225900 | -2.55218300 | -2.17661900 |
| O | -6.17311000 | -1.86771200 | 1.36177600 | H | 7.64592000 | -0.79359000 | -2.30262200 |
| O | 4.81033900 | -1.82252800 | -1.96786000 | H | 8.21715200 | -1.51233600 | -0.77660900 |
| C | 5.96193400 | -2.02377000 | -2.75444400 | | | | |
| H | 5.72677500 | -2.82731100 | -3.44953700 | 64 | | | |
| H | 6.22503000 | -1.12557600 | -3.32394400 | RR-PhOme_ID2_TS2-square_P, E(SCF) = - | | | |
| H | 6.82171000 | -2.32040400 | -2.14371600 | 2714.33335512, E(ZPE) = -2713.852736, E(G) | | | |
| C | -7.50026300 | -1.65843400 | 1.77878500 | = -2713.928981 a.u. | | | |
| H | -7.78857400 | -2.53453100 | 2.35722100 | C | -0.05480000 | 0.63695500 | -1.83782100 |
| H | -7.59129300 | -0.76870000 | 2.41233500 | H | 0.01157200 | -0.20058500 | -2.53792000 |
| H | -8.18284000 | -1.55461400 | 0.92757700 | H | -0.15995800 | 1.56081800 | -2.41247800 |
| | | | | C | 1.14446500 | 0.66853000 | -0.93267600 |
| 64 | | | | H | 2.06812000 | 0.80317000 | -1.50153400 |
| RR-PhOme_ID2_TS2_R, E(SCF) = - | | | | H | 1.07129000 | 1.49253300 | -0.21537200 |
| 2714.34676630, E(ZPE) = -2713.867558, E(G) | | | | N | 1.18426600 | -0.60157300 | -0.17189200 |
| = -2713.942789 a.u. | | | | N | -1.24915100 | 0.41644700 | -0.99205200 |
| C | -0.03656800 | 0.81805600 | -1.86330100 | C | 2.15667600 | -0.58953400 | 0.95666900 |
| H | 0.03373900 | 0.00481400 | -2.59064700 | H | 2.16685100 | -1.60815800 | 1.35472400 |
| H | -0.15191300 | 1.76196800 | -2.40296000 | C | -2.48911600 | 0.09857000 | -1.73656500 |
| C | 1.16932300 | 0.82456900 | -0.96429200 | H | -2.62692000 | 0.84450900 | -2.52610800 |
| H | 2.09141100 | 0.97582700 | -1.53188800 | C | 3.52405600 | -0.14884500 | 0.54454300 |
| H | 1.09468500 | 1.62986800 | -0.22509800 | C | 4.30227800 | -1.01984500 | -0.25055200 |
| N | 1.21158000 | -0.46247700 | -0.23214200 | C | 3.98461300 | 1.11693300 | 0.90467000 |
| N | -1.22078900 | 0.55877600 | -1.01317300 | C | 5.58909300 | -0.53355900 | -0.65578100 |
| C | 2.14062500 | -0.44126000 | 0.92651900 | C | 5.22466400 | 1.54745000 | 0.49632600 |
| H | 2.04361500 | -1.40930400 | 1.42319100 | H | 3.36432800 | 1.76820200 | 1.51286400 |
| C | -2.47334000 | 0.28785800 | -1.75352900 | C | 6.02868300 | 0.71985300 | -0.29426800 |
| H | -2.63630300 | 1.09181400 | -2.47901300 | H | 7.00226800 | 1.07938200 | -0.60832100 |
| C | 3.55927700 | -0.17813000 | 0.53499700 | C | -3.67515500 | 0.09437000 | -0.82769900 |
| C | 4.24299600 | -1.17447300 | -0.19463000 | C | -3.68988100 | -0.74486500 | 0.29793300 |
| C | 4.17087500 | 1.02785100 | 0.87117400 | C | -4.76184100 | 0.91818600 | -1.11758300 |
| C | 5.60032600 | -0.88779600 | -0.54997900 | C | -4.85656900 | -0.73323900 | -1.11585300 |
| C | 5.47586600 | 1.26949300 | 0.50857900 | C | -5.87619100 | 0.90605100 | -0.31400700 |
| H | 3.61978800 | 1.78142000 | 1.42557600 | H | -4.73400400 | 1.56778600 | -1.98552200 |
| C | 6.19419600 | 0.30668800 | -0.20670200 | C | -5.92777900 | 0.07792100 | 0.80595000 |
| H | 7.22133500 | 0.51564800 | -0.48351600 | H | -6.81331600 | 0.08855600 | 1.43049900 |
| C | -3.64992700 | 0.18648200 | -0.83463900 | O | 3.89488700 | -2.19213400 | -0.60480500 |
| C | -3.65475600 | -0.76084000 | 0.20383700 | O | -2.71671400 | -1.56371300 | 0.62781800 |
| C | -4.75634400 | 1.00832500 | -1.05041900 | S | 5.83669600 | 3.17069100 | 0.93523500 |
| C | -4.83476700 | -0.87109600 | 0.99456900 | S | -7.29042100 | 1.95223600 | -0.67255300 |
| C | -5.87785500 | 0.88793600 | -0.26528900 | O | -7.46489100 | 2.82270700 | 0.52543600 |

| | | | |
|----|-------------|-------------|-------------|
| O | -8.44101000 | 1.02483600 | -0.87079100 |
| O | -6.93870600 | 2.71596100 | -1.90092900 |
| O | 7.11395400 | 2.94989600 | 1.67644400 |
| O | 4.78163000 | 3.80066900 | 1.77859600 |
| O | 6.05518800 | 3.89437400 | -0.35244600 |
| H | -1.41608100 | 1.24767500 | -0.42094600 |
| H | 1.45264400 | -1.34571800 | -0.83554800 |
| O | 0.73083000 | -4.16361400 | -0.02038100 |
| H | 1.58888200 | -4.29459800 | 0.44596900 |
| H | 2.63418300 | -2.56107200 | -1.78731000 |
| O | 1.74663800 | -2.65935600 | -2.19606500 |
| H | 1.30474000 | -3.31181400 | -1.62454000 |
| H | 0.29222200 | -5.01793700 | -0.03271900 |
| H | 3.56106600 | -3.42474200 | 0.47959600 |
| O | 3.23251200 | -4.19727600 | 1.00836700 |
| H | 3.40856400 | -3.98549300 | 1.92768700 |
| H | -0.22112500 | -2.67833100 | 0.98245700 |
| H | -0.42855100 | -2.20959700 | 1.62881200 |
| Pd | -0.77593800 | -1.09787500 | 0.30310700 |
| H | 1.74968000 | 0.07447500 | 1.72393000 |
| H | -2.32285100 | -0.87226800 | -2.21593800 |
| O | -4.81655500 | -1.56761100 | 2.18160500 |
| O | 6.30703700 | -1.40257800 | -1.41544600 |
| C | -5.93940000 | -1.59421300 | 3.03339000 |
| H | -5.71815500 | -2.31532600 | 3.81749200 |
| H | -6.12268500 | -0.61508200 | 3.48932700 |
| H | -6.84233100 | -1.91123200 | 2.50049100 |
| C | 7.57082400 | -0.98362600 | -1.86970300 |
| H | 7.97742300 | -1.80110500 | -2.46255000 |
| H | 7.49992700 | -0.08875400 | -2.49863500 |
| H | 8.25304300 | -0.77383100 | -1.03795700 |

62

RR-PhOme_ID2_TS2-square_R_noH2, E(SCF) = -2713.16916299, E(ZPE) = -2712.704152, E(G) = -2712.777520 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.11584100 | 1.40204300 | -1.71241900 |
| H | -0.07168900 | 0.77293600 | -2.60562800 |
| H | -0.26342000 | 2.43837300 | -2.02933300 |
| C | 1.12098300 | 1.24615100 | -0.87204500 |
| H | 2.02206100 | 1.52876100 | -1.42180000 |
| H | 1.05373100 | 1.89315500 | 0.00796400 |
| N | 1.20349500 | -0.15345700 | -0.39134300 |
| N | -1.26802100 | 0.93694300 | -0.90358100 |
| C | 2.07005700 | -0.30070300 | 0.81221700 |
| H | 1.86837000 | -1.29057800 | 1.22352100 |
| C | -2.53449300 | 0.83128500 | -1.66483700 |
| H | -2.73947900 | 1.79577300 | -2.14125900 |
| C | 3.52501300 | -0.13061000 | 0.51658900 |
| C | 4.23289600 | -1.23320500 | -0.01547600 |
| C | 4.15756100 | 1.08755300 | 0.76621900 |
| C | 5.62185500 | -1.02176300 | -0.30028500 |
| C | 5.49410100 | 1.24806600 | 0.48686700 |
| H | 3.59952400 | 1.91480800 | 1.19447100 |
| C | 6.22864900 | 0.18979800 | -0.05767500 |
| H | 7.28060200 | 0.33658900 | -0.27540200 |
| C | -3.68837400 | 0.43978200 | -0.79838800 |
| C | -3.64546100 | -0.75946400 | -0.06758100 |
| C | -4.82429500 | 1.24802300 | -0.77096000 |
| C | -4.80736100 | -1.12749900 | 0.66998400 |
| C | -5.92978800 | 0.87120200 | -0.04686600 |
| H | -4.84473900 | 2.17406100 | -1.33547300 |
| C | -5.92566600 | -0.32127400 | 0.67568100 |
| H | -6.80698500 | -0.60047800 | 1.24136400 |
| O | 3.68524300 | -2.38280600 | -0.23899200 |
| O | -2.61676800 | -1.57313200 | -0.04634000 |
| S | 6.32485100 | 2.80626800 | 0.77604900 |
| S | -7.40387000 | 1.89367100 | -0.00784800 |
| O | -7.61240100 | 2.25748400 | 1.42351500 |
| O | -8.50507700 | 1.04061700 | -0.54041300 |
| O | -7.11156100 | 3.07163900 | -0.87019800 |
| O | 7.50961800 | 2.49378300 | 1.62853700 |
| O | 5.33626100 | 3.68716500 | 1.46017300 |
| O | 6.72251200 | 3.32133100 | -0.56813700 |
| H | -1.40881000 | 1.57151500 | -0.11553900 |
| H | 1.56786400 | -0.75926600 | -1.14105000 |
| O | -0.20903600 | -2.88841800 | 0.22744500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.57423500 | -3.18137500 | 0.77255100 |
| H | 2.50931100 | -2.56998000 | -1.49572300 |
| O | 1.74069200 | -2.49447400 | -2.10812600 |
| H | 1.01410300 | -2.93221800 | -1.64844900 |
| H | -0.99798200 | -3.34457600 | 0.54206400 |
| H | 2.73440700 | -3.22935200 | 0.82612300 |
| O | 2.02522000 | -3.72511800 | 1.52186800 |
| H | 2.24510300 | -3.67277900 | 2.25154600 |
| Pd | -0.72725200 | -0.88340100 | -0.18758900 |
| H | 1.72203000 | 0.43609600 | 1.54054000 |
| H | -2.35094200 | 0.09836600 | -2.45807500 |
| O | -4.71062000 | -2.30287800 | 1.33753700 |
| O | 6.26408800 | -2.10528000 | -0.81209800 |
| C | -5.83214300 | -2.72896500 | 2.07683000 |
| H | -5.56536800 | -3.68470500 | -2.52343700 |
| H | -6.08345000 | -2.02034900 | 2.87343900 |
| H | -6.70938400 | -2.86643300 | 1.43553700 |
| C | 7.63246000 | -1.97234500 | -1.10965700 |
| H | 7.96486400 | -2.93494400 | -1.94444000 |
| H | 7.80959600 | -1.20452100 | -1.87177300 |
| H | 8.21972400 | -1.72363500 | -0.21809400 |

64

RR-PhOme_ID2_TS2-square_R, E(SCF) = -2714.34247164, E(ZPE) = -2713.862075, E(G) = -2713.937026 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.12252800 | 1.47382200 | -1.72444900 |
| H | -0.07932500 | 0.86750900 | -2.63320800 |
| H | -0.27534700 | 2.51720100 | -2.01490000 |
| C | 1.11796700 | 1.30304200 | -0.89178100 |
| H | 2.01756600 | 1.59729000 | -1.43777000 |
| H | 1.05181200 | 1.93391300 | -0.00018800 |
| N | 1.20523800 | -0.10498700 | -0.43537400 |
| N | -1.26987200 | 0.98388700 | -0.92280200 |
| C | 2.05157600 | -0.26598000 | 0.78169100 |
| H | 1.82713300 | -1.25221200 | 1.19014700 |
| C | -2.54060500 | 0.89337300 | -1.67969600 |
| H | -2.75311300 | 1.86924000 | -2.12870700 |
| C | 3.51284900 | -0.11714700 | 0.50812900 |
| C | 4.21687600 | -1.23716600 | 0.00791500 |
| C | 4.15541800 | 1.09811200 | 0.74665700 |
| C | 5.61135100 | -1.04473800 | -0.26343800 |
| C | 5.49777300 | 1.23883400 | 0.48487200 |
| H | 3.60123300 | 1.93854300 | 1.15371500 |
| C | 6.22806800 | 0.16399200 | -0.03216700 |
| H | 7.28454800 | 0.29592400 | -0.23709000 |
| C | -3.68639300 | 0.47218400 | -0.81617000 |
| C | -3.63364700 | -0.75008800 | -0.12537100 |
| C | -4.82366400 | 1.27627600 | -0.75125800 |
| C | -4.78362600 | -1.14133600 | 0.61818600 |
| C | -5.91984600 | 0.87482400 | -0.02597500 |
| H | -4.85128100 | 2.21903700 | -1.28667200 |
| C | -5.90390300 | -0.33876400 | 0.66082200 |
| H | -6.77696100 | -0.63687800 | 1.22980800 |
| O | 3.66032000 | -2.38522000 | -0.20142800 |
| O | -2.60417700 | -1.56307300 | -0.14645800 |
| S | 6.34038400 | 2.79323500 | 0.76063900 |
| S | -7.40307200 | 1.88245200 | 0.04687800 |
| O | -7.63058300 | 2.17326500 | 1.49169300 |
| O | -8.49024500 | 1.04673300 | -0.53937200 |
| O | -7.11284300 | 3.10358500 | -0.75397800 |
| O | 7.52473800 | 2.47840800 | 1.61271000 |
| O | 5.35941500 | 3.68579500 | 1.44058000 |
| O | 6.73850400 | 3.29629300 | -0.58798200 |
| H | -1.40845100 | 1.59595100 | -0.11678200 |
| H | 1.58843400 | -0.69544200 | -1.18836300 |
| O | -0.18570800 | -2.87656300 | 0.06210600 |
| H | 0.55035800 | -3.16175700 | -0.67409200 |
| H | 2.54328400 | -2.52879400 | -1.51830500 |
| O | 1.80245200 | -2.42948800 | -2.16076600 |
| H | 1.05031100 | -2.85349900 | -1.72888700 |
| H | -0.99059200 | -3.34758600 | -0.30885200 |
| H | 2.67888900 | -3.20020500 | 0.86058100 |
| O | 1.95497200 | -3.67590500 | 1.35258200 |
| H | 2.11483800 | -3.53126500 | 2.28817100 |
| H | -0.71679500 | -1.67526800 | 2.95806600 |
| H | -0.60494900 | -0.94506100 | 2.83347800 |

Pd -0.71982300 -0.85530300 -0.26488800
 H 1.70282600 0.47535900 1.50546400
 H -2.35808700 0.18262400 -2.49296400
 O -4.67413700 -2.33424800 1.25178100
 O 6.24798300 -2.14281500 -0.75028000
 C -5.78415600 -2.78487000 1.99399000
 H -5.50817700 -3.75190800 2.40959400
 H -6.02682000 -2.10018900 2.81393500
 H -6.66967800 -2.90729200 1.36111300
 C 7.62101100 -2.02921400 -1.03430700
 H 7.94653600 -3.00054300 -1.40270000
 H 7.81510900 -1.27366900 -1.80443400
 H 8.20133100 -1.77545900 -0.13963200

64

RR-PhOMe_ID2_TS2-square, E(SCF) = -
 2714.32517849, E(ZPE) = -2713.846466, E(G)
 = -2713.921483 a.u.

C -0.06001400 1.19693700 -1.58607500
 H 0.05869700 0.48088500 -2.40427300
 H -0.19572900 2.19385800 -2.01412900
 C 1.11994500 1.13482400 -0.65521800
 H 2.05000000 1.39149300 -1.17015500
 H 0.99579800 1.83074700 0.18093000
 N 1.19012000 -0.23547800 -0.10163800
 N -1.26055500 0.79686800 -0.81829000
 C 2.17584900 -0.38557400 0.99934500
 H 2.05438100 -1.40261500 1.37986600
 C -2.46478600 0.52723700 -1.63648400
 H -2.63357600 1.37866900 -2.30423600
 C 3.58272100 -0.14954600 0.55668000
 C 4.22301100 -1.16239700 -0.19370200
 C 4.22795200 1.04590000 0.87095900
 C 5.57457500 -0.89736400 -0.59425900
 C 5.52162600 1.26523600 0.46049600
 H 3.71147000 1.80927900 1.44529300
 C 6.19948200 0.28667900 -0.27438200
 H 7.22062200 0.47752800 -0.58483700
 C -3.67236100 0.30739500 -0.78283400
 C -3.66812200 -0.70726100 0.18838000
 C -4.80188600 1.10235600 -0.97483900
 C -4.86175200 -0.91513500 0.93750200
 C -5.93943400 0.88325100 -0.23483600
 H -4.78871100 1.89221900 -1.71753500
 C -5.97499000 -0.13120100 0.72131000
 H -6.88026900 -0.28550800 1.29685400
 O 3.64232100 -2.26920500 -0.51478500
 O -2.64699000 -1.49559800 0.42855000
 S 6.38073000 2.78257500 0.86047100
 S -7.41331700 1.87906800 -0.48046300
 O -7.73987900 2.45754900 0.85424200
 O -8.46363500 0.93571200 -0.96111300
 O -7.05127900 2.91097900 -1.49042200
 O 7.54275100 2.39383100 1.71393800
 O 5.39797200 3.64112200 1.58077200
 O 6.81594800 3.36884000 -0.44187000
 H -1.48397400 1.52292200 -0.13509900
 H 1.45840700 -0.86567800 -0.87341900
 O -0.05147100 -3.26221200 -0.38775600
 H 0.66803400 -3.67800200 0.14446100
 H 2.46905400 -2.26718600 -1.84734400
 O 1.64671300 -2.11322300 -2.36191900
 H 0.98031400 -2.65500300 -1.90770800
 H -0.80226400 -3.86205400 -0.38104000
 H 2.81298300 -3.38958200 0.42012500
 O 2.20806500 -4.07168600 0.81104000
 H 2.36505200 -4.06491700 1.75773600
 H -0.33311000 -2.26185600 1.85806700
 H -0.42870000 -1.58945400 2.21174400
 Pd -0.74546800 -0.86408500 0.26966700
 H 1.88338200 0.31153700 1.78936900
 H -2.22649600 -0.34456200 -2.25551700
 O -4.79796000 -1.92112700 1.84085300
 O 6.15890700 -1.90073400 -1.30143200
 C -5.94843900 -2.18605800 2.61106500
 H -5.69897400 -3.01951200 3.26457000
 H -6.23145000 -1.32363200 3.22437400

H -6.79923600 -2.46825000 1.98152400
 C 7.48112400 -1.70765000 -1.74084500
 H 7.76440100 -2.60625300 -2.28631400
 H 7.56438300 -0.84432900 -2.41099300
 H 8.17274000 -1.56861600 -0.90200100

64

RR-PhOMe_ID2_TS2, E(SCF) = -2714.32295973,
 E(ZPE) = -2713.844542, E(G) = -2713.920510
 a.u.

C -0.00887200 0.48808700 -1.89142000
 H 0.04260400 -0.39701600 -2.53156900
 H -0.09741500 1.37411700 -2.52601700
 C 1.19341700 0.55574600 -0.99250000
 H 2.11907900 0.63202400 -1.56937400
 H 1.13859900 1.42694100 -0.33123200
 N 1.20745400 -0.65953400 -0.14696000
 N -1.20214300 0.34997700 -1.02865300
 C 2.17510000 -0.58208400 0.98097400
 H 2.16485200 -1.56876800 1.45246200
 C -2.45581000 0.02149800 -1.74181100
 H -2.59086100 0.73626900 -2.56064200
 C 3.55515300 -0.18580900 -0.56182800
 C 4.32243900 -1.09806000 -0.19443500
 C 4.04429600 1.07703200 0.89311400
 C 5.63328600 -0.66449600 -0.57899900
 C 5.30504600 1.46044400 0.50031900
 H 3.43010000 1.76297200 1.46832900
 C 6.10267300 0.58569000 -0.24410300
 H 7.09444900 0.90398100 -0.54523500
 C -3.63607000 0.07444800 -0.82597100
 C -3.65929200 -0.71840100 0.33333400
 C -4.71284900 0.90050100 -1.14495900
 C -4.83141500 -0.67341900 1.14247800
 C -5.82926600 0.92775300 -0.34395400
 H -4.67745400 1.51900400 -2.03518600
 C -5.89327700 0.13771900 0.80288300
 H -6.78100300 0.17510800 1.42357700
 O 3.88624300 -2.26438200 -0.53777400
 O -2.68826800 -1.52032200 0.70030700
 S 5.95358900 3.08031800 0.89921500
 S -7.22515700 1.98650300 -0.73393100
 O -6.87701400 2.67733500 -2.00600800
 O -7.35882700 2.92120400 0.42025800
 O -8.40027700 1.07822700 -0.86597900
 O 7.19751600 2.84887000 1.69203100
 O 4.89203600 3.77457900 1.68170700
 O 6.23844000 3.74566200 -0.40697800
 H -2.31049600 -0.97142000 -2.18115000
 H 1.77246600 0.14162300 1.69550100
 H -1.34231900 1.21579600 -0.50451300
 H 1.46557800 -1.44479600 -0.76175100
 O -0.25235300 -3.62940900 0.28137700
 H 0.70326400 -3.84826100 0.36874700
 H 2.81138800 -2.40654000 -1.88672600
 O 1.99551200 -2.32643800 -2.43409500
 H 1.69390000 -3.22554300 -2.58330700
 H -0.52468700 -3.95865600 -0.57856400
 H 2.99489400 -3.41358200 0.28007500
 O 2.40102400 -4.13315300 0.61502500
 H 2.69879300 -4.33713700 1.50406000
 H -0.42674700 -2.25324600 2.07031000
 H -0.34609100 -1.55740300 2.38271200
 Pd -0.75351500 -1.08814500 0.36283900
 O 6.34348000 -1.57747700 -1.29316900
 O -4.80383800 -1.47769000 2.23152000
 C -5.93678500 -1.48159400 3.06998600
 H -5.72886700 -2.18845200 3.87058500
 H -6.12034900 -0.49300400 3.50491600
 H -6.83488500 -1.80427200 2.53232700
 C 7.64219600 -1.22107400 -1.70013500
 H 8.04731500 -2.07589800 -2.23884300
 H 7.63503900 -0.35141800 -2.36731800
 H 8.28922900 -0.99994500 -0.84356600

64

RR-PhOMe_ID2_TS3_P, E(SCF) = -
 2714.36326063, E(ZPE) = -2713.879947, E(G)
 = -2713.955915 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.03795900 | 0.68768300 | -1.73981600 |
| H | 0.01079300 | -0.16718500 | -2.42248900 |
| H | -0.06439100 | 1.59756300 | -2.34927100 |
| C | 1.16263300 | 0.68781000 | -0.82613000 |
| H | 2.08612800 | 0.82890500 | -1.39661500 |
| H | 1.08952100 | 1.50539500 | -0.10098800 |
| N | 1.20869000 | -0.58723900 | -0.06706400 |
| N | -1.25030800 | 0.53742800 | -0.92472100 |
| C | 2.17876200 | -0.56256000 | 1.05568600 |
| H | 2.13630600 | -1.54659300 | 1.52387300 |
| C | -2.46221800 | 0.15343900 | -1.66106800 |
| H | -2.64685400 | 0.84789000 | -2.49042500 |
| C | 3.57273900 | -0.18975900 | 0.64057100 |
| C | 4.37664600 | -1.08004300 | -0.06183700 |
| C | 4.05354100 | 1.09113000 | 0.91797000 |
| C | 5.64742800 | -0.63765800 | -0.51818800 |
| C | 5.29963200 | 1.47449400 | 0.48229500 |
| H | 3.43708900 | 1.79268000 | 1.46938300 |
| C | 6.10053400 | 0.60099900 | -0.24417300 |
| H | 7.07757100 | 0.92629400 | -0.58022900 |
| C | -3.65915500 | 0.12211900 | -0.75960700 |
| C | -3.69307800 | -0.71509700 | 0.37558200 |
| C | -4.75555700 | 0.92075100 | -1.08744300 |
| C | -4.90453100 | -0.72263700 | 1.13726700 |
| C | -5.90074800 | 0.89633800 | -0.32883900 |
| H | -4.70929800 | 1.56374600 | -1.96022400 |
| C | -5.97726800 | 0.06915400 | 0.79193700 |
| H | -6.88553300 | 0.06222800 | 1.38339400 |
| O | 3.99220900 | -2.33916800 | -0.39136800 |
| O | -2.73176600 | -1.50807000 | 0.76825700 |
| S | 5.93205400 | 3.12717400 | 0.82470900 |
| S | -7.31348500 | 1.91865700 | -0.73789100 |
| O | -7.53499800 | 2.80534500 | 0.44209300 |
| O | -8.45292300 | 0.97977300 | -0.95599200 |
| O | -6.94128500 | 2.67357600 | -1.96722300 |
| O | 4.85349200 | 3.83086100 | 1.56820300 |
| O | 6.21470000 | 3.72515600 | -0.50961900 |
| O | 7.16533300 | 2.92072900 | 1.63375700 |
| H | -2.26119800 | -0.83226200 | -2.09983500 |
| H | 1.80510900 | 0.15631800 | 1.78824000 |
| H | -1.43107800 | 1.39976900 | -0.41397600 |
| H | 1.49106800 | -1.30758300 | -0.73920600 |
| O | 0.40695800 | -4.05814300 | -0.78155000 |
| H | 1.69214700 | -4.14434300 | 0.47852700 |
| H | 2.92260100 | -2.44263000 | -1.98164300 |
| O | 2.02133700 | -2.36023400 | -2.33817200 |
| H | 2.10195300 | -2.13061100 | -3.26722800 |
| O | 0.85385600 | -3.57494000 | -1.49994700 |
| H | 3.45132900 | -2.79766200 | 0.29678500 |
| O | 2.48473500 | -4.01746300 | 1.04445000 |
| H | 2.16843700 | -4.00018600 | 1.95103500 |
| H | -0.17493800 | -3.39289800 | -0.37615000 |
| H | -0.33262900 | -2.26067600 | 1.36198400 |
| Pd | -0.76236600 | -1.07149700 | 0.42673400 |
| O | 6.34369000 | -1.60438600 | -1.20603600 |
| O | -4.89594900 | -1.55723300 | 2.20893400 |
| C | 7.62747000 | -1.24973300 | -1.67730600 |
| H | 8.02061200 | -2.12612300 | -2.18759000 |
| H | 7.57923100 | -0.41510900 | -2.38388900 |
| H | 8.29690900 | -0.98358100 | -0.85324700 |
| C | -6.05836900 | -1.61578800 | 3.00018900 |
| H | -5.86276100 | -2.33872300 | 3.78996200 |
| H | -6.28909000 | -0.64550800 | 3.45450100 |
| H | -6.92712800 | -1.94769600 | 2.42048900 |

64
 RR-PhOMe_ID2_TS3_R, E(SCF) = -
 2714.33407624, E(ZPE) = -2713.853436, E(G)
 = -2713.930322 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.06656800 | 0.58137000 | -1.86105700 |
| H | -0.00411400 | -0.26803500 | -2.54770200 |
| H | -0.16902500 | 1.49555200 | -2.45144000 |
| C | 1.13531300 | 0.62314100 | -0.95960700 |
| H | 2.05781500 | 0.74840600 | -1.53269500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.06594600 | 1.45592600 | -0.25241000 |
| N | 1.17436200 | -0.63763200 | -0.18338300 |
| N | -1.25940100 | 0.37804100 | -1.00953500 |
| C | 2.14977300 | -0.61588600 | 0.94349000 |
| H | 2.17214700 | -1.63517200 | 1.33843100 |
| C | -2.50356900 | 0.06029300 | -1.74638700 |
| H | -2.64208000 | 0.80073900 | -2.54909800 |
| C | 3.51209700 | -0.15467800 | 0.53377700 |
| C | 4.31047000 | -1.01099100 | -0.25492800 |
| C | 3.95139100 | 1.11776900 | 0.89832100 |
| C | 5.58969100 | -0.50522300 | -0.65555400 |
| C | 5.18682100 | 1.56754300 | 0.49720800 |
| H | 3.31845300 | 1.75858600 | 1.50456900 |
| C | 6.00795100 | 0.75475800 | -0.29009700 |
| H | 6.97694500 | 1.13081800 | -2.54987600 |
| C | -3.68547500 | 0.06768500 | -0.83214700 |
| C | -3.69978200 | -0.76550800 | 0.29799300 |
| C | -4.76895900 | 0.89570700 | -1.12205500 |
| C | -4.86504300 | -0.74533300 | -1.11802300 |
| C | -5.88061000 | 0.89285500 | -0.31465900 |
| H | -4.74078700 | 1.54151100 | -1.99285700 |
| C | -5.93313100 | 0.06877900 | 0.80828800 |
| H | -6.81688500 | 0.08581100 | 1.43524600 |
| O | 3.92702800 | -2.19585500 | -0.60499800 |
| O | -2.72855200 | -1.58558200 | 0.63008500 |
| S | 5.77446900 | 3.19704400 | 0.94849200 |
| S | -7.29004500 | 1.94546000 | -0.67260700 |
| O | -7.45831500 | 2.81890900 | 0.52411800 |
| O | -8.44583600 | 1.02378600 | -0.86753000 |
| O | -6.93631600 | 2.70539300 | -1.90281400 |
| O | 4.70169800 | 3.81168100 | 1.78030600 |
| O | 6.00026500 | 3.92589600 | -0.33472500 |
| O | 7.04441900 | 2.98746400 | 1.70487000 |
| H | -2.34385300 | -0.91508100 | -2.21875700 |
| H | 1.73507800 | 0.04211000 | 1.71154400 |
| H | -1.41903800 | 1.21713400 | -0.44804300 |
| H | 1.43892000 | -1.38707300 | -0.83737900 |
| O | 0.78612000 | -4.12224300 | 0.08006000 |
| H | 1.64556500 | -4.22533500 | 0.53626800 |
| H | 2.76475500 | -2.56271300 | -1.74515000 |
| O | 1.86031700 | -2.72207800 | -2.11978500 |
| H | 1.92668300 | -2.71560300 | -3.07660600 |
| H | 1.02986500 | -3.78833900 | -0.80064600 |
| H | 3.66954200 | -3.41988400 | 0.54464900 |
| O | 3.37396000 | -4.17223800 | 1.11512400 |
| H | 3.56048600 | -3.90421900 | 2.01763100 |
| H | -0.17664600 | -2.69809200 | 0.97937800 |
| H | -0.45593600 | -2.24145600 | 1.61550700 |
| Pd | -0.78732600 | -1.12567300 | 0.30032600 |
| O | 6.32415300 | -1.36138200 | -1.41330800 |
| O | -4.82665500 | -1.57829300 | 2.18588500 |
| C | 7.58350300 | -0.92198300 | -1.86126400 |
| H | 8.00597800 | -1.73256900 | -2.45237800 |
| H | 7.50096100 | -0.02811500 | -2.49004400 |
| H | 8.25791100 | -0.70170100 | -1.02595700 |
| C | -5.95030800 | -1.60185600 | 3.03659600 |
| H | -5.73205200 | -2.32404000 | 3.82055400 |
| H | -6.13116500 | -0.62242600 | 3.49288500 |
| H | -6.85366200 | -1.91583000 | 2.50256300 |

64
 RR-PhOMe_ID2_TS3-square_P, E(SCF) = -
 2714.36215145, E(ZPE) = -2713.878952, E(G)
 = -2713.954549 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.02352000 | -0.78221500 | -1.70678800 |
| H | -0.03302900 | 0.04980400 | -2.41608800 |
| H | 0.05346300 | -1.71202900 | -2.28514800 |
| C | -1.17262800 | -0.75805800 | -0.78801100 |
| H | -2.09815700 | -0.92393300 | -1.34845700 |
| H | -1.09045600 | -1.55093400 | -0.03658600 |
| N | -1.22128900 | 0.54178500 | -0.07354700 |
| N | 1.23833500 | -0.59981000 | -0.90080500 |
| C | -2.19323000 | 0.55500700 | 1.04708600 |
| H | -2.13365700 | 1.54646900 | 1.49756500 |
| C | 2.44596900 | -0.23509300 | -1.65407600 |
| H | 2.62959500 | -0.95603000 | -2.46066600 |
| C | -3.59182400 | 0.19930100 | 0.63241000 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -4.38717200 | 1.09966500 | -0.06832200 | C | 3.70707000 | 0.69364700 | 0.27935200 |
| C | -4.08627000 | -1.07699300 | 0.90885700 | C | 4.83313500 | -1.03046500 | -1.01998800 |
| C | -5.66089800 | 0.70502300 | -0.52758300 | C | 4.91124300 | 0.83224200 | 0.103427100 |
| C | -5.33504700 | -1.44935200 | 0.47246000 | C | 5.97767900 | -0.87441100 | -0.27615100 |
| H | -3.47747300 | -1.78412000 | 1.46171600 | C | 4.81344800 | -1.75836100 | -1.82375500 |
| C | -6.12650300 | -0.56748100 | -0.25509600 | C | 6.01852500 | 0.05994400 | 0.75914300 |
| H | -7.10644800 | -0.88235800 | -0.59261800 | H | 6.92714900 | 0.16756300 | 1.33980900 |
| C | 3.64637400 | -0.16894100 | -0.75917200 | O | -3.79610900 | 2.22421300 | -0.62533600 |
| C | 3.67908900 | 0.70176300 | 0.35082600 | O | 2.70720900 | 1.48050100 | 0.58976300 |
| C | 4.74758000 | -0.96837100 | -1.06845100 | S | -6.17337900 | -2.95935900 | 0.92689300 |
| C | 4.89214200 | 0.73772700 | 1.10883200 | S | 7.42955800 | -1.88091600 | -0.58520400 |
| C | 5.89565500 | -0.91353900 | -0.31585400 | O | 7.61709200 | -2.71667000 | 0.63663000 |
| H | 4.70279600 | -1.63582900 | -1.92267100 | O | 8.55501400 | -0.92426300 | -0.79205500 |
| C | 5.96945200 | -0.05562100 | 0.78168900 | O | 7.12363300 | -2.68896400 | -1.79813800 |
| H | 6.87971500 | -0.02604200 | 1.36949600 | O | -7.34907200 | -2.61494300 | -0.80239000 |
| O | -4.00234100 | 2.35770900 | -0.38879600 | O | -5.13008900 | -3.72756100 | 1.66349900 |
| O | 2.71454700 | 1.50131900 | 0.72273400 | O | -6.58286100 | -3.61599500 | -0.34972500 |
| S | -5.98401900 | -3.09422900 | 0.81734600 | H | 1.49691600 | -1.47634300 | -0.22069000 |
| S | 7.31340900 | -1.93907500 | -0.69966200 | H | -1.43235700 | 1.02540900 | -0.90844300 |
| O | 7.52657600 | -2.80999400 | 0.49361700 | O | -0.42502500 | 3.86508400 | -0.02463300 |
| O | 8.45301500 | -1.00111300 | -0.92058900 | H | -1.35219600 | 4.08083700 | 0.35426200 |
| O | 6.95249700 | -2.71078100 | -1.92182500 | H | -2.55185800 | 2.36783500 | -1.82703600 |
| O | -7.21667000 | -2.87451100 | 1.62424600 | O | -1.70168300 | 0.23058500 | -2.32240600 |
| O | -4.91370100 | -3.80711000 | 1.56434900 | H | -1.14552400 | 2.99560100 | -1.93802000 |
| O | -6.27092300 | -3.69358200 | -0.51563000 | H | 0.14372900 | 4.64057000 | 0.05547800 |
| H | 1.42476300 | -1.44449400 | -0.36313200 | H | -3.29277800 | 3.43086000 | 0.32738000 |
| H | -1.50245400 | 1.24192900 | -0.77319400 | O | -2.82225600 | 4.20256200 | 0.75670700 |
| O | -0.24927300 | 4.02781600 | -0.78033300 | H | -3.03550200 | 4.18388600 | 1.69257600 |
| H | -1.60487100 | 4.17137500 | 0.44155900 | H | 0.05060700 | 2.89934700 | 0.58293400 |
| H | -2.77712200 | 2.51002100 | -1.97448900 | H | 0.33289100 | 2.20424500 | 1.29028800 |
| O | -1.89991900 | 2.32864600 | -2.34361800 | Pd | 0.76920000 | 0.94911100 | 0.29144800 |
| H | -1.33644500 | 3.04838100 | -2.01115600 | H | -1.85658300 | -0.17848700 | 1.74190900 |
| H | 0.34212700 | 4.74898000 | -1.01521400 | H | 2.28773900 | 0.50441400 | -2.21292300 |
| H | -3.40993000 | 2.78785700 | 0.27123100 | O | 4.86161300 | 1.76720100 | 2.01532100 |
| O | -2.40178500 | 4.01453300 | 0.98427600 | O | -6.28216700 | 1.66077900 | -1.37459100 |
| H | -2.10438700 | 4.01476100 | 1.89759200 | C | 6.01950700 | 1.96375600 | 2.79267900 |
| H | 0.29801600 | 3.35558800 | -0.32968400 | H | 5.78546700 | 2.75165400 | 3.50594000 |
| H | 0.30813900 | 2.26055000 | 1.30031500 | H | 6.29755600 | 1.05723400 | 3.34177900 |
| Pd | 0.74690800 | 1.04474200 | 0.40000400 | H | 6.87023200 | 2.27973400 | 2.17874300 |
| H | -1.83539500 | -0.15620100 | 1.79513500 | C | -7.59888300 | 1.37273200 | -1.77818500 |
| H | 2.23883900 | 0.73449100 | -2.12468500 | H | -7.95067100 | 2.23753300 | -2.33804400 |
| O | 4.88105600 | 1.60050000 | 2.15790100 | H | -7.64154900 | 0.48920300 | -2.42547100 |
| O | -6.34864300 | 1.64047000 | -1.21502800 | H | -8.26082000 | 1.21089000 | -0.91984500 |
| C | 6.04584900 | 1.68916800 | 2.94296800 | | | | |
| H | 5.84655100 | 2.42961100 | 3.71540100 | | | | |
| H | 6.28710100 | 0.73252600 | 3.42007000 | | | | |
| H | 6.90939800 | 2.01461400 | 2.35188000 | | | | |
| C | -7.63234200 | 1.29554400 | -1.69258000 | | | | |
| H | -8.01646700 | 2.17465200 | -2.20513800 | | | | |
| H | -7.58703000 | 0.46040900 | -2.39887100 | | | | |
| H | -8.30827900 | 1.03444900 | -0.87211400 | | | | |

64
RR-PhOMe_ID2_TS3-square, E(SCF) = -2714.32126466, E(ZPE) = -2713.843668, E(G) = -2713.918983 a.u.

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 0.09709200 | -1.03526700 | -1.65790800 | C | -0.11726200 | 1.06378600 | -1.67329800 |
| H | 0.00822700 | -0.28019200 | -2.44529100 | H | -0.02608900 | 0.33183300 | -2.48207900 |
| H | 0.20220000 | -2.01463500 | -2.13372100 | H | -0.23266200 | 2.05444400 | -2.12236200 |
| C | -1.10095700 | -0.98097900 | -0.74816400 | C | 1.07989900 | 0.99778700 | -0.76344200 |
| H | -2.02239100 | -1.21666000 | -1.28822400 | H | 2.00081500 | 1.25741600 | -1.29243000 |
| H | -0.99866700 | -1.70291800 | 0.06913900 | H | 0.96569100 | 1.69679400 | 0.07155300 |
| N | -1.17658800 | 0.37294700 | -0.15274600 | N | 1.16625200 | -0.36931500 | -0.19935600 |
| N | 1.29253600 | -0.70474100 | -0.85673900 | N | -1.30894500 | 0.70253800 | -0.87883500 |
| C | -2.18599600 | 0.48109200 | 0.93440500 | C | 2.15985600 | -0.49104500 | 0.90334000 |
| H | -2.13190300 | 1.50884400 | 1.30085600 | H | 2.10556700 | -1.52614000 | 1.24925700 |
| C | 2.50479600 | -0.40733900 | -1.64393100 | C | -2.52736300 | 0.43403500 | -1.66921500 |
| H | 2.67921700 | -1.21299600 | -2.36594400 | H | -2.70170300 | 1.26455600 | -1.36194400 |
| C | -3.57544000 | 0.14075400 | 0.49994700 | C | 3.55463100 | -0.13512400 | 0.49790000 |
| C | -4.29209900 | 1.08244000 | -0.26947300 | C | 4.31127500 | -1.08249500 | -0.22435000 |
| C | -4.13955100 | -1.08391600 | 0.85651100 | C | 4.08644900 | 1.10930000 | 0.83734500 |
| C | -5.62416700 | 0.71855700 | -0.64889800 | C | 5.64743800 | -0.70554500 | -0.57408500 |
| C | -5.41886900 | -1.40255600 | 0.46603400 | C | 5.36981900 | 1.44145100 | 0.47319600 |
| H | -3.56824300 | -1.79121100 | 1.44980900 | H | 3.48737000 | 1.82064600 | 1.39738900 |
| C | -6.16707600 | -0.49535500 | -0.29022400 | C | 6.15615800 | 0.52881100 | -0.23626600 |
| H | -7.17622400 | -0.75968500 | -0.58522100 | H | 7.16806100 | 0.80502100 | -0.51022600 |
| C | 3.70495400 | -0.25029800 | -0.76403400 | C | -3.72003000 | 0.25390300 | -0.78458000 |
| | | | | C | -3.71492700 | -0.73059600 | 0.21895900 |
| | | | | C | -4.84294500 | 1.05618100 | -0.98977800 |
| | | | | C | -4.90710200 | -0.89220400 | -0.98649400 |
| | | | | C | -5.97414200 | 0.88349100 | -0.22901200 |
| | | | | H | -4.82684800 | 1.81885100 | -1.76049700 |
| | | | | C | -6.01122100 | -0.09931200 | 0.76058500 |
| | | | | H | -6.91037200 | -0.22052200 | 1.35331000 |
| | | | | O | 3.84798900 | -2.24615600 | -0.55672200 |

64
RR-PhOMe_ID2_TS3, E(SCF) = -2714.32850411, E(ZPE) = -2713.849649, E(G) = -2713.924840 a.u.

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| O | -2.71347100 | -1.53496400 | 0.47979900 | O | -7.64200200 | 0.69482500 | -0.27246300 |
| S | 6.07604900 | 3.03292400 | 0.89189700 | H | -0.44097100 | 1.70281800 | 1.62188500 |
| S | -7.43676800 | 1.88670800 | -0.49754300 | H | -1.24379900 | -0.03421900 | -1.71189700 |
| O | -7.76894000 | 2.48775700 | 0.82630500 | H | -1.60662500 | 0.15915700 | -1.00900700 |
| O | -8.49478100 | 0.94804100 | -0.97248700 | O | 0.41510900 | 2.12930100 | 1.40220000 |
| O | -7.06147100 | 2.90266300 | -1.51960400 | H | 0.63837000 | 1.78885900 | 0.52011700 |
| O | 5.01180200 | 3.78564900 | 1.61395100 | H | -0.09139200 | -0.29728600 | -2.62456500 |
| O | 6.45781500 | 3.66881500 | -0.40367900 | O | 0.88249500 | -0.34678200 | 2.78420000 |
| O | 7.26569900 | 2.74717400 | 1.74704200 | H | 1.13564100 | 0.53319300 | 2.45582600 |
| H | -2.31656800 | -0.45958600 | -2.26780700 | H | -2.17930600 | -2.56620300 | -0.82604000 |
| H | 1.81048100 | 0.15394300 | 1.71399400 | H | -1.78734400 | -2.03709400 | -2.03295200 |
| H | -1.51026300 | 1.45142700 | -0.21455200 | H | 1.33206400 | -1.45658700 | 1.36315200 |
| H | 1.43995900 | -1.00520300 | -0.95946800 | H | 2.96061100 | -2.94997700 | 0.13426900 |
| O | 0.55318100 | -3.86148400 | -0.10967800 | Pd | -0.23718700 | -0.89941100 | -0.49612400 |
| H | 1.38690200 | -4.09406500 | 0.38199200 | O | 2.58529000 | 2.62790200 | -1.62456700 |
| H | 2.68732700 | -2.45925700 | -1.69901900 | O | -2.96504900 | 2.66672300 | 1.60568300 |
| O | 1.78300600 | -2.52636500 | -2.11244800 | C | 3.32025100 | 3.83067200 | -1.06109600 |
| H | 1.88771400 | -2.64955300 | -3.05815700 | H | 3.83394600 | 4.01602900 | -0.11167800 |
| H | 0.87201000 | -3.49563700 | -0.96962400 | H | 4.05740100 | 3.82823100 | -1.87079400 |
| H | 3.40431300 | -3.47259700 | 0.50153000 | H | 2.60109000 | 4.62764100 | -1.23834800 |
| O | 2.96456600 | -4.22621000 | 0.97398100 | C | -3.61851100 | 3.86852800 | 1.27779000 |
| H | 3.12188100 | -4.08780000 | 1.91073200 | H | -3.05745900 | 4.67046700 | 1.75415900 |
| H | -0.02134600 | -2.85459400 | 0.53375900 | H | -3.63395800 | 4.03777900 | 0.19500400 |
| H | -0.36016700 | -2.26037900 | 1.21347400 | H | -4.64915900 | 3.88472300 | 1.65038500 |
| Pd | -0.78149400 | -0.97418700 | 0.21848400 | | | | |
| O | 6.34438700 | -1.65502100 | -1.25185300 | 61 | | | |
| O | -4.84907300 | -1.86782000 | 1.92549000 | RR-PhOMe_EI_D1_TS1_R, E(SCF) = - | | | |
| C | 7.67168200 | -1.35733500 | -1.61227800 | 2637.90684367, E(ZPE) = -2637.452812, E(G) | | | |
| H | 8.06102000 | -2.23490900 | -2.12536100 | = -2637.526620 a.u. | | | |
| H | 7.72542800 | -0.49660300 | -2.28865300 | C | 0.57416000 | -3.49199800 | 0.78754600 |
| H | 8.29392400 | -1.15220300 | -0.73371600 | H | 1.23373400 | -4.36319800 | 0.73421700 |
| C | -5.99635000 | -2.09176800 | 2.71150600 | H | 0.09834600 | -3.49459800 | 1.76991000 |
| H | -5.75526100 | -2.91033700 | 3.38686300 | C | -0.46978300 | -3.55020200 | -0.30031500 |
| H | -6.26130400 | -1.20831700 | 3.30299300 | H | 0.00213800 | -3.68418300 | -1.27543600 |
| H | -6.85766900 | -2.37783200 | 2.09776300 | H | -1.14303600 | -4.39696700 | -0.13971200 |
| | | | | N | -1.23845800 | -2.27849300 | -0.36898100 |
| | | | | N | 1.36195800 | -2.23347500 | 0.70407000 |
| | | | | C | -2.43249500 | -2.14685000 | 0.48485700 |
| | | | | H | -3.06279000 | -3.03558600 | -3.06910200 |
| | | | | C | 2.52355600 | -2.20532100 | -0.19814200 |
| | | | | H | 2.15476900 | -2.32671600 | -1.22283600 |
| | | | | C | -3.23465600 | -0.92570500 | 0.11669000 |
| | | | | C | -2.65737100 | 0.31103100 | -0.22845300 |
| | | | | C | -4.62704000 | -1.05523600 | 0.15291400 |
| | | | | C | -3.54056600 | 1.39181000 | -0.52817100 |
| | | | | C | -5.44946100 | 0.00592700 | -0.12906300 |
| | | | | H | -5.06866500 | -2.01245300 | 0.40867300 |
| | | | | C | -4.90669100 | 1.24343800 | -0.47504400 |
| | | | | H | -5.56549300 | 2.07280300 | -0.70479200 |
| | | | | C | 3.32395300 | -0.93755500 | -0.04023600 |
| | | | | C | 2.76557300 | 0.32909300 | 0.25939500 |
| | | | | C | 4.70315100 | -1.05687000 | -0.24557600 |
| | | | | C | 3.66224900 | 1.43179200 | 0.33861800 |
| | | | | C | 5.53373300 | 0.03138000 | -0.17150600 |
| | | | | H | 5.12803300 | -2.03033000 | -0.46708900 |
| | | | | C | 5.01236000 | 1.29109800 | 0.12386300 |
| | | | | H | 5.67758300 | 2.14414500 | 0.18593100 |
| | | | | O | -1.37268200 | 0.59153500 | -0.30281700 |
| | | | | O | 1.49977200 | 0.59646500 | 0.49272300 |
| | | | | S | -7.23540700 | -0.16529100 | -0.08955600 |
| | | | | S | 7.29814200 | -0.12158500 | -0.45461200 |
| | | | | O | 7.95531500 | 0.38682900 | 0.78382000 |
| | | | | O | 7.59471900 | 0.73084700 | -1.64225000 |
| | | | | O | 7.55589100 | -1.56763100 | -0.69845300 |
| | | | | O | -7.50900400 | -1.56919100 | 0.32373500 |
| | | | | O | -7.70267100 | 0.13681600 | -1.47337400 |
| | | | | O | -7.71730000 | 0.83891200 | 0.90167900 |
| | | | | H | -0.64345200 | 2.40264400 | -0.24368500 |
| | | | | H | -1.22818200 | -0.43935500 | -3.27162100 |
| | | | | H | -1.63898600 | -0.00599500 | -2.81865400 |
| | | | | O | 0.03317000 | 2.98424500 | 0.14586900 |
| | | | | H | 0.78629000 | 2.37673100 | 0.26910300 |
| | | | | H | -1.45972900 | 1.15116000 | 1.91297200 |
| | | | | O | -1.28422200 | 1.93043500 | 2.45404600 |
| | | | | H | -0.80536800 | 2.49664000 | 1.82205600 |
| | | | | H | -1.53295700 | -2.13657000 | -1.33438800 |
| | | | | H | -2.09550100 | -2.12032100 | 1.52712800 |

H 1.68988200 -2.00063100 1.63978300
 H 3.16834500 -3.06492500 0.01779700
 Pd 0.06040900 -0.78127500 0.12249200
 O 3.05609000 2.60919200 0.63320200
 O -2.90782100 2.54643500 -0.85342000
 C 3.85270400 3.77064000 0.67685300
 H 4.61762200 3.70525700 1.45796800
 H 4.34194800 3.95938200 -0.28489700
 H 3.18246300 4.59754700 0.90373100
 C -3.70169100 3.67835000 -1.12956600
 H -3.01356700 4.49155800 -1.35163700
 H -4.35166000 3.51162600 -1.99492100
 H -4.31899300 3.95590500 -0.26852800

61
 RR-PhOMe_EI_D1_TS1, E(SCF) = -
 2637.88507255, E(ZPE) = -2637.431533, E(G)
 = -2637.502413 a.u.

C 0.46433600 -3.28906500 0.64516000
 H 1.11205700 -4.16794900 0.59342500
 H 0.09787100 -3.21056900 1.67112300
 C -0.68299300 -3.40881200 -0.32211600
 H -0.30846600 -3.57298200 -1.33471200
 H -1.33484800 -4.24780700 -0.05871900
 N -1.45311700 -2.13734000 -0.34806100
 N 1.24407900 -2.05421800 0.36556600
 C -2.39247800 -1.92928500 0.79189300
 H -2.97137900 -2.84893600 0.92992800
 C 2.46624500 -2.18514300 -0.44555000
 H 2.16071500 -2.44198100 -1.46571000
 C -3.31039200 -0.78026300 0.52673400
 C -2.77826500 0.52442200 0.47797900
 C -4.66825700 -1.01066700 0.31253400
 C -3.68762100 1.59082000 0.20938100
 C -5.51933700 0.04082200 0.06148600
 H -5.06078600 -2.02132500 0.34916100
 C -5.02999600 1.34821700 0.01066600
 H -5.71789000 2.16119900 -0.19261900
 C 3.29470100 -0.93258400 -0.38172000
 C 2.74250300 0.35553300 -0.49863100
 C 4.67078500 -1.08454700 -0.19022500
 C 3.63451900 1.46665900 -0.42203200
 C 5.50565000 0.00338000 -0.13370700
 H 5.09099700 -2.07871700 -0.08327100
 C 4.98785600 1.29264200 -0.24771700
 H 5.65545700 2.14431900 -0.18979600
 O -1.51434400 0.76749400 0.65158800
 O 1.47475500 0.65399200 -0.68219600
 S -7.27065400 -0.23021500 -0.20861200
 S 7.27247200 -0.19286000 0.11210900
 O 7.59480300 0.55571100 1.36058700
 O 7.91788900 0.40803200 -1.09040600
 O 7.51287600 -1.65711400 0.23181800
 O -7.48047100 -1.70222700 -0.11814400
 O -7.56719700 0.31708300 -1.56475000
 O -7.97541500 0.52363500 0.68892800
 H -0.41275300 2.21611800 0.89292600
 H -0.91056300 0.20409700 -2.36781900
 H -1.33400900 0.63321000 -1.90513600
 O 0.42306000 2.69660000 1.05474200
 H 1.00817100 2.35563900 0.35853600
 H -0.30186200 0.15900200 2.06315800
 O 0.56897900 0.10239800 2.49735600
 H 0.94967600 0.95082200 2.22068700
 H -2.01247000 -2.12202500 -1.20042200
 H -1.79148500 -1.77435400 1.69251400
 H 1.47215600 -1.59307500 1.25230000
 H 3.06246800 -3.02083600 -0.06163800
 Pd -0.02024100 -0.66395700 -0.48452200
 O 3.02550500 2.67385700 -0.53534300
 O -3.11376800 2.82039500 0.16966400
 C 3.82018000 3.83080200 -0.40001500
 H 4.32573200 3.85948200 0.57094600
 H 4.57051200 3.89789600 -1.19475600
 H 3.14447200 4.68031900 -0.47592200
 C -3.94946100 3.92268100 -0.09578300
 H -3.31288900 4.80536200 -0.09282000

H -4.43408000 3.83510300 -1.07465800
 H -4.72276300 4.03759400 0.67202200

61
 RR-PhOMe_EI_D1_TS2_P, E(SCF) = -
 2637.92494081, E(ZPE) = -2637.465728, E(G)
 = -2637.536543 a.u.

C 0.47539400 -3.12894400 1.09005700
 H 1.13175500 -4.00589000 1.11712200
 H 0.12122100 -2.96721000 2.11095700
 C -0.69097300 -3.39898800 0.16448300
 H -0.33255100 -3.67113300 -0.83067800
 H -1.30015800 -4.22728100 0.54408900
 N -1.52043000 -2.17589700 0.00418000
 N 1.21009100 -1.92347000 0.68294000
 C -2.36060100 -1.88347200 1.19405900
 H -2.94594500 -2.77968800 1.43453600
 C 2.35838800 -2.12956300 -0.20432400
 H 1.97463700 -2.47834800 -1.17275500
 C -3.27819600 -0.73411700 0.92393000
 C -2.99460300 0.56096300 1.33747700
 C -4.42057300 -0.97310500 0.15503700
 C -3.84978600 1.61954000 0.96229500
 C -5.24944600 0.06108100 -0.20342500
 H -4.65544800 -1.98385800 -0.16327600
 C -4.96865900 1.36475000 0.19555000
 H -5.63069500 2.16915100 -0.10123600
 C 3.18188900 -0.88000400 -0.35477800
 C 2.62823200 0.37278000 -0.68898900
 C 4.56160900 -1.00633100 -0.16808100
 C 3.53381800 1.47192600 -0.82611100
 C 5.40491800 0.06728300 -0.31205400
 H 4.97742700 -1.97249300 0.09758900
 C 4.88972800 1.31961400 -0.64317800
 H 5.56289100 2.16222500 -0.74784500
 O -1.93125500 0.91977700 2.08345400
 O 1.35918200 0.63939100 -0.90049900
 S -6.74523900 -0.24234400 -1.15833400
 S 7.17634200 0.16619800 -0.09985100
 O 7.77686800 0.15751200 -1.44041000
 O 7.40437300 -1.50032300 0.37233200
 O 7.57353500 0.92031500 0.90742900
 O -6.69477600 -1.67557200 -1.55279200
 O -6.67509900 0.68969900 -2.31748700
 O -7.87296100 0.07198200 -0.23698200
 H -0.37451300 2.12382600 1.33086600
 H -1.15616900 0.09873300 -1.38023000
 H -1.30766200 0.19422000 2.28230100
 O 0.59243300 2.16861900 1.31432500
 H 0.84086300 1.78587500 0.44677500
 H 0.70313500 -0.03937800 3.78763700
 O 0.50773600 -0.14638300 2.85298700
 H 0.74068100 0.70665700 2.42605300
 H -2.14661700 -2.31552600 -0.78567700
 H -1.69499900 -1.70488600 2.04080200
 H 1.48240200 -1.40274600 1.51626400
 H 3.00302100 -2.92820600 0.18533000
 Pd -0.14289900 -0.69521900 -0.48310400
 O -3.47197400 2.84421600 1.38887100
 O 2.94218400 2.65055900 -1.14796400
 C 3.76887000 3.78048700 -1.29787700
 H 4.30060200 4.01981300 -0.37017500
 H 4.50310700 3.64123500 -2.09920600
 H 3.11594500 4.61188200 -1.55644800
 C -4.27666700 3.94395500 1.01818500
 H -4.32723000 4.05387200 -0.06978700
 H -5.29206600 3.84846300 1.41609100
 H -3.80757400 4.82753100 1.44515500

61
 RR-PhOMe_EI_D1_TS2_R, E(SCF) = -
 2637.89418171, E(ZPE) = -2637.437850, E(G)
 = -2637.507182 a.u.

C 0.46739200 -3.28786300 1.00070400
 H 1.19547100 -4.10156800 1.02020400
 H 0.14784600 -3.11213200 2.03018000
 C -0.70402700 -3.63237200 0.12274600

| | | | | | | | |
|------------------------------|--------------------------|----------------------|-------------------|-----------------------|----------------------|--------------|-------------|
| H | -0.36687700 | -3.91751200 | -0.87602400 | C | -4.07993000 | 1.69663800 | 0.29899300 |
| H | -1.28231700 | -4.46232600 | 0.53841300 | C | -5.67551900 | -0.08545900 | 0.09273700 |
| N | -1.56123800 | -2.42700600 | -0.02703500 | H | -4.93389500 | -2.07205700 | 0.28307300 |
| N | 1.11426700 | -2.03360200 | 0.53086900 | C | -5.37916300 | 1.27707100 | 0.10333900 |
| C | -2.43032800 | -2.13354100 | 1.15765100 | H | -6.17821000 | 1.99301800 | -0.05018000 |
| H | -3.08150700 | -3.00374800 | 1.29914000 | C | 3.40162300 | -0.93071900 | -0.33974300 |
| C | 2.31259100 | -2.19198800 | -0.31773600 | C | 2.92988400 | 0.36992400 | -0.58138900 |
| H | 1.98761500 | -2.57898200 | -1.29084500 | C | 4.75490100 | -1.14285900 | -0.06325800 |
| C | -3.21500100 | -0.88781100 | 0.93892700 | C | 3.87494300 | 1.43748500 | -0.52963800 |
| C | -2.72083700 | 0.33706200 | 1.45440500 | C | 5.64503200 | -0.09842600 | -0.03430600 |
| C | -4.37110900 | -0.94173800 | 0.15858600 | H | 5.11214200 | -2.14836400 | 0.13091500 |
| C | -3.47693800 | 1.51164100 | 1.10460100 | C | 5.20488900 | 1.20507200 | -0.26142000 |
| C | -5.05922300 | 0.20598300 | -0.15314700 | H | 5.91572600 | 2.02215000 | -0.22464200 |
| H | -4.73303400 | -1.89669100 | -0.21335600 | O | -1.79236900 | 1.17182500 | 0.64716600 |
| C | -4.60526300 | 1.40824800 | 0.32211800 | O | 1.69202300 | 0.71080700 | -0.87347800 |
| H | -5.15786400 | 2.33952700 | 0.06549500 | S | -7.37948000 | -0.58620700 | -0.17036900 |
| C | 3.07938700 | -0.90752600 | -0.43021700 | S | 7.38508000 | -0.37531900 | 0.30751400 |
| C | 2.44949600 | 0.31652600 | -0.69390800 | O | 8.11729500 | 0.11185500 | -0.89687500 |
| C | 4.46561100 | -0.95864800 | -0.26193800 | O | 7.53467500 | -1.84061600 | -0.92544400 |
| C | 3.26430500 | 1.48226500 | -0.77933200 | O | 7.69580400 | 0.43027900 | 1.52303600 |
| C | 5.23016900 | 0.17654500 | -0.36438200 | O | -7.38655800 | -2.07398400 | -0.11780600 |
| H | 4.94735800 | -1.90612100 | -0.04624400 | O | -7.75803300 | -0.04870700 | -1.50893600 |
| C | 4.63047800 | 1.40803200 | -0.62017000 | O | -8.16212300 | 0.04016500 | 0.93352400 |
| H | 5.24531400 | 2.29786500 | -0.68687800 | H | -0.33726100 | 2.47751300 | 0.73572500 |
| O | -1.65882900 | 0.43542800 | 2.16402800 | H | -0.86763500 | 0.62629400 | -1.46169500 |
| O | 1.15559700 | 0.50132300 | -0.88218400 | H | -1.14170600 | 0.83869200 | -0.61231600 |
| S | -6.54848600 | 0.16324400 | -1.14151600 | O | 0.58953200 | 2.75777200 | 0.81308000 |
| S | 7.01128100 | 0.12025000 | -0.14340400 | H | 1.05487600 | 2.26658200 | 0.10900300 |
| O | 7.59208700 | 0.63636200 | -1.41559100 | H | -0.45750500 | 0.45260900 | 1.97940200 |
| O | 7.34997600 | -1.30585600 | 0.11557000 | O | 0.41439600 | 0.32352400 | 2.39404900 |
| O | 7.30519500 | 1.01009000 | 1.01605500 | H | 0.87069700 | 1.12233300 | 2.08425200 |
| O | -6.75585800 | -1.26301000 | -1.52161700 | H | -2.00667400 | -1.92594100 | -1.25129100 |
| O | -6.29255700 | 1.04438700 | -2.31937600 | H | -1.69716700 | -1.38279500 | 1.60141000 |
| O | -7.64137700 | 0.69514000 | -0.27385300 | H | 1.46372200 | -1.40658700 | 1.24882900 |
| H | -0.44143100 | 1.70393100 | 1.62270000 | H | 3.03839300 | -2.98221500 | 0.07596400 |
| H | -1.24404800 | -0.03423600 | -1.71131800 | Pd | 0.10892900 | -0.53069000 | -0.65132800 |
| H | -1.60669700 | 0.15945400 | -1.00836100 | O | -3.69280800 | 2.99459100 | 0.31848200 |
| O | 0.41398400 | 2.13108100 | 1.40167600 | O | 3.34536400 | 2.66228500 | -0.76723600 |
| H | 0.63757300 | 1.78839300 | 0.52053900 | C | 4.20617500 | 3.75866600 | -0.69409000 |
| H | -0.09133800 | -0.29680400 | 2.67204100 | H | 4.64934300 | 3.87726600 | 0.30253200 |
| O | 0.88252900 | -0.34601500 | 2.78429600 | H | 5.00988800 | 3.71214000 | -1.43538200 |
| H | 1.13582300 | 0.53395900 | 2.45628300 | C | 3.59802800 | 4.65317800 | -0.90443300 |
| H | -2.17945000 | -2.56654800 | -0.82526800 | C | -4.68603000 | 3.97898600 | 0.14352300 |
| H | -1.78705500 | -2.03664300 | 2.03357500 | H | -5.17058000 | 3.89429400 | -0.83533700 |
| H | 1.33215000 | -1.45691200 | 1.36347600 | H | -5.45214500 | 3.92182900 | 0.92426700 |
| H | 2.96040600 | -2.95023500 | 0.13364800 | H | -4.18418700 | 4.94239800 | 0.20825600 |
| Pd | -0.23735700 | -0.89958700 | -0.49550900 | | | | |
| O | -2.96512500 | 2.66677200 | 1.60571700 | 53 | | | |
| O | 2.58483500 | 2.62799900 | -1.02376900 | RR-PhOMe_EI, E(SCF) = | -2483.85913167, | | |
| C | 3.31958700 | 3.83092100 | -1.05936500 | E(ZPE) = | -2483.469995, E(G) = | -2483.533590 | |
| H | 3.83341000 | 4.01552300 | -0.10987200 | a.u. | | | |
| H | 4.05657500 | 3.82934700 | -1.86920500 | C | -0.63563600 | -3.40776700 | 0.41616600 |
| H | 2.60025400 | 4.62792400 | -1.23578500 | H | -0.40600900 | -3.38246700 | 1.48529000 |
| C | -3.61805400 | 3.86862100 | 1.27693500 | H | -1.24347600 | -4.29511600 | 0.22060800 |
| H | -3.63300200 | 4.03729300 | 0.19405100 | C | 0.63427700 | -3.40765800 | -0.39933800 |
| H | -4.64884200 | 3.88538700 | 1.64912100 | H | 1.24272900 | -4.29446800 | -0.20347000 |
| H | -3.05693100 | 4.67060600 | 1.75312400 | H | 0.40413200 | -3.38352100 | -1.46839600 |
| | | | | N | 1.38309000 | -2.17171800 | -0.07930500 |
| 61 | | | | N | -1.38448400 | -2.17254200 | 0.09415300 |
| RR-PhOMe_EI_D1_TS2, E(SCF) = | -2637.88662444, E(ZPE) = | -2637.431945, E(G) = | -2637.503306 a.u. | C | 2.46121400 | -1.82587200 | -1.02649400 |
| C | 0.42424100 | -3.09377100 | 0.66968100 | H | 3.10081800 | -2.70082800 | -1.18686100 |
| H | 1.03858700 | -3.99731900 | 0.66634000 | C | -2.46952300 | -1.82939900 | 1.03450100 |
| H | 0.02661700 | -2.97496900 | 1.67961000 | H | -1.98713100 | -1.59958700 | 1.99158800 |
| C | -0.69348400 | -3.20625600 | -0.33438200 | C | 3.29160900 | -0.68535400 | -0.52301300 |
| H | -0.29369500 | -3.41188300 | -1.32957800 | C | 2.69852200 | 0.53100200 | -0.13051000 |
| H | -1.37849000 | -4.01793000 | -0.06718300 | C | 4.67860500 | -0.84193900 | -0.49197600 |
| N | -1.42604600 | -1.91444200 | -0.41495800 | C | 3.57860000 | 1.58817900 | 0.25953600 |
| N | 1.25788100 | -1.89978300 | 0.37530100 | C | 5.49662500 | 0.19266600 | -0.10939300 |
| C | -2.32459800 | -1.65634600 | 0.75064800 | H | 5.11948100 | -1.78807100 | -0.78735500 |
| H | -2.81971200 | -2.60203700 | 0.99918200 | C | 4.94459400 | 1.41713200 | 0.26991200 |
| C | 2.50664000 | -2.13602000 | -0.37166800 | H | 5.60137700 | 2.22498600 | 0.57128200 |
| H | 2.22874300 | -2.42922900 | -1.39102800 | C | -3.29626200 | -0.68844000 | -0.52622100 |
| C | -3.36227800 | -0.60939100 | 0.48582100 | C | -2.69953800 | 0.53021300 | 0.14694700 |
| C | -3.02914100 | 0.75616300 | 0.49683000 | C | -4.68253600 | -0.84711100 | 0.47437200 |
| C | -4.68296200 | -1.01663700 | 0.28289300 | C | -3.57527500 | 1.58819800 | -0.25027200 |
| | | | | C | -5.49598200 | 0.18702900 | 0.08123100 |
| | | | | H | -5.12685100 | -1.79551000 | 0.75697800 |

| | | | |
|----|-------------|-------------|-------------|
| C | -4.94068100 | 1.41545900 | -0.28031600 |
| H | -5.59348500 | 2.22321200 | -0.59072100 |
| O | 1.41690800 | 0.78453900 | -0.11842500 |
| O | -1.41785400 | 0.78406500 | 0.15143300 |
| S | 7.27663800 | -0.00528700 | -0.04523200 |
| S | -7.27682500 | -0.00219200 | 0.01491300 |
| O | -7.66758600 | 0.27990500 | -1.39720500 |
| O | -7.83169000 | 1.00634200 | 0.96408900 |
| O | -7.56177900 | -1.40502400 | 0.42657500 |
| O | 7.56323800 | -1.35748900 | -0.60035200 |
| O | 7.65403200 | 0.12312700 | 1.39294700 |
| O | 7.84214800 | 1.09688400 | -0.87631300 |
| H | 1.78998300 | -2.26099400 | 0.85282900 |
| H | 1.97174300 | -1.59484500 | -1.97973600 |
| H | -1.78543100 | -2.26082900 | -0.84069900 |
| H | -3.10965900 | -2.70510200 | 1.18844500 |
| Pd | -0.00075300 | -0.66190800 | 0.01201300 |
| O | -2.94826800 | 2.74280500 | -0.58795000 |
| O | 2.95502200 | 2.74096900 | 0.60988700 |
| C | -3.74931400 | 3.83037800 | -0.98538400 |
| H | -4.33705900 | 3.59525800 | -1.87982700 |
| H | -4.43157200 | 4.14349700 | -0.18722600 |
| H | -3.07060800 | 4.65011500 | -1.21298200 |
| C | 3.76047100 | 3.82831600 | 0.99892300 |
| H | 3.08431100 | 4.64690400 | 1.23796300 |
| H | 4.36073600 | 3.59148900 | 1.88454100 |
| H | 4.43137700 | 4.14393100 | 0.19215000 |

53

RR-PhOMe, E(SCF) = -2483.85913167, E(ZPE) = -2483.469995, E(G) = -2483.533590 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.63563600 | -3.40776700 | 0.41616600 |
| H | -0.40600900 | -3.38246700 | 1.48529000 |
| H | -1.24347600 | -4.29511600 | 0.22060800 |
| C | 0.63427700 | -3.40765800 | -0.39933800 |
| H | 1.24272900 | -4.29446800 | -0.20347000 |
| H | 0.40413200 | -3.38352100 | -1.46839600 |
| N | 1.38309000 | -2.17171800 | -0.07930500 |
| N | -1.38448400 | -2.17254200 | 0.09415300 |
| C | 2.46121400 | -1.82587200 | -1.02649400 |
| H | 3.10081800 | -2.70082800 | -1.18686100 |
| C | -2.46952300 | -1.82939900 | 1.03450100 |
| H | -1.98713100 | -1.59958700 | 1.99158800 |
| C | 3.29160900 | -0.68535400 | -0.52301300 |
| C | 2.69852200 | 0.53100200 | -0.13051000 |
| C | 4.67860500 | -0.84193900 | -0.49197600 |
| C | 3.57860000 | 1.58817900 | 0.25953600 |
| C | 5.49662500 | 0.19266600 | -0.10939300 |
| H | 5.11948100 | -1.78807100 | -0.78735500 |
| C | 4.94459400 | 1.41713200 | 0.26991200 |
| H | 5.60137700 | 2.22498600 | 0.57128200 |
| C | -3.29626200 | -0.68844000 | 0.52622100 |
| C | -2.69953800 | 0.53021300 | 0.14694700 |
| C | -4.68253600 | -0.84711100 | 0.47437200 |
| C | -3.57527500 | 1.58819800 | -0.25027200 |
| C | -5.49598200 | 0.18702900 | 0.08123100 |
| H | -5.12685100 | -1.79551000 | 0.75697800 |
| C | -4.94068100 | 1.41545900 | -0.28031600 |
| H | -5.59348500 | 2.22321200 | -0.59072100 |
| O | 1.41690800 | 0.78453900 | -0.11842500 |
| O | -1.41785400 | 0.78406500 | 0.15143300 |
| S | 7.27663800 | -0.00528700 | -0.04523200 |
| S | -7.27682500 | -0.00219200 | 0.01491300 |
| O | -7.66758600 | 0.27990500 | -1.39720500 |
| O | -7.83169000 | 1.00634200 | 0.96408900 |
| O | -7.56177900 | -1.40502400 | 0.42657500 |
| O | 7.56323800 | -1.35748900 | -0.60035200 |
| O | 7.65403200 | 0.12312700 | 1.39294700 |
| O | 7.84214800 | 1.09688400 | -0.87631300 |
| H | 1.78998300 | -2.26099400 | 0.85282900 |
| H | 1.97174300 | -1.59484500 | -1.97973600 |
| H | -1.78543100 | -2.26082900 | -0.84069900 |
| H | -3.10965900 | -2.70510200 | 1.18844500 |
| Pd | -0.00075300 | -0.66190800 | 0.01201300 |
| O | -2.94826800 | 2.74280500 | -0.58795000 |
| O | 2.95502200 | 2.74096900 | 0.60988700 |
| C | -3.74931400 | 3.83037800 | -0.98538400 |

| | | | |
|---|-------------|------------|-------------|
| H | -4.33705900 | 3.59525800 | -1.87982700 |
| H | -4.43157200 | 4.14349700 | -0.18722600 |
| H | -3.07060800 | 4.65011500 | -1.21298200 |
| C | 3.76047100 | 3.82831600 | 0.99892300 |
| H | 3.08431100 | 4.64690400 | 1.23796300 |
| H | 4.36073600 | 3.59148900 | 1.88454100 |
| H | 4.43137700 | 4.14393100 | 0.19215000 |

77

RR-PhtBu_D1_D2_REF, E(SCF) = -2723.27240819, E(ZPE) = -2722.658977, E(G) = -2722.735413 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.59371400 | -3.78295200 | -0.28785200 |
| H | 0.28602900 | -3.78582500 | -1.33926500 |
| H | 1.20901000 | -4.67033000 | -0.11367700 |
| C | -0.61494200 | -3.75262800 | 0.62107900 |
| H | -1.23727500 | -4.64267500 | 0.49648600 |
| H | -0.30945700 | -3.69241200 | 1.66928200 |
| N | -1.38095400 | -2.52356900 | 0.30783900 |
| N | 1.37128300 | -2.54248100 | -0.05780600 |
| C | -2.43635400 | -2.12103900 | 1.26655500 |
| H | -3.08222900 | -2.97867200 | 1.48278000 |
| C | 2.39926500 | -2.20752700 | -1.06440600 |
| H | 1.86524400 | -1.98229400 | -1.99472700 |
| C | -3.25418700 | -0.99825700 | 0.69676300 |
| C | -2.65254800 | 0.23143700 | 0.34865000 |
| C | -4.61791900 | 0.18307200 | 0.51374300 |
| C | -3.46192200 | 1.30112800 | -0.13022800 |
| C | -5.39831000 | -0.15976700 | 0.02375200 |
| H | -5.07631900 | -2.13573900 | 0.76330100 |
| C | -4.81936500 | 1.06753400 | -0.28197500 |
| H | -5.46408900 | 1.85386600 | -0.65350200 |
| C | 3.25019200 | -1.05847400 | -0.60163200 |
| C | 2.67865200 | 0.18152200 | -0.23016500 |
| C | 4.62487000 | -1.22461300 | -0.56680200 |
| C | 3.52326800 | 1.25269700 | 0.18024800 |
| C | 5.44801000 | -0.18075400 | -0.19457100 |
| H | 5.06775500 | -2.17551000 | -0.84550200 |
| C | 4.89049600 | 1.03943300 | 0.17395200 |
| H | 5.56326200 | 1.83574400 | 0.47418700 |
| O | -1.35517100 | 0.43014600 | 0.48004700 |
| O | 1.37772500 | 0.39827500 | -0.28101500 |
| S | -7.16554400 | -0.37135000 | -0.21248200 |
| S | 7.23166000 | -0.36941600 | -0.15778400 |
| O | 7.64330100 | -0.09497300 | 1.24945600 |
| O | 7.76883300 | 0.64807700 | -1.10972400 |
| O | 7.50835100 | -1.76704600 | -0.58403100 |
| O | -7.46125300 | -1.78659400 | 0.14353600 |
| O | -7.42906100 | -0.06487300 | -1.64793600 |
| O | -7.81977500 | 0.60826800 | 0.70462400 |
| H | -1.81197700 | -2.63189300 | -0.60931500 |
| H | -1.92970400 | -1.82809900 | 2.19385400 |
| H | 1.82533300 | -2.60705400 | 0.85534200 |
| H | 3.03363700 | -3.08180100 | -1.24599600 |
| Pd | 0.00306100 | -1.03096100 | 0.10488300 |
| H | -0.12353400 | 0.57449400 | -3.15654900 |
| H | -2.61620100 | -0.85676200 | -2.85733900 |
| H | -2.69812800 | -0.52774100 | -2.18668300 |
| O | 0.83051200 | 0.61090900 | -3.05051400 |
| H | 0.96771300 | 0.59021700 | -2.08348100 |
| H | -1.05774700 | 0.53728300 | 2.29469200 |
| O | -0.99038700 | 0.49367800 | 3.27037900 |
| H | -0.13874200 | 0.07657100 | 3.42600900 |
| C | -2.83809000 | 2.65080300 | -0.48983600 |
| C | 2.92134700 | 2.57885000 | 0.64830800 |
| C | 2.05301500 | 2.33499400 | 1.88819900 |
| H | 1.59999500 | 3.27764800 | 2.21886200 |
| H | 1.24932500 | 1.62615200 | 1.62735900 |
| H | 2.65982100 | 1.94632400 | 2.71280900 |
| C | 4.00157800 | 3.58704200 | 1.03350600 |
| H | 4.63092500 | 3.22293900 | 1.85195200 |
| H | 4.64453100 | 3.84244800 | 0.18870700 |
| H | 3.52326800 | 4.50798200 | 1.37471100 |
| C | -2.11269900 | 3.25486500 | 0.72119500 |
| H | -2.79092200 | 3.33803600 | 1.57872300 |
| H | -1.25163300 | 2.65364800 | 1.01343000 |
| H | -1.75974800 | 4.26023300 | 0.47523100 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.84190400 | 2.47741900 | -1.63936200 |
| H | -1.40095100 | 3.44359100 | -1.90165200 |
| H | -1.03546000 | 1.79700500 | -1.35537700 |
| H | -2.34224400 | 2.08317000 | -2.53132500 |
| C | -3.89128800 | 3.66118700 | -0.93591800 |
| H | -4.42074900 | 3.33286400 | -1.83695300 |
| H | -4.63001700 | 3.85780500 | -0.15393300 |
| H | -3.39983100 | 4.60717200 | -1.17314800 |
| C | 2.07496900 | 3.22639300 | -0.45434300 |
| H | 2.65639600 | 3.34092000 | -1.37545400 |
| H | 1.18249100 | 2.64103600 | -0.68032000 |
| H | 1.75456000 | 4.22421900 | -0.13582600 |
| 77 | | | |
| RR-PhtBu_D1_TS1_P, E(SCF) = -2723.25055737, | | | |
| E(ZPE) = -2722.634516, E(G) = -2722.707757 | | | |
| a.u. | | | |
| C | 0.57355400 | -4.11477000 | -0.11950600 |
| H | 0.44946700 | -4.37449900 | -1.17392400 |
| H | 1.20001700 | -4.87984600 | 0.35033600 |
| C | -0.74370800 | -3.98073900 | 0.59288700 |
| H | -1.36210200 | -4.87337600 | 0.48595200 |
| H | -0.55863400 | -3.83235600 | 1.65960000 |
| N | -1.47771100 | -2.77365600 | 0.10750100 |
| N | 1.22588700 | -2.79483300 | -0.04643800 |
| C | -2.37131600 | -2.24921600 | 1.18780200 |
| H | -3.10465000 | -2.03523900 | 1.40217200 |
| C | 2.55716900 | -2.71525500 | -0.67120100 |
| H | 2.43633300 | -3.02469200 | -1.71490100 |
| C | -3.05659500 | -0.97023800 | 0.87193200 |
| C | -2.36865400 | 0.25259300 | 1.13982000 |
| C | -4.35238900 | -0.99267300 | 0.38086100 |
| C | -3.11213600 | 1.47287100 | 0.95292800 |
| C | -5.02385600 | 0.18764500 | 0.14907800 |
| H | -4.84406900 | -1.94196800 | 0.18801600 |
| C | -4.39845100 | 1.39522500 | 0.45249200 |
| H | -4.96380400 | 2.30670300 | 0.29012700 |
| C | 3.13184400 | -1.34037900 | -0.57511200 |
| C | 2.49836400 | -0.29013700 | -1.27700000 |
| C | 4.27993100 | -1.10983700 | 0.16219200 |
| C | 3.15040400 | 0.97326800 | -1.36954800 |
| C | 4.85438300 | 0.14474600 | 0.15746300 |
| H | 4.73958600 | -1.91324900 | 0.72876000 |
| C | 4.30902300 | 1.15237100 | -0.62555700 |
| H | 4.81966700 | 2.10784500 | -0.64659400 |
| O | -1.13875800 | 0.22476500 | 1.52501800 |
| O | 1.34027300 | -0.49459800 | -1.87522700 |
| S | -6.69650500 | 0.20465400 | -0.48103900 |
| S | 6.25419800 | 0.51763200 | 1.21568600 |
| O | 5.69252900 | 1.30853600 | 2.34955200 |
| O | 7.20418400 | 1.30964800 | 0.38486700 |
| O | 6.80579500 | -0.79714100 | 1.64502800 |
| O | -7.06757300 | -1.22014100 | -0.71914400 |
| O | -6.66227000 | 1.00888400 | -1.73912200 |
| O | -7.53758100 | 0.85148000 | 0.57045800 |
| H | 0.52249100 | 1.04304400 | 1.46535500 |
| H | -1.25418400 | -0.53732100 | -1.86855000 |
| H | -1.34274200 | -0.18647800 | -1.14316700 |
| O | 1.46650600 | 1.22712700 | 1.65252400 |
| H | 1.90957700 | 1.20626100 | 0.79417100 |
| H | 0.03101700 | -0.98632700 | 2.20445900 |
| O | 0.86957300 | -1.42880500 | 2.46625100 |
| H | 1.48709200 | -0.68201900 | 2.40913200 |
| H | -2.07289000 | -3.04992200 | -0.67358800 |
| H | -1.74332100 | -2.13398600 | 2.07275400 |
| H | 1.27399300 | -2.46793000 | 0.93805800 |
| H | 3.22009100 | -3.43408000 | -0.17794900 |
| Pd | -0.10591900 | -1.47636400 | -0.83963900 |
| C | -2.48240900 | 2.82578200 | 1.27649100 |
| C | 2.61456900 | 2.07365800 | -2.28527800 |
| C | 2.50362600 | 1.53981700 | -3.71641100 |
| H | 1.81409000 | 0.69732600 | -3.77486000 |
| H | 2.14345900 | 2.33109600 | -4.38129000 |
| H | 3.48260100 | 1.21354800 | -4.08118200 |
| C | 1.24909100 | 2.55277600 | -1.79714800 |
| H | 0.85476500 | 3.32259600 | -2.46856800 |
| H | 0.52832100 | 1.73540500 | -1.75362200 |

| | | | |
|---|-------------|------------|-------------|
| H | 1.33194300 | 2.99540600 | -0.79910400 |
| C | 3.53752500 | 3.28819100 | -2.32335800 |
| H | 3.63315600 | 3.76557700 | -1.34380700 |
| H | 4.53854500 | 3.03249100 | -2.68255100 |
| H | 3.11903600 | 4.03015600 | -3.00880400 |
| C | -1.33846800 | 3.08681300 | 0.29802600 |
| H | -0.61958300 | 2.26905400 | 0.24021800 |
| H | -1.72289100 | 3.18934300 | -0.72268200 |
| H | -0.80732600 | 4.01086100 | 0.55371700 |
| C | -3.47062900 | 3.98123000 | 1.14285000 |
| H | -3.84568000 | 4.09173300 | 0.12145100 |
| H | -4.32649400 | 3.86665800 | 1.81475800 |
| H | -2.96460200 | 4.91458400 | 1.40639300 |
| C | -1.96508800 | 2.84614900 | 2.71833000 |
| H | -1.51801600 | 3.82074200 | 2.94044500 |
| H | -2.79073800 | 2.68905700 | 3.41999100 |
| H | -1.21773200 | 2.07201200 | 2.88906500 |

77
RR-PhtBu_D1_TS1_R, E(SCF) = -2723.27269028,
E(ZPE) = -2722.657449, E(G) = -2722.729687
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.79390500 | -3.82469500 | -0.26852500 |
| H | 0.51307800 | -3.86257300 | -1.32588900 |
| H | 1.41297700 | -4.69887100 | -0.05105000 |
| C | -0.43934100 | -3.77819000 | 0.60741600 |
| H | -1.04595400 | -4.68113200 | 0.49905900 |
| H | -0.16225500 | -3.67843400 | 1.66079900 |
| N | -1.20751500 | -2.57148300 | 0.22881100 |
| N | 1.55250700 | -2.57074800 | -0.05645600 |
| C | -2.30214400 | -2.15880300 | -1.13094700 |
| H | -2.94342200 | -3.01859000 | 1.35291300 |
| C | 2.60276000 | -2.25670700 | -1.04858200 |
| H | 2.08646800 | -2.07600600 | -1.99892400 |
| C | -3.11942600 | -1.07061800 | 0.49692800 |
| C | -2.52229800 | 0.14172100 | 0.07807400 |
| C | -4.48711700 | -1.26121500 | 0.35546100 |
| C | -3.33450000 | 1.15918000 | -0.50199400 |
| C | -5.27549000 | -0.26775000 | -0.18116700 |
| H | -4.94404900 | -2.18996000 | 0.68062600 |
| C | -4.69666200 | 0.92334200 | -0.60324400 |
| H | -5.34426300 | 1.68007900 | -1.03022200 |
| C | 3.42346400 | -1.07868200 | -0.61228200 |
| C | 2.81767400 | 0.17104100 | -0.32777100 |
| C | 4.80189200 | -1.22171200 | -0.53203600 |
| C | 3.64549200 | 1.28123600 | 0.02355300 |
| C | 5.59693800 | -0.14742400 | -0.19918700 |
| H | 5.26221100 | -2.18132100 | -0.74495700 |
| C | 5.01369000 | 1.08591200 | 0.07239000 |
| H | 5.66721000 | 1.90946200 | 0.33795900 |
| O | -1.23581400 | 0.37994000 | 0.24740100 |
| O | 1.52465200 | 0.36049700 | -0.40658800 |
| S | -7.05235800 | -0.47146100 | -0.33265300 |
| S | 7.37795900 | -0.30969800 | -0.08859300 |
| O | 7.73364500 | -0.01472600 | 1.33054100 |
| O | 7.94257600 | 0.70001800 | -1.03099700 |
| O | 7.69244900 | -1.71148100 | -0.48416200 |
| O | -7.35331500 | -1.84226300 | 0.16484600 |
| O | -7.36391700 | -0.29440500 | -1.77981500 |
| O | -7.65199000 | 0.60160600 | 0.51198300 |
| H | -1.06797800 | 0.81534000 | 1.99216800 |
| H | -0.76077100 | -1.58691800 | -3.17785400 |
| H | -0.73621400 | -1.05967600 | -2.64266500 |
| O | -1.24449000 | 1.05861300 | 2.92447600 |
| H | -0.85849400 | 0.35440600 | 3.45137400 |
| H | -4.22541900 | 1.47813100 | 1.86766300 |
| O | -4.04709000 | 1.59454700 | 2.80836400 |
| H | -3.09797400 | 1.39032400 | 2.89557800 |
| H | -1.60825800 | -2.72004500 | -0.69950000 |
| H | -1.83706800 | -1.83766500 | 2.06927300 |
| H | 1.98652800 | -2.59931300 | 0.86760700 |
| H | 3.25284700 | -3.12824100 | -1.18219800 |
| Pd | 0.16789000 | -1.06804400 | 0.01000100 |
| C | -2.71174300 | 2.46203700 | -1.01073700 |
| C | 3.01788100 | 2.64349800 | 0.32679400 |
| C | 2.29268400 | 3.17862500 | -0.91281400 |
| H | 1.48998900 | 2.50931200 | -1.22634400 |

| | | | | | | | |
|---|-------------|------------|-------------|----|-------------|-------------|-------------|
| H | 1.86000100 | 4.16128300 | -0.69562100 | Pd | 0.05019600 | -1.15534600 | 0.71844800 |
| H | 2.99329200 | 3.29799200 | -1.74556900 | C | 2.78467600 | 2.73375600 | -0.93693300 |
| C | 2.03120500 | 2.53149200 | 1.49518200 | C | -2.95802300 | 2.53516400 | 1.57612300 |
| H | 1.60447500 | 3.51614600 | 1.71550600 | C | -2.81393400 | 2.26120400 | 3.07759900 |
| H | 1.21351700 | 1.84571500 | 1.26550900 | H | -2.05916400 | 1.49663100 | 3.27078300 |
| H | 2.54213100 | 2.17973000 | 2.39741800 | H | -2.51589400 | 3.17703200 | 3.59793300 |
| C | 4.06877200 | 3.67820000 | 0.71884800 | H | -3.76546100 | 1.92545700 | 3.50110700 |
| H | 4.61833700 | 3.38440600 | 1.61818700 | C | -1.62599600 | 3.04906200 | 1.03412900 |
| H | 4.79122200 | 3.85686900 | -0.08308700 | H | -1.34309800 | 3.96896800 | 1.55618400 |
| H | 3.57258800 | 4.62928600 | 0.93099100 | H | -0.83413600 | 2.31571500 | 1.17917600 |
| C | -1.69590900 | 2.15378000 | -2.11682500 | H | -1.69132500 | 3.28652800 | -0.03322100 |
| H | -0.87373300 | 1.53853200 | -1.74755300 | C | -3.98273300 | 3.65279500 | 1.40782600 |
| H | -2.17996600 | 1.63257300 | -2.94896400 | H | -4.12735100 | 3.92143200 | 0.35716400 |
| H | -1.27740900 | 3.08888900 | -2.50435000 | H | -4.95460900 | 3.39091400 | 1.83513300 |
| C | -3.76294200 | 3.39484500 | -1.60757200 | H | -3.62379800 | 4.54435700 | 1.92894600 |
| H | -4.27947400 | 2.94341800 | -2.45950200 | C | 1.68374800 | 3.03572400 | 0.07776300 |
| H | -4.51154200 | 3.69678600 | -0.86897600 | H | 0.92113700 | 2.25918700 | 0.06657700 |
| H | -3.27013000 | 4.30254000 | -1.96597000 | H | 2.09796000 | 3.09392200 | 1.09024500 |
| C | -2.02514200 | 3.25528000 | 0.12673200 | H | 1.20571700 | 3.99536600 | -0.14728000 |
| H | -1.63678200 | 4.17717100 | -0.25121200 | C | 3.81172800 | 3.85860100 | -0.84429800 |
| H | -2.73587800 | 3.44836500 | 0.92931200 | H | 4.25382900 | 3.93191700 | 0.15363300 |
| H | -1.19285800 | 2.65957700 | 0.54594300 | H | 4.61928300 | 3.74065800 | -1.57270500 |

77

RR-PhtBu_D1_TS1, E(SCF) = -2723.24223837,
E(ZPE) = -2722.627823, E(G) = -2722.700668
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.58096500 | -3.93588800 | 0.66921600 |
| H | -0.43624800 | -3.99057700 | 1.75115200 |
| H | -1.18425700 | -4.79570800 | 0.35947500 |
| C | 0.72754100 | -3.89363500 | -0.07221700 |
| H | 1.35284300 | -4.76167500 | 0.14746600 |
| H | 0.53665800 | -3.88471700 | -1.14907800 |
| N | 1.45018700 | -2.63362200 | 0.25072900 |
| N | -1.27788700 | -2.67390200 | 0.36635200 |
| C | 2.46412600 | -2.32130700 | -0.79457900 |
| H | 3.14199600 | -3.17937100 | -0.86776000 |
| C | -2.56603200 | -2.47205000 | 1.04212800 |
| H | -2.36011700 | -2.49637200 | 2.11782700 |
| C | 3.24262900 | -1.07546700 | -0.55439100 |
| C | 2.58623900 | 0.17519000 | -0.70873900 |
| C | 4.59612800 | -1.15832900 | -0.27100000 |
| C | 3.38953400 | 1.36047200 | -0.65701500 |
| C | 5.34579000 | -0.00688000 | -0.16245900 |
| H | 5.07230200 | -2.12635000 | -0.14908700 |
| C | 4.73875600 | 1.22571900 | -0.37358400 |
| H | 5.36278500 | 2.11037300 | -0.31245100 |
| C | -3.22795600 | -1.19049100 | 0.64621100 |
| C | -2.62346700 | 0.04576600 | 0.98356700 |
| C | -4.46951700 | -1.22538200 | 0.03377800 |
| C | -3.40636500 | 1.23796000 | 0.89484900 |
| C | -5.16252300 | -0.05396900 | -0.18862800 |
| H | -4.91032500 | -2.17579100 | -0.24902800 |
| C | -4.64448400 | 1.14745800 | 0.27498600 |
| H | -5.25184100 | 2.03687000 | 0.15478500 |
| O | 1.29407100 | 0.19158800 | -0.88524300 |
| O | -1.38498500 | 0.09787900 | 1.41791300 |
| S | 7.09249100 | -0.06507000 | 0.22572100 |
| S | -6.71796400 | -0.06152800 | -1.08096100 |
| O | -6.41162700 | 0.48348900 | -2.43603500 |
| O | -7.64264500 | 0.81990600 | -0.31249200 |
| O | -7.16203300 | -1.48281300 | -1.11774500 |
| O | 7.43571700 | -1.50841000 | 0.36984700 |
| O | 7.26028700 | 0.69984000 | 1.49680300 |
| O | 7.79807800 | 0.58604800 | -0.91712000 |
| H | -0.28231700 | 1.06611400 | -1.40441100 |
| H | 1.37686500 | -0.11228000 | 2.22743600 |
| H | 1.38057900 | 0.42622600 | 1.68946000 |
| O | -1.15139400 | 1.22654600 | -1.82319200 |
| H | -1.76831700 | 1.32739200 | -1.08776600 |
| H | 0.17835200 | -1.09427700 | -1.95577900 |
| O | -0.62079900 | -1.49685200 | -2.34486500 |
| H | -1.18661900 | -0.71029600 | -2.41105100 |
| H | 1.94410500 | -2.75928000 | 1.13561900 |
| H | 1.91754200 | -2.25972500 | -1.74030300 |
| H | -1.38951800 | -2.56832800 | -0.65245300 |
| H | -3.22667800 | -3.31398700 | 0.80527000 |

77

RR-PhtBu_D1_TS2_P, E(SCF) = -2723.27650232,
E(ZPE) = -2722.659242, E(G) = -2722.735107
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.58958900 | -3.84026600 | 0.36531700 |
| H | -0.31513300 | -3.98192300 | 1.41612100 |
| H | -1.13917000 | -4.73332000 | 0.04262400 |
| C | 0.63570100 | -3.64662100 | -0.49521300 |
| H | 1.29303800 | -4.51978500 | -0.47393100 |
| H | 0.32110300 | -3.49664000 | -1.53243000 |
| N | 1.39200300 | -2.42345800 | -0.09628600 |
| N | -1.39378100 | -2.62355100 | 0.25455800 |
| C | 2.25215700 | -1.97326000 | -1.22322900 |
| H | 2.82662100 | -2.83692900 | -1.57888200 |
| C | -2.55884100 | -2.51619000 | 1.13576100 |
| H | -2.19579100 | -2.58517600 | 2.16832000 |
| C | 3.19542600 | -0.87356000 | -0.85834800 |
| C | 2.84560200 | 0.46891100 | -1.03109900 |
| C | 4.45941100 | -1.19872600 | -0.38302100 |
| C | 3.76137700 | 1.50465200 | -0.76601400 |
| C | 5.36209800 | -0.19830300 | -0.10318700 |
| H | 4.74560100 | -2.23773100 | -0.25462200 |
| C | 5.01572800 | 1.12950300 | -0.30199700 |
| H | 5.75669500 | 1.88781600 | -0.07969900 |
| C | -3.26004700 | -1.21348600 | 0.89118600 |
| C | -2.61450100 | 0.00603900 | 1.22138100 |
| C | -4.51864900 | -1.21400100 | 0.31306300 |
| C | -3.32301400 | 1.23333900 | 1.02325100 |
| C | -5.18288800 | -0.02526100 | 0.08825100 |
| H | -4.98827200 | -2.15255400 | 0.03516400 |
| C | -4.58998200 | 1.17546100 | 0.45990500 |
| H | -5.14104100 | 2.09151600 | 0.27827000 |
| O | 1.60442800 | 0.77918600 | -1.50507600 |
| O | -1.40657500 | 0.02424700 | 1.72893600 |
| S | 7.00899900 | -0.58605000 | 0.51360500 |
| S | -6.77216300 | 0.01598500 | -0.73729400 |
| O | -6.54748400 | 0.77730500 | -2.00161900 |
| O | -7.70573800 | 0.72201400 | 0.18776200 |
| O | -7.15400400 | -1.40414100 | -0.97548900 |
| O | 7.09810700 | -2.07104200 | 0.53108300 |
| O | 7.07957600 | 0.02164500 | 1.87211200 |
| O | 7.95519300 | 0.04707000 | -0.44659800 |
| H | -1.80031400 | 1.33761000 | -2.16614300 |
| H | 1.11514300 | -0.02555000 | 1.16391700 |
| H | 0.93720600 | 0.31827500 | -0.95796400 |
| O | -2.58858100 | 0.78642900 | -2.15735500 |
| H | -2.98198000 | 0.92683300 | -1.28140100 |
| H | -1.35228300 | -1.98770800 | -3.20870900 |
| O | -2.02324200 | -1.92241100 | -2.52497700 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.20994100 | -0.96669400 | -2.43525000 |
| H | 2.00643900 | -2.66368400 | 0.68137600 |
| H | 1.58336000 | -1.66758800 | -2.03162100 |
| H | -1.68472800 | -2.48592600 | -0.72187700 |
| H | -3.25439900 | -3.34951700 | 0.97154900 |
| Pd | 0.02257300 | -1.07915800 | 0.75449300 |
| C | 3.39631800 | 2.97643700 | -0.96240700 |
| C | -2.69820400 | 2.56671200 | 1.43514100 |
| C | -2.45402300 | 2.56612100 | 2.94722400 |
| H | -1.77181900 | 1.76615600 | 3.23574700 |
| H | -2.02240900 | 3.52349500 | 3.25701600 |
| H | -3.39785700 | 2.43289400 | 3.48533100 |
| C | -1.37666200 | 2.80134800 | 0.69667600 |
| H | -0.90926000 | 3.72420200 | 1.05643000 |
| H | -0.67695500 | 1.97700800 | 0.84629200 |
| H | -1.55157700 | 2.92905900 | -0.37763800 |
| C | -3.60595000 | 3.75126400 | 1.11795900 |
| H | -3.81428300 | 3.83353900 | 0.04655800 |
| H | -4.55892400 | 3.69731800 | 1.65229100 |
| H | -3.10715400 | 4.67394000 | 1.42744600 |
| C | 2.20089000 | 3.34333200 | -0.07866300 |
| H | 1.31326200 | 2.76664900 | -0.33698300 |
| H | 2.43171800 | 3.16400700 | 0.97657300 |
| H | 1.96606200 | 4.40618300 | -0.19499600 |
| C | 4.54687400 | 3.90337000 | -0.58051800 |
| H | 4.82418700 | 3.80346700 | 0.47266700 |
| H | 5.43689400 | 3.72989300 | -1.19219600 |
| H | 4.23461700 | 4.93842200 | -0.74156000 |
| C | 3.06743600 | 3.24196700 | -2.43424400 |
| H | 2.84222000 | 4.30337400 | -2.57783600 |
| H | 3.92283500 | 2.99173800 | -3.06922000 |
| H | 2.20755200 | 2.66360700 | -2.76983100 |

77

RR-PhtBu_D1_TS2, E(SCF) = -2723.24266154,
E(ZPE) = -2722.629535, E(G) = -2722.704062
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.62683300 | -4.02693600 | 0.44347900 |
| H | -0.49811500 | -4.20316700 | 1.51480800 |
| H | -1.17170700 | -4.87723100 | 0.01984100 |
| C | 0.69317600 | -3.84191000 | -0.26338700 |
| H | 1.35739200 | -4.69578800 | -0.11512500 |
| H | 0.50972100 | -3.75102200 | -1.33749100 |
| N | 1.36913700 | -2.57916400 | 0.16531100 |
| N | -1.37374500 | -2.77295300 | 0.27244100 |
| C | 2.30203900 | -2.12711700 | -0.91101500 |
| H | 2.95475400 | -2.97642400 | -1.14371200 |
| C | -2.72097200 | -2.69577700 | 0.86122800 |
| H | -2.61076600 | -2.89018200 | 1.93344800 |
| C | 3.14617800 | -0.92694900 | -0.62121200 |
| C | 2.59729400 | 0.37183700 | -0.71842200 |
| C | 4.50519400 | -1.10265100 | -0.39355900 |
| C | 3.45392500 | 1.50263400 | -0.61483500 |
| C | 5.32772300 | -0.00619000 | -0.26456900 |
| H | 4.92694700 | -2.10082900 | -0.32938200 |
| C | 4.80221700 | 1.27419500 | -0.38892200 |
| H | 5.48491100 | 2.11118000 | -0.29717500 |
| C | -3.33226100 | -1.35101600 | 0.60959200 |
| C | -2.75356900 | -0.21143200 | 1.21683400 |
| C | -4.44638900 | -1.22705000 | -0.20147300 |
| C | -3.41660800 | 1.04607000 | 1.11754900 |
| C | -5.03496700 | 0.00997300 | -0.37541500 |
| H | -4.86765500 | -2.09985100 | -0.68986700 |
| C | -4.53633200 | 1.11637800 | 0.29952000 |
| H | -5.05345500 | 2.06074300 | 0.17284900 |
| O | 1.28536600 | 0.49563700 | -0.83709100 |
| O | -1.63239800 | -0.32172300 | 1.89801100 |
| S | 7.08881100 | -0.19845300 | 0.02163500 |
| S | -6.41060300 | 0.22356400 | -1.50762200 |
| O | -5.85970500 | 0.97425800 | -2.67368600 |
| O | -7.44077200 | 1.00616200 | -0.76703400 |
| O | -6.86520400 | -1.14885700 | -1.86534400 |
| O | 7.32765300 | -1.66301700 | 0.14930500 |
| O | 7.38334100 | 0.55129000 | 1.27674400 |
| O | 7.76435000 | 0.40001900 | -1.16599900 |
| H | -0.42612900 | 1.35164100 | -1.26949600 |
| H | 0.92123500 | -0.01563100 | 1.41505000 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.91376800 | 0.17615400 | 0.49781600 |
| O | -1.33239200 | 1.45846100 | -1.60980700 |
| H | -1.90196700 | 1.38298100 | -0.83239100 |
| H | 0.06477400 | -0.79119200 | -1.81965200 |
| O | -0.70463900 | -1.23186000 | -2.22597800 |
| H | -1.31301800 | -0.48066400 | -2.30463800 |
| H | 1.92986700 | -2.77719400 | 0.99353000 |
| H | 1.68818300 | -1.95185700 | -1.79698300 |
| H | -1.41833600 | -2.51986400 | -0.72553900 |
| H | -3.35405100 | -3.48184500 | 0.43542100 |
| Pd | -0.11755500 | -1.29073000 | 0.94750400 |
| C | 2.90194100 | 2.92166100 | -0.75497400 |
| C | -2.95138100 | 2.24867600 | 1.94323700 |
| C | -3.04432400 | 1.88778300 | 3.42945900 |
| H | -2.39182000 | 1.04907800 | 3.07543700 |
| H | -2.75085900 | 2.74612100 | 4.04214900 |
| H | -4.07153400 | 1.61929500 | 3.69489500 |
| C | -1.51403100 | 2.65062700 | 1.60344300 |
| H | -1.19346500 | 3.46800700 | 2.25797100 |
| H | -0.82142000 | 1.81749300 | 1.73161000 |
| H | -1.44213300 | 3.01644400 | 0.57374600 |
| C | -3.83009700 | 3.47387800 | 1.71074000 |
| H | -3.80274600 | 3.68055800 | 0.66850000 |
| H | -4.87229700 | 3.29281900 | 1.98856100 |
| H | -3.46193400 | 4.29792500 | 2.32795000 |
| C | 1.87233600 | 3.20637700 | 0.34227000 |
| H | 1.00721600 | 2.54865800 | 0.26488100 |
| H | 2.31717300 | 3.07333300 | 1.33412100 |
| H | 1.52144200 | 4.24105200 | 0.26703500 |
| C | 3.99598400 | 3.97906000 | -0.63232300 |
| H | 4.47778000 | 3.96156300 | 0.34964000 |
| H | 4.76810100 | 3.86372100 | -1.39844000 |
| H | 3.54985900 | 4.96888200 | -0.76186300 |
| C | 2.26020200 | 3.09370000 | -2.13519300 |
| H | 1.84701400 | 4.10288100 | -2.23276600 |
| H | 3.00790900 | 2.95907200 | -2.92300500 |
| H | 1.45637100 | 2.37644600 | -2.30065500 |

77

RR-PhtBu_D2_TS2_P, E(SCF) = -2723.26998318,
E(ZPE) = -2722.653224, E(G) = -2722.730955
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.27228200 | -2.54326200 | 0.81983200 |
| H | 0.07284500 | -2.12306000 | 1.76998300 |
| H | -0.53400300 | -3.59266700 | 0.99201100 |
| C | 0.80534800 | -2.42253500 | -0.23042700 |
| H | 1.69305400 | -3.00656700 | -0.03945500 |
| H | 0.43660100 | -2.79424800 | -1.19082000 |
| N | 1.16917600 | -0.99268100 | -0.40099200 |
| N | -1.43092200 | -1.75493100 | 0.37627700 |
| C | 2.12630300 | -0.76294300 | -1.52739200 |
| H | 1.70426500 | -0.01234700 | -2.19809800 |
| C | -2.46361400 | -1.49519900 | 1.39334700 |
| H | -2.79631200 | -2.43389900 | 1.85281400 |
| C | 3.47570400 | -0.36644700 | -1.01427400 |
| C | 3.69114100 | 0.91500100 | -0.49554200 |
| C | 4.50286800 | -1.30095700 | -0.98315900 |
| C | 4.94508200 | 1.29161600 | 0.03020200 |
| C | 5.73073700 | -0.95433100 | -0.46648800 |
| H | 4.34191300 | -2.30124900 | -1.37171800 |
| C | 5.94036600 | 0.32501900 | 0.02779500 |
| H | 6.91909800 | 0.56072300 | 0.42770700 |
| C | -3.63408500 | -0.79071800 | 0.77640000 |
| C | -3.47927600 | 0.49572000 | 0.20687400 |
| C | -4.86968200 | -1.42078400 | 0.76862300 |
| C | -4.61667000 | 1.14256900 | -0.36062300 |
| C | -5.96712800 | -0.79197700 | 0.22114400 |
| H | -4.97797200 | -2.40937200 | 1.20324600 |
| C | -5.82959600 | 0.47409000 | -0.33337600 |
| H | -6.71069700 | 0.93800700 | -0.76193700 |
| O | 2.70233000 | 1.83837400 | -0.48106000 |
| O | -2.31779400 | 1.12195900 | 0.21945600 |
| S | 7.08537700 | -2.13672200 | -0.41854900 |
| S | -7.56430900 | -1.60432900 | 0.15867500 |
| O | -7.41442700 | -2.87148500 | 0.92804400 |
| O | -7.84991500 | -1.83601900 | -1.28792500 |
| O | -8.53662000 | -0.65911000 | 0.78047700 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
| O | 8.16975200 | -1.53805400 | -1.24643000 | S | 7.46965400 | -1.36728600 | -0.63545700 |
| O | 6.54339800 | -3.40008200 | -0.98761200 | S | -7.60747700 | -1.08842800 | 0.45376600 |
| O | 7.46308200 | -2.25402300 | 1.01785600 | O | -7.55527400 | -2.30880200 | 1.30557100 |
| H | -1.99008100 | -0.89100800 | 2.17664800 | O | -8.07016300 | -1.36907600 | -0.93637900 |
| H | 2.21047900 | -1.68505700 | -2.10552100 | O | -8.36242600 | 0.03188500 | 1.08525400 |
| H | -1.86745600 | -2.21357700 | -0.42236300 | O | 8.30569000 | -0.35348100 | -1.34220600 |
| H | 1.64754400 | -0.72290000 | 0.46943900 | O | 7.25938600 | -2.60641600 | -1.43586200 |
| H | 2.47642000 | 0.47517000 | 2.45058500 | O | 7.97021300 | -1.64721700 | 0.74275500 |
| O | 2.46339800 | -0.44953900 | 2.18389500 | H | -1.89454700 | -0.95660500 | 2.08770000 |
| H | 3.39112100 | -0.70515500 | 2.14214600 | H | 2.60260900 | -2.38073100 | -1.64101800 |
| H | -0.05126100 | 2.20845100 | 1.94479000 | H | -2.00138300 | -2.39250100 | -0.45141200 |
| O | -0.91589900 | 2.26534800 | 2.36289200 | H | 1.52511700 | -1.37885200 | 0.65044100 |
| H | -1.50771000 | 1.87604000 | 1.69012600 | H | 1.72508500 | 0.24052700 | 1.82554100 |
| Pd | -0.58529000 | 0.11634400 | -0.24255800 | O | 1.53253600 | -0.52001600 | 2.40740300 |
| H | 1.81751400 | 1.47133500 | -0.66428400 | H | 2.29355700 | -0.59648000 | -0.59864000 |
| H | 0.08045300 | 1.49009300 | -0.67028100 | H | 0.70538000 | 2.23264100 | 0.98579500 |
| C | 5.19074600 | 2.68673600 | 0.60767400 | O | -0.11974400 | 2.57956000 | 1.35671100 |
| C | -4.49071000 | 2.52970400 | -0.99171600 | H | -0.82063000 | 2.04380600 | 0.95076300 |
| C | 6.62669100 | 2.85442300 | 1.09733000 | Pd | -0.47224800 | -0.47224800 | -0.40167700 |
| H | 6.74802400 | 3.86502000 | 1.49587200 | H | 0.93618100 | 0.88406300 | -0.67092300 |
| H | 6.87362300 | 2.15402700 | 1.89989600 | H | 0.24854700 | 0.96852200 | -1.21577500 |
| H | 7.35404000 | 2.72927000 | 0.29026200 | C | 4.45056500 | 2.59142200 | 1.10434700 |
| C | 4.27403700 | 2.92443800 | 1.81284000 | C | -4.11601500 | 2.39539200 | -1.24358300 |
| H | 3.21900400 | 2.85120600 | 1.54716900 | C | 5.83739200 | 3.13277200 | 1.44811500 |
| H | 4.49141600 | 2.20021800 | 2.60496800 | H | 5.72952400 | 4.11373300 | 1.91871400 |
| H | 4.45193500 | 3.92364500 | 2.22191100 | H | 6.36945800 | 2.48760400 | 2.15324300 |
| C | 4.95199200 | 3.75598900 | -0.46292600 | H | 6.46143600 | 3.26146400 | 0.55914700 |
| H | 5.62203200 | 3.59900100 | -1.31355000 | C | 3.67813200 | 2.48712400 | 2.42293400 |
| H | 3.92567900 | 3.75068300 | -0.82684200 | H | 2.63175800 | 2.22650900 | 2.26554400 |
| H | 5.16413600 | 4.74596000 | -0.04774400 | H | 4.13070600 | 1.73447600 | 3.07676900 |
| C | -4.02475800 | 3.54740200 | 0.05405500 | C | 3.70719600 | 3.44708600 | 2.94808100 |
| H | -3.04781500 | 3.28287900 | 0.45992200 | C | 3.78472700 | 3.62161700 | 0.18726600 |
| H | -3.95677800 | 4.54253600 | -0.39783500 | H | 4.35730800 | 3.73455800 | -0.73862200 |
| H | -4.74148300 | 3.60318400 | 0.87975200 | H | 2.76621400 | 3.33320700 | -0.07041500 |
| C | -5.82099700 | 3.03188300 | -1.54762700 | H | 3.75408200 | 4.59707000 | 0.68346300 |
| H | -6.21306700 | 2.37857500 | -2.33263000 | C | -3.47610400 | 3.47838900 | -0.55036200 |
| H | -6.58283300 | 3.13102500 | -0.76875100 | H | -2.50594500 | 3.16481500 | -0.16562300 |
| H | -5.67075300 | 4.02130100 | -1.98858500 | H | -3.33397600 | 4.39217800 | -1.13623000 |
| C | -3.50105000 | 2.48438300 | -2.16013100 | H | -4.12404600 | 3.72140600 | 0.29759800 |
| H | -2.51022900 | 2.16595200 | -1.83386800 | C | -5.40904800 | 2.97999300 | -1.98722300 |
| H | -3.85353900 | 1.79093200 | -2.93037100 | H | -5.92406000 | 2.27880700 | -2.65013600 |
| H | -3.41620800 | 3.47628400 | -2.61621800 | H | -6.10329000 | 3.28345200 | -1.19819500 |
| | | | | H | -5.16942500 | 3.87161200 | -2.57281700 |
| | | | | C | -3.20813500 | 2.07616500 | -2.61580900 |
| 77 | | | | H | -2.24082400 | 1.68877600 | -2.29389800 |
| RR-PhtBu_D2_TS2_P, E(SCF) = -2723.24164119, | | | | H | -3.68051900 | 1.33496200 | -3.26805900 |
| E(ZPE) = -2722.627510, E(G) = -2722.702607 | | | | H | -3.03912900 | 2.98198300 | -3.20677700 |
| a.u. | | | | | | | |
| C | -0.47711200 | -2.97921200 | 0.79801800 | | | | |
| H | -0.10906000 | -2.63854500 | 1.77033400 | 77 | | | |
| H | -0.92877100 | -3.96589000 | 0.92650300 | RR-PhtBu_D2_TS1_P, E(SCF) = -2723.24185376, | | | |
| C | 0.64773900 | -2.99613300 | -0.20819400 | E(ZPE) = -2722.626329, E(G) = -2722.701356 | | | |
| H | 1.43601600 | -3.69561200 | 0.08626600 | a.u. | | | |
| H | 0.28444400 | -3.28783600 | -1.19749900 | C | -0.44136500 | -2.94953800 | 0.75703600 |
| N | 1.17868200 | -1.61790600 | -0.28920500 | H | -0.06636200 | -2.60896200 | 1.72631300 |
| N | -1.48626300 | -1.99822400 | 0.33772200 | H | -0.88974700 | -3.93725500 | 0.88681100 |
| C | 2.27732300 | -1.40280600 | -1.27468300 | C | 0.67208800 | -2.95768400 | -0.26115200 |
| H | 1.85546400 | -0.87363600 | -2.13296400 | H | 1.47389300 | -3.64328800 | 0.02949900 |
| C | -2.46029400 | -1.54771500 | 1.35843200 | H | 0.30351800 | -3.26002000 | -1.24516500 |
| H | -2.87122500 | -2.42010000 | 1.87724700 | N | 1.18048000 | -1.57218700 | -0.35252700 |
| C | 3.46630300 | -0.68163300 | -0.70178200 | N | -1.46163600 | -1.97202000 | 0.30941700 |
| C | 3.33983400 | 0.56844500 | -0.04052400 | C | 2.28724100 | -1.34325300 | -1.32803900 |
| C | 4.71437600 | -1.26207600 | -0.87938800 | H | 1.87789100 | -0.77608700 | -2.16772400 |
| C | 4.52440800 | 1.22871800 | 0.41061200 | C | -2.42441000 | -1.52764300 | 1.34562500 |
| C | 5.85085100 | -0.62425500 | -0.43485100 | H | -2.81448300 | -2.40481600 | 1.87189300 |
| H | 4.80231000 | -2.22103600 | -1.38007200 | C | 3.48089800 | -0.66098500 | -0.72292000 |
| C | 5.74364900 | 0.60585500 | 0.20102500 | C | 3.35079700 | 0.58447800 | -0.04667600 |
| H | 6.65830800 | 1.08181300 | 0.53484800 | C | 4.72241000 | -1.25872600 | -0.88128300 |
| C | -3.56842300 | -0.76857300 | 0.72011100 | C | 4.54002600 | 1.22177400 | 0.43460200 |
| C | -3.29292700 | 0.40976300 | -0.01117300 | C | 5.85843000 | -0.64269700 | -0.40347900 |
| C | -4.87144500 | -1.22313400 | 0.85972300 | H | 4.80669300 | -2.21184100 | -1.39391900 |
| C | -4.37047700 | 1.12980600 | -0.60313300 | C | 5.75357300 | 0.58356900 | 0.24296400 |
| C | -5.91322400 | -0.51694400 | 0.30166900 | H | 6.66809600 | 1.04301100 | 0.60063200 |
| H | -5.07523600 | -2.13110000 | 1.41776100 | C | -3.55288200 | -0.76520500 | 0.72387100 |
| C | -5.65381000 | 0.64199300 | -0.41843300 | C | -3.30283800 | 0.41155400 | -0.01808300 |
| H | -6.49693700 | 1.16560900 | -0.85367900 | C | -4.84821200 | -1.23358800 | 0.88737000 |
| O | 2.15461300 | 1.08625600 | 0.18833200 | C | -4.439701900 | 1.11901200 | -0.59334700 |
| O | -2.06105300 | 0.87181400 | -0.13350300 | C | -5.90626800 | -0.54088000 | 0.34327400 |

| | | | | | | | |
|----|-------------|--------------|-------------|----|--------------|-------------|-------------|
| H | -5.03311200 | -2.14106800 | 1.45261800 | C | -3.44890000 | -0.96755300 | 0.44428100 |
| C | -5.67173100 | 0.61807200 | -0.38510600 | C | -2.73765700 | 0.25283100 | 0.35562700 |
| H | -6.52753900 | 1.13143200 | -0.80774200 | C | -4.76068500 | -1.05828800 | 0.00334100 |
| O | 2.17010300 | 1.10263100 | 0.15279500 | C | -3.38955000 | 1.39253000 | -0.20273200 |
| O | -2.07652700 | 0.88279000 | -0.16391000 | C | -5.39327000 | 0.04921400 | -0.51611400 |
| S | 7.47156700 | -1.39831900 | -0.58714800 | H | -5.29671600 | -1.99897600 | 0.07702700 |
| S | -7.59154300 | -1.131408100 | 0.52472200 | C | -4.70396400 | 1.25098200 | -0.61667800 |
| O | -7.51099200 | -2.34865600 | 1.37814500 | H | -5.22670900 | 2.09867300 | -1.04416000 |
| O | -8.07279200 | -1.42003900 | -0.85720000 | O | 1.47325700 | 0.05972500 | 0.98511400 |
| O | -8.34816200 | -0.01765200 | 1.16598600 | O | -1.50270700 | 0.35886600 | 0.80609600 |
| O | 8.32336700 | -0.39529700 | -1.29187600 | S | 6.75655700 | -0.04364600 | -1.68841500 |
| O | 7.25995800 | -2.64001600 | -1.38418500 | S | -7.08129800 | -0.04349300 | -1.11428900 |
| O | 7.96202800 | -1.67696800 | 0.79555000 | O | -7.56648800 | -1.40928600 | -0.76957000 |
| H | -1.85173800 | -0.92924800 | 2.06299900 | O | -7.00980100 | 0.19141000 | -2.58630700 |
| H | 2.59386300 | -2.131410700 | -1.72736600 | O | -7.82913700 | 1.03584500 | -0.47022600 |
| H | -1.98666700 | -2.37065600 | -0.47149100 | O | 6.81468100 | 1.15057600 | -2.57949000 |
| H | 1.51601800 | -1.31870600 | 0.58732700 | O | 6.85682400 | -1.33007400 | -2.43239800 |
| H | 1.68968500 | 0.28076100 | 1.75919000 | O | 7.72256800 | 0.04823300 | -0.55521900 |
| O | 1.47167200 | -0.46545600 | 2.325300100 | H | -2.463300300 | -2.04355000 | -2.48845400 |
| H | 2.21857900 | -0.53887100 | 2.95337000 | H | 2.85859100 | -3.18413600 | -0.86651200 |
| H | 0.76272400 | 2.24360300 | 0.87534300 | H | -1.83817200 | -2.57086600 | -0.74073900 |
| O | -0.04999700 | 2.64675900 | 1.22133000 | H | 1.62606500 | -2.78129300 | 1.21260600 |
| H | -0.77225400 | 2.10503600 | 0.86655300 | H | 1.94457400 | -1.07529200 | 2.48530000 |
| Pd | -0.48579400 | -0.34306900 | -0.46309800 | O | 2.14908900 | -1.90882900 | 2.94289200 |
| H | 0.79544300 | 0.93682200 | -0.83093700 | H | 3.06408400 | -1.82469700 | 3.22420200 |
| H | 0.15630900 | 1.00704200 | -1.37880500 | O | 0.52941800 | 0.89769900 | 2.58552300 |
| C | 4.46898600 | 2.57920600 | 1.13753900 | H | -0.22927600 | 0.94818500 | 3.18564800 |
| C | -4.16986400 | 2.38665700 | -1.41875300 | H | -0.95283500 | 0.76253900 | 2.56206600 |
| C | 5.85418200 | 3.10453800 | 1.51020900 | Pd | -0.12719600 | -1.13158400 | 0.51446700 |
| H | 5.74824100 | 4.08380600 | 1.98509400 | H | 1.00620700 | 0.56841000 | -1.84083100 |
| H | 6.36675000 | 2.44920100 | 2.22050900 | H | 1.12291500 | 0.45995100 | -2.57455400 |
| H | 6.49558400 | 3.23142800 | 0.63337000 | C | 3.06479700 | 2.42147800 | 1.14983600 |
| C | 3.67035900 | 2.47241800 | 2.44033900 | C | -2.65755700 | 2.72685000 | -0.35891700 |
| H | 2.62536100 | 2.22147700 | 2.25924900 | C | 4.06590100 | 3.56234000 | 0.97106400 |
| H | 4.10371500 | 1.71107600 | 3.09734100 | H | 3.70905200 | 4.43516300 | 1.52473100 |
| H | 3.69679200 | 3.42831600 | 2.97325600 | H | 5.05629900 | 3.31301300 | 1.36105200 |
| C | 3.82775300 | 3.62122700 | 0.21612900 | H | 4.16945500 | 3.85514500 | -0.07768800 |
| H | 4.42214600 | 3.74164000 | -0.69503500 | C | 3.01968400 | 2.11278200 | 2.65038300 |
| H | 2.81502900 | 3.33595200 | -0.06811900 | H | 2.41396400 | 1.23763900 | 2.88409600 |
| H | 3.78765500 | 4.59216300 | 0.72075100 | H | 4.03030100 | 1.91787600 | 3.02203900 |
| C | -3.52316700 | 3.47440400 | -0.55651200 | H | 2.61462200 | 2.96523100 | 3.20531400 |
| H | -2.54379000 | 3.16783300 | -0.18962800 | C | 1.71743000 | 2.94640000 | 0.64081700 |
| H | -3.39863300 | 4.38961100 | -1.14406700 | H | 1.79604400 | 3.21425500 | -0.41871300 |
| H | -4.15730200 | 3.71167900 | 0.30339100 | H | 0.91373500 | 2.21868000 | 0.74060900 |
| C | -5.47840900 | 2.95901100 | -1.95766100 | H | 1.43825700 | 3.85068800 | 1.19242200 |
| H | -5.99836900 | 2.25333000 | -2.61180300 | C | -2.22198800 | 3.26724200 | 1.00565500 |
| H | -6.16089600 | 3.25462000 | -1.15555100 | H | -1.52548500 | 2.59345900 | 1.50432600 |
| H | -5.25814400 | 3.85334800 | -2.54663700 | H | -1.72718800 | 4.23618800 | 0.87856000 |
| C | -3.28141100 | 2.07560100 | -2.62751300 | H | -3.09090100 | 3.41682200 | 1.65430500 |
| H | -2.30519200 | 1.69604300 | -2.32381600 | C | -3.54044400 | 3.79298200 | -1.00338700 |
| H | -3.75938800 | 1.33090600 | -3.27157900 | H | -3.86558000 | 3.50695200 | -2.00790400 |
| H | -3.13039200 | 2.98311600 | -3.22070200 | H | -4.42749000 | 4.01551100 | -4.02962000 |
| | | | | H | -2.96604500 | 4.71867200 | -1.09602000 |
| | | | | C | -1.43611200 | 2.54803900 | -1.26502000 |
| | | | | H | -0.72342200 | 1.84200000 | -0.84039400 |
| | | | | H | -1.74009500 | 2.18909000 | -2.25373900 |
| | | | | H | -0.92500400 | 3.50809400 | -1.39697000 |

77

RR-PhtBu_D2_TS1_R, E(SCF) = -2723.27180187,
E(ZPE) = -2722.657730, E(G) = -2722.732606
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.94002700 | -3.81545700 | 0.63062000 |
| H | -0.81713200 | -3.80888500 | 1.71737900 |
| H | -1.57013600 | -4.66879200 | 0.36344400 |
| C | 0.39895800 | -3.87848800 | -0.06304100 |
| H | 0.94627400 | -4.78869400 | 0.19377700 |
| H | 0.25622100 | -3.86966500 | -1.14768200 |
| N | 1.18598100 | -2.67292700 | 0.28967000 |
| N | -1.58728500 | -2.53935400 | 0.24836300 |
| C | 2.19862000 | -2.32206200 | -0.71191500 |
| H | 1.65825000 | -2.16700900 | -1.65494100 |
| C | -2.79345700 | -2.18070500 | 1.02590700 |
| H | -3.49317600 | -3.02336000 | 1.02066200 |
| C | 3.04537900 | -1.11303500 | -0.40968500 |
| C | 2.62117500 | 0.02129800 | 0.32159600 |
| C | 4.29747300 | -1.11900200 | -1.01643800 |
| C | 3.48011700 | 1.16321500 | 0.38416800 |
| C | 5.12504200 | -0.02539100 | -0.94248500 |
| H | 4.62421900 | -1.99548500 | -1.56682100 |
| C | 4.70855900 | 1.10184800 | -0.24817100 |
| H | 5.37732100 | 1.95351300 | -0.21230300 |

77

RR-PhtBu_D2_TS1, E(SCF) = -2723.23716979,
E(ZPE) = -2722.624938, E(G) = -2722.699409
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.69374300 | -3.23115700 | 0.92203400 |
| H | -0.37252100 | -2.96011200 | 1.93165900 |
| H | -1.25858600 | -4.16493800 | 0.97230500 |
| C | 0.49692300 | -3.33065700 | 0.00200200 |
| H | 1.19039100 | -4.11226500 | 0.32663500 |
| H | 0.18850400 | -3.55398300 | -1.02363900 |
| N | 1.16016400 | -2.00977900 | 0.01668800 |
| N | -1.55204300 | -2.13511700 | 0.41933400 |
| C | 2.30391200 | -1.87535900 | -0.90305500 |
| H | 1.89772300 | -1.61458000 | -1.88713900 |
| C | -2.58418100 | -1.63424800 | 1.35738100 |
| H | -3.10780500 | -2.48983300 | 1.79614700 |
| C | 3.37924700 | -0.91050100 | -0.46358600 |
| C | 3.13889000 | 0.25989100 | 0.31252300 |
| C | 4.66198900 | -1.21630700 | -0.90180100 |

| | | | | | | | |
|--|--------------|--------------|-------------|--|-------------|-------------|-------------|
| C | 4.25660800 | 1.11768600 | 0.59681000 | C | -2.71128500 | -2.39837200 | -0.03163100 |
| C | 5.72343800 | -0.38940000 | -0.61460100 | H | -3.42451600 | -3.15581600 | -0.38080300 |
| H | 4.83638800 | -2.11826400 | -1.48117900 | C | 3.08574000 | -0.50972300 | -1.29800900 |
| C | 5.50838000 | 0.76498300 | 0.12955500 | C | 3.89444400 | -0.89392300 | -0.22803300 |
| H | 6.36385700 | 1.39617800 | 0.34176100 | C | 3.03622600 | 0.82371600 | -1.67950600 |
| C | -3.56346600 | -0.75417000 | 0.64586000 | C | 4.70055600 | 0.03555300 | 0.45636500 |
| C | -3.12369200 | 0.39864100 | -0.04161500 | C | 3.78599700 | 1.75442100 | -0.99617800 |
| C | -4.91043200 | -1.08493100 | 0.67587200 | H | 2.40003200 | 1.13698800 | -2.50035800 |
| C | -4.07728800 | 1.22580400 | -0.70151400 | C | 4.60710600 | 1.36207300 | 0.04861000 |
| C | -5.83371400 | -0.27431600 | 0.05490800 | H | 5.19332100 | 2.12366100 | 0.54755500 |
| H | -5.24310000 | -1.97539200 | 1.19883100 | C | -3.42201800 | -1.09978600 | 0.19716800 |
| C | -5.41160200 | 0.86316800 | -0.62138200 | C | -2.73277700 | 0.00628700 | 0.76029500 |
| H | -6.16445100 | 1.47338200 | -1.10661200 | C | -4.76129700 | -1.00153800 | -0.14728900 |
| O | 1.94952100 | 0.53498000 | 0.76553000 | C | -3.45666300 | 1.22242300 | 0.97551100 |
| O | -1.84718800 | 0.74303600 | -0.05793000 | C | -5.45320500 | 0.17083800 | 0.17083800 |
| S | 7.38393000 | -0.78287300 | -1.15226400 | H | -5.27420800 | -1.85542000 | -0.57898000 |
| S | -7.58178600 | -0.68554800 | 0.07079200 | C | -4.79490700 | 1.26252700 | 0.62294200 |
| O | -7.70883900 | -1.89996300 | 0.92304200 | H | -5.36490700 | 2.17245900 | 0.77360900 |
| O | -7.95565600 | -0.933041500 | -1.35209200 | C | -3.89207200 | -2.22406000 | 0.07781800 |
| O | -8.27633400 | 0.50341000 | 0.64218400 | O | -1.47603300 | -0.06893800 | 1.12350000 |
| O | 7.83835000 | 0.37192600 | -1.98242800 | S | 3.72941200 | 3.49811800 | -1.44610100 |
| O | 7.28158400 | -2.04947300 | -1.93157800 | S | -7.17319800 | 0.33423000 | -0.39882000 |
| O | 8.19895000 | -0.93304400 | 0.09001700 | O | -7.62048700 | -1.02039600 | -1.82048300 |
| H | -2.05165700 | -1.11458300 | 2.16206200 | O | -7.20878000 | 1.32552500 | -1.51543500 |
| H | 2.76182300 | -2.86532900 | -1.01860200 | O | -7.88980700 | 0.82984100 | 0.81296500 |
| H | -2.01762200 | -2.44290800 | -0.43732800 | O | 2.77105600 | 3.59635800 | -2.57976700 |
| H | 1.47462000 | -1.83864200 | 0.98110800 | O | 5.12448400 | 3.85955000 | -1.82043200 |
| H | 1.64173700 | -0.37640800 | 2.23333300 | O | 3.26562000 | 4.21058000 | -0.22278800 |
| O | 1.44940500 | -1.14914500 | 2.81070900 | H | -2.25157800 | -2.77623300 | 0.88964700 |
| H | 2.19805700 | -1.21771400 | 3.40860700 | H | 2.90311700 | -2.29551500 | -2.47267000 |
| H | 0.66792500 | 1.66390400 | 1.50010500 | H | -1.99504600 | -1.77770800 | -1.84056600 |
| O | -0.13874700 | 2.06713700 | 1.86824300 | H | 1.66710600 | -2.80042900 | -0.58656300 |
| H | -0.85344600 | 1.69570700 | 1.32647300 | H | 1.36158300 | -1.99424900 | 1.77013500 |
| Pd | -0.33994100 | -0.60584900 | -0.18329100 | H | 2.83283900 | -5.00390800 | 0.02701600 |
| H | 0.77317700 | 0.86451500 | -0.93502100 | O | 1.92590100 | -4.73836500 | 0.20776000 |
| H | 0.36946800 | 0.65365900 | -1.57064000 | H | 1.40924400 | -5.54746100 | 0.15456000 |
| C | 4.05659400 | 2.41138900 | 1.38858700 | H | 3.36571100 | -2.36062300 | 0.91649500 |
| C | -3.64124400 | 2.46999500 | -1.47666600 | O | 2.01603000 | -2.64742800 | 2.07329700 |
| C | 5.36544100 | 3.17240900 | 1.59125800 | H | 1.74884200 | -3.48462900 | 1.65594200 |
| H | 5.16035100 | 4.09177400 | 2.14711000 | Pd | -0.09633700 | -1.00741500 | -0.06582000 |
| H | 6.09218200 | 2.59333600 | 2.16881100 | H | 1.05029000 | -0.20389800 | 0.64350600 |
| H | 5.82823300 | 3.45942400 | 0.64292000 | C | 5.65388200 | -0.37288700 | 1.58301900 |
| C | 3.50426200 | 2.11490200 | 2.78681400 | C | -2.76186000 | 2.44982400 | 1.56692800 |
| H | 2.51813800 | 1.65492700 | 2.75072700 | C | -2.24701100 | 2.14206200 | 2.97583700 |
| H | 4.17773900 | 1.44200900 | 3.32811900 | H | -1.52222600 | 1.32939600 | 2.96403700 |
| H | 3.42596600 | 3.04321500 | 3.36210100 | H | -1.76976800 | 3.03091700 | 3.40207600 |
| C | 3.11309300 | 3.34490600 | 0.62253600 | H | -3.07662800 | 1.86045300 | 3.63243400 |
| H | 3.57578600 | 3.65736300 | -0.31916200 | C | -1.60232600 | 2.88457200 | 0.66531500 |
| H | 2.16222700 | 2.86373000 | 0.39163300 | H | -0.86110800 | 2.09236600 | 0.55566100 |
| H | 2.91075500 | 4.24572900 | 1.21164000 | H | -1.97364900 | 3.15467600 | -0.32851700 |
| C | -2.94367500 | 3.46599100 | -0.54563900 | H | -1.11125300 | 3.76651000 | 1.08987500 |
| H | -2.052526300 | 3.05387200 | -0.12788900 | C | -3.70675000 | 3.64293100 | 1.68807200 |
| H | -2.69035900 | 4.37555700 | -1.09954300 | H | -4.10078900 | 3.95892600 | 0.71759900 |
| H | -3.60429600 | 3.74918800 | 0.27981200 | H | -4.55141800 | 3.43387800 | 2.35125800 |
| C | -4.82838100 | 3.19791800 | -2.10272600 | H | -3.15804200 | 4.48883500 | 2.11143900 |
| H | -5.36939000 | 2.56898600 | -2.81534900 | C | 4.87725300 | -0.92765500 | 2.78068500 |
| H | -5.53625400 | 3.55469000 | -1.34900900 | H | 4.09944600 | -0.22513600 | 3.09760500 |
| H | -4.46113300 | 4.07109600 | -2.64861100 | H | 4.40160000 | -1.88569200 | 2.57611200 |
| C | -2.70213600 | 2.06976500 | -2.61818600 | H | 5.55958500 | -1.07567600 | 3.62330700 |
| H | -1.81069400 | 1.56436500 | -2.24592300 | C | 6.65091300 | -1.41616500 | 1.07072400 |
| H | -3.21352000 | 1.40176900 | -3.31804800 | H | 7.24780900 | -1.00345300 | 0.25178500 |
| H | -2.38849900 | 2.96023800 | -3.17216300 | H | 7.33552600 | -1.69817600 | 1.87657000 |
| | | | | H | 6.15052100 | -2.31567300 | 0.71349400 |
| | | | | C | 6.46638600 | 0.81560300 | 2.09268900 |
| | | | | H | 7.06446400 | 1.27540800 | 1.30122800 |
| | | | | H | 5.83393300 | 1.58589500 | 2.54285900 |
| | | | | H | 7.15569400 | 0.46587800 | 2.86543000 |
| 77 | | | | 77 | | | |
| RR-PhtBu_D2_TS2W_P, E(SCF) = - | | | | RR-PhtBu_D2_TS2W, E(SCF) = -2723.23301860, | | | |
| 2723.27165739, E(ZPE) = -2722.654017, E(G) | | | | E(ZPE) = -2722.620748, E(G) = -2722.694883 | | | |
| = -2722.730635 a.u. | | | | a.u. | | | |
| C | -0.89213200 | -3.44101400 | -1.37600000 | C | -0.83232900 | -3.73124700 | -1.09633400 |
| H | -0.63814800 | -3.97022800 | -0.45185600 | H | -0.59335700 | -4.25349800 | -0.16492900 |
| H | -1.49969700 | -4.11420100 | -1.99162200 | H | -1.47349400 | -4.38328300 | -1.69799900 |
| C | 0.36103000 | -3.03074800 | -2.10842100 | C | 0.41759400 | -3.34901900 | -1.84347200 |
| H | 0.93279200 | -3.90391200 | -2.43848500 | H | 1.01180200 | -4.22685500 | -2.11531300 |
| H | 0.09349900 | -2.44974900 | -2.99674600 | | | | |
| N | 1.20511400 | -2.16602600 | -1.24268600 | | | | |
| N | -1.62171800 | -2.22345900 | -1.00406000 | | | | |
| C | 2.26412700 | -3.51074500 | -2.04594600 | | | | |
| H | 1.76533900 | -1.00604000 | -2.87671200 | | | | |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 0.14721200 | -2.83018500 | -2.76798900 | N | -1.38023600 | -2.50640900 | 0.18809100 |
| N | 1.23256000 | -2.41686300 | -1.01972600 | C | 2.41282100 | -2.14113600 | -1.14634700 |
| N | -1.52727100 | -2.47826700 | -0.74319100 | H | 3.05203000 | -3.00821400 | -1.34667500 |
| C | 2.21039500 | -1.68625300 | -1.87545800 | C | -2.42851500 | -2.13937500 | 1.16393700 |
| H | 1.65039500 | -1.32028800 | -2.73943700 | H | -1.91074400 | -1.88854200 | 2.09649900 |
| C | -2.70598700 | -2.62256200 | 0.13930200 | C | 3.25129300 | -1.00424100 | -0.64140400 |
| H | -3.40642600 | -3.34296800 | -0.29736900 | C | 2.66125800 | 0.23014200 | -0.28677500 |
| C | 2.90786600 | -0.53348600 | -1.23388100 | C | 4.62747900 | -1.17249700 | -0.57462900 |
| C | 3.93286700 | -0.75479800 | -0.28238900 | C | 3.50824500 | 1.29807000 | 0.16527700 |
| C | 2.53266600 | 0.75350100 | -1.59231700 | C | 5.43960500 | -0.13701800 | -0.16794900 |
| C | 4.68119600 | 0.37295800 | 0.18393000 | H | 5.07246700 | -2.12213400 | -0.85723900 |
| C | 3.18385300 | 1.83989800 | -1.05132400 | C | 4.87346500 | 1.08062600 | 0.19543300 |
| H | 1.71243400 | 0.90784400 | -2.28749800 | H | 5.53848700 | 1.87352000 | 0.51931400 |
| C | 4.26654900 | 1.63664200 | -0.20105000 | C | -3.26071900 | -1.00297400 | 0.64805300 |
| H | 4.79108700 | 2.51114100 | 0.16751000 | C | -2.66460000 | 0.238167300 | 0.28481800 |
| C | -3.37335500 | -1.29642500 | 0.31930500 | C | -4.63520400 | -1.17257800 | 0.55478000 |
| C | -2.65687500 | -0.23561600 | 0.92154200 | C | -3.50361700 | 1.29973400 | -0.16153500 |
| C | -4.67298800 | -1.11353000 | -0.12475000 | C | -5.43964500 | -0.13844200 | 0.12987800 |
| C | -3.28298300 | 1.03897900 | 1.04857600 | H | -5.08517300 | -2.12215400 | -0.85723900 |
| C | -5.28741000 | 0.11049800 | 0.03204000 | C | -4.86795800 | 1.08132200 | -0.21768300 |
| H | -5.21299700 | -1.93281000 | -0.58820300 | H | -5.52649900 | 1.87409500 | -0.55488000 |
| C | -4.59020700 | 1.16554200 | 0.60807000 | O | 1.37081800 | 0.43989100 | -0.32711100 |
| H | -5.09902100 | 2.11890200 | 0.69507900 | O | -1.37500900 | 0.43971800 | 0.38761900 |
| O | 4.13839900 | -1.95812000 | 0.18627200 | S | 7.21617100 | -0.33930400 | -0.05926500 |
| O | -1.44132800 | -0.41988600 | 1.39298200 | S | -7.21636000 | -0.33364500 | 0.01012600 |
| S | 2.70138300 | 3.51263600 | -1.47002000 | O | -7.56951200 | -0.05076000 | -1.41204800 |
| S | -6.97171600 | 0.37645300 | -0.52286600 | O | -7.80598400 | 0.66903000 | 0.94534600 |
| O | -6.94758000 | 1.62805200 | -1.33434600 | O | -7.50735000 | -1.73950500 | 0.40976500 |
| O | -7.79382000 | 0.52173600 | 0.71364700 | O | 7.51177700 | -1.69781400 | -0.59602200 |
| O | -7.33703800 | -0.82607000 | -1.32320300 | O | 7.56164600 | -0.20023200 | 1.38633900 |
| O | 1.44606200 | 3.39534800 | -2.26545000 | O | 7.80821900 | 0.75293800 | -0.88583200 |
| O | 3.83085700 | 4.09211000 | -2.25666400 | H | 1.82119800 | -2.59333300 | 0.75289400 |
| O | 2.50068400 | 4.22315000 | -0.17243700 | H | 1.88634500 | -1.89191700 | -2.07454700 |
| H | -2.33943700 | -3.03575100 | 1.08507800 | H | -1.82073000 | -2.59422900 | -0.72910800 |
| H | 2.93494500 | -2.42745800 | -2.24000600 | H | -3.06983600 | -3.05988800 | 0.18809100 |
| H | -1.82249000 | -2.00405900 | -1.59774000 | Pd | -0.00256900 | -1.00113400 | 0.01681000 |
| H | 1.77873800 | -3.01899500 | -0.39200200 | C | -0.61197900 | -3.74018900 | 0.46704600 |
| H | 1.54487900 | -1.14199700 | 1.45350400 | C | 0.60429300 | -3.74202300 | -0.43299400 |
| H | 3.66708100 | -3.62941900 | -0.05460200 | H | 1.22086500 | -4.63103100 | -0.27611400 |
| O | 3.07774800 | -4.40588200 | 0.06297600 | H | 0.30483400 | -3.71842200 | -1.48488800 |
| H | 3.34554400 | -5.05296200 | -0.59336100 | H | -0.31302300 | -3.71166200 | 1.51893300 |
| H | 3.18154900 | -1.98199100 | 1.40118000 | H | -1.22839000 | -4.62997000 | 0.31360100 |
| O | 2.42554500 | -1.82781100 | 2.07911100 | C | 2.90267500 | 2.63648100 | 0.59300200 |
| H | 2.06052800 | -2.68506600 | 2.33171600 | C | -2.89081500 | 2.63875500 | -0.57715900 |
| Pd | -0.07007300 | -1.32637200 | 0.20217900 | C | -2.14695500 | 3.27533100 | 0.60203600 |
| H | 1.07059300 | -0.39179600 | 0.98677300 | H | -2.83184500 | 3.45131100 | 1.43790500 |
| C | 5.91405600 | 0.18290900 | 1.07107500 | H | -1.33095900 | 2.63990600 | 0.94793900 |
| C | -2.51826000 | 2.22945200 | 1.62689700 | H | -1.73188700 | 4.24307800 | 0.30040600 |
| C | -2.11375800 | 1.94984000 | 3.07688800 | C | -3.95299600 | 3.63609800 | -1.03127300 |
| H | -1.47412900 | 1.07050500 | 3.14784100 | H | -4.50757300 | 3.27814200 | -1.90362500 |
| H | -1.57374200 | 2.80994200 | 3.48629400 | H | -4.66960100 | 3.86534500 | -0.23700700 |
| H | -3.00143500 | 1.78612200 | 3.69633200 | H | -3.46520600 | 4.57313800 | -1.31414100 |
| C | -1.27374100 | 2.50900000 | 0.77556800 | C | 1.96336100 | 2.42999800 | 1.78702800 |
| H | -0.59621100 | 1.65336800 | 0.75859600 | H | 1.15298400 | 1.73971900 | 1.54516300 |
| H | -1.56088500 | 2.74423300 | -0.25435600 | H | 2.51699800 | 2.03465500 | 2.64480600 |
| H | -0.72993600 | 3.37118400 | 1.17574000 | H | 1.52539400 | 3.08888400 | 3.08492900 |
| C | -3.35774400 | 3.50386400 | 1.62840400 | C | 2.13473200 | 3.27285600 | -0.57086500 |
| H | -3.66157100 | 3.79805200 | 0.61957300 | H | 2.80283800 | 3.45113300 | -1.41971000 |
| H | -4.25582800 | 3.40412100 | 2.24487900 | H | 1.31335600 | 2.63646900 | -0.90214600 |
| H | -2.76270400 | 4.32130700 | 2.04459900 | H | 1.72389600 | 4.23944100 | -0.25989000 |
| C | 5.53541700 | -0.41519900 | 2.42805400 | C | 3.97220100 | 3.63549000 | 1.02549200 |
| H | 4.78286000 | 0.20239300 | 2.92860400 | H | 4.54562300 | 3.27874900 | 1.88604900 |
| H | 5.13945700 | -1.42447500 | 2.32406400 | H | 4.67153300 | 3.86659300 | 0.21649100 |
| H | 6.41896800 | -0.45869900 | 3.07369800 | H | 3.48846600 | 4.57145900 | 1.31872900 |
| C | 6.91142300 | -0.73951600 | 0.36347900 | C | -1.92647500 | 2.43393800 | -1.75136800 |
| H | 7.24506300 | -0.29249400 | -0.57850800 | H | -1.11305600 | 1.75515800 | -1.48793100 |
| H | 7.79368000 | -0.89185100 | 0.99385300 | H | -2.45885800 | 2.02687000 | -2.61710000 |
| H | 6.46366000 | -1.71057300 | 0.14960200 | H | -1.49343200 | 3.39574700 | -2.04720000 |
| C | 6.63081500 | 1.50277900 | 1.34399800 | | | | |
| H | 6.94283900 | 1.99861100 | 0.42026600 | | | | |
| H | 6.01124000 | 2.19882900 | 1.91712800 | | | | |
| H | 7.53021400 | 1.30424200 | 1.93366900 | | | | |

69

RR-PhtBu, E(SCF) = -2569.21633981, E(ZPE) =
-2568.667715, E(G) = -2568.736510 a.u.
N 1.37339900 -2.50698500 -0.16084000

45

RS_hs_left, E(SCF) = -2254.85590857, E(ZPE) =
-2254.531522, E(G) = -2254.589531 a.u.
N -1.50289900 -2.54806700 0.50576000
N 1.11642700 -1.81282000 1.02475700
C -2.91087200 -2.32813200 0.09670300
H -3.07697700 -2.99878600 -0.75125000
C 1.67930100 -0.48292400 1.35386400

| | | | |
|----|-------------|-------------|-------------|
| H | 2.16208300 | -0.53144900 | 2.33601300 |
| C | -3.21508400 | -0.92310100 | -0.30847700 |
| C | -2.51760800 | -0.35943400 | -1.40441700 |
| C | -4.23252200 | -0.21224700 | 0.30811100 |
| C | -2.93096600 | 0.90287000 | -1.86620400 |
| C | -4.60500200 | 1.03976600 | -0.15056700 |
| H | -4.75839800 | -0.64643500 | 1.15293700 |
| C | -3.95736500 | 1.58800000 | -1.25137200 |
| H | -2.40929400 | 1.32931900 | -2.71636800 |
| H | -4.25425800 | 2.56555300 | -1.61931800 |
| C | 2.68037300 | -0.03630800 | 0.33309000 |
| C | 2.38979500 | -0.01434300 | -1.05488700 |
| C | 3.92398500 | 0.39809800 | 0.77978900 |
| C | 3.39370800 | 0.47716600 | -1.91972000 |
| C | 4.88543600 | 0.87426100 | -0.08868000 |
| H | 4.14765100 | 0.37351400 | 1.84196400 |
| C | 4.61054400 | 0.91120500 | -1.45222100 |
| H | 3.16810300 | 0.49880700 | -2.98055700 |
| H | 5.35878900 | 1.28165500 | -2.14644700 |
| O | -1.52405000 | -0.98798200 | -1.99777900 |
| O | 1.26346400 | -0.39855900 | -1.59704900 |
| S | -5.92319600 | 1.96271900 | 0.64227800 |
| S | 6.48948600 | 1.40581700 | 0.50395100 |
| O | 6.68008900 | 2.79368900 | -0.00852600 |
| O | 7.48006400 | 0.45208700 | -0.07578700 |
| O | 6.42355100 | 1.33865800 | 1.99088900 |
| O | -6.38483500 | 1.12611300 | 1.78501900 |
| O | -6.97319300 | 2.15310100 | -0.39999900 |
| O | -5.31706900 | 3.25506900 | 1.07516700 |
| H | -1.29775100 | -3.54106000 | 0.40465800 |
| H | -3.57426300 | -2.64333000 | 0.90955000 |
| H | 0.83304300 | 0.20897900 | 1.43938500 |
| Pd | -0.12048300 | -1.49891400 | -0.60588200 |
| C | 0.29608600 | -2.42562700 | 2.10522300 |
| C | -1.17227400 | -2.14232200 | 1.88872800 |
| H | -1.78432400 | -2.68993300 | 2.61304700 |
| H | -1.40094900 | -1.07746000 | 1.98890500 |
| H | 0.46707100 | -3.50382400 | 2.07067000 |
| H | 0.62703400 | -2.06998800 | 3.08421000 |
| H | 1.88996300 | -2.43485200 | 0.80062100 |

45

RS_hs_right, E(SCF) = -2254.85590860,
E(ZPE) = -2254.531524, E(G) = -2254.589531
a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | -1.11616800 | -1.81214300 | 1.02499400 |
| N | 1.50285000 | -2.54796400 | 0.50557500 |
| C | -1.67907300 | -0.48218900 | 1.35389000 |
| H | -2.16173800 | -0.53051000 | 2.33610500 |
| C | 2.91075500 | -2.32829600 | 0.09609300 |
| H | 3.07639700 | -2.99882500 | -0.75204400 |
| C | -2.68030400 | -0.03586600 | 0.33315300 |
| C | -2.38971800 | -0.01380800 | -1.05483200 |
| C | -3.92405300 | 0.39811700 | 0.77984800 |
| C | -3.39378300 | 0.47733200 | -1.91967800 |
| C | -4.88563800 | 0.87401000 | -0.08863600 |
| H | -4.14772700 | 0.37353400 | 1.84202100 |
| C | -4.61077000 | 0.91097700 | -1.45217600 |
| H | -3.16820800 | 0.49903000 | -2.98052100 |
| H | -5.35913200 | 1.28118000 | -2.14640800 |
| C | 3.21509800 | -0.92324500 | -0.30886600 |
| C | 2.51751700 | -0.35930100 | -1.40459800 |
| C | 4.23256100 | -0.21253900 | 0.30786300 |
| C | 2.93093400 | 0.90309500 | -1.86613800 |
| C | 4.60504200 | 1.03955700 | -0.15054400 |
| H | 4.75846100 | -0.64692200 | 1.15258100 |
| C | 3.95735400 | 1.58806600 | -1.25119300 |
| H | 2.40925700 | 1.32972900 | -2.71621000 |
| H | 4.25429800 | 2.56567600 | -1.61894800 |
| O | -1.26317500 | -0.39753300 | -1.59688800 |
| O | 1.52386300 | -0.98765800 | -1.99795100 |
| S | -6.48984200 | 1.40510900 | 0.50397200 |
| S | 5.92339600 | 1.96218800 | 0.64239000 |
| O | 5.31757200 | 3.25470700 | 1.07520100 |
| O | 6.97357200 | 2.15221400 | -0.39977700 |
| O | 6.38463600 | 1.12544200 | 1.78518500 |
| O | -6.42364700 | 1.33867400 | 1.99092900 |

45

RS_hs_TS, E(SCF) = -2254.84826796, E(ZPE) =
-2254.524416, E(G) = -2254.581437 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.35141800 | 2.42509900 | 0.02164000 |
| N | -1.44302500 | 2.18643100 | 0.12018100 |
| C | 2.72086400 | 1.97436300 | 0.36773100 |
| H | 3.41320900 | 2.74080200 | 0.00466300 |
| C | -2.16790100 | 1.25803300 | 1.01002300 |
| H | -2.82694100 | 1.83282300 | 1.67065900 |
| C | 3.20351500 | 0.62448400 | -0.11163100 |
| C | 2.61285700 | -0.18388500 | -1.10667100 |
| C | 4.40294300 | 0.21414200 | 0.46812900 |
| C | 3.30125400 | -1.36158300 | -1.48203900 |
| C | 5.04963400 | -0.94225700 | 0.08839400 |
| H | 4.85497800 | 0.83173300 | 1.23949200 |
| C | 4.49107900 | -1.73561100 | -0.90968200 |
| H | 2.84153200 | -1.97230200 | -2.25179400 |
| H | 4.98709500 | -2.64873000 | -1.22346900 |
| C | -2.99058100 | 0.27159100 | 0.23180900 |
| C | -2.52393300 | -0.38908300 | -0.93488600 |
| C | -4.26484800 | -0.01332400 | 0.71426600 |
| C | -3.39791500 | -1.32258900 | -1.54018500 |
| C | -5.09214100 | -0.93349300 | 0.10484000 |
| H | -4.62410500 | 0.50378500 | 1.59854700 |
| C | -4.64590500 | -1.59406500 | -1.03633400 |
| H | -3.03952100 | -1.82716100 | -2.43121000 |
| H | -5.28691600 | -2.31774400 | -1.53052900 |
| O | 1.48860400 | 0.06619700 | -1.73356700 |
| O | -1.36089900 | -0.21327200 | -1.50879200 |
| S | 6.60176200 | -1.43263400 | 0.83711900 |
| S | -6.72509900 | -1.28685000 | 0.74918300 |
| O | -6.72195200 | -2.73535400 | 1.10732800 |
| O | -7.67988200 | -0.98330800 | -0.35642100 |
| O | -6.90577900 | -0.39839100 | 1.93151100 |
| O | 6.88477600 | -0.43288200 | 1.90476900 |
| O | 7.60977700 | -1.40775800 | -0.26283600 |
| O | 6.38459100 | -2.80808400 | 1.37148500 |
| H | 1.42404100 | 3.16577100 | -0.67257800 |
| H | 2.80206200 | 1.99275500 | 1.45784800 |
| H | -1.42293300 | 0.76483200 | 1.64529400 |
| Pd | 0.02494000 | 1.09018600 | -0.81142600 |
| C | -0.78066600 | 3.33440300 | 0.78615600 |
| C | 0.61810700 | 2.95921900 | 1.19934500 |
| H | 1.14181600 | 3.82162500 | 1.62321200 |
| H | 0.60606100 | 2.16969200 | 1.95446400 |
| H | -0.74889400 | 4.15388800 | 0.06468100 |
| H | -1.36304900 | 3.67084300 | 1.64844500 |
| H | -2.10308000 | 2.54062900 | -0.56912000 |

53

RS_D1_I1_delta_CH_P, E(SCF) = -
2408.88983943, E(ZPE) = -2408.497965, E(G) =
-2408.565428 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.18762500 | 1.08464600 | -0.94493300 |
| N | -1.64674900 | 1.23364400 | -0.97004000 |
| C | 2.47538700 | 0.42595000 | -1.21459400 |
| C | 2.25441400 | -0.54006700 | -1.67682300 |
| H | -2.53946200 | 0.18584200 | -1.49118300 |
| H | -1.90926700 | -0.61278600 | -1.90324000 |
| C | 3.34477100 | 0.18566200 | 0.01796900 |
| C | 3.84042200 | 1.46797200 | 0.64790700 |
| C | 4.38997400 | -0.83029200 | -0.27295000 |
| C | 5.23970600 | 1.56373600 | 1.00120400 |

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 5.66200700 | -0.65263400 | 0.07953200 | O | 6.47110100 | -3.29809800 | -0.31435500 |
| H | 4.08447700 | -1.74904800 | -0.76448200 | O | 4.40298300 | -3.56431600 | -1.66734400 |
| C | 6.09370200 | 0.56263900 | 0.72851900 | O | 4.35483300 | -3.96251200 | -0.78507900 |
| H | 7.14265700 | 0.65633700 | 0.99254000 | H | 3.00805000 | 2.08537800 | -2.12981600 |
| C | -3.45720800 | -0.32658800 | -0.41965300 | H | -1.73849900 | 2.34567800 | 0.63780000 |
| C | -2.98781600 | -0.80776300 | 0.83256300 | H | -3.10090400 | 2.00215600 | -1.35132700 |
| C | -4.82331000 | -0.33241100 | -0.68345700 | Pd | 0.12054500 | 0.64408700 | 0.27719800 |
| C | -3.95829100 | -1.29380700 | 1.74050000 | H | 5.13961800 | 0.97755000 | 2.19900700 |
| C | -5.74628400 | -0.81015100 | 0.22556000 | H | -2.81092300 | -2.02474400 | 2.35140200 |
| H | -5.18090200 | 0.04799700 | -1.63556500 | C | -0.69878000 | 3.12183900 | -0.96483100 |
| C | -5.30053100 | -1.29720600 | 1.45038100 | C | 0.44607600 | 2.60029300 | -1.78516700 |
| H | -6.01393100 | -1.67477600 | 2.17678300 | H | 1.77638800 | 2.51521700 | -0.21807900 |
| O | 3.05552200 | 2.38893300 | 0.86348800 | H | 2.38528000 | 3.00641800 | 1.81840800 |
| O | -1.74020200 | -0.85835300 | 1.22182300 | H | 1.10074200 | -0.67021400 | 0.99252500 |
| S | 6.91733300 | -1.90788800 | -0.22514000 | H | 1.63558100 | -0.46275800 | 0.46394900 |
| S | -7.50005200 | -0.79788500 | -0.13079800 | O | 1.62498000 | 3.53542300 | 2.14687700 |
| O | -7.94642700 | -2.22085300 | -0.06867300 | H | 0.92910500 | 2.89898400 | 2.33283400 |
| O | -7.64544300 | -0.20488400 | -1.49027200 | H | 3.15532900 | 4.05445700 | -0.17824200 |
| O | -8.13073400 | 0.03470200 | 0.93532500 | O | 2.52433100 | 4.78367800 | -0.42158400 |
| O | 7.93397900 | -1.22402800 | -1.06862000 | H | 2.01140400 | 4.75447100 | 0.49888600 |
| O | 6.22289900 | -3.02458300 | -0.91216800 | H | 0.98363500 | 3.42252200 | -2.26719200 |
| O | 7.42718900 | -2.25884800 | 1.12733500 | H | 0.10157600 | 1.91308700 | -2.56336800 |
| H | 3.03644000 | 1.02026000 | -1.94797900 | H | -1.44201700 | 3.63294200 | -3.58149800 |
| H | -2.20497100 | 1.88486500 | -0.42633200 | H | -0.32883300 | 3.82765800 | -0.21796700 |
| H | -3.14003000 | 0.57869600 | -2.32153500 | | | | |
| Pd | -0.23530800 | 0.10998800 | 0.24330600 | 53 | | | |
| H | 5.56735500 | 2.48348200 | 1.47135100 | RS_D1_I1_delta_CH_TS, E(SCF) = - | | | |
| H | -3.59818400 | -1.66598400 | 2.69403200 | 2408.87136030, E(ZPE) = -2408.484256, E(G) | | | |
| C | -0.86357600 | 1.97826100 | -1.97115700 | = -2408.549247 a.u. | | | |
| C | 0.46818700 | 1.31329500 | -2.22379500 | N | 1.24590800 | 1.87745700 | -0.96270700 |
| H | 1.36308800 | 1.99773900 | -0.50830900 | N | -1.51570200 | 1.70531800 | -0.68175400 |
| H | 1.55883800 | 2.32716700 | 2.11153400 | C | 2.56983700 | 1.40187800 | -1.41473600 |
| H | 0.79849400 | -0.75122300 | 1.04572300 | H | 2.41260400 | 0.77642400 | -2.29711600 |
| H | 2.66799700 | -0.25876300 | 0.77460300 | C | -2.41164600 | 0.77556100 | -1.39778100 |
| O | 0.64847000 | 2.49706100 | 2.40224300 | H | -1.79861800 | 0.20617500 | -2.10665500 |
| H | 0.17563400 | 1.69545800 | 2.12783200 | C | 3.29487600 | 0.61210400 | -0.36293200 |
| H | 1.64147200 | 4.26037400 | 0.05027200 | C | 3.63074100 | 1.27630700 | 0.88805400 |
| O | 0.70622000 | 4.03908500 | 0.01008200 | C | 4.06071800 | -0.52304900 | -0.77296900 |
| H | 0.52722200 | 3.63856400 | 0.88065600 | C | 4.50430600 | 0.55812900 | 1.77070900 |
| H | 1.07615800 | 1.93371500 | -2.89254000 | C | 4.91678100 | -1.13002300 | 0.08550700 |
| H | 0.34056600 | 0.33801400 | -2.70360200 | H | 3.90698600 | -0.94085000 | -1.76342300 |
| H | -1.41528200 | 2.07493300 | -2.91293000 | C | 5.12630700 | -0.58386600 | 1.37651500 |
| H | -0.68852500 | 2.97905200 | -1.57281900 | H | 5.80779100 | -1.09052600 | 2.05344000 |
| | | | | C | -3.14788400 | -0.11837600 | -0.44290400 |
| | | | | C | -2.50128800 | -0.85186800 | 0.58561900 |
| | | | | C | -4.52577200 | -0.23718600 | -0.60271300 |
| | | | | C | -3.30813400 | -1.69516400 | -1.38333500 |
| | | | | C | -5.28745700 | -1.06817900 | 0.19282600 |
| | | | | H | -5.01941500 | 0.33632000 | -1.38119600 |
| | | | | C | -4.66404300 | -1.80426200 | 1.19592000 |
| | | | | H | -5.24966200 | -2.46154100 | 1.83136800 |
| | | | | O | 3.11921400 | 2.37932700 | 1.20174000 |
| | | | | O | -1.22094900 | -0.83188100 | 0.86231900 |
| | | | | S | 5.82785300 | -2.60375200 | -0.38204100 |
| | | | | S | -7.06262800 | -1.19102900 | -0.01259200 |
| | | | | O | -7.35102500 | -0.26337700 | -0.23637700 |
| | | | | O | -7.40643300 | -0.34191800 | -1.18748700 |
| | | | | O | -7.65846700 | -0.68954700 | 1.26023200 |
| | | | | O | 7.26577100 | -2.22430000 | -0.29065900 |
| | | | | O | 5.39136400 | -2.93043600 | -1.76554100 |
| | | | | O | 5.44680300 | -3.63976900 | 0.61825600 |
| | | | | H | 3.15728200 | 2.27728700 | -1.72154600 |
| | | | | H | -2.03823900 | 2.10856600 | 0.09249100 |
| | | | | H | -3.13734200 | 1.34887100 | -1.98620100 |
| | | | | Pd | 0.06552000 | 0.50281700 | 0.03567700 |
| | | | | H | 4.69865000 | 0.99666200 | 2.74339900 |
| | | | | H | -2.81033100 | -2.26014400 | 2.16419500 |
| | | | | C | -0.92653300 | 2.80130200 | -1.48857700 |
| | | | | C | 0.40025700 | 2.37966500 | -2.06673400 |
| | | | | H | 1.39728300 | 2.65727800 | -0.31386600 |
| | | | | H | 1.61201200 | 2.60237200 | 2.26495200 |
| | | | | H | 1.30049100 | -0.49107600 | 0.53917100 |
| | | | | H | 2.14326700 | -0.04245100 | 0.18147700 |
| | | | | O | 0.76178600 | 2.98875100 | 2.54911800 |
| | | | | H | 0.11137000 | 2.30590100 | 2.35270400 |
| | | | | H | 2.43808800 | 4.17006500 | 0.50085500 |
| | | | | O | 1.58455600 | 4.59908500 | 0.33838600 |

H 1.07124500 4.31224700 1.11339600
H 0.88674100 3.22390200 -2.56790200
H 0.28219200 1.57355700 -2.79638900
H -1.61707700 3.11642400 -2.27644900
H -0.77162300 3.64949800 -0.81722200

53

RS_D1_I1_lambda_CH_R, E(SCF) = -
2408.89092785, E(ZPE) = -2408.501018, E(G)
= -2408.567414 a.u.

N -1.53667800 2.10642400 0.52161700
N 1.12539500 1.53108400 0.99306500
C -2.64634500 1.50346200 1.31357100
H -2.20669700 1.00191400 2.17943500
C 2.03232500 0.49718100 1.53932200
H 1.39193100 -0.26084700 2.00375900
C -3.45316000 0.54573100 0.50804600
C -4.20150000 1.04043600 -0.59844800
C -3.42857300 -0.81041300 0.80261200
C -4.89348700 0.07270000 -1.37238200
C -4.11990000 -1.72387100 0.02703700
H -2.84583600 -1.16763100 1.64735700
C -4.85184900 -1.26852100 -1.06862500
H -5.39135500 -1.98094900 -1.68593600
C 2.91354100 -0.07212600 0.47573000
C 2.36720400 -0.61835000 -0.70685100
C 4.28902900 -0.09535100 0.67295700
C 3.25428100 -1.19469200 -1.63622900
C 5.13853600 -0.66883200 -0.25168000
H 4.70809200 0.33380300 1.57766400
C 4.61086800 -1.22552200 -1.41176100
H 5.27169500 -1.67848500 -2.14411300
O -4.22821700 2.29391000 -0.89725300
L 1.08142800 -0.65821900 -0.98604600
S -4.09677500 -3.47137800 0.40759400
S 6.91473900 -0.67452000 0.00136900
O 7.48382000 0.15663400 -1.09825700
O 7.33557500 -2.10167300 -0.09094000
O 7.13933000 -0.08658000 1.35083000
O -5.50925600 -3.85246800 0.70619900
O -3.19502800 -3.62747400 1.58417700
O -3.57992400 -4.15694800 -0.81364800
H -3.25643600 2.33903000 1.67916500
H 1.67609500 2.18351800 0.43065900
H 2.64348900 0.94680700 2.32864300
Pd -0.23306200 0.70531500 -0.29699300
H -5.46384900 0.42678100 -2.22555900
H 2.83022300 -1.61888400 -2.53968900
C 0.37038900 2.29101400 2.01679800
C -0.71241700 3.05588400 1.30729500
H -1.94373000 2.61927000 -0.26803100
H -2.99825000 3.06340600 -1.90764000
H -1.61612600 -0.14056900 -1.07510100
H -1.22714600 0.20693000 -1.70195800
O -2.17690700 3.57149800 -2.00334100
H -1.78804800 3.34273300 -2.85028300
H -3.95112600 3.86818300 -0.00235900
O -3.57182000 4.73658600 0.24082400
H -2.94715700 4.88843400 -0.47865000
H -0.27774100 3.77248000 0.60414500
H -1.33843000 3.61550800 2.00726000
H -0.04700800 1.56606400 2.72034700
H 1.04416800 2.94856300 2.57166400

53

RS_D1_I1_lambda_CH_TS, E(SCF) = -
2408.87174525, E(ZPE) = -2408.485668, E(G)
= -2408.551500 a.u.

N -1.23082100 2.01542100 0.65094400
N 1.39386300 1.28013200 1.23627200
C -2.51138800 1.50847200 1.19074500
H -2.29955800 0.94230100 2.10165500
C 2.27715200 0.20738600 1.72915200
H 1.62294200 -0.54246500 2.18928500
C -3.22505100 0.63877800 0.19287300
C -3.69090800 1.26367100 -1.03682600
C -3.86397800 -0.55454600 0.65124500

C -4.56681300 0.47736300 -1.85496600
C -4.72497200 -1.23298000 -0.14712000
H -3.60659700 -0.95857600 1.62881900
C -5.06677000 -0.70924600 -1.41919800
H -5.75126900 -1.27108600 -2.04801700
C 3.09256900 -0.37971000 0.62171000
C 2.46733500 -0.98816100 -0.49484100
C 4.47854300 -0.36102800 0.71098600
C 3.30210600 -1.59206400 -1.45810000
C 5.27280000 -0.94969900 -0.25449400
H 4.95353900 0.11353600 1.56427900
C 4.67267700 -1.57478700 -1.34231800
H 5.28838900 -2.04531000 -2.10278200
O -3.28030000 2.39717400 -1.39249500
O 1.16928500 -1.05932600 -0.67066300
S -5.47475100 -2.77832600 0.37445800
S 7.06043100 -0.89492100 -0.14906400
O 7.51569600 -0.11112300 -1.33428600
O 7.52050100 -2.31297300 -0.20065000
O 7.37897000 -0.22699600 1.14390700
O -6.94355600 -2.53399000 0.33678600
O -4.95562400 -3.04414800 1.74223500
O -5.03886800 -3.78892300 -0.62935600
H -3.13055300 2.37220500 1.46519600
H 1.95697200 1.97083100 0.74026300
H 2.93688900 0.59789200 2.51278800
Pd -0.04274700 0.64535300 -0.06828100
H -4.86193500 0.89322800 -2.81205700
H 2.82324800 -2.06976500 -2.30631500
C 0.59586500 1.94755000 2.28364200
C -0.43067400 2.81987700 1.60575100
H -1.44699600 2.60797600 -0.15404300
H -1.63833200 3.08187800 -2.14651500
H -2.07281800 0.07799300 -0.44880700
H -1.23698600 -0.20411000 -1.100562100
O -0.87276700 3.63648500 -1.92065700
H -0.11804600 3.25447600 -2.37528300
H -3.14107700 4.08545900 -0.47008700
O -2.71026000 4.88631100 -0.12818200
H -1.89242100 4.90781800 -0.64181900
H 0.06828800 3.60227900 1.02693500
H -1.08278800 3.31232600 2.33210800
H 0.11418400 1.16397800 2.87592900
H 1.23353900 2.53079900 2.95575400

53

RS_delta_D2_TS1_P_02_NOT-USED, E(SCF) = -
2408.88728843, E(ZPE) = -2408.497452, E(G)
= -2408.563972 a.u.

N 1.30205000 1.83662600 -0.77069900
N -1.40196300 1.77962900 -0.26522900
C 2.56498000 1.41680100 -1.42223200
H 2.30562000 0.77626200 -2.26950600
C -2.43139300 1.09528000 -1.07962100
H -1.92659200 0.67367800 -1.95624200
C 3.48065800 0.70945200 -0.48040400
C 3.81569900 1.32072500 0.76141700
C 3.99210900 -0.53618900 -0.81868700
C 4.64966800 0.57131300 1.62924500
C 4.82268900 -1.22737500 0.04337000
H 3.72436800 -0.98605400 -1.77021200
C 5.14404100 -0.66283400 1.27672600
H 5.78669700 -1.20605100 1.96362400
C -3.17810900 0.05743100 -0.29687700
C -2.54713600 -0.84763800 0.58599600
C -4.55560600 -0.02399000 -0.48578800
C -3.35526700 -1.80899100 1.22932700
C -5.32242700 -0.97599000 0.15084300
H -5.04332200 0.67765500 -1.15512500
C -4.71029300 -1.87596900 1.01804600
H -5.30322300 -2.62846800 1.52830100
O 3.37008900 2.48792300 1.09219000
O -1.26431300 -0.87620700 0.87660800
S 5.48699000 -2.83193000 -0.38837100
S -7.09540900 -1.06669200 -0.10210100
O -7.36066600 -2.43818800 -0.62354600
O -7.42886100 0.00353500 -1.08242100

O -7.71090000 -0.84223300 1.23762100
O 6.97209700 -2.68749500 -0.35545200
O 4.96625500 -3.14491700 -1.74925300
O 4.99419800 -3.78100200 0.65309800
H 3.02751400 2.32986700 -1.82337500
H -1.81922400 2.03677600 0.62884300
H -3.13920400 1.84657400 -1.44451800
Pd 0.07484100 0.39986000 0.08445700
H 4.90217400 1.01458900 2.58752600
H -2.86314600 -2.50056800 1.90411500
C -0.80044400 2.99284400 -0.88533700
C 0.42178400 2.60809000 -1.67044000
H 1.57344100 2.43817300 0.01622500
H 1.88388200 2.80305800 2.00768100
H 1.05826100 -1.07666700 0.21161200
H 1.59336900 -0.50808100 0.44391900
O 0.96436300 3.06866500 2.22374200
H 0.55902000 2.27552800 2.58431900
H 2.98987300 3.96370000 0.19341900
O 2.57736400 4.71976800 -0.27591900
H 2.03532100 5.14794400 0.39110600
H 0.94756200 3.49803800 -2.02998600
H 0.17394400 1.97771900 -2.52924500
H -1.54090300 3.50091800 -1.50696400
H -0.51673400 3.65946300 -0.06837900

53
RS_delta_D2_TS1_P_CH_P, E(SCF) = -
2408.88983943, E(ZPE) = -2408.497965, E(G)
= -2408.565428 a.u.

N 1.18762500 1.08464600 -0.94493300
N -1.64674900 1.23364400 -0.97004000
C 2.47538700 0.42595000 -1.21459400
H 2.25441400 -0.54006700 -1.67682300
C -2.53946200 0.18584200 -1.49118300
H -1.90926700 -0.61278600 -1.90324000
C 3.34477100 0.18566200 0.01796900
C 3.84042200 1.46797200 0.64790700
C 4.38997400 -0.83029200 -0.27295000
C 5.23970600 1.56373600 1.00120400
C 5.66200700 -0.65263400 0.07953200
H 4.08447700 -1.74904800 -0.76448200
C 6.09370200 0.56263900 0.72851900
H 7.14265700 0.65633700 0.99254000
C -3.45720800 -0.32658800 -0.41965300
C -2.98781600 -0.80776300 0.83256300
C -4.82331000 -0.33241100 -0.68345700
C -3.95829100 -1.29380700 1.74050000
C -5.74628400 -0.81015100 0.22556000
H -5.18090200 0.04799700 -1.63556500
C -5.30053100 -1.29720600 1.45038100
H -6.01393100 -1.67477600 2.17678300
O 3.05552200 2.38893300 0.86348800
O -1.74020200 -0.85835300 1.22182300
S 6.91733300 -1.90788800 -0.22514000
S -7.50005200 -0.79788500 -0.13079800
O -7.94642700 -2.22085300 -0.06867300
O -7.64544300 -0.20488400 -1.49027200
O -8.13073400 0.03470200 0.93532500
O 7.93397900 -1.22402800 -1.06862000
O 6.22289900 -3.02458300 -0.91216800
O 7.42718900 -2.25884800 1.12733500
H 3.03644000 1.02026000 -1.94797900
H -2.20497100 1.88486500 -0.42633200
H -3.14003000 0.57869600 -2.32153500
Pd -0.23530800 0.10998800 0.24330600
H 5.56735500 2.48348200 1.47135100
H -3.59818400 -1.66598400 2.69403200
C -0.86357600 1.97826100 -1.97115700
C 0.46818700 1.31329500 -2.22379500
H 1.36308800 1.99773900 -0.50830900
H 1.55883800 2.32716700 2.11153400
H 0.79849400 -0.75122300 1.04572300
O 2.66799700 -0.25876300 0.77460300
O 0.64847000 2.49706100 2.40224300
H 0.17563400 1.69545800 2.12783200
H 1.64147200 4.26037400 0.05027200

O 0.70622000 4.03908500 0.01008200
H 0.52722200 3.63856400 0.88066500
H 1.07615800 1.93371500 -2.89254000
H 0.34056600 0.33801400 -2.70360200
H -1.41528200 2.07493300 -2.91293000
H -0.68852500 2.97905200 -1.57281900

53
RS_delta_D2_TS1_P_CH_R, E(SCF) = -
2408.88714525, E(ZPE) = -2408.497051, E(G)
= -2408.564853 a.u.

N 1.35266300 1.85841900 -0.88716800
N -1.33285900 1.99558000 -0.22909000
C 2.49763300 1.25734500 -1.61584100
H 2.09628100 0.58541500 -2.37882700
C -2.37679900 1.27047600 -0.97649900
H -1.89752900 0.81878000 -1.85242700
C 3.42429600 0.53458600 -0.69899200
C 3.92941800 1.22240600 0.44167500
C 3.75961300 -0.79179100 -0.93659100
C 4.75645200 0.47463700 1.31645800
C 4.58176200 -1.48563500 -0.06711500
H 3.36101500 -1.30045500 -1.80944500
C 5.06985900 -0.84184200 1.06897500
H 5.70447400 -1.38688000 1.76183800
C -3.09648800 0.24596300 -0.14706600
C -2.49427600 -0.49425300 0.89482500
C -4.42988900 0.00256600 -0.47001100
C -3.28291500 -1.46155700 1.55402200
C -5.17756900 -0.94869100 0.18888500
H -4.89931600 0.57590500 -1.26361100
C -4.59438700 -1.68413300 1.21620500
H -5.17431900 -2.43263700 1.74676000
O 3.61991300 2.45295700 0.67748300
O -1.26361200 -0.34802400 1.34401900
S 4.98180400 -3.20841300 -0.34076500
S -6.89415300 -1.24318300 -0.23888200
O -6.97409100 -2.67970500 -0.63012000
O -7.20367200 -0.31484500 -1.36123000
O -7.67755200 -0.94862500 0.99515300
O 6.47110100 -3.29809800 -0.31435500
O 4.40298300 -3.56431600 -1.66734400
O 4.35483300 -3.96251200 0.78507900
H 3.00805000 2.08537800 -2.12981600
H -1.73849900 2.34567800 0.63780000
H -3.10090400 2.00215600 -1.35132700
Pd 0.12054500 0.64408700 0.27719800
H 5.13961800 0.97755000 2.19900700
H -2.81092300 -2.02474400 2.35140200
C -0.69878000 3.12183900 -0.96483100
C 0.44607600 2.60029300 -1.78516700
H 1.77638800 2.51521700 -0.21807900
H 2.38528000 3.00641800 1.81840800
H 1.10074200 -0.67021400 0.99252500
H 1.63558100 -0.36275800 0.46394900
O 1.62498000 3.53542300 2.14687700
H 0.92910500 2.89898400 2.33283400
H 3.15532900 4.05445700 -0.17824200
O 2.52433100 4.78367800 -0.32158400
H 2.01140400 4.75447100 0.49888600
H 0.98363500 3.42252200 -2.26719200
H 0.10157600 1.91308700 -2.56336800
H -1.44201700 3.63294200 -1.58149800
H -0.32883300 3.82765800 -0.21796700

53
RS_delta_D2_TS1_P_CH_TS, E(SCF) = -
2408.87136030, E(ZPE) = -2408.484256, E(G)
= -2408.549247 a.u.

N 1.24590800 1.87745700 -0.96270700
N -1.51570200 1.70531800 -0.68175400
C 2.56983700 1.40187800 -1.41473600
H 2.41260400 0.77642400 -2.29711600
C -2.41164600 0.77556100 -1.39778100
H -1.79861800 0.20617500 -2.10665500
C 3.29487600 0.61210400 -0.36293200
C 3.63074100 1.27630700 0.88805400

C 4.06071800 -0.52304900 -0.77296900
C 4.50430600 0.55812900 1.77070900
C 4.91678100 -1.13002300 0.08550700
H 3.90698600 -0.94085000 -1.76342300
C 5.12630700 -0.58386600 1.37651500
H 5.80779100 -1.09052600 2.05344000
C -3.14788400 -0.11837600 -0.44290400
C -2.50128800 -0.85186800 0.58561900
C -4.52577200 -0.23718600 -0.60271300
C -3.30813400 -1.69516400 1.38333500
C -5.28745700 -1.06817900 0.19282600
H -5.01941500 0.33632000 -1.38119600
C -4.66404300 -1.80426200 1.19592000
H -5.24966200 -2.46154100 1.83136800
O 3.11921400 2.37932700 1.20174000
O -1.22094900 -0.83188100 0.86231900
S 5.82785300 -2.60375200 -0.38204100
S -7.06262800 -1.19102900 -0.01259200
O -7.35102500 -0.23947700 -0.23637700
O -7.40643300 -0.34191800 -1.18748700
O -7.65846700 -0.68954700 1.26023200
O 7.26577100 -2.22430000 -0.29065900
O 5.39136400 -2.93043600 -1.76554100
O 5.44680300 -3.63976900 0.61825600
H 3.15728200 2.27728700 -1.72154600
H -2.03823900 2.10856600 0.09249100
H -3.13734200 1.34887100 -1.98620100
Pd 0.06552000 0.50281700 0.03567700
H 4.69865000 0.99666200 2.74339900
H -2.81033100 -2.26014400 2.16419500
C -0.92653300 2.80130200 -1.48857700
C 0.40025700 2.37966500 -2.06673400
H 1.39728300 2.65727800 -0.31386600
H 1.61201200 2.60237200 2.26495200
H 1.30049100 -0.49107600 0.53917100
H 2.14326700 -0.04245100 0.18147700
O 0.76178600 2.98875100 2.54911800
H 0.11137000 2.30590100 2.35270400
H 2.43808800 4.17006500 0.50085500
O 1.58455600 4.59908500 0.33838600
H 1.07124500 4.31224700 1.11339600
H 0.88674100 3.22390200 -2.56790200
H 0.28219200 1.57355700 -2.79638900
H -1.61707700 3.11642400 -2.27644900
H -0.77162300 3.64949800 -0.81722200

53
RS_delta_D2_TS1_P, E(SCF) = -2408.91281913,
E(ZPE) = -2408.520622, E(G) = -2408.588411
a.u.
N -1.34118000 -0.76332800 -0.43755100
N 1.32923700 -1.25920000 0.31761500
C -2.53411700 -0.54614400 -1.30995900
H -2.21406000 0.00382800 -2.19686700
C 2.47878000 -1.57956400 -0.54936800
H 2.10608200 -1.65693400 -1.57804000
C -3.66239900 0.14109700 -0.59781200
C -3.54719600 1.41673900 -0.03736000
C -4.88678000 -0.51435000 -0.48468800
C -4.62874500 1.99712600 0.62081200
C -5.95983200 0.06646200 0.15900500
H -5.00324200 -1.50513100 -0.91141300
C -5.82910400 1.32930100 0.71979600
H -6.66823300 1.78803300 1.23185600
C 3.55256500 -0.54005800 -0.41398500
C 3.31101700 0.84102000 -0.61723000
C 4.83222500 -0.96037200 -0.06636600
C 4.39965100 1.72518300 -0.46609500
C 5.88279500 -0.07422500 0.06935800
H 5.01729100 -2.01800700 0.09506400
C 5.65629700 1.28361500 -0.12585700
H 6.47044100 1.99311300 -0.01491100
O -2.40615200 2.14849100 -0.04685900
O 2.15600100 1.36965200 -0.96227600
S -7.53233100 -0.79696800 0.30222200
S 7.51113000 -0.63541200 0.56405400
O 8.46413300 -0.05111700 -0.42279100

O 7.46655800 -2.12370500 0.51977400
O 7.72840400 -0.10286800 1.94104600
O -8.53902700 0.10786200 -0.31873700
O -7.75207300 -0.98129400 1.76378600
O -7.36259700 -2.07919900 -0.43225500
H -2.89350600 -1.51968600 -1.65411100
H 1.68636300 -1.321069600 1.23601600
H 2.89013800 -2.56007200 -0.28072400
Pd 0.37638000 0.39745400 -0.69753500
H -4.49898000 2.98439600 1.04895500
H 4.20871500 2.78214300 -0.62358300
C 0.31201500 -2.31915000 0.45815400
C -0.80353400 -2.14077200 -0.54429000
H -1.60747000 -0.59536900 0.54200800
H -1.26956600 3.32109800 0.62420000
H -0.31560700 1.52187200 -1.56412300
H -1.69545000 1.76062500 -0.60057500
O 1.30990200 3.58467500 0.49876800
H 1.64938200 2.85457300 -0.62358300
H -1.66527200 1.33119700 1.81972200
O -1.57853800 0.47524600 2.26179600
H -0.71344800 0.50316800 2.68114700
H -1.59691300 -2.87354400 -0.35868700
H -0.44909800 -2.28504800 -1.56862100
H 0.75990400 -3.31282700 0.35503700
H -0.09896800 -2.25121900 1.46860600

53
RS_delta_D2_TS1_R, E(SCF) = -2408.91930651,
E(ZPE) = -2408.529715, E(G) = -2408.595619
a.u.
N 1.38349400 1.94267800 0.14973600
N -1.33202000 1.87214100 0.75929300
C 2.40791200 1.63907900 -0.87207900
H 1.86189600 1.42505200 -1.79800100
C -2.42273300 1.78089100 -0.23275600
H -1.96596500 1.82528800 -1.22745500
C 3.27497600 0.49175400 -0.46666600
C 2.71411500 -0.72354000 -0.19059900
C 4.65339500 0.65687600 -0.41449300
C 3.58622200 -1.83514300 0.10097800
C 5.49249000 -0.39995200 -0.11939800
H 5.08458600 1.63143200 -0.62003000
C 4.95085000 -1.65498800 0.13203100
H 5.60395400 -2.49127700 0.36060200
C -3.25611500 0.54506500 -0.05310100
C -2.71329700 -0.73709400 0.18451600
C -4.63805500 0.68295500 -0.16009900
C -3.60369000 -1.82518400 0.27990900
C -5.48990600 -0.39670800 -0.06081500
H -5.06314200 1.66735900 -0.32864200
C -4.96288900 -1.66448000 0.15926700
H -5.62294600 -2.52199200 0.24235100
O 1.41477700 -1.01660300 -0.21953000
O -1.42902400 -1.01257900 0.32469400
S 7.27292500 -0.18430300 -0.05464600
S -7.26734700 -0.19530600 -0.19602500
O -7.68153900 -1.01597800 -1.36982300
O -7.50402400 1.26182100 -0.39078500
O -7.83170100 -0.71183700 1.08356400
O 7.83187500 -1.12075200 -1.07100600
O 7.67581900 -0.54889800 1.33381300
O 7.52702600 1.24665100 -0.37780200
H 3.02093900 2.53017000 -1.04464900
H -1.72921300 1.70187200 1.68143600
H -3.06558100 2.66216700 -0.13337500
Pd 0.03466000 0.40619500 0.30948700
H 3.15164400 -2.81056900 0.29573900
H -3.17255300 -2.80523900 0.46063400
C -0.60618400 3.17058200 0.78169600
C 0.55466000 3.12642900 -0.17668300
H 1.84626100 2.08414200 1.04859400
H 0.52015200 -2.27827900 -1.37904700
H -0.65341400 0.54686800 -2.99481700
H -0.46340700 0.03203100 -2.48116500
O -0.29760000 -2.70872600 -1.67657000
H -0.93199500 -2.29740000 -1.06869800

H 0.87595200 -2.31002200 1.15613900
O 0.26263000 -2.72266100 1.78586400
H -0.57221400 -2.31974400 1.49910900
H 1.14886600 4.04315700 -0.12342500
H 0.21372800 3.00784000 -1.20894600
H -1.28566200 3.99324200 0.54467600
H -0.24224300 3.31904300 1.80049400

53

RS_delta_D2_TS1_V2_P_strange-central-
chelate_weak-lambda, E(SCF) = -
2408.88649816, E(ZPE) = -2408.498043, E(G)
= -2408.564873 a.u.

N 1.17304300 2.22969700 0.43839100
N -1.32506800 2.20595300 -0.18665700
C 2.64207600 2.17422700 0.57239200
H 3.09665600 2.59001000 -0.33071300
C -2.59123700 2.04205100 -0.93091900
H -2.40584300 2.40245100 -1.94818300
C 3.11005400 0.77453300 0.81621200
C 2.42024400 -0.06032300 1.74440300
C 4.22574800 0.30288900 0.13878200
C 2.93174500 -1.37076600 1.91538400
C 4.70297700 -0.97930800 0.34109200
H 4.73122100 0.94796800 -0.57382000
C 4.04656800 -1.81413800 1.24203300
H 4.41046900 -2.82484700 1.40181500
C -3.03225900 0.61618800 -0.92855400
C -2.21616000 -0.35773700 -1.55454100
C -4.21976500 0.23847000 -0.33082800
C -2.67381100 -1.68126800 -1.58927200
C -4.64622100 -1.08223000 -0.36371800
H -4.83078700 0.99007300 0.16199000
C -3.87512600 -2.03772200 -1.00449400
H -4.21722300 -3.06603800 -1.02935200
O 1.35849500 0.33267300 2.37649100
O -1.06190200 -0.04928000 -2.11762300
S 6.16450300 -1.57048300 -0.50621600
S -6.19756800 -1.51342900 0.43054100
O -6.34488100 -2.98622700 0.27200800
O -7.25126700 -0.74067900 -0.28799700
O -6.05415100 -1.08978400 1.85227900
O 7.21286800 -1.74007100 0.54311600
O 6.51613200 -0.52489900 -1.50870700
O 5.78389100 -2.87042700 -1.13243900
H 2.90895600 2.83379100 1.41208700
H -1.44961000 1.90128200 0.79226900
H -3.35572200 2.68141700 -0.47712700
Pd 0.18281000 1.03731800 -0.93347600
H 2.41334600 -2.02235800 2.61227700
H -2.05270000 -2.42282500 -2.07989700
C -0.79138000 3.58362500 -0.18920600
C 0.62037800 3.59932100 0.39348100
H 0.85130400 1.75110500 1.29410800
H 0.08192100 -0.92608400 1.88794800
H 1.42862100 0.17909800 -1.88730400
H 1.66426700 0.02997200 -1.12186600
O -0.59625200 -1.55015900 1.55905900
H -0.50499400 -1.52232400 0.60202700
H -0.22725000 1.15348100 2.81608300
O -1.04492500 1.65507800 2.64297700
H -1.09133200 2.33468700 3.31970700
H 0.64050600 4.01788800 1.40411100
H 1.27125900 4.21335200 -0.23099400
H -0.77984100 3.91575000 -1.22922900
H -1.46631100 4.24189600 0.36584600

53

RS_delta_D2_TS1_V2, E(SCF) = -
2408.87945502, E(ZPE) = -2408.490410, E(G)
= -2408.555825 a.u.

N 1.26750000 1.70874900 0.10148000
N -1.41033500 1.74339900 0.31847600
C 2.61224500 1.58340000 -0.47621500
H 2.49196300 1.61835900 -1.56563500
C -2.68074900 1.87990500 -0.42826000
H -2.41997200 2.23364200 -1.43159100

C 3.39510300 0.37018900 -0.04478000
C 2.81956400 -0.86376200 0.36790600
C 4.77997800 0.49213400 -0.11445000
C 3.71864200 -1.91841300 0.66424800
C 5.62509900 -0.55782200 0.18130900
H 5.21698400 1.43933000 -0.41817100
C 5.08190600 -1.77700300 0.57723900
H 5.73515300 -2.61126800 0.81459200
C -3.45004900 0.59632200 -0.45318100
C -2.88066400 -0.60712600 -0.93706700
C -4.76525500 0.59338400 -0.01386200
C -3.68961900 -1.75327100 -0.97213900
C -5.54648200 -0.54918300 -0.06247400
H -5.19538600 1.51656900 0.36593200
C -5.00153500 -1.72724500 -0.54661000
H -5.61114200 -2.62253700 -0.58334200
O 1.53865200 -1.05999800 0.49088500
O -1.64459100 -0.71141000 -1.38551900
S 7.40368800 -0.36829200 -0.95975200
S -7.24328500 -0.47225500 0.51791400
O -7.81383900 -1.82922500 0.29605200
O -7.90573800 0.58085800 -0.30378400
O -7.16665500 -0.09950900 -1.95975200
O 7.90244700 -0.55465000 1.49815300
O 7.65334800 1.00413100 -0.42104700
O 7.89288900 -1.43798000 -0.81462900
H 3.18150300 2.48198500 -0.20514000
H -1.57849000 1.25775100 1.20253600
H -3.28945300 2.65450600 0.04976200
Pd -0.14965900 0.45196500 -0.67864600
H 3.27993000 -2.86200800 0.97376500
H -3.25009400 -2.67060500 -1.34994100
C -0.69190700 3.01932200 0.61437100
C 0.65566200 3.04047500 -0.07006700
H 1.28282800 1.46689200 1.09957900
H 0.45311100 -2.44787900 0.08567500
H 0.84528400 -0.24342500 -2.36180900
H 1.06594900 -0.76416100 -1.83909700
O -0.29230400 -2.99238900 -0.23697000
H -0.83231300 -2.35265400 -0.72774200
H 0.67582600 -0.36411500 1.88999300
O 0.21326800 0.31851200 2.42654000
H 0.37210900 0.09521000 3.34627300
H 1.29925000 3.82170800 0.34835600
H 0.55117200 3.22299700 -1.14313500
H -1.30113100 3.86663900 0.29766900
H -0.56679500 3.08182100 1.69649400

53

RS_delta_D2_TS1, E(SCF) = -2408.87894046,
E(ZPE) = -2408.489230, E(G) = -2408.553398
a.u.

N 1.23622800 1.50847300 0.27549700
N -1.47836900 1.51401700 0.69884900
C 2.46909900 1.40700500 -0.52101600
H 2.16028800 1.30055900 -1.56773100
C -2.60981400 1.67813800 -0.24309400
H -2.18213700 1.92333400 -1.22137700
C 3.43634400 0.32180900 -0.11787700
C 3.07826600 -0.89662900 0.52522600
C 4.76682600 0.55210500 -0.45781000
C 4.12337500 -1.82670600 0.75325900
C 5.75876800 -0.37697900 -0.21725400
H 5.03971000 1.48864900 -0.93435000
C 5.42672400 -1.58094200 0.39752400
H 6.19633400 -2.32156100 0.59347200
C -3.49253100 0.46622400 -0.28247400
C -2.99674100 -0.85282800 -0.38631800
C -4.86912900 0.67118000 -0.23794600
C -3.93047100 -1.90621500 -0.45073700
C -5.76423700 -0.37485900 -0.31115300
H -5.25396800 1.68188900 -0.14697200
C -5.28446900 -1.67610100 -0.41743200
H -5.97889000 -2.50879500 -0.46818700
O 1.86928400 -1.17783800 0.91636000
O -1.72270300 -1.18593800 -0.43422900
S 7.46932900 -0.03694600 -0.62257600

| | | | |
|----|-------------|-------------|-------------|
| S | -7.53434000 | -0.08932000 | -0.26432200 |
| O | -8.06513600 | -0.62226200 | -1.55173900 |
| O | -7.71029900 | 1.38305000 | -0.12705200 |
| O | -8.03879900 | -0.85066700 | 0.91428500 |
| O | 7.93222300 | -1.18321700 | -1.45830600 |
| O | 8.19532200 | 0.03637600 | 0.67975100 |
| O | 7.47486000 | 1.25844800 | -1.35937300 |
| H | 2.98680300 | 2.37257800 | -0.45614200 |
| H | -1.84549000 | 1.14361600 | 1.57439000 |
| H | -3.20480100 | 2.53978400 | 0.07777500 |
| Pd | -0.21842600 | 0.11550600 | -0.12820800 |
| H | 3.85019300 | -2.75949500 | 1.23669100 |
| H | -3.53926300 | -2.91502800 | -0.52714300 |
| C | -0.69594300 | 2.75040200 | 0.98165300 |
| C | 0.52995700 | 2.79465900 | 0.10816500 |
| H | 1.44143800 | 1.36147400 | 1.27505000 |
| H | 0.68817000 | -2.57208700 | 0.96624300 |
| H | 0.61723500 | -0.84548700 | -1.67077400 |
| H | 0.95510700 | -1.18348800 | -1.05450900 |
| O | -0.09232900 | -3.15820300 | 0.93781000 |
| H | -0.77064400 | -2.62802800 | 0.49162000 |
| H | 1.51891200 | -0.30861900 | 2.39784800 |
| O | 1.42303200 | 0.45831800 | 3.00815800 |
| H | 0.58044200 | 0.33229900 | 3.45142300 |
| H | 1.17829000 | 3.63228400 | 0.38599400 |
| H | 0.26823100 | 2.90400900 | -0.94809700 |
| H | -1.32385500 | 3.63194200 | 0.83907500 |
| H | -0.39913800 | 2.71262200 | 2.03157900 |

53
RS_delta-from-lambda_D1_TS1_V2_lambda-went-to-delta, E(SCF) = -2408.87945503, E(ZPE) = -2408.490411, E(G) = -2408.555836 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.26755000 | 1.70864500 | 0.10140800 |
| N | -1.41027400 | 1.74336500 | 0.31847500 |
| C | 2.61226200 | 1.58327900 | -0.47636900 |
| H | 2.49190300 | 1.61811200 | -1.56578500 |
| C | -2.68079700 | 1.87994600 | -0.42806500 |
| H | -2.42016300 | 2.23378600 | -1.43139500 |
| C | 3.39515700 | 0.37013400 | -0.04483400 |
| C | 2.81961600 | -0.86385900 | 0.36771800 |
| C | 4.78003100 | 0.49214200 | -0.11433500 |
| C | 3.71869800 | -1.91846800 | 0.66419400 |
| C | 5.62516000 | -0.55778500 | 0.18151400 |
| H | 5.21703500 | 1.43936100 | -0.41798600 |
| C | 5.08196800 | -1.77699600 | 0.57735600 |
| H | 5.73522300 | -2.61123800 | 0.81476400 |
| C | -3.45008400 | 0.59636000 | -0.45305900 |
| C | -2.88074900 | -0.60700800 | -0.93721100 |
| C | -4.76523900 | 0.59335300 | -0.01360200 |
| C | -3.68973600 | -1.75312500 | -0.97245300 |
| C | -5.54649000 | -0.54919800 | -0.06234600 |
| H | -5.19533600 | 1.51646300 | 0.36641300 |
| C | -5.00162100 | -1.72715500 | -0.54681700 |
| H | -5.61123800 | -2.62243200 | -0.58372200 |
| O | 1.53869100 | -1.06015800 | 0.49044800 |
| O | -1.64470800 | -0.71122700 | -1.38577200 |
| S | 7.40374500 | -0.36822800 | 0.10363800 |
| S | -7.24326400 | -0.47223200 | 0.51812000 |
| O | -7.81360900 | -1.82944500 | 0.29721700 |
| O | -7.90596600 | 0.58022100 | -0.30422800 |
| O | -7.16657100 | -0.09850000 | 1.95969600 |
| O | 7.90257100 | -0.55483200 | 1.49828700 |
| O | 7.65337400 | 1.00428500 | -0.42063000 |
| O | 7.89291000 | -1.43775100 | -0.81464700 |
| H | 3.18152200 | 2.48190200 | -0.20542900 |
| H | -1.57832700 | 1.25759400 | 1.20248600 |
| H | -3.28944000 | 2.65494400 | 0.05012200 |
| Pd | -0.14969000 | 0.45199900 | -0.67882000 |
| H | 3.27998200 | -2.86209200 | 0.97361800 |
| H | -3.25027900 | -2.67039200 | -1.35049600 |
| C | -0.69181100 | 3.01924300 | 0.61451600 |
| C | 0.65577200 | 3.04042800 | -0.06989800 |
| H | 1.28290000 | 1.46658500 | 1.09946100 |
| H | 0.45309700 | -2.44790000 | 0.08521400 |
| H | 0.84519700 | -0.24353700 | -2.36207500 |
| H | 1.06586700 | -0.76417400 | -1.83927100 |

| | | | |
|---|-------------|-------------|-------------|
| O | -0.29254100 | -2.99229300 | -0.23712800 |
| H | -0.83250000 | -2.35252500 | -0.72790900 |
| O | 0.67563900 | -0.36457200 | 1.88970600 |
| O | 0.21312800 | 0.31802000 | 2.42632700 |
| H | 0.37203000 | 0.09464600 | 3.34603200 |
| H | 1.29940000 | 3.82155900 | 0.34865200 |
| H | 0.55128500 | 3.22312900 | -1.14293500 |
| H | -1.30099300 | 3.86660700 | 0.29786700 |
| H | -0.56673700 | 3.08163700 | 1.69664900 |

56
RS_delta_ID1_TS3-diamond_P, E(SCF) = -2485.36879450, E(ZPE) = -2484.950108, E(G) = -2485.018560 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.57998600 | 0.46377800 | 2.95807800 |
| H | 1.14165000 | 0.40769700 | 3.89786600 |
| H | 0.30997800 | 1.51088500 | 2.78514100 |
| C | -0.64365200 | -0.41918900 | 3.02112900 |
| H | -0.33327200 | -1.46314500 | 3.11481000 |
| H | -1.26086400 | -0.17932900 | 3.89166900 |
| N | -1.44866900 | -0.30211000 | 1.77118700 |
| C | -2.52151800 | 0.72410300 | 1.90500300 |
| H | -3.05936200 | 0.52587700 | 2.83983300 |
| C | -3.47264000 | 0.66724100 | 0.75632700 |
| C | -3.39279200 | 1.56206100 | -0.30881800 |
| C | -4.41464000 | -0.35452800 | 0.70307200 |
| C | -4.22239200 | 1.40503100 | -1.41056100 |
| C | -5.23657100 | -0.50934700 | -0.39573600 |
| H | -4.50025200 | -1.05198000 | 1.53115800 |
| C | -5.13418100 | 0.37061500 | -1.46473200 |
| H | -5.77667800 | 0.25103600 | -2.33053600 |
| O | -2.51335600 | 2.58924000 | -0.24914200 |
| S | -6.46280000 | -1.82583700 | -0.45806900 |
| O | -7.78355100 | -1.13750600 | -0.49066000 |
| O | -6.25507100 | -0.62575100 | -0.77232200 |
| O | -6.17697000 | -2.57685400 | -1.71159400 |
| H | 2.08747400 | 3.43772400 | -1.61206900 |
| O | 1.28087800 | 3.04602600 | -1.26796600 |
| H | 1.41956700 | 2.06783300 | -1.25736500 |
| H | -0.97772100 | 3.18715300 | 0.83232100 |
| O | -0.13452800 | 3.52658300 | 1.16607200 |
| H | 0.45349400 | 3.45257700 | 0.39525300 |
| H | -1.91139100 | -1.19458000 | 1.61000200 |
| H | -2.04812800 | 1.70099700 | 1.99741300 |
| Pd | -0.06783400 | -0.04271100 | 0.19819700 |
| O | -1.09916400 | 2.37759100 | -2.52447300 |
| H | -0.25741200 | 2.80461100 | -2.27267200 |
| H | -2.10823600 | 2.71121100 | -1.14224000 |
| H | -4.14075600 | 2.10934500 | -2.23854500 |
| H | -1.16793300 | -0.08616400 | -0.91708700 |
| H | -0.93205100 | 1.44110700 | -2.34115300 |
| N | 1.38017400 | 0.01924200 | 1.81177400 |
| C | 2.51249200 | 0.87598700 | 1.43745000 |
| H | 3.18121200 | 1.03625900 | 2.29247200 |
| C | 3.27272500 | 0.24679600 | 0.30871300 |
| C | 2.65044600 | -0.00114500 | -0.93596800 |
| C | 4.60121700 | -0.11458800 | 0.49214800 |
| C | 3.41592000 | -0.59863200 | -1.95075400 |
| C | 5.33501000 | -0.70214600 | -0.52187700 |
| H | 5.07874800 | 0.06801000 | 1.44992600 |
| C | 4.73615100 | -0.93954700 | -1.75247400 |
| H | 5.30531600 | -1.40196600 | -2.55280500 |
| O | 1.40043800 | 0.35044500 | -1.21033700 |
| S | 7.05440500 | -1.15458700 | -0.27896800 |
| O | 7.83448600 | -0.33179600 | -1.24805300 |
| O | 7.13821800 | -2.61268200 | -0.57974500 |
| O | 7.36887400 | -0.83387100 | 1.14081100 |
| H | 2.09462100 | 1.84963100 | 1.15763900 |
| H | 2.93276000 | -0.78020700 | -2.90487700 |
| H | 1.72800600 | -0.92277400 | 1.98615600 |

54
RS_delta_ID2_TS1_chain_P, E(SCF) = -2484.16702633, E(ZPE) = -2483.767552, E(G) = -2483.838661 a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.02366000 | -1.06814700 | -1.98164000 |
| H | 0.18217000 | -2.08975000 | -1.63027900 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.28829500 | -1.11757400 | -3.02517900 |
| C | 1.28982100 | -0.23508600 | -1.85438900 |
| H | 2.18739300 | -0.85970700 | -1.92409600 |
| H | 1.33668900 | 0.51332800 | -2.64860200 |
| N | 1.26963000 | 0.49459600 | -0.57406300 |
| C | 2.51822600 | 1.24760500 | -0.29438600 |
| H | 2.26248300 | 2.06984300 | 0.37768100 |
| C | 3.54181400 | 0.34909100 | 0.32589800 |
| C | 3.19022800 | -0.32030900 | 1.53187500 |
| C | 4.78448000 | 0.15489200 | -0.25443600 |
| C | 4.16634200 | -1.16792500 | 2.10001700 |
| C | 5.72059800 | -0.67999100 | 0.33276100 |
| H | 5.03575400 | 0.66546600 | -1.17985600 |
| C | 5.40173400 | -1.34108900 | 1.51534400 |
| H | 3.91272700 | -1.68604800 | 3.01967800 |
| H | 6.13247700 | -1.99953300 | 1.97595100 |
| O | 2.01417300 | -0.16767500 | 2.07097300 |
| S | 7.33412200 | -0.92736300 | -0.40292400 |
| O | 7.45535500 | -2.39380000 | -0.65497200 |
| O | 8.32755900 | -0.44879100 | 0.60337100 |
| O | 7.34732200 | -0.12209200 | -1.65698500 |
| H | 2.87374900 | 1.68712100 | -1.22918900 |
| H | 1.18082700 | -0.16605100 | 0.20360600 |
| O | -0.06583800 | 3.24538400 | 0.34046300 |
| H | 0.30763800 | 3.01203700 | 1.23335800 |
| H | 0.63707200 | -1.23304900 | 1.76265700 |
| O | -0.14023800 | -1.64903100 | 1.32525000 |
| H | -0.06185200 | -2.59136700 | 1.48969300 |
| H | -0.90785800 | 3.69308800 | 0.49305800 |
| H | 1.41147600 | 1.38039200 | 2.41862900 |
| O | 1.08589200 | 2.30883500 | 2.55286900 |
| H | 0.64478400 | 2.32468700 | 3.40512300 |
| Pd | -0.58945700 | 1.38229800 | -0.51211200 |
| N | -1.08173900 | -0.47338300 | -1.17773200 |
| C | -2.40438700 | -0.48689100 | -1.83980700 |
| H | -2.31628500 | 0.16246300 | -2.71746800 |
| C | -3.49985200 | -0.03720200 | -0.92681800 |
| C | -3.47383300 | 1.25356900 | -0.34770200 |
| C | -4.57873700 | -0.87367600 | -0.68389200 |
| C | -4.58370100 | 1.65457300 | 0.41807600 |
| C | -5.64992300 | -0.46735600 | 0.08780000 |
| H | -4.59100300 | -1.87301600 | -1.11501600 |
| C | -5.65269800 | 0.81327800 | 0.62954700 |
| H | -4.56640700 | 2.64946700 | 0.84968500 |
| H | -6.49250500 | 1.14456200 | 1.23247100 |
| O | -2.47877600 | 2.09847100 | -0.51150400 |
| S | -7.05144700 | -1.54925800 | 0.37579400 |
| O | -6.68592800 | -2.86514700 | -0.21882700 |
| O | -8.21153500 | -0.90552100 | -0.30617600 |
| O | -7.22660300 | -1.60729500 | 1.85530800 |
| H | -2.61341500 | -1.50164200 | -2.19461600 |
| H | -1.12432000 | -0.99250500 | -0.29025900 |

54
RS_delta_ID2_TS1_chain_R, E(SCF) = -
2484.18033756, E(ZPE) = -2483.782165, E(G)
= -2483.852533 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.48668300 | 3.24219900 | -0.01156500 |
| H | 0.01615400 | 3.65364400 | 0.88448500 |
| H | 1.15660400 | 4.00281100 | -0.42194400 |
| C | -0.57375000 | 2.84482700 | -1.00744200 |
| H | -1.19758700 | 3.70233100 | -1.27836900 |
| H | -0.12813900 | 2.45490000 | -1.92727700 |
| N | -1.38778500 | 1.76887800 | -0.40899100 |
| C | -2.30681400 | 1.10902300 | -1.35469200 |
| H | -1.68434700 | 0.62863400 | -2.11860400 |
| C | -3.18423400 | 0.12521200 | -0.64941600 |
| C | -2.61860800 | -0.94141900 | 0.08433600 |
| C | -4.56482700 | 0.25436400 | -0.72338900 |
| C | -3.49393500 | -1.85845700 | 0.69345100 |
| C | -5.40567700 | -0.65399500 | -0.10776100 |
| H | -4.99691200 | 1.08172500 | -1.27755300 |
| C | -4.86080100 | -1.72152600 | 0.59652900 |
| H | -3.05649000 | -2.68037100 | 1.24994700 |
| H | -5.51382200 | -2.44036600 | 1.08146400 |
| O | -1.32040800 | -1.13088400 | 0.20953800 |
| S | -7.18869000 | -0.50084400 | -0.23310300 |

| | | | |
|----|-------------|-------------|-------------|
| O | -7.70031500 | -0.50944000 | 1.16735100 |
| O | -7.64446800 | -1.69000200 | -1.00943100 |
| O | -7.44412300 | 0.78578900 | -0.93822500 |
| H | -2.92083800 | 1.86720200 | -1.85384500 |
| H | -1.93057900 | 2.12529700 | 0.39168500 |
| O | 2.14997700 | -1.72600300 | -2.25296200 |
| H | 1.59392700 | -2.22804600 | -1.62550400 |
| H | -2.34404100 | 1.68349600 | 2.70934600 |
| O | -2.83640600 | 2.22468300 | 2.08451400 |
| H | -3.68479700 | 1.77875400 | 1.99324500 |
| H | 2.71423900 | -1.18758700 | -1.68668100 |
| H | -0.27729200 | -2.59500300 | -0.28711900 |
| O | 0.59230400 | -3.03531100 | -0.25865900 |
| H | 1.02416400 | -2.47877700 | 0.41431800 |
| Pd | -0.03411400 | 0.44736200 | 0.36983400 |
| N | 1.25562900 | 2.04242900 | 0.41410900 |
| C | 2.39098300 | 1.69412800 | -0.45890200 |
| H | 1.97774800 | 1.45338900 | -1.44580400 |
| C | 3.22763200 | 0.56355900 | 0.07474600 |
| C | 2.70854300 | -0.55875300 | 0.76733100 |
| C | 4.59412900 | 0.61575500 | -0.20067600 |
| C | 3.62013500 | -1.56795800 | 1.15122100 |
| C | 5.45611500 | -0.39333400 | -0.17002200 |
| H | 4.99707700 | 1.47586500 | -0.72679500 |
| C | 4.95841900 | -1.49787700 | 0.85470800 |
| H | 3.21689000 | -2.42135500 | 1.68707100 |
| H | 5.62699900 | -2.29736000 | 1.15774400 |
| O | 1.44663900 | -0.75800300 | 1.08171400 |
| S | 7.20487700 | -0.31720600 | -0.22162800 |
| O | 7.42402500 | 1.00246300 | -0.87522100 |
| O | 7.46572000 | -1.46942900 | -1.13119500 |
| O | 7.91834200 | -0.45021700 | 1.08058600 |
| H | 3.02609400 | 2.57813900 | -0.58585000 |
| H | 1.60603400 | 2.19003600 | 1.35849200 |

54
RS_delta_ID2_TS1_chain, E(SCF) = -
2484.15303047, E(ZPE) = -2483.754148, E(G)
= -2483.820209 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.76815800 | 3.00020100 | 0.49813500 |
| H | 0.47666300 | 3.17934600 | 1.53513800 |
| H | 1.40739100 | 3.82652200 | 0.17853000 |
| C | -0.46845700 | 2.89201600 | -0.35918500 |
| H | -1.09731700 | 3.78248700 | -0.25382000 |
| H | -0.21538600 | 2.78007900 | -1.41741000 |
| N | -1.19406300 | 1.68144700 | 0.06971400 |
| C | -2.41184100 | 1.39879800 | -0.70125900 |
| H | -2.08117200 | 1.06248000 | -1.69158400 |
| C | -3.35280000 | 0.39478800 | -0.08950700 |
| C | -2.94467900 | -0.71274600 | 0.70578700 |
| C | -4.69524600 | 0.53830200 | -0.42372600 |
| C | -3.94893400 | -1.64267800 | 1.06897500 |
| C | -5.65130700 | -0.38236300 | -0.04037800 |
| H | -5.00836100 | 1.39372600 | -1.01556800 |
| C | -5.26651400 | -1.48960500 | 0.70857600 |
| H | -3.63474000 | -2.49552600 | 1.66349500 |
| H | -6.00597400 | -2.22484900 | 1.01169800 |
| O | -1.72454800 | -0.89332100 | 1.12825000 |
| S | -7.37595100 | -0.16451100 | -0.46720500 |
| O | -8.11362600 | -0.07623500 | 0.82752900 |
| O | -7.76593200 | -1.37222200 | -1.25251300 |
| O | -7.45419200 | 1.09266800 | -1.26376100 |
| H | -2.95017200 | 2.34358000 | -0.85036000 |
| H | -1.41491700 | 1.75258100 | 1.07376000 |
| O | -0.83485000 | -1.22253900 | -1.58649000 |
| H | -0.77328900 | -2.05968400 | -1.07734100 |
| H | -1.44667600 | 0.26123400 | 2.44136000 |
| O | -1.31440200 | 1.12200300 | 2.89955900 |
| H | -2.03170000 | 1.19495300 | 3.53313200 |
| H | -0.19199500 | -1.31415600 | -2.29733800 |
| O | -0.89113200 | -2.43930800 | 0.86454000 |
| H | -0.33896700 | -3.10501100 | 0.39581200 |
| H | 0.54400900 | -2.69811200 | 0.38292900 |
| Pd | 0.21667200 | 0.21016000 | -0.04912100 |
| N | 1.52498900 | 1.71917800 | 0.47156800 |
| C | 2.63966300 | 1.65295500 | -0.49905500 |
| H | 2.19763200 | 1.69290100 | -1.50072900 |

| | | | |
|---|------------|-------------|-------------|
| C | 3.49356600 | 0.43608500 | -0.29239000 |
| C | 2.96686700 | -0.86835300 | -0.13552300 |
| C | 4.87419200 | 0.61484800 | -0.28342600 |
| C | 3.88069900 | -1.93218600 | 0.01316900 |
| C | 5.74767900 | -0.44328700 | -0.14379800 |
| H | 5.28051400 | 1.61541900 | -0.39128900 |
| C | 5.23941000 | -1.72970600 | 0.00388500 |
| H | 3.46843100 | -2.92852500 | 0.13291000 |
| H | 5.91564600 | -2.57096200 | 0.11923600 |
| O | 1.68795900 | -1.17232100 | -0.12282700 |
| S | 7.52260300 | -0.19162700 | -0.14698500 |
| O | 7.73127500 | 1.27621200 | -0.28928800 |
| O | 8.04105700 | -0.96939300 | -1.30925500 |
| O | 8.01559000 | -0.72659300 | 1.15500400 |
| H | 3.26288600 | 2.54642000 | -0.38140900 |
| H | 1.90219100 | 1.53747700 | 1.39987200 |

54

RS_delta_ID2_TS1_N-trigo-square_Htr_TS,
E(SCF) = -2484.16320653, E(ZPE) = -
2483.767317, E(G) = -2483.834773 a.u.

| | | | |
|----|-------------|-------------|--------------|
| C | 0.36031100 | -2.44914100 | 0.56680600 |
| H | -0.04776600 | -2.37066300 | 1.57652100 |
| H | 0.87375400 | -3.40932400 | 0.48400800 |
| C | -0.76132500 | -2.33430000 | -0.43679600 |
| H | -1.54313600 | -3.07145900 | -0.22502400 |
| H | -0.40822900 | -2.50044400 | -0.145812600 |
| N | -1.29599900 | -0.96006500 | -0.34982900 |
| N | 1.32839900 | -1.32883800 | 0.39740500 |
| C | -2.46169600 | -0.68541800 | -1.23532800 |
| H | -2.09280900 | -0.14791600 | -2.11259800 |
| C | 2.55233000 | -1.64618600 | -0.37315400 |
| H | 2.24075800 | -1.83868400 | -1.40605400 |
| C | -3.56833100 | 0.05760900 | -0.54164600 |
| C | -3.37000500 | 1.32564500 | 0.05741600 |
| C | -4.82602100 | -0.53317500 | -0.48209500 |
| C | -4.46640100 | 1.92810600 | 0.70052200 |
| C | -5.88973500 | 0.08592500 | 0.14592800 |
| H | -4.98239400 | -1.50865700 | -0.93282800 |
| C | -5.70384500 | 1.32596900 | 0.74429600 |
| H | -4.30371700 | 2.89580900 | 1.16373700 |
| H | -6.53281100 | 1.81514500 | 1.24651400 |
| C | 3.57557900 | -0.55168100 | -0.27181500 |
| C | 3.27356000 | 0.81660200 | -0.47063300 |
| C | 4.88785900 | -0.91983300 | 0.01512000 |
| C | 4.33302500 | 1.74314500 | -0.39712700 |
| C | 5.90687000 | 0.00683200 | 0.08503900 |
| H | 5.12235300 | -1.96588100 | 0.18631300 |
| C | 5.62147600 | 1.35158600 | -0.12591100 |
| H | 4.09136000 | 2.78874300 | -0.55445800 |
| H | 6.41440400 | 2.09083200 | -0.06955700 |
| O | -2.19874700 | 1.92902300 | 0.08559900 |
| O | 2.07562200 | 1.30141800 | -0.72669700 |
| S | -7.49647500 | -0.70537500 | 0.23974600 |
| S | 7.59047600 | -0.48252400 | 0.46039800 |
| O | 7.55911200 | -1.95930000 | 0.64970300 |
| O | 8.40790100 | -0.06264300 | -0.71417500 |
| O | 7.96219700 | 0.25763800 | 1.70034300 |
| O | -7.75270100 | -0.93737800 | 1.69092600 |
| O | -8.46441800 | 0.25879500 | -0.35776800 |
| O | -7.37918600 | -1.97004800 | -0.53817900 |
| H | 2.98390100 | -2.57476500 | 0.01484300 |
| H | -2.85111300 | -1.64432500 | -1.58957600 |
| H | -1.56315000 | -0.77085000 | 0.62619600 |
| O | -0.60088400 | 1.63801200 | -1.69942800 |
| H | -1.38505400 | 1.84444500 | -0.96029900 |
| H | -1.61709000 | 1.03548100 | 1.72358100 |
| O | -1.44013800 | 0.26944600 | 2.29954700 |
| H | -2.17111500 | 0.25070000 | 2.92309300 |
| H | -0.05102000 | 2.41778200 | -1.83486100 |
| H | -0.46756200 | 2.84215700 | 0.79129700 |
| O | 0.42256100 | 3.17937100 | 0.96544400 |
| H | 1.01924600 | 2.58349600 | 0.48486100 |
| Pd | 0.40027900 | 0.19354600 | -0.60125200 |
| H | 1.61506000 | -1.00080000 | 1.31839800 |

54

RS_delta_ID2_TS1_N-trigo-square_P_Htr_P,
E(SCF) = -2484.16559814, E(ZPE) = -
2483.766813, E(G) = -2483.835516 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.26010600 | -2.16812200 | 0.86218000 |
| H | -0.14767900 | -1.97618600 | 1.85716800 |
| H | 0.69895100 | -3.16907400 | 0.86448700 |
| C | -0.84242500 | -2.05891700 | -0.16109400 |
| H | -1.66208400 | -2.74546800 | 0.07722200 |
| H | -0.47788100 | -2.30285200 | -1.16244000 |
| N | -1.32086600 | -0.65899300 | -0.17735200 |
| N | 1.30249500 | -1.13995200 | 0.61024400 |
| C | -2.39375200 | -0.39419300 | -1.17950400 |
| H | -1.98131400 | 0.27673500 | -1.93716800 |
| C | 2.44817500 | -1.57362800 | -0.21795100 |
| H | 2.06664400 | -1.76867400 | -1.22824900 |
| C | -3.63184500 | 0.17769700 | -0.55949100 |
| C | -3.64747300 | 1.44286800 | 0.04611400 |
| C | -4.80574400 | -0.56973900 | -0.56742500 |
| C | -4.82136600 | 1.90725300 | 0.64022600 |
| C | -5.96684000 | -0.09539900 | 0.00931300 |
| H | -4.81149300 | -1.54935800 | -1.03430100 |
| C | -5.97262700 | 1.14975600 | 0.62269600 |
| H | -4.80366900 | 2.88551200 | 1.10716000 |
| H | -6.88040300 | 1.52701000 | 1.08179400 |
| C | 3.55949900 | -0.56275300 | -0.20961000 |
| C | 3.35565700 | 0.82358800 | -0.41010500 |
| C | 4.85599700 | -1.03395400 | -0.02023300 |
| C | 4.49042700 | 1.66011700 | -0.42314800 |
| C | 5.95124600 | -0.19515000 | -0.04395800 |
| H | 5.01648500 | -2.09491900 | 0.14482600 |
| C | 5.76069600 | 1.16778500 | -0.24545300 |
| H | 4.32338600 | 2.72103600 | -0.57843600 |
| H | 6.61267200 | 1.84019300 | -0.26276700 |
| O | -2.56414400 | 2.23742900 | 0.15393100 |
| O | 2.18867800 | 1.40480100 | -0.59599500 |
| S | -7.47121100 | -1.08111300 | 0.00594500 |
| S | 7.60856800 | -0.82583400 | 0.22123200 |
| O | 7.47826100 | -2.30704400 | 0.30756900 |
| O | 8.40794900 | -0.37846600 | -0.95530400 |
| O | 8.08293500 | -0.20944300 | 1.49427000 |
| O | -7.76225000 | -1.37109500 | 1.43817800 |
| O | -8.51109100 | -0.22185400 | -0.62574700 |
| O | -7.15858600 | -2.30135000 | -0.78594300 |
| H | 2.83016200 | -2.52610400 | 0.16612200 |
| H | -2.64160700 | -1.33655400 | -1.67300000 |
| H | -1.65638000 | -0.41443900 | 0.76466300 |
| O | -0.54845600 | 1.88033600 | -1.41205300 |
| H | -1.82813700 | 2.09257000 | -0.52794500 |
| H | -1.83006200 | 1.46778000 | 1.88227200 |
| O | -1.61128100 | 0.68446600 | 2.41176800 |
| H | -2.30355600 | 0.63192300 | 3.07627300 |
| H | 0.05333700 | 2.60508200 | -1.60733000 |
| H | 0.19626600 | 3.26911100 | 0.70542500 |
| O | 1.10282100 | 3.52738800 | 0.90072500 |
| H | 1.62781400 | 2.86101200 | 0.41954200 |
| Pd | 0.42227400 | 0.43469400 | -0.38720900 |
| H | 1.66769800 | -0.81905900 | 1.50469900 |

54

RS_delta_ID2_TS1_N-trigo-square_P, E(SCF) =
-2484.16371030, E(ZPE) = -2483.764598, E(G)
= -2483.832945 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.35119500 | 2.44946800 | 0.53521200 |
| H | 0.06156000 | 2.38104200 | 1.54360800 |
| H | -0.86880700 | 3.40660200 | 0.44606800 |
| C | 0.76475600 | 2.32638600 | -0.47335500 |
| H | 1.55047500 | 3.06138600 | -0.26874100 |
| H | 0.40768700 | 2.48831400 | -1.49392800 |
| N | 1.29234100 | 0.95045300 | -0.37823700 |
| N | -1.31817800 | 1.32478600 | 0.38017700 |
| C | 2.46927700 | 0.66611700 | -1.24701700 |
| H | 2.11380400 | 0.10674400 | -2.11661300 |
| C | -2.55246200 | 1.64120200 | -0.37525200 |
| H | -2.25266700 | 1.83660500 | -1.41108900 |
| C | 3.57416000 | -0.05275700 | -0.52809100 |
| C | 3.35873800 | -1.31034700 | 0.09578600 |
| C | 4.83215300 | 0.53491000 | -0.47670900 |

C 4.45683800 -1.90590100 0.75062200
C 5.89202300 -0.07889700 0.16494700
H 4.99480700 1.50030000 -0.94697800
C 5.69677000 -1.30836300 0.78376500
H 4.29096700 -2.86426500 1.23254400
H 6.52297900 -1.79259800 1.29578600
C -3.57617700 0.548842400 -0.26516400
C -3.27777300 -0.82007600 -0.46527900
C -4.88664400 0.91935400 0.02656500
C -4.33801700 -1.74511800 -0.38667200
C -5.90685900 -0.00552300 0.10052000
H -5.11875800 1.96592600 0.19772400
C -5.62466500 -1.35091100 -0.11088100
H -4.09891000 -2.79113100 -0.54468000
H -6.41872300 -2.08867400 -0.05123900
O 2.18450800 -1.88670900 0.12029300
O -2.08147800 -1.30619800 -0.72601300
S 7.50258400 0.70164200 0.24619600
S -7.58866600 0.48732000 0.47970700
O -7.55410800 1.96432700 0.66627200
O -8.40952000 0.06670500 -0.69214900
O -7.95822100 -0.25011800 1.72185400
O 7.76674300 0.95094500 1.69369200
O 8.46546000 -0.27464700 -0.34137300
O 7.39341900 1.95835600 -0.54672000
H -2.97830800 2.56902000 0.02055600
H 2.85152200 1.62052100 -1.62119200
H 1.54808000 0.76701600 0.60180900
O 0.54082000 -1.67710800 -1.77075300
H 1.28860000 -1.90271000 -1.11140300
H 1.60981100 -0.99885900 1.71459800
O 1.41368700 -0.24150000 2.29904600
H 2.14473000 -0.20921300 2.92178500
H -0.02653600 -2.44945800 -1.87991200
H 0.55559800 -2.81941700 0.79877200
O -0.32642500 -3.18343900 0.97198400
H -0.94429500 -2.58364300 0.52709400
Pd -0.40756900 -0.19919100 -0.62458400
H -1.59192500 0.99649900 1.30522000

54
RS_delta_ID2_TS1_N-trigo-square R, E(SCF) =
-2484.18574380, E(ZPE) = -2483.787515, E(G)
= -2483.856981 a.u.
C -0.72379000 3.07536300 0.66461800
H -0.36399400 3.16952600 1.69155000
H -1.39495800 3.91345600 0.45977500
C 0.44795200 3.06069900 -0.28066000
H 1.05190000 3.96687900 -0.17264000
H 0.11682500 3.00334600 -1.32161700
N 1.25574000 1.85563700 -0.00118700
N -1.45900200 1.78521300 0.58248900
C 2.28259600 1.59355800 -1.02219000
H 1.75093700 1.42600600 -1.96659000
C -2.53681900 1.70951000 -0.42429800
H -2.06736600 1.74937600 -1.41368200
C 3.15575600 0.43148900 -0.66794100
C 2.61400400 -0.83531600 -0.36646000
C 4.53603000 0.59620300 -0.68139000
C 3.50522100 -1.89413700 -0.11488100
C 5.39303400 -0.45709600 -0.43016600
H 4.95465800 1.57254200 -0.90397000
C 4.86883900 -1.71241400 -0.14628600
H 3.08154200 -2.86711200 0.11571600
H 5.53384900 -2.54632100 0.05470500
C -3.37749000 0.47785500 -0.24342900
C -2.83879900 -0.80584700 0.01852700
C -4.75678500 0.62285100 -0.36404800
C -3.74380900 -1.88316900 0.12926100
C -5.61840500 -0.44906100 -0.25782700
H -5.17226700 1.60760600 -0.55458900
C -5.10062900 -1.71461500 -0.00337600
H -3.32723000 -2.86547200 0.32801000
H -5.76589100 -2.56724800 0.08836500
O 1.31800800 -1.09782000 -0.30807100
O -1.56245300 -1.08351700 0.17204400
S 7.17294900 -0.23262800 -0.44383000

S -7.39343200 -0.22433700 -0.36845600
O -7.60385500 1.17348300 -0.83776300
O -7.87484100 -1.24539900 -1.34233900
O -7.92346900 -0.46054900 1.00626800
O 7.63560300 -0.57311000 0.93238500
O 7.69423800 -1.18302600 -1.46746600
O 7.40695700 1.19406200 -0.80010000
H -3.17463100 2.59556400 -0.33282000
H 2.89989400 2.49000700 -1.15125600
H 1.68356200 1.90328100 0.93738300
O -0.15442900 -3.47303300 -0.00067800
H 0.58031000 -2.89800100 -0.26511500
H 1.69979600 0.34963600 2.75244800
O 1.91106500 1.30455500 2.74223000
H 2.75125600 1.38833300 3.19895300
H -0.84539000 -2.80063000 0.13641300
H 1.20059200 -1.52909400 1.57737400
O 1.27767200 -1.44847100 2.54567600
H 0.41734900 -1.71858200 2.87963200
Pd -0.09629400 0.32924300 0.11525800
H -1.86808200 1.58460600 1.49333700

54
RS_delta_ID2_TS1_N-trigo-square, E(SCF) = -
2484.15312830, E(ZPE) = -2483.754438, E(G)
= -2483.822641 a.u.
C -0.59848000 2.77884000 0.88378700
H -0.24311400 2.75260900 1.91599900
H -1.20976000 3.67556600 0.76073300
C 0.57758400 2.77865400 -0.05903800
H 1.25782900 3.60761200 0.16126200
H 0.25537600 2.87285600 -1.09996300
N 1.26721500 1.48029800 0.08381700
N -1.42552600 1.55848600 0.67276000
C 2.40083900 1.28359200 -0.84363900
H 1.96823400 1.00514800 -1.81176500
C -2.58955700 1.71916600 -0.22712900
H -2.19671800 1.92393700 -1.22901700
C 3.40189900 0.27695000 -0.35770400
C 3.01941800 -0.99573800 0.13682300
C 4.75052400 0.60854700 -0.42990200
C 4.04893000 -1.86870900 0.54858000
C 5.73716100 -0.27363400 -0.03419600
H 5.04276000 1.58522500 -0.80358300
C 5.37737800 -1.52272600 0.46006000
H 3.75391000 -2.83888800 0.93531700
H 6.14490100 -2.21984300 0.78238900
C -3.49679400 0.52345600 -0.19617600
C -3.03330100 -0.80971000 -0.27616900
C -4.86670600 0.75813900 -0.10985700
C -3.99001300 -1.84392600 -0.26716000
C -5.78555800 -0.27028000 -0.11752300
H -5.22810600 1.77933800 -0.04121400
C -5.33720800 -1.58466400 -0.19277500
H -3.62228200 -2.86306400 -0.32375600
H -6.04958600 -2.40349600 -0.19099000
O 1.76743200 -1.36927800 0.24819000
O -1.76838500 -1.16972300 -0.36468600
S 7.47284900 0.15307400 -0.16328700
S -7.54455000 0.05667500 0.00592600
O -7.69068600 1.53822100 -0.02579400
O -8.16555200 -0.61688800 -1.17006600
O -7.98333800 -0.54386100 1.29885800
O 8.04268400 -0.01650100 1.20468000
O 8.05859300 -0.81009000 -1.14074600
O 7.51962300 1.56331100 -0.64080000
H -3.15677900 2.60209300 0.08735100
H 2.90455200 2.24675400 -0.98392700
H 1.57971700 1.34726700 1.05552400
O 0.50694500 -1.20762100 -2.07135100
H 1.08785700 -1.63678900 -1.41051300
H 1.44571700 -0.63316900 1.97899600
O 1.39030500 0.06841000 2.65603400
H 2.07953600 -0.13688700 3.29281200
H -0.28372100 -1.75830600 -2.12416800
H 0.60261700 -2.71375200 0.78899900
O -0.23114600 -3.19185500 0.94232200

H -0.90065700 -2.61250000 0.54297500
Pd -0.22786200 0.11443800 -0.16602200
H -1.76375600 1.22591800 1.57427700

54

RS_delta_ID2_TS1_P_02, E(SCF) = -
2484.17017201, E(ZPE) = -2483.770219, E(G)
= -2483.838390 a.u.

C -0.05916400 0.89328300 1.64461500
H 0.20755000 0.31014000 2.52855100
H -0.29759200 1.91083500 1.96350100
C 1.08004200 0.86983000 0.66262300
H 1.99992800 1.24258500 1.12556600
H 0.86829600 1.49215000 -0.21219300
N 1.25821200 -0.52329700 0.19739500
N -1.25822500 0.24716300 1.04424800
C 2.30405900 -0.64842900 -0.85165800
H 2.20335600 -1.64248900 -1.28877600
C -2.19543000 -1.14667900 0.33674800
H -1.67612900 1.52824700 -0.54940100
C 3.68588200 -0.45060000 -0.32072700
C 4.25874000 -1.48290000 0.47370900
C 4.39553800 0.70962100 -0.59305800
C 5.57376800 -1.26057500 0.95052100
C 5.67766000 0.89498600 -0.10691800
H 3.94190300 1.48922600 -1.19953900
C 6.26364500 -0.10432100 0.66660000
H 6.02763300 -2.04025800 1.55459900
H 7.27081600 0.03385000 1.04942800
C -3.48568200 0.45898700 -0.00762200
C -3.55487100 -0.84727000 -0.55099600
C -4.66428800 1.17249700 0.19475400
C -4.83060500 -1.34966900 -0.88699100
C -5.89820500 0.65747600 -0.14300700
H -4.61703300 2.16845500 0.62463000
C -5.97647800 -0.61905600 -0.69091600
H -4.87478000 -2.34830700 -1.30783200
H -6.94119300 -1.03773400 -0.95992400
O 3.61159700 -2.56555300 0.76728200
O -2.53287600 -1.64269100 -0.77022300
S 6.60874300 2.37563000 -0.48410200
S -7.40349800 1.58303000 0.15682000
O -8.10664500 1.65766500 -1.15613300
O -8.17342300 0.79745700 1.16479600
O -6.97386600 2.91542700 0.66492900
O 7.76367200 1.94313500 -1.32650300
O 5.67300800 3.28071800 -1.21061400
O 7.05246800 2.93382400 0.82739400
H -2.41024200 2.00625100 0.98061700
H 2.06617200 0.08004000 -1.63139900
H 1.52976900 -1.08666600 1.01509800
O -0.05734800 -2.61113200 -1.18492900
H 0.55445200 -3.25214300 -1.22451600
H 2.63470600 -2.27418100 2.18228900
O 1.89825800 -1.91962000 2.73198300
H 2.31832600 -1.41442000 3.43212800
H -0.85123300 -3.09192000 -1.94825200
H 2.42049500 -3.50241900 0.05322600
O 1.71413900 -4.05799000 -0.37022100
H 1.39595100 -4.65511800 0.31080000
Pd -0.64512700 -1.15630300 -0.29356900
H -1.77865900 -0.22497000 1.78208400

54

RS_delta_ID2_TS1_P_Htr_P, E(SCF) = -
2484.16897791, E(ZPE) = -2483.769831, E(G)
= -2483.838164 a.u.

C 0.02757500 -0.76633000 1.67752400
H -0.22936700 -0.18090900 2.56323700
H 0.23230500 -1.79088500 2.00110100
C -1.11599500 -0.72799400 0.69660100
H -2.03465300 -1.09034300 1.17127000
H -0.91580500 -1.36156900 -0.17274800
N -1.28256600 0.66131400 0.21387700
N 1.24048500 -0.15200400 1.08599800
C -2.29804200 0.78407800 -0.85823700
H -2.18654800 1.77546900 -1.29769200

C 2.14438700 -1.07268200 0.36849000
H 1.60788700 -1.43334200 -0.51684100
C -3.69644400 0.52957800 -0.38323700
C -4.42492300 1.49931200 0.31389200
C -4.29046100 -0.71000600 -0.60725200
C -5.70895500 1.20884500 0.77391300
C -5.56210800 -0.99172200 -0.15289700
H -3.74232200 -1.47433000 -1.14979400
C -6.27524100 -0.02585000 0.54497900
H -6.24816900 1.98105200 1.31045800
H -7.27582500 -0.24210900 -0.90400300
C 3.44754100 -0.41587200 0.00989600
C 3.54393800 0.88586600 -0.54701300
C 4.61004700 -1.15529100 0.21229100
C 4.83020100 1.35019800 -0.89172400
C 5.85604100 -0.67560300 -0.13503300
H 4.53912300 -2.14650500 0.65022100
C 5.96286700 0.59453900 -0.69356200
H 4.90177000 2.34260000 -1.32268600
H 6.93640800 0.98709400 -0.97059000
O -3.95249600 2.72933600 0.61504800
O 2.54690500 1.70540800 -0.77266400
S -6.31630600 -2.59760700 -2.42778900
S 7.33926700 -1.63196500 0.16991600
O 6.88211600 -2.95410400 0.68202100
O 8.04440400 -1.72652700 -1.14124600
O 8.12659200 -0.86158200 1.17704700
O -5.29603000 -3.39929500 -1.17565400
O -6.63587600 -3.13948100 0.90234700
O -7.53594200 -2.32340300 -1.25765900
H 2.34724000 -1.94579300 0.99935600
H -2.02865300 0.06934700 -1.63962400
H -1.56401900 1.23216400 1.02336700
O 0.00634900 2.59673300 -1.66126800
H -1.03406500 3.54085900 -0.82284700
H -2.93753300 2.45657500 2.30955700
O -2.13819000 2.05366500 2.68242900
H -2.44055500 1.52583800 3.42622500
H 0.80690900 3.00855900 -2.00234400
H -3.14291900 3.02693800 0.12702500
O -1.77493900 3.96681400 -0.30300000
H -1.36191100 4.38831300 0.45430400
Pd 0.63940000 1.26295700 -0.29295600
H 1.77576700 0.29535800 1.82685900

54

RS_delta_ID2_TS1_P_Htr_TS, E(SCF) = -
2484.16026658, E(ZPE) = -2483.767218, E(G)
= -2483.835251 a.u.

C 0.04607800 -1.14104600 1.45531400
H -0.27429400 -0.67956200 2.39154600
H 0.29687600 -2.18492900 1.66098200
C -1.05074000 -1.03639900 0.43006200
H -1.97546600 -1.49155500 0.80157100
H -0.77327300 -1.54803200 -0.49590200
N -1.25944000 0.39269100 0.10818600
N 1.24854300 -0.40058500 0.98944900
C -2.29653400 0.59246100 -0.93882300
H -2.12852500 1.56438300 -1.40013600
C 2.23549800 -1.19481100 0.22719300
H 1.75841500 -1.48955500 -0.71458700
C -3.68399600 0.47599900 -0.39101200
C -4.21121000 1.50693000 0.41542900
C -4.44687700 -0.65853500 -0.64205800
C -5.49073200 1.32685100 0.96569300
C -5.71093000 -0.80641600 -0.10443400
H -4.04407300 -1.44624800 -1.27240900
C -6.22924300 0.19219500 0.71182000
H -5.88781300 2.11870000 1.59185000
H -7.21965000 0.08008700 1.14193000
C 3.51763900 -0.44492900 0.00035200
C 3.57237700 0.91711100 -0.38856100
C 4.70572600 -1.15634600 0.14824500
C 4.84765100 1.47695500 -0.62462200
C 5.93790000 -0.58351000 -0.08866300
H 4.66762900 -2.19499000 0.46201500
C 6.00319300 0.74968200 -0.48205400

| | | | |
|----|-------------|-------------|-------------|
| H | 4.88197900 | 2.51904400 | -0.92358100 |
| H | 6.96605500 | 1.21568900 | -0.66740200 |
| O | -3.54421300 | 2.60940300 | 0.71060000 |
| O | 2.54364200 | 1.71702700 | -0.54070500 |
| S | -6.68881400 | -2.27601900 | -0.42696300 |
| S | 7.45101400 | -1.52757100 | 0.08448400 |
| O | 7.05158400 | -2.84942400 | 0.64315500 |
| O | 8.03296000 | -1.62863700 | -1.28596000 |
| O | 8.32061700 | -0.74356100 | 1.00828200 |
| O | -6.84737700 | -2.95852000 | 0.88958800 |
| O | -7.98844500 | -1.79102900 | -0.97313800 |
| O | -5.90758700 | -3.07962900 | -1.40766700 |
| H | 2.45393500 | -2.11477100 | 0.78042100 |
| H | -2.11998200 | -0.15951200 | -1.71173800 |
| H | -1.54447000 | 0.86914300 | 0.97580000 |
| O | 0.04389500 | 2.62068300 | -1.49998900 |
| H | -0.83767300 | 3.21595500 | -1.03398600 |
| H | -2.55227200 | 2.23655200 | 2.18325600 |
| O | -1.84080800 | 1.77625400 | 2.67267300 |
| H | -2.27947400 | 1.31178600 | 3.38956500 |
| H | 0.80416600 | 3.18684200 | -1.66749500 |
| H | -2.68628000 | 3.10990300 | 0.02599300 |
| O | -1.85881500 | 3.74083400 | -0.56077100 |
| H | -1.63831600 | 4.51898000 | -0.04424200 |
| Pd | 0.64721700 | 1.12336900 | -0.23668700 |
| H | 1.72317600 | -0.00454400 | 1.79855000 |

54
RS_delta_ID2_TS1_P, E(SCF) = -
2484.17011834, E(ZPE) = -2483.770167, E(G)
= -2483.837639 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.06060000 | -0.92673200 | 1.61220000 |
| H | -0.20588800 | -0.35668400 | 2.50322500 |
| H | 0.29976500 | -1.94794100 | 1.91855100 |
| C | -1.07908800 | -0.89419000 | 0.63113600 |
| H | -1.99870700 | -1.27319000 | 1.08961300 |
| H | -0.86685200 | -1.50339900 | -0.25120400 |
| N | -1.25811400 | 0.50430300 | 0.18265600 |
| N | 1.25881000 | -0.27264600 | 1.01858200 |
| C | -2.31170700 | 0.64362000 | -0.85725000 |
| H | -2.20649800 | 1.63849900 | -1.29362100 |
| C | 2.20148600 | -1.16355400 | 0.30619700 |
| H | 1.68747700 | -1.53592800 | -0.58562400 |
| C | -3.68890800 | 0.45123600 | -0.31543800 |
| C | -4.23920900 | 1.47497500 | 0.50700700 |
| C | -4.41617700 | -0.69392300 | -0.60316500 |
| C | -5.54753900 | 1.25348500 | 1.00339300 |
| C | -5.69575700 | -0.87391600 | -0.10406900 |
| H | -3.98286300 | -1.46288900 | -1.23604500 |
| C | -6.25437500 | 0.11166700 | 0.70775500 |
| H | -5.98356100 | 2.02552000 | 1.63292100 |
| H | -7.25868200 | -0.02486800 | 1.10096400 |
| C | 3.49152700 | -0.46739900 | -0.02379600 |
| C | 3.55618200 | 0.84032600 | -0.56293800 |
| C | 4.67191100 | -1.17478900 | 0.18839600 |
| C | 4.83166900 | 1.35285600 | -0.88534700 |
| C | 5.90565900 | -0.64982400 | -0.13588600 |
| H | 4.62640400 | -2.17349100 | 0.61419800 |
| C | 5.98166300 | 0.62807800 | -0.68013800 |
| H | 4.87405200 | 2.35214100 | -1.30178900 |
| H | 6.94623500 | 1.05269000 | -0.93805300 |
| O | -3.57913700 | 2.54817300 | 0.80562400 |
| O | 2.53171400 | 1.62964200 | -0.78880900 |
| S | -6.64777200 | -2.33901700 | -0.48572700 |
| S | 7.41315300 | -1.56949200 | 0.17113900 |
| O | 6.98885300 | -2.90229000 | 0.67733500 |
| O | 8.12309100 | -1.64105200 | -1.13862500 |
| O | 8.17690500 | -0.77969100 | 1.18007000 |
| O | -5.80479100 | -3.15466400 | -1.41180300 |
| O | -6.90535500 | -3.02134200 | 0.82163900 |
| O | -7.91442700 | -1.85569500 | -1.12347900 |
| H | 2.41568100 | -2.02980400 | 0.94124100 |
| H | -2.08575800 | -0.08490800 | -1.64407000 |
| H | -1.52216600 | 1.06178800 | 1.00755400 |
| O | 0.05669900 | 2.60920200 | -1.68527800 |
| H | -0.54523100 | 3.25098300 | -1.21181100 |
| H | -2.58715100 | 2.25104700 | 2.20205500 |

| | | | |
|----|-------------|------------|-------------|
| O | -1.84535600 | 1.89059200 | 2.74111900 |
| H | -2.25816600 | 1.39999200 | 3.45523900 |
| H | 0.85036800 | 3.08710100 | -1.95215900 |
| H | -2.41307800 | 3.47781500 | 0.04507500 |
| O | -1.69231900 | 4.04836100 | -0.33549900 |
| H | -1.36878900 | 4.58541100 | 0.39150100 |
| Pd | 0.64483500 | 1.14102800 | -0.31067300 |
| H | 1.77540000 | 0.19599600 | 1.76121800 |

54
RS_delta_ID2_TS1_R, E(SCF) = -
2484.18029934, E(ZPE) = -2483.781990, E(G)
= -2483.850783 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.47871100 | 3.23156900 | 0.05439200 |
| H | -0.00530000 | 3.61872600 | 0.95938000 |
| H | -1.14840900 | 4.00382700 | -0.33397700 |
| C | 0.57719800 | 2.85848000 | -0.95549500 |
| H | 1.20241500 | 3.72104400 | -1.20588400 |
| H | 0.12652400 | 2.49470900 | -1.88340200 |
| N | 1.39026700 | 1.76317200 | -0.39160900 |
| N | -1.24880100 | 2.02275800 | 0.45031700 |
| C | 2.29682000 | 1.12078400 | -1.36205200 |
| H | 1.66452800 | 0.65530700 | -2.12691000 |
| C | -2.38448700 | 1.69759600 | -0.43140300 |
| H | -1.97109700 | 1.47813700 | -1.42326200 |
| C | 3.18015600 | 0.12548200 | -0.68135900 |
| C | 2.61922800 | -0.95384800 | 0.03738200 |
| C | 4.55979800 | 0.26654100 | -0.74827100 |
| C | 3.49884900 | -1.87255600 | 0.63753000 |
| C | 5.40501900 | -0.64551400 | -0.14379000 |
| H | 4.98746700 | 1.10344200 | -1.29144800 |
| C | 4.86525000 | -1.72172700 | 0.55103200 |
| H | 3.06568600 | -2.70417600 | 1.18276200 |
| H | 5.52202300 | -2.44150000 | 1.02948900 |
| C | -3.22386100 | 0.55780200 | 0.07647000 |
| C | -2.70787700 | -0.58142600 | 0.74333600 |
| C | -4.59027000 | 0.62159700 | -0.19540500 |
| C | -3.62284500 | -1.59549900 | 1.10532900 |
| C | -5.45558300 | -0.39315600 | -0.15146400 |
| H | -4.98962300 | 1.49387500 | -0.70384100 |
| C | -4.96206700 | -1.51220300 | 0.81523000 |
| H | -3.22230600 | -2.46263800 | 1.62080100 |
| H | -5.63240800 | -2.31640200 | 1.10134200 |
| O | 1.32156500 | -1.14963300 | 0.15814700 |
| O | -1.44566000 | -0.79208800 | 1.04987900 |
| S | 7.18621400 | -0.44116900 | -0.20615500 |
| S | -7.21156800 | -0.27647900 | -0.19536900 |
| O | -7.39265500 | 0.97532600 | -0.98097600 |
| O | -7.55724000 | -1.50509400 | -0.96521700 |
| O | -7.88487900 | -0.23373200 | 1.13442900 |
| O | 7.43673600 | 0.71679900 | -1.10815200 |
| O | 7.61549400 | -0.18686200 | 1.19971300 |
| O | 7.72617100 | -1.72429600 | -0.73928500 |
| H | -3.01711200 | 2.58608800 | -0.53821200 |
| H | 2.90617300 | 1.88759100 | -1.85347900 |
| H | 1.94413500 | 2.09047100 | 0.41333300 |
| O | -2.15574800 | -1.68204400 | -2.30054600 |
| H | -1.60153500 | -2.19744600 | -1.68235800 |
| H | 2.35235000 | 1.26005700 | 2.59086900 |
| O | 2.86635100 | 1.93080000 | 2.12968700 |
| H | 3.70571600 | 1.49881100 | 1.93679100 |
| H | -2.72368900 | -1.15771900 | -1.72477800 |
| H | 0.27333700 | -2.60519300 | -0.36309700 |
| O | -0.59868700 | -3.04046900 | -0.33839600 |
| H | -1.02452200 | -2.49383800 | 0.34667600 |
| Pd | 0.03671100 | 0.42668600 | 0.36356200 |
| H | -1.59891400 | 2.14695200 | 1.39817900 |

54
RS_delta_ID2_TS1, E(SCF) = -2484.15302227,
E(ZPE) = -2483.754246, E(G) = -2483.820856
a.u.

| | | | |
|---|-------------|------------|-------------|
| C | -0.76615000 | 2.99756300 | 0.49905800 |
| H | -0.47607200 | 3.17334600 | 1.53703100 |
| H | -1.40465900 | 3.82507200 | 0.18113800 |
| C | 0.47174900 | 2.89181600 | -0.35673800 |
| H | 1.10136200 | 3.78113600 | -0.24627800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.22034600 | 2.78490100 | -1.41588000 |
| N | 1.19550900 | 1.67863000 | 0.06788400 |
| N | -1.52347500 | 1.71684800 | 0.46736700 |
| C | 2.41361500 | 1.39684400 | -0.70309200 |
| H | 2.08323000 | 1.06054600 | -1.69352000 |
| C | -2.63933600 | 1.65449000 | -0.50220000 |
| H | -2.19836100 | 1.69686800 | -1.50421800 |
| C | 3.35394000 | 0.39307300 | -0.09028200 |
| C | 2.94377100 | -0.71755600 | 0.69966000 |
| C | 4.69776000 | 0.54013700 | -0.41737200 |
| C | 3.94837300 | -1.64540300 | 1.06725700 |
| C | 5.65382000 | -0.37912100 | -0.03070900 |
| H | 5.01205700 | 1.39748000 | -1.00578300 |
| C | 5.26752900 | -1.48847200 | 0.71435300 |
| H | 3.63298400 | -2.50020300 | 1.65829700 |
| H | 6.00706700 | -2.22250100 | 1.02021600 |
| C | -3.49360000 | 0.43761900 | -0.29692600 |
| C | -2.96687200 | -0.86742500 | -0.14517100 |
| C | -4.87409600 | 0.61699800 | -0.28213000 |
| C | -3.88042000 | -1.93093100 | 0.00686400 |
| C | -5.74741800 | -0.44094100 | -0.13958000 |
| H | -5.28035400 | 1.61794300 | -0.38682000 |
| C | -5.23906700 | -1.72769100 | 0.00472400 |
| H | -3.46809400 | -2.92762100 | 0.12349800 |
| H | -5.91502300 | -2.56875600 | 0.12295800 |
| O | 1.72143600 | -0.90260800 | 1.11368500 |
| O | -1.68803100 | -1.17203900 | -0.14024800 |
| S | 7.37958400 | -0.15900700 | -0.45194200 |
| S | -7.52227800 | -0.18846100 | -0.13313800 |
| O | -7.73127400 | 1.27945300 | -0.27358200 |
| O | -8.04777200 | -0.96546300 | -1.29275500 |
| O | -8.00790000 | -0.72359600 | 1.17150600 |
| O | 7.45973500 | 1.10230900 | -1.24175800 |
| O | 8.11424600 | -0.07753500 | 0.84493000 |
| O | 7.77123900 | -1.36273300 | -1.24260500 |
| H | -3.26171900 | 2.54808200 | -0.38123200 |
| H | 2.95181500 | 2.34172400 | -0.85176700 |
| H | 1.41482100 | 1.74478900 | 1.07259800 |
| O | 0.83523900 | -1.21753600 | -1.60419400 |
| H | 0.77760000 | -2.05615800 | -1.09713200 |
| H | 1.42808900 | 0.24305400 | 2.43232600 |
| O | 1.28834400 | 1.09997700 | 2.89537300 |
| H | 1.99789000 | 1.16951500 | 3.53802700 |
| H | 0.18916600 | -1.30872200 | -2.31218800 |
| H | 0.88697800 | -2.44834900 | 0.84204600 |
| O | 0.33496100 | -3.11032700 | 0.36824000 |
| H | -0.54708700 | -2.70132800 | 0.35516000 |
| Pd | -0.21602000 | 0.20921400 | -0.05924200 |
| H | -1.89962500 | 1.53124700 | 1.39546200 |

56
RS_delta_ID2_TS2-square_P, E(SCF) = -
2485.33249918, E(ZPE) = -2484.916675, E(G)
= -2484.985842 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.10098500 | -0.58851600 | 1.84010700 |
| H | -0.13510300 | 0.08587700 | 2.66656700 |
| H | 0.32902300 | -1.57109600 | 2.26015700 |
| C | -1.05596300 | -0.64897900 | 0.88202500 |
| H | -1.96556000 | -0.97810300 | 1.39207000 |
| H | -0.86263600 | -1.34900700 | 0.60419100 |
| N | -1.24049500 | 0.69573700 | 0.29406900 |
| N | 1.29847900 | -0.03317000 | 1.15466600 |
| C | -2.29886200 | 0.74165100 | -0.75530500 |
| H | -2.32311900 | 1.77096200 | -1.11987700 |
| C | 2.17908600 | -1.02115000 | 0.49460100 |
| H | 1.61596700 | -1.46109000 | -0.33605800 |
| C | -3.64709200 | 0.32113200 | -0.26659800 |
| C | -4.44607600 | 1.24470900 | 0.46395700 |
| C | -4.11620400 | -0.95971200 | -0.53144300 |
| C | -5.71605600 | 0.78493900 | 0.89318000 |
| C | -5.35925900 | -1.37498800 | -0.09378600 |
| H | -3.49827300 | -1.65287000 | -1.09582600 |
| C | -6.15947300 | -0.48803800 | 0.62443000 |
| H | -6.33845200 | 1.48103900 | 1.44688000 |
| H | -7.13890200 | -0.80716000 | 0.96936500 |
| C | 3.47447500 | -0.41072200 | 0.04632200 |
| C | 3.56438500 | 0.85996400 | -0.56838800 |

| | | | |
|----|-------------|-------------|-------------|
| C | 4.63354000 | -1.16095900 | 0.22936100 |
| C | 4.83990600 | 1.29666100 | -0.98605100 |
| C | 5.86713200 | -0.71237500 | -0.19178400 |
| H | 4.56917200 | -2.13173100 | 0.71159800 |
| C | 5.96653200 | 0.53399400 | -0.80248100 |
| H | 4.89993000 | 2.27067600 | -1.45903200 |
| H | 6.93211800 | 0.90214300 | -1.13464200 |
| O | -4.05422800 | 2.45208400 | 0.72136500 |
| O | 2.56707100 | 1.68968000 | -0.78602900 |
| S | -5.96615700 | -3.02423500 | -0.43254300 |
| S | 7.35232600 | -1.67298600 | 0.10032100 |
| O | 8.15346000 | -0.89423500 | 1.08897900 |
| O | 6.89545700 | -2.98724400 | 0.63092600 |
| O | 8.03545700 | -1.78069600 | -1.22048400 |
| O | -6.23783100 | -3.64576800 | 0.89742500 |
| O | -7.21323600 | -2.85337700 | -1.23538600 |
| O | -4.88479300 | -3.71955900 | -1.18676100 |
| H | 2.38875000 | -1.82786400 | 1.20455200 |
| H | -1.95946400 | 0.09805900 | -1.57184400 |
| H | -1.47995100 | 1.36515700 | 1.04073700 |
| O | -0.79151700 | 4.25928500 | -0.33209900 |
| H | -1.68280400 | 4.35919400 | -0.72299700 |
| H | -2.74275200 | 2.83760700 | 1.62174200 |
| O | -1.81690300 | 2.97370900 | 1.97935200 |
| H | -1.87043900 | 3.13273000 | 2.92392400 |
| H | -0.97941000 | 3.94490500 | 0.56977100 |
| H | -3.76296900 | 3.60019600 | -0.50815300 |
| O | -3.46359400 | 4.30262000 | -1.13645200 |
| H | -3.72645700 | 3.99985300 | -2.00848700 |
| H | 0.00741800 | 2.69953400 | -1.19032200 |
| H | 0.21407000 | 2.13086300 | -1.76040500 |
| Pd | 0.66501500 | 1.26639400 | -0.29726500 |
| H | 1.85748600 | 0.48591600 | 1.83009100 |

54
RS_delta_ID2_TS2-square_R_noH2, E(SCF) = -
2484.16609790, E(ZPE) = -2483.765343, E(G)
= -2483.830994 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.03931200 | 0.77552800 | -2.15944200 |
| H | -0.20211400 | 0.16363700 | -3.03048800 |
| H | 0.25694300 | 1.79037200 | -2.50468800 |
| C | -1.09542200 | 0.76857500 | -1.17597600 |
| H | -2.01987300 | 1.12147900 | -1.64086900 |
| H | -0.87337300 | 1.44033600 | -0.34227200 |
| N | -1.26695800 | -0.58990800 | -0.60223300 |
| N | 1.24569600 | 0.17407600 | -1.53627700 |
| C | -2.03455700 | -0.54855500 | 0.67993600 |
| H | -1.85532600 | -1.49014600 | 1.19449800 |
| C | 2.07114400 | 1.04523500 | -0.68234100 |
| H | 1.46768400 | 1.32637300 | 0.18832000 |
| C | -3.50198800 | -0.33560800 | 0.50127400 |
| C | -4.35685900 | -1.47133500 | 0.41009900 |
| C | -4.02888100 | 0.94932100 | 0.44905000 |
| C | -5.74050700 | -1.21013000 | 0.24711500 |
| C | -5.38354000 | 1.16519400 | 0.28085100 |
| H | -3.36942800 | 1.80698700 | 0.54775400 |
| C | -6.23917000 | 0.06947100 | 0.18112200 |
| H | -6.40605500 | -2.06503000 | 0.17909000 |
| H | -7.30595200 | 0.23066000 | 0.05470000 |
| C | 3.35900500 | 0.37462900 | -0.28657200 |
| C | 3.50525100 | -1.02212400 | -0.08829400 |
| C | 4.45887800 | 1.20740300 | -0.09518600 |
| C | 4.78361100 | -1.49188000 | 0.29014300 |
| C | 5.68967400 | 0.72123800 | 0.28896700 |
| H | 4.34771000 | 2.27591100 | -0.25304500 |
| C | 5.85057300 | -0.64875200 | 0.47525800 |
| H | 4.89166700 | -2.56149900 | 0.43362300 |
| H | 6.81657000 | -1.04885500 | 0.76806300 |
| O | -3.91302400 | -2.68748300 | 0.47847600 |
| O | 2.57140600 | -1.93595300 | -0.24059300 |
| S | -6.06494300 | 2.81842900 | 0.22118500 |
| S | 7.09278700 | 1.81263200 | 0.51415100 |
| O | 8.10496200 | 1.39247100 | -0.49817800 |
| O | 6.58408700 | 3.19393400 | 0.28662700 |
| O | 7.56487100 | 1.58657500 | 1.91066300 |
| O | -6.79670800 | 2.91768600 | -1.07625500 |
| O | -6.98430800 | 2.93341700 | 1.39179900 |

| | | | |
|----|-------------|-------------|-------------|
| O | -4.90506800 | 3.75114900 | 0.30434000 |
| H | 2.29769400 | 1.96663700 | -1.23091800 |
| H | -1.58007400 | 0.24334000 | 1.28084000 |
| H | -1.75550300 | -1.21021900 | -1.25690600 |
| O | -0.00263500 | -3.23153500 | 0.44470800 |
| H | -0.53606600 | -3.23448600 | 1.27089800 |
| H | -2.85929200 | -3.18203300 | -0.68780900 |
| O | -2.08032600 | -3.34436600 | -1.28721400 |
| H | -2.36160600 | -3.96647800 | -1.96123100 |
| H | -0.66401200 | -3.51167600 | -0.23076900 |
| H | -2.80584000 | -3.27861800 | 1.67736700 |
| O | -2.04139400 | -3.61516700 | 2.20722300 |
| H | -2.18818600 | -3.31541300 | 3.10719100 |
| Pd | 0.64113900 | -1.39710800 | -0.42070200 |
| H | 1.84129700 | -0.19611400 | -2.27564400 |

56

RS_delta_ID2_TS2-square_R, E(SCF) = -
 2485.34044064, E(ZPE) = -2484.925053, E(G)
 = -2484.992358 a.u.

| | | | |
|----|-------------|--------------|-------------|
| C | 0.02010200 | -0.73636400 | 2.24507300 |
| H | -0.22315400 | -0.10577800 | 3.10211200 |
| H | 0.23259200 | -1.74483000 | 2.61182100 |
| C | -1.10984300 | -0.74610900 | 1.25566900 |
| H | -2.03815800 | -1.08300900 | 1.72442800 |
| H | -0.88723800 | -1.44009600 | 0.44059200 |
| N | -1.27160700 | 0.59884700 | 0.64695400 |
| N | 1.23109600 | -0.15094800 | 1.61619200 |
| C | -2.00255600 | 0.52631900 | -0.65487700 |
| H | -1.80763500 | 1.45637700 | -1.18450900 |
| C | 2.04680800 | -1.03448300 | 0.76684100 |
| H | 1.43379000 | -1.32842300 | -0.09377200 |
| C | -3.47452600 | 0.31858000 | -0.51272300 |
| C | -4.32935500 | 1.45755500 | -0.47797300 |
| C | -4.00470100 | -0.96370600 | -0.43721100 |
| C | -5.71709400 | 1.20289100 | -0.34234000 |
| C | -5.36372800 | -1.17286500 | -0.29899500 |
| H | -3.34516600 | -1.82504000 | -0.49431200 |
| C | -6.21942000 | -0.071383700 | -0.25136300 |
| H | -6.38286800 | 2.05994000 | -0.31662900 |
| H | -7.28934300 | -0.23069100 | -0.14779700 |
| C | 3.33115900 | -0.37261100 | 0.34332900 |
| C | 3.48851700 | 1.02377300 | 0.14707600 |
| C | 4.41738300 | -1.21644900 | 0.12384800 |
| C | 4.76093100 | 1.47945900 | -0.26685200 |
| C | 5.64348600 | -0.74285900 | -0.28974500 |
| H | 4.29869800 | -2.28412000 | 0.28213700 |
| C | 5.81438300 | 0.62559900 | -0.47855600 |
| H | 4.87640100 | 2.54804500 | -0.41221900 |
| H | 6.77641100 | 1.01533100 | -0.79654000 |
| O | -3.88062800 | 2.67037700 | -0.57133600 |
| O | 2.57127500 | 1.94820900 | 0.33328900 |
| S | -6.04953800 | -2.82250700 | -0.20290500 |
| S | 7.03105100 | -1.84851300 | -0.54094100 |
| O | 8.05718600 | -1.45104500 | 0.46656100 |
| O | 6.50835000 | -3.22609600 | -0.32304500 |
| O | 7.49266200 | -1.61295100 | -1.93929200 |
| O | -6.77426700 | -2.89496600 | 1.10032800 |
| O | -6.97572600 | -2.95616700 | -1.36592500 |
| O | -4.89288100 | -3.76010200 | -0.27442000 |
| H | 2.27816700 | -1.94851700 | 1.32585800 |
| H | -1.53016500 | -0.27831800 | -1.22481700 |
| H | -1.78186600 | 1.23049200 | 1.27328900 |
| O | -0.00005800 | 3.24327000 | -0.39809100 |
| H | -0.50452600 | 3.23028100 | -1.24318200 |
| H | -2.88412700 | 3.19413800 | 0.63706800 |
| O | -2.13033600 | 3.36274900 | 1.26576900 |
| H | -2.43713700 | 3.99418100 | 1.91963800 |
| H | -0.68570700 | 3.52327900 | 0.25280000 |
| H | -2.73158300 | 3.21950600 | -1.75210100 |
| O | -1.95091800 | 3.54241000 | -2.26710500 |
| H | -2.05176000 | 3.19023800 | -3.15436500 |
| H | 0.93704400 | 1.09963300 | -2.62067500 |
| H | 1.24019800 | 0.48520800 | -2.31586900 |
| Pd | 0.63585700 | 1.41362700 | 0.48813600 |
| H | 1.83055900 | 0.22148300 | 2.35122800 |

56

RS_delta_ID2_TS2-square, E(SCF) = -
 2485.32424314, E(ZPE) = -2484.910941, E(G)
 = -2484.980976 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.02597100 | -0.66882900 | 1.87237300 |
| H | -0.27682700 | -0.01120800 | 2.69060800 |
| H | 0.25515500 | -1.65094400 | 2.29376100 |
| C | -1.06910900 | -0.74885600 | 0.84515500 |
| H | -1.99893200 | -1.11220900 | 1.29280900 |
| H | -0.80322300 | -1.42967700 | 0.03061000 |
| N | -1.25573600 | 0.59676300 | 0.26378000 |
| N | 1.24656000 | -0.07556300 | 1.26447700 |
| C | -2.24709200 | 0.62855500 | -0.84545200 |
| H | -2.18182100 | 1.62552900 | -1.28593500 |
| C | 2.17831500 | -1.03525900 | 0.64460900 |
| H | 1.64284400 | -1.52606200 | -0.17550900 |
| C | -3.64105600 | 0.34342700 | -0.39059900 |
| C | -4.38892300 | 1.38379400 | 0.22903500 |
| C | -4.19439200 | -0.91802700 | -0.47348400 |
| C | -5.70185000 | 1.05602900 | 0.64889600 |
| C | -5.47924800 | -1.20226100 | -0.13973400 |
| H | -3.61324900 | -1.69979900 | -1.04587400 |
| C | -6.23049600 | -0.20150800 | -0.27348400 |
| H | -6.28710900 | 1.83942700 | 1.12029200 |
| H | -7.24105400 | -0.41764100 | 0.80825900 |
| C | 3.45717000 | -0.39835100 | 0.17954000 |
| C | 3.54460300 | 0.90041300 | -0.37596800 |
| C | 4.61034900 | -1.17501400 | 0.27072300 |
| C | 4.81075900 | 1.33621600 | -0.82450800 |
| C | 5.83303300 | -0.72692100 | -0.18016800 |
| H | 4.54898800 | -2.16874500 | 0.70429700 |
| C | 5.93009500 | 0.54748800 | -0.73015600 |
| H | 4.86805900 | 2.33189300 | -1.25038800 |
| H | 6.88653300 | 0.91616000 | -1.08720800 |
| O | -3.90694300 | 2.57386400 | 0.40247800 |
| O | 2.55815800 | 1.76118200 | -0.49989200 |
| S | -6.19525400 | -2.82612700 | -0.36637500 |
| S | 7.30438600 | -1.74114600 | -0.03648300 |
| O | 8.20874300 | -1.01923600 | 0.90473600 |
| O | 6.84804400 | -3.05687700 | 0.49116000 |
| O | 7.87456900 | -1.82932500 | -1.41124000 |
| O | -6.51954700 | -3.33138700 | 1.00047300 |
| O | -7.42116300 | -2.62992200 | -1.19545900 |
| O | -5.15647900 | -3.64509000 | -1.05373800 |
| H | 2.41569200 | -1.80971900 | 1.38274300 |
| H | -1.91144800 | -0.09784900 | -1.59093100 |
| H | -1.56360900 | 1.24410800 | 1.00321500 |
| O | -0.17642500 | 3.67225700 | -0.09669800 |
| H | -0.94307400 | 3.88667300 | -0.66739700 |
| H | -2.71638400 | 2.85410200 | 1.53766300 |
| O | -1.84201000 | 2.87688500 | 2.00778400 |
| H | -2.01592900 | 3.04907700 | 2.93536700 |
| H | -0.58720500 | 3.56407600 | 0.78010800 |
| H | -3.16458800 | 3.55446800 | -0.78585100 |
| O | -2.60498900 | 4.14787800 | -1.34584500 |
| H | -2.84103400 | 3.95647400 | -2.25618800 |
| H | 0.14001900 | 2.15750200 | -2.07492900 |
| H | 0.45985800 | 1.48757200 | -2.26376300 |
| Pd | 0.65151600 | 1.25099700 | -0.18765600 |
| H | 1.75224900 | 0.45170000 | 1.97412700 |

56

RS_delta_ID2_TS3-square_P, E(SCF) = -
 2485.36301199, E(ZPE) = -2484.944417, E(G)
 = -2485.013589 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.04364000 | -0.65957800 | 1.58681500 |
| H | -0.19648000 | -0.02612800 | 2.44509000 |
| H | 0.198548700 | -1.67815400 | 1.96106900 |
| C | -1.11319700 | -0.62913800 | 0.61649000 |
| H | -2.02645600 | -0.96062300 | 1.12221500 |
| H | -0.94582600 | -1.29795400 | -0.23368000 |
| N | -1.27523800 | 0.74342700 | 0.08098300 |
| N | 1.27235400 | -0.12481600 | 0.97714600 |
| C | -2.38803800 | 0.85851100 | -0.89655800 |
| H | -2.39300500 | 1.89243400 | -1.24361700 |
| C | 2.11850800 | -1.09514100 | 0.26371800 |
| H | 1.55834800 | -1.44246600 | -0.61362700 |

| | | | |
|----|-------------|-------------|-------------|
| C | -3.71634500 | 0.44407900 | -0.33513700 |
| C | -4.43953200 | 1.27172800 | 0.52810200 |
| C | -4.22514100 | -0.82144400 | -0.61587800 |
| C | -5.61396400 | 0.81551400 | 1.11825600 |
| C | -5.39735500 | -1.26663600 | -0.03937400 |
| H | -3.68266000 | -1.47756300 | -1.28944400 |
| C | -6.09072200 | -0.44875100 | 0.84232800 |
| H | -6.14624000 | 1.48104300 | 1.78781700 |
| H | -7.00970600 | -0.79804300 | 1.30069900 |
| C | 3.43577100 | -0.48845300 | -0.12541500 |
| C | 3.54568100 | 0.73025900 | -0.84948400 |
| C | 4.59125300 | -1.17911000 | 0.22648100 |
| C | 4.85099200 | 1.15909300 | -1.19015000 |
| C | 5.85105200 | -0.73494400 | -0.12246200 |
| H | 4.50293900 | -2.10345100 | 0.78902600 |
| C | 5.97453000 | 0.45095800 | -0.83983400 |
| H | 4.93464700 | 2.08536400 | -1.74915800 |
| H | 6.95749500 | 0.81628800 | -1.12177900 |
| O | -4.02338600 | 2.52075900 | 0.87112900 |
| O | 2.55602900 | 1.48737400 | -1.24584400 |
| S | -6.03821600 | -2.91218000 | -0.39411900 |
| S | 7.32200300 | -1.62794100 | 0.37011900 |
| O | 8.05042100 | -0.73383900 | 1.31841400 |
| O | 6.84904200 | -2.88686800 | 1.01215600 |
| O | 8.09858800 | -1.87061000 | -0.88080300 |
| O | -6.04022200 | -3.62457200 | 0.91371100 |
| O | -7.40994300 | -2.69623100 | -0.93123100 |
| O | -5.10542300 | -3.50855700 | -1.38719800 |
| H | 2.29995100 | -1.97510500 | 0.89396100 |
| H | -2.12977800 | 0.23299600 | -1.75425200 |
| H | -1.45969000 | 1.36714400 | 0.87562600 |
| O | -0.48884000 | 4.21457200 | 0.34118600 |
| H | -2.02692600 | 4.36658300 | -0.53384700 |
| H | -2.64571700 | 2.68874500 | 2.17600200 |
| O | -1.68921700 | 2.64260600 | 2.34918000 |
| H | -1.57559000 | 2.54371100 | 3.29773800 |
| H | -0.76205900 | 3.77860100 | 1.16911000 |
| H | -3.65943200 | 3.04433000 | 0.11430900 |
| O | -2.95828900 | 4.28061100 | -0.83625000 |
| H | -2.94071000 | 4.29250800 | -1.79600900 |
| H | 0.00352300 | 3.52368200 | -0.13606400 |
| H | 0.11978400 | 2.12636200 | -1.77584300 |
| Pd | 0.63907900 | 1.22747800 | -0.60007000 |
| H | 1.83720000 | 0.32373800 | 1.69198700 |

56
RS_delta_ID2_TS3-square, E(SCF) = -
2485.32700607, E(ZPE) = -2484.912772, E(G)
= -2484.979801 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.10214600 | -0.63605800 | 1.89055000 |
| H | -0.16054800 | 0.01888200 | 2.72495000 |
| H | 0.32017600 | -1.62734700 | 2.29796500 |
| C | -1.03475600 | -0.69078700 | 0.90612300 |
| H | -1.94854800 | -1.04814300 | 1.38950900 |
| H | -0.81105900 | -1.37233000 | 0.07939900 |
| N | -1.23787300 | 0.65690500 | 0.32906200 |
| N | 1.30815800 | -0.06059400 | 1.24840400 |
| C | -2.26007700 | 0.66833000 | -0.75683100 |
| H | -2.26195500 | 1.67700500 | -1.17301000 |
| C | 2.18601800 | -1.01959700 | 0.55286600 |
| H | 1.62072700 | -1.43075200 | -0.29169100 |
| C | -3.63102700 | 0.28956900 | -0.29964400 |
| C | -4.44068600 | 1.26509800 | 0.34468400 |
| C | -4.11726500 | -0.99266300 | -0.52110400 |
| C | -5.73576200 | 0.85506800 | 0.74410400 |
| C | -5.38775800 | -1.35889800 | -0.11829600 |
| H | -3.49337100 | -1.72486200 | -1.02654400 |
| C | -6.19626700 | -0.42140100 | 0.52109200 |
| H | -6.36566800 | 1.59104800 | 1.23392100 |
| H | -7.19617600 | -0.70219400 | 0.83931300 |
| C | 3.47708100 | -0.39133100 | 0.11086000 |
| C | 3.57198700 | 0.90765200 | -0.44753600 |
| C | 4.62936300 | -1.16458100 | 0.23208300 |
| C | 4.85048500 | 1.34342900 | -0.86439000 |
| C | 5.86233000 | -0.71608700 | -0.19162900 |
| H | 4.55941100 | -2.15707500 | 0.66734600 |
| C | 5.96883500 | 0.55701900 | -0.74329800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 4.91666800 | 2.33794700 | -1.29228200 |
| H | 6.93284700 | 0.92656900 | -1.07882900 |
| O | -4.03343000 | 2.47983900 | 0.55108100 |
| O | 2.58821200 | 1.76177700 | -0.61197400 |
| S | -6.01854600 | -3.00884800 | -0.40657100 |
| S | 7.33104400 | -1.72660300 | -0.01304900 |
| O | 8.21948900 | -0.99746200 | 0.93837400 |
| O | 6.86788400 | -3.03942200 | 0.51684400 |
| O | 7.92751700 | -1.82615700 | -1.37637400 |
| O | -6.32614000 | -3.57530700 | 0.93993700 |
| O | -7.24706800 | -2.84567900 | -1.23891500 |
| O | -4.93571800 | -3.75068400 | -1.11285500 |
| H | 2.40655400 | -1.85565500 | 1.22604000 |
| H | -1.89823300 | -0.01272900 | -1.53193700 |
| H | -1.53356200 | 1.30701700 | 1.07002200 |
| O | -0.72567700 | 4.10115200 | -0.40208800 |
| H | -1.59853800 | 4.23201700 | -0.86124800 |
| H | -2.76802800 | 2.91478100 | 1.49703200 |
| O | -1.85158300 | 3.09281300 | 1.84643100 |
| H | -1.93233800 | 3.40309200 | 2.75079700 |
| H | -0.98471600 | 3.87206500 | 0.52328500 |
| H | -3.64232000 | 3.56628400 | -0.68613300 |
| O | 3.24259800 | 4.24885300 | -1.28427300 |
| H | -3.50269600 | 4.01268000 | -2.17758200 |
| H | -0.14723100 | 3.00767500 | -0.88911000 |
| H | 0.19233200 | 2.29370700 | -1.45018400 |
| Pd | 0.67278000 | 1.29946100 | -0.18279900 |
| H | 1.86145200 | 0.42390100 | 1.95208300 |

54
RS_delta_SR_lambda_ID2_TS1_N-trigo-
square_Htr_TS, E(SCF) = -2484.16320653,
E(ZPE) = -2483.767317, E(G) = -2483.834773
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.36031100 | -2.44914100 | 0.56680600 |
| H | -0.04776600 | -2.37066300 | 1.57652100 |
| H | 0.87375400 | -3.40932400 | 0.48400800 |
| C | -0.76132500 | -2.33430000 | -0.43679600 |
| H | -1.54313600 | -3.07145900 | -0.22502400 |
| H | -0.40822900 | -2.50044400 | -1.45812600 |
| N | -1.29599900 | -0.96006500 | -0.34982900 |
| N | 1.32839900 | -1.32883800 | 0.39740500 |
| C | -2.46169600 | -0.68541800 | -1.23532800 |
| H | -2.09280900 | -0.14791600 | -2.11259800 |
| C | 2.55233000 | -1.64618600 | -0.37315400 |
| H | 2.24075800 | -1.83868400 | -1.40605400 |
| C | -3.56833100 | 0.05760900 | -0.54164600 |
| C | -3.37000500 | 1.32564500 | 0.05741600 |
| C | -4.82602100 | -0.53317500 | -0.48209500 |
| C | -4.46640100 | 1.92810600 | 0.70052200 |
| C | -5.88973500 | 0.08592500 | 0.14592800 |
| H | -4.98239400 | -1.50865700 | -0.93282800 |
| C | -5.70384500 | 1.32596900 | 0.74429600 |
| H | -4.30371700 | 2.89580900 | 1.16373700 |
| H | -6.53281100 | 1.81514500 | 1.24651400 |
| C | 3.57557900 | -0.55168100 | -0.27181500 |
| C | 3.27356000 | 0.81660200 | -0.47063300 |
| C | 4.88785900 | -0.91983300 | 0.01512000 |
| C | 4.33302500 | 1.74314500 | -0.39712700 |
| C | 5.90687000 | 0.00683200 | 0.08503900 |
| H | 5.12235300 | -1.96588100 | 0.18631300 |
| C | 5.62147600 | 1.35158600 | -0.12591100 |
| H | 4.09136000 | 2.78874300 | -0.55445800 |
| H | 6.41440400 | 2.09083200 | -0.06955700 |
| O | -2.19874700 | 1.92902300 | 0.08559900 |
| O | 2.07562200 | 1.30141800 | -0.72669700 |
| S | -7.49647500 | -0.70537500 | 0.23974600 |
| S | 7.59047600 | -0.48252400 | 0.46039800 |
| O | 7.55911200 | -1.95930000 | 0.64970300 |
| O | 8.40790100 | -0.06264300 | -0.71417500 |
| O | 7.96219700 | 0.25763800 | 1.70034300 |
| O | -7.75270100 | -0.93737800 | 1.69092600 |
| O | -8.46441800 | 0.25879500 | -0.35776800 |
| O | -7.37918600 | -1.97004800 | -0.53817900 |
| H | 2.98390100 | -2.57476500 | 0.01484300 |
| H | -2.85111300 | -1.64432500 | -1.58957600 |
| H | -1.56315000 | -0.77085000 | 0.62619600 |

| | | | |
|----|-------------|-------------|-------------|
| O | -0.60088400 | 1.63801200 | -1.69942800 |
| H | -1.38505400 | 1.84444500 | -0.96029900 |
| H | -1.61709000 | 1.03548100 | 1.72358100 |
| O | -1.44013800 | 0.26944600 | 2.29954700 |
| H | -2.17111500 | 0.25070000 | 2.92309300 |
| H | -0.05102000 | 2.41778200 | -1.83486100 |
| H | -0.46756200 | 2.84215700 | 0.79129700 |
| O | 0.42256100 | 3.17937100 | 0.96544400 |
| H | 1.01924600 | 2.58349600 | 0.48486100 |
| Pd | 0.40027900 | 0.19354600 | -0.60125200 |
| H | 1.61506000 | -1.00080000 | 1.31839800 |

54

RS_delta_SR_lambda_ID2_TS1_N-trigo-
square_P_Htr_P, E(SCF) = -2484.16559814,
E(ZPE) = -2483.766813, E(G) = -2483.835516
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.26010600 | -2.16812200 | 0.86218000 |
| H | -0.14767900 | -1.97618600 | 1.85716800 |
| H | 0.69895100 | -3.16907400 | 0.86448700 |
| C | -0.84242500 | -2.05891700 | -0.16109400 |
| H | -1.66208400 | -2.74546800 | 0.07722200 |
| H | -0.47788100 | -2.30285200 | -1.16244000 |
| N | -1.32086600 | -0.65899300 | -0.17735200 |
| N | 1.30249500 | -1.13995200 | 0.61024400 |
| C | -2.39375200 | -0.39419300 | -1.17950400 |
| H | -1.98131400 | 0.27673500 | -1.93716800 |
| C | 2.44817500 | -1.57362800 | -0.21795100 |
| H | 2.06664400 | -1.76067400 | -1.22824900 |
| C | -3.63184500 | 0.17769700 | -0.55949100 |
| C | -3.64747300 | 1.44286800 | 0.04611400 |
| C | -4.80574400 | -0.56973900 | -0.56742500 |
| C | -4.82136600 | 1.90725300 | 0.64022600 |
| C | -5.96684000 | -0.09539900 | 0.00931300 |
| H | -4.81149300 | -1.54935800 | -1.03430100 |
| C | -5.97262700 | 1.14975600 | 0.62269600 |
| H | -4.80366900 | 2.88551200 | 1.10716000 |
| H | -6.88040300 | 1.52701000 | 1.08179400 |
| C | 3.55949900 | -0.56275300 | -0.20961000 |
| C | 3.35565700 | 0.82358800 | -0.41010500 |
| C | 4.85599700 | -1.03395400 | -0.02023300 |
| C | 4.49042700 | 1.66011700 | -0.42314800 |
| C | 5.95124600 | -0.19515000 | -0.04395800 |
| H | 5.01648500 | -2.09491900 | 0.14482600 |
| C | 5.76069600 | 1.16778500 | -0.24545300 |
| H | 4.32338600 | 2.72103600 | -0.57843600 |
| H | 6.61267200 | 1.84019300 | -0.26276700 |
| O | -2.56414400 | 2.23742900 | 0.15393100 |
| O | 2.18867800 | 1.40480100 | -0.59599500 |
| S | -7.47121100 | -1.08111300 | 0.00594500 |
| S | 7.60856800 | -0.82583400 | 0.22123200 |
| O | 7.47826100 | -2.30704400 | 0.30756900 |
| O | 8.40794900 | -0.37846600 | -0.95530400 |
| O | 8.08293500 | -0.20944300 | 1.49427000 |
| O | -7.76225000 | -1.37109500 | 1.43817800 |
| O | -8.51109100 | -0.22185400 | -0.62574700 |
| O | -7.15858600 | -2.30135000 | -0.78594300 |
| H | 2.83016200 | -2.52610400 | 0.16612200 |
| H | -2.64160700 | -1.33655400 | -1.67300000 |
| H | -1.65638000 | -0.41443900 | 0.76466300 |
| O | -0.54845600 | 1.88033600 | -1.41205300 |
| H | -1.82813700 | 2.09257000 | -0.52794500 |
| H | -1.83006200 | 1.46778000 | 1.88227200 |
| O | -1.61128100 | 0.68446600 | 2.41176800 |
| H | -2.30355600 | 0.63192300 | 3.07627300 |
| H | 0.05333700 | 2.60508200 | -1.60733000 |
| H | 0.19626600 | 3.26911100 | 0.70542500 |
| O | 1.10282100 | 3.52738800 | 0.90072500 |
| H | 1.62781400 | 2.86101200 | 0.41954200 |
| Pd | 0.42227400 | 0.43469400 | -0.38720900 |
| H | 1.66769800 | -0.81905900 | 1.50469900 |

54

RS_delta_SR_lambda_ID2_TS1_N-trigo-
square_P, E(SCF) = -2484.16371030, E(ZPE) =
-2483.764598, E(G) = -2483.832945 a.u.

| | | | |
|---|-------------|------------|------------|
| C | -0.35119500 | 2.44946800 | 0.53521200 |
|---|-------------|------------|------------|

| | | | |
|----|-------------|--------------|-------------|
| H | 0.06156000 | 2.38104200 | 1.54360800 |
| H | -0.86880700 | 3.40660200 | 0.44606800 |
| C | 0.76475600 | 2.32638600 | -0.47335500 |
| H | 1.55047500 | 3.06138600 | -0.26874100 |
| H | 0.40768700 | 2.48831400 | -1.49392800 |
| N | 1.29234100 | 0.95045300 | -0.37823700 |
| N | -1.31817800 | 1.32478600 | 0.38017700 |
| C | 2.46927700 | 0.66611700 | -1.24701700 |
| H | 2.11380400 | 0.10674400 | -2.11661300 |
| C | -2.55246200 | 1.64120200 | -0.37525200 |
| H | -2.25266700 | 1.83660500 | -1.41108900 |
| C | 3.57416000 | -0.05275700 | -0.52809100 |
| C | 3.35873800 | -1.31034700 | 0.09578600 |
| C | 4.83215300 | 0.53491000 | -0.47670900 |
| C | 4.45683800 | -1.90590100 | 0.73062200 |
| C | 5.89202300 | -0.07889700 | 0.16494700 |
| H | 4.99480700 | 1.50030000 | -0.94697800 |
| C | 5.69677000 | -1.30836300 | 0.78376500 |
| H | 4.29096700 | -2.86426500 | 0.23254400 |
| H | 6.52297900 | -1.79259800 | 1.29578600 |
| C | -3.57617700 | 0.54842400 | -0.26516400 |
| C | -3.27777300 | -0.82007600 | -0.46527900 |
| C | -4.88664400 | 0.91935400 | 0.02656500 |
| C | -4.33801700 | -1.74511800 | -0.38667200 |
| C | -5.90685900 | -0.00552300 | 0.10052000 |
| H | -5.11875800 | 1.96592600 | 0.19772400 |
| C | -5.62466500 | -1.35091100 | -0.11088100 |
| H | -4.09891000 | -2.79113100 | -0.54468000 |
| H | -6.41872300 | -2.08867400 | -0.05123900 |
| O | 2.18450800 | -1.88670900 | 0.12029300 |
| O | -2.08147800 | -1.30619800 | -0.72601300 |
| S | 7.50258400 | 0.70164200 | 0.24619600 |
| S | -7.58866600 | 0.48732000 | 0.47970700 |
| O | -7.55410800 | 1.96432700 | 0.66627200 |
| O | -8.40952000 | 0.06670500 | -0.69214900 |
| O | -7.95822100 | -0.25011800 | 1.72185400 |
| O | 7.76674300 | 0.95094500 | 1.69369200 |
| O | 8.46546000 | -0.27464700 | -0.34137300 |
| O | 7.39341900 | 1.95835600 | -0.54672000 |
| H | -2.97830800 | 2.56902000 | 0.02055600 |
| H | 2.85152200 | 1.62052100 | -1.62119200 |
| H | 1.54808000 | 0.76701600 | 0.60180900 |
| O | 0.54082000 | -1.707710800 | -1.77075300 |
| H | 1.28860000 | -1.90271000 | -1.11140300 |
| H | 1.60981100 | -0.99885900 | 1.71459800 |
| O | 1.41368700 | -0.24150000 | 2.29904600 |
| H | 2.14473000 | -0.20921300 | 2.92178500 |
| H | -0.02653600 | -2.44945800 | -1.87991200 |
| H | 0.55559800 | -2.81941700 | 0.79877200 |
| O | -0.32642500 | -3.18343900 | 0.97198400 |
| H | -0.94429500 | -2.58364300 | 0.52709400 |
| Pd | -0.40756900 | -0.19919100 | -0.62458400 |
| H | -1.59192500 | 0.99649900 | 1.30522000 |

54

RS_delta_SR_lambda_ID2_TS1_N-trigo-
square_R, E(SCF) = -2484.18574380, E(ZPE) =
-2483.787515, E(G) = -2483.856981 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.72379000 | 3.07536300 | 0.66461800 |
| H | -0.36399400 | 3.16952600 | 1.69155000 |
| H | -1.39495800 | 3.91345600 | 0.45977500 |
| C | 0.44795200 | 3.06069900 | -0.28066000 |
| H | 1.05190000 | 3.96687900 | -0.17264000 |
| H | 0.11682500 | 3.00334600 | -1.32161700 |
| N | 1.25574000 | 1.85563700 | -0.00118700 |
| N | -1.45900200 | 1.78521300 | 0.58248900 |
| C | 2.28259600 | 1.59355800 | -1.02219000 |
| H | 1.75093700 | 1.42600600 | -1.96659000 |
| C | -2.53681900 | 1.70951000 | -0.42429800 |
| H | -2.06736600 | 1.74937600 | -1.41368200 |
| C | 3.15575600 | 0.43148900 | -0.66794100 |
| C | 2.61400400 | -0.83531600 | -0.36646000 |
| C | 4.53603000 | 0.59620300 | -0.68139000 |
| C | 3.50522100 | -1.89413700 | -0.11488100 |
| C | 5.39303400 | -0.45709600 | -0.43016600 |
| H | 4.95465800 | 1.57254200 | -0.90397000 |
| C | 4.86883900 | -1.71241400 | -0.14628600 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.08154200 | -2.86711200 | 0.11571600 |
| H | 5.53384900 | -2.54632100 | 0.05470500 |
| C | -3.37749000 | 0.47785500 | -0.24342900 |
| C | -2.83879900 | -0.80584700 | 0.01852700 |
| C | -4.75678500 | 0.62285100 | -0.36404800 |
| C | -3.74380900 | -1.88316900 | 0.12926100 |
| C | -5.61840500 | -0.44906100 | -0.25782700 |
| H | -5.17226700 | 1.60760600 | -0.55458900 |
| C | -5.10062900 | -1.71461500 | -0.00337600 |
| H | -3.32723000 | -2.86547200 | 0.32801000 |
| H | -5.76589100 | -2.56724800 | 0.08836500 |
| O | 1.31800800 | -1.09782000 | -0.30807100 |
| O | -1.56245300 | -1.08351700 | 0.17204400 |
| S | 7.17294900 | -0.23262800 | -0.44383000 |
| S | -7.39343200 | 0.22433700 | -0.36254500 |
| O | -7.60385500 | 1.17348300 | -0.83776300 |
| O | -7.87484100 | -1.24539900 | -1.34233900 |
| O | -7.92346900 | -0.46054900 | 1.00626800 |
| O | 7.63560300 | -0.57311000 | 0.93238500 |
| O | 7.69423800 | -1.18302600 | -1.46746600 |
| O | 7.40695700 | 1.19406200 | -0.80010000 |
| H | -3.17463100 | 2.59556400 | -0.33282000 |
| H | 2.89989400 | 2.49000700 | -1.15125600 |
| H | 1.68356200 | 1.90328100 | 0.93738300 |
| O | -0.15442900 | -3.47303300 | -0.00067800 |
| H | 0.58031000 | -2.89800100 | -0.26511500 |
| H | 1.69979600 | 0.34963600 | 2.75244800 |
| O | 1.91106500 | 1.30455500 | 2.74223000 |
| H | 2.75125600 | 1.38833300 | 3.19895300 |
| H | -0.84539000 | -2.80063000 | 0.13641300 |
| H | 1.20059200 | -1.52909400 | 1.57737400 |
| O | 1.27767200 | -1.44847100 | 2.54567600 |
| H | 0.41734900 | -1.71858200 | 2.87963200 |
| Pd | -0.09629400 | 0.32924300 | 0.11525800 |
| H | -1.86808200 | 1.58460600 | 1.49333700 |

54

RS_delta_SR_lambda_ID2_TS1_N-trigo-square,
E(SCF) = -2484.15312830, E(ZPE) = -
2483.754438, E(G) = -2483.822641 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.59848000 | 2.77884000 | 0.88378700 |
| H | -0.24311400 | 2.75260900 | 1.91599900 |
| H | -1.20976000 | 3.67556600 | 0.76073300 |
| C | 0.57758400 | 2.77865400 | -0.05903800 |
| H | 1.25782900 | 3.60761200 | 0.16126200 |
| H | 0.25537600 | 2.87285600 | -1.09996300 |
| N | 1.26721500 | 1.48029800 | 0.08381700 |
| N | -1.42552600 | 1.55848600 | 0.67276000 |
| C | 2.40083900 | 1.28359200 | -0.84363900 |
| H | 1.96823400 | 1.00514800 | -1.81176500 |
| C | -2.58955700 | 1.71916600 | -0.22712900 |
| H | -2.19671800 | 1.92393700 | -1.22901700 |
| C | 3.40189900 | 0.27695000 | -0.35770400 |
| C | 3.01941800 | -0.99573800 | 0.13682300 |
| C | 4.75052400 | 0.60854700 | -0.42990200 |
| C | 4.04893000 | -1.86870900 | 0.54858000 |
| C | 5.73716100 | -0.27363400 | -0.03419600 |
| H | 5.04276000 | 1.58522500 | -0.80358300 |
| C | 5.37737800 | -1.52272600 | 0.46006000 |
| H | 3.75391900 | -2.83888800 | 0.93531700 |
| H | 6.14490100 | -2.21984300 | 0.78238900 |
| C | -3.49679400 | 0.52345600 | -0.19617600 |
| C | -3.03330100 | -0.80971000 | -0.27616900 |
| C | -4.86670600 | 0.75813900 | -0.10985700 |
| C | -3.99001300 | -1.84392600 | -0.26716000 |
| C | -5.78555800 | -0.27028000 | -0.11752300 |
| H | -5.22810600 | 1.77933800 | -0.04121400 |
| C | -5.33720800 | -1.58466400 | -0.19277500 |
| H | -3.62228200 | -2.86306400 | -0.32375600 |
| H | -6.04958600 | -2.40349600 | -0.19099000 |
| O | 1.76743200 | -1.36927800 | 0.24819000 |
| O | -1.76838500 | -1.16972300 | -0.36468600 |
| S | 7.47284900 | 0.15307400 | -0.16328700 |
| S | -7.54455000 | 0.05667500 | 0.00592600 |
| O | -7.69068600 | 1.53822100 | -0.02579400 |
| O | -8.16555200 | -0.61688800 | -1.17006600 |
| O | -7.98333800 | -0.54386100 | 1.29885800 |

| | | | |
|----|-------------|-------------|-------------|
| O | 8.04268400 | -0.01650100 | 1.20468000 |
| O | 8.05859300 | -0.81009000 | -1.14074600 |
| O | 7.51962300 | 1.56331100 | -0.64080000 |
| H | -3.15677900 | 2.60209300 | 0.08735100 |
| H | 2.90455200 | 2.24675400 | -0.98392700 |
| H | 1.57971700 | 1.34726700 | 1.05552400 |
| O | 0.50694500 | -1.20762100 | -2.07135100 |
| H | 1.08785700 | -1.63678900 | -1.41051300 |
| H | 1.44571700 | -0.63316900 | 1.97899600 |
| O | 1.39030500 | 0.06841000 | 2.65603400 |
| H | 2.07953600 | -0.13688700 | 3.29281200 |
| H | -0.28372100 | -1.75830600 | -2.12416800 |
| H | 0.60261700 | -2.71375200 | 0.78899900 |
| O | -0.23114600 | -3.19185500 | 0.94232200 |
| H | -0.90065700 | -2.61250000 | 0.54297500 |
| Pd | -0.22786200 | 0.11443800 | -0.16602200 |
| H | -1.76375600 | 1.22591800 | 1.57427700 |

45

RS_EI_P, E(SCF) = -2254.86057616, E(ZPE) =
-2254.536696, E(G) = -2254.594519 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.35778700 | 1.68754500 | 0.66166600 |
| N | 1.37298700 | 1.77712600 | 0.13124500 |
| C | -2.42575100 | 1.57883500 | -0.35470500 |
| H | -3.07330800 | 2.46037400 | -0.29080200 |
| C | 2.43348400 | 1.48978400 | -0.85612000 |
| H | 3.06254100 | 2.37801700 | -0.98211700 |
| C | -3.25327200 | 0.34381300 | -0.15215900 |
| C | -2.68548600 | -0.93706300 | 0.07249100 |
| C | -4.63727700 | 0.47667500 | -0.21273400 |
| C | -3.57766300 | -2.02629100 | 0.20370400 |
| C | -5.48282400 | -0.60580100 | -0.08250800 |
| H | -5.07058200 | 1.45912600 | -0.37367100 |
| C | -4.93976800 | -1.86947500 | 0.12955800 |
| H | -3.14089000 | -3.00525000 | 0.37044000 |
| H | -5.59240000 | -2.73038700 | 0.23692400 |
| C | 3.27319100 | 0.32173400 | -0.45289500 |
| C | 2.68549500 | -0.94567000 | -0.21985800 |
| C | 4.65192300 | 0.47069800 | -0.37203100 |
| C | 3.55345000 | -2.02303400 | 0.05692000 |
| C | 5.47814600 | -0.60026800 | -0.09115900 |
| H | 5.09545700 | 1.44628900 | -0.54542500 |
| C | 4.91744700 | -1.85635100 | 0.11740500 |
| H | 3.10559800 | -2.99676400 | 0.22455100 |
| H | 5.55856300 | -2.70515600 | 0.33502400 |
| O | -1.40757600 | -1.20406100 | 0.16267100 |
| O | 1.39878700 | -1.18442800 | -0.27539900 |
| S | -7.26218800 | -0.40797000 | -0.12235500 |
| S | 7.25572700 | -0.40314300 | 0.01626300 |
| O | 7.83319800 | -1.33081800 | -0.99930700 |
| O | 7.62932900 | -0.78925000 | 1.40812800 |
| O | 7.53309100 | 1.02981200 | -0.28171300 |
| O | -7.51455500 | 1.01986400 | -0.46465400 |
| O | -7.74627000 | -0.77023800 | 1.24220100 |
| O | -7.75816800 | -1.35334500 | -1.16420900 |
| H | -1.77724600 | 1.51197900 | 1.57260000 |
| H | -1.94436500 | 1.60019000 | -1.33910400 |
| H | 1.92067300 | 1.30873100 | -1.80790100 |
| Pd | 0.02534900 | 0.22736600 | 0.22092200 |
| C | 0.55074900 | 2.95995300 | -0.20996700 |
| C | -0.64329200 | 2.99015000 | 0.70834300 |
| H | -0.31307700 | 3.13914600 | 1.73876300 |
| H | -1.31993800 | 3.80979200 | 0.45202100 |
| H | 1.13705200 | 3.87993400 | -0.12659600 |
| H | 0.24486800 | 2.85176900 | -1.25388900 |
| H | 1.80396800 | 1.91204200 | 1.04641700 |

45

RS_EI_TS, E(SCF) = -2254.85349501, E(ZPE) =
-2254.529759, E(G) = -2254.585579 a.u.

| | | | |
|---|-------------|------------|-------------|
| N | -1.34185300 | 1.94704000 | 0.48823300 |
| N | 1.34233600 | 1.94765200 | 0.48758300 |
| C | -2.67004600 | 1.97653700 | -0.16846500 |
| H | -3.33984900 | 2.63332500 | 0.39748400 |
| C | 2.67058100 | 1.97730600 | -0.16901600 |
| H | 3.34033800 | 2.63397500 | 0.39712400 |
| C | -3.26694600 | 0.61404500 | -0.29180200 |

| | | | |
|----|-------------|-------------|-------------|
| C | -2.60020300 | -0.38906800 | -1.03792300 |
| C | -4.51026300 | 0.35218700 | 0.26776700 |
| C | -3.26549500 | -1.61997200 | -1.21291700 |
| C | -5.13304100 | -0.86928900 | 0.09313200 |
| H | -5.01292300 | 1.12325500 | 0.84326300 |
| C | -4.50460300 | -1.85423600 | -0.66188500 |
| H | -2.76272700 | -0.35246200 | -1.79416000 |
| H | -4.99057700 | -2.81424400 | -0.80821500 |
| C | 3.26737700 | 0.61478200 | -0.29248000 |
| C | 2.60065600 | -0.38797400 | -1.03908700 |
| C | 4.51036700 | 0.35246200 | 0.26757900 |
| C | 3.26563200 | -1.61902400 | -1.21409000 |
| C | 5.13281200 | -0.86920000 | 0.09298700 |
| H | 5.01299800 | 1.12324300 | 0.84348400 |
| C | 4.50442400 | -1.85378300 | -0.66253500 |
| H | 2.76287400 | -2.38434900 | -1.79569000 |
| H | 4.99015800 | -2.81392100 | -0.80881300 |
| O | -1.42422700 | -0.22092200 | -1.59086100 |
| O | 1.42489800 | -0.21924100 | -1.59237800 |
| S | -6.74136300 | -1.20356000 | 0.81047700 |
| S | 6.74068700 | -1.20417000 | 0.81102100 |
| O | 7.65273200 | -1.48454000 | -0.33607300 |
| O | 6.55810100 | -2.39596700 | 1.68974700 |
| O | 7.12041600 | 0.02148300 | 1.56776500 |
| O | -7.12107200 | 0.02241700 | 1.56670800 |
| O | -6.55959500 | -2.39517800 | 1.68961700 |
| O | -7.65295200 | -1.48394100 | -0.33698100 |
| H | -1.44732600 | 1.48415400 | 1.39054100 |
| H | -2.50644300 | 2.42963800 | -1.15254100 |
| H | 2.50707800 | 2.43054200 | -1.15304100 |
| Pd | 0.00025200 | 0.82819500 | -0.58088600 |
| C | 0.76700900 | 3.30189200 | 0.68365300 |
| C | -0.76690800 | 3.30149200 | 0.68427800 |
| H | -1.17269400 | 3.73764400 | 1.60009900 |
| H | -1.12199300 | 3.91034600 | -0.14842000 |
| H | 1.17330900 | 3.73850700 | 1.59903300 |
| H | 1.12115600 | 3.91065100 | -0.14952000 |
| H | 1.44792100 | 1.48484500 | 1.38992300 |

53
RS_lambda_D2_TS1_P_02_half-apical, E(SCF) =
-2408.89365368, E(ZPE) = -2408.504452, E(G)
= -2408.571330 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.26810000 | 2.10866100 | -0.61942000 |
| N | -1.25276800 | 1.31213600 | -1.28423200 |
| C | 2.62767600 | 1.90253300 | -1.18435300 |
| H | 2.54032200 | 1.39334000 | -2.14848800 |
| C | -2.23443000 | 0.39669000 | -1.89498100 |
| H | -1.67938700 | -0.25466900 | -2.57888900 |
| C | 3.48308000 | 1.13700100 | -0.23050500 |
| C | 3.52474000 | 1.56124700 | 1.13275100 |
| C | 4.18960900 | 0.02013600 | -0.65092200 |
| C | 4.31065100 | 0.77454000 | 2.01230500 |
| C | 4.94937700 | -0.72040300 | 0.23858000 |
| H | 4.13460700 | -0.29421700 | -1.68927700 |
| C | 5.00550700 | -0.33007100 | 1.57519500 |
| H | 5.59367900 | -0.91239900 | 2.27849900 |
| C | -2.96282400 | -0.38295100 | -0.85077100 |
| C | -2.23450500 | -1.21828800 | 0.02933400 |
| C | -4.34077700 | -0.31348100 | -0.75105000 |
| C | -2.95335300 | -1.98459100 | 0.95766200 |
| C | -5.03098900 | -1.07563000 | 0.17998100 |
| H | -4.88877100 | 0.34099800 | -1.42357100 |
| C | -4.33158400 | -1.92006100 | 1.02698300 |
| H | -4.87471900 | -2.51672400 | 1.75092600 |
| O | 2.84578200 | 2.57955700 | 1.54172900 |
| O | -0.92226800 | -1.33510700 | -0.02127900 |
| S | 5.88896500 | -2.14263500 | -0.30449400 |
| S | -6.82111600 | -0.95905000 | 0.24590600 |
| O | -7.24492800 | -1.79526900 | 1.40224600 |
| O | -7.31251600 | -1.48140200 | -1.06178400 |
| O | -7.12761800 | 0.48859100 | 0.42834300 |
| O | 7.32869400 | -1.76061800 | -0.19487200 |
| O | 5.46883100 | -2.40439700 | -1.71058000 |
| O | 5.53253000 | -3.25519300 | 0.62395900 |
| H | 3.04446100 | 2.90298700 | -1.36827900 |
| H | -1.69840700 | 1.87332700 | -0.54023800 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.94180800 | 0.98412400 | -2.49022300 |
| Pd | 0.20664800 | 0.33489400 | -0.24863900 |
| H | 4.34672200 | 1.07219000 | 3.05591300 |
| H | -2.39373100 | -2.63184300 | 1.62394900 |
| C | -0.55885100 | 2.20395700 | -2.23370900 |
| C | 0.41546700 | 3.01782700 | -1.42676900 |
| H | 1.46552400 | 2.53246100 | 0.30055700 |
| H | 1.38757000 | 2.31723600 | 2.43757000 |
| H | 1.21689200 | -0.61079600 | 0.89381600 |
| H | 1.77410800 | -0.35739800 | 0.35977100 |
| O | 0.47486600 | 2.17156200 | 2.78514500 |
| H | 0.46698700 | 1.26436000 | 3.10076200 |
| H | -2.19311600 | 3.47433800 | 1.47869500 |
| O | -1.76075800 | 2.66892500 | 1.18718500 |
| H | -0.98763900 | 2.54300800 | 1.77646600 |
| H | -0.13125100 | 3.66564000 | -0.73791400 |
| H | 1.03376100 | 3.65086500 | -2.06734000 |
| H | -0.04702500 | 1.57958000 | -2.97170800 |
| H | -1.28116400 | 2.83591000 | -2.75973300 |

53
RS_lambda_D2_TS1_P_CH_P, E(SCF) = -
2408.89295434, E(ZPE) = -2408.501205, E(G)
= -2408.569041 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.21587700 | 1.50325000 | 1.17004000 |
| N | 1.44569400 | 0.55661200 | 1.53849800 |
| C | -2.42877600 | 0.70653400 | 1.43116500 |
| H | -2.12260700 | -0.21119400 | 1.94031800 |
| C | 2.23320900 | -0.67947400 | 1.43945800 |
| H | 1.51399200 | -1.49522000 | 1.29224200 |
| C | -3.21309600 | 0.32192200 | 0.18687600 |
| C | -3.84057600 | 1.48985000 | -0.53551500 |
| C | -4.10599600 | -0.84289600 | 0.41012400 |
| C | -5.06837800 | 1.23910400 | -1.26332900 |
| C | -5.27379500 | -0.95498900 | -0.22334200 |
| H | -3.75858000 | -1.63831300 | 1.06236200 |
| C | -5.74739000 | 0.09072400 | -1.09774900 |
| H | -6.69097800 | -0.06156800 | -1.61319600 |
| C | 3.21956300 | -0.60589900 | 0.31450500 |
| C | 2.80916100 | -0.35372800 | -1.02139200 |
| C | 4.56298100 | -0.83320100 | 0.58945200 |
| C | 3.81325400 | -0.36584000 | -2.01647600 |
| C | 5.52173800 | -0.83735700 | -0.40548300 |
| H | 4.87078700 | -1.02298100 | 1.61331700 |
| C | 5.13430800 | -0.60445700 | -1.72136100 |
| H | 5.87741300 | -0.60505000 | -2.51316600 |
| O | -3.29993800 | 2.59124600 | -0.53002600 |
| O | 1.57687400 | -0.14675800 | -1.41057800 |
| S | -6.32519300 | -2.40368000 | -0.02972600 |
| S | 7.24762200 | -1.13762100 | -0.03574100 |
| O | 7.98454500 | 0.08482600 | -0.47189800 |
| O | 7.63508800 | -2.33970600 | -0.83037900 |
| O | 7.32540200 | -1.36511800 | 1.43508300 |
| O | -7.61523100 | -1.86722100 | 0.48134700 |
| O | -5.62642000 | -3.29390600 | 0.93022600 |
| O | -6.43644900 | -2.97043000 | -1.40046800 |
| H | -3.07474700 | 1.26273800 | 2.12193800 |
| H | 2.08024900 | 1.35309000 | 1.56297500 |
| H | 2.76183600 | -0.87729400 | 2.38069300 |
| Pd | 0.16755900 | 0.69108400 | -0.18942800 |
| H | -5.44966100 | 2.04376000 | -1.88118900 |
| H | 3.50077200 | -0.17751500 | -3.03830500 |
| C | 0.52299500 | 0.62465600 | 2.67920100 |
| C | -0.45696500 | 1.74283200 | 1.47226100 |
| H | -1.49061900 | 2.42023700 | 0.80648200 |
| H | -1.98489400 | 3.26397300 | -1.77889000 |
| H | -2.45465700 | -0.02621600 | -0.55014100 |
| H | -0.81751100 | 0.76291600 | -1.41816200 |
| O | -1.07851600 | 3.44871100 | -2.07318900 |
| H | -0.64484300 | 2.58725400 | -1.95663100 |
| H | -1.05216700 | 5.11347100 | 0.73927400 |
| O | -0.53846400 | 4.32772200 | 0.53936300 |
| H | -0.64107000 | 4.19170800 | -0.42146900 |
| H | 0.07359700 | 2.68851700 | 2.29462600 |
| H | -1.14480700 | 1.85990800 | 3.27102300 |
| H | 0.00995900 | -0.33996500 | 2.74626500 |
| H | 1.05467900 | 0.77767700 | 3.62479200 |

53

RS_lambda_D2_TS1_P_CH_R, E(SCF) = -
2408.89092785, E(ZPE) = -2408.501018, E(G)
= -2408.567414 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.53667800 | 2.10642400 | 0.52161700 |
| N | 1.12539500 | 1.53108400 | 0.99306500 |
| C | -2.64634500 | 1.50346200 | 1.31357100 |
| H | -2.20669700 | 1.00191400 | 2.17943500 |
| C | 2.03232500 | 0.49718100 | 1.53932200 |
| H | 1.39193100 | -0.26084700 | 2.00375900 |
| C | -3.45316000 | 0.54573100 | 0.50804600 |
| C | -4.20150000 | 1.04043600 | -0.59844800 |
| C | -3.42857300 | -0.81041300 | 0.80261200 |
| C | -4.89348700 | 0.07270000 | -1.37238200 |
| C | -4.11990000 | -1.72387100 | 0.02703700 |
| H | -2.84583600 | -1.16763100 | 1.64735700 |
| C | -4.85184900 | -1.26823100 | -1.06862500 |
| H | -5.39135500 | -1.19484900 | -1.63622900 |
| C | 2.91354100 | -0.07212600 | 0.47573000 |
| C | 2.36720400 | -0.61835000 | -0.70685100 |
| C | 4.28902900 | -0.09535100 | 0.67295700 |
| C | 3.25428100 | -1.19469200 | -1.63622900 |
| C | 5.13853600 | -0.66883200 | -0.25168000 |
| H | 4.70809200 | 0.33380300 | 1.57766400 |
| C | 4.61086800 | -1.22552200 | -1.41176100 |
| H | 5.27169500 | -1.67848500 | -2.14411300 |
| O | -4.22821700 | 2.29391000 | -0.89725300 |
| O | 1.08142800 | -0.65821900 | -0.98604600 |
| S | -4.09677500 | -3.47137800 | 0.40759400 |
| S | 6.91473900 | -0.67452000 | 0.00136900 |
| O | 7.48382000 | 0.15663400 | -1.09825700 |
| O | 7.33557500 | -2.10167300 | -0.09094000 |
| O | 7.13933000 | -0.08658000 | 1.35083000 |
| O | -5.50925600 | -3.85246800 | 0.70619900 |
| O | -3.19502800 | -3.62747400 | 1.58417700 |
| O | -3.57992400 | -4.15694800 | -0.81364800 |
| H | -3.25643600 | 2.33903000 | 1.67916500 |
| H | 1.67609500 | 2.18351800 | 0.43065900 |
| H | 2.64348900 | 0.94680700 | 2.32864300 |
| Pd | -0.23306200 | 0.70531500 | -0.29699300 |
| H | -5.46384900 | 0.42678100 | -2.22555900 |
| H | 2.83022300 | -1.61888400 | -2.53968900 |
| C | 0.37038900 | 2.29101400 | 2.01679800 |
| C | -0.71241700 | 3.05588400 | 1.30729500 |
| H | -1.94373000 | 2.61927000 | -0.26803100 |
| H | -2.99825000 | 3.03840600 | -1.90764000 |
| H | -1.61612600 | -0.14056900 | -1.07510100 |
| H | -1.22714600 | 0.20693000 | -1.70195800 |
| O | -2.17690700 | 3.57149800 | -2.00334100 |
| H | -1.78804800 | 3.34273300 | -2.85028300 |
| H | -3.95112600 | 3.86818300 | -0.00235900 |
| O | -3.57182000 | 4.73658600 | 0.24082400 |
| H | -2.94715700 | 4.88843400 | -0.47865000 |
| H | -0.27774100 | 3.77248000 | 0.60414500 |
| H | -1.33843000 | 3.61550800 | 2.00726000 |
| H | -0.04700800 | 1.56606400 | 2.72034700 |
| H | 1.04416800 | 2.94856300 | 2.57166400 |

53

RS_lambda_D2_TS1_P_CH_TS, E(SCF) = -
2408.87174525, E(ZPE) = -2408.485668, E(G)
= -2408.551500 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | -1.23082100 | 2.01542100 | 0.65094400 |
| N | 1.39386300 | 1.28013200 | 1.23627200 |
| C | -2.51138800 | 1.50847200 | 1.19074500 |
| H | -2.29955800 | 0.94230100 | 2.10165500 |
| C | 2.27715200 | 0.27386600 | 1.72915200 |
| H | 1.62294200 | -0.54246500 | 2.18928500 |
| C | -3.22505100 | 0.63877800 | 0.19287300 |
| C | -3.69090800 | 1.26367100 | -1.03682600 |
| C | -3.86397800 | -0.55454600 | 0.65124500 |
| C | -4.56681300 | 0.47736300 | -1.85496600 |
| C | -4.72497200 | -1.23298000 | -0.14712000 |
| H | -3.60659700 | -0.95057600 | 1.62881900 |
| C | -5.06677000 | -0.70924600 | -1.41919800 |
| H | -5.75126900 | -1.27108600 | -2.04801700 |

| | | | |
|----|-------------|-------------|-------------|
| C | 3.09256900 | -0.37971000 | 0.62171000 |
| C | 2.46733500 | -0.98816100 | -0.49484100 |
| C | 4.47854300 | -0.36102800 | 0.71098600 |
| C | 3.30210600 | -1.59206400 | -1.45810000 |
| C | 5.27280000 | -0.94969900 | -0.25449400 |
| H | 4.95353900 | 0.11353600 | 1.56427900 |
| C | 4.67267700 | -1.57478700 | -1.34231800 |
| H | 5.28838900 | -2.04531000 | -2.10278200 |
| O | -3.28030000 | 2.39717400 | -1.39249500 |
| O | 1.16928500 | -1.05932600 | -0.67066300 |
| S | -5.47475100 | -2.77832600 | 0.37445800 |
| S | 7.06043100 | -0.89492100 | -0.14906400 |
| O | 7.51569600 | -0.11112300 | -1.33428600 |
| O | 7.52050100 | -2.31297300 | -0.20066500 |
| O | 7.37897000 | -0.22699600 | 1.14390700 |
| O | -6.94355600 | -2.53399000 | 0.33678600 |
| O | -4.95562400 | -3.04414800 | 1.74223500 |
| O | -5.03886800 | -3.78892300 | -0.62935600 |
| H | -3.13055300 | 2.37220500 | 1.26451900 |
| H | 1.95697200 | 1.97083100 | 0.74026300 |
| H | 2.93688900 | 0.59789200 | 2.51278800 |
| Pd | -0.04274700 | 0.46535300 | -0.06828100 |
| H | -4.86193500 | 0.89322800 | -2.81205700 |
| H | 2.82324800 | -2.06976500 | -2.30631500 |
| C | 0.59586500 | 1.94755000 | 2.28364200 |
| C | -0.43067400 | 2.81987700 | 1.60575100 |
| H | -1.44699600 | 2.60797600 | -0.15404300 |
| H | -1.63833200 | 3.08187800 | -2.14651500 |
| H | -2.07281800 | 0.07799300 | -0.44880700 |
| H | -1.23698600 | -0.20411000 | -1.00562100 |
| O | -0.87276700 | 3.63648500 | -1.92065700 |
| H | -0.11804600 | 3.25447600 | -2.37528300 |
| H | -3.14107700 | 4.08545900 | -0.47008700 |
| O | -2.71026000 | 4.88631100 | -0.12818200 |
| H | -1.89242100 | 4.90781800 | -0.64181900 |
| H | 0.06828800 | 3.60227900 | 1.02693500 |
| H | -1.08278800 | 3.31232600 | 2.33210800 |
| H | 0.11418400 | 1.16397800 | 2.87592900 |
| H | 1.23353900 | 2.53079900 | 2.95575400 |

53

RS_lambda_D2_TS1_P, E(SCF) = -
2408.89092709, E(ZPE) = -2408.501039, E(G)
= -2408.567484 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.53711300 | 2.10640100 | -0.52093300 |
| N | -1.12512500 | 1.53155000 | -0.99238600 |
| C | 2.646661700 | 1.50381900 | -1.31333100 |
| H | 2.20686500 | 1.00268000 | -2.17938700 |
| C | -2.03204500 | 0.49787300 | -1.53916700 |
| H | -1.39162800 | -0.25995200 | -2.00389800 |
| C | 3.45339300 | 0.54571400 | -0.50821400 |
| C | 4.20200800 | 1.03999600 | 0.59827900 |
| C | 3.42810000 | -0.81040200 | -0.80282700 |
| C | 4.89355000 | 0.07188900 | 1.37214800 |
| C | 4.11896700 | -1.72424100 | -0.02730200 |
| H | 2.84510900 | -1.16727400 | -1.64754200 |
| C | 4.85118300 | -1.26901200 | 1.06836900 |
| H | 5.39026700 | -1.98205300 | 1.68567700 |
| C | -2.91330800 | -0.07181200 | -0.47582600 |
| C | -2.36697000 | -0.61855400 | 0.70651000 |
| C | -4.28880800 | -0.09473000 | -0.67296500 |
| C | -3.25406300 | -1.19493800 | 1.63582600 |
| C | -5.13833000 | -0.66836000 | 0.25157000 |
| H | -4.70787600 | 0.33478000 | -1.57750000 |
| C | -4.61068000 | -1.22546700 | 1.41145200 |
| H | -5.27154500 | -1.67850100 | 2.14372500 |
| O | 4.22941500 | 2.29346800 | 0.89714400 |
| O | -1.08112800 | -0.65893500 | 0.98542900 |
| S | 4.09494300 | -3.47174500 | -0.40780600 |
| S | -6.91456100 | -0.67367900 | -0.00137100 |
| O | -7.48337900 | 0.15764600 | 1.09825800 |
| O | -7.33572300 | -2.10073800 | 0.09100700 |
| O | -7.13910500 | -0.08572500 | -1.35083100 |
| O | 5.50713400 | -3.85352000 | -0.70699700 |
| O | 3.19263100 | -3.62739300 | -1.58399400 |
| O | 3.57828400 | -4.15697900 | 0.81369600 |
| H | 3.25670300 | 2.33951700 | -1.67860700 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.67586800 | 2.18365500 | -0.42963400 |
| H | -2.64314700 | 0.94786100 | -2.32832600 |
| Pd | 0.23342200 | 0.70494300 | 0.29706800 |
| H | 5.46409700 | 0.42563700 | 2.22533500 |
| H | -2.83000300 | -1.61948600 | 2.53911800 |
| C | -0.37017500 | 2.29205600 | -2.01573200 |
| C | 0.71277600 | 3.05639000 | -1.30590100 |
| H | 1.94438100 | 2.61880500 | 0.26889800 |
| H | 2.99978900 | 3.03874600 | 1.90736700 |
| H | 1.61615100 | -0.14224900 | 1.07460700 |
| H | 1.22783100 | 0.20558200 | 1.70163100 |
| O | 2.17851500 | 3.57175800 | 2.00418800 |
| H | 1.78794100 | 3.33842300 | 2.84910900 |
| H | 3.95212300 | 3.86773300 | 0.00333500 |
| O | 3.57330600 | 4.73567500 | -0.24227800 |
| H | 2.94844400 | 4.88998800 | 0.47643900 |
| H | 0.27824700 | 3.77255600 | -0.60221400 |
| H | 1.33871200 | 3.61641400 | -2.00560700 |
| H | 0.04707000 | 1.56749600 | -2.71978500 |
| H | -1.04395900 | 2.95000100 | -2.57012300 |

53
RS_lambda_D2_TS1_R, E(SCF) = -
2408.91645969, E(ZPE) = -2408.527821, E(G)
= -2408.595825 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.23388500 | 1.95493100 | 0.69103600 |
| N | -1.43456300 | 1.88241700 | -0.10669200 |
| C | 2.34670200 | 1.75684300 | -0.24996200 |
| H | 1.92338600 | 1.75753700 | -1.26200700 |
| C | -2.38509400 | 1.40037600 | -1.12986000 |
| H | -1.77685000 | 1.04735000 | -1.97089100 |
| C | 3.15085500 | 0.50713700 | -0.01504400 |
| C | 2.63535900 | -0.69917300 | 0.50736800 |
| C | 4.48938900 | 0.55624700 | -0.39913200 |
| C | 3.51025400 | -1.79800900 | 0.61703600 |
| C | 5.32225800 | -0.53675300 | -0.29383100 |
| H | 4.89444200 | 1.48240800 | -0.79580300 |
| C | 4.82518900 | -1.72659300 | 0.22460400 |
| H | 5.47194000 | -2.59261900 | 0.32080400 |
| C | -3.26901200 | 0.32002400 | -0.59522500 |
| C | -2.71500700 | -0.86800600 | -0.06658100 |
| C | -4.64894800 | 0.46245600 | -0.66893000 |
| C | -3.60172000 | -1.88654000 | 0.33225000 |
| C | -5.49892600 | -0.54752800 | -0.26163700 |
| H | -5.07261500 | 1.37944100 | -1.06655400 |
| C | -4.96552100 | -1.73245600 | 0.23387600 |
| H | -5.62763400 | -2.53203600 | 0.55174900 |
| O | 1.39810000 | -0.87714200 | 0.95372200 |
| O | -1.42330800 | -1.08374300 | 0.04513900 |
| S | 7.04848100 | -0.44009700 | -0.77443900 |
| S | -7.27977800 | -0.35891200 | -0.35494100 |
| O | -7.77930600 | -0.49701300 | 1.04385100 |
| O | -7.76257800 | -1.45965900 | -1.23786900 |
| O | -7.52190500 | 0.99466900 | -0.92734300 |
| O | 7.83071200 | -0.64991800 | 0.47775800 |
| O | 7.23980000 | 0.91575700 | -1.35886500 |
| O | 7.25555000 | -1.53692200 | -1.76220800 |
| H | 3.01525300 | 2.62378200 | -0.18980100 |
| H | -1.96024800 | 2.14891000 | 0.72692500 |
| H | -2.99268100 | 2.23970500 | -1.48581700 |
| Pd | -0.09428500 | 0.42195300 | 0.42168300 |
| H | 3.11099600 | -2.71698900 | 1.03368700 |
| H | -3.17228400 | -2.80221500 | 0.72635800 |
| C | -0.59279200 | 3.01948800 | -0.54198500 |
| C | 0.49147600 | 3.22345800 | 0.48679600 |
| H | 1.57778300 | 1.88782500 | 1.65633100 |
| H | 0.78413800 | -2.63872500 | 0.56281200 |
| H | 0.86212600 | -0.24362400 | -2.51602700 |
| H | 0.77860800 | -0.90979200 | -2.18086500 |
| O | 0.19852000 | -3.30925300 | 0.17307200 |
| H | -0.57739200 | -2.75033000 | -0.00571600 |
| H | 1.63075200 | -0.05198300 | 2.70008300 |
| O | 1.91670700 | 0.70018400 | 3.24813500 |
| H | 1.33046000 | 0.69837000 | 4.00856700 |
| H | 0.04927100 | 3.50099400 | 1.44615200 |
| H | 1.17336300 | 4.02448300 | 0.18817400 |
| H | -0.17000400 | 2.75596100 | -1.51558000 |

| | | | |
|---|-------------|------------|-------------|
| H | -1.19529700 | 3.92294300 | -0.67190600 |
|---|-------------|------------|-------------|

53
RS_lambda_D2_TS1, E(SCF) = -2408.87614687,
E(ZPE) = -2408.487192, E(G) = -2408.553185
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.17429600 | 1.66815900 | 0.75268500 |
| N | -1.45252700 | 1.86569100 | 0.01865300 |
| C | 2.54533100 | 1.72122900 | 0.22423600 |
| H | 2.47920200 | 2.02841700 | -0.82671200 |
| C | -2.54620000 | 1.73872400 | -0.96930700 |
| H | -2.06982100 | 1.74222800 | -1.95506300 |
| C | 3.36772800 | 0.46103700 | 0.35590300 |
| C | 2.92710800 | -0.75308300 | 0.95072900 |
| C | 4.66223500 | 0.55053800 | -0.14597400 |
| C | 3.85457300 | -1.82454900 | 0.97524200 |
| C | 5.54161700 | -0.51159100 | -0.09691900 |
| H | 4.99465200 | 1.48151300 | -0.59780300 |
| C | 5.12830400 | -1.71260700 | -0.47407500 |
| H | 5.80867600 | -2.55794400 | 0.51252700 |
| C | -3.35174700 | 0.50143700 | -0.74100500 |
| C | -2.73747800 | -0.76920900 | -0.77925300 |
| C | -4.71887400 | 0.59621400 | -0.51671300 |
| C | -3.54950400 | -1.90466500 | -0.61356200 |
| C | -5.49744200 | -0.53292600 | -0.35165400 |
| H | -5.19128300 | 1.57271300 | -0.47577500 |
| C | -4.90615300 | -1.78936100 | -0.40945200 |
| H | -5.51264800 | -2.68007000 | -0.28056400 |
| O | 1.72440100 | -0.92380900 | 1.41748100 |
| O | -1.44614500 | -0.94905600 | -0.99047300 |
| S | 7.20738600 | -0.36716900 | -0.73989000 |
| S | -7.26836500 | -0.40360500 | -0.08742100 |
| O | -7.55005200 | -1.16890200 | 1.15999900 |
| O | -7.90395800 | -1.01980900 | -1.28715500 |
| O | -7.55738500 | 1.05117600 | 0.04152700 |
| O | 8.11780600 | -0.49166600 | 0.43665000 |
| O | 7.28751800 | 0.96952600 | -1.39399400 |
| O | 7.37541900 | -1.49496200 | -1.70196700 |
| H | 3.06641200 | 2.53506500 | 0.74743300 |
| H | -1.84688000 | 1.81919800 | 0.96041600 |
| H | -3.18834700 | 2.62338200 | -0.90087700 |
| Pd | -0.10086600 | 0.34479100 | -0.20671800 |
| H | 3.51233100 | -2.75691900 | 1.41393500 |
| H | -3.07471600 | -2.87943600 | -0.65261200 |
| C | -0.63258200 | 3.08987200 | -0.12497500 |
| C | 0.50498300 | 2.99798500 | 0.85589400 |
| H | 1.18911800 | 1.26173800 | 1.69205900 |
| H | 0.48947800 | -2.25652600 | 1.19389600 |
| H | 1.14527600 | -0.63838100 | -1.42412900 |
| H | 1.25231100 | -1.00376100 | -0.74588200 |
| O | -0.29641100 | -2.80569000 | 1.00261600 |
| H | -0.73829900 | -2.33697000 | 0.27823700 |
| H | 0.89510100 | -0.24821600 | 2.80554300 |
| O | 0.43131200 | 0.41584300 | 3.36099700 |
| H | -0.50342300 | 0.22358000 | 3.24781200 |
| H | 0.12907000 | 3.09054500 | 1.87856000 |
| H | 1.22526900 | 3.80161800 | 0.69378600 |
| H | -0.26683700 | 3.11640000 | -1.15461800 |
| H | -1.24295400 | 3.98148100 | 0.04743100 |

53
RS_lambda_D2_TS2_R, E(SCF) = -
2408.88496167, E(ZPE) = -2408.496190, E(G)
= -2408.566190 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.80068900 | -1.55263400 | 1.02563400 |
| H | -0.52581600 | -1.30453300 | 2.05449200 |
| H | -1.65836700 | -2.23102000 | 1.06106400 |
| N | -1.16825500 | -0.28963500 | 0.34231700 |
| C | -2.10774300 | -0.47632000 | -0.81488500 |
| H | -1.70978600 | 0.08333300 | -1.66481600 |
| C | -3.48446100 | -0.00830600 | -0.49181300 |
| C | -3.67065700 | 1.39149700 | -0.30795400 |
| C | -4.54819900 | -0.88449000 | -0.39192300 |
| C | -4.98683400 | 1.83081600 | -0.05415700 |
| C | -5.83054100 | -0.41929000 | -0.12980800 |
| H | -4.37771000 | -1.94993900 | -0.53084600 |
| C | -6.04067500 | 0.94209500 | 0.03610800 |

| | | | |
|----|-------------|-------------|-------------|
| H | -7.04503500 | 1.29842600 | 0.23755600 |
| O | -2.65760600 | 2.20488800 | -0.34614500 |
| S | -7.17426400 | -1.59409100 | 0.00598600 |
| O | -7.19548600 | -2.35215500 | -1.27955100 |
| O | -6.84443800 | -2.47106800 | 1.16818000 |
| O | -8.40805200 | -0.78682700 | 0.22295700 |
| H | -2.10204500 | -1.53346900 | -1.08916400 |
| H | -1.59462000 | 0.33762800 | 1.03539000 |
| H | -2.15224500 | 2.23387400 | 1.38762200 |
| O | -1.82841600 | 1.87006700 | 2.23838600 |
| H | -2.59567800 | 1.85785900 | 2.81621500 |
| H | -2.97034400 | 3.92011300 | -0.06690200 |
| O | -3.11345700 | 4.85786300 | 0.19245900 |
| H | -3.49664600 | 4.80371200 | 1.07076100 |
| Pd | 0.59122200 | 0.63417500 | -0.24209800 |
| H | -0.65693500 | 1.97642200 | -0.60362800 |
| H | 0.08723300 | 2.28662400 | -0.71944000 |
| H | -5.15346500 | 2.89611900 | 0.07547000 |
| N | 1.45291600 | -1.14893200 | 0.28111600 |
| C | 2.58118700 | -1.47966700 | -0.61781500 |
| H | 2.17645700 | -1.47253300 | -1.63564700 |
| C | 3.71140700 | -0.51777200 | -0.44600200 |
| C | 3.50480100 | 0.87219400 | -0.59147900 |
| C | 4.98609700 | -1.00004400 | -0.17467300 |
| C | 4.62228800 | 1.72005500 | -0.46716300 |
| C | 6.06756000 | -0.14880400 | -0.06257200 |
| H | 5.14154900 | -2.06794600 | -0.05796100 |
| C | 5.87929000 | 1.22063100 | -0.21703800 |
| H | 6.72439100 | 1.89618000 | -0.12862800 |
| O | 2.34416800 | 1.42403000 | -0.87154500 |
| S | 7.71346400 | -0.77625100 | 0.27752900 |
| O | 8.14151300 | -0.12933000 | 1.55098400 |
| O | 8.55379100 | -0.35759400 | -0.88073300 |
| O | 7.57553600 | -2.25451800 | 0.39261800 |
| H | 1.81801400 | -1.02761400 | 1.228101300 |
| H | 2.92021100 | -2.49779100 | -0.39910400 |
| H | 4.45978000 | 2.78621300 | -0.58098100 |
| C | 0.36969600 | -2.16266500 | 0.30485100 |
| H | 0.11935400 | -2.39436000 | -0.73393900 |
| H | 0.72007700 | -3.08053900 | 0.78387500 |

53
RS_lambda_D2_TS2_TS, E(SCF) = -
2408.88289934, E(ZPE) = -2408.495169, E(G)
= -2408.562157 a.u.

| | | | |
|----|-------------|-------------|--------------|
| C | -0.66680800 | -1.77923000 | 1.29593100 |
| H | -0.35650900 | -1.43988200 | 2.28872800 |
| H | -1.47394700 | -2.50489700 | 1.42849400 |
| N | -1.14939800 | -0.58746100 | 0.55667500 |
| C | -2.15434200 | -0.88027200 | -0.51484900 |
| H | -1.70666100 | -0.63532400 | -1.48240700 |
| C | -3.44357700 | -0.14284200 | -0.32635800 |
| C | -3.45848400 | 1.27036500 | -0.22964200 |
| C | -4.63736200 | -0.84545000 | -0.30281900 |
| C | -4.70683100 | 1.90637300 | -0.13304000 |
| C | -5.85727400 | -0.19367100 | -0.20588800 |
| H | -4.61351500 | -1.92970500 | -0.37458200 |
| C | -5.88635500 | 1.18883800 | -0.11923900 |
| H | -6.84066200 | 1.69825900 | -0.04675400 |
| O | -2.35457500 | 1.98994100 | -0.19034400 |
| S | -7.36600900 | -1.16233200 | -0.15098800 |
| O | -7.30204100 | -2.08846200 | -1.31756000 |
| O | -7.33815400 | -1.89043100 | 1.15114200 |
| O | -8.48466300 | -0.18381000 | -0.24377700 |
| H | -2.34413700 | -1.95674600 | -0.52420400 |
| H | -1.55114900 | 0.05641900 | 1.24790700 |
| H | -1.93147300 | 2.00020100 | 1.64870100 |
| O | -1.68219100 | 1.55450200 | 2.47962100 |
| H | -2.45731900 | 1.61851600 | 3.04367900 |
| H | -2.49265700 | 3.76819700 | 0.13761400 |
| O | -2.55566200 | 4.69870600 | 0.43250000 |
| H | -3.06969000 | 4.65788000 | 1.24218900 |
| Pd | 0.52429100 | 0.35487100 | -0.24966800 |
| H | -1.01402100 | 1.62974500 | -0.61164700 |
| H | -0.20739700 | 1.72296100 | -0.97035400 |
| H | -4.72197500 | 2.98970600 | -0.060909100 |
| N | 1.52903500 | -1.32108600 | 0.42637700 |

| | | | |
|---|------------|-------------|-------------|
| C | 2.64493200 | -1.66126100 | -0.47973800 |
| H | 2.20663600 | -1.78291100 | -1.47676100 |
| C | 3.70227400 | -0.60583500 | -0.45508500 |
| C | 3.38694700 | 0.73448700 | -0.77666400 |
| C | 5.01183100 | -0.95221800 | -0.14677000 |
| C | 4.44168900 | 1.66857200 | -0.79877500 |
| C | 6.02753800 | -0.01653700 | -0.17253800 |
| H | 5.24959400 | -1.98037100 | 0.10816400 |
| C | 5.73485300 | 1.30142600 | -0.50697500 |
| H | 6.52799400 | 2.04232400 | -0.52996300 |
| O | 2.18305300 | 1.15610200 | -1.09207700 |
| S | 7.71691000 | -0.46471500 | 0.22755000 |
| O | 8.08171300 | 0.34276600 | 1.42716100 |
| O | 8.52910400 | -0.09841000 | -0.96825900 |
| O | 7.70282000 | -1.92956800 | 0.49581000 |
| H | 1.91346300 | -1.10061800 | 1.34638600 |
| H | 3.07078400 | -2.62568200 | -0.18210700 |
| H | 4.19919000 | 2.69462300 | -1.05313600 |
| C | 0.50405200 | -2.37976400 | -0.56648500 |
| H | 0.21766400 | -2.69463800 | -0.44152100 |
| H | 0.91276400 | -3.24810900 | 1.09109300 |

53
RS_lambda_D2_TS2W_P, E(SCF) = -
2408.91802109, E(ZPE) = -2408.525004, E(G)
= -2408.590066 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 2.15815500 | -1.70216300 | 1.34072100 |
| N | -0.35837900 | -0.34373100 | 1.45554700 |
| C | 3.40090200 | -1.26209500 | 0.64562900 |
| H | 4.14667200 | -1.00995800 | 1.40885700 |
| C | -1.10931800 | 0.59798300 | 0.61499800 |
| H | -0.42645200 | 0.90848900 | -0.18910700 |
| C | 3.23178400 | -0.10244300 | -0.28642800 |
| C | 2.96434400 | -0.26770400 | -1.65318100 |
| C | 3.34485700 | 1.19310200 | 0.20652600 |
| C | 2.75229100 | 0.85156000 | -2.45854400 |
| C | 3.13272400 | 2.29827300 | -0.59413600 |
| H | 3.60092300 | 1.34024200 | 1.25237200 |
| C | 2.81905700 | 2.12436100 | -1.93447800 |
| H | 2.64859500 | 2.98792900 | -2.56683600 |
| C | -2.35838100 | -0.02465300 | 0.06932800 |
| C | -2.33965600 | -1.23561000 | -0.67539900 |
| C | -3.56492200 | 0.63632000 | 0.27198900 |
| C | -3.57596800 | -1.68902800 | -1.19370200 |
| C | -4.75617400 | 0.16513100 | -0.24495600 |
| H | -3.57515900 | 1.55631900 | 0.84899900 |
| C | -4.75306000 | -1.01097300 | -0.98864000 |
| H | -5.68170200 | -1.39421100 | -1.40108500 |
| O | 2.92612800 | -1.45425400 | -2.28455300 |
| O | -1.28014900 | -1.95021300 | -0.94776300 |
| S | 3.13094900 | 3.93981500 | 0.13471900 |
| S | -6.29817000 | 1.03025400 | 0.02961600 |
| O | -7.19141000 | 0.07105000 | 0.74423400 |
| O | -6.82279500 | 1.38136300 | -1.32304000 |
| O | -5.96280800 | 2.22880600 | 0.84923900 |
| O | 3.54297400 | 4.87069800 | -0.95062500 |
| O | 4.09804700 | 3.88560800 | 1.26499600 |
| O | 1.72754700 | 4.16620400 | 0.58752200 |
| H | 3.77871000 | -2.14326300 | 0.12328500 |
| H | -0.99087700 | -0.75652100 | 2.13826800 |
| H | -1.37020500 | 1.50192800 | 1.18115700 |
| Pd | 0.43676000 | -1.88689500 | 0.16909500 |
| H | 2.53921400 | 0.69110200 | -3.50919500 |
| H | -3.56202100 | -2.60873900 | -1.76943900 |
| C | 0.80594200 | 0.23558500 | 2.13808500 |
| C | 1.77037900 | -0.86822900 | 2.51023800 |
| H | 2.37283500 | -2.64991300 | 1.67194500 |
| H | 4.21394500 | -4.44098700 | -1.75152100 |
| H | 1.06369500 | -3.00861100 | -0.72798200 |
| H | 2.99671500 | -2.22281500 | -1.68998700 |
| O | 3.41882400 | -4.12219500 | -1.31205600 |
| H | 2.68795300 | -4.57977000 | -1.74121600 |
| H | 3.86742200 | -4.71616900 | 1.93481500 |
| O | 3.05580300 | -4.45062100 | 1.49589300 |
| H | 3.25931000 | -4.46887500 | 0.54413100 |
| H | 1.28804900 | -1.53706200 | 3.22827700 |
| H | 2.66155800 | -0.45432600 | 2.99535100 |

```

H 1.26849800    0.94557200    1.44987000
H 0.51238400    0.79591900    3.03268600

53
RS_lambda_D2_TS2W_R_half-apical, E(SCF) = -
2408.88736033, E(ZPE) = -2408.497562, E(G)
= -2408.563316 a.u.
N 2.48917500   -1.65219400    1.51143300
N -0.22328000  -1.07918100    1.64668500
C 3.41555200   -0.45723800    1.56903500
H 3.28255300   0.01375100    2.54528300
C -1.14152000   0.04446200    1.35587300
H -0.51152800   0.89557300    1.06724200
C 3.18113300   0.54258500    0.48365400
C 3.67974300   0.27961400   -0.82320600
C 2.43444200   1.68584500    0.73625500
C 3.37416500   1.23394300   -1.82576000
C 2.13633200   2.58484300   -0.27015800
H 2.06899300   1.88497900    1.74038000
C 2.61088500   2.34646600   -1.55873700
H 2.37729700   3.04762500   -2.35480000
C -2.12685600  -0.33005300    0.29599300
C -1.70309200  -1.70309200   -0.94338900
C -3.48313300  -0.13769200    0.53310100
C -2.68936400  -1.15844400   -1.90297700
C -4.43058500  -0.43032100   -0.42714700
H -3.80827900  0.26000800    1.48927000
C -4.02471300  -0.94283800   -1.65447800
H -4.76351600  -1.18035700   -2.41334500
O 4.32619100   -0.80495100   -1.09441500
O -0.44677800  -1.06300500   -1.28288800
S 1.10436900   4.01283200    0.40491200
S -6.18107600  -0.20340900   -0.10521700
O -6.78066800  -1.56818200   -0.15478100
O -6.68568400  0.67654100   -1.19751400
O -6.27545600  0.42425200    1.24174300
O 1.89031700   5.20393500   -0.39500500
O 0.82062900   4.00885000    1.50433800
O -0.12401900  3.81763000   -0.78590200
H 4.43520500   -0.84749600    1.53353700
H -0.77767400  -1.93137300    1.75332900
H -1.67035200  0.31765200    2.27496700
Pd 1.00867200  -1.45447000    0.05238500
H 3.74213500   1.04379500   -2.82923800
H -2.35862400  -1.56292300   -2.85316100
C 0.61702000   -0.89745900    2.85479100
C 1.75628000   -1.87743300    2.78046500
H 3.05677600   -2.47396700    1.26835900
H 4.40281400   -2.06781600   -2.37259300
H 1.78249700   -2.20447400   -1.37325900
H 2.36252300   -1.67436100   -1.17036800
O 4.48306900   -2.96856500   -2.74909100
H 3.82323900   -3.01414000   -3.44400100
H 4.60924800   -2.27147300   -0.17896900
O 4.55224000   -3.18231500    0.18921800
H 4.39901800   -3.70044400   -0.61126800
H 1.37657400   -2.90182700    2.77168000
H 2.42683000   -1.77414200    3.63790000
H 0.97887000   0.13358400    2.84914500
H 0.01607300   -1.03399100    3.75671200

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53
RS_lambda_D2_TS2W, E(SCF) = -2408.88433222,
E(ZPE) = -2408.496466, E(G) = -2408.563325
a.u.
N 2.32374900   -1.69541400    1.60141300
N -0.34970000  -0.89623100    1.68414400
C 3.34417500   -0.59192100    1.49628900
H 3.35027100   -0.05168200    2.44582900
C -1.15438400   0.24319500    1.19826400
H -0.45053000   0.95559700    0.74702700
C 3.11906200   0.37156200    0.37353400
C 3.38166600   -0.03241000   -0.95344300
C 2.66814000   1.66034000    0.62612800
C 3.18975000   0.90099700   -1.98368300
C 2.45945000   2.55457300   -0.40706100
H 2.46726200   1.98014000    1.64465300

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```

C 2.73230400    2.17438600   -1.71595700
H 2.56943400    2.87750900   -2.52684100
C -2.20047200   -0.22534400    0.23666100
C -1.86764400   -1.00782600   -0.89439400
C -3.52743400    0.12050000    0.46628700
C -2.91555000   -1.38097000   -1.76125800
C -4.53460600   -0.25913000   -0.39779600
H -3.78206100    0.70863600    1.34237600
C -4.21873400   -1.01403200   -1.52246000
H -5.00366600   -1.32248800   -2.20603600
C 3.70551700    -1.28386500   -1.21307800
O -0.65268400   -1.39208300   -1.21744300
S 1.82684200    4.20236000   -0.08059300
S -6.24464100    0.17946400   -0.08453300
O -6.98295400   -1.11188700   -0.04323300
O -6.68343800    0.98239000   -1.26212900
O -6.24615800    0.95829500    1.18475400
O 2.91049400    5.14802600   -0.47398800
O 1.51981600    4.24057600    1.21307800
O 0.61368700    4.34192100   -0.93585000
H 4.32297200   -1.06745400    1.40174900
H -0.98425300   -1.65402500    1.93999800
H -1.63101200   0.74912300    2.04913900
Pd 0.82479200   -1.62110100    0.14080500
H 3.38666900    0.58424100   -3.00239300
H -2.65760700   -1.97801100   -2.62920200
C 0.53743600    -0.60158300   -0.02303000
C 1.59148600   -1.67603400    2.89134800
H 2.81953500   -2.58465100    1.48365200
H 4.10431800   -2.71193900   -2.36415500
H 1.67068700   -2.40412900   -1.13600500
H 2.42121800   -1.92898100   -1.08313900
O 4.25308100   -3.65942200   -2.53053800
H 3.58433000   -3.90927600   -3.17200000
H 4.34969400   -2.61943500   -0.09217200
O 4.33758300   -3.47605500    0.37598300
H 4.20700100   -4.08496400   -0.36342400
H 1.12634300   -2.65550500    3.02634000
H 2.27976600   -1.51136200    3.72522400
H 0.98642100   0.37994100    2.65575200
H -0.03821800  -0.54244700    3.75749100

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54
RS_lambda_ID1_TS2-diamond_R_noH2_Htr_W-
reor_P, E(SCF) = -2484.16963151, E(ZPE) = -
2483.769607, E(G) = -2483.837860 a.u.
C -0.02591600   -2.38122000   -0.12274200
H -0.51024800   -2.61691200   -1.07306900
H 0.38672900   -3.31008800    0.28011000
C -1.03052200   -1.77971000    0.82550000
H -1.87764200   -2.45715600    0.97706500
H -0.58342400   -1.57441800    1.80091200
N -1.49057800   -0.48676200    0.26499600
C -2.47558600    0.22837400    1.13893600
H -2.67612200   -0.40785000    2.00395400
C -3.75407700    0.50148600    0.41414600
C -3.94419600    1.64685200   -0.37529800
C -4.77936200   -0.43996800    0.49375300
C -5.17036600    1.82096900   -1.02998500
C -5.97575800   -0.26289400   -0.16740800
H -4.63539500   -1.32928400    1.10009700
C -6.17201300    0.88397000   -0.92971600
H -7.11336100    1.03689600   -1.44740400
O -3.04225800    2.61456600   -0.54025400
S -7.30202600   -1.46704800   -0.03109600
O -8.41400000   -0.76399400    0.66915000
O -6.74507500   -2.60366600    0.75202000
O -7.65338400   -1.83600100   -1.41296600
H 2.31802400    4.56588900   -0.46144100
O 1.83251700    3.92562000    0.06288400
H 2.08932600    3.03671700   -0.26578900
H 0.18721900    2.58766000    1.89807500
O 0.83069100    2.92114300    2.55133100
H 1.40322400    3.45437200    1.98125700
H -1.95020700   -0.67335500   -0.62735200
H -2.00329400   1.14079800    1.50565200
Pd 0.27741100    0.49226200   -0.19588400

```

O -0.57196700 2.28802800 0.17513800
H -0.00412100 2.99802600 -0.15818000
H -2.10642500 2.42058400 -0.22040000
H -5.30350100 2.71688000 -1.62572600
N 1.05820900 -1.40699600 -0.40642800
C 2.21972000 -1.48692700 0.50330200
H 2.54632200 -2.53036100 0.57533500
C 3.37252500 -0.64593400 0.03852100
C 3.23352200 0.67901200 -0.43436400
C 4.64642500 -1.19964500 0.13548200
C 4.40714000 1.37954800 -0.78018500
C 5.78030900 -0.49002300 -0.19999400
H 4.75663000 -2.22003000 0.48938200
C 5.65442100 0.81628800 -0.65894700
H 6.53750800 1.38604100 -0.93044100
O 2.09089800 1.32002900 -0.59007800
S 7.41340800 -1.21303600 -0.03680400
O 8.13350100 -0.36388800 0.95551500
O 8.03032400 -1.14420900 -1.39272800
O 7.20150900 -2.60891800 0.43646800
H 1.87473600 -1.18737400 1.49983700
H 4.29646600 2.39445200 -1.14824000
H 1.39144900 -1.54863900 -1.35776200

54
RS_lambda_ID2_TS1_chain_P, E(SCF) = -
2484.17026088, E(ZPE) = -2483.770278, E(G)
= -2483.839711 a.u.

C 0.05711400 0.89806000 1.63969100
H -0.21085900 0.31578000 2.52385900
H 0.29542700 1.91582900 1.95798500
C -1.08066200 0.87387300 0.65617100
H -2.00090100 1.24825600 1.11713700
H -0.86702900 1.49474700 -0.21921200
N -1.25927800 -0.51976000 0.19287300
C -2.30392000 -0.64497400 -0.85749300
H -2.19999000 -1.63723900 -1.29783300
C -3.68676500 -0.45129600 -0.32733900
C -4.26033600 -1.48743800 0.46173200
C -4.39641900 0.71016700 -0.59473800
C -5.57570000 -1.26760900 0.93834800
C -5.67892900 0.89303000 -0.10859300
H -3.94249700 1.49270700 -1.19699100
C -6.26539400 -0.10992300 0.65968300
H -6.03000100 -2.05022100 1.53827300
H -7.27294200 0.02631500 1.04222100
O -3.61322800 -2.57169600 0.75102100
S -6.60924300 2.37624100 -0.47763700
O -7.76762800 1.94800900 -1.31735800
O -5.67476900 3.28242900 -1.20438400
O -7.04752500 2.93059400 0.83730700
H -2.06707000 0.08605900 -1.63513200
H -1.53244100 -1.08185900 1.01105300
O 0.06021500 -2.61678400 -1.67966400
H -0.54305600 -3.26163400 -1.21311900
H -2.63722300 -2.28121800 2.16608900
O -1.90529700 -1.92366600 2.72008200
H -2.33158500 -1.42051900 3.41795200
H 0.85681900 -3.09147600 -1.94620800
H -2.42358700 -3.49447900 0.01758800
O -1.69337100 -4.06352900 -0.34352600
H -1.37441100 -4.58600500 0.39613900
Pd 0.64480200 -1.15588800 -0.29330900
N 1.25670000 0.25095000 1.04142400
C 2.19475200 1.14886800 0.33294400
H 1.67657900 1.52856000 -0.55465100
C 3.48528400 0.46007700 -0.00843800
C 3.55482800 -0.84521000 -0.54853600
C 4.66386200 1.17378400 0.19348500
C 4.83076500 -1.35096900 -0.88209700
C 5.89802400 0.65762600 -0.14167200
H 4.61646600 2.17075500 0.62099900
C 5.97659100 -0.62012800 -0.68660500
H 4.87514900 -2.35062100 -1.30050200
H 6.94149100 -1.03967500 -0.95360900
O 2.53300100 -1.64352200 -0.76668400
S 7.40334000 1.58343300 0.15730700

O 8.10670200 1.65641400 -1.15560400
O 8.17301500 0.79894800 1.16634200
O 6.97378100 2.91651000 0.66375000
H 2.40902700 2.00981500 0.97515400
H 1.77652900 -0.21957500 1.78073500

54
RS_lambda_ID2_TS1_chain_R, E(SCF) = -
2484.18028011, E(ZPE) = -2483.782121, E(G)
= -2483.851974 a.u.

C 0.48202000 3.24387200 0.04442600
H 0.00828100 3.63915700 0.94572000
H 1.15245100 4.01236300 -0.35009700
C -0.57374700 2.86325200 -0.96298100
H -1.19827200 3.72430700 -1.22035500
H -0.12321800 2.49177500 -1.88794100
N -1.38773600 1.77320300 -0.39035200
C -2.29789300 1.12616100 -1.35418100
H -1.66839200 0.65635800 -2.11870600
C -3.17926300 0.13394900 -0.66630000
C -2.61584500 -0.94293000 0.05417200
C -4.55933300 0.27252900 -0.73186800
C -3.49321600 -1.86081200 0.65887400
C -5.40224800 -0.63634900 -0.11944600
H -4.98935000 1.10848900 -1.27460200
C -4.85986500 -1.71387100 0.57150700
H -3.05794400 -2.69024100 -1.20577600
H -5.51474800 -2.43254000 1.05412200
O -1.31785600 -1.13652800 0.17389700
S -7.18520700 -0.46902500 -0.23024500
O -7.65542200 -1.65021200 -1.00987900
O -7.43565600 0.82366100 -0.92580200
O -7.68545400 -0.48189600 1.17420300
H -2.90847600 1.89070900 -1.84761100
H -1.93950700 2.10758200 0.41306200
O 2.14577500 -1.68326600 -2.27360500
H 1.59526800 -2.19854900 -1.65213900
H -2.36728000 1.30386700 2.59449500
O -2.87095900 0.97675300 1.22514300
H -3.71165600 1.55045100 1.92534200
H 2.71282400 -1.15447400 -1.70103000
H -0.27369000 -2.60078100 -0.32485400
O 0.59809800 -3.03642400 -0.29729500
H 1.02532400 -2.48281100 0.38121000
Pd -0.03419100 0.44120700 0.37232300
N 1.25126900 2.03793900 0.45143400
C 2.39065800 1.70866600 -0.42373900
H 1.98143300 1.48723500 -1.41691200
C 3.22726300 0.56888200 0.08927500
C 2.70864200 -0.56711800 0.75948800
C 4.59374200 0.62742800 -0.18476200
C 3.62082600 -1.58271100 1.12440100
C 5.45609000 -0.38844500 0.16570300
H 4.99620000 1.49795800 -0.69387300
C 4.95915800 -1.50599000 0.82943100
H 3.21829100 -2.44656300 1.64379000
H 5.62832200 -2.31057600 1.11721400
O 1.44631000 -0.77323400 1.06870900
S 7.20532800 -0.30262200 -0.22184800
O 7.47187200 -1.44627100 -1.14040600
O 7.91688300 -0.44390800 1.08054900
O 7.42094300 1.02321800 -0.86392000
H 3.02464000 2.59623400 -0.53018400
H 1.59741200 2.16863800 1.39986300

54
RS_lambda_ID2_TS1_chain, E(SCF) = -
2484.15295377, E(ZPE) = -2483.754004, E(G)
= -2483.820608 a.u.

C 0.78675200 3.02307500 0.47044800
H 0.50792600 3.21985800 1.50768400
H 1.42858300 3.83961200 0.13154500
C -0.45974100 2.91167000 -0.37194100
H -1.08101300 3.80815200 -0.27271600
H -0.21867600 2.78272900 -1.43103200
N -1.18941000 1.71212000 0.08115900
C -2.41819800 1.43086300 -0.67207200

H -0.95678300 -2.42750600 0.85409000
H 0.71969600 -0.64375600 2.36034100
O 0.17536600 -0.78936400 3.14912500
H -0.27065100 -1.61518800 2.90450600
H 1.79332800 2.15401200 -0.89869100
H 1.93898600 1.48516800 1.94296600
H -2.01890800 1.75178100 1.35842900
Pd 0.01995700 0.45399600 -0.15479200
H 3.05601700 -2.79427000 -0.14309900
H -3.16324500 -2.75789900 -0.61366600
O 0.35194400 -2.42208700 -1.90275100
H -0.49710500 -2.08261900 -1.57843700
H 0.95366800 -2.07008100 -1.23061500
H -1.70812100 1.78675800 -1.54630700

56

RS_lambda_ID2_TS1_H2-out, E(SCF) = -
2485.32776092, E(ZPE) = -2484.912311, E(G)
= -2484.978944 a.u.

C -0.54778500 3.24661500 -0.45808600
H -0.14603200 3.54734400 -1.42764900
H -1.20442200 4.04382300 -0.09843800
C 0.55972900 2.97202900 0.51314200
H 1.18614400 3.85475400 0.66684700
H 0.15054900 2.68158700 1.48480600
N 1.37875300 1.82722300 0.03631400
N -1.32144500 2.00077500 -0.67163500
C 2.29714500 1.40662600 1.13604900
H 2.86663600 2.29296000 1.43941200
C -2.38249400 1.71205900 0.31186700
H -3.00007300 2.60893500 0.43165700
C 3.22607700 0.29951600 0.79085800
C 2.71982500 -1.02001900 0.71626200
C 4.57668400 0.54832600 0.59197500
C 3.64551300 -2.05232700 0.44468500
C 5.45750200 -0.48036000 0.31329500
H 4.95201300 1.56542800 0.65306000
C 4.98103800 -1.78644200 0.24096400
H 5.66871100 -2.59827300 0.02379900
C -3.25451800 0.56639200 -0.11671700
C -2.77715900 -0.58402400 -0.78135800
C -4.60697800 0.64227700 0.20941800
C -3.69510400 -1.10208400 -1.07062300
C -5.48634000 -0.37863500 -0.07982200
H -4.98422900 1.52932500 0.70872200
C -5.02157900 -1.51867700 -0.72585600
H -5.70474400 -2.32781700 -0.96285100
O 1.44624900 -1.26536900 0.84589600
O -1.52617000 -0.79707800 -1.16719100
S 7.18795600 -0.15642100 -0.01453900
S -7.22268200 -0.26610000 0.35971900
O -7.97403500 -0.41730200 -0.91898300
O -7.40411400 1.07099300 0.98864200
O -7.47422000 -1.39333800 1.30219300
O 7.41676100 -0.55094000 -1.43594400
O 7.95847800 -1.00960900 0.93620200
O 7.38765000 1.30145500 0.21913800
H 0.08260700 -2.55541800 0.90285400
H 3.84154400 0.36994900 -2.72064200
H 4.16285900 0.27595200 -2.04879100
O -0.83755500 -2.85009400 0.77662100
H -1.13213400 -2.30778300 0.02710400
H 0.15333800 -0.52639500 1.98112400
O -0.69315600 -0.37463200 2.44403800
H -1.20622400 -1.13761300 2.14443300
H 1.94928900 2.12390000 -0.75699700
H 1.65276600 1.12845500 1.97449200
H -1.89616300 1.49975600 1.27060300
Pd -0.01592100 0.43165700 -0.66775500
H 3.26922300 -3.06961100 0.38947000
H -3.31356900 -2.49124500 -1.57941900
O 1.13368100 -1.30193400 -1.78688400
H 0.36740700 -1.74234000 -2.17493800
H 1.29463300 -1.74983600 -0.93400800
H -1.74117900 2.02742500 -1.59971300

54

RS_lambda_ID2_TS1_N-trigo-square_P, E(SCF)
= -2484.17555396, E(ZPE) = -2483.775412,
E(G) = -2483.842910 a.u.

C -0.10149200 2.16476300 0.01354200
H -0.38308600 3.14283200 0.41317800
H 0.12413500 2.28296300 -1.04975100
C 1.06346700 1.56391800 0.75393200
H 0.81865000 1.45474600 1.81449300
H 1.95784600 2.18989000 0.68141000
N 1.32916300 0.20579100 0.21825300
N -1.23704000 1.21504500 0.11931000
C 2.32878700 0.15672000 -0.89695100
H 1.96659900 -0.55875600 -1.63883500
C -2.37754700 1.52559500 -0.76977000
H -2.00720900 1.41909200 -1.79519700
C 3.68166600 -0.23371300 -0.40551800
C 3.85733400 -1.55975000 0.09193400
C 4.73763200 0.65892900 -0.42471300
C 5.14815500 -1.89611900 0.55191300
C 5.99579000 0.29131100 0.03419400
H 4.57617900 1.66460300 -0.80745700
C 6.19291600 -0.99413100 0.51860600
H 5.29911600 -2.90061800 0.93533200
H 7.17574900 -1.27802000 0.87892800
C -3.54705600 0.63394300 -0.49644700
C -3.42472100 -0.77184200 -0.55360900
C -4.78376700 1.20241600 -0.21510300
C -4.58335400 -1.54427300 -0.35376200
C -5.90640800 0.42372900 -0.01478700
H -4.87655600 2.28253300 -0.16218300
C -5.80066500 -0.96018500 -0.08914700
H -4.49131400 -2.62400300 -0.41031600
H -6.67810800 -1.58022000 0.06433500
O 2.87528500 -2.40556900 0.15603200
O -2.29313200 -1.40088100 -0.81067700
S 7.33697300 1.47412400 -0.04413700
S -7.49242000 1.16483700 0.37770900
O -8.44774600 0.65153400 -0.64499900
O -7.82844800 0.69556500 1.75267900
O -7.28917700 2.63765000 0.29931300
O 7.58731100 1.72926400 -1.49396400
O 6.85453400 2.69667100 0.66350800
O 8.49683300 0.83151400 0.63615200
H -2.66702000 2.57219200 -0.62694900
H 2.34723300 1.13703800 -1.37829600
H 1.66269300 -0.37239500 0.99872100
O 0.44018100 -2.42593200 -0.82841500
H 1.37653600 -2.47351800 -0.47138800
H 2.19947700 -2.14031200 1.79678400
O 1.73718400 -1.62789200 2.49502800
H 2.38639200 -1.49872300 3.19053600
H -0.09862000 -3.18154200 -0.50593900
H -1.87961600 -4.21417800 0.71653000
O -1.65511100 -3.98336800 -0.18801400
H -2.09888300 -3.12638100 -0.36470100
Pd -0.47829600 -0.62439300 -0.30048600
H -1.57241700 1.19929500 1.08402200

54

RS_lambda_ID2_TS1_N-trigo-square_R, E(SCF)
= -2484.18275443, E(ZPE) = -2483.784349,
E(G) = -2483.852572 a.u.

C -0.59953100 3.12362900 -0.27431300
H -1.20519300 4.03419600 -0.26605500
H -0.22034200 2.98311000 -1.28991200
C 0.52780200 3.20289400 0.72369900
H 0.12807600 3.36980100 1.72634000
H 1.20426200 4.02957900 0.49045200
N 1.26631900 1.91599800 0.75489200
N -1.42922000 1.93935300 0.05236000
C 2.35503800 1.80797900 -0.22873200
H 1.90763800 1.87714200 -1.22732400
C -2.39819700 1.57323300 -1.00114200
H -1.80545000 1.31340900 -1.88543600
C 3.17668400 0.55537100 -0.09108700
C 2.66764200 -0.69763500 0.30851300
C 4.52707000 0.65518900 -0.41893900

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 3.54837000 | -1.79425900 | 0.34369300 | S | -7.30304900 | -0.22250400 | 0.78374900 |
| C | 5.37137600 | -0.43402100 | -0.38276300 | O | -8.20141500 | -0.62681800 | -0.33556400 |
| H | 4.93253600 | 1.61699500 | -0.71765900 | O | -7.37066900 | -1.16779900 | 1.93417500 |
| C | 4.87592000 | -1.67144800 | 0.00954900 | O | -7.47890000 | 1.20015600 | 1.18645200 |
| H | 3.14233800 | -2.74956800 | 0.66232100 | O | 7.53107500 | 1.44556800 | 0.22758900 |
| H | 5.53134800 | -2.53532900 | 0.04904100 | O | 7.82092000 | -0.48568900 | 1.76460000 |
| C | -3.28404500 | 0.44541300 | -0.57661300 | O | 8.08359600 | -0.80157500 | -0.67742400 |
| C | -2.74756100 | -0.79182600 | -0.16191500 | H | -3.29446800 | 2.78491100 | -0.39525800 |
| C | -4.66341300 | 0.60321700 | -0.64391200 | H | 3.00105000 | 2.36363400 | -0.46064200 |
| C | -3.64070500 | -1.83560000 | 0.13610800 | H | 1.42169100 | 0.95001500 | 1.12185600 |
| C | -5.52317700 | -0.43354800 | -0.33949200 | O | 0.81586900 | -0.76494800 | -2.45580800 |
| H | -5.07844900 | 1.55625000 | -0.95625500 | H | 1.25421600 | -1.31869300 | -1.77471300 |
| C | -5.00335900 | -1.66295800 | 0.04844000 | H | 1.09140700 | -1.00841400 | 1.68512300 |
| H | -3.22096000 | -2.78949700 | 0.43961000 | O | 0.94509000 | -0.43888100 | 2.46632400 |
| H | -5.67196500 | -2.48434700 | 0.28580300 | H | 1.56438100 | -0.75309400 | 3.12982500 |
| O | 1.41465300 | -0.93300500 | 0.68904300 | H | 0.10629700 | -1.29837500 | -2.83095800 |
| O | -1.45184100 | -1.03587300 | -0.05981800 | H | 0.33306900 | -2.67426200 | -0.00367500 |
| S | 7.11530700 | -0.26863100 | -0.77631500 | O | -0.54693600 | -3.07316100 | -0.11728500 |
| S | -7.30278700 | -0.21609300 | -0.41745400 | H | -1.04815100 | -2.38578800 | -2.58637200 |
| O | -7.80013100 | -1.27054900 | -1.34629900 | Pd | -0.26973700 | 0.33484500 | -0.61306200 |
| O | -7.79828000 | -0.40892600 | 0.97584900 | H | -1.67006000 | 1.70424300 | 1.04174000 |
| O | -7.52637000 | 1.16424600 | -0.92900800 | | | | |
| O | 7.29981800 | 1.13106300 | -1.24831700 | 54 | | | |
| O | 7.84466600 | -0.55630400 | 0.49193900 | RS_lambda_ID2_TS2_R_noH2_Htr_P, E(SCF) = - | | | |
| O | 7.38974000 | -1.28413000 | -1.83217900 | 2484.16780743, E(ZPE) = -2483.767817, E(G) | | | |
| H | -3.00607700 | 2.44871000 | -1.25465500 | = -2483.834574 a.u. | | | |
| H | 3.01477400 | 2.67632800 | -0.11812200 | C | -0.08588800 | -1.54115700 | 0.41984200 |
| H | 1.63670700 | 1.74089300 | 1.69740800 | H | 0.07290900 | -2.52182900 | 0.87736100 |
| O | 0.34907400 | -2.75846500 | -1.33442200 | H | -0.34743900 | -1.70799300 | -0.62901700 |
| H | 0.95923200 | -2.37580700 | -0.68854400 | C | -1.16595400 | -0.76780200 | 1.13578100 |
| H | 1.64433100 | -0.27057900 | 2.59112300 | H | -0.88156900 | -0.60558400 | 2.17828400 |
| O | 1.82280600 | 0.45491700 | 3.21130900 | H | -2.11361300 | -1.31443000 | 1.13426200 |
| H | 2.67426000 | 0.24500200 | 3.60401700 | N | -1.31034000 | 0.56491700 | 0.50292900 |
| H | -0.47391200 | -2.30675200 | -1.08342300 | N | 1.15629300 | -0.73901400 | 0.44600400 |
| H | 0.47150000 | -2.30200500 | 1.78784000 | C | -2.14217100 | 0.55856800 | -0.73414300 |
| O | -0.39921700 | -2.61410500 | 2.07423900 | H | -1.91897300 | 1.47963300 | -1.27021500 |
| H | -0.96911800 | -2.18617400 | 1.41283100 | C | 2.18233800 | -1.15820400 | -0.52728900 |
| Pd | -0.08299900 | 0.43008200 | 0.37006100 | H | 1.76445900 | -0.95441100 | -1.52054300 |
| H | -1.93640300 | 2.10825300 | 0.92209000 | C | -3.60788300 | 0.41828200 | -0.45538600 |
| | | | | C | -4.40618500 | 1.52721500 | -0.15182400 |
| | | | | C | -4.19948600 | -0.84344500 | -0.45527000 |
| | | | | C | -5.74389800 | 1.34869500 | 0.19355200 |
| | | | | C | -5.52731000 | -1.01311700 | -0.12056400 |
| | | | | H | -3.60889000 | -1.71380600 | -0.72528700 |
| | | | | C | -6.30140900 | 0.08833400 | 0.21726200 |
| | | | | H | -6.33391200 | 2.22605800 | 0.43177000 |
| | | | | H | -7.34508200 | -0.04185300 | 0.48316400 |
| | | | | C | 3.47930600 | -0.44403400 | -0.30468300 |
| | | | | C | 3.54835700 | 0.97091900 | -0.22595300 |
| | | | | C | 4.64677200 | -1.19503200 | -0.22386700 |
| | | | | C | 4.83100400 | 1.54860000 | -0.08968900 |
| | | | | C | 5.88625300 | -0.60190100 | -0.08720700 |
| | | | | H | 4.58790600 | -2.27790200 | -0.27516400 |
| | | | | C | 5.97184800 | 0.78589900 | -0.02586800 |
| | | | | H | 4.88480200 | 2.63063900 | -0.03455700 |
| | | | | H | 6.94044500 | 1.26452800 | 0.08359900 |
| | | | | O | -3.94004000 | 2.80101300 | -0.12801000 |
| | | | | O | 2.52573700 | 1.78304900 | -0.29055700 |
| | | | | S | -6.27849400 | -2.64895100 | -0.11045000 |
| | | | | S | 7.38384800 | -1.58017200 | 0.00099400 |
| | | | | O | 8.04143500 | -1.21125900 | 1.28879300 |
| | | | | O | 6.95331000 | -3.00589500 | -0.04195600 |
| | | | | O | 8.20392500 | -1.18559300 | -1.18144000 |
| | | | | O | -6.74211900 | -2.86294200 | -1.28850200 |
| | | | | O | -7.40440700 | -2.57555900 | -1.08228700 |
| | | | | O | -5.20558000 | -3.59267800 | -0.52355400 |
| | | | | H | 2.34051400 | -2.24029600 | -0.45266100 |
| | | | | H | -1.79609200 | -0.26124700 | -1.36625200 |
| | | | | H | -1.71255000 | 1.23048900 | 1.17403000 |
| | | | | O | 0.01359700 | 3.14567500 | -0.12409400 |
| | | | | H | -1.14963000 | 3.53856700 | -1.19694700 |
| | | | | H | -2.91933600 | 3.14253000 | 1.46553100 |
| | | | | O | -2.11204500 | 2.96175200 | 1.97490700 |
| | | | | H | -2.31800300 | 3.16169700 | 2.89118400 |
| | | | | H | -0.48742900 | 3.32480000 | 0.68486900 |
| | | | | H | -3.23850500 | 3.00648600 | -0.80024900 |
| | | | | O | -2.00046900 | 3.76106600 | -1.68210300 |

H -1.84755000 3.59564300 -2.61486700
Pd 0.61734500 1.22761600 0.12685500
H 1.56142600 -0.78734600 1.38134300

54

RS_lambda_ID2_TS2_R_noH2_Htr_TS, E(SCF) = -
2484.16183605, E(ZPE) = -2483.767406, E(G)
= -2483.832684 a.u.

C -0.03276600 -1.61541400 0.44943400
H 0.15591000 -2.57776800 0.93293600
H -0.29799700 -1.81587500 -0.59213000
C -1.12021700 -0.84336700 1.15365500
H -0.83601300 -0.65573200 2.19195200
H -2.06213800 -1.40014900 1.16319000
N -1.28275300 -0.47097500 0.48683300
N 1.19344500 -0.78531800 0.44206200
C -2.14147400 0.41231700 -0.73369500
H -1.89133000 1.27897000 -1.34168000
C 2.23004600 -1.243254800 -0.51355000
H 1.81048300 -1.06752700 -1.51429700
C -3.60431600 0.37116400 -0.42085900
C -4.30525500 1.54839100 -0.10026000
C -4.28502600 -0.84325300 -0.42830000
C -5.65850300 1.45168000 0.24555800
C -5.62280900 -0.91836400 -0.09582000
H -3.75805500 -1.75189700 -0.70451900
C -6.31013400 0.23809600 0.25134000
H -6.18327400 2.36623000 0.49889000
H -7.36091000 0.18484200 0.51740400
C 3.51388200 -0.48151200 -0.31544700
C 3.55534200 0.93489100 -0.29185700
C 4.69546300 -1.20610800 -0.20350800
C 4.82381200 1.54530600 -0.17940300
C 5.92203500 -0.58200800 -0.09154200
H 4.65868300 -2.29098800 -0.21242300
C 5.97970000 0.80837500 -0.08623300
H 4.85519000 2.62942200 -0.16750900
H 6.93869200 1.31005200 0.00164200
O -3.74145800 2.75749200 -0.07457300
O 2.51361400 1.72196400 -0.38873700
S -6.49868700 -2.48659800 -0.11649300
S 7.43868900 -1.52584900 0.04406600
O 8.06347700 -1.11830800 1.33644900
O 7.03808300 -2.96054700 0.02084100
O 8.27073400 -1.13510800 -1.13077100
O -7.03136100 -2.66882400 1.26327500
O -7.58154400 -2.33065800 -1.12865200
O -5.48979100 -3.51414300 -0.49367900
H 2.40297900 -2.29977300 -0.39251900
H -1.84793000 -0.47070400 -1.30411800
H -1.67736700 1.14966100 1.14805900
O 0.000732400 3.09638100 -0.19226300
H -0.93578200 3.30544400 -0.92239800
H -2.72375900 3.08209200 1.41256500
O -1.91688000 2.95735600 1.94949400
H -2.13950300 3.21451800 2.84711200
H -0.36546400 3.31673500 0.67662500
H -2.95093900 3.03156800 -0.80733600
O -1.95779100 3.56019600 -1.48655200
H -1.93023400 3.36108900 -2.42408800
Pd 0.62806900 1.14752200 0.06596300
H 1.59879300 -0.78694900 1.37917900

54

RS_lambda_ID2_TS2_R_noH2, E(SCF) = -
2484.17648560, E(ZPE) = -2483.775900, E(G)
= -2483.841976 a.u.

C -0.04921800 -1.60188000 0.46574400
H 0.14694400 -2.56897400 0.93587200
H -0.33129400 -1.78875700 -0.57360700
C -1.11716200 -0.83007600 1.19649700
H -0.81547800 -0.65867400 2.23248500
H -2.06524800 -1.37549400 1.21177700
N -1.27571800 0.49271900 0.54512900
N 1.18236400 -0.77700300 0.44914500
C -2.16055100 0.45349800 -0.66273800
H -1.95460700 1.36120900 -1.23070200

C 2.21123100 -1.22400100 -0.51407600
H 1.78676000 -1.06460600 -1.51195200
C -3.61268300 0.35819000 -0.33030600
C -4.31556800 1.54624700 0.01589800
C -4.27468700 -0.86218600 -0.38236500
C -5.69118300 1.40619400 0.31961600
C -5.62034500 -0.96125100 -0.08032100
H -3.73352600 -1.75779900 -0.67624800
C -6.32529700 0.18637100 0.27535500
H -6.23929900 2.30457600 0.58596800
H -7.38270100 0.11411800 0.51346900
C 3.50247700 -0.49379700 -0.32193100
C 3.55248200 0.92081300 -0.30122900
C 4.67971300 -1.22537000 -0.21128900
C 4.82153900 1.52753300 -0.19208600
C 5.90892500 -0.60592100 -0.10417200
H 4.63769200 -2.30999800 -0.21775000
C 5.97382400 0.78394300 -0.10140600
H 4.85800200 2.61118900 -0.15623500
H 6.93567700 1.28052100 -0.01682400
O -3.73922300 2.70753300 0.04788500
O 2.51017300 1.70981400 -0.39902200
S -6.47921200 -2.52918000 -0.14520600
S 7.42222800 -1.55687900 0.02972600
O 8.04852900 -1.15194200 1.32184900
O 7.01468700 -2.98934300 0.00595800
O 8.25371500 -1.14685200 -1.14577100
O -7.02592800 -2.76887200 1.21187200
O -7.56136300 -2.36226700 -1.17078000
O -5.46157500 -3.54194700 -0.55730500
H 2.37201800 -2.30036400 -0.38982000
H -1.83909900 -0.39194300 -1.27464800
H -1.66469600 1.16373400 1.21481400
O 0.05190300 3.16639400 -0.11028900
H -0.56160900 3.34436600 -0.86388200
H -2.67280300 3.07489700 1.25086800
O -1.84658800 3.11704000 1.80331900
H -2.05068600 3.59457700 2.60975300
H -0.51221200 3.33922700 0.67927500
H -2.74310200 3.38016100 -1.16228500
O -2.02279300 3.78674600 -1.70800000
H -2.20670900 3.55481800 -2.62091800
Pd 0.63769500 1.15068200 0.09436200
H 1.59390800 -0.78001800 1.38422100

56

RS_lambda_ID2_TS2-square_P, E(SCF) = -
2485.33476568, E(ZPE) = -2484.919326, E(G)
= -2484.988303 a.u.

C -0.12532200 -1.34642700 0.61579500
H 0.03356000 -2.22217500 1.25026400
H -0.46633200 -1.69629500 -0.36271900
C -1.10099900 -0.37858200 1.22365800
H -0.73401300 -0.02409500 2.19084000
H -2.07828700 -0.84089300 1.38565800
N -1.22675100 0.80829100 0.34080800
N 1.14974300 -0.62067800 0.41118600
C -2.22647100 0.65571500 -0.76100500
H -2.20462600 1.60142000 -1.30834400
C -2.14604800 -1.33675100 -0.41672100
H 1.71549500 -1.41383900 -1.42108900
C -3.60372800 0.34316800 -0.27817300
C -4.35590000 1.35996300 0.37084000
C -4.13740400 -0.92614100 -0.45598200
C -5.65857500 1.00868600 0.80266400
C -5.41213400 -1.23555400 -0.01872400
H -3.54881000 -1.69456700 -0.95095600
C -6.17071600 -0.25427200 0.61636000
H -6.24800400 1.77583400 1.29509600
H -7.17325700 -0.49053900 0.96149500
C 3.45937600 -0.62549400 -0.41423600
C 3.54359800 0.72638700 -0.81487200
C 4.61137200 -1.30746600 -0.04294300
C 4.81603900 1.32836600 -0.83852200
C 5.84937100 -0.69654400 -0.07853900
H 4.54443500 -2.34407300 0.27201300
C 5.94713900 0.63011400 -0.48421700

| | | | |
|----|-------------|-------------|-------------|
| H | 4.87690500 | 2.36522200 | -1.15000100 |
| H | 6.91681800 | 1.11749600 | -0.51236600 |
| O | -3.87976500 | 2.54891700 | 0.56182100 |
| O | 2.51373800 | 1.44880500 | -1.20237100 |
| S | -6.10524400 | -2.86816000 | -0.25488300 |
| S | 7.33310700 | -1.57500100 | 0.41627900 |
| O | 7.86027300 | -0.84130400 | 1.60276800 |
| O | 6.90391200 | -2.96483700 | 0.73432200 |
| O | 8.25688500 | -1.50197000 | -0.75155500 |
| O | -6.42351900 | -3.38516900 | 1.10880800 |
| O | -7.33291400 | -2.68396700 | -1.08406700 |
| O | -5.05448000 | -3.66819700 | -0.94613300 |
| H | 2.26781400 | -2.35207600 | -0.02496700 |
| H | -1.86478900 | -0.12540400 | -1.43493700 |
| H | -1.50883000 | 1.59996500 | 0.93097900 |
| O | -0.45799300 | 4.38909000 | 0.42598400 |
| H | -1.25066800 | 4.51612700 | -0.13344800 |
| H | -2.80272300 | 2.83516400 | 1.81795000 |
| O | -1.93477800 | 2.89702100 | 2.29238900 |
| H | -2.10132100 | 2.77032000 | 3.22850000 |
| H | -0.81650000 | 3.98437100 | 1.23446000 |
| H | -3.26700000 | 3.66601100 | -0.56531100 |
| O | -2.81443900 | 4.39601100 | -1.05478500 |
| H | -2.80833600 | 4.13491100 | -1.97815900 |
| H | 0.17381500 | 2.91746300 | -0.71493200 |
| H | 0.22536500 | 2.53971700 | -1.45240000 |
| Pd | 0.67081900 | 1.19195400 | -0.42119700 |
| H | 1.56936600 | -0.41975500 | 1.32136600 |

56
RS_lambda_ID2_TS2-square_R, E(SCF) = -
2485.35047714, E(ZPE) = -2484.934476, E(G)
= -2485.001907 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.04730700 | -1.62081700 | 0.44219100 |
| H | 0.14790300 | -2.59911400 | 0.88886300 |
| H | -0.32303700 | -1.78159500 | -0.60366600 |
| C | -1.12030300 | -0.86851200 | 1.18586200 |
| H | -0.82122000 | -0.71596200 | 2.22551900 |
| H | -2.06612200 | -1.41799600 | 1.18885300 |
| N | -1.28258200 | 0.46556900 | 0.55882100 |
| N | 1.18250100 | -0.79352900 | 0.45250200 |
| C | -2.16094300 | 0.44007800 | -0.65465200 |
| H | -1.94509100 | 1.34879200 | -1.21677500 |
| C | 2.21603300 | -1.21399200 | -0.51714900 |
| H | 1.79583600 | -1.03006000 | -1.51289800 |
| C | -3.61550900 | 0.35400400 | -0.33117600 |
| C | -4.31609300 | 1.54886700 | -0.00419400 |
| C | -4.28199400 | -0.86448300 | -0.37230100 |
| C | -5.69365000 | 1.41751800 | 0.29433100 |
| C | -5.62929500 | -0.95500300 | -0.07523600 |
| H | -3.74335600 | -1.76555700 | -0.65372200 |
| C | -6.33180200 | 0.19944100 | 0.26294400 |
| H | -6.23967600 | 2.32119200 | 0.54669500 |
| H | -7.39057300 | 0.13386500 | 0.49684300 |
| C | 3.50587000 | -0.48812500 | -0.30078200 |
| C | 3.55512900 | 0.92525400 | -0.23676900 |
| C | 4.68301600 | -1.22245500 | -0.20943000 |
| C | 4.82379800 | 1.52816500 | -0.10524500 |
| C | 5.91174400 | -0.60661200 | -0.07981900 |
| H | 4.64096200 | -2.30642500 | -0.24776900 |
| C | 5.97613200 | 0.78263100 | -0.03464600 |
| H | 4.86004700 | 2.61117000 | -0.06151100 |
| H | 6.93737700 | 1.27676100 | 0.06914600 |
| O | -3.73543300 | 2.70850800 | 0.01727400 |
| O | 2.51304200 | 1.71696000 | -0.31246200 |
| S | -6.49254600 | -2.52138400 | -0.13050700 |
| S | 7.42520000 | -1.56139100 | 0.02413700 |
| O | 8.06831800 | -1.17058900 | 1.31220100 |
| O | 7.01502400 | -2.99290900 | -0.00931800 |
| O | 8.24275000 | -1.16229600 | -1.15779900 |
| O | -7.03171200 | -2.74620000 | 1.24311000 |
| O | -7.58030400 | -2.36188400 | -1.14016800 |
| O | -5.47952400 | -3.54042900 | -0.52738700 |
| H | 2.37731200 | -2.29309600 | -0.42029800 |
| H | -1.84161800 | -0.40331000 | -1.27049900 |
| H | -1.68155100 | 1.12237800 | 1.23697600 |
| O | 0.05220900 | 3.16205300 | -0.02463900 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.53640900 | 3.34573600 | -0.79637500 |
| H | -2.70210300 | 3.04701600 | 1.25503600 |
| O | -1.89438300 | 3.06874200 | 1.83618000 |
| H | -2.11868800 | 3.53865700 | 2.64175700 |
| H | -0.53780000 | 3.31649500 | 0.74974300 |
| H | -2.70188600 | 3.36062400 | -1.17750400 |
| O | -1.96367000 | 3.75646500 | -1.70702900 |
| H | -2.11467200 | 3.50326000 | -2.62054500 |
| H | 0.10014100 | 1.14608300 | -2.81164000 |
| H | 0.39161400 | 0.53179000 | -3.12824500 |
| Pd | 0.63480600 | 1.14142500 | 0.14418300 |
| H | 1.59014900 | -0.81924700 | 1.38896400 |

56
RS_lambda_ID2_TS2-square, E(SCF) = -
2485.32664519, E(ZPE) = -2484.912902, E(G)
= -2484.981927 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.12064200 | -1.47384000 | 0.48994500 |
| H | 0.03510800 | -2.36196400 | 1.10846600 |
| H | -0.41373900 | -1.80371900 | -0.51038200 |
| C | -1.14271600 | -0.54504800 | 1.08177600 |
| H | -0.82340000 | -0.20656100 | 2.07163400 |
| H | -2.11479800 | -1.03298600 | 1.19304100 |
| N | -1.25937400 | 0.65875600 | 0.22090300 |
| N | 1.14285200 | -0.71392100 | 0.35533200 |
| C | -2.26755900 | 0.52778200 | -0.87052300 |
| H | -2.17920800 | 1.43470100 | -1.47396200 |
| C | 2.18602900 | -1.38113900 | -0.45157400 |
| H | 1.78776800 | -1.45638200 | -1.46907900 |
| C | -3.65518000 | 0.36754900 | -0.34229500 |
| C | -4.24759800 | 1.45950900 | 0.35002300 |
| C | -4.34022700 | -0.82876900 | -0.49785700 |
| C | -5.56179000 | 1.26396400 | 0.83904800 |
| C | -5.62210800 | -0.98645700 | -0.00293700 |
| H | -3.86664600 | -1.65745800 | -1.01740400 |
| C | -6.22900400 | 0.07272000 | 0.66823400 |
| H | -6.03130400 | 2.09000800 | 1.36421100 |
| H | -7.23588800 | -0.04703300 | 1.05798400 |
| C | 3.48216600 | -0.63879600 | -0.40063300 |
| C | 3.55152500 | 0.73174200 | -0.74046400 |
| C | 4.64217000 | -1.31930300 | -0.05015600 |
| C | 4.81891700 | 1.34739500 | -0.73487900 |
| C | 5.87290800 | -0.69382200 | -0.05195200 |
| H | 4.58690700 | -2.36849800 | 0.22247900 |
| C | 5.95662500 | 0.64890500 | -0.40504300 |
| H | 4.86878000 | 2.39662800 | -1.00374600 |
| H | 6.92047500 | 1.14852500 | -0.40965900 |
| O | -3.61644300 | 2.57577700 | 0.53355300 |
| O | 2.51839300 | 1.46506600 | -1.08865000 |
| S | -6.51503300 | -2.52384500 | -0.20343800 |
| S | 7.36326800 | -1.57784900 | 0.41066600 |
| O | 7.90364500 | -0.86452600 | 1.60362400 |
| O | 6.93942600 | -2.97384700 | 0.70909100 |
| O | 8.27447300 | -1.48404300 | -0.76583200 |
| O | -6.84560500 | -2.99445200 | 1.17420100 |
| O | -7.73921400 | -2.19430300 | -0.99141400 |
| O | -5.59468000 | -3.44863900 | -0.92445200 |
| H | 2.32724300 | -2.39887400 | -0.07092500 |
| H | -1.97949700 | -0.32007800 | -1.49774100 |
| H | -1.54786600 | 1.43996200 | 0.81865900 |
| O | 0.28950500 | 3.52019500 | 0.52449400 |
| H | -0.43111200 | 3.91024100 | -0.00944800 |
| H | -2.55299600 | 2.77574300 | 1.86538900 |
| O | -1.69353000 | 2.73187100 | 2.35040400 |
| H | -1.89038200 | 2.53285000 | 3.26789300 |
| H | -0.16629000 | 3.29345800 | 1.35309300 |
| H | -2.67199800 | 3.57893300 | -0.46565700 |
| O | -2.01242200 | 4.20907000 | -0.84666800 |
| H | -2.21721100 | 4.29347400 | -1.78001500 |
| H | -0.03830000 | 2.63858500 | -1.73481900 |
| H | 0.18418700 | 2.10288000 | -2.23645300 |
| Pd | 0.64877700 | 1.10663200 | -0.45195000 |
| H | 1.52083300 | -0.52526700 | 1.28577400 |

56

RS_lambda_ID2_TS2-trigo_P, E(SCF) = -
 2485.32763018, E(ZPE) = -2484.912577, E(G)
 = -2484.985709 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.07207800 | -0.00881400 | 1.96495800 |
| H | 0.11613700 | 0.84901300 | 2.61357500 |
| H | -0.28086000 | -0.87769000 | 2.59382600 |
| C | 1.11960100 | -0.24027500 | 1.07880100 |
| H | 2.02071300 | -0.39370900 | 1.68005800 |
| H | 0.99116400 | -1.12166200 | 0.44270100 |
| N | 1.27700900 | 0.93947100 | 0.19774700 |
| C | 2.36113100 | 0.78779800 | -0.81308600 |
| H | 2.47158500 | 1.77097200 | -1.28161900 |
| C | 3.65629900 | 0.30050000 | -0.24913500 |
| C | 4.38489800 | 1.13239600 | 0.64492300 |
| C | 4.12821900 | -0.96307100 | -0.58361100 |
| C | 5.60870100 | 0.61546900 | 1.13882000 |
| C | 5.32655000 | -1.43508500 | -0.08063800 |
| H | 3.55271000 | -1.58853900 | -1.25831500 |
| C | 6.06381900 | -0.63443100 | 0.78917600 |
| H | 6.18078900 | 1.24243600 | 1.81582000 |
| H | 7.00615200 | -1.00025500 | 1.18717600 |
| O | 3.95667100 | 2.29808800 | 0.99988200 |
| S | 5.93487600 | -3.06306000 | -0.50256600 |
| O | 5.97400500 | -3.83777200 | 0.77375600 |
| O | 7.29894700 | -2.86337100 | -1.07513100 |
| O | 4.97051900 | -3.62697100 | -1.48999400 |
| H | 1.99624100 | 0.09086300 | -1.57277500 |
| H | 1.48008400 | 1.75418200 | 0.79387300 |
| O | 0.46852400 | 4.28990300 | -1.32516200 |
| H | 1.34625500 | 4.37580700 | -0.89584000 |
| H | 2.61410900 | 2.74061900 | 2.04999100 |
| O | 1.70083300 | 3.01841200 | 2.28454200 |
| H | 1.61955600 | 3.86844000 | 1.83591600 |
| H | -0.16380000 | 4.60529900 | -0.67430000 |
| H | 3.37755700 | 3.65629400 | 0.19825300 |
| O | 2.88538400 | 4.47843700 | -0.04903900 |
| H | 3.53941200 | 5.12043100 | -0.33239500 |
| H | -0.01382900 | 2.45921200 | -1.77684100 |
| H | -0.12301700 | 1.74434000 | -2.18111900 |
| Pd | -0.62586800 | 1.27073100 | -0.56154100 |
| N | -1.26307700 | 0.32048100 | 1.13733600 |
| C | -2.07519200 | -0.83306700 | 0.69307100 |
| H | -1.46449400 | -1.41628800 | -0.00559000 |
| C | -3.37968300 | -0.40204900 | 0.09051300 |
| C | -3.49899600 | 0.68864800 | -0.80209000 |
| C | -4.51398000 | -1.14008100 | 0.41926900 |
| C | -4.77954200 | 0.97031200 | -1.32420300 |
| C | -5.75237900 | -0.84884800 | -0.11140400 |
| H | -4.42545200 | -1.97155200 | 1.11143000 |
| C | -5.88137400 | 0.22189500 | -0.99065100 |
| H | -4.86373900 | 1.80899900 | -2.00653800 |
| H | -6.85182300 | 0.46721500 | -1.41070300 |
| O | -2.52333400 | 1.47957600 | -1.19303300 |
| S | -7.20564600 | -1.79953100 | 0.33538100 |
| O | -8.12403200 | -0.84349600 | 1.01901000 |
| O | -6.72858900 | -2.88869500 | 1.23202500 |
| O | -7.77081300 | -2.30537000 | -0.94850000 |
| H | -2.27339500 | -1.47219700 | 1.55959000 |
| H | -1.86819200 | 0.95284200 | 1.65894600 |

54
 RS_lambda_ID2_TS2-trigo_R_noH2, E(SCF) = -
 2484.17029036, E(ZPE) = -2483.770079, E(G)
 = -2483.838439 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.05910900 | -0.86353200 | 1.67374500 |
| H | 0.20741100 | -0.27169300 | 2.55168900 |
| H | -0.29910600 | -1.87759800 | 2.00231400 |
| C | 1.08248600 | -0.85245000 | 0.69408400 |
| H | 2.00206600 | -1.21552000 | 1.16492200 |
| H | 0.87459800 | -1.48882800 | -0.17169200 |
| N | 1.25896800 | 0.53296300 | 0.20611300 |
| C | 2.31124500 | 0.64554800 | -0.83741900 |
| H | 2.21923200 | 1.63896600 | -1.27873600 |
| C | 3.68905200 | 0.44192200 | -0.29727900 |
| C | 4.25687100 | 1.46631900 | 0.51089400 |
| C | 4.40090500 | -0.71473400 | -0.57784800 |
| C | 5.56787200 | 1.23884000 | 0.99531900 |

| | | | |
|----|-------------|-------------|-------------|
| C | 5.68046800 | -0.90444800 | -0.08602100 |
| H | 3.95126200 | -1.48787100 | -1.19528300 |
| C | 6.26062600 | 0.08630700 | 0.70264600 |
| H | 6.01740600 | 2.01177700 | 1.61115700 |
| H | 7.26537000 | -0.05502700 | 1.09059500 |
| O | 3.60888100 | 2.54928600 | 0.80488700 |
| S | 6.62088200 | -2.37176900 | -0.49161700 |
| O | 7.09922700 | -2.93350400 | 0.80595800 |
| O | 7.75213200 | -1.91917100 | -1.35568700 |
| O | 5.68122500 | -3.28294500 | -1.20535700 |
| H | 2.07386100 | -0.08577800 | -1.61467400 |
| H | 1.51631600 | 1.11695800 | 1.01439300 |
| O | -0.05454000 | 2.57697200 | -1.72588200 |
| H | 0.57115500 | 3.21375100 | -1.27923500 |
| H | 2.58749000 | 2.29929100 | 2.19868700 |
| O | 1.87973800 | 1.89629900 | 2.75259100 |
| H | 1.30493400 | 2.62124100 | 3.00941900 |
| H | -0.84724400 | 3.06536900 | -1.97887500 |
| H | 2.43619100 | 3.43872400 | 0.02987200 |
| O | 1.68891400 | 3.98360700 | -0.33895100 |
| H | 2.08200700 | 4.79107100 | -0.67717100 |
| Pd | -0.64352700 | 1.15120500 | -0.30377800 |
| N | -1.25735500 | -0.22376800 | 1.06362000 |
| C | -2.19831400 | -1.13353300 | 0.37489100 |
| H | -1.68041100 | -1.53321100 | -0.50413700 |
| C | -3.48744900 | -0.45065100 | 0.01748400 |
| C | -3.55386300 | 0.84314800 | -0.55523900 |
| C | -4.66743400 | -1.15761100 | 0.23426600 |
| C | -4.82830500 | 1.33998800 | -0.90330900 |
| C | -5.90086700 | -0.64668100 | -0.11196300 |
| H | -4.62111800 | -2.14232000 | 0.68904800 |
| C | -5.97533400 | 0.61446500 | -0.69514900 |
| H | -4.87066300 | 2.32924200 | -1.34592000 |
| H | -6.93850100 | 1.03032800 | -0.97361000 |
| O | -2.53022400 | 1.63194700 | -0.78947800 |
| S | -7.40375400 | -1.58778000 | 0.15033100 |
| O | -8.32237800 | -0.68860300 | 0.90623800 |
| O | -7.00551700 | -2.79731300 | 0.92290600 |
| O | -7.92493500 | -1.92150100 | -1.20946700 |
| H | -2.41427900 | -1.98009500 | 1.03533400 |
| H | -1.77434900 | 0.26425900 | 1.79345200 |

56
 RS_lambda_ID2_TS2-trigo_R, E(SCF) = -
 2485.34433995, E(ZPE) = -2484.927884, E(G)
 = -2484.997354 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.04728100 | -0.79185900 | 1.74881300 |
| H | 0.22783200 | -0.17686700 | 2.60813000 |
| H | -0.28610900 | -1.79619800 | 2.10700900 |
| C | 1.08673600 | -0.80978200 | 0.76021000 |
| H | 2.00879900 | -1.16167600 | 1.23457600 |
| H | 0.87362800 | -1.47048900 | -0.08607500 |
| N | 1.26259100 | 0.56155500 | 0.23451100 |
| C | 2.29996700 | 0.64513400 | -0.82655200 |
| H | 2.21029300 | 1.63141900 | -1.28450100 |
| C | 3.68419200 | 0.43953100 | -0.30414600 |
| C | 4.27910100 | 1.47857100 | 0.46494500 |
| C | 4.37581700 | -0.73437300 | -0.56379200 |
| C | 5.59724400 | 1.24872900 | 0.92923400 |
| C | 5.66184500 | -0.92640000 | -0.09085000 |
| H | 3.90535500 | -1.51874600 | -1.15083000 |
| C | 6.26940800 | 0.07918300 | 0.65739100 |
| H | 6.06843400 | 2.03328700 | 1.51336700 |
| H | 7.28010300 | -0.06442300 | 1.02882700 |
| O | 3.64973100 | 2.57677400 | 0.74236700 |
| S | 6.57103900 | -2.42377000 | -0.45375700 |
| O | 7.00808800 | -2.97529200 | 0.86277400 |
| O | 7.73093500 | -2.01541900 | -1.30120100 |
| O | 5.62225700 | -3.32271300 | -1.17094300 |
| H | 2.04405500 | -0.09829100 | -1.58656100 |
| H | 1.53460500 | 1.16218300 | 1.02526800 |
| O | -0.06210600 | 2.56917500 | -1.72773200 |
| H | 0.57711100 | 3.21124900 | -1.30873500 |
| H | 2.64323100 | 2.36732300 | 2.15559000 |
| O | 1.94065000 | 1.98498800 | 2.73016300 |
| H | 1.37656700 | 2.72163300 | 2.97726000 |
| H | -0.85347300 | 3.05933300 | -1.98161500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.46621100 | 3.45535100 | -0.03340300 |
| O | 1.71392100 | 3.99341900 | -0.39995700 |
| H | 2.10100900 | 4.79758300 | -0.75257300 |
| H | -0.42877600 | -0.29501700 | -2.81305800 |
| H | -0.31360100 | -1.02939500 | -2.71355500 |
| Pd | -0.64290500 | 1.18211100 | -0.26272100 |
| N | -1.24995100 | -0.16691200 | 1.13242100 |
| C | -2.18616500 | -1.09357000 | 0.46172100 |
| H | -1.66288000 | -1.51502900 | -0.40365300 |
| C | -3.47561300 | -0.42598800 | 0.07574700 |
| C | -3.54915000 | 0.86151900 | -0.51010300 |
| C | -4.65012600 | -1.14689300 | 0.27739900 |
| C | -4.82431500 | 1.33844200 | -0.88318800 |
| C | -5.88383900 | -0.65612800 | -0.09507700 |
| H | -4.59878800 | -2.12720400 | 0.74113100 |
| C | -5.96517500 | 0.59991800 | -0.68838200 |
| H | -4.87196500 | 2.32362900 | -1.33423000 |
| H | -6.92887200 | 1.00074300 | -0.98636700 |
| O | -2.53334400 | 1.86394800 | -0.73286600 |
| S | -7.37896200 | -1.61365800 | 0.15144600 |
| O | -8.31333500 | -0.72589400 | 0.90158600 |
| O | -6.97505900 | -2.82097200 | 0.92451900 |
| O | -7.88493200 | -1.94000200 | -1.21366000 |
| H | -2.40432700 | -1.92352400 | 1.14223400 |
| H | -1.76684900 | 0.33205800 | 1.85478400 |

56
RS_lambda_ID2_TS2-trigo, E(SCF) = -
2485.32076414, E(ZPE) = -2484.906105, E(G)
= -2484.974593 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.01870200 | -0.04931700 | 1.91879500 |
| H | 0.21056800 | 0.80336300 | 2.56094000 |
| H | -0.22668800 | -0.91663700 | 2.55019400 |
| C | 1.14272400 | -0.30204000 | 0.99728200 |
| H | 2.05890000 | -0.46595400 | 1.57350900 |
| H | 0.98401200 | -1.18156200 | 0.36546000 |
| N | 1.28777800 | 0.87498300 | 0.11254300 |
| C | 2.36676700 | 0.73635200 | -0.90118500 |
| H | 2.41473000 | 1.70036200 | -1.41788700 |
| C | 3.68863600 | 0.35405100 | -0.31925000 |
| C | 4.34334500 | 1.25351100 | 0.56581600 |
| C | 4.24553000 | -0.88186400 | -0.61214900 |
| C | 5.58614600 | 0.82774100 | 1.09695000 |
| C | 5.46168600 | -1.26637300 | -0.07574100 |
| H | 3.72306500 | -1.56224400 | -1.27876000 |
| C | 6.12628200 | -0.39996000 | 0.78979500 |
| H | 6.10262800 | 1.50451200 | 1.77066800 |
| H | 7.08009700 | -0.69496800 | 1.21773300 |
| O | 3.82888400 | 2.39603600 | 0.88279700 |
| S | 6.17299700 | -2.86768100 | -0.43610200 |
| O | 6.20846800 | -3.60958600 | 0.85942200 |
| O | 7.54360700 | -2.60630200 | -0.96675400 |
| O | 5.27567800 | -3.50576500 | -1.44140100 |
| H | 2.03947700 | -0.01830300 | -1.62181300 |
| H | 1.49976400 | 1.68459700 | 0.71021600 |
| O | -0.11475500 | 3.65630000 | -0.95473700 |
| H | 0.76862400 | 3.97837400 | -0.67272200 |
| H | 2.53666200 | 2.69653600 | 2.06024100 |
| O | 1.61975200 | 2.87436700 | 2.36381200 |
| H | 1.41747900 | 3.71908500 | 1.94524100 |
| H | -0.75567200 | 4.22313800 | -0.51860400 |
| H | 3.01519700 | 3.65259200 | 0.10530400 |
| O | 2.38311300 | 4.38446700 | -0.10432300 |
| H | 2.88305000 | 5.06686900 | -0.55651900 |
| H | -0.16747000 | 1.94163700 | -2.37958300 |
| H | -0.08100300 | 1.17466900 | -2.49348400 |
| Pd | -0.62052300 | 1.21801500 | -0.61119800 |
| N | -1.22797000 | 0.30749700 | 1.12921700 |
| C | -2.09086200 | -0.83021900 | 0.75279900 |
| H | -1.50639300 | -1.47783700 | 0.09023800 |
| C | -3.38551100 | -0.39886600 | 0.12760500 |
| C | -3.49958100 | 0.67756300 | -0.78342900 |
| C | -4.52136400 | -1.13785700 | 0.45052500 |
| C | -4.77550400 | 0.94289200 | -1.32680800 |
| C | -5.75426100 | -0.86332100 | -0.10117400 |
| H | -4.43753600 | -1.95917800 | 1.15538200 |
| C | -5.87805200 | 0.19458300 | -0.99667800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.85497000 | 1.77099000 | -2.02253800 |
| H | -6.84378000 | 0.42811100 | -1.43392300 |
| O | -2.52716900 | 1.47351100 | -1.16797000 |
| S | -7.20765100 | -1.81446400 | 0.34358900 |
| O | -8.12844600 | -0.85893800 | 1.02505500 |
| O | -6.73210500 | -2.90283900 | 1.24215500 |
| O | -7.77024800 | -2.32174900 | -0.94091900 |
| H | -2.31000100 | -1.40889400 | 1.65721000 |
| H | -1.78877600 | 0.97173300 | 1.66046200 |

56
RS_lambda_ID2_TS3-square_P, E(SCF) = -
2485.36463172, E(ZPE) = -2484.945803, E(G)
= -2485.015125 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.15289700 | -1.32089600 | 0.53749500 |
| H | -0.09155900 | -2.22277400 | 1.15621400 |
| H | -0.46268600 | -1.63409700 | -0.46508600 |
| C | -1.13841400 | -0.33883200 | 1.11971500 |
| H | -0.77978800 | 0.01418800 | 2.09105900 |
| H | -2.11494300 | -0.80492400 | 1.28124500 |
| N | -1.26144700 | 0.86037000 | 0.24838700 |
| N | 1.14764600 | -0.64948800 | 0.41567300 |
| C | -2.25696000 | 0.71804700 | -0.84988900 |
| H | -2.22259200 | 1.65131400 | -1.41471000 |
| C | 2.13091000 | -1.32399900 | -0.44264500 |
| H | 1.69866800 | -1.34849600 | -1.45089400 |
| C | -3.64317500 | 0.39988400 | -0.37391200 |
| C | -4.44646700 | 1.35731100 | 0.25201400 |
| C | -4.14224000 | -0.89346500 | -0.50749100 |
| C | -5.69454600 | 1.00376400 | 0.75689000 |
| C | -5.38597700 | -1.23775400 | -0.01853200 |
| H | -3.53827300 | -1.65172300 | -0.99712100 |
| C | -6.16324800 | -0.28617400 | 0.62748000 |
| H | -6.28837300 | 1.76907000 | 1.24294800 |
| H | -7.13887100 | -0.55465400 | 1.01835000 |
| C | 3.44413400 | -0.60390100 | -0.42679500 |
| C | 3.54946900 | 0.75421700 | -0.82740300 |
| C | 4.58547400 | -1.29798500 | -0.04355600 |
| C | 4.84236600 | 1.32438900 | -0.83950300 |
| C | 5.83627300 | -0.71032500 | -0.05897400 |
| H | 4.49815300 | -2.33476400 | 0.26736900 |
| C | 5.95873900 | 0.61414900 | -0.46627300 |
| H | 4.92543100 | 2.35950900 | -1.15409300 |
| H | 6.93576500 | 1.08790700 | -0.48469300 |
| O | -4.05700800 | 2.64336400 | 0.44905700 |
| O | 2.55146000 | 1.50495600 | -1.22118900 |
| S | -6.02545900 | -2.90957000 | -0.21059800 |
| S | 7.29659700 | -1.60925700 | 0.45531000 |
| O | 7.82780100 | -0.88276200 | 1.64620000 |
| O | 6.84456100 | -2.99262500 | 0.77530900 |
| O | 8.23999800 | -1.55937400 | -0.69973200 |
| O | -6.31609000 | -3.38489300 | 1.17029600 |
| O | -7.25495400 | -2.76980000 | -1.03921900 |
| O | -4.94730100 | -3.68195800 | -0.88374200 |
| H | 2.27557000 | -2.36413800 | -0.12406800 |
| H | -1.90646200 | -0.06776700 | -1.52264200 |
| H | -1.54946400 | 1.62815900 | 0.85937900 |
| O | -0.43070700 | 4.39135100 | 0.75476600 |
| H | -1.72009200 | 4.36591700 | -0.50824600 |
| H | -2.96961700 | 2.86783900 | 2.03612200 |
| O | -2.06409300 | 2.79944400 | 2.38261000 |
| H | -2.13208100 | 2.59331100 | 3.31809400 |
| H | -0.88212600 | 3.94999300 | 1.49667300 |
| H | -3.48975200 | 3.02580000 | -0.26392200 |
| O | -2.49315400 | 4.17802600 | -1.08432900 |
| H | -2.14085800 | 4.06375800 | -1.97060600 |
| H | 0.13342500 | 3.69747100 | 0.37355300 |
| H | 0.22676700 | 2.58744500 | -1.19139200 |
| Pd | 0.66295500 | 1.25541100 | -0.48110600 |
| H | 1.55147100 | -0.51858900 | 1.34155500 |

56
RS_lambda_ID2_TS3-square, E(SCF) = -
2485.32950081, E(ZPE) = -2484.915990, E(G)
= -2484.984453 a.u.

| | | | |
|---|-------------|-------------|------------|
| C | -0.09513300 | -1.42116900 | 0.52865200 |
| H | 0.04679400 | -2.32772200 | 1.12388200 |

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| H | -0.41742000 | -1.72485200 | -0.47188100 | O | 4.14322000 | 2.48586300 | 0.90748000 |
| C | -1.09324100 | -0.49023500 | 1.16040000 | S | 5.89604100 | -3.00038400 | -0.49939000 |
| H | -0.74242300 | -0.17405500 | 2.14698700 | O | 6.07716300 | -3.69767300 | 0.80363900 |
| H | -2.06497500 | -0.97387300 | 1.29166200 | O | 7.18039500 | -2.80098300 | -1.22680600 |
| N | -1.22663200 | 0.73329300 | 0.32936100 | O | 4.83057300 | -3.60181000 | -1.34508700 |
| N | 1.17634200 | -0.68274600 | 0.38411500 | H | 2.06624400 | 0.28146600 | -1.66565800 |
| C | -2.23273600 | 0.61886000 | -0.76991200 | H | 1.47356300 | 1.49349000 | 0.95158800 |
| H | -2.19780300 | 1.57102400 | -1.30571000 | O | 0.49190900 | 4.43009400 | -0.21185500 |
| C | 2.18394900 | -1.34272800 | -0.46964100 | H | 2.20159500 | 4.40915600 | -0.63978300 |
| H | 1.76105200 | -1.37278800 | -1.48033600 | H | 2.87300600 | 2.45266100 | 2.31133800 |
| C | -3.61226400 | 0.32969900 | -0.27818500 | O | 2.04092200 | 2.13408600 | 2.69990300 |
| C | -4.33058800 | 1.35211800 | 0.39815500 | H | 1.64947600 | 2.89375600 | 3.13781000 |
| C | -4.17711500 | -0.92462300 | -0.46351800 | H | 0.27496900 | 4.43529400 | 0.72505700 |
| C | -5.63475600 | 1.02795900 | 0.84208300 | H | 3.76165100 | 3.03024500 | 0.17335500 |
| C | -5.45186300 | -1.21085600 | -0.00956700 | O | 3.15961800 | 4.27166200 | -0.80291500 |
| H | -3.61188100 | -1.69972100 | -0.97507300 | H | 3.28404000 | 4.29832000 | -1.75444700 |
| C | -6.17900500 | -0.22099900 | 0.64709600 | H | 0.09592200 | 3.60596300 | -0.55495500 |
| H | -6.19860600 | 1.80176900 | 1.35366900 | H | -0.11148700 | 2.14137200 | -1.74360400 |
| H | -7.18142600 | -0.43912100 | 1.00418000 | Pd | -0.64097600 | 1.29721600 | -0.52782200 |
| C | 3.48816200 | -0.61339100 | -0.42776800 | N | -1.29075100 | 0.00231900 | 1.07888400 |
| C | 3.56318100 | 0.75510200 | -0.77855200 | C | -2.11193500 | -1.00592900 | 0.38951900 |
| C | 4.64349700 | -1.29776900 | -0.07096800 | H | -1.52931200 | -1.38343800 | -0.46036100 |
| C | 4.83599700 | 1.36142600 | -0.77774300 | C | -3.42784600 | -0.43399800 | -0.05351400 |
| C | 5.87823400 | -0.67832900 | -0.07304600 | C | -3.53898300 | 0.76368800 | -0.81130600 |
| H | 4.58164100 | -2.34522900 | 0.20754200 | C | -4.58021600 | -1.13980100 | 0.27908600 |
| C | 5.96950000 | 0.66118400 | -0.43667800 | C | -4.84121700 | 1.15906900 | -1.20067100 |
| H | 4.89267800 | 2.40818900 | -1.05589100 | C | -5.83692300 | -0.72742300 | -0.11614800 |
| H | 6.93595500 | 1.15602400 | -0.44235900 | H | -4.49220800 | -2.04646700 | 0.86979300 |
| O | -3.81960600 | 2.52703900 | 0.60276800 | C | -5.96078400 | 0.43582800 | -0.86989100 |
| O | 2.53524000 | 1.48869600 | -1.13942000 | H | -4.92490500 | 2.07009500 | -1.78412200 |
| S | -6.18231400 | -2.82702500 | -0.24793700 | H | -6.94170600 | 0.77558800 | -1.18864600 |
| S | 7.36241400 | -1.56240400 | 0.40508900 | O | -2.55319100 | 1.53236700 | -1.19443100 |
| O | 7.89394500 | -0.84707300 | 1.60142000 | S | -7.30324600 | -1.66338200 | 0.30503900 |
| O | 6.93562600 | -2.95771700 | 0.70406100 | O | -8.21038600 | -0.71327200 | 1.01342400 |
| O | 8.28612300 | -1.47357700 | -0.76245000 | O | -6.84821500 | -2.78650800 | 1.17254800 |
| O | -6.50176100 | -3.34227700 | 1.11610000 | O | -7.88139400 | -2.13012300 | -0.98972600 |
| O | -7.41152700 | -2.61255800 | -1.06741500 | H | -2.29606800 | -1.86044100 | 1.05305400 |
| O | -5.15442300 | -3.64713700 | -0.94994300 | H | -1.87399000 | 0.47202700 | 1.76490900 |
| H | 2.32323800 | -2.37710400 | -0.13619200 | | | | |
| H | -1.89043700 | -0.16021800 | -1.45607600 | 56 | | | |
| H | -1.52306500 | 1.49120700 | 0.95037600 | RS_lambda_ID2_TS3-trigo, E(SCF) = - | | | |
| O | -0.49978200 | 4.16978100 | 0.19714800 | 2485.32012581, E(ZPE) = -2484.907540, E(G) | | | |
| H | -1.33518800 | 4.40652200 | -0.28891100 | = -2484.977515 a.u. | | | |
| H | -2.71452600 | 2.86095400 | 1.80493700 | C | -0.05888200 | -0.49535200 | 1.79862400 |
| O | -1.81664900 | 2.96233700 | 2.21700000 | H | 0.16317200 | 0.21591300 | 2.59781100 |
| H | -1.92235000 | 3.05872100 | 3.16544100 | H | -0.25238500 | -1.47072000 | 2.25394200 |
| H | -0.82044500 | 3.83201200 | 1.06677400 | C | 1.10940500 | -0.55529000 | 0.85128300 |
| H | -3.33858200 | 3.72253500 | -0.48250000 | H | 2.02022200 | -0.83949700 | 1.38764200 |
| O | -2.90062500 | 4.48860900 | -0.93385200 | H | 0.95068300 | -1.29005300 | 0.05527300 |
| H | -3.00617100 | 4.34411600 | -1.87690900 | N | 1.26906400 | 0.77349100 | 0.21961100 |
| H | -0.00090200 | 3.14023000 | -0.48518800 | C | 2.36168300 | 0.81429100 | -0.79121600 |
| H | 0.25213400 | 2.57232000 | -1.21397700 | H | 2.39773700 | 1.84138300 | -1.16179200 |
| Pd | 0.67724000 | 1.17712300 | -0.39283100 | C | 3.68889900 | 0.38387300 | -0.25512500 |
| H | 1.58269500 | -0.53302200 | 1.30881800 | C | 4.40911600 | 1.24851300 | 0.61392300 |
| | | | | C | 4.19805000 | -0.86513400 | -0.58460300 |
| | | | | C | 5.64915500 | 0.76961900 | 1.10342800 |
| | | | | C | 5.41217700 | -1.30190100 | -0.08775200 |
| | | | | H | 3.63300500 | -1.51610000 | -1.24605600 |
| | | | | C | 6.13592900 | -0.47160200 | 0.76530000 |
| | | | | H | 6.21184600 | 1.42144600 | 1.76454300 |
| | | | | H | 7.09074100 | -0.80738500 | 1.15979600 |
| | | | | O | 3.96749800 | 2.41908700 | 0.95352600 |
| | | | | S | 6.06809000 | -2.91200800 | -0.51137900 |
| | | | | O | 6.21221100 | -3.65321200 | 0.77649500 |
| | | | | O | 7.38743900 | -2.66590000 | -1.16519100 |
| | | | | O | 5.07561500 | -3.53881500 | -1.43024600 |
| | | | | H | 2.05287600 | 0.17115800 | -1.62015900 |
| | | | | H | 1.47014500 | 1.45582800 | 0.96538200 |
| | | | | O | 0.35630400 | 4.17395900 | -0.97333300 |
| | | | | H | 1.34400400 | 4.24130300 | -0.76623900 |
| | | | | H | 2.66205200 | 2.60121000 | 2.06166900 |
| | | | | O | 1.77175600 | 2.55568400 | 2.48424500 |
| | | | | H | 1.40594500 | 3.44080300 | 2.41352900 |
| | | | | H | -0.12991100 | 4.41931000 | -0.17669200 |
| | | | | H | 3.33487900 | 3.58306000 | 0.00769800 |
| | | | | O | 2.89053200 | 4.34373700 | -0.46267400 |
| | | | | H | 3.45775500 | 4.58705200 | -1.19760100 |

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|--|-------------|-------------|-------------|--|--|--|--|
| 56 | | | | | | | |
| RS_lambda_ID2_TS3-trigo_P, E(SCF) = - | | | | | | | |
| 2485.35829832, E(ZPE) = -2484.941043, E(G) | | | | | | | |
| = -2485.011888 a.u. | | | | | | | |
| C | -0.06798300 | -0.49458700 | 1.73336100 | | | | |
| H | 0.15493600 | 0.17926400 | 2.56393100 | | | | |
| H | -0.22053100 | -1.49690700 | 2.14932100 | | | | |
| C | 1.10431700 | -0.50088500 | 0.78151500 | | | | |
| H | 2.01089500 | -0.79756300 | 1.32050100 | | | | |
| H | 0.95553800 | -1.21489600 | -0.03495800 | | | | |
| N | 1.26928800 | 0.84434100 | 0.17990500 | | | | |
| C | 2.36894900 | 0.90146900 | -0.81858000 | | | | |
| H | 2.41329400 | 1.93151400 | -1.17588100 | | | | |
| C | 3.69566300 | 0.43144100 | -0.29506300 | | | | |
| C | 4.48928000 | 1.22452800 | 0.53842800 | | | | |
| C | 4.14294600 | -0.85108600 | -0.60360300 | | | | |
| C | 5.66974200 | 0.71739600 | 1.07455200 | | | | |
| C | 5.32087300 | -1.34590100 | -0.08186400 | | | | |
| H | 3.54780500 | -1.48157900 | -1.25689500 | | | | |
| C | 6.08536400 | -0.56130900 | 0.77048900 | | | | |
| H | 6.25616400 | 1.35777600 | 1.72318800 | | | | |
| H | 7.00913400 | -0.94963200 | 1.18610300 | | | | |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.04138600 | 2.97370900 | -1.28310300 |
| H | -0.11810800 | 2.11262100 | -1.77348400 |
| Pd | -0.63613500 | 1.25459600 | -0.44143300 |
| N | -1.26669500 | 0.00150100 | 1.09653400 |
| C | -2.11895500 | -1.02682500 | 0.46662100 |
| H | -1.54787500 | -1.46691600 | -0.35940800 |
| C | -3.42897500 | -0.45459500 | 0.00883300 |
| C | -3.53527900 | 0.76427500 | -0.70745000 |
| C | -4.58204900 | -1.18223000 | 0.29081500 |
| C | -4.82713900 | 1.16619900 | -1.11571200 |
| C | -5.83040400 | -0.76574500 | -0.12217700 |
| H | -4.50114800 | -2.10663100 | 0.85426200 |
| C | -5.94715200 | 0.42266500 | -0.83677900 |
| H | -4.90374400 | 2.09730100 | -1.66695500 |
| H | -6.92308400 | 0.70759900 | -1.16617000 |
| O | -2.54587800 | 1.56136100 | -1.03348600 |
| S | -7.30209900 | -1.71954200 | 0.24306000 |
| O | -8.21931500 | -0.79379300 | 0.96914900 |
| O | -6.85676800 | -2.87043800 | 1.07755300 |
| O | -7.85614800 | -2.13966400 | -1.07710000 |
| H | -2.30880900 | -1.82813700 | 1.18926100 |
| H | -1.84105100 | 0.52541300 | 1.75327300 |

54

RS_lambda_SR_delta_ID2_TS1_N-trigo-square_P, E(SCF) = -2484.17555396, E(ZPE) = -2483.775412, E(G) = -2483.842910 a.u.

| | | | |
|---|-------------|--------------|-------------|
| C | -0.10149200 | 2.16476300 | 0.01354200 |
| H | -0.38308600 | 3.14283200 | 0.41317800 |
| H | 0.12413500 | 2.28296300 | -1.04975100 |
| C | 1.06346700 | 1.56391800 | 0.75393200 |
| H | 0.81865000 | 1.45474600 | 1.81449300 |
| H | 1.95784600 | 2.18989000 | 0.68141000 |
| N | 1.32916300 | 0.20579100 | 0.21825300 |
| N | -1.23704000 | 1.21504500 | 0.11931000 |
| C | 2.32878700 | 0.15672000 | -0.89695100 |
| H | 1.96659900 | -0.55875600 | -1.63883500 |
| C | -2.37754700 | 1.52559500 | -0.76977000 |
| H | -2.00720900 | 1.41909200 | -1.79519700 |
| C | 3.68166600 | -0.23371300 | -0.40551800 |
| C | 3.85733400 | -1.55975000 | 0.09193400 |
| C | 4.73763200 | 0.65892900 | -0.42471300 |
| C | 5.14815500 | -1.89611900 | 0.55191300 |
| C | 5.99579000 | 0.29131100 | 0.03419400 |
| H | 4.57617900 | 1.66460300 | -0.80745700 |
| C | 6.19291600 | -0.99413100 | 0.51860600 |
| H | 5.29911600 | -2.90061800 | 0.93533200 |
| H | 7.17574900 | -1.27802000 | 0.87892800 |
| C | -3.54705600 | 0.63394300 | -0.49644700 |
| C | -3.42472100 | -0.77184200 | -0.55360900 |
| C | -4.78376700 | 1.20241600 | -0.21510300 |
| C | -4.58335400 | -1.54427300 | -0.35376200 |
| C | -5.90640800 | 0.42372900 | -0.01478700 |
| H | -4.87655600 | 2.28253300 | -0.16218300 |
| C | -5.80066500 | -0.96018500 | -0.08914700 |
| H | -4.49131400 | -2.62400300 | -0.41031600 |
| H | -6.67810800 | -1.58022000 | 0.06433500 |
| O | 2.87528500 | -2.40556900 | 0.15603200 |
| O | -2.29313200 | -1.40088100 | -0.81067700 |
| S | 7.33697300 | 1.47412400 | -0.04413700 |
| S | -7.49242000 | 1.16483700 | 0.37770900 |
| O | -8.44774600 | 0.65153400 | -0.64499900 |
| O | -7.82844800 | 0.69556500 | 1.75267900 |
| O | -7.28917700 | 2.63765000 | 0.29931300 |
| O | 7.58731100 | 1.72926400 | -1.49396400 |
| O | 6.85453400 | 2.69667100 | 0.66350800 |
| O | 8.49683300 | 0.83151400 | 0.63615200 |
| H | -2.66702000 | 2.57219200 | -0.62694900 |
| H | 2.34723300 | 1.13703800 | -1.37829600 |
| H | 1.66269300 | -0.37239500 | 0.99872100 |
| O | 0.44018100 | -2.42593200 | -0.82841500 |
| H | 1.37653600 | -2.471351800 | -0.47138800 |
| H | 2.19947700 | -2.14031200 | 1.79678400 |
| O | 1.73718400 | -1.62789200 | 2.49502800 |
| H | 2.38639200 | -1.49872300 | 3.19053600 |
| H | -0.09862000 | -3.18154200 | -0.50593900 |
| H | -1.87961600 | -4.21417800 | 0.71653000 |

| | | | |
|----|-------------|-------------|-------------|
| O | -1.65511100 | -3.98336800 | -0.18801400 |
| H | -2.09888300 | -3.12638100 | -0.36470100 |
| Pd | -0.47829600 | -0.62439300 | -0.30048600 |
| H | -1.57241700 | 1.19929500 | 1.08402200 |

54

RS_lambda_SR_delta_ID2_TS1_N-trigo-square_R, E(SCF) = -2484.18275443, E(ZPE) = -2483.784349, E(G) = -2483.852572 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.59953100 | 3.12362900 | -0.27431300 |
| H | -1.20519300 | 4.03419600 | -0.26605500 |
| H | -0.22034200 | 2.98311000 | -1.28991200 |
| C | 0.52780200 | 3.20289400 | 0.72369900 |
| H | 0.12807600 | 3.36980100 | 1.72634000 |
| H | 1.20426200 | 4.02957900 | 0.49045200 |
| N | 1.26631900 | 1.91599800 | 0.75489200 |
| N | -1.42922000 | 1.93935300 | 0.05236000 |
| C | 2.35503800 | 1.80797900 | -0.22873200 |
| H | 1.90763800 | 1.87714200 | -1.22732400 |
| C | -2.39819700 | 1.57323300 | -1.00114200 |
| H | -1.80545000 | 1.31340900 | -1.88543600 |
| C | 3.17668400 | 0.55537100 | -0.09108700 |
| C | 2.66764200 | -0.69763500 | 0.30851300 |
| C | 4.52707000 | 0.65518900 | -0.41893900 |
| C | 3.54837000 | -1.79425900 | 0.34369300 |
| C | 5.37137600 | -0.43402100 | -0.38276300 |
| H | 4.93253600 | 1.61699500 | -0.71765900 |
| C | 4.87592000 | -1.67144800 | 0.00954900 |
| H | 3.14233800 | -2.74956800 | 0.66232100 |
| H | 5.53134800 | -2.53532900 | 0.04904100 |
| C | -3.28404500 | 0.44541300 | -0.57661300 |
| C | -2.74756100 | -0.79182600 | -0.16191500 |
| C | -4.66341300 | 0.60321700 | -0.64391200 |
| C | -3.64070500 | -1.83560000 | 0.13610800 |
| C | -5.52317700 | -0.43354800 | -0.33949200 |
| H | -5.07844900 | 1.55625000 | -0.95625500 |
| C | -5.00335900 | -1.66295800 | 0.04844000 |
| H | -3.22096000 | -2.78949700 | 0.43961000 |
| H | -5.67196500 | -2.48434700 | 0.28580300 |
| O | 1.41465300 | -0.93300500 | 0.68904300 |
| O | -1.45184100 | -1.03587300 | -0.05981800 |
| S | 7.11530700 | -0.26863100 | -0.77631500 |
| S | -7.30278700 | -0.21609300 | -0.41745400 |
| O | -7.80013100 | -1.27054900 | -1.34629900 |
| O | -7.79828000 | -0.40892600 | 0.97584900 |
| O | -7.52637000 | 1.16424600 | -0.92900800 |
| O | 7.29981800 | 1.13106300 | -1.24831700 |
| O | 7.84466600 | -0.55630400 | 0.49193900 |
| O | 7.38974000 | -1.28413000 | -1.83217900 |
| H | -3.00607700 | 2.44871000 | -1.25465500 |
| H | 3.01477400 | 2.67632800 | -0.11812200 |
| H | 1.63670700 | 1.74089300 | 1.69740800 |
| O | 0.34907400 | -2.75846500 | -1.33442200 |
| H | 0.95923200 | -2.37580700 | -0.68854400 |
| H | 1.64433100 | -0.27057900 | 2.59112300 |
| O | 1.82280600 | 0.45491700 | 3.21130900 |
| H | 2.67426000 | 0.24500200 | 3.60401700 |
| H | -0.47391200 | -2.30675200 | -1.08342300 |
| O | 0.47150000 | -2.30200500 | 1.78784000 |
| O | -0.39921700 | -2.61410500 | -2.07423900 |
| H | -0.96911800 | -2.18617400 | 1.41283100 |
| Pd | -0.08299900 | 0.43008200 | 0.37006100 |
| H | -1.93640300 | 2.10825300 | 0.92209000 |

54

RS_lambda_SR_delta_ID2_TS1_N-trigo-square, E(SCF) = -2484.14950849, E(ZPE) = -2483.751030, E(G) = -2483.817694 a.u.

| | | | |
|---|-------------|------------|-------------|
| C | -0.60256100 | 3.05106200 | -0.10906200 |
| H | -1.10712200 | 3.93955800 | 0.28360600 |
| H | -0.44382800 | 3.19071400 | -1.18104700 |
| C | 0.69698900 | 2.79113600 | 0.60679400 |
| H | 0.52902600 | 2.78874000 | 1.68726500 |
| H | 1.42649700 | 3.57276800 | 0.38885700 |
| N | 1.23831400 | 1.44914300 | 0.24439100 |
| N | -1.45959200 | 1.85345000 | 0.05346400 |
| C | 2.46912100 | 1.41572700 | -0.58603900 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.16075200 | 1.35932500 | -1.63598300 |
| C | -2.72635200 | 1.90192300 | -0.70765600 |
| H | -2.44612200 | 2.03527700 | -1.75759000 |
| C | 3.39000900 | 0.29173800 | -0.20157400 |
| C | 2.92561500 | -1.02935900 | 0.02675000 |
| C | 4.74584500 | 0.57321100 | -0.07248200 |
| C | 3.88283600 | -2.00171400 | 0.38650500 |
| C | 5.66151500 | -0.40398300 | 0.26737700 |
| H | 5.10151200 | 1.58637400 | -0.23469800 |
| C | 5.22090800 | -1.70271400 | 0.49800300 |
| H | 3.52381500 | -3.00958000 | 0.56861700 |
| H | 5.93115300 | -2.47620400 | 0.77373100 |
| C | -3.54362700 | 0.66768900 | -0.50629600 |
| C | -3.02743900 | -0.59621600 | -0.86699500 |
| C | -4.83072200 | 0.76392700 | 0.00490600 |
| C | -3.86540500 | -1.71701400 | -0.73380000 |
| C | -5.63243300 | -0.35324200 | 0.14115200 |
| H | -5.22217900 | 1.73334200 | 0.29621100 |
| C | -5.14587700 | -1.59741100 | -0.24190100 |
| H | -3.47254400 | -2.68480500 | -1.02759000 |
| H | -5.77281100 | -2.47780700 | -0.14249400 |
| O | 1.65901800 | -1.36122000 | -0.05977100 |
| O | -1.80932300 | -0.76989000 | -1.34578700 |
| S | 7.40880800 | -0.02858300 | 0.40599800 |
| S | -7.30304900 | -0.22250400 | 0.78374900 |
| O | -8.20141500 | -0.62681800 | -0.33556400 |
| O | -7.37066900 | -1.16779900 | 1.93417500 |
| O | -7.47890000 | 1.20015600 | 1.18645200 |
| O | 7.53107500 | 1.44556800 | 0.22758900 |
| O | 7.82092000 | -0.48568900 | 1.76460000 |
| O | 8.08359600 | -0.80157500 | -0.67742400 |
| H | -3.29446800 | 2.78491100 | -0.39525800 |
| H | 3.00105000 | 2.36363400 | -0.46064200 |
| H | 1.42169100 | 0.95001500 | 1.12185600 |
| O | 0.81586900 | -0.76494800 | -2.45580800 |
| H | 1.25421600 | -1.31869300 | -1.77471300 |
| H | 1.09140700 | -1.00841400 | 1.68512300 |
| O | 0.94509000 | -0.43888100 | 2.46632400 |
| H | 1.56438100 | -0.75309400 | 3.12982500 |
| H | 0.10629700 | -1.29837500 | -2.83095800 |
| H | 0.33306900 | -2.67426200 | -0.00367500 |
| O | -0.54693600 | -3.07316100 | -0.11728500 |
| H | -1.04815100 | -2.38578800 | -0.58637200 |
| Pd | -0.26973700 | 0.33484500 | -0.61306200 |
| H | -1.67006000 | 1.70424300 | 1.04174000 |

45

RS N-dissoc_CO-coord, E(SCF) = -
2254.81321819, E(ZPE) = -2254.490417, E(G)
= -2254.548445 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 0.18781600 | -0.15934200 | 1.19556700 |
| N | -1.65729500 | -2.50475200 | 1.97171100 |
| C | 1.51961200 | -0.68753800 | 1.58597500 |
| H | 1.83957700 | -0.18865400 | 2.50797700 |
| C | -2.79986700 | -2.32688800 | 1.09708000 |
| H | -3.68622600 | -2.19209400 | 1.72903800 |
| C | 2.53187800 | -0.47903900 | 0.51224600 |
| C | 2.33968800 | -1.09561500 | -0.74521500 |
| C | 3.66807600 | 0.28162300 | 0.74821000 |
| C | 3.34610300 | -0.93169700 | -1.71779300 |
| C | 4.64048700 | 0.43004000 | -0.22388200 |
| H | 3.80946000 | 0.75404700 | 1.71540700 |
| C | 4.47434300 | -0.18640300 | -1.45996600 |
| H | 3.20434800 | -1.41071700 | -2.68065900 |
| H | 5.23601600 | -0.07361800 | -2.22552400 |
| C | -2.80481200 | -1.18720000 | 0.07699300 |
| C | -2.57337100 | -1.39025700 | -1.33926500 |
| C | -3.47661400 | 0.01322100 | 0.44674600 |
| C | -3.03432500 | -0.40953500 | -2.27463200 |
| C | -3.87353600 | 0.93266000 | -0.47036500 |
| H | -3.73275400 | 0.17254000 | 1.49045600 |
| C | -3.66970500 | 0.71123600 | -1.85342800 |
| H | -2.84990200 | -0.60362500 | -3.32493400 |
| H | -4.01677700 | 1.45084800 | -2.56739000 |
| O | 1.29199400 | -1.83135700 | -1.01816800 |
| O | -1.80287300 | -2.35786000 | -1.71979900 |
| S | 6.10479400 | 1.42176900 | 0.07082100 |

| | | | |
|----|-------------|-------------|-------------|
| S | -4.73158100 | 2.43472800 | 0.03366900 |
| O | -3.87884100 | 3.54588800 | -0.46856700 |
| O | -4.81990500 | 2.37802400 | 1.51543100 |
| O | -6.05423600 | 2.36829800 | -0.64415300 |
| O | 6.02599000 | 1.86679900 | 1.49020500 |
| O | 6.03334200 | 2.55489900 | -0.89728200 |
| O | 7.26756500 | 0.42583500 | -0.19418100 |
| H | 0.32467900 | 0.79048800 | 0.85143900 |
| H | 1.39410400 | -1.75193900 | 1.81066800 |
| H | -2.93804000 | -3.26593800 | 0.55575800 |
| Pd | -0.59060900 | -1.23587000 | -0.42039600 |
| C | -1.24001400 | -1.45047900 | 2.86726300 |
| C | -0.76644000 | -0.09348700 | 2.32379100 |
| H | -1.60379400 | 0.51646700 | 1.98787100 |
| H | -0.29349300 | 0.44283400 | 3.15573800 |
| H | -2.07031700 | -1.22350100 | 3.54759300 |
| H | -0.44761900 | -1.86777500 | 3.49568100 |
| H | -0.87961500 | -2.94269500 | 1.49591100 |

45

RS N-dissoc_TS, E(SCF) = -2254.79454680,
E(ZPE) = -2254.472712, E(G) = -2254.529974
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -0.58382300 | 1.87322000 | 1.23326100 |
| N | 2.21758200 | 2.03887600 | 1.77100500 |
| C | -2.06223600 | 1.97924200 | 1.12991200 |
| H | -2.49737400 | 1.95499600 | 2.13398000 |
| C | 2.82439900 | 2.24010600 | 0.45399800 |
| H | 3.85471900 | 2.61187100 | 0.54357500 |
| C | -2.68432000 | 0.95058400 | 0.25149200 |
| C | -2.33818900 | 0.96423400 | -1.12221400 |
| C | -3.62384000 | 0.05510400 | 0.71929400 |
| C | -2.99272900 | 0.07158400 | -1.98097600 |
| C | -4.25437100 | -0.82912900 | -0.14895700 |
| H | -3.88167300 | 0.05168400 | 1.77521700 |
| C | -3.94404000 | -0.80974700 | -1.49855400 |
| H | -2.73376600 | 0.08907200 | -3.03402600 |
| H | -4.44621900 | -1.50010400 | -2.16685700 |
| C | 2.84770400 | 0.92121300 | -0.32019700 |
| C | 2.34911400 | 0.67478200 | -1.61950100 |
| C | 3.51307500 | -0.13745400 | 0.34568700 |
| C | 2.58778500 | -0.59392600 | -2.21946900 |
| C | 3.72581500 | -1.34442600 | -0.25987400 |
| H | 3.90840500 | 0.01275700 | 1.34503600 |
| C | 3.26783500 | -1.57603800 | -1.56712300 |
| H | 2.19638100 | -0.74187400 | -3.21954200 |
| H | 3.44771500 | -2.53585400 | -2.03980000 |
| O | -1.44450900 | 1.81592400 | -1.58451500 |
| O | 1.58117400 | 1.53044500 | -2.23903500 |
| S | -5.47338700 | -1.96940700 | 0.50957700 |
| S | 4.60744500 | -2.66808300 | 0.58473000 |
| O | 5.77061900 | -2.97959800 | -0.29041000 |
| O | 3.63183800 | -3.78950700 | 0.66769800 |
| O | 4.99588900 | -2.12447800 | 1.91224400 |
| O | -4.76651000 | -2.76372100 | 1.55495300 |
| O | -5.92863700 | -2.79552100 | -0.64245100 |
| O | -6.55802000 | -1.12037100 | 1.08206100 |
| H | -0.33129400 | 1.14075000 | 1.89491800 |
| H | -2.25790500 | 2.97027700 | 0.70699300 |
| H | 2.27939200 | 3.01335600 | -0.09683800 |
| Pd | 0.34688800 | 1.49282200 | -0.62060600 |
| C | 1.36361100 | 3.06447600 | 2.32758000 |
| C | -0.01108700 | 3.16714100 | 1.67962400 |
| H | -0.68835300 | 3.63449400 | 2.40381700 |
| H | -0.00033700 | 3.82205400 | 0.80261400 |
| H | 1.22754200 | 2.80478300 | 3.38085700 |
| H | 1.80428000 | 4.07407800 | 2.31043100 |
| H | 2.91447400 | 1.77114800 | 2.45070300 |

45

RS N-dissoc, E(SCF) = -2254.80703749,
E(ZPE) = -2254.485070, E(G) = -2254.543491
a.u.

| | | | |
|---|-------------|------------|------------|
| N | -0.19493100 | 1.16369900 | 1.44220500 |
| N | 3.12580400 | 2.13747400 | 1.80278300 |
| C | -1.63672300 | 1.50255100 | 1.58462600 |
| H | -1.96832000 | 1.21501600 | 2.58826500 |

| | | | |
|----|-------------|-------------|-------------|
| C | 3.03823500 | 2.32185000 | 0.36448600 |
| H | 4.00967400 | 2.71099300 | 0.03420500 |
| C | -2.50312000 | 0.88381100 | 0.54571500 |
| C | -2.31043500 | 1.28614900 | -0.79454000 |
| C | -3.51585500 | -0.00358200 | 0.86898900 |
| C | -3.19556500 | 0.79342300 | -1.76915900 |
| C | -4.36934800 | -0.48613600 | -0.10920100 |
| H | -3.65757600 | -0.31581700 | 1.89908300 |
| C | -4.21080300 | -0.07468700 | -1.42789800 |
| H | -3.05667800 | 1.11265300 | -2.79649400 |
| H | -4.88593800 | -0.44759900 | -2.19208300 |
| C | 2.78464300 | 1.00895100 | -0.35074400 |
| C | 2.31136500 | 0.91621900 | -1.71577700 |
| C | 3.36304500 | -0.15914100 | 0.20485600 |
| C | 2.45980900 | -0.31401500 | -2.42115200 |
| C | 3.46307600 | -1.32358400 | -0.49659700 |
| H | 3.78367300 | -0.08956200 | 1.20248000 |
| C | 3.02787100 | -1.40033000 | -1.83297000 |
| H | 2.09172500 | -0.34280800 | -3.44017800 |
| H | 3.13664000 | -2.33645400 | -2.36822600 |
| O | -1.35012000 | 2.12195400 | -1.11994100 |
| O | 1.60853000 | 1.88142900 | -2.22056200 |
| S | -5.68513000 | -1.63620900 | 0.29361100 |
| S | 4.21106200 | -2.75768700 | 0.30677200 |
| O | 4.10510200 | -3.86619700 | -0.67790900 |
| O | 3.40356800 | -2.98028100 | 1.53710800 |
| O | 5.61510900 | -2.36233800 | 0.60163200 |
| O | -5.60196800 | -1.85989800 | 1.76381700 |
| O | -5.40855600 | -2.86874300 | -0.49959900 |
| O | -6.95267900 | -0.96991700 | -0.12354400 |
| H | -0.07400700 | 0.17991600 | 1.68357100 |
| H | -1.69046500 | 2.59395800 | 1.51253800 |
| H | 2.30093500 | 3.07971800 | 0.06049000 |
| Pd | 0.50047000 | 1.44303100 | -0.51319600 |
| C | 2.05180400 | 1.50263700 | 2.54631300 |
| C | 0.61358100 | 1.98770600 | 2.37567100 |
| H | 0.11493100 | 1.97126900 | 3.35204000 |
| H | 0.57958100 | 3.02088000 | 2.01566000 |
| H | 2.06606300 | 0.41901200 | 2.36951500 |
| H | 2.31593400 | 1.62000500 | 3.59888800 |
| H | 3.39980100 | 3.00454300 | 2.24246700 |

45
RR-hs_RS_I1, E(SCF) = -2254.80820340,
E(ZPE) = -2254.486205, E(G) = -2254.545442
a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 0.19868300 | -1.21255600 | 1.42928600 |
| N | -3.11981200 | -2.18263700 | 1.79703200 |
| C | 1.64229700 | -1.55266000 | 1.55105500 |
| H | 1.98101300 | -1.29224400 | 2.55965400 |
| C | -3.04402700 | -2.33114700 | 0.35407300 |
| H | -4.02457700 | -2.69447300 | 0.02064100 |
| C | 2.49889800 | -0.90429300 | 0.52243100 |
| C | 2.29877000 | -1.27563900 | -0.82576900 |
| C | 3.50841100 | -0.01884000 | 0.86057300 |
| C | 3.17398700 | -0.75328000 | -1.79415400 |
| C | 4.35171000 | 0.49322700 | -0.11143500 |
| H | 3.65485500 | 0.26890000 | 1.89711300 |
| C | 4.18603700 | 0.11285000 | -1.43870100 |
| H | 3.02994600 | -1.04774400 | -2.82817200 |
| H | 4.85330400 | 0.50862200 | -2.19831800 |
| C | -2.77149900 | -1.00681500 | -0.33260300 |
| C | -2.32623100 | -0.89811000 | -1.70482000 |
| C | -3.33557000 | 0.16129800 | 0.25186500 |
| C | -2.48186500 | 0.34357900 | -2.39518600 |
| C | -3.45123600 | 1.32702700 | -0.43704400 |
| H | -3.73594500 | 0.09518400 | 1.25654300 |
| C | -3.03842500 | 1.41902400 | -1.78512400 |
| H | -2.13118100 | 0.38266800 | -3.41987700 |
| H | -3.15388100 | 2.35840000 | -2.31581100 |
| O | 1.34053800 | -2.10848100 | -1.16321200 |
| O | -1.63638600 | -1.85680200 | -2.23459700 |
| S | 5.66758700 | 1.63607400 | 0.31072300 |
| S | -4.17505500 | 2.78777200 | 0.32776900 |
| O | -5.35611900 | 3.12029600 | -0.51442400 |
| O | -3.10689900 | 3.82211400 | 0.25790800 |
| O | -4.52858200 | 2.39563800 | 1.71653500 |

| | | | |
|----|-------------|-------------|-------------|
| O | 5.58032200 | 1.84025400 | 1.78359200 |
| O | 5.39552400 | 2.87940100 | -0.46703200 |
| O | 6.93577700 | 0.97366200 | -0.11107700 |
| H | 0.07835800 | -0.23572200 | 1.69728600 |
| H | 1.69680800 | -2.64158400 | 1.44800400 |
| H | -2.32223700 | -3.09412100 | 0.02654800 |
| Pd | -0.50899200 | -1.44708400 | -0.52784800 |
| C | -2.03484900 | -1.57898200 | 2.55059500 |
| C | -0.60021300 | -2.06161500 | 2.34876500 |
| H | -0.08990100 | -2.07287400 | 3.31918300 |
| H | -0.57214400 | -3.08456000 | 1.96020500 |
| H | -2.04714300 | -0.49022100 | 2.41315900 |
| H | -2.28840300 | -1.73301700 | 3.60111400 |
| H | -3.39841200 | -3.05895600 | 2.21498700 |

45
RR-hs_RS_TS1, E(SCF) = -2254.81249592,
E(ZPE) = -2254.490504, E(G) = -2254.547779
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -0.08466100 | -1.31966300 | 1.53193600 |
| N | -2.74334500 | -2.71322200 | 1.01750400 |
| C | 1.36844800 | -1.58332100 | 1.71022300 |
| H | 1.68516400 | -1.19475100 | 2.68408700 |
| C | -3.60107400 | -1.96622400 | 0.10912300 |
| H | -4.55288200 | -1.66438300 | 0.57409100 |
| C | 2.22556700 | -1.04099100 | 0.62048700 |
| C | 2.05101100 | -1.56949100 | -0.68461000 |
| C | 3.22383600 | -0.12042100 | 0.86910800 |
| C | 2.94424900 | -1.15808200 | -1.68534000 |
| C | 4.08730500 | 0.28337000 | -0.14258900 |
| H | 3.34608100 | 0.27765400 | 1.87341700 |
| C | 3.94875000 | -0.24653800 | -1.41532400 |
| H | 2.82242700 | -1.57107900 | -2.68114300 |
| H | 4.63162700 | 0.06735200 | -2.19671000 |
| C | -2.93691100 | -0.72182600 | -0.43463700 |
| C | -2.28201400 | -0.69563900 | -1.72227100 |
| C | -3.22751000 | 0.52505000 | 0.17106700 |
| C | -2.00680400 | 0.56395900 | -2.33492500 |
| C | -2.91098600 | 1.70754300 | -0.43020900 |
| H | -3.75858200 | 0.54803800 | 1.11771000 |
| C | -2.31967000 | 1.72975900 | -1.70940100 |
| H | -1.53685800 | 0.54778000 | -3.31156000 |
| H | -2.10149200 | 2.68294200 | -2.17956800 |
| O | 1.10018400 | -2.43771800 | -0.94157600 |
| O | -1.80971500 | -1.79645400 | -2.22148300 |
| S | 5.35507300 | 1.49578100 | 0.23011900 |
| S | -3.28593700 | 3.27948600 | 0.36491100 |
| O | -4.22717600 | 3.96842900 | -0.55967100 |
| O | -1.97441900 | 3.97422900 | 0.47641700 |
| O | -3.88888400 | 2.94001000 | 1.67996900 |
| O | 4.62959700 | 2.73129500 | 0.64559700 |
| O | 6.13777400 | 1.67564300 | -1.02418900 |
| O | 6.16366600 | 0.91662800 | 1.34202400 |
| H | -0.25507600 | -0.33069900 | 1.71740000 |
| H | 1.46609100 | -2.67333300 | 1.73902200 |
| H | -3.84139500 | -2.62711800 | -0.72715500 |
| Pd | -0.74843200 | -1.62971100 | -0.42956000 |
| C | -2.36357300 | -2.06178700 | 2.26773700 |
| C | -0.86977700 | -2.12812800 | 2.49913100 |
| H | -0.62086800 | -1.80647300 | 3.51704000 |
| H | -0.53527200 | -3.16295600 | 2.38494600 |
| H | -2.68671800 | -1.01734600 | 2.26720100 |
| H | -2.85927800 | -2.52598100 | 3.12676200 |
| H | -3.11853000 | -3.63691700 | 1.18550600 |

45
RR-hs_RS_TS3, E(SCF) = -2254.79454680,
E(ZPE) = -2254.472712, E(G) = -2254.529974
a.u.

| | | | |
|---|-------------|------------|-------------|
| N | -0.58382300 | 1.87322000 | 1.23326100 |
| N | 2.21758200 | 2.03887600 | 1.77100500 |
| C | -2.06223600 | 1.97924200 | 1.12991200 |
| H | -2.49737400 | 1.95499600 | 2.13398000 |
| C | 2.82439900 | 2.24010600 | 0.45399800 |
| H | 3.85471900 | 2.61187100 | 0.54357500 |
| C | -2.68432000 | 0.95058400 | 0.25149200 |
| C | -2.33818900 | 0.96423400 | -1.12221400 |

| | | | |
|----|-------------|-------------|-------------|
| C | -3.62384000 | 0.05510400 | 0.71929400 |
| C | -2.99272900 | 0.07158400 | -1.98097600 |
| C | -4.25437100 | -0.82912900 | -0.14895700 |
| H | -3.88167300 | 0.05168400 | 1.77521700 |
| C | -3.94404000 | -0.80974700 | -1.49855400 |
| H | -2.73376600 | 0.08907200 | -3.03402600 |
| H | -4.44621900 | -1.50010400 | -2.16685700 |
| C | 2.84770400 | 0.92121300 | -0.30197000 |
| C | 2.34911400 | 0.67478200 | -1.61950100 |
| C | 3.51307500 | -0.13745400 | 0.34568700 |
| C | 2.58778500 | -0.59392600 | -2.21946900 |
| C | 3.72581500 | -1.34442600 | -0.25987400 |
| H | 3.90840500 | 0.01275700 | 1.34503600 |
| C | 3.26783500 | -1.57603800 | -1.56712300 |
| H | 2.19638100 | -0.74187400 | -3.21954200 |
| H | 3.44771500 | -2.53585400 | -2.03980000 |
| O | -1.44450900 | 1.81592400 | -1.58451500 |
| O | 1.58117400 | 1.53044500 | -2.23903500 |
| S | -5.47338700 | -1.96940700 | 0.50957700 |
| S | 4.60744500 | -2.66808300 | 0.58473000 |
| O | 5.77061900 | -2.97959800 | -0.29041000 |
| O | 3.63183800 | -3.78950700 | 0.66769800 |
| O | 4.99588900 | -1.12447800 | 1.91224400 |
| O | -4.76651000 | -2.76372100 | 1.55495300 |
| O | -5.92863700 | -2.79552100 | -0.64245100 |
| O | -6.55802000 | -1.12037100 | 1.08206100 |
| H | -0.33129400 | 1.14075000 | 1.89491800 |
| H | -2.25790500 | 2.97027700 | 0.70699300 |
| H | 2.27939200 | 3.01335600 | -0.09683800 |
| Pd | 0.34688800 | 1.49282200 | -0.62060600 |
| C | 1.36361100 | 3.06447600 | 2.32758000 |
| C | -0.01108700 | 3.16714100 | 1.67962400 |
| H | -0.68835300 | 3.63449400 | 2.40381700 |
| H | -0.00033700 | 3.82205400 | 0.80261400 |
| H | 1.22754200 | 2.80478300 | 3.38885700 |
| H | 1.80428000 | 4.07407800 | 2.31043100 |
| H | 2.91447400 | 1.77114800 | 2.45070300 |

45

RR-hs_RS_I2, E(SCF) = -2254.80845463,
E(ZPE) = -2254.486600, E(G) = -2254.545269
a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 0.23602000 | -1.19075100 | 1.42686700 |
| N | -2.98974400 | -2.34972700 | 1.79482400 |
| C | 1.67822000 | -1.53572000 | 1.54210900 |
| H | 2.02117900 | -1.28264900 | 2.55121000 |
| C | -3.01591100 | -2.36416600 | 0.34023800 |
| H | -4.00968800 | -2.72370900 | 0.05101100 |
| C | 2.53268800 | -0.88151500 | 0.51544700 |
| C | 2.32440400 | -1.23853100 | -0.83507200 |
| C | 3.54850300 | -0.00487800 | 0.85748100 |
| C | 3.19722800 | -0.71063900 | -1.80262400 |
| C | 4.38988100 | 0.51244100 | -0.11335300 |
| H | 3.70154800 | 0.27173300 | 1.89608100 |
| C | 4.21575000 | 0.14640200 | -1.44356500 |
| H | 3.04667700 | -0.99423300 | -2.83873800 |
| H | 4.88136500 | 0.54622100 | -2.20251800 |
| C | -2.77606400 | -1.02140000 | -0.33982300 |
| C | -2.31317400 | -0.88543100 | -1.70204600 |
| C | -3.38218500 | 0.12376300 | 0.24470200 |
| C | -2.48850300 | 0.35928600 | -2.38258500 |
| C | -3.52010100 | 1.29412700 | -0.43322300 |
| H | -3.80107900 | 0.05361300 | 1.24240200 |
| C | -3.08380300 | 1.41330200 | -1.77126500 |
| H | -2.12318400 | 0.41843600 | -3.40128100 |
| H | -3.21595300 | 2.35483300 | -2.29411500 |
| O | 1.36221400 | -2.06516500 | -1.17657700 |
| O | -1.59787500 | -1.82447200 | -2.23570700 |
| S | 5.71409100 | 1.64318000 | 0.31513800 |
| S | -4.30111400 | 2.72333200 | 0.33599100 |
| O | -5.47103500 | 3.03626700 | -0.52858600 |
| O | -3.25997600 | 3.78654800 | 0.30715800 |
| O | -4.67514900 | 2.29859400 | 1.70977800 |
| O | 5.63066500 | 1.83613500 | 1.78973500 |
| O | 5.44870500 | 2.89432200 | -0.45228200 |
| O | 6.97721000 | 0.97588000 | -0.11404600 |
| H | 0.12134300 | -0.21255200 | 1.69182300 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.73016600 | -2.62414100 | 1.43199300 |
| H | -2.31884700 | -3.11621200 | -0.04261500 |
| Pd | -0.48744600 | -1.42419400 | -0.52424400 |
| C | -1.99679300 | -1.57169500 | 2.51877800 |
| C | -0.55819600 | -2.03293900 | 2.35652000 |
| H | -0.05716200 | -2.01753700 | 3.33106400 |
| H | -0.51561200 | -3.06163200 | 1.98675900 |
| H | -2.02941900 | -0.49125800 | 2.29849900 |
| H | -2.26226800 | -1.66225000 | 3.57366900 |
| H | -3.90785900 | -2.14589300 | 2.16399400 |

45

RR-hs_RS_TS2, E(SCF) = -2254.80535224,
E(ZPE) = -2254.484560, E(G) = -2254.542863
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 0.17443400 | -1.19710500 | 1.44385100 |
| N | -3.05736500 | -2.25192100 | 1.73721100 |
| C | 1.62048300 | -1.51907500 | 1.58264800 |
| H | 1.95004300 | -1.22892500 | 2.58631100 |
| C | -3.08804500 | -2.33415200 | 0.30260800 |
| H | -4.10515700 | -2.63067700 | 0.01873800 |
| C | 2.48186500 | -0.89303800 | 0.54410900 |
| C | 2.29135700 | -1.29568800 | -0.79648700 |
| C | 3.49312500 | -0.00464100 | 0.86916800 |
| C | 3.17619600 | -0.79938400 | -1.76993400 |
| C | 4.34677500 | 0.48038400 | -0.10767500 |
| H | 3.63408200 | 0.30851400 | 1.89991700 |
| C | 4.18940700 | 0.07043800 | -1.42705200 |
| H | 3.03896800 | -1.11782000 | -2.79777900 |
| H | 4.86445900 | 0.44532400 | -2.19037600 |
| C | -2.78164000 | -1.00397300 | -0.36727700 |
| C | -2.30349700 | -0.88052200 | -1.72587700 |
| C | -3.34239100 | 0.16094600 | 0.22498700 |
| C | -2.43179800 | 0.37282400 | -2.40160900 |
| C | -3.42939300 | 1.33881300 | -0.44680800 |
| H | -3.76176900 | 0.08198000 | 1.22150700 |
| C | -2.98829500 | 1.44502000 | -1.78557200 |
| H | -2.06040900 | 0.42430400 | -3.41850100 |
| H | -3.08172800 | 2.39369600 | -2.30391400 |
| O | 1.33415100 | -2.13401900 | -1.12222100 |
| O | -1.60992100 | -1.83958500 | -2.25052100 |
| S | 5.66266700 | 1.62882500 | 0.29826500 |
| S | -4.14748700 | 2.79796900 | 0.32625600 |
| O | -5.31134900 | 3.15666300 | -0.52906400 |
| O | -3.06589500 | 3.82001200 | 0.28716900 |
| O | -4.52692800 | 2.39158500 | 1.70406800 |
| O | 5.57887800 | 1.84952400 | 1.76897400 |
| O | 5.38783800 | 2.86347100 | -0.49240300 |
| O | 6.93035900 | 0.96285200 | -0.11932900 |
| H | 0.04174100 | -0.21571500 | 1.68922600 |
| H | 1.68600500 | -2.60989000 | 1.51053900 |
| H | -2.43241600 | -3.11965000 | -0.10109500 |
| Pd | -0.52084600 | -1.45880700 | -0.51406300 |
| C | -2.06632000 | -1.58740100 | 2.53443900 |
| C | -0.61546100 | -2.03113200 | 2.38473400 |
| H | -0.12221600 | -1.98411000 | 3.36327700 |
| H | -0.55556200 | -3.06651300 | 2.03710300 |
| H | -2.08637500 | -0.49019100 | 2.40991300 |
| H | -2.35295000 | -1.75872000 | 3.57323500 |
| H | -3.81143500 | -2.68985300 | 2.22926300 |

48

RS_W-inside_P, E(SCF) = -2331.26459262,
E(ZPE) = -2330.915342, E(G) = -2330.976341
a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | -1.77999900 | 2.16083500 | -0.24382500 |
| C | -2.08537400 | 1.03588500 | -1.16273100 |
| H | -1.13592100 | 0.57911200 | -1.45804400 |
| C | -2.98808300 | 0.01486200 | -0.53051700 |
| C | -2.50609900 | -1.10826900 | 0.19689000 |
| C | -4.36085900 | 0.19449400 | -0.67002600 |
| C | -3.46828600 | -1.99217400 | 0.73443900 |
| C | -5.27779400 | -0.68573400 | -0.12988200 |
| H | -4.72524500 | 1.04747600 | -1.23598200 |
| C | -4.81947100 | -1.79160000 | 0.57755200 |
| H | -3.09838200 | -2.85077500 | 1.73481100 |
| H | -5.52684400 | -2.49511800 | 1.00580400 |

| | | | |
|----|-------------|-------------|-------------|
| O | -1.24177900 | -1.41741600 | 0.38874300 |
| S | -7.04086800 | -0.41015500 | -0.29383300 |
| O | -7.54127200 | -0.13876200 | 1.08559200 |
| O | -7.60406600 | -1.66980400 | -0.85996100 |
| O | -7.19454200 | 0.75787000 | -1.20528700 |
| H | -2.59815100 | 2.75885100 | -0.19980500 |
| H | -2.55019600 | 1.41355400 | -2.08221800 |
| Pd | 0.14505500 | 0.06133000 | 0.57553900 |
| C | -0.60505000 | 2.97003500 | -0.61868800 |
| C | 0.49887200 | 3.00794300 | 0.43141100 |
| H | 1.16461000 | 3.84781300 | 0.20398400 |
| H | 0.06711400 | 3.20189500 | 1.41427400 |
| H | -0.20791700 | 2.62674000 | -1.57968600 |
| H | -0.91210900 | 4.00630500 | -0.77792600 |
| O | -1.08453000 | 0.98293500 | 2.02967400 |
| H | -1.58729500 | 1.52259300 | 1.34057400 |
| H | -1.69673000 | 0.33894700 | 2.40582600 |
| N | 1.33435300 | 1.77807400 | 0.53893300 |
| C | 2.36202000 | 1.71219800 | -0.53206600 |
| H | 2.98786400 | 2.60952300 | -0.47834100 |
| C | 3.20354300 | 0.48684900 | -0.44606800 |
| C | 2.58525000 | -0.76920200 | -0.61558900 |
| C | 4.57575700 | 0.56605200 | -0.26436200 |
| C | 3.39911200 | -1.91354900 | -0.64365800 |
| C | 5.35788400 | -0.57507500 | -0.27880500 |
| H | 5.04958200 | 1.53265000 | -0.12407300 |
| C | 4.76465600 | -1.81548700 | -0.48319100 |
| H | 2.92237100 | -2.87666000 | -0.78982900 |
| H | 5.37967400 | -2.70979100 | -0.50251600 |
| O | 1.28395700 | -0.88672800 | -0.78679600 |
| S | 7.13555900 | -0.48381400 | -0.05099300 |
| O | 7.44262900 | -1.35922900 | 1.11631200 |
| O | 7.44613900 | 0.95089000 | 0.19969200 |
| O | 7.73533000 | -0.99692100 | -1.31612500 |
| H | 1.82422100 | 1.73543500 | -1.48514200 |
| H | 1.82389700 | 1.81536500 | 1.43196500 |

48

RS W-inside R, E(SCF) = -2331.29751380,
E(ZPE) = -2330.949679, E(G) = -2331.012590
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.44480700 | 1.74571600 | -0.11343700 |
| C | -2.53129800 | 1.40988800 | -1.05579700 |
| H | -2.04438400 | 1.17613300 | -2.00962800 |
| C | -3.36237900 | 0.26795400 | -0.56795600 |
| C | -2.77261500 | -0.98933600 | -0.28540000 |
| C | -4.73724000 | 0.42901000 | -0.45159600 |
| C | -3.63806100 | -2.04559800 | 0.07166500 |
| C | -5.55970200 | -0.62048300 | -0.09012500 |
| H | -5.18215400 | 1.39668500 | -0.66186200 |
| C | -4.99870100 | -1.86756500 | 0.16666400 |
| H | -3.19003700 | -3.01213100 | 0.27682400 |
| H | -5.63676000 | -2.69988700 | 0.44826000 |
| O | -1.48961200 | -1.23650400 | -0.36340000 |
| S | -7.33015600 | -0.40158500 | 0.07279200 |
| O | -7.65123800 | -0.70073000 | 1.49886800 |
| O | -7.95429800 | -1.38220300 | -0.86248200 |
| O | -7.60887500 | 1.01384400 | -0.29907000 |
| H | -1.85067800 | 1.92583000 | 0.80545000 |
| H | -3.16235300 | 2.29175700 | -1.21330700 |
| Pd | -0.09750900 | 0.19990300 | 0.02077200 |
| C | -0.62969000 | 2.90953000 | -0.52955200 |
| C | 0.58474600 | 2.97377200 | 0.36125900 |
| H | 1.25971300 | 3.77712200 | 0.05286300 |
| H | 0.27866000 | 3.17339500 | 1.39210200 |
| H | -0.34369600 | 2.74888100 | -1.57261600 |
| H | -1.21445800 | 3.83308300 | -0.47914900 |
| O | 1.95618200 | 1.00905800 | 3.10449500 |
| H | 1.33394300 | 0.30987000 | 3.32612700 |
| H | 2.82387900 | 0.62268500 | 3.25459000 |
| N | 1.28861000 | 1.66928400 | 0.36538000 |
| C | 2.35938100 | 1.50879900 | -0.63435200 |
| H | 3.00665800 | 2.39329300 | -0.61369300 |
| C | 3.18748900 | 0.28931500 | -0.35058000 |
| C | 2.61531600 | -0.97541300 | -0.05527700 |
| C | 4.57170600 | 0.41842500 | -0.39681600 |
| C | 3.50398100 | -2.05333200 | 0.16083300 |

| | | | |
|---|------------|-------------|-------------|
| C | 5.41486100 | -0.65396300 | -0.18470600 |
| H | 5.00822200 | 1.38923600 | -0.61098400 |
| C | 4.86782600 | -1.90158300 | 0.09819000 |
| H | 3.06392500 | -3.01965500 | 0.38359300 |
| H | 5.51804200 | -2.75349300 | 0.27183800 |
| O | 1.33519100 | -1.23498000 | 0.02862100 |
| S | 7.19472400 | -0.46195900 | -0.22145500 |
| O | 7.67073900 | -0.76807700 | 1.15978300 |
| O | 7.45341200 | 0.94949700 | -0.62278300 |
| O | 7.69463600 | -1.45151000 | -1.21967700 |
| H | 1.89247300 | 1.47373600 | -1.62607900 |
| H | 1.68190500 | 1.50595300 | 1.30156300 |

48

RS W-inside TS, E(SCF) = -2331.25704001,
E(ZPE) = -2330.910054, E(G) = -2330.971454
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.56623800 | 1.96790400 | -0.24315500 |
| C | -2.21869500 | 1.14583900 | -1.26328200 |
| H | -1.42595100 | 0.68958500 | -1.86880600 |
| C | -3.06892200 | 0.08846500 | -0.61820000 |
| C | -2.50910600 | -1.03344900 | 0.05140700 |
| C | -4.45065800 | 0.22847900 | -0.66745900 |
| C | -3.40409300 | -1.95494900 | 0.63559100 |
| C | -5.30415200 | -0.69681000 | -0.09485100 |
| H | -4.87604100 | 1.08458800 | -1.18286800 |
| C | -4.76930600 | -1.79741900 | 0.56296300 |
| H | -2.97286900 | -2.81142100 | 1.14319100 |
| H | -5.42639100 | -2.53040200 | 1.02088500 |
| O | -1.22628500 | -1.30920100 | 0.12908000 |
| S | -7.08190500 | -0.47665800 | -0.14467100 |
| O | -7.50410800 | -0.22951000 | 1.26550900 |
| O | -7.63927600 | -1.75028900 | -0.68450300 |
| O | -7.33103000 | 0.69097000 | -1.03560600 |
| H | -2.27029300 | 2.43706400 | 0.31869200 |
| H | -2.84245500 | 1.74144000 | -1.94586700 |
| Pd | 0.10945000 | 0.18500700 | 0.39148100 |
| C | -0.55133300 | 2.91995200 | -0.68585700 |
| C | 0.52096700 | 3.06918500 | 0.37634000 |
| H | 1.17338100 | 3.92088700 | 0.15616300 |
| H | 0.04941400 | 3.25334800 | 1.34400700 |
| H | -0.11344400 | 2.54883400 | -1.61796400 |
| H | -0.96813400 | 3.90870800 | -0.91219300 |
| O | -0.84407700 | 0.71899300 | 2.42285400 |
| H | -1.75874500 | 0.97017000 | 2.24907500 |
| H | -0.89581600 | -0.08105300 | 2.95758800 |
| N | 1.35456700 | 1.84005300 | 0.51117300 |
| C | 2.45342800 | 1.80661800 | -0.48696400 |
| H | 3.10578200 | 2.67073700 | -0.32223000 |
| C | 3.24477700 | 0.54533900 | -0.44656400 |
| C | 2.59403900 | -0.67057700 | -0.75137100 |
| C | 4.60599700 | 0.55931700 | -0.18621900 |
| C | 3.37585000 | -1.83729100 | -0.82945000 |
| C | 5.35325100 | -0.60397200 | -0.25212500 |
| H | 5.10078300 | 1.49537700 | 0.05370800 |
| C | 4.73177400 | -1.80232200 | -0.58607300 |
| H | 2.87893200 | -2.76839200 | -1.07983200 |
| H | 5.31809500 | -2.71421200 | -0.64575700 |
| O | 1.30532400 | -0.72987400 | -0.99837900 |
| S | 7.11339500 | -0.59834000 | -0.08973000 |
| O | 7.30627500 | -1.51320100 | 1.25179800 |
| O | 7.47170600 | 0.81439400 | 0.39698800 |
| O | 7.77220700 | -1.10998000 | -1.14667400 |
| H | 1.98371200 | 1.92675600 | -1.46848900 |
| H | 1.77437000 | 1.83613800 | 1.43967300 |

45

RS, E(SCF) = -2254.86059075, E(ZPE) = -
2254.536712, E(G) = -2254.594688 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | -1.37387800 | 1.77737700 | 0.13345200 |
| N | 1.35504600 | 1.69182700 | 0.67446400 |
| C | -2.42834500 | 1.48383800 | -0.85858200 |
| H | -3.05667500 | 2.37115400 | -0.99419600 |
| C | 2.42489000 | 1.57998900 | -0.33934000 |
| H | 3.07203300 | 2.46196100 | -0.27707600 |
| C | -3.27034000 | 0.31831300 | -0.45296700 |
| C | -2.68401000 | -0.94753900 | -0.20813300 |

| | | | |
|----|-------------|-------------|-------------|
| C | -4.64951600 | 0.46773500 | -0.38147800 |
| C | -3.55367000 | -2.02293500 | 0.07109500 |
| C | -5.47742900 | -0.60128400 | -0.09830200 |
| H | -5.09194500 | 1.44213000 | -0.56415500 |
| C | -4.91800500 | -1.85590300 | 0.12229600 |
| H | -3.10684700 | -2.99546300 | 0.24819000 |
| H | -5.56038200 | -2.70315200 | 0.34225700 |
| C | 3.25267700 | 0.34587700 | -0.13227500 |
| C | 2.68615100 | -0.93434500 | 0.09879600 |
| C | 4.63648700 | 0.47907500 | -0.19781600 |
| C | 3.57959700 | -2.02215500 | 0.23465900 |
| C | 5.48314300 | -0.60162000 | -0.06204500 |
| H | 5.06870200 | 1.46130700 | -0.36207400 |
| C | 4.94131100 | -1.86514500 | 0.15426800 |
| H | 3.14392500 | -3.00036200 | 0.40853800 |
| H | 5.59542100 | -2.72423500 | 0.26722500 |
| O | -1.39704400 | -1.18666700 | -0.25469800 |
| O | 1.40864000 | -1.20189400 | 0.19345500 |
| S | -7.25568900 | -0.40369500 | -0.00467600 |
| S | 7.26146100 | -0.41056400 | -0.15184400 |
| O | 7.70493300 | -1.22897600 | -1.31789900 |
| O | 7.79680900 | -0.93411300 | 1.13852600 |
| O | 7.51387000 | 1.04611000 | -0.33639100 |
| O | -7.53084400 | 1.02806500 | -0.31034400 |
| O | -7.63945300 | -0.78433800 | 1.38593000 |
| O | -7.82578000 | -1.33535800 | -1.02074500 |
| H | -1.81027200 | 1.91638600 | 1.04542000 |
| H | -1.90975200 | 1.29674700 | -1.80606500 |
| H | 1.94535800 | 1.59823800 | -1.32471400 |
| Pd | -0.02571100 | 0.22881500 | 0.23720600 |
| C | 0.63944300 | 2.99399600 | 0.71372000 |
| C | -0.55098700 | 2.95941500 | -0.20914900 |
| H | -1.13825400 | 3.87929900 | -0.13184800 |
| H | -0.24096200 | 2.84734900 | -1.25144700 |
| H | 0.30513400 | 3.14649400 | 1.74230000 |
| H | 1.31645900 | 3.81318900 | 0.45688700 |
| H | 1.77280400 | 1.52068300 | 1.58701700 |

53
RS_delta_hs_D1_TS1_I1_P, E(SCF) = -
2408.92362684, E(ZPE) = -2408.529927, E(G)
= -2408.595630 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.97149500 | 0.64608000 | -1.55468700 |
| H | 0.93817800 | 1.60041500 | -2.09104900 |
| H | 1.47299400 | 0.82683700 | -0.60119100 |
| C | 1.71393300 | -0.38380700 | -2.37978000 |
| H | 1.19285600 | -0.52628000 | -3.32996800 |
| H | 2.72704900 | -0.04361800 | -2.61411200 |
| N | 1.73658100 | -1.71384100 | -1.70529100 |
| C | 2.91869700 | -1.95317100 | -0.81165700 |
| H | 2.74646200 | -2.91432000 | -0.32386700 |
| C | 3.20102600 | -0.84996200 | 0.16134100 |
| C | 2.59363300 | -0.74182600 | 1.41757800 |
| C | 4.09191600 | 0.15404400 | -0.22118000 |
| C | 2.81316200 | 0.39190800 | 2.20233100 |
| C | 4.31164500 | 1.26777400 | 0.55916400 |
| H | 4.61144100 | 0.07367700 | -1.17071000 |
| C | 3.65386600 | 1.39493400 | 1.77662300 |
| H | 3.81283400 | 2.27215400 | 2.39436400 |
| O | 1.76531300 | -1.66119900 | 1.94693300 |
| S | 5.45651500 | 2.55151600 | 0.03118100 |
| O | 6.58640100 | 2.50119900 | 1.00033600 |
| O | 4.68853600 | 3.82448100 | 0.11056700 |
| O | 5.85714700 | 2.19135500 | -1.35550900 |
| H | 0.02816000 | -3.51510500 | -0.71638200 |
| H | 0.88972900 | -4.40278900 | 0.64089200 |
| H | 1.80214800 | -2.42137500 | -2.43201300 |
| H | 3.79613100 | -2.07400600 | -1.45521700 |
| Pd | -0.16061900 | -1.96168400 | -0.88240900 |
| H | 2.30934500 | 0.45389300 | 3.16001300 |
| H | 1.78168100 | -2.54451300 | 1.51737600 |
| O | 1.19762100 | -4.28916200 | 1.55098600 |
| H | 0.39460000 | -3.95907900 | 2.00366100 |
| H | -0.23582400 | -1.98171400 | 2.52549500 |
| O | -0.90599800 | -2.67853100 | 2.51059800 |
| H | -1.37515900 | -2.52240300 | 1.66380500 |
| N | -0.37954800 | 0.14343300 | -1.26394800 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.05457900 | 0.75752000 | -0.11198000 |
| H | -1.02145600 | 1.85195100 | -0.18050300 |
| C | -2.48340800 | 0.30749100 | -0.02640400 |
| C | -2.84618300 | -1.06079200 | 0.03400100 |
| C | -3.47910700 | 1.27808600 | 0.01720400 |
| C | -4.21781300 | -1.36793200 | 0.13737300 |
| C | -4.81587100 | 0.94866700 | 0.12481200 |
| H | -3.20113800 | 2.32645400 | -0.02974900 |
| C | -5.18374200 | -0.39023000 | 0.18838400 |
| H | -4.48969800 | -2.41711000 | 0.18265100 |
| H | -6.23137000 | -0.66293700 | 0.26985200 |
| O | -2.00056700 | -2.07395100 | 0.02854600 |
| S | -6.08628700 | 2.21247800 | 0.17661500 |
| O | -6.83133700 | 1.99062300 | 1.44945900 |
| O | -6.94185000 | 1.98374200 | -1.19831600 |
| O | -5.37330700 | 3.51985000 | 0.14035400 |
| H | -0.48180000 | 0.47191600 | 0.78076700 |
| H | -0.96924100 | 0.25441000 | -2.08694800 |

53
RS_delta_hs_D1_TS1_P_I1, E(SCF) = -
2408.89303230, E(ZPE) = -2408.501514, E(G)
= -2408.566851 a.u.

| | | | |
|----|-------------|-------------|--------------|
| C | 0.89634100 | 0.75079000 | -1.52397200 |
| H | 0.76965900 | 1.73677900 | -1.97942500 |
| H | 1.46458900 | 0.86670600 | -0.59829000 |
| C | 1.57475900 | 0.67465300 | -2.46657600 |
| H | 1.00997800 | -0.27704300 | -3.39911500 |
| H | 2.58500900 | 0.12904800 | -2.71207200 |
| N | 1.61195000 | -1.57345900 | -1.86813700 |
| C | 2.87599900 | 2.87443200 | -1.874370100 |
| H | 2.73698000 | -2.86601600 | -0.66678900 |
| C | 3.22554700 | -0.85608000 | -0.07448400 |
| C | 2.55523800 | -0.86245900 | 1.18335800 |
| C | 4.17056900 | 0.11985000 | -0.36374500 |
| C | 2.86947800 | 0.19833900 | 2.07403500 |
| C | 4.45426600 | 1.13622700 | 0.52954700 |
| H | 4.69003800 | 0.10363900 | -1.31833300 |
| C | 3.78648700 | 1.17094700 | 1.75363700 |
| H | 3.99715300 | 1.97168800 | 2.45693100 |
| O | 1.69054600 | -1.76366200 | 1.48519000 |
| S | 5.65848800 | 2.40068800 | 0.14667400 |
| O | 6.73881800 | 2.27830400 | 1.16996300 |
| O | 4.93712300 | 3.70371700 | 0.24844300 |
| O | 6.13768300 | 2.11127400 | -1.23506500 |
| H | -0.14688100 | -3.58253700 | -0.95885800 |
| O | 0.19014500 | -3.51041600 | -0.21127100 |
| H | 1.57791100 | -2.24372400 | -2.63311000 |
| H | 3.67624700 | -1.94007700 | -1.84860500 |
| Pd | -0.17330800 | -1.82495900 | -0.82545100 |
| H | 2.35283000 | 0.21908900 | 3.02893900 |
| H | 1.47171100 | -3.53161800 | 1.47635800 |
| O | 0.92356700 | -4.34175200 | 1.53481600 |
| H | 0.19722900 | -4.02044600 | 2.09223300 |
| H | 0.18481600 | -1.88082700 | 2.45088400 |
| O | -0.67705400 | -2.23328600 | -2.75790100 |
| H | -1.23196400 | -2.16083400 | 1.96302900 |
| N | -0.42545900 | 0.17967900 | -1.17393400 |
| C | -1.10312800 | 0.82991500 | -0.02828300 |
| H | -1.06893400 | 1.91553900 | -0.16567100 |
| C | -2.52276500 | 0.37124600 | 0.06675500 |
| C | -2.82787700 | -1.00184300 | 0.16254300 |
| C | -3.55345300 | 1.30342400 | 0.05859000 |
| C | -4.17720500 | -1.38064500 | 0.24935900 |
| C | -4.87333400 | 0.91008800 | 0.15806900 |
| H | -3.32179300 | 2.36058100 | -0.02193800 |
| C | -5.18322500 | -0.44123300 | 0.25630800 |
| H | -4.40214200 | -2.43893500 | 0.32023400 |
| H | -6.21985200 | -0.75467700 | 0.32822800 |
| O | -1.91184800 | -1.95790300 | 0.21016200 |
| S | -6.20541500 | 2.11450700 | 0.13942600 |
| O | -6.96626600 | 1.89326900 | 1.40153500 |
| O | -7.01402000 | 1.80261100 | -1.07335600 |
| O | -5.55128200 | 3.45020000 | 0.07741800 |
| H | -0.51725900 | 0.58640400 | 0.86639500 |
| H | -1.04224000 | 0.23807900 | -1.98680900 |

53
 RS_delta_hs_D1_TS1_P_V2_TS2_P, E(SCF) = -
 2408.92362684, E(ZPE) = -2408.529927, E(G)
 = -2408.595630 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.97149500 | 0.64608000 | -1.55468700 |
| H | 0.93817800 | 1.60041500 | -2.09104900 |
| H | 1.47299400 | 0.82683700 | -0.60119100 |
| C | 1.71393300 | -0.38380700 | -2.37978000 |
| H | 1.19285600 | -0.52628000 | -3.32996800 |
| H | 2.72704900 | -0.04361800 | -2.61411200 |
| N | 1.73658100 | -1.71384100 | -1.70529100 |
| C | 2.91869700 | -1.95317100 | -0.81165700 |
| H | 2.74646200 | -2.91432000 | -0.32386700 |
| C | 3.20102600 | -0.84996200 | 0.16134100 |
| C | 2.59363300 | -0.71382600 | 1.41757800 |
| C | 4.09191600 | 0.15404400 | -0.22118000 |
| C | 2.81316200 | 0.39190800 | 2.20233100 |
| C | 4.31164500 | 1.26777400 | 0.55916400 |
| H | 4.61144100 | 0.07367700 | -1.17071000 |
| C | 3.65386600 | 1.39493400 | 1.77662300 |
| H | 3.81283400 | 2.27215400 | 2.39436400 |
| O | 1.76531300 | -1.66119900 | 1.94693300 |
| S | 5.45651500 | 2.55151600 | 0.03118100 |
| O | 6.58640100 | 2.50119900 | 1.00033600 |
| O | 4.68853600 | 3.82448100 | 0.11056700 |
| O | 5.85714700 | 2.19135500 | -1.35550900 |
| H | 0.02816000 | -3.51510500 | -0.71638200 |
| H | 0.88972900 | -4.40278900 | 0.64089200 |
| H | 1.80214800 | -2.42137500 | -2.43201300 |
| H | 3.79613100 | -2.07400600 | -1.45521700 |
| Pd | -0.16061900 | -1.96168400 | -0.88240900 |
| H | 2.30934500 | 0.45389300 | 3.16001300 |
| H | 1.78168100 | -2.54451300 | 1.51737600 |
| O | 1.19762100 | -4.28916200 | 1.55098600 |
| H | 0.39460000 | -0.95907900 | 2.00366100 |
| H | -0.23582400 | -1.98171400 | 2.52549500 |
| O | -0.90599800 | -2.67853100 | 2.51059800 |
| H | -1.37515900 | -2.52240300 | 1.66380500 |
| N | -0.37954800 | 0.14343300 | -1.26394800 |
| C | -1.05457900 | 0.75752000 | -0.11198000 |
| H | -1.02145600 | 1.85195100 | -0.18050300 |
| C | -2.48340800 | 0.30749100 | -0.02640400 |
| C | -2.84618300 | -1.06079200 | 0.03400100 |
| C | -3.47910700 | 1.27808600 | 0.01720400 |
| C | -4.21781300 | -1.36793200 | 0.13737300 |
| C | -4.81587100 | 0.94866700 | 0.12481200 |
| H | -3.20113800 | 2.32645400 | -0.02974900 |
| C | -5.18374200 | -0.39023000 | 0.18838400 |
| H | -4.48969800 | -2.41711000 | 0.18265100 |
| H | -6.23137000 | -0.66293700 | 0.26985200 |
| O | -2.00056700 | -2.07395100 | 0.02854600 |
| S | -6.08628700 | 2.21247800 | 0.17661500 |
| O | -6.83133700 | 1.99062300 | 1.44945900 |
| O | -6.94185000 | 1.98374200 | -1.02416800 |
| O | -5.37330700 | 3.51985000 | 0.14035400 |
| H | -0.48180000 | 0.47191600 | 0.78076700 |
| H | -0.96924100 | 0.25441000 | -2.08694800 |

53
 RS_delta_hs_D1_TS1_P_V2_TS2, E(SCF) = -
 2408.88702139, E(ZPE) = -2408.497106, E(G)
 = -2408.560726 a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.90699600 | 0.74470900 | -1.45190200 |
| H | 0.80692400 | 1.74048800 | -1.89403300 |
| H | 1.47815000 | 0.83557300 | -0.52538100 |
| C | 1.57275500 | -0.20993200 | -2.41097400 |
| O | 0.99693600 | -0.26370200 | -3.33812400 |
| H | 2.58101100 | 0.12686300 | -2.66568900 |
| N | 1.60860600 | -1.58478300 | -1.83486600 |
| C | 2.87373000 | -1.89542800 | -1.07596400 |
| H | 2.73942700 | -2.89138300 | -0.64944800 |
| C | 3.23819300 | -0.88522500 | -0.04070500 |
| C | 2.61239000 | -0.89696300 | 1.23761500 |
| C | 4.16673000 | 0.10124200 | -0.35308400 |
| C | 2.93207500 | 0.17268300 | 2.11300500 |
| C | 4.46526000 | 1.12237400 | 0.35287900 |
| H | 4.66161200 | 0.08696900 | -1.32042300 |

| | | | |
|----|-------------|--------------|-------------|
| C | 3.82548700 | 1.15799400 | 1.76694700 |
| H | 4.04350800 | 1.96319500 | 2.46254300 |
| O | 1.77553900 | -1.80999500 | 1.59306100 |
| S | 5.62883800 | 2.41107200 | 0.09992900 |
| O | 6.67603400 | 2.40050800 | 1.16356900 |
| O | 4.85108000 | 3.68553300 | 0.09359900 |
| O | 6.16536200 | 2.05440900 | -1.24416600 |
| H | -0.06550700 | -3.52914800 | -0.84223000 |
| H | 0.26006100 | -3.67362300 | 0.04651000 |
| H | 1.57960900 | -2.24261900 | -2.61019300 |
| H | 3.67353700 | -1.95751900 | -1.82180800 |
| Pd | -0.18748300 | -1.84767300 | -0.81301100 |
| H | 2.44209800 | 0.18679700 | 3.08174800 |
| H | 1.40511100 | -3.34140700 | 1.31314800 |
| O | 0.77490800 | -4.117763100 | 1.18982200 |
| H | 0.09433000 | -3.88743600 | 1.85823600 |
| H | 0.18911500 | -1.89950600 | 2.53080300 |
| O | -0.66051300 | -2.32779600 | 2.76065400 |
| H | -1.22007700 | -2.14355200 | 0.12632300 |
| N | -0.42032700 | 0.19205900 | -1.11167400 |
| C | -1.08825800 | 0.81824100 | 0.04869400 |
| H | -1.04829500 | 1.90849400 | -0.04988800 |
| C | -2.51196500 | 0.36485800 | 0.12632300 |
| C | -2.82670900 | -1.00886800 | 0.20949100 |
| C | -3.53674600 | 1.30282400 | 0.09999000 |
| C | -4.18139600 | -1.37541000 | 0.27469500 |
| C | -4.86201100 | 0.91934500 | 0.17090000 |
| H | -3.29586300 | 2.35860900 | 0.02752100 |
| C | -5.18222200 | -0.43012100 | 0.25985400 |
| H | -4.41568600 | -2.43230900 | 0.33899500 |
| H | -6.22200400 | -0.73747500 | 0.31001700 |
| O | -1.91708800 | -1.96918100 | 0.26681300 |
| S | -6.18363700 | 2.13212500 | 0.09967500 |
| O | -7.01794400 | 1.89701700 | 1.31237000 |
| O | -6.92502500 | 1.84760400 | -1.16242400 |
| O | -5.52023500 | 3.46521300 | 0.09624400 |
| H | -0.50688500 | 0.54172900 | 0.93706700 |
| H | -1.03683900 | 0.28285400 | -1.92071500 |

53
 RS_delta_hs_D1_TS1_P_V2, E(SCF) = -
 2408.89303230, E(ZPE) = -2408.501514, E(G)
 = -2408.566851 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.89634100 | 0.75079000 | -1.52397200 |
| H | 0.76965900 | 1.73677900 | -1.97942500 |
| H | 1.46458900 | 0.86670600 | -0.59829000 |
| C | 1.57475900 | -0.20765300 | -2.46657600 |
| H | 1.00997800 | -0.27704300 | -3.39911500 |
| H | 2.58500900 | 0.12904800 | -2.71207200 |
| N | 1.61195000 | -1.57345900 | -1.86813700 |
| C | 2.87599900 | -1.87443200 | -1.10370100 |
| H | 2.73698000 | -2.86601600 | -0.66678900 |
| C | 3.22554700 | -0.85608000 | -0.07448400 |
| C | 2.55523800 | -0.86245900 | 1.18335800 |
| C | 4.17056900 | 0.11985000 | -0.36374500 |
| C | 2.86947800 | 0.19833900 | 2.07403500 |
| C | 4.45426600 | 1.13622700 | 0.52954700 |
| H | 4.69003800 | 0.10363900 | -1.31833300 |
| C | 3.78648700 | 1.17094700 | 1.75363700 |
| H | 3.99715300 | 1.97168800 | 2.45693100 |
| O | 1.69054600 | -1.76366200 | 1.48519000 |
| S | 5.65848800 | 2.40068800 | 0.14667400 |
| O | 6.73881800 | 2.27830400 | 1.16996300 |
| O | 4.93712300 | 3.70371700 | 0.24844300 |
| O | 6.13768300 | 2.11127400 | -1.23506500 |
| H | -0.14688100 | -3.58253700 | -0.95885800 |
| H | 0.19014500 | -3.51041600 | -0.21127100 |
| H | 1.57791100 | -2.24372400 | -2.63311000 |
| H | 3.67624700 | -1.94007700 | -1.84860500 |
| Pd | -0.17330800 | -1.82495900 | -0.82545100 |
| H | 2.35283000 | 0.21908900 | 3.02893900 |
| H | 1.47171100 | -3.53161800 | 1.47635800 |
| O | 0.92356700 | -4.34175200 | 1.53481600 |
| H | 0.19722900 | -4.02044600 | 2.09223300 |
| H | 0.18481600 | -1.88082700 | 2.45088400 |
| O | -0.67705400 | -2.23328600 | 2.75790100 |
| H | -1.23196400 | -2.16083400 | 1.96302900 |

N -0.42545900 0.17967900 -1.17393400
 C -1.10312800 0.82991500 -0.02828300
 H -1.06893400 1.91553900 -0.16567100
 C -2.52276500 0.37124600 0.06675500
 C -2.82787700 -1.00184300 0.16254300
 C -3.55345300 1.30342400 0.05859000
 C -4.17720500 -1.38064500 0.24935900
 C -4.87333400 0.91008800 0.15806900
 H -3.32179300 2.36058100 -0.02193800
 C -5.18322500 -0.44123300 0.25630800
 H -4.40214200 -2.43893500 0.32023400
 H -6.21985200 -0.75467700 0.32822800
 O -1.91184800 -1.95790300 0.21016200
 S -6.20541500 2.11450700 0.13942600
 O -6.96626600 1.81926900 1.40153500
 O -7.01402000 1.80261100 -1.07335600
 O -5.55128200 3.45020000 0.07741800
 H -0.51725900 0.58640400 0.86639500
 H -1.04224000 0.23807900 -1.98680900

53

RS_delta_hs_Dl_TS1_P, E(SCF) = -
 2408.89099175, E(ZPE) = -2408.500204, E(G)
 = -2408.564720 a.u.

C 0.85596800 -0.81791900 1.56759700
 H 0.73318600 -1.81025100 2.01110400
 H 1.44276500 -0.91984000 0.65094700
 C 1.50402400 0.13835400 2.53475400
 H 0.92868700 0.17424100 3.46253200
 H 2.51930800 -0.17931200 2.78432200
 N 1.51562800 1.51764600 1.96645700
 C 2.79396700 1.88751800 1.26011500
 H 2.63599900 2.89171200 0.86018700
 C 3.21468700 0.93410800 0.19696900
 C 2.57593800 0.96090100 -1.07687200
 C 4.22479800 0.01759100 0.45956200
 C 3.01850300 -0.00017900 -2.02542700
 C 4.62065400 -0.91201000 -0.48397600
 H 4.71333400 0.01855500 1.43034500
 C 4.00635500 -0.91086000 -1.73550100
 H 4.31305000 -1.63483100 -2.48507600
 O 1.62509800 1.78629900 -1.34542900
 S 5.93520500 -2.07737300 -0.15009200
 O 7.05579100 -1.71840700 -1.06922200
 O 5.37748300 -3.42887200 -0.44963100
 O 6.29029700 -1.90271100 1.28721500
 H -0.06178700 3.51575000 0.96152700
 H 0.09447500 3.43756800 0.16688100
 H 1.41633100 2.17108400 2.74003300
 H 3.56734000 1.94564300 2.03342600
 Pd -0.17474200 1.73150200 0.78148200
 H 2.54716700 0.00288600 -3.00377300
 H 0.57005700 3.18196900 -1.90446600
 O -0.17910100 3.80407500 -1.93512500
 H -0.94379100 3.24868600 -1.72586700
 H 0.42252100 0.97839000 -2.39559600
 O -0.35396300 0.58917100 -2.85408400
 H -1.08332300 0.91515500 -2.31223800
 N -0.46480400 -0.25607400 1.20201900
 C -1.15956600 -0.95949700 0.10024300
 H -1.19203700 -2.02952000 0.32963900
 C -2.54755600 -0.42929400 -0.07485800
 C -2.75698200 0.93584600 -0.35857000
 C -3.63940800 -1.28139300 0.02811300
 C -4.07034800 1.38855600 -0.54881100
 C -4.92632600 -0.81658500 -0.16378600
 C -3.48515300 -2.33112900 0.25622700
 C -5.13911900 0.52367800 -0.46196200
 H -4.21857400 2.43885300 -0.77363300
 H -6.14908000 0.89094700 -0.61371300
 O -1.75828500 1.79937000 -0.49571700
 S -6.34019400 -1.91566600 -0.01579100
 O -7.04643600 -1.84372600 -1.32595100
 O -7.15837100 -1.36677700 1.10283000
 O -5.78267500 -3.26457700 0.27544500
 H -0.54843100 -0.81701800 -0.79858400
 H -1.07210100 -0.26463700 2.02424100

53

RS_delta_hs_Dl_TS1_R, E(SCF) = -
 2408.91403740, E(ZPE) = -2408.524916, E(G)
 = -2408.591296 a.u.

C 0.32999600 2.98823200 -1.22941000
 H 0.57602300 3.97169200 -0.82360500
 H 0.59579900 2.99375700 -2.28839700
 C -1.14499000 2.71726100 -1.04184000
 H -1.74599600 3.54099000 -1.44093400
 H -1.45499900 1.79621600 -1.54380000
 N -1.38588200 2.54477000 0.40821300
 C -2.79532300 2.28658100 0.79099700
 H -2.86287400 2.54201200 1.85209200
 C -3.23915500 0.87502900 0.58553500
 C -2.57775600 -0.16088400 1.28201900
 C -4.34497500 0.58353200 -0.19687200
 C -3.10878000 -1.45922400 1.20548800
 C -4.83806300 -0.70767200 -0.27930200
 H -4.85107300 1.37722700 -0.73807100
 C -4.22065000 -1.72764800 0.43162100
 H -4.61402600 -2.73786900 0.37949800
 O -1.49481000 0.07229000 2.00139300
 S -6.26600100 -1.09028300 -1.29842500
 O -7.25184400 -1.73610800 -0.38667900
 O -5.77571200 -2.02136700 -2.35450600
 O -6.73877900 0.21242500 -1.84206900
 H 2.30331700 1.46602200 3.24145400
 H 1.96057800 0.81148600 3.10800500
 H -1.07930600 3.38817400 0.89162700
 H -3.44431900 2.97345000 0.23772300
 Pd -0.07562000 1.03130100 0.87228900
 H -2.61184600 -2.24809700 1.76236300
 H -0.66511800 -1.23658600 3.05600300
 O 0.07420500 -1.81484200 3.31556500
 H 0.71076500 -1.57532100 2.62137200
 H -1.36502700 -1.93591600 -0.34696200
 O -0.45676100 -2.14150400 -0.59850500
 H 0.08508000 -1.64875000 0.04394000
 N 1.15248500 1.98180200 -0.49510800
 C 1.77317500 0.93682500 -1.34770700
 H 2.26035300 1.41633800 -2.20309200
 C 2.78510700 0.15250300 -0.57324300
 C 2.42998800 -0.54306800 0.60143600
 C 4.09876400 0.09864600 -1.02512600
 C 3.42654600 -1.27007300 1.27318900
 C 5.06169600 -0.62965700 -0.35415600
 H 4.37926300 0.63954100 -1.92342600
 C 4.71762600 -1.32437500 0.79963400
 H 3.14530800 -1.79541900 2.18050100
 H 5.47083700 -1.89230400 1.33646500
 O 1.20350600 -0.56111100 1.09651000
 S 6.74777200 -0.71756000 -0.96372500
 O 6.95775800 -2.13538800 -1.37456000
 O 7.61445900 -0.32384700 0.18312400
 O 6.82107400 0.23491300 -2.10528700
 H 0.96230400 0.30917700 -1.73249000
 H 1.90488600 2.46407500 -0.00634400

53

RS_delta_hs_Dl_TS1, E(SCF) = -
 2408.88751891, E(ZPE) = -2408.497980, E(G)
 = -2408.561881 a.u.

C -0.60322000 -1.48485400 -1.37376000
 H -0.44257000 -2.54546800 -1.59135000
 H -1.18561900 -1.40468600 -0.45094200
 C -1.29457100 -0.78817400 -2.51706100
 H -0.75028900 -0.96632800 -3.44676800
 H -2.30884500 -1.16914700 -2.65240000
 N -1.32234600 0.68885300 -2.28563900
 C -2.66531400 1.24524000 -1.93688800
 H -2.53475500 2.33082400 -1.91956000
 C -3.22633500 0.75610600 -0.64872800
 C -2.67920600 1.23336100 0.57211400
 C -4.31140800 -0.10950100 -0.64284300
 C -3.32217700 0.82054500 1.76438200
 C -4.89462800 -0.52163100 0.54096700

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -4.72184600 | -0.46616100 | -1.58330500 | N | -0.46233700 | -0.31315500 | 1.22632700 |
| C | -4.39721500 | -0.03793400 | 1.74793100 | C | -1.16980600 | -1.05562500 | 0.16126600 |
| H | -4.86062500 | -0.34185600 | 2.68206500 | H | -1.21824900 | -2.11401200 | 0.43852200 |
| O | -1.62876400 | 1.99747500 | 0.59805300 | C | -2.55234300 | -0.51867200 | -0.04388300 |
| S | -6.30673000 | -1.62236800 | 0.54793400 | C | -2.75836300 | 0.83635800 | -0.38380800 |
| O | -7.43406400 | -0.84547200 | 1.14220100 | C | -3.64582500 | -1.36726000 | 0.07489500 |
| O | -5.91903200 | -2.78754600 | 1.39549600 | C | -4.07186300 | 1.27400600 | -0.61303200 |
| O | -6.54895900 | -1.99564100 | -0.87444700 | C | -4.93114600 | -0.91542500 | -0.15372400 |
| H | 0.20322500 | 3.18848300 | -1.61865600 | H | -3.49289700 | -2.40736900 | 0.34458400 |
| H | -0.13975000 | 3.30471600 | -0.94246000 | C | -5.14121600 | 0.41237300 | -0.50560500 |
| H | -1.03898100 | 1.14231000 | -3.15162500 | H | -4.21935300 | 2.31425200 | -0.88175400 |
| H | -3.34320100 | 0.99770800 | -2.76060400 | H | -6.14922800 | 0.77203300 | -0.68657200 |
| Pd | 0.13993700 | 1.17793500 | -0.91130400 | O | -1.76241700 | 1.69886900 | -0.53189400 |
| H | -2.93913100 | 1.19988200 | 2.70698100 | S | -6.34309400 | -2.01131000 | 0.02071500 |
| H | -0.58309700 | 3.32287000 | 3.58784000 | O | -5.78465100 | -3.54781600 | 0.33630300 |
| O | 0.22682000 | 3.83710400 | 1.55128300 | O | -7.05579100 | -1.96655100 | -1.28753200 |
| H | 0.92418100 | 3.21999000 | 1.28258900 | O | -7.15890700 | -1.44251500 | 1.13162600 |
| H | -0.70988500 | 1.09055900 | 1.99917000 | H | -0.55660200 | -0.96794500 | -0.74298800 |
| O | -0.08120200 | 0.62013600 | 2.57776100 | H | -1.05891900 | -0.25900200 | 0.02560000 |
| H | 0.75486300 | 0.85530500 | 2.15241200 | O | 0.16756000 | 3.72691300 | 0.47639200 |
| N | 0.68737200 | -0.79786800 | -1.14436700 | H | -0.51564500 | 4.23940600 | 0.92185700 |
| C | 1.44893900 | -1.28330300 | 0.02667800 | | | | |
| H | 1.64513200 | -2.35394900 | -0.09652400 | | | | |
| C | 2.73716800 | -0.53943200 | 0.18119400 | | | | |
| C | 2.72828600 | 0.85687200 | 0.37940300 | | | | |
| C | 3.94714600 | -1.21930900 | 0.15932400 | | | | |
| C | 3.95113000 | 1.51706000 | 0.56304200 | | | | |
| C | 5.14274300 | -0.55217700 | 0.34926600 | | | | |
| H | 3.95843700 | -2.29311400 | 0.00337500 | | | | |
| C | 5.14075300 | 0.82164200 | 0.55631500 | | | | |
| H | 3.93218400 | 2.58972900 | 0.71995900 | | | | |
| H | 6.07832200 | 1.34785600 | 0.70512700 | | | | |
| O | 1.60371400 | 1.55814500 | 0.43948100 | | | | |
| S | 6.70974900 | -1.43039300 | 0.30271300 | | | | |
| O | 7.39656900 | -1.09644800 | 1.58207500 | | | | |
| O | 7.43391500 | -0.89971000 | -0.88728200 | | | | |
| O | 6.36835400 | -2.87392700 | 0.18111400 | | | | |
| H | 0.79533900 | -1.15231100 | 0.89608500 | | | | |
| H | 1.27498500 | -0.87494800 | -1.97561300 | | | | |

54

RS_delta_hs_ID1_TS1_R, E(SCF) = -
 2484.18255609, E(ZPE) = -2483.783733, E(G)
 = -2483.853068 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.19901200 | 1.58392800 | -2.81644000 |
| H | 0.41176700 | 2.63704800 | -3.02189500 |
| H | 0.52403300 | 1.00657700 | -3.68571300 |
| C | -1.27990100 | 1.40416600 | -2.56551500 |
| H | -1.87177200 | 1.77838300 | -3.40694900 |
| H | -1.53901900 | 0.35331100 | -2.40711900 |
| N | -1.60492700 | 2.14231900 | -1.32409800 |
| C | -3.02243200 | 2.07282700 | -0.88804600 |
| H | -3.17951500 | 2.95360200 | -0.25940400 |
| C | -3.36300900 | 0.83975300 | -0.11660400 |
| C | -2.68318800 | 0.58292700 | 1.09527100 |
| C | -4.38919300 | 0.00321900 | -0.52494200 |
| C | -3.10466300 | -0.50259800 | 1.87760000 |
| C | -4.77869800 | -1.07259300 | 0.25437200 |
| H | -4.90724700 | 0.19690600 | -1.45928600 |
| C | -4.13980900 | -1.31510400 | 1.46373600 |
| H | -4.44970300 | -2.15443100 | 2.07866900 |
| O | -1.68341800 | 1.35246900 | 1.49490900 |
| S | -6.11004500 | -2.15728400 | -0.26675600 |
| O | -5.51904400 | -3.52450400 | -0.33281800 |
| O | -6.55740300 | -1.65119100 | -1.59382600 |
| O | -7.16234600 | -2.04492300 | 0.78391100 |
| H | 2.52324300 | 3.34026700 | 0.17340100 |
| H | -1.36891700 | 3.12400300 | -1.46445000 |
| H | -3.67023000 | 2.16650800 | -1.76594300 |
| Pd | -0.25164400 | 1.37553400 | 0.01909500 |
| H | -2.58711400 | -0.69245900 | 2.81239900 |
| H | 1.46644800 | 3.61280700 | 2.33817300 |
| O | 2.12794700 | 3.05025300 | 1.92693300 |
| H | 1.70727800 | 2.17075500 | 1.85795900 |
| H | -0.84237700 | 1.11432300 | 3.11542300 |
| O | -0.12864200 | 0.88452400 | 3.73966600 |
| H | 0.53527100 | 0.55759300 | 3.11381300 |
| N | 0.98545500 | 1.20708800 | -1.61500900 |
| C | 1.51226200 | -0.17049600 | -1.62878900 |
| H | 2.00525200 | -0.35189700 | -2.59057500 |
| C | 2.50071900 | -0.40868400 | -0.52607500 |
| C | 2.25212900 | -0.05734800 | 0.81781100 |
| C | 3.70616100 | -1.02335200 | -0.85085400 |
| C | 3.23992800 | -0.35407000 | 1.77524500 |
| C | 4.65627600 | -1.31719600 | 0.10650000 |
| H | 3.90547300 | -1.28929500 | -1.88409200 |
| C | 4.41945900 | -0.97180400 | 1.43165700 |
| H | 3.04132300 | -0.07130200 | 2.80480900 |
| H | 5.16224100 | -1.18827200 | 2.19273700 |
| O | 1.15148700 | 0.53414300 | 1.25403400 |
| S | 6.21786600 | -2.08067900 | -0.33844800 |
| O | 6.10733600 | -2.44039000 | -1.77923100 |
| O | 6.35854400 | -3.26893900 | 0.55057700 |
| O | 7.26260100 | -1.04945300 | -0.07457900 |
| H | 0.65720400 | -0.85514400 | -1.57376000 |

54

RS_delta_hs_ID1_TS1_P, E(SCF) = -
 2484.16936119, E(ZPE) = -2483.769190, E(G)
 = -2483.836060 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.86099200 | -0.86713900 | 1.59478300 |
| H | 0.74272600 | -1.84397900 | 2.07309900 |
| H | 1.43139200 | -1.00034200 | 0.67243900 |
| C | 1.53192500 | 0.11969800 | 2.51695300 |
| H | 0.97783700 | 0.18536800 | 3.45629700 |
| H | 2.55194300 | -0.19401500 | 2.75295100 |
| N | 1.52707100 | 1.47588400 | 1.90235200 |
| C | 2.77781700 | 1.83298000 | 1.14674200 |
| H | 2.58122300 | 2.81000100 | 0.70107700 |
| C | 3.19987200 | 0.83793600 | 0.11970400 |
| C | 2.58428000 | 0.82559100 | -1.16783100 |
| C | 4.20311000 | -0.07292500 | 0.42583000 |
| C | 3.03451300 | -0.17500600 | -2.07220700 |
| C | 4.60881500 | -1.03851500 | -0.47719400 |
| H | 4.67852100 | -0.03852500 | 1.40256700 |
| C | 4.01304800 | -1.07981000 | -1.73670100 |
| H | 4.32682800 | -1.83135000 | -2.45559200 |
| O | 1.64965900 | 1.64794900 | -1.49092600 |
| S | 5.92138000 | -2.18770700 | -0.08689900 |
| O | 5.37774500 | -3.54962100 | -0.36553200 |
| O | 6.24584100 | -1.97708900 | 1.35301900 |
| O | 7.06090000 | -1.84586800 | -0.98968300 |
| H | 0.04764000 | 3.87589300 | -0.49938500 |
| H | 1.43616300 | 2.16285100 | 2.64732900 |
| H | 3.56999300 | 1.94902800 | 1.89476900 |
| Pd | -0.17400000 | 1.64315600 | 0.74939800 |
| H | 2.57849500 | -0.20266500 | -3.05762300 |
| H | 0.56136700 | 2.91746500 | -2.14560000 |
| O | -0.20108000 | 3.53136600 | -2.13791300 |
| H | -0.95457700 | 2.94870000 | -1.94661200 |
| H | 0.42729900 | 0.74537500 | -2.44192200 |
| O | -0.36861500 | 0.34118600 | -2.85113100 |
| H | -1.07249600 | 0.66708600 | -2.27651900 |

H 1.75879800 1.87604800 -1.48373000
 O 2.66151800 3.35411400 -0.79599200
 H 3.60537500 3.47208600 -0.92405600

54

RS_delta_hs_ID1_TS1, E(SCF) = -
 2484.15998810, E(ZPE) = -2483.760527, E(G)
 = -2483.826901 a.u.

C 0.46146200 -1.84311200 1.26133800
 H 0.25163900 -2.89097400 1.50102400
 H 1.01568900 -1.81192600 0.31918200
 C 1.23804000 -1.17613800 2.37258100
 H 0.78042500 -1.39619400 3.33911500
 H 2.26270400 -1.55129800 2.40058900
 N 1.24323200 0.31012000 2.19869500
 C 2.58160800 0.92983800 1.97985000
 H 2.40856500 2.00693200 2.05191000
 C 3.22537900 0.58489300 0.68236800
 C 2.70790400 1.13792600 -0.51928900
 C 4.36900600 -0.20127200 0.65634500
 C 3.44130800 0.89443300 -1.70455400
 C 5.04421700 -0.44905500 -0.52474100
 H 4.75774200 -0.61727200 1.58171100
 C 4.57553200 0.11483300 -1.70736900
 H 5.10988300 -0.06024100 -2.63664600
 O 1.60843400 1.83378200 -0.54020900
 S 6.51827300 -1.46453700 -0.55667200
 O 6.21375700 -2.60725400 -1.46686600
 O 6.75639900 -1.89313400 0.85066800
 O 7.60893700 -0.59704500 -1.09088700
 H -0.12806700 3.58243100 0.67262400
 H 0.86997200 0.72868300 3.04816700
 H 3.22812000 0.63017800 2.81170400
 Pd -0.12415600 0.84047900 0.77091600
 H 3.08175600 1.33916700 -2.62764800
 H 0.58771500 3.22323500 -1.19498400
 O -0.24258600 3.73573800 -1.16330100
 H -0.91764500 3.03482900 -1.18673800
 H 0.83187700 1.06700400 -2.10628300
 O 0.23255700 0.65254500 -2.75310200
 H -0.60953000 0.73149100 -2.28052600
 N -0.79430400 -1.08962800 1.05068100
 C -1.60847600 -1.54855800 -0.09338000
 H -1.88845200 -2.59664700 0.05959700
 C -2.83406100 -0.70806700 -0.26583300
 C -2.71412000 0.67050200 -0.54288800
 C -4.09526000 -1.28299800 -0.18998200
 C -3.88220900 1.41277400 -0.76850300
 C -5.23561000 -0.53259400 -0.40855500
 H -4.19403200 -2.34090300 0.03243500
 C -5.12437600 0.81940900 -0.70835500
 H -3.77859300 2.46871200 -0.99398400
 H -6.01779700 1.40946200 -0.88615100
 O -1.53864800 1.27583100 -0.63174100
 S -6.86754600 -1.27404800 -0.29712500
 O -6.64367600 -2.71825500 -0.01428000
 O -7.51226100 -1.02973400 -1.61843900
 O -7.56183700 -0.56275200 0.81376700
 H -0.95744300 -1.49761300 -0.97263800
 H -1.36669500 -1.12259400 1.89471100
 O -0.06713200 3.15890700 1.55487400
 H -0.90441100 3.34947400 1.98773800

53

RS_delta_D1_TS1_P_CH_P, E(SCF) = -
 2408.89124697, E(ZPE) = -2408.499868, E(G)
 = -2408.568636 a.u.

N -1.41310800 1.68860500 0.31228300
 N 1.37817200 1.69311800 -0.25971400
 C -2.39963700 0.94622800 1.10925100
 H -2.97641300 1.63300200 1.74260500
 C 2.37203300 1.23234000 0.73556500
 H 3.02414300 2.07301000 0.99874700
 C -3.33868000 0.17067700 0.23481400
 C -2.87849000 -0.80778000 -0.68079400
 C -4.70516400 0.38808500 0.36909000
 C -3.84812300 -1.53362600 -1.40172100

C -5.63487200 -0.33557800 -0.35282100
 H -5.05696300 1.14304600 1.06552800
 C -5.19645900 -1.31224700 -1.23937100
 H -3.49142000 -2.28750100 -2.09564000
 H -5.91630500 -1.88965100 -1.81139500
 C 3.21164800 0.06707000 0.22049600
 C 3.13515900 -1.18205300 1.07278400
 C 4.56957900 0.45461000 -0.23398700
 C 4.29706600 -2.04253800 1.08884700
 C 5.61024400 -0.36863000 -0.10177900
 H 4.69583200 1.41861100 -0.71843200
 C 5.46370500 -1.64685100 0.54782000
 H 4.20443200 -2.98504500 1.61550000
 H 6.33522600 -2.29116000 0.61213900
 O -1.61346700 -1.11207400 -0.89035500
 O 2.10233900 -1.47747100 1.66647800
 S -7.39318000 -0.05555200 -0.15070900
 S 7.24885700 0.07036600 -0.70551700
 O 8.12297000 0.00472100 0.60471900
 O 7.56922000 -0.97618600 -1.71269400
 O 7.12055200 1.43308300 -1.27892800
 O -7.52598800 1.07270200 0.81305000
 O -7.91655400 0.27468800 -1.50829600
 O -7.95496000 -1.33495000 0.37244600
 H -1.90001800 2.24789700 -0.38630900
 H -1.82604400 0.29182300 1.77574900
 H 1.82851100 0.94029300 1.63476900
 Pd -0.11103800 0.26850400 -0.66752100
 C 0.66267100 2.91605200 0.19873800
 C -0.50231300 2.54494400 1.08513600
 H -1.00448200 3.44795100 1.44971100
 H -0.17350000 1.96932900 1.95603300
 H 0.29945700 3.43121900 -0.69382900
 H 1.35350400 3.58985400 0.71540000
 H 1.86905000 1.92421400 -1.12104500
 H 0.46365700 -2.49565400 1.06522600
 H 0.87258000 -0.73444700 -1.37138600
 H 2.68715300 -0.30627100 -0.68823800
 O -0.35971400 -2.94872600 0.84339900
 H -0.80789400 -2.34123200 0.22542300
 H 0.73305100 -0.59575400 2.60745100
 O 0.10339700 -0.07863900 3.13617900
 H 0.35535100 -0.24523300 4.04755000

53

RS_delta_D1_TS1_P_CH_TS, E(SCF) = -
 2408.87467379, E(ZPE) = -2408.487788, E(G)
 = -2408.552869 a.u.

N -1.34580200 1.68770400 -0.86497800
 N 1.41552100 1.67364600 -1.30527700
 C -2.39318800 1.62005500 0.17159400
 H -3.10276500 2.44449200 0.03283300
 C 2.43538500 2.06714800 -0.29458800
 H 3.14896400 2.74877800 -0.77011000
 C -3.12342400 0.31417800 0.12581100
 C -2.44132300 -0.91052500 0.31028900
 C -4.50027000 0.30836000 -0.05911500
 C -3.20335600 -2.09217200 0.33081700
 C -5.22779700 -0.86690600 -0.04005000
 H -5.02263600 1.24841000 -0.20868600
 C -4.56993500 -2.07412600 0.16281800
 H -2.67610600 -3.02768900 0.48384600
 H -5.13229000 -3.00242900 0.18204100
 C 3.13926800 0.86464500 0.27142500
 C 3.02661900 0.58829900 1.69950800
 C 4.23367000 0.30721900 -0.46190100
 C 3.87459400 -0.45713600 2.20144000
 C 5.02245100 -0.65235900 0.08017000
 H 4.40163100 0.62051000 -1.48891500
 C 4.82720000 -1.04092200 1.42980800
 H 3.74907000 -0.73382200 3.24285400
 H 5.46330700 -1.81524300 1.84828200
 O -1.13755300 -1.01247200 0.49161100
 O 2.16205800 1.13313800 2.42469900
 S -6.99721100 -0.86540100 -0.33182500
 S 6.34254600 -1.42952800 -0.85549300
 O 7.59192100 -1.12433600 -0.10464500

| | | | |
|----|-------------|-------------|-------------|
| O | 6.01714500 | -2.88296100 | -0.85755600 |
| O | 6.30109200 | -0.81352100 | -2.20819000 |
| O | -7.41568100 | 0.56402800 | -0.33178000 |
| O | -7.19193400 | -1.52567500 | -1.65550800 |
| O | -7.59765400 | -1.64975300 | 0.78482200 |
| H | -1.76258400 | 1.48682500 | -1.77423900 |
| H | -1.88338200 | 1.77657500 | 1.12898000 |
| H | 1.91612500 | 2.60929000 | 0.49719600 |
| Pd | 0.14204200 | 0.25845600 | -0.46360500 |
| C | 0.58675800 | 2.80370000 | -1.80366600 |
| C | -0.62286300 | 2.97640900 | -0.91874900 |
| H | -1.27103900 | 3.77373600 | -1.29697600 |
| H | -0.33602700 | 3.22628500 | 0.10725400 |
| H | 0.27728900 | 2.55575200 | -2.82147200 |
| H | 1.18048600 | 3.72084500 | -1.84929900 |
| H | 1.89307700 | 1.24983200 | -2.09896800 |
| H | 0.85768400 | -0.21311700 | 2.87551800 |
| H | 1.36223100 | -0.81705000 | -0.14155000 |
| H | 2.12201900 | -0.11170600 | 0.04308200 |
| O | 0.22478200 | -0.93852900 | 2.99735200 |
| H | -0.25824400 | -0.98896700 | 2.15383300 |
| H | 0.75554000 | 2.22911100 | 2.32567300 |
| O | -0.03588700 | 2.80240300 | 2.30119700 |
| H | 0.04129800 | 3.36626000 | 3.07385400 |

53
RS_delta_D1_TS1_P, E(SCF) = -2408.89327305,
E(ZPE) = -2408.503419, E(G) = -2408.568532
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.31164300 | 1.74991600 | -0.19589700 |
| N | 1.43753800 | 1.76257700 | -0.58675700 |
| C | -2.41191900 | 1.40960400 | 0.73501300 |
| H | -3.03311900 | 2.30035700 | 0.87709500 |
| C | 2.44024900 | 1.86731300 | 0.52453000 |
| H | 3.03720300 | 2.76283100 | 0.31674700 |
| C | -3.24701200 | 0.29027000 | 0.20324300 |
| C | -2.66142700 | -0.94393700 | -0.14236600 |
| C | -4.62245700 | 0.44967100 | 0.08804900 |
| C | -3.49986300 | -1.98199700 | -0.58029600 |
| C | -5.43138500 | -0.58589400 | -0.33718300 |
| H | -5.07642500 | 1.40114500 | 0.34566300 |
| C | -4.86353200 | -1.81144800 | -0.66434900 |
| H | -3.03962300 | -2.92881200 | -0.84019200 |
| H | -5.49345600 | -2.62891500 | -1.00078300 |
| C | 3.31973300 | 0.67057700 | 0.62717200 |
| C | 2.92932600 | -0.42040200 | 1.45505200 |
| C | 4.50046700 | 0.61852700 | -0.10135600 |
| C | 3.80388900 | -1.53808900 | 1.48414400 |
| C | 5.32702900 | -0.48876700 | -0.05094500 |
| H | 4.78555100 | 1.46115500 | -0.72603100 |
| C | 4.96748700 | -1.56955200 | 0.75218800 |
| H | 3.51930300 | -2.38063300 | 2.10758900 |
| H | 5.61223200 | -2.44278700 | 0.79478900 |
| O | -1.36541300 | -1.19442000 | -0.04790700 |
| O | 1.81804700 | -0.42356700 | 2.10740300 |
| S | -7.21012500 | -0.38029500 | -0.46949500 |
| S | 6.84710600 | -0.56010000 | -0.99158000 |
| O | 7.94871800 | -0.71231300 | 0.00432400 |
| O | 6.72880400 | -1.75309000 | -1.88125700 |
| O | 6.92722000 | 0.72059200 | -1.75024900 |
| O | -7.49123100 | 1.03018500 | -0.08539100 |
| O | -7.54674700 | -0.67690000 | -1.89093400 |
| O | -7.80187100 | -1.37202700 | 0.47310800 |
| H | -1.70253500 | 1.86609100 | -1.13375200 |
| H | -1.93628100 | 1.17053100 | 1.69115500 |
| H | 1.88018200 | 2.03697400 | 1.44550200 |
| Pd | 0.03879000 | 0.22059300 | -0.36172300 |
| C | 0.64999600 | 3.01637800 | -0.74586200 |
| C | -0.54326200 | 2.96309100 | 0.16824600 |
| H | -1.17190400 | 3.85157800 | 0.06518000 |
| H | -0.25365700 | 2.85478100 | 1.21785200 |
| H | 0.32758600 | 3.07872100 | -1.78783400 |
| H | 1.27725100 | 3.88624800 | -0.53531200 |
| H | 1.95852800 | 1.59292800 | -1.44612500 |
| H | 0.79297500 | -1.88230300 | 2.08306700 |
| H | 1.14246500 | -1.04861000 | -0.97316000 |
| H | 1.24269300 | -1.10038800 | -0.16759300 |

| | | | |
|---|-------------|-------------|------------|
| O | 0.16999500 | -2.62141000 | 1.92085300 |
| H | -0.47100700 | -2.24927900 | 1.29540600 |
| H | 0.69334600 | 0.73431700 | 2.70328000 |
| O | -0.01998400 | 1.34848300 | 2.99442900 |
| H | 0.16715800 | 1.53930100 | 3.91575300 |

53
RS_delta_D1_TS1_R, E(SCF) = -2408.91554390,
E(ZPE) = -2408.526837, E(G) = -2408.593915
a.u.

| | | | |
|----|--------------|-------------|-------------|
| N | -1.43109400 | 1.97128700 | -0.06248600 |
| N | 1.29276600 | 1.91566900 | -0.60995500 |
| C | -2.48732800 | 1.64447500 | 0.91879400 |
| H | -3.11712800 | 2.52638900 | 1.07794200 |
| C | 2.37963900 | 1.78557400 | 0.38443500 |
| H | 3.01667700 | 2.67526200 | 0.33600500 |
| C | -3.32696100 | 0.49054200 | 0.47686000 |
| C | -2.74328500 | -0.76620500 | 0.20127500 |
| C | -4.70559200 | 0.64195000 | 0.39611400 |
| C | -3.60355700 | -1.83455000 | -0.11548100 |
| C | -5.52893300 | -0.41957500 | 0.07541500 |
| H | -5.15076300 | 1.61026200 | 0.60211800 |
| C | -4.966821600 | -1.66643700 | -0.17652700 |
| H | -3.15946700 | -2.80526900 | -0.31078100 |
| H | -5.60748500 | -2.50775400 | -0.42543600 |
| C | 3.21875600 | 0.56653500 | 0.13431900 |
| C | 2.67123200 | -0.71241100 | -0.10615100 |
| C | 4.60281300 | 0.71067100 | 0.17471200 |
| C | 3.55780600 | -1.79125000 | -0.28622000 |
| C | 5.45284500 | -0.36191600 | 0.00116600 |
| H | 5.03077100 | 1.69299700 | 0.34720400 |
| C | 4.92152400 | -1.62566800 | -0.22767500 |
| H | 3.12293900 | -2.76930600 | -0.47075400 |
| H | 5.58061200 | -2.47563700 | -0.37217900 |
| O | -1.44765300 | -1.00020500 | 0.25434000 |
| O | 1.37974100 | -0.98759200 | -0.17678300 |
| S | -7.30732900 | -0.21677500 | -0.03843500 |
| S | 7.23464900 | -0.15755500 | 0.06905100 |
| O | 7.69178400 | -0.97656100 | 1.22789400 |
| O | 7.75210600 | -0.67476700 | -1.22966700 |
| O | 7.47556800 | 1.29984500 | 0.25458100 |
| O | -7.58731600 | 1.19496200 | 0.34378100 |
| O | -7.66160700 | -0.51718100 | -1.45563200 |
| O | -7.89142300 | -1.20567500 | 0.91238400 |
| H | -1.86445400 | 2.13341800 | -0.97229100 |
| H | -1.97126600 | 1.43049100 | 1.86150800 |
| H | 1.91693500 | 1.77095000 | 1.37738500 |
| Pd | -0.07917000 | 0.43741500 | -0.20554400 |
| C | 0.57304300 | 3.21777300 | -0.60583100 |
| C | -0.61490000 | 3.14787400 | 0.31748000 |
| H | -1.20990600 | 4.06450700 | 0.26983400 |
| H | -0.30264100 | 3.00431200 | 1.35517400 |
| H | 0.23807700 | 3.40320400 | -1.62855900 |
| H | 1.24887600 | 4.02869700 | -0.32241100 |
| H | 1.69654100 | 1.77119600 | -1.53395200 |
| H | 0.61876300 | -2.55351500 | -1.14535600 |
| H | 1.60053600 | -0.41152700 | -3.33319700 |
| H | 1.48604600 | -0.72683100 | -2.66162400 |
| O | -0.21864600 | -3.01349600 | -1.30525600 |
| H | -0.81517100 | -2.45931200 | -0.77098800 |
| H | 0.99153600 | -2.09234900 | 1.29262300 |
| O | 1.01754300 | -2.63823600 | 2.09845000 |
| H | 1.94884100 | -2.66369900 | 2.33113400 |

53
RS_delta_D1_TS1-trigo_P, E(SCF) = -
2408.89390929, E(ZPE) = -2408.502954, E(G) =
-2408.566676 a.u.

| | | | |
|---|-------------|-------------|--------------|
| N | -1.31231800 | 1.66317700 | 0.34005600 |
| N | 1.44632900 | 1.63259400 | -0.04339300 |
| C | -2.39760800 | 1.06153100 | 1.14797900 |
| H | -2.95493600 | 1.86582900 | 1.63969800 |
| C | 2.39472700 | 1.25819900 | 1.05792000 |
| H | 2.92435500 | 2.17520600 | 1.33965200 |
| C | -3.31960000 | 0.25058000 | 0.29635200 |
| C | -2.82814900 | -0.80652500 | -0.480578500 |
| C | -4.68364700 | 0.51519400 | 0.31389200 |

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|---|-------------|-------------|-------------|
| H | 1.11420400 | -1.39787800 | -0.86421500 |
| O | 0.25352400 | -3.17545600 | 1.12740600 |
| H | -0.50458000 | -2.72636000 | 0.72217000 |
| H | 0.69077600 | 0.25291000 | 2.51571700 |
| O | 0.12534800 | 0.86711600 | 3.03355800 |
| H | 0.32816600 | 0.68358000 | 3.95315800 |

53

RS_delta_D1_TS2_P, E(SCF) = -2408.92288383,
E(ZPE) = -2408.529627, E(G) = -2408.595894
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.36879400 | -1.42041200 | 0.88066900 |
| N | -1.45131800 | -1.45105900 | 0.45303000 |
| C | 2.44424600 | -0.58514600 | 1.43394200 |
| H | 3.03809600 | -1.15016700 | 2.16307000 |
| C | -2.40393800 | -0.77469000 | 1.37883900 |
| H | -2.92879300 | -1.55201600 | 1.94634000 |
| C | 3.33660600 | -0.08279100 | 0.33915100 |
| C | 2.83307200 | 0.70258400 | -0.72412300 |
| C | 4.69190400 | -0.38934200 | 0.37890800 |
| C | 3.74473900 | 1.15888400 | -1.69315300 |
| C | 5.56688300 | 0.06866900 | -0.58737700 |
| H | 5.07769600 | -0.99688300 | 1.19178900 |
| C | 5.08566100 | 0.85454600 | -1.62759300 |
| H | 3.35324400 | 1.76731000 | -2.50134800 |
| H | 5.76522700 | 1.21878000 | -2.39185500 |
| C | -3.41890300 | 0.06209700 | 0.66526800 |
| C | -3.25876800 | 1.43628700 | 0.47796200 |
| C | -4.59396600 | -0.53401500 | 0.21485200 |
| C | -4.27051100 | 2.19111700 | -0.10294500 |
| C | -5.58693500 | 0.21325400 | -0.38658100 |
| H | -4.74336200 | -1.60135500 | 0.34986600 |
| C | -5.43395100 | 1.58526500 | -0.53097500 |
| H | -4.11574400 | 3.25690900 | -0.22318700 |
| H | -6.21859400 | 2.17485300 | -0.99248800 |
| O | 1.56874400 | 1.07493800 | -0.84516400 |
| O | -2.13750900 | 2.09266300 | 0.89046100 |
| S | 7.31417400 | -0.33211900 | -0.52521700 |
| S | -7.12137400 | -0.56223200 | -0.92574800 |
| O | -8.16480000 | -0.06435800 | 0.01318600 |
| O | -7.33441100 | -0.09452600 | -2.32258600 |
| O | -6.89215900 | -2.02813300 | -0.82432100 |
| O | 8.02917300 | 0.97244600 | -0.41826100 |
| O | 7.49722800 | -1.19617300 | 0.67404300 |
| O | 7.61666800 | -1.03878500 | -1.80337900 |
| H | 1.78279800 | -2.14024600 | 0.29018900 |
| H | 1.96030400 | 0.23674000 | 1.97554300 |
| H | -1.82184900 | -0.18346000 | 2.09064900 |
| Pd | 0.04244500 | -0.19340600 | -0.30475200 |
| C | -0.73258900 | -2.56954600 | 1.12578200 |
| C | 0.47707600 | -2.04827900 | 1.86386000 |
| H | 0.97435700 | -2.85883300 | 2.40901600 |
| H | 0.19138700 | -1.28434500 | 2.59237500 |
| H | -0.41650000 | -3.27008900 | 0.34899600 |
| H | -1.41014000 | -3.10103700 | 1.80077800 |
| H | -1.99571500 | -1.83697400 | -0.31581300 |
| H | 0.79231700 | 3.73600900 | 0.82324700 |
| H | -0.97532500 | 0.65897600 | -1.13994800 |
| H | -1.35209200 | 1.61395100 | 0.55341100 |
| O | 1.13278300 | 2.90168300 | 1.15406800 |
| H | 1.25661300 | 2.32997100 | 0.36568400 |
| H | -1.25160800 | 1.90727200 | 2.84878000 |
| O | -0.38096600 | 1.69949500 | 3.20815900 |
| H | 0.21635500 | 2.09983900 | 2.54851200 |

53

RS_delta_D1_TS2_R_checking-H-bond, E(SCF) =
-2408.89388757, E(ZPE) = -2408.502593, E(G)
= -2408.567961 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.31648500 | -1.65907700 | 0.34519400 |
| N | -1.44189900 | -1.63885500 | -0.04677000 |
| C | 2.40842300 | -1.06413400 | 1.14857500 |
| H | 2.96954100 | -1.87279500 | 1.62863900 |
| C | -2.40584200 | -1.27992200 | 1.04602800 |
| H | -2.94081300 | -2.20067400 | 1.30443900 |
| C | 3.32346400 | -0.24569600 | 0.29678200 |
| C | 2.82445500 | 0.81926500 | -0.47949900 |

| | | | |
|----|-------------|-------------|-------------|
| C | 4.68756500 | -0.51023700 | 0.29918000 |
| C | 3.73786900 | 1.59755200 | -1.20942600 |
| C | 5.56970900 | 0.27692900 | -0.42425400 |
| H | 5.07394800 | -1.33615600 | 0.88783100 |
| C | 5.08867200 | 1.33457300 | -1.17422400 |
| H | 3.34601100 | 2.42007600 | -1.79720800 |
| H | 5.77734100 | 1.95132100 | -1.74294600 |
| C | -3.38629800 | -0.22494200 | 0.65793800 |
| C | -3.07078200 | 1.15167300 | 0.82741000 |
| C | -4.63008900 | -0.60505900 | 0.16652900 |
| C | -4.07810600 | 2.08541700 | 0.47882500 |
| C | -5.58676400 | 0.33274800 | -0.17081400 |
| H | -4.86426600 | -1.66002400 | 0.05206800 |
| C | -5.30121100 | 1.68717600 | -0.00635000 |
| H | -3.84952900 | 3.13907200 | 0.60497100 |
| H | -6.05146700 | 2.42935100 | -0.26356800 |
| O | 1.54441200 | 1.15184700 | -0.53928100 |
| O | -1.90719500 | 1.53508600 | 1.24130000 |
| S | 7.33170600 | -0.07534500 | -0.41453700 |
| S | -7.18893600 | -0.15715500 | -0.79977200 |
| O | -8.19536300 | 0.42344800 | 0.13664200 |
| O | -7.29445800 | 0.42799600 | -2.16916000 |
| O | -7.19566100 | -1.64751500 | -0.80575200 |
| O | 7.98106700 | 1.15959200 | 0.10982900 |
| O | 7.51523700 | -1.25474200 | 0.47503100 |
| O | 7.69854300 | -0.35054800 | -1.83308800 |
| H | 1.72046200 | -2.11586200 | -0.47518800 |
| H | 1.91780000 | -0.47259700 | 1.93047000 |
| H | -1.81612800 | -0.98232800 | 1.91512900 |
| Pd | 0.05785300 | -0.20882300 | -0.36445300 |
| C | -0.72821100 | -2.91587600 | 0.22793400 |
| C | 0.47721800 | -2.63172600 | 1.07981000 |
| H | 1.04682700 | -3.53980800 | 1.29405000 |
| H | O.20141100 | -2.17151500 | 2.03240000 |
| H | -0.41876200 | -3.33804700 | -0.73081800 |
| H | -1.39988700 | -3.63059800 | 0.71028100 |
| H | -1.98413200 | -1.74584400 | -0.90272100 |
| H | -0.52515100 | 2.77791100 | 1.15330700 |
| H | -0.96516100 | 0.93558600 | -1.23918400 |
| H | -1.09762000 | 1.14684200 | -0.44398500 |
| O | 0.38597000 | 3.12548900 | 1.17117900 |
| H | 0.86014000 | 2.56863400 | 0.53000500 |
| H | -0.67991000 | 0.86226900 | 2.43851000 |
| O | 0.14420000 | 0.78919300 | 2.96087300 |
| H | 0.61724400 | 1.57481300 | 2.65108500 |

53

RS_delta_D1_TS2, E(SCF) = -2408.89331762,
E(ZPE) = -2408.502917, E(G) = -2408.567613
a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.33889500 | -1.65938600 | 0.33309500 |
| N | -1.43086200 | -1.57851600 | -0.09127900 |
| C | 2.40912300 | -1.05178100 | 1.15351700 |
| H | 2.95413900 | -1.84551000 | 1.67582500 |
| C | -2.38734000 | -1.17902200 | 0.99068300 |
| H | -2.90523900 | -2.09020900 | 1.30993000 |
| C | 3.35257700 | -0.25613100 | 0.31026200 |
| C | 2.88600500 | 0.80450600 | -0.49385400 |
| C | 4.71276400 | -0.53758000 | 0.35013400 |
| C | 3.82987700 | 1.55781100 | -1.21260900 |
| C | 5.62374100 | 0.21610300 | -0.36351900 |
| H | 5.07323300 | -1.35871700 | 0.96162900 |
| C | 5.17539400 | 1.27606600 | -1.14287200 |
| H | 3.46419600 | 2.37662700 | -1.82232800 |
| H | 5.88559500 | 1.87360900 | -1.70568900 |
| C | -3.40043100 | -0.16390400 | 0.56701600 |
| C | -3.11785600 | 1.22255800 | 0.61374300 |
| C | -4.66714800 | -0.59903000 | 0.18903600 |
| C | -4.16013500 | 2.11479500 | 0.29217900 |
| C | -5.66477400 | 0.29751400 | -0.13867800 |
| H | -4.88606700 | -1.66260200 | 0.16015100 |
| C | -5.40729900 | 1.66377100 | -0.07549000 |
| H | -3.94468400 | 3.17733500 | 0.33470800 |
| H | -6.19236200 | 2.37197800 | -0.32255200 |
| O | 1.61413800 | 1.15424700 | -0.59220200 |
| O | -1.91870400 | 1.66349600 | 0.90390400 |
| S | 7.37922800 | -0.15214400 | -0.30692300 |

| | | | |
|----|-------------|-------------|-------------|
| S | -7.29194600 | -0.26661600 | -0.63752100 |
| O | -8.24968900 | 0.32625800 | 0.33971700 |
| O | -7.49971400 | 0.25643700 | -2.01884400 |
| O | -7.24751000 | -1.75418400 | -0.57969700 |
| O | 8.03730100 | 1.08862800 | 0.19271400 |
| O | 7.52750200 | -1.30591100 | 0.62222500 |
| O | 7.77172300 | -0.47696600 | -1.70827900 |
| H | 1.76271600 | -2.14147000 | -0.46137100 |
| H | 1.90227700 | -0.43385300 | 1.90432100 |
| H | -1.79676900 | -0.82262600 | 1.83696800 |
| Pd | 0.10203800 | -0.18628000 | -0.41157500 |
| C | -0.74221400 | -2.86389900 | 0.20704000 |
| C | 0.46357400 | -2.59844000 | 1.06634400 |
| H | 0.99988700 | -3.52148700 | 1.30269000 |
| H | 0.18636600 | -2.12094400 | 2.01031300 |
| H | -0.43319400 | -3.30210300 | -0.74459700 |
| H | -1.43071700 | -3.56138400 | 0.69162800 |
| H | -1.97069800 | -1.68979700 | -0.94755300 |
| H | -0.47995200 | 2.97842800 | 0.86989600 |
| H | -0.90136700 | 0.99259600 | -1.14097200 |
| H | -1.13442100 | 1.19223300 | -0.30746500 |
| O | 0.45067000 | 3.24905500 | 0.93366700 |
| H | 0.91965700 | 2.63056500 | 0.34453200 |
| H | -0.74341600 | 1.11729100 | 2.29939400 |
| O | 0.04599900 | 1.11053200 | 2.87174800 |
| H | 0.53544600 | 1.86160900 | 2.50415500 |

54
RS_delta_ID1_TS1_P_Htr_P, E(SCF) = -
2484.17110169, E(ZPE) = -2483.771246, E(G)
= -2483.837531 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.32652100 | -2.12725000 | 1.43917200 |
| H | 0.74847200 | -3.06489600 | 1.81225400 |
| H | 0.11414300 | -1.48700900 | 2.30098600 |
| C | -0.91449400 | -2.36377000 | 0.61898700 |
| H | -0.66748100 | -2.95331500 | -0.26725400 |
| H | -1.67110200 | -2.91218900 | 1.18708100 |
| N | -1.45372200 | -1.05783500 | 0.15505300 |
| N | 1.29450100 | -1.41528500 | 0.57924200 |
| C | -2.33211600 | -0.38914000 | 1.17284900 |
| H | -2.65601300 | -1.15968700 | 1.87998700 |
| C | 2.44876300 | -0.83442800 | 1.29381200 |
| H | 2.91264400 | -1.60135000 | 1.92369500 |
| C | -3.54546100 | 0.23516900 | 0.55900400 |
| C | -3.59406400 | 1.59215500 | 0.21982400 |
| C | -4.67484100 | -0.55381700 | 0.34758500 |
| C | -4.78071700 | 2.13366100 | -0.27582900 |
| C | -5.83447200 | -0.01300800 | -0.16808900 |
| H | -4.65047900 | -1.60797700 | 0.60818600 |
| C | -5.89143700 | 1.34126600 | -0.47293500 |
| H | -6.80720200 | 1.76952000 | -0.86711900 |
| C | 3.46375800 | -0.28175200 | 0.34153500 |
| C | 3.11600600 | 0.68788600 | -0.62322700 |
| C | 4.78697600 | -0.69596300 | 0.44508800 |
| C | 4.13717000 | 1.21841900 | -1.43028700 |
| C | 5.77379800 | -0.16475300 | -0.36192100 |
| H | 5.05721300 | -1.44901500 | 1.17867900 |
| C | 5.44437700 | 0.80945000 | -1.29697600 |
| H | 6.21489900 | 1.23446200 | -1.93246300 |
| O | -2.52438800 | 2.40077500 | 0.37503100 |
| O | 1.89068800 | 1.15801800 | -0.79447700 |
| S | -7.28497400 | -1.03739300 | -0.46219500 |
| S | 7.48379800 | -0.68255600 | -0.19641700 |
| O | 8.22284600 | 0.51247700 | 0.30315000 |
| O | 7.92076700 | -1.08801200 | -1.56276400 |
| O | 7.47978800 | -1.81138100 | 0.77456500 |
| O | -6.93338400 | -2.39681600 | 0.02904100 |
| O | -7.51254000 | -0.98605500 | -1.93352600 |
| O | -8.38772400 | -0.40082500 | 0.31034500 |
| H | 1.68045600 | 3.93767800 | 0.87229300 |
| O | 1.63464500 | 3.03794700 | 1.20362500 |
| H | 1.69984700 | 2.46108500 | 0.41522500 |
| H | -1.38108800 | 2.42523200 | 1.94565600 |
| O | -0.68475600 | 2.28394700 | 2.60597400 |
| H | 0.13262200 | 2.55866000 | 2.15026600 |
| H | -2.01459200 | -1.21998000 | -0.67925500 |
| H | -1.74151900 | 0.34205600 | 1.72858500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.04744400 | -0.05882200 | 1.95748500 |
| Pd | 0.23213500 | 0.06518000 | -0.37634100 |
| O | -0.86155300 | 1.50511000 | -1.26890700 |
| H | -0.22307100 | 2.14253700 | -1.60572100 |
| H | -1.78281300 | 2.09039500 | -0.27720900 |
| H | -4.79866400 | 3.18995700 | -0.51879200 |
| H | 3.86121900 | 1.96977300 | -2.16196100 |
| H | 1.64650200 | -2.06061900 | -0.12922100 |

54
RS_delta_ID1_TS1_P_Htr_TS, E(SCF) = -
2484.16762240, E(ZPE) = -2483.771618, E(G)
= -2483.839217 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.40447800 | -2.54634700 | 0.91652800 |
| H | 0.89397700 | -3.49967700 | 1.13153600 |
| H | 0.12276000 | -2.09089900 | 1.86961800 |
| C | -0.79287200 | -2.72276700 | 0.02082300 |
| H | -0.48449700 | -3.13345900 | -0.94341400 |
| H | -1.52243400 | -3.40675700 | 0.46384400 |
| N | -1.40688500 | -1.39241400 | -0.22889000 |
| N | 1.33784100 | -1.62092700 | 0.23676100 |
| C | -2.26047900 | -0.94090300 | 0.92094500 |
| H | -2.67359000 | -1.84090100 | 0.46840600 |
| C | 2.39066000 | -1.05244500 | 1.10636300 |
| H | 2.87736700 | -1.86301500 | 1.65933800 |
| C | -3.39393800 | -0.04290200 | 0.53403300 |
| C | -3.24678800 | 1.35986800 | 0.48522200 |
| C | -4.64061600 | -0.61051600 | 0.28356500 |
| C | -4.38530100 | 2.13666200 | 0.21395700 |
| C | -5.73984300 | 0.17262200 | -0.00671700 |
| H | -4.75883200 | -1.68935700 | 0.32707700 |
| C | -5.61028100 | 1.55706700 | -0.03071400 |
| H | -6.47435200 | 2.17741800 | -0.24748900 |
| C | 3.41061000 | -0.30285400 | 0.30768900 |
| C | 3.03879700 | 0.74786600 | -0.55801400 |
| C | 4.75545500 | -0.62406100 | 0.45248900 |
| C | 4.05512100 | 1.44138700 | -1.23623300 |
| C | 5.73879200 | 0.07427900 | -0.21972400 |
| H | 5.04402700 | -1.43641300 | 1.11197100 |
| C | 5.38184100 | 1.11875400 | -1.06440400 |
| H | 6.14920100 | 1.67066300 | -1.59782500 |
| O | -2.06903000 | 1.93832700 | 0.65569200 |
| O | 1.78941500 | 1.13742000 | -0.75350100 |
| S | -7.34288600 | -0.56408000 | -0.34066000 |
| S | 7.47467300 | -0.33128600 | -0.01176100 |
| O | 8.11202400 | 0.89646400 | 0.54411000 |
| O | 7.98090800 | -0.66475400 | -1.37383300 |
| O | 7.51826400 | -1.48661800 | 0.92617700 |
| O | -7.15414600 | -2.03632300 | -0.22218500 |
| O | -7.70390100 | -0.13181700 | -1.72116400 |
| O | -8.26987600 | -0.01034800 | 0.68715200 |
| H | -0.17526400 | 3.11524200 | 0.81269300 |
| O | 0.76745700 | 3.11649500 | 1.02143700 |
| H | 1.16434400 | 2.49076500 | 0.38670000 |
| H | -1.12539900 | 1.50000900 | 2.23769200 |
| O | -0.45131600 | 1.34641300 | 2.92569600 |
| H | 0.28156300 | 1.88030300 | 2.58462400 |
| H | -1.99984400 | -1.45140600 | -1.05509100 |
| H | -1.60532900 | -0.46494800 | 1.65229100 |
| H | 1.87820900 | -0.41205300 | 1.83388300 |
| Pd | 0.21861200 | -0.12371800 | -0.58231200 |
| O | -0.94286400 | 1.37394500 | -1.38482400 |
| H | -0.35889600 | 2.05249200 | -1.74104600 |
| H | -1.44431700 | 1.73524000 | -0.44810400 |
| H | -4.26672600 | 3.21467100 | 0.18932700 |
| H | 3.75980500 | 2.24904600 | -1.89689500 |
| H | 1.78749600 | -2.11227500 | -0.53775100 |

54
RS_delta_ID1_TS1_P, E(SCF) = -
2484.16922472, E(ZPE) = -2483.769139, E(G)
= -2483.836428 a.u.

| | | | |
|---|-------------|------------|-------------|
| C | -0.42416600 | 2.66752700 | 0.80609700 |
| H | -0.95068000 | 3.61275700 | 0.95933300 |
| H | -0.15479400 | 2.27035600 | 1.78795900 |
| C | 0.78742300 | 2.83662300 | -0.07041400 |
| H | 0.49232200 | 3.20168000 | -1.05693200 |

| | | | | | | | |
|----|-------------|--------------|-------------|--|-------------|-------------|-------------|
| H | 1.49236000 | 3.55329700 | 0.36058900 | C | -3.60558100 | -1.82873300 | -0.16148500 |
| N | 1.43426700 | 1.51058500 | -0.25216100 | C | -5.52282200 | -0.40214500 | 0.00621600 |
| N | -1.31395500 | 1.68020200 | 0.15315900 | H | -5.13592700 | 1.63513700 | 0.49618600 |
| C | 2.27010400 | 1.12625300 | 0.93563500 | C | -4.97015200 | -1.65640300 | -0.22286100 |
| H | 2.72887800 | 2.04935000 | 1.30824600 | H | -5.61397200 | -2.49804700 | -0.45780900 |
| C | -2.35101400 | 1.10600500 | 1.03962500 | O | 1.40396900 | -0.99881900 | -0.38078100 |
| H | -2.85911700 | 1.92242600 | 1.56402300 | O | -1.44448500 | -1.00019100 | -0.19628200 |
| C | 3.34724000 | 0.13644900 | 0.63177300 | S | 7.25656000 | -0.19578800 | -0.00601100 |
| C | 3.10940100 | -1.25950200 | 0.71352300 | S | -7.30301900 | -0.19579200 | -0.09620600 |
| C | 4.61569600 | 0.60886200 | 0.31022200 | O | -7.87677900 | -1.12431900 | 0.91904700 |
| C | 4.20972500 | -2.11545000 | 0.48185700 | O | -7.67597100 | -0.57706500 | -1.48828500 |
| C | 5.66651300 | -0.25434100 | 0.06859100 | O | -7.56955400 | 1.23719900 | 0.20668100 |
| H | 4.79189700 | 1.67968500 | 0.25666900 | O | 7.50045800 | 1.26076900 | 0.18306300 |
| C | 5.45577700 | -1.62751100 | 0.16287200 | O | 7.79107800 | -0.71435000 | -1.29743800 |
| H | 6.27899300 | -2.31306400 | -0.01505900 | O | 7.69431400 | -1.01680500 | -1.01680500 |
| C | -3.35185700 | 0.30675000 | 0.26531100 | H | 0.90019300 | -2.25738900 | 0.95572700 |
| C | -2.95554600 | -0.74065900 | -0.59321100 | O | 0.31153700 | -2.56235500 | 1.66894700 |
| C | -4.70574400 | 0.57907500 | 0.42714500 | H | -0.54169900 | -2.23313800 | 1.33520900 |
| C | -3.95562400 | -1.246432900 | -1.24649300 | H | 0.36473300 | 0.40878000 | 2.65922300 |
| C | -5.67273000 | -0.16413800 | -0.21966000 | O | 0.84574400 | -0.22857300 | 3.19504000 |
| H | -5.01481800 | 1.38889100 | 1.08045100 | H | 0.68350000 | -1.07964800 | 2.74428100 |
| C | -5.29068600 | -1.20521100 | -1.05735100 | H | 1.68266200 | 1.72391000 | -1.70251800 |
| H | -6.04508400 | -1.79175400 | -1.57199800 | H | 1.98501600 | 1.80872800 | 1.20209900 |
| O | 1.92011800 | -1.74234900 | 0.94651400 | H | -1.96702900 | 1.47132200 | 1.76320000 |
| O | -1.69620700 | -1.08694100 | -0.80750700 | Pd | -0.05859000 | 0.42283300 | -0.31865700 |
| S | 7.29068100 | 0.35811900 | -0.37381800 | O | -0.29795500 | -2.71411100 | -1.82030400 |
| S | -7.41843700 | 0.18891700 | 0.00283100 | H | -0.91358200 | -2.28323100 | -1.20606200 |
| O | -8.01547200 | -1.05894600 | 0.55822200 | H | 0.53538500 | -2.29315600 | -1.55643700 |
| O | -7.94350700 | 0.51270600 | -1.35451500 | H | 3.14208300 | -2.79109200 | -0.59741100 |
| O | -7.48862400 | 1.33930300 | 0.94510300 | H | -3.16253000 | -2.80369000 | -0.33838000 |
| O | 7.20602300 | 1.84411000 | -0.30439600 | H | -1.84079700 | 2.09845800 | -1.08828300 |
| O | 7.55718900 | -0.14332300 | -1.75397100 | | | | |
| O | 8.23681800 | -0.21769400 | 0.62533100 | | | | |
| O | 0.29452800 | -2.86354100 | 0.98104100 | 54 | | | |
| O | -0.65501300 | -3.06018200 | 1.01533300 | RS_delta_ID1_TS1_V2_R_W-shift-for-new-Ref, | | | |
| H | -1.05590300 | -2.45321700 | 0.36770700 | E(SCF) = -2484.18422533, E(ZPE) = - | | | |
| H | 0.78642200 | -1.07157700 | 2.27074200 | 2483.785016, E(G) = -2483.853874 a.u. | | | |
| O | 0.02465200 | -0.90894000 | 2.86253300 | C | 0.48697900 | 3.27972000 | -0.78710200 |
| H | -0.58710000 | -1.59626700 | 2.56301100 | H | 0.07361700 | 3.48703100 | -1.77598800 |
| H | 2.05251200 | 1.55326300 | -1.06097700 | H | 1.16859300 | 4.09452600 | -0.52989000 |
| H | 1.59585300 | 0.75747300 | 1.70973300 | C | -0.62530600 | 3.15859500 | 0.22232300 |
| H | -1.81609200 | 0.50521700 | 1.78482200 | H | -1.23110300 | 4.06858300 | 0.25449700 |
| Pd | -0.15531000 | 0.20172200 | -0.62046500 | H | -0.23223100 | 2.98253200 | 1.22694500 |
| O | 1.02350200 | -1.33406400 | -1.43939800 | N | -1.45701700 | 1.98605100 | -0.13570200 |
| H | 0.43058900 | -1.99041900 | -1.82567800 | N | 1.22693600 | 1.99260100 | -0.88086900 |
| H | 1.38170000 | -1.70882500 | -0.57895400 | C | -2.42127900 | 1.59422000 | 0.91386600 |
| H | 4.03585900 | -3.18450500 | 0.55220200 | H | -1.82404200 | 1.32405500 | 1.79205400 |
| H | -3.64067000 | -2.28469100 | -1.90203700 | C | 2.33640800 | 1.84822200 | 0.08016700 |
| H | -1.77438200 | 2.12431100 | -0.64361900 | H | 1.89998400 | 1.85970700 | 1.08591300 |
| | | | | C | -3.29643500 | 0.46548300 | 0.47256200 |
| | | | | C | -2.74377900 | -0.76589800 | 0.06371700 |
| | | | | C | -4.67732600 | 0.61357100 | 0.51788700 |
| | | | | C | -3.62216000 | -1.81616700 | -0.25145900 |
| | | | | C | -5.52344000 | -0.42961800 | 0.19646400 |
| | | | | H | -5.10472600 | 1.56226000 | 0.82666300 |
| | | | | C | -4.98776300 | -1.65379000 | -0.18538900 |
| | | | | H | -3.19124200 | -2.76700000 | -0.54851400 |
| | | | | H | -5.64595000 | -2.47997300 | -0.43479600 |
| | | | | C | 3.16215600 | 0.61269400 | -0.14896600 |
| | | | | C | 2.63349800 | -0.63646400 | -0.54726800 |
| | | | | C | 4.53004000 | 0.71497600 | 0.10494200 |
| | | | | C | 3.52355200 | -1.72409100 | -0.66253800 |
| | | | | C | 5.37722900 | -0.36648400 | -0.00374600 |
| | | | | H | 4.94398900 | 1.67233200 | 0.40608600 |
| | | | | C | 4.86523400 | -1.59818000 | -0.39812100 |
| | | | | H | 3.10598800 | -2.67709300 | -0.97254400 |
| | | | | H | 5.52197500 | -2.45682000 | -0.49215400 |
| | | | | O | -1.44223600 | -0.99464800 | -0.01489000 |
| | | | | O | 1.36385300 | -0.88512900 | -0.81144400 |
| | | | | S | -7.30610800 | -0.22597200 | 0.24593300 |
| | | | | S | 7.13680700 | -0.20508200 | 0.31432200 |
| | | | | O | 7.45705600 | -1.23657600 | 1.34126300 |
| | | | | O | 7.80844400 | -0.47284600 | -0.98927100 |
| | | | | O | 7.34006600 | 1.18714100 | 0.79977000 |
| | | | | O | -7.81163100 | -1.29943200 | 1.14788600 |
| | | | | O | -7.54818400 | 1.14407600 | 0.77627900 |
| | | | | O | -7.77502300 | -0.39864000 | -1.15909500 |
| | | | | H | 2.98516600 | 2.72796900 | 0.00542800 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|--|--|--|
| 54 | | | | | | | |
| RS_delta_ID1_TS1_R, E(SCF) = - | | | | | | | |
| 2484.18406122, E(ZPE) = -2483.783619, E(G) | | | | | | | |
| = -2483.849669 a.u. | | | | | | | |
| C | -0.58620900 | 3.14196900 | 0.17012300 | | | | |
| H | -1.18222200 | 4.05736600 | 0.11250600 | | | | |
| H | -0.25720800 | 3.02234900 | 1.20581700 | | | | |
| C | 0.58554300 | 3.19359400 | -0.77512500 | | | | |
| H | 0.23332100 | 3.36417600 | -1.79454100 | | | | |
| H | 1.26804800 | 4.00683900 | -0.51642800 | | | | |
| N | 1.30422700 | 1.89004400 | -0.77169100 | | | | |
| N | -1.40796600 | 1.95803000 | -0.17417800 | | | | |
| C | 2.41642600 | 1.78186700 | 0.19519400 | | | | |
| H | 3.05708400 | 2.66477200 | 0.09716400 | | | | |
| C | -2.47076000 | 1.66326400 | 0.80942100 | | | | |
| H | -3.09519100 | 2.55333900 | 0.94112400 | | | | |
| C | 3.24402400 | 0.54988300 | -0.02968600 | | | | |
| C | 2.69401500 | -0.72772500 | -0.27203100 | | | | |
| C | 4.62834400 | 0.68536400 | 0.04073400 | | | | |
| C | 3.57883200 | -1.81439100 | -0.41221500 | | | | |
| C | 5.47563300 | -0.39311100 | -0.10119500 | | | | |
| H | 5.05875100 | 1.66670800 | 0.21307800 | | | | |
| C | 4.94129600 | -1.65663700 | -0.32653500 | | | | |
| H | 5.59780100 | -2.51290100 | -0.44303900 | | | | |
| C | -3.31688100 | 0.50446700 | 0.39121900 | | | | |
| C | -2.74517900 | -0.75942400 | 0.13944200 | | | | |
| C | -4.69529900 | 0.66113200 | 0.30898300 | | | | |

| | | | |
|----|-------------|-------------|-------------|
| H | -3.03582400 | 2.46028300 | 1.18272500 |
| H | -1.96902500 | 2.17998100 | -0.99729200 |
| O | 2.10219100 | -0.90206200 | 2.72273000 |
| H | 1.50143500 | -1.51846400 | 2.26159400 |
| H | 0.41397200 | -2.10925300 | -2.04067900 |
| O | -0.44458000 | -2.51314500 | -2.23749100 |
| H | -0.98879200 | -2.13411900 | -1.52744900 |
| H | 2.70530700 | -0.59987500 | 2.03452900 |
| H | -0.41485200 | -2.21761800 | 1.05221600 |
| O | 0.45055000 | -2.64225900 | 1.18581700 |
| H | 0.90630800 | -2.34312500 | 0.38067400 |
| Pd | -0.10826400 | 0.48618300 | -0.49634700 |
| H | 1.60128400 | 1.89338000 | -1.82259100 |

54

RS_delta_ID1_TS1, E(SCF) = -2484.16060502,
E(ZPE) = -2483.761185, E(G) = -2483.827386
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.50259400 | 2.93754600 | 0.49684500 |
| H | -1.07130300 | 3.87075700 | 0.53720600 |
| H | -0.20628900 | 2.68038400 | 1.51704800 |
| C | 0.69075400 | 3.05272700 | -0.41227600 |
| H | 0.36650900 | 3.28562700 | -1.42893100 |
| H | 1.36810600 | 3.84589500 | -0.08409200 |
| N | 1.39820400 | 1.74542100 | -0.45457800 |
| N | -1.34747400 | 1.83568900 | -0.01028300 |
| C | 2.35481100 | 1.56634100 | 0.67946600 |
| H | 2.91957600 | 2.49847500 | 0.78840100 |
| C | -2.38546000 | 1.37732900 | 0.93684200 |
| H | -2.95689300 | 2.24572100 | 1.28305500 |
| C | 3.30082800 | 0.43419100 | 0.46066000 |
| C | 2.82997800 | -0.90028300 | 0.48759400 |
| C | 4.64867900 | 0.69242700 | 0.24546400 |
| C | 3.77665500 | -1.92897500 | 0.29677700 |
| C | 5.55523100 | -0.33539000 | 0.02560000 |
| H | 5.00451900 | 1.71809200 | 0.22801300 |
| C | 5.10943600 | -1.65337500 | 0.09185800 |
| H | 5.81751600 | -2.46417100 | -0.05070600 |
| C | -3.31146600 | 0.38623000 | 0.30596900 |
| C | -2.82392100 | -0.79250700 | -0.29693300 |
| C | -4.68258200 | 0.60884200 | 0.35620000 |
| C | -3.75561900 | -1.71556400 | -0.80295400 |
| C | -5.58116200 | -0.31030700 | -0.14804600 |
| H | -5.06114000 | 1.51984400 | 0.80867200 |
| C | -5.10981200 | -1.48476800 | -0.72299600 |
| H | -5.80983500 | -2.21282600 | -1.12063400 |
| O | 1.56472900 | -1.18059200 | 0.65614200 |
| O | -1.54209400 | -1.09562300 | -0.39787400 |
| S | 7.29328200 | -0.00237300 | -0.21722900 |
| S | -7.35026100 | -0.01899600 | -0.06940300 |
| O | -7.90802300 | -1.13014100 | 0.75351000 |
| O | -7.83229700 | -0.06085600 | -1.47971600 |
| O | -7.51972900 | 1.31751000 | 0.56462000 |
| O | 7.45075100 | 1.47635100 | -0.12528600 |
| O | 7.59968500 | -0.53589400 | -1.57662200 |
| O | 8.03005400 | -0.73367900 | 0.85383300 |
| H | 0.49987400 | -2.66634100 | 1.09640500 |
| O | -0.37416200 | -3.07881200 | 1.22106700 |
| H | -0.92839800 | -2.53882700 | 0.63033200 |
| H | 0.55031300 | -0.61410000 | 2.16517800 |
| O | -0.13643900 | -0.62718200 | 2.85691900 |
| H | -0.57103700 | -1.46858900 | 2.65749700 |
| H | 1.93520700 | 1.68962000 | -1.31891500 |
| H | 1.76149800 | 1.43397200 | 1.58849400 |
| H | -1.85091800 | 0.95142700 | 1.79442300 |
| Pd | -0.07632600 | 0.28572400 | -0.46740200 |
| O | 0.91944800 | -1.37187500 | -1.93755900 |
| H | 0.11093800 | -1.84702900 | -2.16213900 |
| H | 1.23889200 | -1.78738100 | -1.11523400 |
| H | 3.41846900 | -2.95389500 | 0.31680000 |
| H | -3.37106000 | -2.62181000 | -1.25824400 |
| H | -1.79490300 | 2.12556300 | -0.88108800 |

56

RS_delta_ID1_TS2-diamond_P, E(SCF) = -
2485.33432770, E(ZPE) = -2484.917290, E(G)
= -2484.984467 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.58177100 | -0.11024700 | 2.96551200 |
| H | 1.20417200 | -0.37573900 | 3.82483600 |
| H | 0.29849700 | 0.94268700 | 3.04014800 |
| C | -0.61630100 | -1.00889200 | 2.84572700 |
| H | -0.29505100 | -2.04571400 | 2.72075400 |
| H | -1.24650700 | -0.96125100 | 3.73639900 |
| N | -1.40261700 | -0.62380100 | 1.63796300 |
| C | -2.51540200 | 0.32547300 | 1.97042400 |
| H | -3.01880100 | -0.09362100 | 2.84969300 |
| C | -3.48103700 | 0.48767700 | 0.85009800 |
| C | -3.44057700 | 1.65561600 | 0.03670900 |
| C | -4.41942100 | -0.50940100 | 0.61369700 |
| C | -4.37752700 | 1.70664500 | -1.03288500 |
| C | -5.32020200 | -0.41954200 | -0.43025200 |
| H | -4.45644800 | -1.38153300 | 1.26282000 |
| C | -5.28708400 | 0.70213700 | -1.25824300 |
| H | -5.98975900 | 0.78128200 | -2.08298000 |
| O | -2.59808400 | 2.60770300 | 0.22960400 |
| S | -6.51182300 | -1.71477400 | -0.74496400 |
| O | -7.85193100 | -1.05689700 | -0.76018000 |
| O | -6.36210400 | -2.69650700 | 0.36711500 |
| O | -6.15791300 | -2.29248800 | -2.07598700 |
| H | 2.05672400 | 3.81880300 | -1.12916500 |
| O | 1.27754700 | 3.32942600 | -0.85539800 |
| H | 1.47465000 | 2.37847300 | -0.99475300 |
| H | -1.07320900 | 2.74123100 | 1.11907500 |
| O | -0.19759700 | 2.86105500 | 1.54757900 |
| H | 0.37321700 | 3.17126400 | 0.82689100 |
| H | -1.83683200 | -1.46435600 | 1.25824100 |
| H | -2.06678300 | 1.27692700 | 2.25728400 |
| Pd | -0.00793200 | 0.01720700 | 0.19022800 |
| O | -1.18975700 | 2.62337900 | -2.08685400 |
| H | -0.33975300 | 3.02660600 | -1.85029500 |
| H | -1.74674300 | 2.77288700 | -1.29055300 |
| H | -4.35774200 | 2.58449600 | -1.67227400 |
| H | -1.25418400 | -0.09984100 | -1.05724700 |
| H | -1.06195700 | 0.69860500 | -1.12523900 |
| N | 1.34357900 | -0.26775400 | 1.70887000 |
| C | 2.53163500 | 0.60545500 | 1.57489200 |
| H | 3.14229400 | 0.51002100 | 2.47852100 |
| C | 3.32291800 | 0.20554500 | 0.37284300 |
| C | 2.71547200 | 0.21523400 | -0.89674500 |
| C | 4.64614900 | -0.19518300 | 0.49719900 |
| C | 3.47559200 | -0.16733600 | -2.00970300 |
| C | 5.38269100 | -0.56290000 | -0.61236800 |
| H | 5.11569200 | -0.21621700 | 1.47544500 |
| C | 4.79469700 | -0.54219900 | -1.87097100 |
| H | 5.37207400 | -0.83439300 | -2.74231600 |
| O | 1.46254500 | 0.62089100 | -1.08846300 |
| S | 7.09053800 | -1.09873200 | -0.44994600 |
| O | 7.88763300 | -0.17244500 | -1.30217200 |
| O | 7.11943600 | -2.50168600 | -0.95129800 |
| O | 7.41653700 | -0.98957300 | 0.99798200 |
| H | 2.16127500 | 1.63351500 | 1.52160500 |
| H | 2.99900900 | -0.15137800 | -2.98334300 |
| H | 1.65412500 | -1.23865200 | 1.62563600 |

54

RS_delta_ID1_TS2-diamond_R_noH2, E(SCF) = -
2484.17446563, E(ZPE) = -2483.774125, E(G)
= -2483.841809 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.14353500 | -2.24940000 | 0.44521000 |
| H | 0.47307900 | -3.29145800 | 0.43982100 |
| H | -0.09185800 | -1.97422900 | 1.47684300 |
| C | -1.03731800 | -2.02836100 | -0.46115900 |
| H | -0.77466500 | -2.27816900 | -1.49161600 |
| H | -1.89120100 | -2.64696200 | -0.16917100 |
| N | -1.39607700 | -0.58710400 | -0.41786000 |
| C | -2.23480300 | -0.21859500 | 0.78872500 |
| H | -2.28372000 | -1.09966000 | 1.43225300 |
| C | -3.60163600 | 0.21568400 | 0.38927800 |
| C | -3.80600800 | 1.56772900 | -0.00209700 |
| C | -4.65327200 | -0.69293800 | 0.37966500 |
| C | -5.12355900 | 1.92648300 | -0.37809600 |
| C | -5.92397600 | -0.30895000 | -0.00330500 |
| H | -4.48109000 | -1.72075800 | 0.68764900 |
| C | -6.15161500 | 1.01384200 | -0.38073900 |

| | | | |
|----|-------------|-------------|--------------|
| H | -7.15025500 | 1.32178200 | -0.67718000 |
| O | -2.84855500 | 2.43952800 | -0.00848100 |
| S | -7.28868400 | -1.46635500 | -0.00991300 |
| O | -8.30476100 | -0.91662900 | 0.93526000 |
| O | -6.72845700 | -2.77300800 | 0.43774000 |
| O | -7.79237300 | -1.50300800 | -1.41447700 |
| H | 1.56061300 | 4.55112400 | 0.44524500 |
| O | 1.11390900 | 3.70869300 | 0.55534600 |
| H | 1.75979200 | 3.00325100 | 0.33562100 |
| H | -1.81056500 | 2.82042000 | 1.47276400 |
| O | -1.17249500 | 2.97487600 | 2.19572600 |
| H | -0.36436200 | 3.27501300 | 1.75368100 |
| H | -1.94555100 | -0.36562800 | -1.24683900 |
| H | -1.71479500 | 0.56838700 | 1.33931200 |
| Pd | 0.40017600 | 0.44480300 | -0.427588900 |
| O | -0.52144300 | 2.22516400 | -1.04898800 |
| H | -0.02248100 | 2.95955100 | -0.63390100 |
| H | -1.46393400 | 2.28015800 | -0.67688900 |
| H | -5.29821600 | 2.95716100 | -0.67050500 |
| N | 1.23573400 | -1.35685800 | -0.01079600 |
| C | 2.33717700 | -1.19668300 | 0.96243200 |
| H | 2.66095200 | -2.18622800 | 1.30254300 |
| C | 3.49709900 | -0.46403900 | 0.36607400 |
| C | 3.33722900 | 0.80302700 | -0.23303700 |
| C | 4.76653900 | -1.02485200 | 0.44868000 |
| C | 4.48312300 | 1.46039800 | -0.71287200 |
| C | 5.87998300 | -0.35886200 | -0.02344500 |
| H | 4.89281000 | -2.00108800 | 0.90616500 |
| C | 5.73305800 | 0.89482500 | -0.60519300 |
| H | 6.60364700 | 1.42450300 | -0.97887900 |
| O | 2.17564300 | 1.42277700 | -0.35158400 |
| S | 7.51455500 | -1.09249500 | 0.08561000 |
| O | 8.36455300 | -0.08327400 | 0.77909600 |
| O | 7.94967800 | -1.33032900 | -1.32089500 |
| O | 7.34946000 | -2.35122500 | 0.86343500 |
| H | 1.91279900 | -0.67063200 | 1.82465500 |
| H | 4.35097800 | 2.43579200 | -1.16852700 |
| H | 1.62377400 | -1.72630800 | -0.88088100 |

56
RS_delta_ID1_TS2-diamond_R, E(SCF) = -
2485.34723744, E(ZPE) = -2484.931483, E(G)
= -2485.000680 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.14487200 | -2.25085100 | 0.45247400 |
| H | 0.47404800 | -3.29296200 | 0.44118500 |
| H | -0.09224500 | -1.98208100 | 1.48539300 |
| C | -1.03421600 | -2.02386400 | -0.45478400 |
| H | -0.76795300 | -2.26473400 | -1.48702600 |
| H | -1.88813500 | -2.64606200 | -0.17061600 |
| N | -1.39474600 | -0.58358800 | -0.40122000 |
| C | -2.23183600 | -0.22231500 | 0.80877800 |
| H | -2.27912300 | -1.10649200 | 1.44814100 |
| C | -3.59943400 | 0.21307300 | 0.41347100 |
| C | -3.80406300 | 1.56589200 | 0.02488000 |
| C | -4.65153500 | -0.69497100 | 0.40554100 |
| C | -5.12219900 | 1.92568900 | -0.34790100 |
| C | -5.92301800 | -0.30972200 | 0.02653400 |
| H | -4.47896100 | -1.72324400 | 0.71174800 |
| C | -6.15076800 | 1.01359300 | -0.34895400 |
| H | -7.14995400 | 1.32240700 | -0.64262000 |
| O | -2.84622900 | 2.43734800 | 0.01797000 |
| S | -7.28847700 | -1.46629300 | 0.02216100 |
| O | -8.30390100 | -0.91412600 | 0.96657300 |
| O | -6.72898200 | -2.77251200 | 0.47196300 |
| O | -7.79245200 | -1.50504800 | -1.38223900 |
| H | 1.56447900 | 4.55915900 | 0.44850900 |
| O | 1.11796700 | 3.71718200 | 0.56272000 |
| H | 1.76403800 | 3.01051700 | 0.34719100 |
| H | -1.80154900 | 2.81859600 | 1.49482700 |
| O | -1.15959000 | 2.97405300 | 2.21406700 |
| H | -0.35559400 | 3.27918600 | 1.76793400 |
| H | -1.94710100 | -0.35835000 | -1.22793800 |
| H | -1.71121800 | 0.56268900 | 1.36173900 |
| Pd | 0.40351300 | 0.44611300 | -0.45319000 |
| O | -0.52170900 | 2.22750500 | -1.02760000 |
| H | -0.02220100 | 2.96534000 | -0.61909900 |
| H | -1.46327700 | 2.28213500 | -0.65247800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -5.29709300 | 2.95678800 | -0.63865300 |
| H | -0.32737800 | -0.37136800 | -3.67657300 |
| H | -0.40298400 | 0.23932900 | -3.33912200 |
| N | 1.23820200 | -1.35606600 | 0.00387100 |
| C | 2.33838500 | -1.20180300 | 0.97940000 |
| H | 2.66126800 | -2.19330600 | 1.31457100 |
| C | 3.49931300 | -0.46650400 | 0.38823200 |
| C | 3.34052900 | 0.80318300 | -0.20552000 |
| C | 4.76853400 | -1.02791600 | 0.46998700 |
| C | 4.48700400 | 1.46229300 | -0.68137800 |
| C | 5.88271200 | -0.35995800 | 0.00242700 |
| H | 4.89406300 | -2.00608000 | 0.92353400 |
| C | 5.73671300 | 0.89605200 | -0.57451300 |
| H | 6.60784600 | 1.42714900 | -0.94487400 |
| O | 2.17922800 | 1.42398500 | -0.32300000 |
| S | 7.51690300 | -1.09472300 | 0.11030300 |
| O | 8.36776400 | -0.08642800 | 0.80401200 |
| O | 7.95124600 | -1.33204100 | -1.29653600 |
| O | 7.35126900 | -2.35178900 | 0.86745200 |
| H | 1.91308800 | -0.68012500 | 1.84384600 |
| H | 4.35552000 | 2.43954400 | -1.13324900 |
| H | 1.62692100 | -1.71998300 | -0.86833300 |

56
RS_delta_ID1_TS2-diamond, E(SCF) = -
2485.32044865, E(ZPE) = -2484.905386, E(G)
= -2484.969704 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.57399100 | 1.15764500 | 2.68739500 |
| H | 1.20432700 | 1.27101600 | 3.57412300 |
| H | 0.27617900 | 2.14655700 | 2.32650500 |
| C | -0.61213500 | 0.27529900 | 2.95174200 |
| H | -0.27719800 | -0.72209300 | 3.24710800 |
| H | -1.23511600 | 0.66857700 | 3.75800300 |
| N | -1.40945400 | 0.14373300 | 1.69947000 |
| C | -2.53186500 | 1.13117900 | 1.66216000 |
| H | -3.00991700 | 1.08590400 | 2.64884000 |
| C | -3.52456400 | 0.83645100 | 0.59276700 |
| C | -3.64078200 | 1.69979800 | -0.53099100 |
| C | -4.34662400 | -0.27685000 | 0.72071000 |
| C | -4.60821200 | 1.33139800 | -1.50651400 |
| C | -5.27138200 | -0.60602300 | -0.25157900 |
| H | 4.26870100 | -0.91173800 | 1.60088300 |
| C | -5.39661400 | 0.21430800 | -1.37271300 |
| H | -6.12194500 | -0.03583100 | -2.14164200 |
| O | -2.89216400 | 2.73613800 | -0.69787900 |
| S | -6.31213200 | -2.05140000 | -0.09953700 |
| O | -7.72175700 | -1.55963800 | -0.12030200 |
| O | -5.94415000 | -2.69411400 | 1.19466100 |
| O | -6.00355300 | -2.91143200 | -1.28041700 |
| H | 1.88401700 | 3.22389300 | -2.51915800 |
| O | 1.26859000 | 2.81115000 | -1.90902000 |
| H | 1.56689900 | 1.88950700 | -1.77622800 |
| H | -1.29796400 | 3.25665600 | 0.00774200 |
| O | -0.42050800 | 3.53804200 | 0.34079900 |
| H | 0.18312900 | 3.40277400 | -0.40519400 |
| H | -1.83095800 | -0.78415700 | 1.68594200 |
| H | -2.10017900 | 2.12501500 | 1.54363700 |
| Pd | -0.02089000 | 0.15156400 | 0.09997600 |
| O | -1.10022000 | 1.26301000 | -2.07301500 |
| H | -0.34571600 | 1.82423200 | -2.30802400 |
| H | -1.75699700 | 1.89117200 | -1.69616000 |
| H | -4.70323200 | 1.97191700 | -2.37846900 |
| H | -1.13562500 | -1.42349400 | -0.93932500 |
| H | -1.43124800 | -0.80724900 | -1.28254800 |
| N | 1.33086800 | 0.50112900 | 1.60277100 |
| C | 2.53883200 | 1.21864000 | 1.13675900 |
| H | 3.14359900 | 1.48626200 | 2.00993200 |
| C | 3.32311300 | 0.34358900 | 0.21578000 |
| C | 2.70766000 | -0.16742000 | -0.94315900 |
| C | 4.64169600 | 0.01453100 | 0.49661800 |
| C | 3.45662500 | -0.99080300 | -1.79476400 |
| C | 5.36863800 | -0.78900700 | -0.36102800 |
| H | 5.11436500 | 0.39606200 | 1.39568300 |
| C | 4.77310600 | -1.28621200 | -1.51422600 |
| H | 5.34247700 | -1.91932000 | -2.18723600 |
| O | 1.46368900 | 0.14752600 | -1.28600600 |
| S | 7.08346200 | -1.20090900 | -0.01071700 |

O 7.87010100 -0.63723700 -1.14377000
 O 7.13775900 -2.68917300 0.03675100
 O 7.40017700 -0.56237600 1.29554700
 H 2.20035700 2.14516900 0.66264300
 H 2.97527400 -1.37590600 -2.68659000
 H 1.62134500 -0.42828100 1.91647000

56

RS_delta_ID1_TS3-diamond_img15, E(SCF) = -
 2485.32316054, E(ZPE) = -2484.909456, E(G)
 = -2484.974426 a.u.

C 0.59124200 -0.69279000 2.79761700
 H 1.18277100 -1.18129300 3.60260500
 H 0.37184300 0.32363800 3.14063900
 C -0.66444000 -1.46956300 2.48729600
 H -0.40564000 -2.47385300 2.15282600
 H -1.29745000 -1.55960500 3.36915400
 N -1.41540600 -0.81101900 1.37471200
 C -2.41588600 0.19207500 1.85528800
 H -2.86550800 -0.21553700 2.76846100
 C -3.47786800 0.45928500 0.84060300
 C -3.52749100 1.71020200 0.15521800
 C -4.43084000 -0.51416900 0.56715000
 C -4.55066500 1.86195300 -0.81688700
 C -5.41550100 -0.32981200 -0.38005900
 H -4.40396400 -1.45701400 1.10942300
 C -5.46023900 0.87096500 -1.10808800
 H -6.22385400 1.02514800 -1.83845400
 O -2.68097600 2.66966100 0.37373700
 S -6.62455600 -1.60531500 -0.74802400
 O -7.96409200 -0.98828300 -0.52216800
 O -6.33542100 -2.72967700 0.18523000
 O -6.41544900 -1.97287800 -2.18687600
 H 1.86354000 3.85975400 -0.93063900
 O 1.18405900 3.24650900 -0.62805000
 H 1.51163600 2.33635600 -0.81329800
 H -1.28810400 3.16400400 1.45784400
 O -0.42643000 3.40730600 1.87798200
 H 0.20453800 3.32087600 1.06456400
 H -1.93797800 -1.54308800 0.87560100
 H -1.88752600 1.11610700 2.10958300
 Pd 0.02998300 -0.08317300 0.04547400
 O -1.16449900 2.36845100 -1.69052600
 H -0.32155800 2.83697000 -1.51061000
 H -1.77748400 2.64787000 -0.95371300
 H -4.57857500 2.80037300 -1.35668300
 H -1.10644700 0.12619900 -1.17967700
 H -0.98392500 1.05317100 -1.29932000
 N 1.36679300 -0.59522900 1.54755800
 C 2.49957300 0.36661200 1.57799000
 H 3.07917600 0.23497900 2.49061500
 C 3.36298000 0.13772100 0.37337900
 C 2.79657700 0.24003200 -0.91530700
 C 4.69543300 -0.21512300 0.52518700
 C 3.62404300 -0.03269600 -2.02386500
 C 5.48354900 -0.47011900 -0.58031400
 H 5.12052700 -0.30342300 1.51523500
 C 4.94837800 -0.37398600 -1.85491900
 H 5.56562800 -0.57632100 -2.72196200
 O 1.54504000 0.61834700 -1.12893000
 S 7.21205400 -0.92449600 -0.39719100
 O 7.98454500 0.13527800 -1.10713300
 O 7.35389700 -2.26314400 -1.04142600
 O 7.47306000 -0.95829000 1.07532900
 H 2.03646200 1.37519500 1.59969300
 H 3.18263200 0.04334700 -3.01027600
 H 1.73742900 -1.51693400 1.31216800

53

RS_lambda_hs_D1_TS1_P, E(SCF) = -
 2408.92137030, E(ZPE) = -2408.527931, E(G)
 = -2408.594332 a.u.

C 0.29550000 0.02210700 -2.97328100
 H 0.18072200 -0.60988600 -3.85704700
 H 0.22612500 1.06494800 -3.30101100
 C 1.63710000 -0.22743100 -2.33439600
 H 2.44520000 -0.03911400 -3.04989600

H 1.78691200 0.44198900 -1.48557200
 N 1.71642300 -1.62171800 -1.82399000
 C 3.01884900 -1.90274300 -1.14473500
 H 2.97328200 -2.93235800 -0.78638300
 C 3.36612900 -0.94547600 -0.04320800
 C 2.90745500 -1.08503200 1.27010300
 C 4.22457900 0.11782600 -0.32247700
 C 3.30065200 -0.18063800 2.25494600
 C 4.61043700 1.01317200 0.65185700
 H 4.61093800 0.24149700 -1.32943900
 C 4.14068200 0.86686100 1.95035500
 H 4.44008500 1.56867200 2.72113800
 O 2.11930200 -2.10704200 1.68259900
 S 5.69604600 2.39389100 0.25792700
 O 4.86979700 3.61592400 0.46343900
 O 6.10801600 2.19476600 -1.15730200
 O 6.82800500 2.29752700 1.22009500
 H 0.45309100 -3.14769400 0.02960300
 H 1.58464200 -2.47189500 0.43337200
 H 1.66785300 -2.25430500 -2.62214900
 H 3.80679700 -1.85490600 -1.90410000
 Pd -0.07812900 -1.91994900 -0.80955200
 H 2.92360600 -0.32230200 3.26173400
 H -1.35658500 -3.02666400 2.93361400
 O -1.80973000 -3.71613500 2.42873900
 H -1.92565900 -3.27602300 1.56781200
 H 0.48046900 -1.40256700 2.59196200
 O -0.43798900 -1.12332600 2.72159200
 H -0.83487400 -1.24639800 1.84263700
 N -0.79764100 -0.32223100 -2.04709500
 C -1.22851300 0.71741600 -1.09704400
 H -1.36946400 1.67296500 -1.61677800
 C -2.51572700 0.32321800 -0.42877900
 C -2.71810600 -0.93279300 0.19207100
 C -3.54813900 1.25724600 -0.41337600
 C -3.96125000 -1.16738600 0.81218100
 C -4.75583200 1.00441000 0.20408700
 H -3.40139900 2.21777100 -0.89727700
 C -4.95878500 -0.22155600 0.82640700
 H -4.10619600 -2.12966200 1.29238100
 H -5.90461200 -0.43453300 1.31453800
 O -1.82385100 -1.90679800 0.26936600
 S -6.07572000 2.21903400 0.20044200
 O -6.38480400 2.48876800 1.63398100
 O -7.21703900 1.57737100 -0.51332300
 O -5.53947800 3.41023800 -0.51442300
 H -0.42250600 0.86428500 0.36595600
 H -1.60919900 -0.61078000 -2.58648300

53

RS_lambda_hs_D1_TS1_R, E(SCF) = -
 2408.91090224, E(ZPE) = -2408.521044, E(G)
 = -2408.587998 a.u.

C -0.27411300 -2.36511300 -2.34296700
 H -0.45207900 -3.44253100 -2.34498300
 H -0.59584400 -1.97540100 -3.31153700
 C 1.19297400 -2.09671700 -2.10500200
 H 1.81010300 -2.62912500 -2.83591400
 H 1.42912500 -1.03104000 -2.17325700
 N 1.50508000 -2.54230200 -0.72905100
 C 2.91380700 -2.36140800 -0.30226900
 H 3.05442500 -3.04356700 0.54140600
 C 3.24684400 -0.96733600 0.11695600
 C 2.55943900 -0.40048700 1.21275400
 C 4.27911300 -0.26826000 -0.48853000
 C 2.98766500 0.84537700 1.69414500
 C 4.67199600 0.97031500 -0.01163600
 H 4.80424200 -0.70342500 -1.33307900
 C 4.02679200 1.52093800 1.08878100
 H 4.34015600 2.48762000 1.47043200
 O 1.54998200 -1.02987100 1.79320500
 S 5.97569800 1.89816600 -0.82570200
 O 5.30372100 3.06734300 -1.46300300
 O 6.58466100 0.96913300 -1.81763300
 O 6.92258900 2.30514200 0.25119900
 H 0.67315300 -4.33683800 1.99034700
 H 0.77625300 -3.66179100 2.30032100

| | | | |
|----|-------------|-------------|-------------|
| H | 1.27875600 | -3.53352800 | -0.65076900 |
| H | 3.57574400 | -2.68610900 | -1.11221300 |
| Pd | 0.12917100 | -1.50644000 | 0.39337300 |
| H | 2.47129000 | 1.26989000 | 2.54868100 |
| H | 0.68661400 | -0.49122800 | 3.35650100 |
| O | -0.08001900 | -0.25892500 | 3.91071100 |
| H | -0.77290200 | -0.24146300 | 3.23066600 |
| H | -0.30925100 | 1.27500200 | 1.29705100 |
| O | -0.12992400 | 2.20495800 | 1.07696300 |
| H | -1.00225800 | 2.56870000 | 0.90233300 |
| N | -1.10063400 | -1.78281900 | -1.24843200 |
| C | -1.67466500 | -0.44985800 | -1.54833400 |
| H | -2.13983500 | -0.47520400 | -2.53926700 |
| C | -2.69960700 | -0.04970000 | -0.53177000 |
| C | -2.42618600 | -0.04514700 | 0.85304700 |
| C | -3.95231600 | 0.36006400 | -0.97765700 |
| C | -3.43585800 | 0.39675700 | 1.72733600 |
| C | -4.92800700 | 0.79043600 | -0.10165100 |
| H | -4.17160200 | 0.35143800 | -2.04071400 |
| C | -4.66220500 | 0.81211900 | 1.26221800 |
| H | -3.21326400 | 0.40606400 | 2.78952300 |
| H | -5.42287400 | 1.15078100 | 1.95858900 |
| O | -1.27026500 | -0.39898600 | 1.38719200 |
| S | -6.54139700 | 1.30660500 | -0.69331800 |
| O | -6.73864600 | 2.69214100 | -0.18025300 |
| O | -7.51640200 | 0.34224000 | -0.10814100 |
| O | -6.47427700 | 1.23747400 | -2.17906000 |
| H | -0.83821000 | 0.25754900 | -1.59419100 |
| H | -1.86892500 | -2.41710200 | -1.04037600 |

53

RS_lambda_hs_D1_TS1, E(SCF) = -
2408.88562550, E(ZPE) = -2408.496792, E(G)
= -2408.561788 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.22505400 | -1.51062100 | -2.83868700 |
| H | 0.19087500 | -2.49261500 | -3.31441300 |
| H | 0.04917300 | -0.75585700 | -3.60942200 |
| C | 1.55207800 | -1.29962000 | -2.16068700 |
| H | 2.38285900 | -1.39046400 | -2.86765900 |
| H | 1.61204400 | -0.30758900 | -1.70692600 |
| N | 1.68019000 | -2.29602300 | -1.07289900 |
| C | 2.92078700 | -2.14488300 | -0.25267300 |
| H | 2.83916100 | -2.88300600 | 0.54927800 |
| C | 3.15777800 | -0.77111500 | 0.27874800 |
| C | 2.30142900 | -0.21548200 | 1.26830100 |
| C | 4.25611000 | -0.05370300 | -0.17930800 |
| C | 2.65760100 | 1.05928200 | 1.77609200 |
| C | 4.56643400 | 1.19390400 | 0.32740700 |
| H | 4.89690500 | -0.48447800 | -0.94337100 |
| C | 3.75518200 | 1.74677600 | 1.31559900 |
| H | 3.99655200 | 2.72250300 | 1.72705200 |
| O | 1.24129000 | -0.83174200 | 1.68932000 |
| S | 5.96869200 | 2.12348100 | -0.28203700 |
| O | 5.40537100 | 3.34357500 | -0.93212500 |
| O | 6.67313400 | 1.22990500 | -1.24491000 |
| O | 6.79730400 | 2.45772000 | 0.91316200 |
| H | 0.30084800 | -3.60695400 | 1.27466700 |
| H | 0.61194000 | -2.97478300 | 1.61142000 |
| H | 1.70080300 | -3.22892700 | -1.48536300 |
| H | 3.76475300 | -2.43671900 | -0.88714900 |
| Pd | -0.10600900 | -2.19162200 | -0.05574600 |
| H | 2.02368300 | 1.48711800 | 2.54656600 |
| H | 0.01166000 | -1.13600100 | 3.06080900 |
| O | -0.81266500 | -1.45476700 | 3.46987100 |
| H | -1.34116400 | -1.71206900 | 2.69791000 |
| H | -0.03016800 | 0.53697800 | 1.56788800 |
| O | -0.59911800 | 1.32653100 | 1.46456100 |
| H | -1.48780900 | 0.97447400 | 1.34639500 |
| N | -0.86663000 | -1.47485400 | -1.82687900 |
| C | -1.42619200 | -0.13742800 | -1.55668100 |
| H | -1.72457000 | 0.31191200 | -2.51013600 |
| C | -2.61114600 | -0.16023500 | -0.63344300 |
| C | -2.73400500 | -1.01266400 | 0.48781700 |
| C | -3.60229300 | 0.79217300 | -0.86732600 |
| C | -3.85255000 | -0.84040900 | 1.32950900 |
| C | -4.68616500 | 0.94037400 | -0.02978200 |
| H | -3.51771900 | 1.44703500 | -1.72900300 |

| | | | |
|---|-------------|-------------|-------------|
| C | -4.80826800 | 0.11452900 | 1.08237400 |
| H | -3.93058900 | -1.49435200 | 2.19159900 |
| H | -5.65559000 | 0.22241100 | 1.75162200 |
| O | -1.89135500 | -1.96970900 | 0.83286000 |
| S | -5.95830600 | 2.16189300 | -0.36348700 |
| O | -6.05419900 | 2.99359400 | 0.86910900 |
| O | -7.20378800 | 1.38447200 | -0.62263000 |
| O | -5.48970100 | 2.92693300 | -1.55124800 |
| H | -0.61839500 | 0.47941000 | -1.14363700 |
| H | -1.62111800 | -2.09062100 | -2.12428600 |

54

RS_lambda_hs_ID1_TS1_P, E(SCF) = -
2484.16277260, E(ZPE) = -2483.762687, E(G)
= -2483.828266 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.31552200 | -1.21113400 | 2.92165500 |
| H | -0.27502700 | -2.15027200 | 3.47723200 |
| H | -0.17908300 | -0.39110100 | 3.63223700 |
| C | -1.62016400 | -1.08391500 | 2.18611100 |
| H | -2.47294000 | -1.13708400 | 2.87005600 |
| H | -1.68001400 | -0.12512800 | 1.66753900 |
| N | -1.70010100 | -2.15228700 | 1.16160100 |
| C | -2.83964700 | -1.98718900 | 0.20018000 |
| H | -2.63413600 | -2.68043100 | -0.61823200 |
| C | -3.05781500 | -0.59271900 | -0.29169900 |
| C | -2.11974400 | 0.04374300 | -1.15618400 |
| C | -4.21047200 | 0.09975500 | 0.09997200 |
| C | -2.45909200 | 1.34650100 | -1.60938700 |
| C | -4.49986700 | 1.35289100 | -0.34720700 |
| H | -4.91182800 | -0.41301300 | 0.76973100 |
| C | -3.61023900 | 1.98442000 | -1.21313100 |
| H | -3.83225300 | 2.98263100 | -1.57972700 |
| O | -1.01276900 | -0.52050400 | -1.50294400 |
| S | -5.98799900 | 2.20413000 | 0.15988500 |
| O | -6.75335600 | 2.49247800 | -1.08976100 |
| O | -5.54106100 | 3.45545300 | 0.84139900 |
| O | -6.70843600 | 1.27402800 | 1.07595800 |
| H | -0.12756000 | -3.07521500 | -2.13696500 |
| H | -1.82948900 | -3.04650500 | 1.63290700 |
| H | -3.74584800 | -2.32729000 | 0.71242800 |
| Pd | 0.16784400 | -2.23914600 | 0.29015800 |
| H | -1.76653400 | 1.83874700 | -2.28510900 |
| O | 0.01423300 | -1.23171700 | -2.76428600 |
| O | 0.65354100 | -1.88597700 | -3.11952500 |
| H | 1.38194500 | -1.84885000 | -2.47687600 |
| H | 0.30332800 | 0.69939500 | -1.70156300 |
| O | 0.99957600 | 1.37379200 | -1.86225500 |
| H | 1.74310000 | 1.10118100 | -1.31361400 |
| N | 0.80336700 | -1.23707400 | 1.94262500 |
| C | 1.30502200 | 0.07723400 | 1.50386700 |
| H | 1.52018600 | 0.68674600 | 2.38847400 |
| C | 2.54796800 | -0.02644100 | 0.66326300 |
| C | 2.77915300 | -1.03749300 | -0.30146900 |
| C | 3.49023500 | 0.99141000 | 0.81453900 |
| C | 3.95213600 | -0.94326000 | -1.08120400 |
| C | 4.62471400 | 1.06041200 | 0.03588600 |
| H | 3.32444200 | 1.76235800 | 1.56087600 |
| C | 4.85332900 | 0.08041600 | -0.92495900 |
| H | 4.11490500 | -1.71815500 | -1.82300800 |
| H | 5.74289800 | 0.12247900 | -1.54517700 |
| O | 1.99332700 | -2.06468800 | -0.55517200 |
| S | 5.82106700 | 2.38028000 | 0.25071100 |
| O | 5.88071900 | 3.08930500 | -1.05903700 |
| O | 7.10726800 | 1.70775200 | 0.59084500 |
| O | 5.29814200 | 3.23182500 | 1.35401900 |
| H | 0.49232000 | 0.57248200 | 0.95714300 |
| H | 1.58114500 | -1.75699700 | 2.34564300 |
| O | -0.47073000 | -3.51707100 | -1.31843300 |
| H | -0.02631900 | -4.36948300 | -1.25822300 |

54

RS_lambda_hs_ID1_TS1_R, E(SCF) = -
2484.18394025, E(ZPE) = -2483.784154, E(G)
= -2483.851581 a.u.

| | | | |
|---|------------|-------------|------------|
| C | 0.35803700 | -1.20841900 | 2.91947000 |
| H | 0.51537200 | -2.24860900 | 3.21423300 |
| H | 0.71374900 | -0.57429400 | 3.73477800 |

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | -1.11029700 | -0.98217400 | 2.64415000 | O | 6.54982700 | 1.63201800 | -1.20893700 |
| H | -1.71538400 | -1.27846300 | 3.50789500 | H | 0.25881500 | -3.43895600 | 1.99161900 |
| H | -1.32492000 | 0.06841300 | 2.42588300 | H | 1.67091100 | -2.97754800 | -1.84785700 |
| N | -1.46007900 | -1.78123300 | 1.45572400 | H | 3.76530600 | -2.17278200 | -1.24617600 |
| C | -2.87345400 | -1.71559800 | 1.02621300 | Pd | -0.04483100 | -1.98926100 | -0.29781100 |
| H | -3.05141100 | -2.63943600 | 0.46462300 | H | 1.90318100 | 1.31217500 | 2.58132700 |
| C | -3.21071900 | -0.53478100 | 0.17288200 | H | 0.23088700 | -1.62984600 | -2.87257500 |
| C | -2.53727800 | -0.36211900 | -1.05456300 | O | -0.47490800 | -2.23417600 | 3.17486100 |
| C | -4.23231800 | 0.33338900 | 0.52438500 | H | -1.17684300 | -2.06033300 | 2.52240600 |
| C | -2.95180700 | 0.66670600 | -1.90921000 | H | -0.11191400 | 0.35482600 | 1.80682600 |
| C | -4.61830200 | 1.35487300 | -0.32647900 | O | -0.71109400 | 1.10145700 | 2.01037500 |
| H | -4.74729600 | 0.20703000 | 1.47151300 | H | -1.57726400 | 0.81888100 | 1.69783700 |
| C | -3.98289500 | 1.51094400 | -1.55142700 | N | -0.89334600 | -1.20537700 | -2.01140800 |
| H | -4.29109600 | 2.30713200 | -2.22188500 | C | -1.45358900 | 0.10669600 | -1.64029000 |
| O | -1.53711100 | -1.16185400 | -1.40873900 | H | -1.79712000 | 0.61364800 | -2.54947600 |
| S | -5.94075900 | 2.48359400 | 0.12286200 | C | -2.60166100 | 0.01753200 | -0.67201800 |
| O | -6.98977100 | 2.31779300 | -0.92354300 | C | -2.66314200 | -0.88260000 | 0.42017900 |
| O | -5.33336600 | 3.84503600 | 0.10728300 | C | -3.62811100 | 0.94624000 | -0.83465100 |
| O | -6.39788000 | 2.06555800 | 1.47669200 | C | -3.75788800 | -0.77878000 | -1.04311500 |
| H | -0.75834000 | -4.41122000 | 0.03756800 | C | -4.68804900 | 1.03150000 | 0.04275400 |
| H | -1.22110600 | -2.77308800 | 1.60363000 | H | -3.59226300 | 1.63377900 | -1.67404500 |
| H | -3.51912500 | -1.74191100 | 1.91082900 | C | -4.74839700 | 0.16200900 | 1.12578300 |
| Pd | -0.09063000 | -1.15580700 | 0.06439800 | H | -3.78742700 | -1.45992800 | 2.14361800 |
| H | -2.43771000 | 0.78362900 | -2.85717100 | H | -5.57527000 | 0.21945300 | 1.82627400 |
| H | -1.52515000 | -3.05833300 | -1.53843900 | O | -1.77975300 | -1.81899200 | 0.69974300 |
| O | -1.07245800 | -3.90899200 | -1.68829500 | S | -6.00346400 | 2.22834200 | -0.19856600 |
| H | -0.33938800 | -3.61923200 | -2.25764900 | O | -6.06022700 | 3.02839600 | 1.05766800 |
| H | -0.48493800 | -1.58698100 | -3.01634100 | O | -7.24180200 | 1.42687200 | -0.41686000 |
| O | 0.34663600 | -1.99877000 | -3.30472200 | O | -5.61321800 | 3.03420100 | -1.38778800 |
| H | 0.97170200 | -1.54052800 | -2.71286500 | H | -0.63157500 | 0.70610800 | -1.22890500 |
| N | 1.16629000 | -0.97302000 | 1.68910300 | H | -1.65330600 | -1.80642800 | -2.32232600 |
| C | 1.78458600 | 0.36980300 | 1.58951700 | O | 0.57996000 | -3.79126600 | 1.13416500 |
| H | 2.28493300 | 0.60237800 | 2.53566000 | H | 0.01290700 | -4.54175100 | 0.93349600 |
| C | 2.78517700 | 0.43577300 | 0.47542200 | | | | |
| C | 2.48120900 | 0.02506100 | -0.84433000 | 53 | | | |
| C | 4.05225900 | 0.93763600 | 0.75723400 | RS_lambda_D1_TS1_P_CH_TS, E(SCF) = - | | | |
| C | 3.48612000 | 0.16495600 | -1.82348100 | 2408.87058397, E(ZPE) = -2408.482942, E(G) | | | |
| C | 5.01837600 | 1.06485700 | -0.21980100 | = -2408.547177 a.u. | | | |
| H | 4.29067400 | 1.24605800 | 1.77042700 | N | 1.45212900 | 2.09170600 | 0.23344400 |
| C | 4.72676600 | 0.67292000 | -1.52222900 | N | -1.23139700 | 2.07710600 | -0.61267500 |
| H | 3.24589200 | -0.14838800 | -2.83446500 | C | 2.39217000 | 1.63137600 | 1.29237500 |
| H | 5.48017800 | 0.76613800 | -2.29832400 | H | 3.10374000 | 2.43794000 | 1.49751200 |
| O | 1.32556900 | -0.46643100 | -1.22948200 | C | -2.30244200 | 1.65826600 | 0.30726700 |
| S | 6.64586900 | 1.71404700 | 0.15864600 | H | -3.01709700 | 2.48092300 | 0.42984900 |
| O | 6.82432400 | 2.90400800 | -0.72271600 | C | 3.10967300 | 0.36307100 | 0.93627000 |
| O | 7.60963500 | 0.62252700 | -0.16561100 | C | 2.87063900 | -0.81820700 | 1.76419100 |
| O | 6.62703500 | 2.06073400 | 1.60700800 | C | 4.30081200 | 0.44078100 | 0.15167000 |
| H | 0.96936300 | 1.09137700 | 1.46541200 | C | 3.75598500 | -1.92712500 | 1.53617800 |
| H | 1.91279400 | -1.66408900 | 1.64654400 | C | 5.10665200 | -0.63766200 | -0.00488200 |
| O | -0.79492500 | -4.53189000 | 1.00971500 | H | 4.54014300 | 1.36771300 | -0.36268200 |
| H | 0.06070700 | -4.88763300 | 1.26070900 | C | 4.82095800 | -1.83537600 | 0.69901200 |
| | | | | H | 3.55963100 | -2.83617200 | 2.09432300 |
| | | | | H | 5.47840600 | -2.68922300 | 0.56431300 |
| | | | | C | -3.03850800 | 0.44359800 | -0.18973500 |
| | | | | C | -2.41322300 | -0.69948900 | -0.74574600 |
| | | | | C | -4.42438800 | 0.44557500 | -0.04245200 |
| | | | | C | -3.23586300 | -1.79136400 | -1.09511800 |
| | | | | C | -5.20523900 | -0.63509700 | -0.39490600 |
| | | | | H | -4.91059400 | 1.32404300 | 0.37065000 |
| | | | | C | -4.59857400 | -1.76774600 | -0.92648100 |
| | | | | H | -2.74402300 | -2.66525600 | -1.50946600 |
| | | | | H | -5.19770800 | -2.62798800 | -1.20808100 |
| | | | | O | 1.87899800 | -0.90909600 | 2.52319400 |
| | | | | O | -1.12158400 | -0.86042300 | -0.97206900 |
| | | | | S | 6.56600800 | -0.57978700 | -1.04729000 |
| | | | | S | -6.98963800 | -0.58556600 | -0.22712900 |
| | | | | O | -7.36003000 | -1.79506200 | 0.56222700 |
| | | | | O | -7.53198700 | -0.62942800 | -1.61633900 |
| | | | | O | -7.30396000 | 0.68872300 | 0.47673700 |
| | | | | O | 6.36315500 | -1.64441000 | -2.06923000 |
| | | | | O | 7.71163300 | -0.86992400 | -0.14051600 |
| | | | | O | 6.60121300 | 0.79108800 | -1.62259800 |
| | | | | H | 1.98849300 | 2.46943600 | -0.54861900 |
| | | | | H | 1.79719900 | 1.46669800 | 2.19164600 |
| | | | | H | -1.83933400 | 1.47284600 | 1.28418800 |
| | | | | Pd | 0.23550000 | 0.58027000 | -0.51062800 |
| | | | | C | -0.56768700 | 3.36077900 | -0.28565800 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|--|--|--|
| 54 | | | | | | | |
| RS_lambda_hs_ID1_TS1, E(SCF) = - | | | | | | | |
| 2484.15903107, E(ZPE) = -2483.760623, E(G) | | | | | | | |
| = -2483.826862 a.u. | | | | | | | |
| C | 0.16270100 | -1.17206800 | -3.05875900 | | | | |
| H | 0.10928500 | -2.11988000 | -3.59827300 | | | | |
| H | -0.03394700 | -3.36813300 | -3.77316600 | | | | |
| C | 1.51951200 | -1.01332900 | -2.42090400 | | | | |
| H | 2.32059000 | -1.07782900 | -3.16430700 | | | | |
| H | 1.61016500 | -0.04758700 | -1.91831800 | | | | |
| N | 1.67267900 | -2.06516600 | -1.39165600 | | | | |
| C | 2.91868800 | -1.96962100 | -0.58100200 | | | | |
| H | 2.85342600 | -2.78375500 | 0.14555100 | | | | |
| C | 3.11725400 | -0.65183000 | 0.09053900 | | | | |
| C | 2.24360400 | -0.23364600 | 1.13060700 | | | | |
| C | 4.19575900 | 0.14263600 | -0.27126800 | | | | |
| C | 2.55500800 | 0.98761100 | 1.77644000 | | | | |
| C | 4.46537100 | 1.33581000 | 0.36601800 | | | | |
| H | 4.85342800 | -0.18260200 | -1.07887600 | | | | |
| C | 3.63474100 | 1.75257800 | 1.40235700 | | | | |
| H | 3.84372400 | 2.68556700 | 1.91766200 | | | | |
| O | 1.20404300 | -0.92862400 | 1.48459200 | | | | |
| S | 5.86393100 | 2.35152600 | -0.09860100 | | | | |
| O | 6.71217000 | 2.47391500 | 1.12360800 | | | | |
| O | 5.29912100 | 3.66682300 | -0.52210600 | | | | |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.52079500 | 3.13654300 | 0.73105800 |
| H | 1.05727400 | 4.06503600 | 0.94626200 |
| H | 0.10009500 | 2.76648400 | 1.67009100 |
| H | -0.14214100 | 3.75078700 | -1.21307400 |
| H | -1.29495900 | 4.09221800 | 0.08157300 |
| H | -1.61260100 | 2.12854000 | -1.55448100 |
| H | 0.41777800 | -2.02314900 | 1.71504000 |
| H | 1.39302300 | -0.60844500 | -0.50819600 |
| H | 2.14049900 | -0.16904400 | 0.03070900 |
| O | -0.46335700 | -2.31298500 | 1.42634100 |
| H | -0.57842300 | -1.92213000 | 0.54147600 |
| H | 0.23931300 | 0.01511400 | 2.91401900 |
| O | -0.72231400 | 0.15458500 | 2.95848000 |
| H | -1.04343500 | -0.63689700 | 2.49907200 |

53

RS_lambda_D1_TS1_P, E(SCF) = -
 2408.88829293, E(ZPE) = -2408.496868, E(G)
 = -2408.562633 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.44819900 | 1.73041300 | 0.30009000 |
| N | -1.23997500 | 2.01501400 | -0.45473900 |
| C | 2.36786200 | 1.17651000 | 1.34533300 |
| H | 2.93740900 | 2.02673800 | 1.73858900 |
| C | -2.32179900 | 1.60934100 | 0.46681400 |
| H | -2.93763400 | 2.48604500 | 0.69296200 |
| C | 3.29816200 | 0.10785100 | 0.88375200 |
| C | 2.90973900 | -1.25812600 | 0.97997100 |
| C | 4.56916200 | 0.44825400 | 0.43606900 |
| C | 3.87423200 | -2.22303300 | 0.60201900 |
| C | 5.48115800 | -0.51978400 | 0.06299200 |
| H | 4.85858200 | 1.49427200 | 0.38349200 |
| C | 5.12333100 | -1.86366400 | 0.15280200 |
| H | 3.59014000 | -3.26860500 | 0.66668400 |
| H | 5.83717100 | -2.62967900 | -0.13572900 |
| C | -3.18734700 | 0.53121900 | -0.12177600 |
| C | -2.68997000 | -0.55175300 | -0.87832300 |
| C | -4.55336600 | 0.59403200 | 0.14617800 |
| C | -3.60301100 | -1.53253600 | -1.31224700 |
| C | -5.42808300 | -0.37828600 | -0.28821200 |
| H | -4.94522100 | 1.42992300 | 0.71719000 |
| C | -4.94385000 | -1.45368700 | -1.02506800 |
| H | -3.20502100 | -2.36204000 | -1.88708000 |
| H | -5.62225100 | -2.22568900 | -1.37393000 |
| O | 1.71114400 | -1.60209000 | 1.33545500 |
| O | -1.42745600 | -0.74551200 | -1.23473400 |
| S | 7.10949200 | -0.08304700 | -0.53954600 |
| S | -7.18509700 | -0.27102400 | 0.06013100 |
| O | -7.53465800 | -1.53143100 | 0.77479400 |
| O | -7.85537800 | -0.16834300 | -1.26772400 |
| O | -7.36382800 | 0.94514500 | 0.90008700 |
| O | 7.17723200 | -0.58669900 | -1.94321100 |
| O | 8.08249700 | -0.77735200 | 0.35343800 |
| O | 7.20153200 | 1.40188400 | -0.45226100 |
| H | 2.01828700 | 2.11081900 | -0.45657600 |
| H | 1.72573600 | 0.80703500 | 2.14720900 |
| H | -1.85365200 | 1.27357500 | 1.40035900 |
| Pd | 0.05739700 | 0.43730200 | -0.56980300 |
| C | -0.46147900 | 3.21697800 | -0.06593100 |
| C | 0.62554100 | 2.82052900 | 0.89036900 |
| H | 1.25554400 | 3.67551100 | 1.15072400 |
| H | 0.19794900 | 2.43008000 | 1.81798200 |
| H | -0.03525500 | 3.63353700 | -0.98045100 |
| H | -1.12024300 | 3.96986000 | 0.37524700 |
| H | -1.64264500 | 2.16256300 | -1.37908200 |
| H | 0.21377300 | -2.68231600 | 0.81132900 |
| H | 1.17007000 | -0.80092800 | -1.06684800 |
| H | 1.08047000 | -0.99880700 | -0.25620800 |
| O | -0.71454900 | -2.89980800 | 0.60852000 |
| H | -0.94039300 | -2.32125500 | -0.13863400 |
| H | 0.27243100 | -0.83770100 | 2.25488000 |
| O | -0.65042000 | -0.66309600 | 2.52428100 |
| H | -1.11399500 | -1.36635000 | 2.04656200 |

53

RS_lambda_D1_TS1_R, E(SCF) = -
 2408.91866586, E(ZPE) = -2408.530347, E(G)
 = -2408.597141 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.36978000 | 1.93324000 | -0.06061100 |
| N | -1.35026400 | 1.85495400 | -0.62216600 |
| C | 2.442724800 | 1.64428900 | 0.93150100 |
| H | 3.04274900 | 2.53909000 | 1.07261200 |
| C | -2.44448100 | 1.75644100 | 0.36852600 |
| H | -3.07469300 | 2.64891700 | 0.29273000 |
| C | 3.28321800 | 0.49496300 | 0.51006000 |
| C | 2.71658900 | -0.77301100 | 0.26765400 |
| C | 4.65719200 | 0.66645200 | 0.39525200 |
| C | 3.57958000 | -1.83331300 | -0.05755400 |
| C | 5.48750200 | -0.38842400 | -0.07008100 |
| H | 5.09224000 | 1.64449900 | 0.57399800 |
| C | 4.94084700 | -1.64668100 | -0.15154400 |
| H | 3.14332400 | -2.81188000 | -0.23079700 |
| H | 5.58695700 | -2.48094700 | -0.40602700 |
| C | -3.28783200 | 0.53762500 | 0.13834900 |
| C | -2.74080300 | -0.74746800 | -0.06799400 |
| C | -4.67134100 | 0.68944200 | 0.15784900 |
| C | -3.63040200 | -1.82782300 | -0.22531500 |
| C | -5.52371800 | -0.38366600 | 0.00119500 |
| H | -5.09642100 | 1.67748600 | 0.30248600 |
| C | -4.99341300 | -1.65500100 | -0.18808500 |
| H | -3.19809400 | -2.81217600 | -0.37688000 |
| H | -5.65423200 | -2.50670600 | -0.31390200 |
| O | 1.41938800 | -1.01909000 | 0.34869100 |
| O | -1.45010600 | -1.02676900 | -0.11253500 |
| S | 7.26286900 | -0.16444500 | -0.07188600 |
| S | -7.30472100 | -0.17054100 | 0.03460000 |
| O | -7.78796600 | -0.98081700 | 1.18914500 |
| O | -7.80198700 | -0.69244900 | -1.27052700 |
| O | -7.54252700 | 1.28917300 | 0.20717300 |
| O | 7.60952000 | -0.54698000 | -1.47032300 |
| O | 7.86823900 | -1.08309600 | 0.93416700 |
| O | 7.52110300 | 1.27236300 | 0.22035400 |
| H | 1.80398500 | 2.06664400 | -0.97552600 |
| H | 1.91243800 | 1.44051700 | 1.87684500 |
| H | -1.98879400 | 1.76326800 | 1.36476300 |
| Pd | 0.01915600 | 0.39164200 | -0.16659100 |
| C | -0.63087200 | 3.15700000 | -0.65644400 |
| C | 0.54831000 | 3.11840800 | 0.27872600 |
| H | 1.14173500 | 4.03455800 | 0.20866400 |
| H | 0.22814700 | 3.00419000 | 1.31764700 |
| H | -0.28683300 | 3.30754600 | -1.68190200 |
| H | -1.30983600 | 3.97626800 | -0.40708300 |
| H | -1.74779500 | 1.67779000 | -1.54296100 |
| H | 0.81551200 | -2.45247600 | -0.83264000 |
| H | 2.12994600 | -0.05359800 | -3.05973200 |
| H | 2.02338600 | -0.37982600 | -2.39186100 |
| O | 0.17979800 | -2.93356300 | -1.38753100 |
| H | -0.63808000 | -2.47316200 | -1.14069700 |
| H | 0.53190600 | -2.11629400 | 1.67773300 |
| O | -0.28807300 | -2.47754600 | 2.04999700 |
| H | -0.93056600 | -2.13400700 | 1.40930200 |

53

RS_lambda_D1_TS1-trigo_02, E(SCF) = -
 2408.88420975, E(ZPE) = -2408.494414, E(G)
 = -2408.557754 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | -1.25425300 | 2.03561000 | -0.59842500 |
| N | 1.43769100 | 1.89837200 | 0.13659400 |
| C | -2.33355000 | 1.67585300 | 0.34055400 |
| H | -2.97599300 | 2.55143400 | 0.48245400 |
| C | 2.42880600 | 1.47521600 | 1.17322600 |
| H | 3.04240100 | 2.35215600 | 1.40815100 |
| C | -3.16301200 | 0.52936800 | -0.16009400 |
| C | -2.63776200 | -0.57543500 | -0.86390200 |
| C | -4.52242700 | 0.55142300 | 0.14273200 |
| C | -3.51937800 | -1.61644300 | -1.21522600 |
| C | -5.36585800 | -0.48065200 | -0.20788600 |
| H | -4.93338700 | 1.40220000 | 0.67705100 |
| C | -4.85541800 | -1.57506900 | -0.89734000 |
| H | -3.10183800 | -2.46213400 | -1.75155300 |
| H | -5.50787600 | -2.39424600 | -1.18201500 |
| C | 3.28662000 | 0.32545300 | 0.78717500 |
| C | 2.72722300 | -0.97750300 | 0.86690300 |
| C | 4.61033900 | 0.50650100 | 0.41713600 |
| C | 3.57723400 | -2.06177000 | 0.54816200 |

| | | | |
|----|-------------|-------------|-------------|
| C | 5.41537900 | -0.57541800 | 0.10532000 |
| H | 5.02781600 | 1.50824900 | 0.36812300 |
| C | 4.88988300 | -1.86283500 | 0.18068000 |
| H | 3.16052800 | -3.06328300 | 0.59729600 |
| H | 5.51779300 | -2.71401000 | -0.06589300 |
| O | -1.37587700 | -0.73571100 | -1.23830900 |
| O | 1.47880700 | -1.14518800 | 1.15900700 |
| S | -7.11959200 | -0.41410100 | 0.16821900 |
| S | 7.13359500 | -0.35022800 | -0.34405500 |
| O | 7.93573300 | -0.94066700 | 0.76809400 |
| O | 7.32644700 | -1.08705400 | -1.62709800 |
| O | 7.33516200 | 1.11997600 | -0.48382000 |
| O | -7.31783500 | 0.81259200 | 0.98856000 |
| O | -7.81279700 | -0.35251500 | -1.15051700 |
| O | -7.42502900 | -1.66983700 | 0.91065900 |
| H | -1.64678800 | 2.09781600 | -1.53660200 |
| H | -1.86816300 | 1.42807800 | 1.30159800 |
| H | 1.84123200 | 1.22684000 | 2.06126500 |
| Pd | 0.08940000 | 0.48954400 | -0.61675500 |
| C | 0.58213700 | 2.98506300 | 0.67835700 |
| C | -0.51774500 | 3.28686500 | -0.29496800 |
| H | -0.10787000 | 3.65805400 | -1.23637200 |
| H | -1.20293700 | 4.04237700 | 0.09902700 |
| H | 1.18095700 | 3.87457700 | 0.89325600 |
| H | 0.16984300 | 2.62463300 | 1.62533500 |
| H | 1.95529200 | 2.25270800 | -0.66899800 |
| H | 1.35144500 | -0.66495300 | -1.67894500 |
| H | 1.29300400 | -1.04731300 | -1.00375800 |
| H | 0.24127900 | -2.42379400 | 0.85330500 |
| O | -0.63257300 | -2.81434300 | 0.64602300 |
| H | -0.92130900 | -2.29063600 | -0.11795300 |
| H | 0.08005800 | -0.46941800 | 2.13461600 |
| O | -0.83800200 | -0.40911100 | 2.46262800 |
| H | -1.22309300 | -1.20579300 | 2.07076300 |

53
RS_lambda_D1_TS1-trigo_P, E(SCF) = -
2408.88829264, E(ZPE) = -2408.496859, E(G)
= -2408.562471 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.23979600 | 2.01496400 | -0.45466600 |
| N | 1.44826700 | 1.73025700 | 0.30032300 |
| C | -2.32161100 | 1.60926400 | 0.46690000 |
| H | -2.93741100 | 2.48597400 | 0.69313300 |
| C | 2.36768500 | 1.17622400 | 1.34574800 |
| H | 2.93715500 | 2.02640000 | 1.73921800 |
| C | -3.18720900 | 0.53124100 | -0.12181100 |
| C | -2.68987000 | -0.55172300 | -0.87840200 |
| C | -4.55324000 | 0.59412200 | 0.14606800 |
| C | -3.60296600 | -1.53231400 | -1.31259700 |
| C | -5.42801100 | -0.37806900 | -0.28851600 |
| H | -4.94506900 | 1.43000700 | 0.71710200 |
| C | -4.94381300 | -1.45341800 | -1.02545400 |
| H | -3.20502100 | -2.36178100 | -1.88751600 |
| H | -5.62224200 | -2.22530800 | -1.37451000 |
| C | 3.29804200 | 0.10762400 | 0.88416000 |
| C | 2.90966900 | -1.25837400 | 0.98016600 |
| C | 4.56902300 | 0.44813700 | 0.43650300 |
| C | 3.87422100 | -2.22317700 | 0.60210000 |
| C | 5.48109400 | -0.51980200 | 0.06334600 |
| H | 4.85839500 | 1.49418000 | 0.38411100 |
| C | 5.12330000 | -1.86370200 | 0.15290100 |
| H | 3.59017500 | -3.26876700 | 0.66661900 |
| H | 5.83715600 | -2.62966600 | -0.13571300 |
| O | -1.42729600 | -0.74568400 | -1.23455800 |
| O | 1.71108600 | -1.60250300 | 1.33554700 |
| S | -7.18500400 | -0.27090600 | 0.06001500 |
| S | 7.10912000 | -0.08284300 | -0.53987500 |
| O | 7.20199700 | -1.40189700 | -0.45015600 |
| O | 8.08257300 | -0.77919400 | 0.35101400 |
| O | 7.17533000 | -0.58406600 | -1.94448000 |
| O | -7.36372000 | 0.94531500 | 0.89990000 |
| O | -7.85546700 | -0.16835500 | -1.26775000 |
| O | -7.53432100 | -1.53130800 | 0.77480300 |
| H | -1.64247400 | 2.16243600 | -1.37902100 |
| H | -1.85343800 | 1.27341900 | 1.40040500 |
| H | 1.72536400 | 0.80667400 | 2.14743200 |
| Pd | 0.05751600 | 0.43717500 | -0.56968200 |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.62567000 | 2.82051500 | 0.89044800 |
| C | -0.46129800 | 3.21691400 | -0.06593100 |
| H | -0.03502400 | 3.63339700 | -0.98046200 |
| H | -1.12005300 | 3.96986100 | 0.37516200 |
| H | 1.25574400 | 3.67548000 | 1.15069300 |
| H | 0.19803600 | 2.43025600 | 1.81811700 |
| H | 2.01856600 | 2.11059100 | -0.45621900 |
| H | 1.17005000 | -0.80112400 | -1.06678600 |
| H | 1.08046900 | -0.99910800 | -0.25614500 |
| H | 0.21349300 | -2.68231200 | 0.81175400 |
| O | -0.71478200 | -2.89991600 | 0.60862900 |
| H | -0.94063600 | -2.32133800 | -0.13823000 |
| H | 0.27276000 | -0.83799300 | 2.25508900 |
| O | -0.65002600 | -0.66278200 | 2.52438300 |
| H | -1.11399200 | -1.36589700 | 2.04686400 |

53
RS_lambda_D1_TS1-trigo_R, E(SCF) = -
2408.91745983, E(ZPE) = -2408.526881, E(G)
= -2408.592681 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.29389800 | 1.93734900 | -0.61714400 |
| N | 1.39212700 | 1.93538600 | 0.08850300 |
| C | -2.41045900 | 1.74122600 | 0.33172400 |
| H | -3.04869000 | 2.63161500 | 0.31578900 |
| C | 2.42372300 | 1.53814200 | 1.07110100 |
| H | 3.04284500 | 2.40674600 | 1.32011300 |
| C | -3.24130500 | 0.53660500 | -0.00157900 |
| C | -2.69180800 | -0.70925900 | -0.38586200 |
| C | -4.62323900 | 0.66186800 | 0.11381800 |
| C | -3.58598900 | -1.77629200 | -0.61633900 |
| C | -5.47529300 | -0.39828700 | -0.11410700 |
| H | -5.04846400 | 1.61986100 | 0.39689400 |
| C | -4.94544500 | -1.63009200 | -0.48357100 |
| H | -3.16050900 | -2.73005300 | -0.91180100 |
| H | -5.60380300 | -2.47260300 | -0.66987600 |
| C | 3.27435700 | 0.43311100 | 0.53640900 |
| C | 2.68920900 | -0.80036000 | 0.18232600 |
| C | 4.64585900 | 0.60614800 | 0.40934500 |
| C | 3.53192400 | -1.82940200 | -0.26838600 |
| C | 5.45652000 | -0.41773800 | -0.04300700 |
| H | 5.09501700 | 1.55774500 | 0.67491000 |
| C | 4.89319000 | -1.64411100 | -0.37451500 |
| H | 3.07900400 | -2.77967500 | -0.53355800 |
| H | 5.52493900 | -2.45226700 | -0.72967000 |
| O | -1.41185600 | -0.95941200 | -0.56203200 |
| O | 1.39122000 | -1.03355500 | 0.28532900 |
| S | -7.25354400 | -0.20227100 | 0.00302200 |
| S | 7.23012500 | -0.19276000 | -0.20678000 |
| O | 7.50249600 | 1.22059400 | 0.17385100 |
| O | 7.85229000 | -1.17816400 | 0.72318900 |
| O | 7.54425700 | -0.48332900 | -1.63471800 |
| O | -7.48369800 | 1.17055500 | 0.53260500 |
| O | -7.77678700 | -0.38608900 | -1.38196100 |
| O | -7.72233700 | -1.27146400 | 0.93025300 |
| H | -1.66460500 | 1.86773700 | -1.56293300 |
| H | -1.97705300 | 1.67440200 | 1.33669200 |
| H | 1.88669800 | 1.23771800 | 1.97809900 |
| Pd | 0.04531100 | 0.42397500 | -0.25786000 |
| C | 0.55910200 | 3.08271400 | 0.51195100 |
| C | -0.57107600 | 3.22957200 | -0.47472500 |
| H | -0.17458300 | 3.48845200 | -1.45866900 |
| H | -1.26146600 | 4.02126500 | -0.17272600 |
| H | 1.15606900 | 3.99769900 | 0.56842200 |
| H | 0.18597400 | 2.86235900 | 1.51548200 |
| H | 1.85478000 | 2.15973900 | -0.79356900 |
| H | 1.08497100 | -1.57630700 | -2.91906700 |
| H | 1.18750400 | -1.67188300 | -2.18181100 |
| H | 0.60571500 | -2.79504400 | 0.24518800 |
| O | -0.22181000 | -3.30594100 | 0.26793900 |
| H | -0.82504500 | -2.64595300 | -0.12351300 |
| H | 0.47584700 | -1.17571600 | 2.10387700 |
| O | -0.16740700 | -1.63644500 | -2.66391600 |
| H | -0.43890800 | -2.35439900 | 2.06945700 |

53

RS_lambda_D1_TS1-trigo, E(SCF) = -
 2408.88421518, E(ZPE) = -2408.494600, E(G)
 = -2408.558543 a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | -1.24773500 | 2.05144100 | -0.60728200 |
| N | 1.44045300 | 1.90062000 | 0.14233100 |
| C | -2.33255800 | 1.69052700 | 0.32472500 |
| H | -2.97374100 | 2.56701600 | 0.46684300 |
| C | 2.42199200 | 1.46779800 | 1.18410500 |
| H | 3.03624200 | 2.34138900 | 1.42962100 |
| C | -3.16206800 | 0.54694100 | -0.18273200 |
| C | -2.63637700 | -0.55494100 | -0.89071800 |
| C | -4.52104600 | 0.56560600 | 0.12325200 |
| C | -3.51760400 | -1.59442700 | -1.24761200 |
| C | -5.36344500 | -0.46583900 | -0.23147200 |
| H | -4.93334700 | 1.41451000 | 0.65977400 |
| C | -4.85231000 | -1.55762700 | -0.92448500 |
| H | -3.09999800 | -2.43649700 | -1.78953600 |
| H | -5.50498600 | -2.37554500 | -1.21222600 |
| C | 3.27959300 | 0.31827200 | 0.79668300 |
| C | 2.71553200 | -0.98340300 | 0.86129900 |
| C | 4.60687200 | 0.49792800 | 0.43866800 |
| C | 3.56403000 | -2.06796000 | 0.53908600 |
| C | 5.41065700 | -0.58408900 | 0.12461800 |
| H | 5.02877100 | 1.49833900 | 0.40355800 |
| C | 4.87968400 | -1.87023900 | 0.18209500 |
| H | 3.14344100 | -3.06836600 | 0.57638100 |
| H | 5.50685700 | -2.72105900 | -0.06783800 |
| O | -1.37444800 | -0.71373300 | -1.26564500 |
| O | 1.46464300 | -1.14939500 | 1.14376200 |
| S | -7.10592200 | -0.43392600 | 0.19796700 |
| S | 7.12869000 | -0.36158600 | -0.32627500 |
| O | 7.35634000 | 1.11029200 | -0.37552900 |
| O | 7.92908800 | -1.03632100 | 0.73784600 |
| O | 7.29662500 | -1.01834300 | -1.65557700 |
| O | -7.34322000 | 0.87778900 | 0.86108300 |
| O | -7.84369900 | -0.58008300 | -1.08906900 |
| O | -7.31815300 | -1.59501100 | 1.10884500 |
| H | -1.63550800 | 2.11990900 | -1.54700300 |
| H | -1.87254800 | 1.43759800 | 1.28709600 |
| H | 1.82652100 | 1.21564900 | 2.06577700 |
| Pd | 0.09154200 | 0.50154300 | -0.62774300 |
| C | 0.58583700 | 2.98825800 | 0.68386800 |
| C | -0.50797900 | 3.29837900 | -0.29381600 |
| H | -0.09173100 | 3.67231100 | -1.23128600 |
| H | -1.19226800 | 4.05475900 | 0.10014300 |
| H | 1.18671500 | 3.87476200 | 0.90546800 |
| H | 0.16747000 | 2.62575100 | 1.62735200 |
| H | 1.96576600 | 2.25715000 | -0.65727600 |
| H | 1.35467500 | -0.65176000 | -1.69459300 |
| H | 1.29657700 | -1.03573200 | -1.02061300 |
| H | 0.22645100 | -2.42093300 | 0.82335200 |
| O | -0.64742600 | -2.80793700 | 0.60942100 |
| H | -0.92999900 | -2.27953400 | -0.15353600 |
| O | 0.06519900 | -0.47496200 | 2.11802200 |
| O | -0.85456200 | -0.41087600 | 2.44055600 |
| H | -1.24117700 | -1.20413100 | 2.04336300 |

53

RS_lambda_D1_TS1, E(SCF) = -2408.88417738,
 E(ZPE) = -2408.495041, E(G) = -2408.559990
 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.41052300 | 1.99699200 | -0.00272200 |
| N | -1.27882000 | 2.09958300 | -0.77338200 |
| C | 2.35788800 | 1.58692100 | 1.08223400 |
| H | 3.00578400 | 2.44670300 | 1.28551800 |
| C | -2.33838100 | 1.74738400 | 0.18824100 |
| H | -3.01532400 | 2.60355800 | 0.28433700 |
| C | 3.17235500 | 0.37916400 | 0.78446900 |
| C | 2.54740500 | -0.89175800 | 0.89099000 |
| C | 4.51768600 | 0.48011900 | 0.46600400 |
| C | 3.35298200 | -2.02750700 | 0.64566200 |
| C | 5.27994300 | -0.65113200 | 0.23014700 |
| H | 4.98613600 | 1.45774500 | 0.39752400 |
| C | 4.68809700 | -1.90711000 | 0.32729000 |
| H | 2.88573400 | -3.00547900 | 0.71305900 |
| H | 5.28257700 | -2.79608800 | 0.13815300 |
| C | -3.12786700 | 0.54061700 | -0.23457600 |

| | | | |
|----|-------------|-------------|-------------|
| C | -2.59507900 | -0.55384400 | -0.94998800 |
| C | -4.46458600 | 0.50182400 | 0.15725400 |
| C | -3.44504100 | -1.64572300 | -1.21767200 |
| C | -5.27732900 | -0.57624900 | -0.11814600 |
| H | -4.88312900 | 1.34611400 | 0.69599800 |
| C | -4.75775800 | -1.66214800 | -0.81440400 |
| H | -3.02434200 | -2.78037700 | -1.76858700 |
| H | -5.38655900 | -2.51658400 | -1.04264100 |
| O | 1.27874600 | -0.99526800 | 1.13492800 |
| O | -1.36157600 | -0.65162700 | -1.42662200 |
| S | 7.02311800 | -0.52993900 | -0.15966200 |
| S | -6.99549700 | -0.60433900 | 0.40039600 |
| O | -7.11569700 | -1.75570800 | 1.33970600 |
| O | -7.79091500 | -0.80319800 | -0.84482600 |
| O | 7.25204100 | 0.70525200 | -0.50521500 |
| O | 7.21555900 | -1.28367900 | -1.43301800 |
| O | 7.74939700 | -1.16118400 | 0.98146600 |
| O | 7.31668000 | 0.92477400 | -0.29668200 |
| H | 1.96060200 | 2.33373300 | -0.79379800 |
| H | 1.73558300 | 1.41673400 | 1.96408800 |
| H | -1.86065000 | 1.57701400 | 1.16055800 |
| Pd | 0.08916100 | 0.57649800 | -0.78562700 |
| C | -0.55045600 | 3.36346000 | -0.50321500 |
| C | 0.54239200 | 3.09918800 | 0.48980900 |
| H | 1.13553300 | 3.99828200 | 0.67834400 |
| H | 0.12259900 | 2.76771300 | 1.44331100 |
| H | -0.13695500 | 3.70691800 | -1.45352400 |
| H | -1.24294800 | 4.12689900 | -0.13731000 |
| H | -1.68279600 | 2.13894400 | -1.70767000 |
| H | 0.30647600 | -2.36631300 | 0.51034600 |
| H | 1.39073300 | -0.53158100 | -1.78410500 |
| H | 1.31991600 | -0.91924700 | -1.11103600 |
| O | -0.29018600 | -2.95381700 | 0.00125100 |
| H | -0.70878800 | -2.34137200 | -0.62236700 |
| O | 0.13037600 | -0.11540800 | 2.12187500 |
| O | -0.56236300 | 0.40244800 | 2.58876800 |
| H | -0.70017200 | -0.04956300 | 3.42366700 |

53

RS_lambda_D1_TS2_P, E(SCF) = -
 2408.92437648, E(ZPE) = -2408.531430, E(G)
 = -2408.597627 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | -1.50263000 | 0.16990200 | 1.63968500 |
| N | 1.22044600 | -0.65702900 | 1.62522700 |
| C | -2.60887400 | 1.16046200 | 1.62541400 |
| H | -3.14909400 | 1.07209500 | 2.57696900 |
| C | 2.37064200 | 0.25928900 | 1.55549400 |
| H | 2.99352500 | 0.16092400 | 2.45373800 |
| C | -3.55890300 | 0.94940900 | 0.49212100 |
| C | -3.64968500 | 1.82144600 | -0.59972100 |
| C | -4.39733400 | -0.16284300 | 0.52711400 |
| C | -4.57536800 | 1.55683600 | -1.61378100 |
| C | -5.29662600 | -0.42400400 | -0.48421100 |
| H | -4.35956900 | -0.83717300 | 1.37877500 |
| C | -5.38484000 | 0.44554700 | -1.56479200 |
| H | -4.62859300 | 2.24900400 | -2.44641000 |
| H | -6.09433100 | 0.25153500 | -2.36225200 |
| C | 3.20512500 | -0.03244200 | 0.34165000 |
| C | 2.67555700 | -0.02489200 | -0.97309400 |
| C | 4.55625400 | -0.30764200 | 0.52814900 |
| C | 3.56508000 | -0.28565700 | -2.03560100 |
| C | 5.40513500 | -0.55951100 | -0.53124600 |
| H | 4.96020800 | -0.32017000 | 1.53565100 |
| C | 4.90003600 | -0.54145200 | -1.82629600 |
| H | 3.15494100 | -0.27127900 | -3.03992900 |
| H | 5.55656400 | -0.73791900 | -2.66827000 |
| O | -2.92520700 | 2.94138800 | -0.75113700 |
| O | 1.42339100 | 0.24119300 | -1.29160600 |
| S | -6.36328500 | -1.86941500 | -0.42897100 |
| S | 7.14540100 | -0.89892600 | -0.27025500 |
| O | 7.88439700 | 0.16935800 | -1.00373500 |
| O | 7.39003200 | -2.25212500 | -0.84850100 |
| O | 7.36209200 | -0.84791800 | 1.20256700 |
| O | -6.01290900 | -2.67208700 | -1.63421400 |
| O | -7.75697300 | -1.34456200 | -0.47864700 |
| O | -6.04454400 | -2.56292900 | 0.84860200 |
| H | -1.91580000 | -0.76218600 | 1.68987200 |

H -2.14248600 2.14596000 1.60754700
H 1.98450200 1.28660500 1.54225200
Pd -0.11674200 0.10881100 0.07247700
C 0.45431300 -0.65345100 2.88084100
C -0.65401600 0.37038600 2.84187300
H -1.26174900 0.30623200 3.75153700
H -0.25378200 1.38649400 2.78117200
H 0.02322000 -1.65038100 3.00453000
H 1.10177700 -0.46876000 3.74548700
H 1.55552500 -1.59713100 1.43791900
H 1.34901400 3.42449100 -1.98578300
H -1.08415600 0.71446200 -0.98519300
H -2.15692900 3.03723600 -0.14467800
O 1.37220100 2.99848600 -1.12567600
H 1.33877400 2.03368700 -1.30221500
H -0.59513000 4.49633300 0.89920900
O -0.65191000 3.57147200 0.64744500
H 0.09156900 3.41089000 0.02507900

53
RS_lambda_D1_TS2_R_checking-H-bond, E(SCF)
= -2408.88829300, E(ZPE) = -2408.496862,
E(G) = -2408.562464 a.u.
N 1.44831500 1.73058200 0.30027700
N -1.23978500 2.01516700 -0.45483900
C 2.36780400 1.17665800 1.34567000
H 2.93739000 2.02685000 1.73894200
C -2.32170300 1.60954600 0.46660800
H -2.93759700 2.48624800 0.69260000
C 3.29802800 0.10789400 0.88418300
C 2.90945200 -1.25803400 0.98033700
C 4.56906000 0.44816200 0.43647500
C 3.87379900 -2.22303400 0.60224000
C 5.48094100 -0.51995800 0.06334300
H 4.85860700 1.49415100 0.38397600
C 5.12291800 -1.86379900 0.15298100
H 3.58956100 -3.26857100 0.66683400
H 5.83662900 -2.62989400 -0.13565200
C -3.18716500 0.53133900 -0.12197900
C -2.68969400 -0.55169400 -0.87839300
C -4.55319400 0.59409200 0.14592100
C -3.60268400 -1.53248100 -1.31239100
C -5.42785300 -0.37829200 -0.28846200
H -4.94511400 1.43001400 0.71684100
C -4.94353800 -1.45369000 -1.02525400
H -3.20464800 -2.36198800 -1.88719100
H -5.62188200 -2.22572500 -1.37415700
O 1.71083200 -1.60189600 1.33584900
O -1.42712400 -0.74551100 -1.23457400
S 7.10906300 -0.08331300 -0.53984300
S -7.18486100 -0.27122600 0.05999800
O -7.53416000 -1.53166600 0.77473300
O -7.85526900 -0.16867100 -1.26779800
O -7.36367200 0.94495200 0.89992600
O 7.17527100 -0.58468200 -1.94440000
O 8.08236100 -0.77972200 0.35117300
O 7.20213900 1.40142300 -0.45026900
H 2.01854300 2.11095900 -0.45629400
H 1.72556200 0.80726800 2.14749300
H -1.85366400 1.27385500 1.40023600
Pd 0.05758800 0.43742400 -0.56968600
C -0.46131100 3.21714400 -0.06603200
C 0.62561600 2.82076800 0.89039600
H 1.25561300 3.67576500 1.15072100
H 0.19795100 2.43042900 1.81802000
H -0.03499300 3.63361900 -0.98054800
H -1.12010500 3.97008000 0.37501200
H -1.64235100 2.16268900 -1.37923300
H 0.21365000 -2.68213500 0.81189300
H 1.17010500 -0.80093900 -1.06675400
H 1.08044600 -0.99885600 -0.25613300
O -0.71459000 -2.89994000 0.60876200
H -0.94066000 -2.32143100 -0.13808000
H 0.27212300 -0.83721200 2.25490800
O -0.65075100 -0.66254100 2.52421600
H -1.11428700 -1.36599800 2.04678100

53
RS_lambda_D1_TS2_R_trigo, E(SCF) = -
2408.88829300, E(ZPE) = -2408.496862, E(G)
= -2408.562464 a.u.
N 1.44831500 1.73058200 0.30027700
N -1.23978500 2.01516700 -0.45483900
C 2.36780400 1.17665800 1.34567000
H 2.93739000 2.02685000 1.73894200
C -2.32170300 1.60954600 0.46660800
H -2.93759700 2.48624800 0.69260000
C 3.29802800 0.10789400 0.88418300
C 2.90945200 -1.25803400 0.98033700
C 4.56906000 0.44816200 0.43647500
C 3.87379900 -2.22303400 0.60224000
C 5.48094100 -0.51995800 0.06334300
H 4.85860700 1.49415100 0.38397600
C 5.12291800 -1.86379900 0.15298100
H 3.58956100 -3.26857100 0.66683400
H 5.83662900 -2.62989400 -0.13565200
C -3.18716500 0.53133900 -0.12197900
C -2.68969400 -0.55169400 -0.87839300
C -4.55319400 0.59409200 0.14592100
C -3.60268400 -1.53248100 -1.31239100
C -5.42785300 -0.37829200 -0.28846200
H -4.94511400 1.43001400 0.71684100
C -4.94353800 -1.45369000 -1.02525400
H -3.20464800 -2.36198800 -1.88719100
H -5.62188200 -2.22572500 -1.37415700
O 1.71083200 -1.60189600 1.33584900
O -1.42712400 -0.74551100 -1.23457400
S 7.10906300 -0.08331300 -0.53984300
S -7.18486100 -0.27122600 0.05999800
O -7.53416000 -1.53166600 0.77473300
O -7.85526900 -0.16867100 -1.26779800
O -7.36367200 0.94495200 0.89992600
O 7.17527100 -0.58468200 -1.94440000
O 8.08236100 -0.77972200 0.35117300
O 7.20213900 1.40142300 -0.45026900
H 2.01854300 2.11095900 -0.45629400
H 1.72556200 0.80726800 2.14749300
H -1.85366400 1.27385500 1.40023600
Pd 0.05758800 0.43742400 -0.56968600
C -0.46131100 3.21714400 -0.06603200
C 0.62561600 2.82076800 0.89039600
H 1.25561300 3.67576500 1.15072100
H 0.19795100 2.43042900 1.81802000
H -0.03499300 3.63361900 -0.98054800
H -1.12010500 3.97008000 0.37501200
H -1.64235100 2.16268900 -1.37923300
H 0.21365000 -2.68213500 0.81189300
H 1.17010500 -0.80093900 -1.06675400
H 1.08044600 -0.99885600 -0.25613300
O -0.71459000 -2.89994000 0.60876200
H -0.94066000 -2.32143100 -0.13808000
H 0.27212300 -0.83721200 2.25490800
O -0.65075100 -0.66254100 2.52421600
H -1.11428700 -1.36599800 2.04678100

53
RS_lambda_D1_TS2, E(SCF) = -2408.88782872,
E(ZPE) = -2408.497237, E(G) = -2408.562005
a.u.
N 1.44050900 1.65757900 0.25884600
N -1.25323800 2.04241000 -0.48253200
C 2.32445200 1.03934200 1.29485600
H 2.86030700 1.86161600 1.78354400
C -2.35183100 1.67248500 0.42802400
H -2.96083200 2.56086900 0.62776700
C 3.30350400 0.03101800 0.79090800
C 2.95856600 -1.34338100 0.73871800
C 4.59482400 0.43646300 0.46935200
C 3.96794500 -2.25391900 0.36300800
C 5.55716800 -0.47696900 0.08680600
H 4.85941100 1.48882200 0.52468400
C 5.23843300 -1.83152100 0.04525700
H 3.70750900 -3.30647000 0.32290600
H 5.99598100 -2.55272300 -0.24650000

| | | | |
|----|-------------|-------------|-------------|
| C | -3.23023200 | 0.58621300 | -0.12825800 |
| C | -2.76261200 | -0.51193600 | -0.88369700 |
| C | -4.58627200 | 0.65780800 | 0.18619600 |
| C | -3.69529900 | -1.49926000 | -1.26062500 |
| C | -5.47929200 | -0.31916500 | -0.19619500 |
| H | -4.95490200 | 1.50567900 | 0.75513900 |
| C | -5.02441700 | -1.41156100 | -0.92688700 |
| H | -3.32122900 | -2.34125900 | -1.83371700 |
| H | -5.71611300 | -2.18937100 | -1.23402100 |
| O | 1.73737500 | -1.74922900 | 0.97283900 |
| O | -1.51928200 | -0.71111200 | -1.29678800 |
| S | 7.21819800 | 0.04404700 | -0.33899900 |
| S | -7.22437900 | -0.19148700 | 0.20118000 |
| O | -7.56556700 | -1.43811500 | 0.94351600 |
| O | -7.93085100 | -0.10118100 | -1.10882900 |
| O | -7.36927900 | 1.03815100 | 1.02803600 |
| O | 7.44442500 | -0.41793400 | -1.73922400 |
| O | 8.12453100 | -0.63495400 | 0.63177400 |
| O | 7.23282900 | 1.52773700 | -0.20175900 |
| H | 2.02962600 | 2.03815900 | -0.48249600 |
| H | 1.65578200 | 0.59457500 | 2.03520700 |
| H | -1.90210500 | 1.36679300 | 1.37960600 |
| Pd | 0.00583600 | 0.42165000 | -0.62551500 |
| C | -0.43231800 | 3.20692600 | -0.07071500 |
| C | 0.64771500 | 2.75704500 | 0.87191800 |
| H | 1.30116300 | 3.58904700 | 1.14878600 |
| H | 0.21347100 | 2.36026100 | 1.79414400 |
| H | 0.00392800 | 3.63052400 | -0.97730400 |
| H | -1.06053100 | 3.97315600 | 0.39183400 |
| H | -1.64495400 | 2.21889200 | -1.40597400 |
| H | 0.21445100 | -2.90438900 | 0.36026400 |
| H | 1.04273200 | -0.83871300 | -1.09151700 |
| H | 1.06555500 | -1.05586800 | -0.24618600 |
| O | -0.72532800 | -3.07097600 | 0.17964700 |
| H | -0.97550100 | -2.39037100 | -0.46918800 |
| H | 0.31661300 | -1.24265200 | 2.08859900 |
| O | -0.59621800 | -1.18599600 | 2.42680800 |
| H | -1.05387200 | -1.79201000 | 1.82555900 |

56
RS_lambda_ID1_TS1_H2-out_P, E(SCF) = -
2485.33389308, E(ZPE) = -2484.917910, E(G)
= -2484.985523 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.49015000 | 3.20176800 | -0.15709900 |
| H | -0.08797300 | 3.59895300 | -1.09110000 |
| H | -1.10548900 | 3.97760800 | 0.30735400 |
| C | 0.61548500 | 2.76934600 | 0.75789900 |
| H | 1.28475700 | 3.60183700 | 0.99037200 |
| H | 0.20250100 | 2.40745400 | 1.70350500 |
| N | 1.38041100 | 1.63637200 | 0.16515600 |
| N | -1.31965400 | 2.02605500 | -0.50677600 |
| C | 2.21410300 | 1.03956100 | 1.25980200 |
| H | 2.71739200 | 1.88113700 | 1.75166800 |
| C | -2.34257400 | 1.61445500 | 0.47429000 |
| H | -2.92313900 | 2.49523700 | 0.76984300 |
| C | 3.23631000 | 0.03110100 | 0.86137100 |
| C | 2.91930500 | -1.35138100 | 0.84894500 |
| C | 4.53373700 | 0.45267200 | 0.59304300 |
| C | 3.97077300 | -2.25047600 | 0.56009600 |
| C | 5.53501800 | -0.44985100 | 0.29132300 |
| H | 4.77038900 | 1.51305400 | 0.61472800 |
| C | 5.24553400 | -1.81150400 | 0.28367000 |
| H | 6.03005000 | -2.52676600 | 0.05488000 |
| C | -3.27204300 | 0.57634300 | -0.09117500 |
| C | -2.86544000 | -0.46990000 | -0.94931300 |
| C | -4.60726500 | 0.64257200 | 0.30185700 |
| C | -3.83330700 | -1.41072800 | -1.35164000 |
| C | -5.53626100 | -0.29081500 | -0.10419200 |
| H | -4.93054400 | 1.45090300 | 0.95029200 |
| C | -5.14104500 | -1.33010700 | -0.93895000 |
| H | -5.86327800 | -2.07081600 | -1.26670600 |
| O | 1.69892400 | -1.78061300 | 1.02926300 |
| O | -1.63995400 | -0.66240100 | -1.42028300 |
| S | 7.19447500 | 0.09645800 | -0.10116600 |
| S | -7.25120000 | -0.18265700 | 0.41347800 |
| O | -8.04518000 | -0.04399300 | -0.84308600 |
| O | -7.34063900 | 1.01375100 | 1.29483700 |

| | | | |
|----|-------------|-------------|-------------|
| O | -7.53975100 | -1.45835200 | 1.12900700 |
| O | 7.47966800 | -0.41444500 | -1.47413100 |
| O | 8.08821700 | -0.51781100 | 0.92361000 |
| O | 7.16706500 | 1.58461700 | -0.03087200 |
| H | -0.05935900 | -2.81868000 | 0.62895700 |
| H | 3.95763400 | 0.00615100 | -2.75389800 |
| H | 4.28474400 | -0.07704000 | -2.36292100 |
| O | -1.00718900 | -2.89910100 | 0.44213500 |
| H | -1.18267300 | -2.24985600 | -0.25859100 |
| H | 0.28827500 | -0.98662900 | 1.96275500 |
| O | -0.56978400 | -0.73087500 | -2.35782800 |
| H | -1.17053000 | -1.35868900 | 1.93393400 |
| H | 2.01014400 | 1.99446300 | -0.55424400 |
| H | 1.50969900 | 0.62104100 | 1.97974500 |
| H | -1.81893700 | 1.23830400 | 1.36083000 |
| Pd | -0.08616100 | 0.45037900 | -0.79375800 |
| H | 3.73685900 | -3.31031700 | 0.55040400 |
| H | -3.50424500 | -2.21315500 | -2.00351300 |
| O | 1.10061200 | -0.18286400 | -1.37336000 |
| H | 0.54966200 | -1.78000000 | -1.89330000 |
| H | 1.30569000 | -1.61680100 | -0.48899400 |
| H | -1.78488400 | 2.20570700 | -1.39569600 |

56
RS_lambda_ID1_TS1_H2-out_R, E(SCF) = -
2485.35791418, E(ZPE) = -2484.943225, E(G)
= -2485.012185 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.62498500 | 3.23478900 | -0.56719300 |
| H | -0.26434000 | 3.43799300 | -1.57766300 |
| H | -1.31550300 | 4.03541500 | -0.29118200 |
| C | 0.53780000 | 3.16132800 | 0.38819600 |
| H | 1.12985500 | 4.08084700 | 0.36412100 |
| H | 0.19940800 | 3.00501300 | 1.41611500 |
| N | 1.36647100 | 1.99159600 | 0.01492700 |
| N | -1.33541900 | 1.92766000 | -0.60907100 |
| C | 2.43714200 | 1.68219000 | 0.98712000 |
| H | 3.06946200 | 2.56604100 | 1.12091900 |
| C | -2.45168000 | 1.77937900 | 0.35155400 |
| H | -3.08777600 | 2.66920700 | 0.29663700 |
| C | 3.26696700 | 0.52095400 | 0.54299200 |
| C | 2.67949200 | -0.74261000 | 0.33407900 |
| C | 4.63377400 | 0.67845100 | 0.35379300 |
| C | 3.51205400 | -1.81819900 | -0.00763000 |
| C | 5.43558200 | -0.38983200 | -0.00174000 |
| H | 5.08804100 | 1.65321600 | 0.50082500 |
| C | 4.86896700 | -1.64555600 | -0.17752500 |
| H | 5.49381200 | -2.49007100 | -0.44900400 |
| C | -3.28106600 | 0.56393900 | 0.05731400 |
| C | -2.72505900 | -0.70845800 | -0.19539200 |
| C | -4.66602700 | 0.70648700 | 0.06140100 |
| C | -3.60393600 | -1.78497000 | -0.41801700 |
| C | -5.50905500 | -0.36310800 | -0.15693400 |
| H | -5.09941300 | 1.68514700 | 0.24082800 |
| C | -4.96847700 | -1.62163100 | -0.39521400 |
| H | -5.62128200 | -2.46991600 | -0.57397700 |
| O | 1.37662500 | -0.96573700 | 0.46366400 |
| O | -1.43019400 | -0.97792400 | -0.23621700 |
| S | 7.19053300 | -0.16080400 | -0.30962400 |
| S | -7.29230100 | -0.16345100 | -0.12904100 |
| O | -7.78062000 | -0.68603600 | -1.43366100 |
| O | -7.54142600 | 1.29378000 | 0.04685700 |
| O | -7.77235500 | -0.98012400 | 1.02231800 |
| O | 7.35886100 | -0.30266700 | -1.78444700 |
| O | 7.88117900 | -1.24074100 | 0.44898300 |
| O | 7.51777800 | 1.20473900 | 0.18421300 |
| H | 0.47694300 | -2.71484700 | 1.15004300 |
| H | 2.58711700 | 0.10650700 | -2.92415000 |
| H | 2.91110200 | 0.00728800 | -2.25477300 |
| O | -0.40845200 | -3.00980100 | 1.41134400 |
| H | -0.95678300 | -2.42750600 | 0.85409000 |
| H | 0.71969600 | -0.64375600 | 2.36034100 |
| O | 0.17536600 | -0.78936400 | 3.14912500 |
| H | -0.27065100 | -1.61518800 | 2.90450600 |
| H | 1.79332800 | 2.15401200 | -0.89869100 |
| H | 1.93898600 | 1.48516800 | 1.94296600 |
| H | -2.01890800 | 1.75178100 | 1.35842900 |
| Pd | 0.01995700 | 0.45399600 | -0.15479200 |

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|---|-------------|-------------|-------------|
| H | 3.05601700 | -2.79427000 | -0.14309900 |
| H | -3.16324500 | -2.75789900 | -0.61366600 |
| C | 0.35194400 | -2.42208700 | -1.90275100 |
| H | -0.49710500 | -2.08261900 | -1.57843700 |
| H | 0.95366800 | -2.07008100 | -1.23061500 |
| H | -1.70812100 | 1.78675800 | -1.54630700 |

56
 RS_lambda_ID1 TS1_H2-out, E(SCF) = -
 2485.32776092, E(ZPE) = -2484.912311, E(G)
 = -2484.978944 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.54778500 | 3.24661500 | -0.45808600 |
| H | -0.14603200 | 3.54734400 | -1.42764900 |
| H | -1.20442200 | 4.04382300 | -0.09843800 |
| C | 0.55972900 | 2.97202900 | 0.51314200 |
| H | 1.18614400 | 3.85475400 | 0.66684700 |
| H | 0.15054900 | 2.68158700 | 1.48480600 |
| N | 1.37875300 | 1.82722300 | 0.03631400 |
| N | -1.32144500 | 2.00077500 | -0.67163500 |
| C | 2.29714500 | 1.40662600 | 1.13604900 |
| H | 2.86663600 | 2.29296000 | 1.43941200 |
| C | -2.38249400 | 1.71205900 | 0.31186700 |
| H | -3.00007300 | 2.60893500 | 0.43165700 |
| C | 3.22607700 | 0.29951600 | 0.79085800 |
| C | 2.71982500 | -1.02001900 | 0.71626200 |
| C | 4.57668400 | 0.54832600 | 0.59197500 |
| C | 3.64551300 | -2.05232700 | 0.44468500 |
| C | 5.45750200 | -0.48036000 | 0.31329500 |
| H | 4.95201300 | 1.56542800 | 0.65306000 |
| C | 4.98103800 | -1.78644200 | 0.24096400 |
| H | 5.66871100 | -2.59827300 | 0.02379900 |
| C | -3.25451800 | 0.56639200 | -0.11671700 |
| C | -2.77715900 | -0.58402400 | -0.78135800 |
| C | -4.60697800 | 0.64227700 | 0.20941800 |
| C | -3.69510400 | -1.61208400 | -1.07062300 |
| C | -5.48634000 | -0.37863500 | -0.07982200 |
| H | -4.98422900 | 1.52932500 | 0.70872200 |
| C | -5.02157900 | -1.51867700 | -0.72585600 |
| H | -5.70474400 | -2.32781700 | -0.96285100 |
| O | 1.44624900 | -1.26536900 | 0.84589600 |
| O | -1.52617000 | -0.79707800 | -1.16719100 |
| S | 7.18795600 | -0.15642100 | -0.01453900 |
| S | -7.22268200 | -0.26610000 | 0.35971900 |
| O | -7.97403500 | -0.41730200 | -0.91898300 |
| O | -7.40411400 | 1.07099300 | 0.98864200 |
| O | -7.47422000 | -1.39333800 | 1.30219300 |
| O | 7.41676100 | -0.55094000 | -1.43594400 |
| O | 7.95847800 | -1.00960900 | 0.93620200 |
| O | 7.38765000 | 1.30145500 | 0.21913800 |
| H | 0.08260700 | -2.55541800 | 0.90285400 |
| H | 3.84154400 | 0.36994900 | -2.72064200 |
| H | 4.16285900 | 0.27595200 | -2.04879100 |
| O | -0.83755500 | -2.85009400 | 0.77662100 |
| H | -1.13213400 | -2.30778300 | 0.02710400 |
| H | 0.15333800 | -0.52639500 | 1.98112400 |
| O | -0.69315600 | -0.37463200 | 2.44403800 |
| H | -1.20622400 | -1.13761300 | 2.14443300 |
| H | 1.94928900 | 2.12390000 | -0.75699700 |
| H | 1.65276600 | 1.12845500 | 1.97449200 |
| H | -1.89616300 | 1.49975600 | 1.27060300 |
| Pd | -0.01592100 | 0.43165700 | -0.66775500 |
| H | 3.26922300 | -3.06961100 | 0.38947000 |
| H | -3.31356900 | -2.49124500 | -1.57941900 |
| O | 1.13368100 | -1.30193400 | -1.78688400 |
| H | 0.36740700 | -1.74234000 | -2.17493800 |
| H | 1.29463300 | -1.74983600 | -0.93400800 |
| H | -1.74117900 | 2.02742500 | -1.59971300 |

54
 RS_lambda_ID1 TS1_P, E(SCF) = -
 2484.15957074, E(ZPE) = -2483.758897, E(G)
 = -2483.824927 a.u.

| | | | |
|---|-------------|------------|-------------|
| C | -0.47790400 | 3.22058700 | -0.13700100 |
| H | -0.08383700 | 3.63466600 | -1.06711500 |
| H | -1.09486900 | 3.98553500 | 0.34306600 |
| C | 0.63592100 | 2.78070800 | 0.76467600 |
| H | 1.30216300 | 3.61342100 | 1.00518600 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.23084700 | 2.40300200 | 1.70756100 |
| N | 1.40267200 | 1.66140400 | 0.14857000 |
| N | -1.30280500 | 2.04535800 | -0.49990100 |
| C | 2.24893400 | 1.05111300 | 1.22520800 |
| H | 2.76415000 | 1.88620200 | 1.71588900 |
| C | -2.31785400 | 1.61472200 | 0.48097000 |
| H | -2.90260700 | 2.48800300 | 0.79018500 |
| C | 3.25960800 | 0.03522300 | 0.81355800 |
| C | 2.93689300 | -1.34613900 | 0.82391600 |
| C | 4.55686300 | 0.44609200 | 0.52838400 |
| C | 3.98541700 | -2.25556800 | 0.56151000 |
| C | 5.55393200 | -0.46680500 | 0.24381800 |
| H | 4.80000500 | 1.50519200 | 0.53611100 |
| C | 5.26114100 | -1.82743200 | 0.27361000 |
| H | 6.04418500 | -2.55074600 | 0.06893000 |
| C | -3.24352800 | 0.57763500 | -0.09288900 |
| C | -2.83538600 | -0.45246800 | -0.96986100 |
| C | -4.57611800 | 0.62723200 | 0.31159000 |
| C | -3.79976100 | -1.39297300 | -1.38122300 |
| C | -5.50100900 | -0.30709600 | -0.10182300 |
| H | -4.90014400 | 1.42204600 | 0.97629700 |
| C | -5.10482500 | -1.32882100 | -0.95752900 |
| H | -5.82391600 | -2.06990400 | -1.29119300 |
| O | 1.71186900 | -1.76526700 | 1.00059100 |
| O | -1.61136500 | -0.63114900 | -1.44988300 |
| S | 7.22198000 | 0.06268200 | -0.13669000 |
| S | -7.21320600 | -0.22088000 | -0.42862900 |
| O | -8.01477500 | -0.03309800 | -0.81467800 |
| O | -7.29920300 | 0.93889800 | 1.35799100 |
| O | -7.49614500 | -1.52494200 | 1.09299800 |
| O | 7.51893500 | -0.46381600 | -1.50108300 |
| O | 8.09842000 | -0.54906400 | 0.90455300 |
| O | 7.20716300 | 1.55158000 | -0.08098400 |
| H | -0.01959400 | -2.79091800 | 0.58725200 |
| O | -0.96537100 | -2.88205800 | 0.39296500 |
| H | -1.14426300 | -2.22825900 | -0.30252800 |
| H | 0.30780100 | -0.97232600 | 1.93892800 |
| O | -0.55306300 | -0.72449800 | 2.33299200 |
| H | -1.14746800 | -1.35491200 | 1.90407400 |
| H | 2.02246900 | 2.03583000 | -0.57050300 |
| H | 1.55172000 | 0.63188000 | 1.95187900 |
| H | -1.78647900 | 1.23101500 | 1.35967300 |
| Pd | -0.06140200 | 0.48182000 | -0.81483800 |
| H | 3.74763100 | -3.31446000 | 0.57677600 |
| H | -3.46964500 | -2.18249000 | -2.04814100 |
| O | 1.14422900 | -1.13384100 | -1.40761000 |
| H | 0.60586600 | -1.72834600 | -1.94354800 |
| H | 1.33519600 | -1.57790300 | -0.52557800 |
| H | -1.77363100 | 2.23556100 | -1.38366100 |

54
 RS_lambda_ID1 TS1_R, E(SCF) = -
 2484.18323342, E(ZPE) = -2483.783573, E(G)
 = -2483.851200 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.63599100 | 3.24416700 | -0.61735900 |
| H | -0.29360100 | 3.44904000 | -1.63381500 |
| H | -1.32181100 | 4.04401200 | -0.32734100 |
| C | 0.54359800 | 3.16922600 | 0.31672800 |
| H | 1.13384400 | 4.08964500 | 0.28547200 |
| H | 0.22336100 | 3.00964700 | 1.34989400 |
| N | 1.36824400 | 2.00188500 | -0.07325700 |
| N | -1.34615400 | 1.93665900 | -0.64903300 |
| C | 2.44401100 | 1.68722600 | 0.89115100 |
| H | 3.07262800 | 2.57287900 | 1.03130100 |
| C | -2.44011500 | 1.78235500 | 0.33526700 |
| H | -3.07959300 | 2.67069100 | 0.29711000 |
| C | 3.28119800 | 0.53356600 | 0.44018300 |
| C | 2.70209500 | -0.72718000 | 0.19560100 |
| C | 4.65576600 | 0.69016000 | 0.31192800 |
| C | 3.54565300 | -1.79445000 | -0.14807100 |
| C | 5.46939600 | -0.37195100 | -0.03136900 |
| H | 5.10503900 | 1.66134800 | 0.49279500 |
| C | 4.90840700 | -1.62295300 | -0.25479600 |
| H | 5.54312900 | -2.46215800 | -0.52095700 |
| C | -3.27307600 | 0.56540600 | 0.05708700 |
| C | -2.72106600 | -0.70348200 | -0.22203700 |
| C | -4.65777400 | 0.70289000 | 0.10567600 |

| | | | |
|----|-------------|-------------|-------------|
| C | -3.60346400 | -1.78136800 | -0.42404900 |
| C | -5.50386400 | -0.36790200 | -0.09356800 |
| H | -5.08883700 | 1.67867500 | 0.30548200 |
| C | -4.96715000 | -1.62293900 | -0.35774000 |
| H | -5.62258400 | -2.47214600 | -0.52200900 |
| O | 1.39912500 | -0.96321900 | 0.30419500 |
| O | -1.42761100 | -0.96859800 | -0.30779300 |
| S | 7.24644400 | -0.16593400 | -0.19223400 |
| S | -7.28598900 | -0.17353000 | -0.01084700 |
| O | -7.81030100 | -0.68554100 | -1.30884800 |
| O | -7.53350400 | 1.28137200 | 0.18550300 |
| O | -7.73078200 | -1.00166400 | 1.14645700 |
| O | 7.57175200 | -0.54892100 | -1.59531300 |
| O | 7.85170600 | -1.09350200 | 0.80517800 |
| O | 7.52184000 | 1.26730200 | 0.10040200 |
| H | 0.53106200 | -2.73565000 | 0.95734100 |
| O | -0.34386200 | -3.04908400 | 1.23230000 |
| H | -0.91296200 | -2.45020900 | 0.71454900 |
| H | 0.78497000 | -0.70266200 | 2.23512300 |
| O | 0.26926400 | -0.88765300 | 3.03448200 |
| H | -0.17064800 | -1.71171300 | 2.77332300 |
| H | 1.78826800 | 2.17107400 | -0.98834400 |
| H | 1.94914000 | 1.48178600 | 1.84722000 |
| H | -1.98500700 | 1.75304100 | 1.33215500 |
| Pd | 0.02232100 | 0.46437600 | -0.24043700 |
| H | 3.09338100 | -2.76683700 | -0.31880900 |
| H | -3.16619700 | -2.75133500 | -0.64076900 |
| O | 0.32048100 | -2.35856500 | -2.05521500 |
| H | -0.52198100 | -2.04057000 | -1.69385200 |
| H | 0.93850200 | -2.02044200 | -1.39051300 |
| H | -1.73938900 | 1.80016700 | -1.57850300 |

54

RS_lambda_ID1_TS1_trigo_P, E(SCF) = -
2484.15957074, E(ZPE) = -2483.758897, E(G)
= -2483.824927 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.47790400 | 3.22058700 | -0.13700100 |
| H | -0.08383700 | 3.63466600 | -1.06711500 |
| H | -1.09486900 | 3.98553500 | 0.34306600 |
| C | 0.63592100 | 2.78070800 | 0.76467600 |
| H | 1.30216300 | 3.61342100 | 1.00518600 |
| H | 0.23084700 | 2.40300200 | 1.70756100 |
| N | 1.40267200 | 1.66140400 | 0.14857000 |
| N | -1.30280500 | 2.04535800 | -0.49990100 |
| C | 2.24893400 | 1.05111300 | 1.22520800 |
| H | 2.76415000 | 1.88620200 | 1.71588900 |
| C | -2.31785400 | 1.61472200 | 0.48097000 |
| H | -2.90260700 | 2.48800300 | 0.79018500 |
| C | 3.25960800 | 0.03522300 | 0.81355800 |
| C | 2.93689300 | -1.34613900 | 0.82391600 |
| C | 4.55686300 | 0.44609200 | 0.52838400 |
| C | 3.98541700 | -2.25556800 | 0.56151000 |
| C | 5.55393200 | -0.46680500 | 0.24381800 |
| H | 4.80000500 | 1.50519200 | 0.53611100 |
| C | 5.26114100 | -1.82743200 | 0.27361000 |
| H | 6.04418500 | -2.55074600 | 0.06593000 |
| C | -3.24352800 | 0.57763500 | -0.09288900 |
| C | -2.83538600 | -0.45246800 | -0.96986100 |
| C | -4.57611800 | 0.62723200 | 0.31159000 |
| C | -3.79976100 | -1.39297300 | -1.38122300 |
| C | -5.50100900 | -0.30709600 | -0.10182300 |
| H | -4.90014400 | 1.42204600 | 0.97629700 |
| C | -5.10482500 | -1.32882100 | -0.95752900 |
| H | -5.82391600 | -2.06990400 | -1.29119300 |
| O | 1.71186900 | -1.76526700 | 1.00059100 |
| O | -1.61136500 | -0.63114900 | -1.44988300 |
| S | 7.22198000 | 0.06268200 | -0.13669000 |
| S | -7.21320600 | -0.22088000 | 0.42862900 |
| O | -8.01477500 | -0.03309800 | -0.81467800 |
| O | -7.29920300 | 0.93889800 | 1.35799100 |
| O | -7.49614500 | -1.52494200 | 1.09299800 |
| O | 7.51893500 | -0.46381600 | -1.50108300 |
| O | 8.09842000 | -0.54906400 | 0.90455300 |
| O | 7.20716300 | 1.55158000 | -0.08098400 |
| H | -0.01959400 | -2.79091800 | 0.58725200 |
| O | -0.96537100 | -2.88205800 | 0.39296500 |
| H | -1.14426300 | -2.22825900 | -0.30252800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.30780100 | -0.97232600 | 1.93892800 |
| O | -0.55306300 | -0.72449800 | 2.33299200 |
| H | -1.14746800 | -1.35491200 | 1.90407400 |
| H | 2.02246900 | 2.03583000 | -0.57050300 |
| H | 1.55172000 | 0.63188000 | 1.95187900 |
| H | -1.78647900 | 1.23101500 | 1.35967300 |
| Pd | -0.06140200 | 0.48182000 | -0.81483800 |
| H | 3.74763100 | -3.31446000 | 0.57677600 |
| H | -3.46964500 | -2.18249000 | -2.04814100 |
| O | 1.14422900 | -1.13384100 | -1.40761000 |
| H | 0.60586600 | -1.72834600 | -1.94354800 |
| H | 1.33519600 | -1.57790300 | -0.52557800 |
| H | -1.77363100 | 2.23556100 | -1.38366100 |

54

RS_lambda_ID1_TS1_trigo_R, E(SCF) = -
2484.18323342, E(ZPE) = -2483.783573, E(G)
= -2483.851200 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.63599100 | 3.24416700 | -0.61735900 |
| H | -0.29360100 | 3.44904000 | -1.63381500 |
| H | -1.32181100 | 4.04401200 | -0.32734100 |
| C | 0.54359800 | 3.16922600 | 0.31672800 |
| C | 1.13384400 | 4.08964500 | 0.28547200 |
| H | 0.22336100 | 3.00964700 | 1.34989400 |
| N | 1.36824400 | 2.00188500 | -0.07325700 |
| N | -1.34615400 | 1.93665900 | -0.64903300 |
| C | 2.44401100 | 1.68722600 | 0.89115100 |
| H | 3.07262800 | 2.57287900 | 1.03130100 |
| C | -2.44011500 | 1.78235500 | 0.33526700 |
| H | -3.07959300 | 2.67069100 | 0.29711000 |
| C | 3.28119800 | 0.53356600 | 0.44018300 |
| C | 2.70209500 | -0.72718000 | 0.19560100 |
| C | 4.65576600 | 0.69016000 | 0.31192800 |
| C | 3.54565300 | -1.79445000 | -0.14807100 |
| C | 5.46939600 | -0.37195100 | -0.03136900 |
| H | 5.10503900 | 1.66134800 | 0.49279500 |
| C | 4.90840700 | -1.62295300 | -0.25479600 |
| H | 5.54312900 | -2.46215800 | -0.52095700 |
| C | -3.27307600 | 0.56540600 | 0.05708700 |
| C | -2.72106600 | -0.70348200 | -0.22203700 |
| C | -4.65777400 | 0.70289000 | 0.10567600 |
| C | -3.60346400 | -1.78136800 | -0.42404900 |
| C | -5.50386400 | -0.36790200 | -0.09356800 |
| H | -5.08883700 | 1.67867500 | 0.30548200 |
| C | -4.96715000 | -1.62293900 | -0.35774000 |
| H | -5.62258400 | -2.47214600 | -0.52200900 |
| O | 1.39912500 | -0.96321900 | 0.30419500 |
| O | -1.42761100 | -0.96859800 | -0.30779300 |
| S | 7.24644400 | -0.16593400 | -0.19223400 |
| S | -7.28598900 | -0.17353000 | -0.01084700 |
| O | -7.81030100 | -0.68554100 | -1.30884800 |
| O | -7.53350400 | 1.28137200 | 0.18550300 |
| O | -7.73078200 | -1.00166400 | 1.14645700 |
| O | 7.57175200 | -0.54892100 | -1.59531300 |
| O | 7.85170600 | -1.09350200 | 0.80517800 |
| O | 7.52184000 | 1.26730200 | 0.10040200 |
| H | 0.53106200 | -2.73565000 | 0.95734100 |
| O | -0.34386200 | -3.04908400 | 1.23230000 |
| H | -0.91296200 | -2.45020900 | 0.71454900 |
| H | 0.78497000 | -0.70266200 | 2.23512300 |
| O | 0.26926400 | -0.88765300 | 3.03448200 |
| H | -0.17064800 | -1.71171300 | 2.77332300 |
| H | 1.78826800 | 2.17107400 | -0.98834400 |
| H | 1.94914000 | 1.48178600 | 1.84722000 |
| H | -1.98500700 | 1.75304100 | 1.33215500 |
| Pd | 0.02232100 | 0.46437600 | -0.24043700 |
| H | 3.09338100 | -2.76683700 | -0.31880900 |
| H | -3.16619700 | -2.75133500 | -0.64076900 |
| O | 0.32048100 | -2.35856500 | -2.05521500 |
| H | -0.52198100 | -2.04057000 | -1.69385200 |
| H | 0.93850200 | -2.02044200 | -1.39051300 |
| H | -1.73938900 | 1.80016700 | -1.57850300 |

54

RS_lambda_ID1_TS1_trigo, E(SCF) = -
2484.15348498, E(ZPE) = -2483.753270, E(G)
= -2483.818334 a.u.

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -0.55806800 | 3.28349800 | -0.43153600 | C | -5.89138500 | 1.05969400 | -0.92003700 |
| H | -0.17124600 | 3.61346100 | -1.39780000 | H | -6.78867600 | 1.27633000 | -1.49024400 |
| H | -1.21896400 | 4.06409300 | -0.04439600 | C | 3.44257800 | -0.34421600 | 0.26890700 |
| C | 0.56455700 | 2.99840300 | 0.51995600 | C | 3.05042500 | 0.54718600 | -0.76594100 |
| H | 1.18232200 | 3.88480800 | 0.68797100 | C | 4.75374400 | -0.73013600 | 0.37799000 |
| H | 0.17050000 | 2.67874700 | 1.48878800 | C | 4.05138500 | 1.01410700 | -1.63101400 |
| N | 1.39010100 | 1.87579100 | 0.00338800 | C | 5.72536900 | -0.25256500 | -0.48529900 |
| N | -1.32056300 | 2.03443400 | -0.66682800 | H | 5.03650600 | -1.42285400 | 1.16631200 |
| C | 2.34090600 | 1.44602200 | 1.07078200 | C | 5.36880200 | 0.62966800 | -1.49214400 |
| H | 2.92611200 | 2.32750800 | 1.35759500 | H | 6.12828400 | 1.00136500 | -2.17046800 |
| C | -2.37145200 | 1.71704000 | 0.31812900 | O | -2.80832300 | 2.71140700 | 0.04100200 |
| H | -2.99974000 | 2.60373100 | 0.45662200 | O | 1.82092600 | 0.99647400 | -0.95941200 |
| C | 3.25097800 | 0.32613000 | 0.71217800 | S | -6.99546600 | -1.44183700 | -0.55799100 |
| C | 2.73178800 | -0.99045700 | 0.68210500 | S | 7.42373500 | -0.79323900 | -0.27482300 |
| C | 4.60315900 | 0.55323200 | 0.49802800 | C | 7.39981600 | -0.27800800 | -0.41010600 |
| C | 3.64677500 | -2.04286300 | 0.45947800 | O | 7.82416600 | -0.35575800 | 1.09313000 |
| C | 5.47297700 | -0.49487700 | 0.25802300 | O | 8.20145800 | -0.12244900 | -1.35235400 |
| H | 4.99067500 | 1.56708700 | 0.52777700 | O | -6.98321600 | -1.76647100 | -2.01222800 |
| C | 4.98570200 | -1.79887600 | 0.24998600 | O | -8.26904900 | -0.80210100 | -0.12547800 |
| H | 5.66731800 | -2.62559300 | 0.07294300 | O | -6.59394800 | -2.58975200 | 0.29944500 |
| C | -3.23213400 | 0.56673200 | -0.12026100 | H | 2.11928100 | 3.79264000 | 0.73234600 |
| C | -2.74521700 | -0.56912300 | -0.80322200 | O | 1.61937300 | 3.02021600 | 1.00685300 |
| C | -4.58229900 | 0.62046800 | 0.21940600 | H | 1.67236700 | 2.39830000 | 0.25880500 |
| C | -3.65338600 | -1.60437300 | -1.09891000 | H | -1.62478500 | 3.29622400 | 1.53141800 |
| C | -5.45129000 | -0.40783000 | -0.07532200 | O | -0.93473800 | 3.42031500 | 2.19869500 |
| H | -4.96618200 | 1.49562000 | 0.73445300 | H | -0.09240700 | 3.28354300 | 1.72884600 |
| C | -4.97774500 | -1.53287300 | -0.74108400 | C | -1.90069700 | -1.40866300 | 0.31012300 |
| H | -5.65236500 | -2.34786300 | -0.98258100 | H | -1.91372300 | 1.11558800 | 1.76858900 |
| O | 1.45366000 | -1.21530000 | 0.80605900 | H | 2.07393000 | -0.09435100 | 1.94200800 |
| O | -1.49532200 | -0.76207000 | -1.20093800 | Pd | 0.17084300 | 0.10374500 | -0.18813600 |
| S | 7.21796700 | -0.20907400 | -0.02741300 | H | -5.01928700 | 2.99816100 | -1.22984300 |
| S | -7.18338300 | -0.32621700 | 0.38737800 | H | 3.75369500 | 1.69920600 | -2.41736400 |
| O | -7.94947900 | -0.48697600 | -0.88142600 | O | -0.86050500 | 1.62584600 | -1.00584900 |
| O | -7.37909800 | 1.00598200 | 1.02254800 | H | -0.20054500 | 2.20470300 | -1.40113500 |
| O | -7.40360500 | -1.45997200 | 1.33006700 | H | -1.92888300 | 2.31643000 | -0.36033800 |
| O | 7.50822700 | -0.75396900 | -1.38604900 | H | 1.61198000 | -2.03508100 | -0.18478300 |
| O | 7.93958300 | -0.95649000 | 1.04352000 | | | | |
| O | 7.41543800 | 1.26526500 | 0.06069200 | | | | |
| H | 0.13087100 | -2.52432100 | 0.83091500 | 54 | | | |
| O | -0.78007900 | -2.84236000 | 0.69075400 | RS_lambda_ID1_TS1_V2_P_02_Htr_TS, E(SCF) = | | | |
| H | -1.08155200 | -2.28988800 | -0.04870100 | -2484.16482396, E(ZPE) = -2483.767643, E(G) | | | |
| H | 0.16362400 | -0.50709600 | 1.95385700 | = -2483.833799 a.u. | | | |
| O | -0.68506100 | -0.37982600 | 2.42021400 | C | 0.39167700 | -2.29360200 | 1.52290700 |
| H | -1.18454100 | -1.14649300 | 2.10779100 | H | -0.03720900 | -3.07982100 | 0.89810600 |
| H | 1.93381500 | 2.19821300 | -0.79785300 | H | 0.98747400 | -2.77239900 | 2.30368700 |
| H | 1.71942300 | 1.17132900 | 1.92798400 | C | -0.70060100 | -1.44746100 | 2.10739500 |
| H | -1.87594200 | 1.49531000 | 1.26996500 | H | -1.39245400 | -2.05414600 | 2.69958500 |
| Pd | 0.00312000 | 0.47762700 | -0.69413900 | H | -0.29266500 | -0.67195900 | 2.76257200 |
| H | 3.25946900 | -3.05739100 | 0.44570100 | N | -1.42646600 | -0.75712300 | 1.01100700 |
| H | -3.26542100 | -2.47195500 | -1.62251300 | N | 1.25157300 | -1.45749300 | 0.65089100 |
| O | 1.22726000 | -1.17728000 | -1.84786600 | C | -2.47250100 | 0.14096000 | 1.58684200 |
| H | 0.51138400 | -1.62691200 | -2.31225800 | H | -2.89098800 | -0.38748100 | 2.45261600 |
| H | 1.35960300 | -1.67309300 | -1.01836700 | C | 2.44062900 | -0.84921700 | 1.29546900 |
| H | -1.74649300 | 2.07538500 | -1.59140300 | H | 2.93832700 | -1.60604600 | 1.90983800 |
| | | | | C | -3.58177600 | 0.48375500 | 0.64885200 |
| | | | | C | -3.65661600 | 1.76370800 | 0.05170300 |
| | | | | C | -4.59377400 | -0.44653000 | -0.43072700 |
| | | | | C | -4.79424600 | 2.04987200 | -0.73168300 |
| | | | | C | -5.68045400 | -0.14919400 | -0.36662600 |
| | | | | H | -4.54184400 | -1.42212400 | 0.90779600 |
| | | | | C | -5.78059900 | 1.11446200 | -0.94340500 |
| | | | | H | -6.64063700 | 1.35817600 | -1.55991400 |
| | | | | C | 3.40123900 | -0.33848300 | 0.26367100 |
| | | | | C | 2.99283300 | 0.50345400 | -0.79742200 |
| | | | | C | 4.73789800 | -0.69593600 | -0.36436400 |
| | | | | C | 3.96516600 | 0.95072900 | -1.70243100 |
| | | | | C | 5.68390300 | -0.23326300 | -0.53430100 |
| | | | | H | 5.04799000 | -1.35047800 | 1.17468400 |
| | | | | C | 5.29209800 | 0.59669900 | -1.57183600 |
| | | | | H | 6.03211800 | 0.95498300 | -2.27809700 |
| | | | | O | -2.70322100 | 2.65233500 | 0.18742000 |
| | | | | O | 1.75104300 | 0.93074900 | -0.97752600 |
| | | | | S | -6.97160000 | -1.35569900 | -0.66866300 |
| | | | | S | 7.39615000 | -0.73722800 | -0.33725900 |
| | | | | O | 7.40164500 | -2.22191200 | -0.47293000 |
| | | | | O | 7.79590500 | -0.29091700 | 1.02751700 |
| | | | | O | 8.15028800 | -0.04991300 | -1.42074300 |
| | | | | O | -6.94601600 | -1.62157900 | -2.13651200 |

| | | | | | | | |
|---|-------------|-------------|-------------|--|--|--|--|
| 54 | | | | | | | |
| RS_lambda_ID1_TS1_V2_P_02_Htr_P, E(SCF) = - | | | | | | | |
| 2484.16512524, E(ZPE) = -2483.766884, E(G) | | | | | | | |
| = -2483.834278 a.u. | | | | | | | |
| C | 0.37086200 | -2.29359500 | 1.42442900 | | | | |
| H | -0.05672900 | -3.06546700 | 0.78072400 | | | | |
| H | 0.93413300 | -2.79398200 | 2.21669800 | | | | |
| C | -0.72445200 | -1.43953100 | 1.99611100 | | | | |
| H | -1.43504100 | -2.04500900 | 2.56761100 | | | | |
| H | -0.31970400 | -0.67816400 | 2.66946400 | | | | |
| N | -1.42240800 | -0.72396300 | 0.89697100 | | | | |
| N | 1.26594200 | -1.46508900 | 0.58476200 | | | | |
| C | -2.43774300 | 0.20741700 | 1.46541000 | | | | |
| H | -2.83056400 | -0.26382200 | 2.37475000 | | | | |
| C | 2.44045300 | -0.87584000 | 1.26720900 | | | | |
| H | 2.92519800 | -1.64265500 | 1.88060000 | | | | |
| C | -3.59044800 | 0.50357500 | 0.55988900 | | | | |
| C | -3.74811300 | 1.75304100 | -0.05318400 | | | | |
| C | -4.58972300 | -0.45501100 | 0.40496400 | | | | |
| C | -4.91371800 | 2.02004600 | -0.77422200 | | | | |
| C | -5.72344200 | -0.18941500 | -0.33464100 | | | | |
| H | -4.49447900 | -1.42143000 | 0.89288500 | | | | |

O -8.24496700 -0.71190000 -0.23426800
O -6.61908200 -2.55383400 0.14328000
H 2.07555000 3.81673400 0.61176100
O 1.69003200 3.00330200 0.94606900
H 1.71490900 2.37599900 0.20026000
H -1.52412400 3.03521100 1.58039200
O -0.83819800 3.15422500 2.26201800
H 0.00800500 3.10987600 1.78411700
H -1.89309100 -1.45715300 0.43181600
H -1.96140400 1.03185800 1.95805300
H 2.08592300 -0.05830900 1.96533800
Pd 0.13177800 0.06942100 -0.12406100
H -4.85983700 3.03552600 -1.18077500
H 3.63987300 1.59776700 -2.50963800
O -0.59876200 1.59975000 -1.203701200
H -0.25005400 2.21870900 -1.39038100
H -1.64593300 2.13341700 -0.47173200
H 1.58201700 -2.02851500 -0.12568200

54
RS_lambda_ID1_TS1_V2_P_02, E(SCF) = -
2484.16498333, E(ZPE) = -2483.765714, E(G)
= -2483.834012 a.u.
C 0.39752500 -2.22355000 1.64397300
H -0.03117300 -3.03738000 1.05552400
H 1.00363600 -2.66532100 2.43833600
C -0.69505400 -1.35990500 2.20104300
H -1.38051200 -1.94501600 2.82162900
H -0.28794200 -0.55526000 2.82043200
N -1.43019500 -0.72010800 1.08078300
N 1.24468500 -1.41776500 0.73115800
C -2.48260500 0.19103100 1.62363800
H -2.90487800 -0.31463100 2.50139000
C 2.43711800 -0.77844300 1.34157600
H 2.93860900 -1.50727500 1.98571900
C -3.58303700 0.50904400 0.66777900
C -3.66200900 1.78662900 0.05785100
C -4.57738200 -0.43738400 0.44237800
C -4.79310100 2.04269800 -0.75156800
C -5.65426200 -0.16607900 -0.37797600
H -4.52078100 -1.40729000 0.93094500
C -5.76027300 1.09009900 -0.97135300
H -6.61194400 1.31466300 -1.60668700
C 3.38959000 -0.31635400 0.28049800
C 2.96990500 0.47046400 -0.81713500
C 4.72722900 -0.66869200 0.38550700
C 3.93015100 0.86555400 -1.75828000
C 5.66252300 -0.25406400 -0.54705100
H 5.04641900 -1.27949700 1.22581400
C 5.25821100 0.51673100 -1.62481400
H 5.99023700 0.83596100 -2.35762300
O -2.72980900 2.68551100 0.20130700
O 1.72637300 0.89350100 -0.99953200
S -6.91653400 -1.39756900 -0.69240400
S 7.37637200 -0.75317700 -0.34948700
O 7.38386600 -2.23951800 -0.46591400
O 7.78019700 -0.28802600 1.00759800
O 8.12487300 -0.07906800 -1.44509600
O -6.83980200 -1.70130300 -2.15177200
O -8.21470700 -0.76517900 -0.31751700
O -6.57476100 -2.57066800 0.16074800
H 2.04399200 3.86797800 0.42513300
O 1.68953000 3.06530500 0.81506000
H 1.71749000 2.39498000 0.10845200
H -1.50763600 3.06422500 1.53606600
O -0.80792500 3.20193500 2.20192000
H 0.02864000 3.14899400 1.70889000
H -1.89162400 -1.44626100 0.53030300
H -1.97208900 1.09107300 1.97179700
H 2.08581100 0.04126000 1.97818000
Pd 0.11603700 0.06897500 -0.09653600
H -4.86666900 3.02251300 -1.21254200
H 3.59549900 1.46891200 -2.59487100
O -0.90927100 1.57556400 -1.08185100
H -0.25642700 2.17992600 -1.45314000
H -1.60335800 2.11819800 -0.53763900
H 1.57246800 -2.01766800 -0.02476100

54
RS_lambda_ID1_TS1_V2_P, E(SCF) = -
2484.15932093, E(ZPE) = -2483.759218, E(G)
= -2483.826245 a.u.
C -0.47795600 3.55731600 -0.05241200
H 0.05231300 4.03123100 -0.88100200
H -1.18001500 4.28563100 0.36398400
C 0.48539500 3.07373000 0.99287000
H 1.07977300 3.90061700 1.39266800
H -0.05444700 2.61206600 1.82427900
N 1.36748600 2.01804100 0.43063600
N -1.20911200 2.39382300 -0.60814000
C 2.18284900 1.43674800 1.54384400
H 2.84579800 2.23693300 1.89603800
C -2.36794200 1.94175600 0.17716300
H -3.08198100 2.77133000 0.24262600
C 2.96626600 0.22126200 1.19707000
C 2.43629900 -1.06112000 1.51269400
C 4.20982800 0.34323700 0.59785200
C 3.25528600 -2.17604200 1.19949000
C 4.96703200 -0.76922200 0.27217900
H 4.60214700 1.33225200 0.37376500
C 4.48182200 -2.03554700 0.59294800
H 5.07460300 -2.91488000 0.35779700
C -3.06325100 0.73068100 -0.38760800
C -2.49678800 -0.17714300 -1.31215000
C -4.34531300 0.48664000 0.09804200
C -3.26620800 -1.29797300 -1.68965200
C -5.07892400 -0.61373900 -0.29157400
H -4.78515900 1.18424700 0.80466800
C -4.53125500 -1.51402000 -1.19900800
H -5.09875000 -2.38387300 -1.51413400
O 1.26793400 -1.22622100 2.04206500
O -1.31399400 -0.04889200 -1.88706900
S 6.59391300 -0.60227300 -0.45027100
S -6.72407600 -0.91093500 0.36060400
O -7.02501400 0.23447100 1.26281600
O -6.64468200 -2.21445800 1.08070600
O -7.62729600 -0.97314400 -0.82423800
O 7.56955000 -0.98581700 0.61455900
O 6.72510200 0.82592500 -0.85932400
O 6.63724100 -1.54190600 -1.60963800
H 0.35787200 -2.18755600 0.98396900
O -0.01368200 -2.59179000 0.15589100
H -0.94275600 -2.34215800 0.13280300
O -0.07407100 -0.19198500 2.40029000
O -0.87292900 0.34733300 2.60806600
H -1.18462200 0.01768600 3.45334500
H 2.01401900 2.44606400 -0.23307100
H 1.48026400 1.21029100 2.34606300
H -2.01258900 1.72198900 1.18931800
Pd 0.10143300 0.85835400 -0.80055400
O 1.35078600 -0.79389100 -1.27799000
H 1.23823900 -0.92236200 -2.22735900
O 0.87532500 -1.55721200 -0.85031700
H 2.87044400 -3.16292500 1.44108500
H -2.81885000 -1.98866900 -2.39655300
H -1.51647000 2.60981100 -1.55481300

54
RS_lambda_ID1_TS1_V2_R, E(SCF) = -
2484.18039334, E(ZPE) = -2483.781793, E(G)
= -2483.851249 a.u.
C -0.64886500 3.03453900 -1.11468100
H -0.25687700 3.05022200 -2.13355300
H -1.34445500 3.87108100 -1.01111200
C 0.48253800 3.13633800 -0.12561100
H 1.07119300 4.04361900 -0.28907900
H 0.11227100 3.15624500 0.90301300
N 1.32581700 1.92881500 -0.26685300
N -1.36367800 1.74104500 -0.93582700
C 2.35400000 1.79018500 0.78614000
H 2.96874300 2.69623400 0.81291400
C -2.47815400 1.77997700 0.03721500
H -3.11628000 2.63989500 -0.19327100
C 3.21261600 0.59099800 0.54798500

| | | | |
|----|-------------|-------------|-------------|
| C | 2.64346200 | -0.69811400 | 0.51233200 |
| C | 4.58238500 | 0.74311700 | 0.37718700 |
| C | 3.50002000 | -1.79752900 | 0.34552600 |
| C | 5.40628400 | -0.35134000 | 0.19997300 |
| H | 5.01839900 | 1.73685000 | 0.39167200 |
| C | 4.85880500 | -1.62798900 | 0.19149200 |
| H | 5.50189400 | -2.49155700 | 0.05596400 |
| C | -3.30677900 | 0.53070400 | 0.00684400 |
| C | -2.75030000 | -0.76874500 | -0.02460300 |
| C | -4.69033000 | 0.67718600 | 0.05278300 |
| C | -3.63997600 | -1.86302300 | 0.00090800 |
| C | -5.53882700 | -0.40930200 | 0.08556100 |
| H | -5.11836900 | 1.67447300 | 0.07012800 |
| C | -5.00191000 | -1.69231700 | 0.05568800 |
| H | -5.65745100 | -2.55762600 | 0.07538700 |
| O | 1.34016600 | -0.91573700 | 0.65254200 |
| O | -1.46490500 | -1.04524900 | -0.07495400 |
| S | 7.17439000 | -0.15249200 | -0.04440300 |
| S | -7.31910200 | -0.19763200 | 0.12172300 |
| O | -7.55751600 | 1.26717800 | 0.24650300 |
| O | -7.79760700 | -0.97003300 | 1.30404000 |
| O | -7.82461600 | -0.76124700 | -1.16375200 |
| O | 7.82544900 | -0.92772500 | 1.04935400 |
| O | 7.43802900 | 1.31014000 | 0.03906500 |
| O | 7.45960800 | -0.72181500 | -1.39222400 |
| H | 0.73516400 | -2.61353000 | 0.12037800 |
| O | 0.17454000 | -3.20735300 | -0.41254900 |
| H | -0.65819800 | -2.70176000 | -0.38499800 |
| H | 0.55883000 | -0.58674600 | 2.33987000 |
| O | 0.10150600 | -0.31606900 | 3.15593600 |
| H | 0.80743100 | -0.15824100 | 3.78702000 |
| H | 1.78901000 | 1.94201900 | -1.17677900 |
| H | 1.81517800 | 1.72134200 | 1.73717900 |
| H | -2.04073500 | 1.95849200 | 1.02684800 |
| Pd | -0.01249500 | 0.36899100 | -0.22088500 |
| O | 1.16625700 | -1.87071600 | -2.72201400 |
| H | 1.22678400 | -0.99068600 | -2.33552200 |
| H | 0.82490100 | -2.41983100 | -1.99020800 |
| H | 3.06507700 | -2.79141100 | 0.32754500 |
| H | -3.20802000 | -2.85843900 | -0.02091400 |
| H | -1.73640000 | 1.43925200 | -1.83414900 |

54
RS_lambda_ID1_TS1_V2, E(SCF) = -
2484.15587318, E(ZPE) = -2483.756135, E(G) =
-2483.821023 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.63201800 | 3.42621700 | -0.61520200 |
| H | -0.22727500 | 3.74162600 | -1.57891700 |
| H | -1.32281300 | 4.19961300 | -0.26597700 |
| C | 0.47175400 | 3.19851500 | 0.37652800 |
| H | 1.06485200 | 4.10456000 | 0.52813400 |
| H | 0.05760400 | 2.90459300 | 1.34457200 |
| N | 1.33645900 | 2.07553500 | -0.07399300 |
| N | -1.35586100 | 2.15251500 | -0.84206900 |
| C | 2.22563000 | 1.65179900 | 1.05073900 |
| H | 2.88386300 | 2.49658600 | 1.28371900 |
| C | -2.39643700 | 1.81354700 | 0.14149600 |
| H | -3.09715900 | 2.65400400 | 0.21165900 |
| C | 3.02818400 | 0.42349200 | 0.80508800 |
| C | 2.37639100 | -0.83759600 | 0.84618600 |
| C | 4.39556100 | 0.50119000 | 0.59413000 |
| C | 3.19393600 | -1.98618400 | 0.73710100 |
| C | 5.16236000 | -0.64150400 | 0.44024300 |
| H | 4.88191800 | 1.47192800 | 0.55655500 |
| C | 4.55118000 | -1.88916200 | 0.52779800 |
| H | 5.15020700 | -2.78953200 | 0.42763000 |
| C | -3.15900100 | 0.56701500 | -0.21667700 |
| C | -2.62509700 | -0.52976700 | -0.93178300 |
| C | -4.46783600 | 0.48890300 | 0.25415600 |
| C | -3.45368200 | -1.65384900 | -1.12809000 |
| C | -5.25525600 | -0.62504000 | 0.05573800 |
| H | -4.88484600 | 1.32903600 | 0.80130800 |
| C | -4.74041400 | -1.70645000 | -0.65069300 |
| H | -5.34913800 | -2.58856300 | -0.82078900 |
| O | 1.08479400 | -0.93416900 | 0.95196200 |
| O | -1.41614800 | -0.59630500 | -1.46738500 |
| S | 6.93064900 | -0.54246900 | 0.18487500 |

| | | | |
|----|-------------|-------------|--------------|
| S | -6.94625700 | -0.68208500 | 0.65125600 |
| O | -7.13368100 | 0.54339600 | 1.47624700 |
| O | -7.05619700 | -1.94119500 | 1.44142300 |
| O | -7.80770700 | -0.70094400 | -0.56629300 |
| O | 7.56441700 | -1.14894900 | 1.39345100 |
| O | 7.24723600 | 0.90669100 | 0.03525600 |
| O | 7.21805100 | -1.32859100 | -1.905102100 |
| H | 0.46204400 | -2.31135700 | 0.03177500 |
| O | 0.17381400 | -2.82291900 | -0.75986500 |
| H | -0.58349000 | -2.29909100 | -1.07336700 |
| H | -0.00579500 | -0.05399100 | -2.01790000 |
| O | -0.63073000 | 0.49218300 | 2.54522400 |
| H | -0.74025700 | 0.02489200 | 3.37591900 |
| H | 1.92205300 | 2.38738500 | -0.84906200 |
| H | 1.56004900 | 1.50034800 | 1.90457900 |
| H | -1.90728900 | 1.69271800 | 1.11530400 |
| Pd | 0.03494800 | 0.65225000 | -0.84670100 |
| O | 1.55509200 | -0.73538300 | -1.94133100 |
| H | 1.33227700 | -0.64357500 | -2.01790000 |
| H | 1.23401200 | -1.62637200 | -1.67925600 |
| H | 2.71513100 | -2.95928800 | 0.79502500 |
| H | -3.03667700 | -2.48836300 | -1.68268300 |
| H | -1.77443700 | 2.16857700 | -1.77016200 |

54
RS_lambda_ID1_TS1, E(SCF) = -2484.15348498,
E(ZPE) = -2483.753270, E(G) = -2483.818334
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.55806800 | 3.28349800 | -0.43153600 |
| H | -0.17124600 | 3.61346100 | -1.39780000 |
| H | -1.21896400 | 4.06409300 | -0.04439600 |
| C | 0.56455700 | 2.99840300 | 0.51995600 |
| H | 1.18232200 | 3.88480800 | 0.68797100 |
| H | 0.17050000 | 2.67874700 | 1.48878800 |
| N | 1.39010100 | 1.87579100 | 0.00338800 |
| N | -1.32056300 | 2.03443400 | -0.66682800 |
| C | 2.34090600 | 1.44602200 | 1.07078200 |
| H | 2.92611200 | 2.32750800 | 1.35759500 |
| C | -2.37145200 | 1.71704000 | 0.31812900 |
| H | -2.99974000 | 2.60373100 | 0.45662200 |
| C | 3.25097800 | 0.32613000 | 0.71217800 |
| C | 2.73178800 | -0.99045700 | 0.68210500 |
| C | 4.60315900 | 0.55323200 | 0.49828500 |
| C | 3.64677500 | -2.04286300 | 0.45947800 |
| C | 5.47297700 | -0.49487700 | 0.25802300 |
| H | 4.99067500 | 1.56708700 | 0.52777700 |
| C | 4.98870200 | -1.79887600 | 0.24998600 |
| H | 5.66731800 | -2.62559300 | 0.07294300 |
| C | -3.23213400 | 0.56673200 | -0.12026100 |
| C | -2.74521700 | -0.56912300 | -0.80322200 |
| C | -4.58229900 | 0.62046800 | 0.21940600 |
| C | -3.65338600 | -1.60437300 | -1.09891000 |
| C | -5.45129000 | -0.40783000 | -0.07532200 |
| H | -4.96618200 | 1.49562000 | 0.73445300 |
| C | -4.97774500 | -1.53287300 | -0.74108400 |
| H | -5.65236500 | -2.34786300 | -0.98258100 |
| O | 1.45366000 | -1.21530000 | 0.80605900 |
| O | -1.49532200 | -0.76207000 | -1.20093800 |
| S | 7.21796700 | -0.20907400 | -0.02741300 |
| S | -7.18338300 | -0.32621700 | 0.38737800 |
| O | -7.94947900 | -0.48697600 | -0.88142600 |
| O | -7.37909800 | 1.00598200 | 1.02254800 |
| O | -7.40360500 | -1.45997200 | 1.33006700 |
| O | 7.50822700 | -0.75396900 | -1.38604900 |
| O | 7.93958300 | -0.95649000 | 1.04352000 |
| O | 7.41543800 | 1.26526500 | 0.06069200 |
| H | 0.13087100 | -2.52432100 | 0.83091500 |
| O | -0.78007900 | -2.84236000 | 0.69075400 |
| H | -1.08155200 | -2.28988800 | -0.04870100 |
| H | 0.16362400 | -0.50709600 | 1.95385700 |
| O | -0.68506100 | -0.37982600 | 2.42021400 |
| H | -1.18454100 | -1.14649300 | 2.10779100 |
| H | 1.93381500 | 2.19821300 | -0.79785300 |
| H | 1.71942300 | 1.17132900 | 1.92798400 |
| H | -1.87594200 | 1.49531000 | 1.26996500 |
| Pd | 0.00312000 | 0.674762700 | -0.69413900 |
| H | 3.25946900 | -3.05739100 | 0.44570100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.26542100 | -2.47195500 | -1.62251300 |
| O | 1.22726000 | -1.17728000 | -1.84786600 |
| H | 0.51138400 | -1.62691200 | -2.31225800 |
| H | 1.35960300 | -1.67309300 | -1.01836700 |
| H | -1.74649300 | 2.07538500 | -1.59140300 |

56

RS_lambda_ID1_TS2-diamond_P, E(SCF) = -2485.32903036, E(ZPE) = -2484.912656, E(G) = -2484.980403 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.62582600 | 0.15453500 | 3.13653400 |
| H | 0.33782800 | -0.82434500 | 3.52498200 |
| H | 1.34447500 | 0.59049300 | 3.83299600 |
| C | -0.58368700 | 1.02965900 | 2.97560600 |
| H | -1.15099000 | 1.09769200 | 3.90890700 |
| H | -0.30985000 | 2.04054900 | 2.65821300 |
| N | -1.43113300 | 0.46263300 | 1.89695500 |
| C | -2.71512900 | 1.22138500 | 1.77461400 |
| H | -3.24598500 | 1.06919000 | 2.72219700 |
| C | -3.55061500 | 0.80125500 | 0.61979400 |
| C | -3.54594600 | 1.60002700 | -0.56200600 |
| C | -4.31758100 | -0.35344000 | 0.69711100 |
| C | -4.34548500 | 1.12734800 | -1.63847700 |
| C | -5.07859800 | -0.78248700 | -0.37413600 |
| H | -4.31807300 | -0.94148300 | 1.61184300 |
| C | -5.08917600 | -0.02486600 | -1.54499500 |
| H | -5.68515900 | -0.35497200 | -2.39117400 |
| O | -2.83228500 | 2.66372200 | -0.67093100 |
| S | -6.07493200 | -2.26395400 | -0.27490900 |
| O | -7.49913000 | -1.81924400 | -0.33979000 |
| O | -5.73224900 | -2.90885500 | 1.02503600 |
| O | -5.69534700 | -3.09768400 | -1.45310100 |
| H | 2.02703500 | 3.37048900 | -1.88653300 |
| O | 1.21394700 | 2.96627900 | -1.57429400 |
| H | 1.38995800 | 2.00680400 | -1.49034200 |
| H | -1.36084600 | 3.27385400 | 0.19095200 |
| O | -0.54204400 | 3.60496900 | 0.61527000 |
| H | 0.14481000 | 3.47490200 | -0.05756000 |
| H | -1.67074600 | -0.50326100 | 2.13075500 |
| H | -2.44967900 | 2.27540000 | 1.69874800 |
| Pd | -0.10062300 | 0.28200000 | 0.29988000 |
| O | -1.26116900 | 2.44292100 | -2.90041000 |
| H | -0.40748300 | 2.77758800 | -2.58460800 |
| H | -1.88930000 | 2.63810900 | -2.17182100 |
| H | -4.35382900 | 1.71548400 | -2.55169500 |
| H | -1.41793200 | 0.15527800 | -0.86614900 |
| H | -1.08380300 | 0.87791400 | -1.07288900 |
| N | 1.26542000 | -0.06354100 | 1.80853500 |
| C | 2.48210700 | 0.74538500 | 1.52583600 |
| H | 3.11619500 | 0.74751700 | 2.41720800 |
| C | 3.23238400 | 0.14070700 | 0.38179200 |
| C | 2.60435800 | -0.10050400 | -0.85544900 |
| C | 4.56285000 | -0.22400900 | 0.55374400 |
| C | 3.35096800 | -0.69988700 | -1.88109500 |
| C | 5.28465700 | -0.80077100 | -0.47172800 |
| H | 5.04917200 | -0.05506000 | 1.50933000 |
| C | 4.67379200 | -1.03409400 | -1.69783200 |
| H | 5.23483000 | -1.49428200 | -2.50474200 |
| O | 1.34998100 | 0.24537100 | -1.12689600 |
| S | 7.00687100 | -1.25989800 | -0.24375200 |
| O | 7.77621800 | -0.43528000 | -1.21787600 |
| O | 7.07809900 | -2.71642500 | -0.54942600 |
| O | 7.32885300 | -0.94259200 | 1.17409000 |
| H | 2.16237900 | 1.77647800 | 1.34171200 |
| H | 2.85539000 | -0.88135300 | -2.82816600 |
| H | 1.53587300 | -1.04390200 | 1.73426800 |

54

RS_lambda_ID1_TS2-diamond_R_noH2_Htr_W-reor_P, E(SCF) = -2484.16963151, E(ZPE) = -2483.769607, E(G) = -2483.837860 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.02591600 | -2.38122000 | -0.12274200 |
| H | -0.51024800 | -2.61691200 | -1.07306900 |
| H | 0.38672900 | -3.31008800 | 0.28011000 |
| C | -1.03052200 | -1.77971000 | 0.82550000 |
| H | -1.87764200 | -2.45715600 | 0.97706500 |
| H | -0.58342400 | -1.57441800 | 1.80091200 |

| | | | |
|----|-------------|-------------|--------------|
| N | -1.49057800 | -0.48676200 | 0.26499600 |
| C | -2.47558600 | 0.22837400 | 1.13893600 |
| H | -2.67612200 | -0.40785000 | 2.00395400 |
| C | -3.75407700 | 0.50148600 | 0.41414600 |
| C | -3.94419600 | 1.64685200 | -0.37529800 |
| C | -4.77936200 | -0.43996800 | 0.49375300 |
| C | -5.17036600 | 1.82096900 | -1.02998500 |
| C | -5.97575800 | -0.26289400 | -0.16740800 |
| H | -4.63539500 | -1.32928400 | 1.10009700 |
| C | -6.17201300 | 0.88397000 | -0.92971600 |
| H | -7.11336100 | 1.03689600 | -1.44740400 |
| O | -3.04225800 | 2.61456600 | -0.54025400 |
| S | -7.30202600 | -1.46704800 | -0.03109600 |
| O | -8.41400000 | -0.76399400 | 0.66915000 |
| O | -6.74507500 | -2.60366600 | 0.75202000 |
| O | -7.65338400 | -1.83600100 | -1.43129600 |
| H | 2.31802400 | 4.56588900 | -0.46144100 |
| O | 1.83251700 | 3.92562000 | 0.06288400 |
| H | 2.08932600 | 3.26571700 | -0.26578900 |
| H | 0.18721900 | 2.58766000 | 1.89807500 |
| O | 0.83069100 | 2.92114300 | 2.55133100 |
| H | 1.40322400 | 3.45437200 | 1.98125700 |
| H | -1.95020700 | -0.67355500 | -0.623735200 |
| H | -2.00329400 | 1.14079800 | 1.50565200 |
| Pd | 0.27741100 | 0.49226200 | -0.19588400 |
| O | -0.57196700 | 2.28802800 | 0.17513800 |
| H | -0.00412100 | -2.99802600 | -0.15818000 |
| H | -2.10642500 | 2.42058400 | -0.22040000 |
| H | -5.30350100 | 2.71688000 | -1.62572600 |
| N | 1.05820900 | -1.40699600 | -0.40642800 |
| C | 2.21972000 | -1.48692700 | -0.50330200 |
| H | 2.54632200 | -2.53036100 | 0.57533500 |
| C | 3.37252500 | -0.64593400 | 0.03852100 |
| C | 3.23352200 | 0.67901200 | -0.43436400 |
| C | 4.64642500 | -1.19964500 | -0.13548200 |
| C | 4.40714000 | 1.37954800 | -0.78018500 |
| C | 5.78030900 | -0.49002300 | -0.19999400 |
| H | 4.75663000 | -2.22003000 | 0.48938200 |
| C | 5.65442100 | 0.81628800 | -0.65894700 |
| H | 6.53750800 | 1.38604100 | -0.93044100 |
| O | 2.09089800 | 1.32002900 | -0.59007800 |
| S | 7.41340800 | -1.21303600 | -0.03680400 |
| O | 8.13350100 | -0.36388800 | 0.95551500 |
| O | 8.03032400 | -1.14420900 | -1.39272800 |
| O | 7.20150900 | -2.60891800 | 0.43646800 |
| H | 1.87473600 | -1.18737400 | 1.49983700 |
| H | 4.29646600 | 2.39445200 | -1.14824000 |
| H | 1.39144900 | -1.54863900 | -1.35776200 |

54

RS_lambda_ID1_TS2-diamond_R_noH2, E(SCF) = -2484.16802963, E(ZPE) = -2483.768114, E(G) = -2483.835086 a.u.

| | | | |
|---|-------------|-------------|--------------|
| C | 0.27691300 | -2.68869400 | 0.53716700 |
| H | -0.19075500 | -3.17375400 | -0.32238700 |
| H | 0.82160300 | -3.45145300 | 1.09942600 |
| C | -0.76335100 | -2.01910900 | 1.38525900 |
| H | -1.50375800 | -2.73972600 | 1.74524400 |
| H | -0.31141800 | -1.54243300 | 2.25959700 |
| N | -1.42639700 | -0.95055000 | 0.59674800 |
| C | -2.37219900 | -0.18025800 | 1.46758300 |
| H | -2.69795300 | -0.86856700 | 2.25622900 |
| C | -3.57215600 | 0.34396000 | 0.75364000 |
| C | -3.69208400 | 1.72794400 | 0.46339600 |
| C | -4.61112100 | -0.53069500 | 0.45124600 |
| C | -4.91021400 | 2.15463500 | -0.12056500 |
| C | -5.77553200 | -0.08515400 | -0.14147100 |
| H | -4.51662100 | -1.58548800 | 0.69922100 |
| C | -5.92115400 | 1.27355800 | -0.41980900 |
| H | -6.84079500 | 1.63292100 | -0.87236500 |
| O | -2.73485000 | 2.57101600 | 0.69913400 |
| S | -7.11249000 | -1.20714600 | -0.53867200 |
| O | -8.31120900 | -0.69313100 | 0.18654500 |
| O | -6.68174500 | -2.55282600 | -0.06479500 |
| O | -7.28138400 | -1.14083500 | -2.02034300 |
| H | 1.63125500 | 4.26344500 | -0.428357200 |
| O | 1.23706400 | 3.48179100 | -0.09116300 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.74319900 | 2.70772700 | -0.41174800 |
| H | -1.29831600 | 2.90089600 | 1.83930600 |
| O | -0.44766500 | 3.08000400 | 2.27987400 |
| H | 0.16711900 | 3.28063000 | 1.55874600 |
| H | -1.97036000 | -1.38354600 | -0.15122300 |
| H | -1.80359100 | 0.62172700 | 1.94213400 |
| Pd | 0.17671800 | 0.06747200 | -0.28971200 |
| O | -0.82870500 | 1.81972000 | -0.78274500 |
| H | -0.18610600 | 2.55614400 | -0.74664800 |
| H | -1.58765100 | 2.11050700 | -0.16559600 |
| H | -5.01694200 | 3.21279000 | -0.33738700 |
| N | 1.21127900 | -1.66413000 | 0.01226500 |
| C | 2.37212100 | -1.35488700 | 0.87633600 |
| H | 2.81649700 | -2.29520100 | 1.21951400 |
| C | 3.40858300 | -0.55920000 | 0.14138000 |
| C | 3.09048900 | 0.53621500 | -0.68841600 |
| C | 4.74439900 | -0.90813300 | 0.32025900 |
| C | 4.14932400 | 1.23448200 | -1.29910600 |
| C | 5.76634300 | -0.20375800 | -0.28060500 |
| H | 4.99404800 | -1.75550100 | 0.95090700 |
| C | 5.46169500 | 0.88065300 | -1.09542600 |
| H | 6.25777300 | 1.43938500 | -1.57705100 |
| O | 1.86782700 | 0.97879800 | -0.93960200 |
| S | 7.48370400 | -0.66001800 | -0.03169400 |
| O | 8.13255000 | 0.53075800 | 0.58797600 |
| O | 8.02488700 | -0.95844200 | -1.38839300 |
| O | 7.46828800 | -1.84858100 | 0.86453800 |
| H | 1.99532500 | -0.83005400 | 1.76077800 |
| H | 3.89358000 | 2.07397800 | -1.93741500 |
| H | 1.56844900 | -1.97720100 | -0.88961700 |

56
RS_lambda_ID1_TS2-diamond_R, E(SCF) = -
2485.34229864, E(ZPE) = -2484.927501, E(G)
= -2484.996295 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.31767500 | -2.43530000 | 1.23555600 |
| H | -0.14794200 | -3.09695800 | 0.50260100 |
| H | 0.89163800 | -3.05403000 | 1.92939300 |
| C | -0.73356300 | -1.63751800 | 1.94888300 |
| H | -1.45609600 | -2.29254800 | 2.44539900 |
| H | -0.29305200 | -0.98671900 | 2.70913700 |
| N | -1.42148500 | -0.76454100 | 0.96581000 |
| C | -2.44759400 | 0.08452300 | 1.64805100 |
| H | -2.80742000 | -0.49482500 | 2.50666300 |
| C | -3.60017200 | 0.44713900 | 0.77430500 |
| C | -3.74535700 | 1.77155800 | 0.28720000 |
| C | -4.55405300 | -0.52110100 | 0.47878900 |
| C | -4.89747700 | 2.04263500 | -0.49120700 |
| C | -5.65174500 | -0.22973100 | -0.30567400 |
| H | -4.44118700 | -1.52863600 | 0.87292800 |
| C | -5.82033600 | 1.06817700 | -0.78659300 |
| H | -6.68662300 | 1.30591800 | -1.39717400 |
| O | -2.85790500 | 2.69210600 | 0.50723200 |
| S | -6.86904500 | -1.47907200 | -0.70894400 |
| O | -8.16869500 | -0.98456800 | -0.16721000 |
| O | -6.40865600 | -2.73558600 | -0.05304000 |
| O | -6.88137300 | -1.57349000 | -2.19842600 |
| H | 1.59141400 | 4.31739400 | -0.56084700 |
| O | 1.19325800 | 3.57196300 | -0.10522200 |
| H | 1.71298900 | 2.77665300 | -0.34134800 |
| H | -1.50691600 | 3.22827300 | 1.67750500 |
| O | -0.69519200 | 3.49612800 | 2.14519400 |
| H | -0.02342800 | 3.57858800 | 1.45248900 |
| H | -1.90472100 | -1.35486000 | 0.28639300 |
| H | -1.93859700 | 0.96934300 | 2.03385500 |
| Pd | 0.16937500 | 0.15858000 | -0.03747700 |
| O | -0.83235000 | 1.84139100 | -0.74849600 |
| H | -0.19667200 | 2.58480700 | -0.73880900 |
| H | -1.63478500 | 2.17686800 | -0.21681900 |
| H | -5.02119800 | 3.05366400 | -0.86623600 |
| H | -2.73666000 | -0.42777000 | -2.48817600 |
| H | -2.53783300 | 0.08045500 | -1.97318100 |
| N | 1.21690200 | -1.51579900 | 0.49444400 |
| C | 2.43625900 | -1.09458500 | 1.22322700 |
| H | 2.89259800 | -1.97714500 | 1.68305200 |
| C | 3.42755200 | -0.45269200 | 0.30138000 |
| C | 3.06710300 | 0.55368500 | -0.61836000 |

| | | | |
|---|------------|-------------|-------------|
| C | 4.75784000 | -0.85379100 | 0.38176400 |
| C | 4.08105900 | 1.12375400 | -1.40972700 |
| C | 5.73796900 | -0.27518500 | -0.39787200 |
| H | 5.03715300 | -1.63566300 | 1.08090500 |
| C | 5.39193500 | 0.72360400 | -1.30087700 |
| H | 6.15302900 | 1.18269500 | -1.92348200 |
| O | 1.84218300 | 1.02521900 | -0.78774100 |
| S | 7.44304500 | -0.82924800 | -0.30743300 |
| O | 8.25923800 | 0.40017800 | -0.09784100 |
| O | 7.72560700 | -1.48077900 | -1.61860000 |
| O | 7.50839400 | -1.77651300 | 0.83918900 |
| H | 2.12309500 | -0.42801300 | 2.03400200 |
| H | 3.79273800 | 1.89847700 | -2.11235000 |
| H | 1.51667900 | -1.97455600 | -0.36507100 |

56
RS_lambda_ID1_TS2-diamond, E(SCF) = -
2485.31381434, E(ZPE) = -2484.899025, E(G)
= -2484.966415 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.57322200 | 0.67022400 | 3.01116400 |
| H | 0.25935800 | -0.23381000 | 3.53893000 |
| H | 1.29511800 | 1.19233500 | 3.64201500 |
| C | -0.61285500 | 1.53080100 | 2.70047400 |
| H | -1.18125000 | 1.76910300 | 3.60534700 |
| H | -0.31709500 | 2.46801100 | 2.22072800 |
| N | -1.47088800 | 0.81460900 | 1.72534900 |
| C | -2.72979500 | 1.58176100 | 1.48747400 |
| H | -3.25166600 | 1.61851900 | 2.45204500 |
| C | -3.58855500 | 0.98441900 | 0.43085200 |
| C | -3.64906200 | 1.60662900 | -0.84688700 |
| C | -4.30323400 | -0.17625500 | 0.69601700 |
| C | -4.45703800 | 0.95509800 | -1.82044600 |
| C | -5.06394300 | -0.78893100 | -0.28231500 |
| H | -4.25941400 | -0.62443600 | 1.68626200 |
| C | -5.13880000 | -0.20666400 | -1.54645900 |
| H | -5.73780200 | -0.68000900 | -2.32024100 |
| O | -2.98942700 | 2.67548900 | -1.13614800 |
| S | -5.99073200 | -2.27780400 | 0.06032200 |
| O | -7.43442300 | -1.92174900 | -0.09941000 |
| O | -5.64851400 | -2.67254100 | 1.45769000 |
| O | -5.55183300 | -3.28638500 | -0.94850100 |
| H | 2.18275200 | 3.02309100 | -2.30380800 |
| O | 1.39560100 | 2.68365900 | -1.87375100 |
| H | 1.56184900 | 1.74480200 | -1.66842200 |
| H | -1.41885500 | 3.33767800 | -0.41415500 |
| O | -0.59730100 | 3.71445200 | -0.03763300 |
| H | 0.11400900 | 3.43744000 | -0.63431900 |
| H | -1.73832100 | -0.08985000 | 2.11965000 |
| H | -2.43616600 | 2.59560200 | 1.21965100 |
| Pd | -0.14322400 | 0.32006800 | 0.18628200 |
| O | -1.01633500 | 1.33032100 | -2.35908800 |
| H | -0.24927100 | 1.89808500 | -2.52105300 |
| H | -1.73289200 | 1.93720400 | -2.06770700 |
| H | -4.50993200 | 1.40518200 | -2.80746300 |
| H | -1.55938300 | -1.05548500 | -0.76397500 |
| H | -1.53077100 | -0.52403400 | -1.31374500 |
| N | 1.22047100 | 0.24360200 | 1.74255600 |
| C | 2.44565600 | 0.98674300 | 1.34579200 |
| H | 3.06235900 | 1.13876700 | 2.23668100 |
| C | 3.21284800 | 0.19147500 | 0.34028900 |
| C | 2.58774900 | -0.29106600 | -0.82849000 |
| C | 4.55014700 | -0.10422400 | 0.57196600 |
| C | 3.34853700 | -1.05681500 | -1.72792500 |
| C | 5.28677700 | -0.83997100 | -0.33626200 |
| H | 5.03172500 | 0.25478600 | 1.47615500 |
| C | 4.67949600 | -1.31442800 | -1.49185500 |
| H | 5.25623300 | -1.89581500 | -2.20409300 |
| O | 1.33418500 | -0.01257400 | -1.15717200 |
| S | 7.01919300 | -1.21463700 | -0.04031600 |
| O | 7.75363700 | -0.65567100 | -1.21627400 |
| O | 7.10251100 | -2.70499500 | 0.03114400 |
| O | 7.36830200 | -0.54402800 | 1.24625300 |
| H | 2.13127400 | 1.97117700 | 0.98158400 |
| H | 2.85875400 | -1.41990600 | -2.62223800 |
| H | 1.47711700 | -0.74060300 | 1.82056400 |

56

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RS_lambda_ID1_TS2_trigo_P, E(SCF) = -
2485.33476568, E(ZPE) = -2484.919326, E(G)
= -2484.988303 a.u.
C -0.12532200 -1.34642700 0.61579500
H 0.03356000 -2.22217500 1.25026400
H -0.46633200 -1.69629500 -0.36271900
C -1.10099900 -0.37858200 1.22365800
H -0.73401300 -0.02409500 2.19084000
H -2.07828700 -0.84089300 1.38565800
N -1.22675100 0.80829100 0.34080800
N 1.14974300 -0.62067800 0.41118600
C -2.22647100 0.65571500 -0.76100500
H -2.20462600 1.60142000 -1.30834400
C 2.14604800 -1.33675100 -0.41672100
H 1.71549500 -1.41383900 -1.42108900
C -3.60372800 0.34316800 -0.27817300
C -4.35590000 1.35996300 0.37084000
C -4.13740400 -0.92614100 -0.45598200
C -5.65857500 1.00868600 0.80266400
C -5.41213400 -1.23555400 -0.01872400
H -3.54881000 -1.69456700 -0.95095600
C -6.17071600 -0.25427200 0.61636000
H -6.24800400 -1.77583400 1.29509600
H -7.17325700 -0.49053900 0.96149500
C 3.45937600 -0.62549400 -0.41423600
C 3.54359800 0.72638700 -0.81487200
C 4.61137200 -1.30746600 -0.04294300
C 4.81603900 1.32836600 -0.83852200
C 5.84937100 -0.69654400 -0.07853900
H 4.54443500 -2.34407300 0.27201300
C 5.94713900 0.63011400 -0.48421700
H 4.87690500 2.36522200 -1.15000100
H 6.91681800 1.11749600 -0.51236600
O -3.87976500 2.54891700 0.56182100
O 2.51373800 1.44880500 -1.20237100
S -6.10524400 -2.86816000 -0.25488300
S 7.33310700 -1.57500100 0.41627900
O 7.86027300 -0.84130400 1.60276800
O 6.90391200 -2.96483700 0.73432200
O 8.25688500 -1.50197000 -0.75155500
O -6.42351900 -3.38516900 1.10880800
O -7.33291400 -2.68396700 -1.08406700
O -5.05448000 -3.66819700 -0.94613300
H 2.26781400 -2.35207600 -0.02496700
H -1.86478900 -0.12540400 -1.43493700
H -1.50883000 1.59996500 0.93097900
O -0.45799300 4.38909000 0.42598400
H -1.25066800 4.51612700 -0.13344800
H -2.80272300 2.83516400 1.81795000
O -1.93477800 2.89702100 2.29238900
H -2.10132100 2.77032000 3.22850000
H -0.81650000 3.98437100 1.23446000
H -3.26700000 3.66601100 -0.56531100
O -2.81443900 4.39611700 -1.05478500
H -2.80833600 4.13491100 -1.97815900
H 0.17381500 2.91746300 -0.71493200
H 0.22536500 2.53971700 -1.45240000
Pd 0.67081900 1.19195400 -0.42119700
H 1.56936600 -0.41975500 1.32136600

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54
RS_lambda_ID1_TS2_trigo_R_noH2, E(SCF) = -
2484.16258809, E(ZPE) = -2483.763298, E(G)
= -2483.831840 a.u.
C 0.39964700 -2.70954400 0.96771400
H -0.10481900 -3.32913700 0.22371400
H 0.98760000 -3.36743100 1.61269700
C -0.61038000 -1.92601400 1.75599300
H -1.31937700 -2.59273200 2.25624900
H -0.12805000 -1.31499500 2.52377300
N -1.32549600 -1.00285500 0.84124900
N 1.28782600 -1.77448800 0.23409800
C -2.28495500 -0.14491300 1.60056500
H -2.64875900 -0.74651700 2.44221000
C 2.49221500 -1.34074700 0.97423700
H 2.99322500 -2.22924000 1.37308100
C -3.44670200 0.31758100 0.78452900

```

```

C -3.54494900 1.66196200 0.35285100
C -4.46669600 -0.58369500 0.49625600
C -4.70431600 2.02764500 -0.36574900
C -5.58240300 -0.20074100 -0.22089800
H -4.39685100 -1.60837500 0.85363000
C -5.69538800 1.11860500 -0.65348500
H -6.57306600 1.42859100 -1.21262500
C 3.45803400 -0.58051900 0.11247000
C 3.06234500 0.37911200 -0.84816100
C 4.81542200 -0.81422000 0.31937100
C 4.07769400 1.06041700 -1.55240700
C 5.78842100 -0.12714300 -0.37457700
H 5.12236800 -1.55489300 1.05145100
C 5.40953900 0.81911800 -1.32192600
H 6.16567000 1.36375300 -1.87864000
O -2.60140300 2.53315100 0.58534500
O 1.82342600 0.69346300 -1.15727400
S -6.87616100 -1.37376700 -0.62388800
S 7.53058000 -0.43081800 -0.09175700
O 8.07130500 -0.95040500 -1.38452800
O 7.59757100 -1.44552700 1.00474200
O 8.12201400 0.87595400 0.28665700
O -8.15364800 -0.74581800 -0.17889000
O -6.55096800 -2.62202800 0.12171300
O -6.82099800 -1.55151200 -2.10459800
H -1.96881100 4.24249500 -0.02299900
O -1.23570200 4.88117300 -0.01823400
H -0.77460900 4.62889200 0.79578900
H -1.44376100 2.91147800 1.89709400
O -0.62422800 3.26948900 2.29727100
H -0.85191100 3.49015100 3.20309100
H -1.86358200 -1.55765100 0.17374800
H -1.71915600 0.69206100 2.01314000
H 2.15208900 -0.74939500 1.83163700
Pd 0.23137000 -0.10223000 -0.24371500
H -4.78502400 3.05776400 -0.69756000
H 3.76516900 1.79408900 -2.28735800
O -0.70724700 1.64660900 -0.86340100
H -0.01437400 2.30175400 -1.01101800
H -1.40257900 2.05305700 -0.24629900
H 1.59239600 -2.21648800 -0.63211200

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56
RS_lambda_ID1_TS2_trigo_R, E(SCF) = -
2485.33713963, E(ZPE) = -2484.922122, E(G)
= -2484.991352 a.u.
C 0.39307000 -2.68410900 1.04855600
H -0.13091900 -3.31135100 0.32456600
H 0.98586700 -3.33704000 1.69412200
C -0.59525700 -1.87677400 1.84013900
H -1.30116700 -2.52756300 2.36515000
H -0.09442700 -1.25589900 2.58775500
N -1.31750200 -0.96602900 0.91932500
N 1.27746100 -1.77086400 0.28336000
C -2.26630100 -0.09138900 1.67230400
H -2.62708000 -0.67700100 2.52648700
C 2.49575100 -1.33505900 0.99835000
H 2.99746800 -2.22171500 1.40054500
C -3.42756800 0.35599500 0.84800100
C -3.51686200 1.68605500 0.37479000
C -4.43763900 -0.55590500 0.56281900
C -4.65920800 2.02802500 -0.38156900
C -5.53506700 -0.19818400 -0.19440400
H -4.37067100 -1.57123900 0.94652800
C -5.63946400 1.10690000 -0.66996500
H -6.50165000 1.39650400 -1.26316300
C 3.45445400 -0.58969200 0.11587900
C 3.05321700 0.35346600 -0.85841600
C 4.81315100 -0.81780500 0.32091200
C 4.06476300 1.02730300 -1.57536600
C 5.78221200 -0.13951300 -0.38677400
H 5.12421800 -1.54667400 1.06304000
C 5.39795600 0.79264200 -1.34588800
H 6.15097200 1.33144700 -1.91237700
O -2.57659900 2.56367400 0.59783900
O 1.81250500 0.65788100 -1.17094900
S -6.79933100 -1.39475000 -0.61923500

```

S 7.52603000 -0.44360700 -0.10470800
O 8.06678100 -0.95865400 -1.39566200
O 7.59872300 -1.44321600 0.99696700
O 8.11274600 0.87648300 0.26601600
O -8.10094900 -0.77630200 -0.23491100
O -6.48654800 -2.62424200 0.16182400
O -6.68532800 -1.60008600 -2.09349000
H -1.93929900 4.26458600 -0.03127200
H -2.80589600 -0.70716300 -2.22482600
H -2.46709100 -0.05228200 -2.08397400
O -1.20249900 4.89897300 -0.03416300
H -0.73819600 4.64831300 0.77860400
H -1.40859100 2.94629200 1.89671400
O -0.58390100 3.30242800 2.28841200
H -0.80270500 3.52854900 3.19507400
H -1.86703000 -1.53083600 0.26932500
H -1.69455700 0.75064500 2.06600100
H 2.17278500 -0.73149200 1.85390200
Pd 0.22803100 -0.09761400 -0.21199300
H -4.73329800 3.04737100 -0.74664100
H 3.74806800 1.74965900 -2.31968000
O -0.70129700 1.64843200 -0.86137000
H -0.00351700 2.29455200 -1.02556300
H -1.38677100 2.07156600 -0.24573800
H 1.56484600 -2.23172000 -0.57890000

56
RS_lambda_ID1_TS2_trigo, E(SCF) = -
2485.31348973, E(ZPE) = -2484.898748, E(G)
= -2484.966710 a.u.
C 0.37680600 -3.27761700 1.22129600
H -0.19372800 -3.99838600 0.63241300
H 1.09651700 -3.82924800 1.83212000
C -0.54099100 -2.44968900 2.07401200
H -1.11757000 -3.08212900 2.75604800
H 0.02434100 -1.73309400 2.67699300
N -1.44453800 -1.66321500 1.20177100
N 1.08644800 -2.39487000 0.26693300
C -2.35741600 -0.81983600 2.02921200
H -3.01325600 -1.50355800 2.58132900
C 2.29097400 -1.74219400 0.80091500
H 2.97288000 -2.52350600 1.15724300
C -3.14691700 0.15500600 1.23020100
C -2.69934500 1.49940700 1.14420400
C -4.28388200 -0.25750000 0.55022600
C -3.46538500 2.37462700 0.33797400
C -5.00484400 0.62117000 -0.23748600
H -4.62090000 -1.28761900 0.63662300
C -4.57933200 1.94360500 -0.34541000
H -5.13780800 2.63842100 -0.96557800
C 3.00771500 -0.87388700 -0.19435200
C 2.40562200 -0.31993500 -1.34754100
C 4.34008600 -0.58105700 0.08191300
C 3.18814700 0.52887000 -2.15747800
C 5.08809500 0.23932800 -0.73468300
H 4.80786800 -1.01124500 0.96242800
C 4.50476400 0.79453100 -1.86931700
H 5.08660500 1.44092500 -2.51852000
O -1.62170000 1.90685900 1.74259800
O 1.17238100 -0.56151900 -1.74949800
S -6.43153900 0.07440400 -1.17001900
S 6.80428400 0.60959400 -0.35996800
O 7.58033900 0.18225500 -1.55872600
O 7.13850800 -0.17309100 0.86136400
O 6.86137600 2.08357800 -0.14316900
O -7.51618000 1.05842400 -0.88558700
O -6.74757900 -1.29671400 -0.67829200
O -6.02010500 0.09085500 -2.60556200
H -0.55824700 3.42084400 2.05980800
H -1.95155100 -0.39124200 -1.58060400
H -1.61837700 0.29199900 -1.50692900
O 0.31113500 3.81572500 2.25270600
H 0.83494000 3.02906000 2.45714300
H -0.17491100 1.09719700 2.38335700
O 0.74807800 0.89310200 2.65701500
H 0.71114700 0.77674900 3.61000500
H -2.03185300 -2.31482600 0.67762800

H -1.73525100 -0.29624600 2.75522900
H 1.98002000 -1.15228000 1.66998200
Pd -0.19288000 -0.91252500 -0.33437100
H -3.13204000 3.40500600 0.25690100
H 2.71340600 0.95254500 -3.03574200
O -0.13747800 1.70045700 -0.49469800
H 0.80198000 1.88376600 -0.39774900
H -0.55252700 1.93483800 0.36497400
H 1.32873900 -2.91763300 -0.57250800

56
RS_lambda_ID1_TS3-diamond_P_Htr-to-
Ophen_P_it-is-a-Dl-with-3W, E(SCF) = -
2485.36501938, E(ZPE) = -2484.945579, E(G)
= -2485.014445 a.u.
C 0.49168500 -2.56248800 1.78522900
H 0.02561700 -3.40153700 1.26190700
H 1.14495600 -2.98127300 2.55948100
C -0.57745300 -1.71040100 2.42318300
H -1.17800000 -2.31019300 3.11625500
H -0.13903000 -0.88561600 2.99200500
N -1.44537600 -1.10185900 1.38329000
C -2.50001600 -0.27356200 0.22301800
H -3.03644900 -0.91037700 2.73962000
C -3.46899700 0.28751300 1.03515600
C -3.51751100 1.64452900 0.70538400
C -4.36778900 -0.57710400 0.41474600
C -4.44479800 2.09831200 -0.23400000
C -5.27885500 -0.12514700 -0.51643000
H -4.36554400 -1.63158900 0.67634200
C -5.31486900 1.22406300 -0.84532200
H -6.02919200 1.58797500 -1.57604400
O -2.74021600 2.59400300 1.26670700
S -6.46276100 -1.24741500 -1.27490000
O -7.79959700 -0.78652600 -0.80601700
O -6.10769700 -2.60686200 -0.78554700
O -6.28608700 -1.08692200 -2.74497700
H 2.00004500 3.43009900 0.28655300
O 1.14402600 2.99397000 0.27182900
H 1.25321100 2.18117100 -0.27684100
H -0.18586500 2.75593100 3.24145200
O -0.34505300 2.18941600 2.48197100
H 0.27626900 2.48732000 1.78536500
H -1.90545800 -1.85332200 0.86779500
H -1.98722000 0.49623500 2.59907900
Pd -0.08339900 -0.23737600 0.05168200
O -1.28168600 4.14998300 -0.69921900
H -0.39813400 3.84407400 -0.43584100
H -1.86675700 3.71934700 -0.05939500
H -4.45651800 3.15595100 -0.47355100
H -1.05561200 0.89873800 -0.39075600
H -1.94684800 2.26550000 1.75060000
N 1.25750100 -1.79366000 0.79297300
C 2.39685500 -1.02189700 1.31350800
H 3.02445500 -1.65371900 1.95555700
C 3.23813000 -0.46524000 0.20020000
C 2.70941600 0.31174800 -0.86010300
C 4.60976200 -0.69794200 0.24839800
C 3.61613700 0.82152900 -1.81181400
C 5.47570700 -0.18622500 -0.69732300
H 5.01639400 -1.29831200 1.05655800
C 4.96921800 0.59001200 -1.73312500
H 5.63723100 1.00053000 -2.48378800
O 1.43876300 0.63217900 -1.02583600
S 7.24431400 -0.44952900 -0.57064700
O 7.82924400 0.88125700 -0.23315300
O 7.68691500 -0.93798100 -1.90801600
O 7.43639400 -1.45678000 -0.50983900
H 1.99730200 -0.21974600 1.94719600
H 3.20343400 1.42041000 -2.61695700
H 1.59855200 -2.41979000 0.07006600

56
RS_lambda_ID1_TS3-diamond_P_Htr-to-
Ophen_R_it-is-a-Dl-with-3W, E(SCF) = -
2485.33060968, E(ZPE) = -2484.914258, E(G)
= -2484.983678 a.u.

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 0.41368600 | -3.10002800 | 0.40637600 | H | -6.24236300 | 2.03832600 | -0.77067300 |
| H | -0.04020000 | -3.57895000 | -0.46350300 | O | -2.13350600 | 1.88441200 | 1.06215500 |
| H | 1.04526600 | -3.83824100 | 0.90656200 | S | -7.14631400 | -0.69396500 | -0.72131100 |
| C | -0.64770100 | -2.57544900 | 1.32717900 | O | -8.25911600 | 0.06000700 | -0.07567700 |
| H | -1.31353900 | -3.37672700 | 1.66055400 | O | -7.07795700 | -2.11702500 | -0.28636600 |
| H | -0.20858600 | -2.11772100 | 2.21847300 | O | -7.14580000 | -0.54072200 | -2.20534900 |
| N | -1.42559100 | -1.52045500 | 0.62997100 | H | 2.15215900 | 3.68405000 | 0.10080500 |
| C | -2.39808800 | -0.89043300 | 1.57182000 | O | 1.31871900 | 3.20972400 | 0.15631100 |
| H | -2.86891500 | -1.70682000 | 2.13221100 | H | 1.43043400 | 2.39555400 | -0.37923900 |
| C | -3.43785800 | -0.06489300 | 0.89577200 | H | -0.66531800 | 1.89586700 | 2.19713800 |
| C | -3.25338100 | 1.33474500 | 0.76818300 | O | 0.23456000 | 2.01327200 | 2.54771100 |
| C | -4.60680200 | -0.66416300 | 0.44216100 | H | 0.70112400 | 2.46470300 | 1.82531600 |
| C | -4.29686400 | 2.06911500 | 0.15843200 | H | -1.94399900 | -1.94750900 | -0.16638300 |
| C | -5.60699400 | 0.08000000 | -0.15358800 | H | -1.82467700 | -0.30282300 | 2.24533300 |
| H | -4.74694100 | -1.73057500 | 0.56406900 | Pd | 0.04784900 | -0.30088700 | -0.20080000 |
| C | -5.44286600 | 1.45666200 | -0.29328900 | O | -1.30393300 | 4.34066900 | 0.07553600 |
| H | -6.22687600 | 2.04705500 | -0.75820700 | H | -0.36872200 | 4.09256700 | 0.01170400 |
| O | -2.16012100 | 1.91491900 | 1.16259100 | H | -1.71383600 | 3.54153100 | 0.46010800 |
| S | -7.10234700 | -0.69345500 | -0.76350300 | H | -4.14837400 | 3.12012000 | -0.02146000 |
| O | -8.23570600 | 0.03669700 | -0.12743800 | H | -0.85840400 | 1.06349700 | -0.74728900 |
| O | -7.02686400 | -2.12409900 | -0.34700500 | H | -1.10160700 | 1.21359400 | 0.06547200 |
| O | -7.08106200 | -0.52334100 | -2.24582700 | N | 1.25057700 | -1.97077300 | -0.10528600 |
| H | 2.15533200 | 3.69332100 | 0.07655800 | C | 2.40092300 | -1.59861800 | -0.17433900 |
| O | 1.32584300 | 3.21440200 | 0.14606700 | H | 2.95193100 | -2.50643900 | 1.01099900 |
| H | 1.43298300 | 2.39935700 | -0.38811400 | C | 3.32720600 | -0.65223700 | 0.03776700 |
| H | -0.64403900 | 1.88488800 | 2.19995200 | C | 2.88292700 | 0.42567300 | -0.75418600 |
| O | 0.26331400 | 1.99201800 | 2.53743800 | C | 4.69622600 | -0.85066700 | -0.20159000 |
| H | 0.72120800 | 2.45470200 | 1.81705300 | C | 3.85228600 | 1.25660700 | -1.34774100 |
| H | -1.95545100 | -1.94478900 | -0.13319100 | C | 5.62796300 | -0.01587600 | -0.37716100 |
| H | -1.81193100 | -0.29058300 | 2.27171100 | H | 5.04390400 | -1.68365300 | 0.80435000 |
| Pd | 0.03556800 | 4.30691400 | -0.25222200 | C | 5.19784900 | 1.04768000 | -1.16198800 |
| O | -1.31998600 | 4.28834500 | 0.02394200 | H | 5.92067900 | 1.70706700 | -1.63141600 |
| H | -0.37953500 | 4.05702300 | -0.02018900 | O | 1.61780400 | 0.74265200 | -1.00288100 |
| H | -1.71773400 | 3.51103300 | 0.46539600 | S | 7.38793600 | -0.30090900 | -0.16588900 |
| H | -4.16511900 | 3.14150900 | 0.05180900 | O | 7.94021600 | 0.97292200 | 0.37540200 |
| H | -0.90574700 | 1.03834200 | -0.77038200 | O | 7.91244000 | -0.61493300 | -1.52560500 |
| H | -1.05340700 | 1.18257900 | 0.04850500 | O | 7.50811500 | -1.44138700 | 0.78287400 |
| N | 1.23676100 | -1.97058000 | -0.09129500 | H | 2.00711700 | -1.17344000 | 1.67389000 |
| C | 2.39403400 | -1.59862300 | 0.74913000 | H | 3.49919800 | 2.07653600 | -1.96468600 |
| H | 2.94570100 | -2.50771300 | 1.01030200 | H | 1.60286000 | -2.19660200 | -1.03431900 |
| C | 3.31525500 | -0.65271600 | 0.03665200 | | | | |
| C | 2.86552000 | 0.42037800 | -0.75794500 | | | | |
| C | 4.68536200 | -0.84764300 | 0.19583400 | | | | |
| C | 3.82997600 | 1.24966500 | -1.36119400 | | | | |
| C | 5.61253500 | -0.01367600 | -0.39100000 | | | | |
| H | 5.03735100 | -1.67710700 | 0.80090100 | | | | |
| C | 5.17673600 | 1.04443100 | -1.17999200 | | | | |
| H | 5.89608600 | 1.70233800 | -1.65672500 | | | | |
| O | 1.59785700 | 0.73456700 | -1.00115100 | | | | |
| S | 7.37427800 | -0.29234700 | -0.18399600 | | | | |
| O | 7.92282700 | 0.98389600 | 0.35515700 | | | | |
| O | 7.89599000 | -0.60519300 | -1.54491300 | | | | |
| O | 7.50051000 | -1.43169800 | 0.76519500 | | | | |
| H | 2.00741000 | -1.17513600 | 1.68322700 | | | | |
| H | 3.47285800 | 2.06493300 | -1.98193600 | | | | |
| H | 1.58231200 | -2.19639900 | -1.02317600 | | | | |

56

RS_lambda_ID1_TS3-diamond_P, E(SCF) = -2485.36722633, E(ZPE) = -2484.947436, E(G) = -2485.015399 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.49153800 | -2.61766900 | 1.84220100 |
| H | 0.03120100 | -3.45652200 | 1.31360900 |
| H | 1.16139300 | -3.03851000 | 2.60087200 |
| C | -0.58454000 | -1.79424800 | 2.50893800 |
| H | -1.17053000 | -2.41924400 | 3.19225200 |
| H | -0.15061500 | -0.97925600 | 3.09596800 |
| N | -1.46671500 | -1.17523700 | 1.48850600 |
| C | -2.56157200 | -0.40871200 | 2.13773700 |
| H | -3.09882500 | -1.08834300 | 2.81090800 |
| C | -3.49998400 | 0.17517800 | 1.13465900 |
| C | -3.46745300 | 1.53462300 | 0.81582000 |
| C | -4.38195200 | -0.65330000 | 0.45179300 |
| C | -4.29466700 | 2.03188100 | -0.19074600 |
| C | -5.19687400 | -0.15868600 | -0.54787100 |
| H | -4.43207800 | -1.71009500 | 0.69897900 |
| C | -5.14659800 | 1.18913300 | -0.87452100 |
| H | -5.78637900 | 1.58213500 | -1.65752200 |
| O | -2.64474600 | 2.34791200 | 1.50794300 |
| S | -6.32724300 | -1.23562300 | -1.44105300 |
| O | -7.68351000 | -0.65808000 | -1.22750800 |
| O | -6.16386600 | -2.58611200 | -0.83847600 |
| O | -5.89715900 | -1.17273700 | -2.86595500 |
| H | 1.71815200 | 3.74852400 | -0.58231600 |
| O | 0.96603700 | 3.22905200 | -0.28809000 |
| H | 1.10440900 | 2.30997800 | -0.62705600 |
| H | -0.67461300 | 2.17992000 | 2.10088900 |
| O | 0.18561100 | 2.52114500 | 2.38416600 |
| H | 0.60906300 | 2.77395600 | 1.54703700 |
| H | -1.89776500 | -1.92171800 | 0.94133200 |
| H | -2.09973400 | 0.36567300 | 2.75059300 |
| Pd | -0.11904700 | -0.23509500 | 0.19061300 |
| O | -1.57606300 | 4.25595300 | -0.03867800 |

56

RS_lambda_ID1_TS3-diamond_P_Htr-to-Ophen, E(SCF) = -2485.33055641, E(ZPE) = -2484.915274, E(G) = -2484.983897 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.42401900 | -3.09845600 | 0.38627500 |
| H | -0.02516300 | -3.57717800 | -0.48627800 |
| H | 1.05013100 | -3.83843300 | 0.89111600 |
| C | -0.64351500 | -2.57426400 | 1.30059200 |
| H | -1.30903500 | -3.37704500 | 1.63143000 |
| H | -0.20930100 | -2.11547300 | 2.19376600 |
| N | -1.42090800 | -1.52105800 | 0.60004500 |
| C | -2.40247900 | -0.90280100 | 1.53837100 |
| H | -2.87333900 | -1.72307200 | 2.09292000 |
| C | -3.44533300 | -0.07985500 | 0.86249500 |
| C | -3.25140800 | 1.31173500 | 0.70373900 |
| C | -4.62932500 | -0.67317700 | 0.44064100 |
| C | -4.29360300 | 2.05209500 | 0.10761800 |
| C | -5.63123600 | 0.07458700 | -0.14749300 |
| H | -4.77924900 | -1.73999300 | -0.58242300 |
| C | -5.45635700 | 1.44642400 | -0.31151800 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|------------|-------------|-------------|
| H | -0.67638700 | 3.91727600 | -0.23167700 | O | 1.36981600 | 0.02364200 | -1.17971800 |
| H | -2.40147500 | 3.13374400 | 0.95900900 | S | 7.08645200 | -1.12264000 | -0.14435900 |
| H | -4.26635600 | 3.09068800 | -0.42460000 | O | 7.81087000 | -0.39364400 | -0.22383000 |
| H | -1.09002300 | 0.91584900 | -0.20003000 | O | 7.22771900 | -2.60171200 | -0.26423400 |
| H | -1.94827700 | 4.51585200 | -0.88461200 | O | 7.40361600 | -0.61436000 | 1.21834100 |
| N | 1.23313200 | -1.82285100 | 0.85122300 | H | 2.08965700 | 1.81174100 | 1.13110400 |
| C | 2.39250700 | -0.67126700 | 1.36231800 | H | 2.93470000 | -1.21117200 | -2.74918900 |
| H | 3.03949400 | -1.73456500 | 1.95558700 | H | 1.60450900 | -0.98060500 | 1.80095700 |
| C | 3.20034600 | -0.47106400 | 0.24818700 | | | | |
| C | 2.64627800 | 0.35281300 | -0.76267100 | | | | |
| C | 4.57207100 | -0.71044100 | 0.24442600 | | | | |
| C | 3.52943700 | 0.91274500 | -1.70891100 | | | | |
| C | 5.41353400 | -0.15656300 | -0.69949200 | | | | |
| H | 4.99949400 | -1.34983900 | 1.01078700 | | | | |
| C | 4.88228300 | 0.67127500 | -1.68143500 | | | | |
| H | 5.53138800 | 1.11538900 | -2.42960200 | | | | |
| O | 1.37021100 | 0.66091700 | -0.89777600 | | | | |
| S | 7.17624900 | -0.48050600 | -0.68128200 | | | | |
| O | 7.83428200 | 0.84576900 | -0.49907500 | | | | |
| O | 7.49379000 | -1.09020900 | -2.00519900 | | | | |
| O | 7.41537500 | -1.40892500 | 0.45854000 | | | | |
| H | 2.01580500 | -0.30173000 | 2.04334600 | | | | |
| H | 3.09630900 | 1.55013300 | -2.47349000 | | | | |
| H | 1.54764700 | -2.42793500 | 0.09906800 | | | | |

56
RS_lambda_ID1_TS3-diamond, E(SCF) = -
2485.32266579, E(ZPE) = -2484.907835, E(G)
= -2484.973634 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.62479600 | 0.29555100 | 3.07197700 |
| H | 0.30793600 | -0.65232900 | 3.51265200 |
| H | 1.32728000 | 0.76469600 | 3.76539400 |
| C | -0.56637400 | 1.17591700 | 2.82822500 |
| H | -1.12704100 | 1.34534300 | 3.75316200 |
| H | -0.26730700 | 2.14696200 | 2.42235000 |
| N | -1.43884500 | 0.54514300 | 1.80391100 |
| C | -2.67903800 | 1.36268800 | 1.63262300 |
| H | -3.20172900 | 1.32866400 | 2.59670100 |
| C | -3.56963200 | 0.91070300 | 0.53179400 |
| C | -3.62499800 | 1.66152700 | -0.67480000 |
| C | -4.33639100 | -0.23594700 | 0.68922100 |
| C | -4.47720900 | 1.15751800 | -1.68998600 |
| C | -5.15070100 | -0.70204100 | -0.32627400 |
| H | -4.29185200 | -0.78732400 | 1.62519800 |
| C | -5.21848600 | 0.01145400 | -1.52134100 |
| H | -5.85611900 | -0.34541700 | -2.32506400 |
| O | -2.91350500 | 2.72633900 | -0.87271900 |
| S | -6.14826800 | -2.17372600 | -0.12484000 |
| O | -7.57129500 | -1.72194300 | -0.14962200 |
| O | -5.75580500 | -2.76819700 | 1.18473800 |
| O | -5.82082900 | -3.05551200 | -1.28341100 |
| H | 2.00196100 | 3.09734300 | -2.19063000 |
| O | 1.26008700 | 2.71046100 | -1.71920100 |
| H | 1.47617000 | 1.76718400 | -1.55712700 |
| H | -1.38926700 | 3.37425100 | -0.05915600 |
| O | -0.55748600 | 3.72399000 | 0.31896900 |
| H | 0.13468000 | 3.45706200 | -0.30445700 |
| H | -1.72285700 | -0.37912800 | 2.13360600 |
| H | -2.35294800 | 2.38801600 | 1.46522800 |
| Pd | -0.10805800 | 0.15870000 | 0.23453100 |
| O | -1.15841600 | 1.71147500 | -2.46452700 |
| H | -0.32000500 | 2.21945700 | -2.42608500 |
| H | -1.86234700 | 2.27693200 | -2.01981200 |
| H | -4.52774200 | 1.71308000 | -2.62201800 |
| H | -1.32014800 | 0.06702200 | -0.91492700 |
| H | -1.07159500 | 0.77973600 | -1.48282700 |
| N | 1.28857400 | -0.01242100 | 1.78262600 |
| C | 2.46006700 | 0.82322900 | 1.42468300 |
| H | 3.09472800 | 0.95437000 | 2.30682800 |
| C | 3.24204400 | 0.14371100 | 0.34276400 |
| C | 2.63136700 | -0.24902400 | -0.86605900 |
| C | 4.58805500 | -0.13631600 | 0.54988600 |
| C | 3.41465700 | -0.91356500 | -1.82350400 |
| C | 5.34425300 | -0.77702600 | -0.41123800 |
| H | 5.05856900 | 0.15609900 | 1.48293100 |
| C | 4.75034200 | -1.16619600 | -1.60591900 |
| H | 5.33770200 | -1.67675700 | -2.36241800 |

56
RS_lambda_ID1_TS3_trigo_P, E(SCF) = -
2485.35275672, E(ZPE) = -2484.935129, E(G)
= -2485.006310 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.51434400 | -3.13025200 | 1.26501900 |
| H | 0.07342900 | -3.90042900 | 0.62758600 |
| H | 1.17365500 | -3.63330100 | 1.98291800 |
| C | -0.57434900 | -2.39830500 | 2.01207700 |
| H | -1.15173000 | -3.09652500 | 2.62707600 |
| H | -0.13494200 | -1.66065900 | 2.68907000 |
| N | -1.47218600 | -1.65460000 | 1.08694600 |
| N | 1.26496200 | -2.21731000 | 0.38844100 |
| C | -2.37678000 | -0.76581000 | 1.87212900 |
| H | -2.98587500 | -1.39400900 | 2.53312000 |
| C | 2.32913500 | -1.42643800 | 1.01535100 |
| H | 3.02136600 | -2.08086000 | 1.56159900 |
| C | -3.25616200 | 0.08244100 | 1.01412700 |
| C | -2.88277000 | 1.37932300 | 0.65262000 |
| C | -4.44082200 | -0.43663300 | 0.50565100 |
| C | -3.67650100 | 2.11994400 | -0.21692700 |
| C | -5.22578600 | 0.30048300 | -0.36030800 |
| H | -4.75313600 | -1.44031300 | 0.77939700 |
| C | -4.83988600 | 1.58079600 | -0.72919500 |
| H | -5.45559400 | 2.15848400 | -1.41037300 |
| C | 3.11463700 | -0.62153200 | 0.01096100 |
| C | 2.54427500 | 0.17557800 | -1.01841700 |
| C | 4.50047500 | -0.63166800 | 0.15859900 |
| C | 3.42913400 | 0.92231500 | -1.82774500 |
| C | 5.33912700 | 0.11284000 | -0.64494100 |
| H | 4.94187400 | -1.24585900 | 0.93750100 |
| C | 4.79063800 | 0.90141800 | -1.64996600 |
| H | 5.43511700 | 1.49140400 | -2.29420900 |
| O | -1.74466900 | 1.91890000 | 1.16515300 |
| O | 1.26328700 | 0.29600100 | -1.30488600 |
| S | -6.75781400 | -0.37481400 | -1.02288900 |
| S | 7.11685500 | 0.07569700 | -0.42641300 |
| O | 7.67790300 | -0.43551300 | -1.71086300 |
| O | 7.37628400 | -0.83537200 | 0.72331800 |
| O | 7.52603600 | 1.48464900 | -0.15505300 |
| O | -7.83339800 | 0.53950400 | -0.54805000 |
| O | -6.86950300 | -1.75080600 | -0.46904800 |
| O | -6.59469700 | -0.34820200 | -2.50265900 |
| H | -1.26114300 | 3.76402100 | 2.24854900 |
| H | -1.24438600 | 0.24922400 | -0.80006300 |
| H | 0.46207700 | 1.91255000 | -0.99101200 |
| O | -0.44023100 | 4.19465400 | 2.51276400 |
| H | 0.18262400 | 3.44916000 | 2.53899600 |
| H | 0.12371700 | 1.32286600 | 1.88218800 |
| O | 0.90487700 | 1.67645700 | 2.33700700 |
| H | 0.93205800 | 1.21946300 | 3.18249600 |
| H | -2.05023000 | -2.32536300 | 0.58059000 |
| H | -1.74152700 | -0.14342500 | 2.50383200 |
| H | 1.86119400 | -0.76975900 | 1.75857400 |
| Pd | -0.17443800 | -0.74598200 | -0.28821100 |
| H | -3.36295700 | 3.12323900 | -0.48595900 |
| H | 2.98324500 | 1.53051100 | -2.60824500 |
| O | -0.03351500 | 2.72797900 | -0.75480000 |
| H | 0.62668000 | 3.36766400 | -0.47418700 |
| H | -1.19903800 | 2.31585000 | 0.43645500 |
| H | 1.66233500 | -2.74251700 | -0.38437000 |

56
RS_lambda_ID1_TS3_trigo_R, E(SCF) = -
2485.32341550, E(ZPE) = -2484.909193, E(G)
= -2484.977673 a.u.

| | | | |
|---|-------------|-------------|------------|
| C | 0.36820900 | -3.42511500 | 0.97640500 |
| H | -0.19014100 | -4.11004400 | 0.33522000 |
| H | 1.08704700 | -4.01130900 | 1.55515900 |

| | | | | | | | |
|----|-------------|-------------|-------------|--|-------------|--------------|-------------|
| C | -0.56310200 | -2.66441600 | 1.87609500 | H | -5.53826100 | 2.36085100 | -1.09619900 |
| H | -1.14300900 | -3.34275000 | 2.50829900 | C | 3.12352200 | -0.69447700 | -0.04554300 |
| H | -0.00400000 | -1.99275100 | 2.53253700 | C | 2.56748100 | -0.09928900 | -1.20515800 |
| N | -1.46542400 | -1.81650400 | 1.05764000 | C | 4.48863500 | -0.55726700 | 0.19659900 |
| N | 1.07874000 | -2.47220100 | 0.08725100 | C | 3.44062300 | 0.61910300 | -2.05181200 |
| C | -2.30341200 | -0.94397000 | 1.93874300 | C | 5.31722800 | 0.15185700 | -0.64650200 |
| H | -2.96169600 | -1.60742700 | 2.51174200 | H | 4.91827100 | -1.02238700 | -1.07882400 |
| C | 2.27191600 | -1.83893400 | 0.67336600 | C | 4.78136200 | 0.74570900 | -1.78482900 |
| H | 2.96332400 | -2.63236300 | 0.97904100 | H | 5.42111300 | 1.30568800 | -2.45963700 |
| C | -3.08586800 | 0.07923200 | 1.19584700 | O | -1.77627800 | 2.03553200 | 1.34792400 |
| C | -2.58601800 | 1.40742300 | 1.11255000 | O | 1.31041500 | -0.16556100 | -1.59620900 |
| C | -4.26865800 | -0.27168500 | 0.55861100 | S | -6.68678800 | -0.27644800 | -1.01221600 |
| C | -3.35637700 | 2.33091500 | 0.36470200 | S | 7.06987200 | 0.31755100 | -0.30943800 |
| C | -4.98750400 | 0.65169400 | -0.17742000 | O | 7.77101900 | -0.28411200 | -1.48051100 |
| H | -4.64358800 | -1.28910600 | 0.67311700 | O | 7.31975700 | -0.42103200 | 0.95957400 |
| C | -4.51743200 | 1.95995700 | -0.27257300 | O | 7.32534400 | 1.78221200 | -0.19024000 |
| H | -5.07700800 | 2.69062000 | -0.84915700 | O | -7.81579100 | 0.57788700 | -0.54173800 |
| C | 2.97930000 | -0.88979900 | -0.25408500 | O | -6.78069600 | -1.68259500 | -0.52861900 |
| C | 2.37320700 | -2.37320700 | -1.34861500 | O | -6.48858000 | -0.144823900 | -2.13681200 |
| C | 4.31012800 | -0.61311400 | 0.04766500 | H | -0.95858800 | 3.67691700 | 1.92866000 |
| C | 3.14588500 | 0.70405700 | -2.06616700 | H | -1.27804700 | 0.15845100 | -1.03480700 |
| C | 5.04941800 | 0.29350000 | -0.68091000 | H | -0.76695600 | 1.00959400 | -0.94351300 |
| H | 4.78387900 | -1.12474900 | 0.848019800 | O | -0.13291300 | 4.14482500 | 2.13681200 |
| C | 4.45857100 | 0.95786900 | -1.75050400 | H | 0.47755700 | 3.40554800 | 2.26947900 |
| H | 5.03104800 | 1.67600500 | -2.32876400 | H | -0.25451200 | 1.37355300 | 2.02948300 |
| O | -1.46374000 | 1.75871400 | 1.65528000 | O | 0.68562400 | 1.31771900 | 2.30992000 |
| O | 1.14670500 | -0.44917700 | -1.79200700 | H | 0.66284800 | 1.12920600 | 3.25194900 |
| S | -6.48714800 | 0.19184100 | -1.03938700 | H | -1.99916400 | -2.27904700 | 0.62077600 |
| S | 6.76447300 | 0.63450400 | -0.27566900 | H | -1.70202000 | -0.10181800 | 2.54437800 |
| O | 7.54329000 | 0.30363000 | -1.50286400 | H | 1.89146100 | -0.75025300 | 1.71989700 |
| O | 7.09743500 | -0.24204100 | 0.88069100 | Pd | -0.12254500 | -0.82948600 | -0.34345900 |
| O | 6.81982100 | 2.08654300 | 0.05756900 | H | -3.49669000 | 3.32594000 | -0.09220500 |
| O | -7.53839800 | 1.14712000 | -0.58266300 | H | 3.00596100 | 1.07435700 | -2.93540600 |
| O | -6.77369800 | -1.21718700 | -0.64811000 | O | -0.46728200 | 2.25359500 | -0.84737600 |
| O | -6.18883900 | 0.33907200 | -2.49482100 | H | 0.49297700 | 2.30328500 | -0.74805400 |
| H | -0.50382500 | 3.18293700 | 2.41176100 | H | -0.88947800 | 2.39862000 | 0.06187700 |
| H | -1.56830600 | 0.05559000 | -0.96867200 | H | 1.59628900 | -2.76206200 | -0.38454500 |
| H | -0.94445200 | 0.58931400 | -0.92664100 | | | | |
| O | 0.32310200 | 3.57456100 | 2.74476500 | | | | |
| H | 0.92647600 | 2.82215900 | 2.69257800 | 54 | | | |
| H | -0.03134200 | 0.88643400 | 2.16503200 | RS lambda_ID2_TS1_chain (2), E(SCF) = - | | | |
| O | 0.88356800 | 0.62372600 | 2.41982400 | 2484.15295377, E(ZPE) = -2483.754004, E(G) | | | |
| H | 0.84344300 | 0.44820500 | 3.36394700 | = -2483.820608 a.u. | | | |
| H | -2.09842400 | -2.42209000 | 0.53216700 | C | 0.78675200 | 3.02307500 | 0.47044800 |
| H | -1.62320400 | -0.45801900 | 2.63968200 | H | 0.50792600 | 3.21985800 | 1.50768400 |
| H | 1.95320500 | -1.30332300 | 1.57532200 | H | 1.42858300 | 3.83961200 | 0.13154500 |
| Pd | -0.23207800 | -0.98967200 | -0.43828100 | C | -0.45974100 | 2.91167000 | -0.37194100 |
| H | -2.98512800 | 3.34874800 | 0.28930100 | H | -1.08101300 | 3.80815200 | -0.27271600 |
| H | 2.66342900 | 1.21105500 | -2.89491800 | H | -0.21867600 | 2.78272900 | -1.43103200 |
| O | 0.01485100 | 2.46417100 | -0.57533200 | N | -1.18941000 | 1.71212000 | 0.08115900 |
| H | 0.91996700 | 2.17504800 | -0.42396100 | C | -2.41819800 | 1.43086300 | -0.67207200 |
| H | -0.43800500 | 2.33345000 | 0.28510200 | H | -2.10209300 | 1.09603900 | -1.66766500 |
| H | 1.34313500 | -2.94424600 | -0.77541400 | C | -3.35244200 | 0.42489100 | -0.05180500 |
| | | | | C | -2.93927600 | -0.67047400 | 0.75759600 |
| | | | | C | -4.69305900 | 0.54871800 | -0.40074500 |
| | | | | C | -3.93794700 | -1.60254100 | 1.12934900 |
| | | | | C | -5.64398800 | -0.37438600 | -0.00958500 |
| | | | | H | -5.00912200 | 1.39282200 | -1.00732600 |
| | | | | C | -5.25373000 | -1.46894900 | 0.75478500 |
| | | | | H | -3.61993200 | -2.44393600 | 1.73804400 |
| | | | | H | -5.98822100 | -2.20622000 | 1.06434700 |
| | | | | O | -1.71878500 | -0.84014700 | 1.18431000 |
| | | | | S | -7.35420000 | -0.21665200 | -0.51534700 |
| | | | | O | -7.60563600 | -1.32866400 | -1.47966200 |
| | | | | O | -7.48255300 | 1.12902700 | -1.14331400 |
| | | | | O | -8.16803200 | -0.35810900 | 0.72748100 |
| | | | | H | -2.95789900 | 2.37633000 | -0.81235800 |
| | | | | H | -1.39800100 | 1.79773100 | 1.08674100 |
| | | | | O | -0.86640100 | -1.21294300 | -1.54452900 |
| | | | | H | -0.80343900 | -2.04436800 | -1.02624700 |
| | | | | H | -1.42214700 | 0.33008200 | 2.47258500 |
| | | | | O | -1.27819800 | 1.19613300 | 2.91782600 |
| | | | | H | -1.98567700 | 1.28174800 | 3.56072900 |
| | | | | H | -0.23058600 | -1.31526400 | -2.26021500 |
| | | | | H | -0.90257000 | -2.39741300 | 0.92583400 |
| | | | | O | -0.36347500 | -3.07355000 | 0.45676900 |
| | | | | H | 0.52285600 | -2.67466200 | -0.42762700 |
| | | | | Pd | 0.21029700 | 0.22995500 | -0.03520000 |

| | | | | | | | |
|--|-------------|-------------|-------------|--|--|--|--|
| 56 | | | | | | | |
| RS lambda_ID1_TS3_trigo, E(SCF) = - | | | | | | | |
| 2485.31363983, E(ZPE) = -2484.900732, E(G) | | | | | | | |
| = -2484.970883 a.u. | | | | | | | |
| C | 0.49821300 | -3.12139200 | 1.31168900 | | | | |
| H | 0.02437900 | -3.89333000 | 0.70178200 | | | | |
| H | 1.18995400 | -3.61417500 | 2.00180600 | | | | |
| C | -0.53790600 | -2.33774900 | 2.06632300 | | | | |
| H | -1.12966000 | -2.98979200 | 2.71565500 | | | | |
| H | -0.05923800 | -1.58580000 | 2.69974200 | | | | |
| N | -1.42074300 | -1.60327200 | 1.12212200 | | | | |
| N | 1.22644000 | -2.22065300 | 0.39382500 | | | | |
| C | -2.33441900 | -0.71407100 | 1.90054300 | | | | |
| H | -2.93419700 | -1.36394300 | 2.54951500 | | | | |
| C | 2.32777100 | -1.44286600 | 0.98872900 | | | | |
| H | 2.99468900 | -2.12343800 | 1.53072300 | | | | |
| C | -3.21442500 | 0.15263700 | 1.07184400 | | | | |
| C | -2.87207300 | 1.51250200 | 0.86650400 | | | | |
| C | -4.37150600 | -0.37167700 | 0.51088100 | | | | |
| C | -3.75095400 | 2.28335700 | 0.07432700 | | | | |
| C | -5.20595300 | 0.40560600 | -0.26974300 | | | | |
| H | -4.63378200 | -1.41154900 | 0.68874300 | | | | |
| C | -4.88626700 | 1.74267100 | -0.48620000 | | | | |

| | | | |
|---|------------|-------------|-------------|
| N | 1.53416100 | 1.73626700 | 0.45488100 |
| C | 2.64066900 | 1.64901300 | -0.52338900 |
| H | 2.19102700 | 1.67860600 | -1.52204700 |
| C | 3.48721700 | 0.42864000 | -0.30689500 |
| C | 2.95179500 | -0.86983400 | -0.13148500 |
| C | 4.86920800 | 0.59699400 | -0.30697000 |
| C | 3.85820700 | -1.93881200 | 0.02523000 |
| C | 5.73529500 | -0.46603700 | -0.15856800 |
| H | 5.28265700 | 1.59302600 | -0.42897200 |
| C | 5.21829800 | -1.74677200 | 0.00688500 |
| H | 3.43896700 | -2.93045400 | 0.15901900 |
| H | 5.88873200 | -2.59163800 | 0.12928100 |
| O | 1.67068100 | -1.16393800 | -0.10866500 |
| S | 7.51212200 | -0.22861400 | -0.17229900 |
| O | 8.01870300 | -1.02039100 | -1.33029200 |
| O | 8.00670700 | -0.75664100 | 1.13187000 |
| O | 7.73225700 | 1.23613500 | -0.32807400 |
| H | 3.27149500 | 2.53930100 | -0.42305100 |
| H | 1.91698300 | 1.56388200 | 1.38266000 |

54

RS_lambda_ID2_TS1_chain_P (2), E(SCF) = -2484.17026088, E(ZPE) = -2483.770278, E(G) = -2483.839711 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.05711400 | 0.89806000 | 1.63969100 |
| H | -0.21085900 | 0.31578000 | 2.52385900 |
| H | 0.29542700 | 1.91582900 | 1.95798500 |
| C | -1.08066200 | 0.87387300 | 0.65617100 |
| H | -2.00090100 | 1.24825600 | 1.11713700 |
| H | -0.86702900 | 1.49474700 | -0.21921200 |
| N | -1.25927800 | -0.51976000 | 0.19287300 |
| C | -2.30392000 | -0.64497400 | -0.85749300 |
| H | -2.19999000 | -1.63723900 | -1.29783300 |
| C | -3.68676500 | -0.45129600 | -0.32733900 |
| C | -4.26033600 | -1.48743800 | 0.46173200 |
| C | -4.39641900 | 0.71016700 | -0.59473800 |
| C | -5.57570000 | -1.26760900 | 0.93834800 |
| C | -5.67892900 | 0.89303000 | -0.10859300 |
| H | -3.94249700 | 1.49270700 | -1.19699100 |
| C | -6.26539400 | -0.10992300 | 0.65968300 |
| H | -6.03000100 | -2.05022100 | 1.53827300 |
| H | -7.27294200 | 0.02631500 | 1.04222100 |
| O | -3.61322800 | -2.57169600 | 0.75102100 |
| S | -6.60924300 | 2.37624100 | -0.47763700 |
| O | -7.76762800 | 1.94800900 | -1.31735800 |
| O | -5.67476900 | 3.28242900 | -1.20438400 |
| O | -7.04752500 | 2.93059400 | 0.83730700 |
| H | -2.06707000 | 0.08605900 | -1.63513200 |
| H | -1.53244100 | -1.08185900 | 1.01105300 |
| O | 0.06021500 | -2.61678400 | -1.67966400 |
| H | -0.54305600 | -3.26163400 | -1.21311900 |
| H | -2.63722300 | -2.28121800 | 2.16608900 |
| O | -1.90529700 | -1.92366600 | 2.72008200 |
| H | -2.33158500 | -1.42051900 | 3.41795200 |
| H | 0.85681900 | -3.09147600 | -1.94620800 |
| H | -2.42358700 | -3.49447900 | 0.01758800 |
| O | -1.69337100 | -4.06352900 | -0.34352600 |
| H | -1.37441100 | -4.58600500 | 0.39613900 |
| Pd | 0.64480200 | -1.15588800 | -0.29330900 |
| N | 1.25670000 | 0.25095000 | 1.04142400 |
| C | 2.19475200 | 1.14886800 | 0.33294400 |
| H | 1.67657900 | 1.52856000 | -0.55465100 |
| C | 3.48528400 | 0.46007700 | -0.00843800 |
| C | 3.55482800 | -0.84752100 | -0.54853600 |
| C | 4.66386200 | 1.17378400 | 0.19348500 |
| C | 4.83076500 | -1.35096900 | -0.88209700 |
| C | 5.89802400 | 0.65762600 | -0.14167200 |
| H | 4.61646600 | 2.17075500 | 0.12099900 |
| C | 5.97659100 | -0.62012800 | -0.68660500 |
| H | 4.87514900 | -2.35062100 | -1.30050200 |
| H | 6.94149100 | -1.03967500 | -0.95360900 |
| O | 2.53300100 | -1.64352200 | -0.76668400 |
| S | 7.40334000 | 1.58343300 | 0.15730700 |
| O | 8.10670200 | 1.65641400 | -1.15560400 |
| O | 8.17301500 | 0.79894800 | 1.16634200 |
| O | 6.97378100 | 2.91651000 | 0.66375000 |
| H | 2.40902700 | 2.00981500 | 0.97515400 |

| | | | |
|---|------------|-------------|------------|
| H | 1.77652900 | -0.21957500 | 1.78073500 |
|---|------------|-------------|------------|

54

RS_lambda_ID2_TS1_chain_P, E(SCF) = -2484.16702633, E(ZPE) = -2483.767552, E(G) = -2483.838661 a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | 0.02366000 | -1.06814700 | -1.98164000 |
| H | 0.18217000 | -2.08975000 | -1.63027900 |
| H | -0.28829500 | -1.11757400 | -3.02517900 |
| C | 1.28982100 | -0.23508600 | -1.85438900 |
| H | 2.18739300 | -0.85970700 | -1.92409600 |
| H | 1.33668900 | 0.51332800 | -2.64860200 |
| N | 1.26963000 | 0.49459600 | -0.57406300 |
| C | 2.51822600 | 1.24760500 | -0.29438600 |
| H | 2.26248300 | 2.06984300 | 0.37768100 |
| C | 3.54181400 | 0.34909100 | 0.32589800 |
| C | 3.19022800 | -0.32030900 | 1.53187500 |
| C | 4.78448000 | 0.15489200 | -0.25443600 |
| C | 4.16634200 | -1.16792500 | -2.10001700 |
| C | 5.72059800 | -0.67999100 | 0.33276100 |
| H | 5.03575400 | 0.66546600 | -1.17985600 |
| C | 5.40173400 | -1.34108900 | 1.51534400 |
| H | 3.91272700 | -1.68604800 | 3.01768000 |
| H | 6.13247700 | -1.99953300 | 1.97595100 |
| O | 2.01417300 | -0.16767500 | 2.07097300 |
| S | 7.33412200 | -0.92736300 | -0.40292400 |
| O | 7.45535500 | -2.39380000 | -0.65497200 |
| O | 8.32755900 | -0.44879100 | 0.60337100 |
| O | 7.34732200 | -0.12209200 | -1.65698500 |
| H | 2.87374900 | 1.68712100 | -1.22918900 |
| H | 1.18082700 | -0.16605100 | 0.20360600 |
| O | -0.06583800 | 3.24538400 | 0.34046300 |
| H | 0.30763800 | 3.01203700 | 1.23335800 |
| H | 0.63707200 | -1.23304900 | 1.76265700 |
| O | -0.14023800 | -1.64903100 | 1.32525000 |
| H | -0.06185200 | -2.59136700 | 1.48969300 |
| H | -0.90785800 | 3.69308800 | 0.49305800 |
| H | 1.41147600 | 1.38039200 | 2.41862900 |
| O | 1.08589200 | 2.30883500 | 2.55286900 |
| H | 0.64478400 | 2.32468700 | 3.40512300 |
| Pd | -0.58945700 | 1.38229800 | -0.51211200 |
| N | -1.08173900 | -0.47338300 | -1.17773200 |
| C | -2.40438700 | -0.48689100 | -1.83980700 |
| H | -2.31628500 | 0.16246300 | -2.71746800 |
| C | -3.49985200 | -0.03720200 | -0.92681800 |
| C | -3.47383300 | 1.25356900 | -0.34770200 |
| C | -4.57873700 | -0.87687600 | -0.68389200 |
| C | -4.58370100 | 1.65457300 | 0.41807600 |
| C | -5.64992300 | -0.46735600 | 0.08780000 |
| H | -4.59100300 | -1.87301600 | -1.11501600 |
| C | -5.65269800 | 0.81327800 | 0.62954700 |
| H | -4.56640700 | 2.64946700 | 0.84968500 |
| H | -6.49250500 | 1.14456200 | 1.23247100 |
| O | -2.47877600 | 2.09847100 | -0.51150400 |
| S | -7.05144700 | -1.54925800 | 0.37574000 |
| O | -6.68592800 | -2.86514700 | -0.21882700 |
| O | -8.21153500 | -0.90552100 | -0.30617600 |
| O | -7.22660300 | -1.60729500 | 1.85530800 |
| H | -2.61341500 | -1.50164200 | -2.19461600 |
| H | -1.12432000 | -0.99250500 | -0.29025900 |

54

RS_lambda_ID2_TS1_chain_R (2), E(SCF) = -2484.18028011, E(ZPE) = -2483.782121, E(G) = -2483.851974 a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.48202000 | 3.24387200 | 0.04442600 |
| H | 0.00828100 | 3.63915700 | 0.94572000 |
| H | 1.15245100 | 4.01236300 | -0.35009700 |
| C | -0.57374700 | 2.86325200 | -0.96298100 |
| H | -1.19827200 | 3.72430700 | -1.22035500 |
| H | -0.12321800 | 2.49177500 | -1.88794100 |
| N | -1.38773600 | 1.77320300 | -0.39035200 |
| C | -2.29789300 | 1.12616100 | -1.35418100 |
| H | -1.66839200 | 0.65635800 | -2.11870600 |
| C | -3.17926300 | 0.13394900 | -0.66630000 |
| C | -2.61584500 | -0.94293000 | 0.05417200 |
| C | -4.55933300 | 0.27252900 | -0.73186800 |

C -3.49321600 -1.86081200 0.65887400
C -5.40224800 -0.63634900 -0.11944600
H -4.98935000 -1.10848900 -1.27460200
C -4.85986500 -1.71387100 0.57150700
H -3.05794400 -2.69024100 1.20577700
H -5.51474800 -2.43254000 1.05412200
O -1.31785600 -1.13652800 0.17389700
S -7.18520700 -0.46902500 -0.23024500
O -7.65542200 -1.65021200 -1.00987900
O -7.43565600 0.82366100 -0.92580200
O -7.68545400 -0.48189600 1.17420300
H -2.90847600 1.89070900 -1.84761100
H -1.93950700 2.10758200 0.41306200
O 2.14577500 -1.68326600 -2.27360500
H 1.59526800 -2.19549000 -1.65213900
H -2.36728000 1.30386700 2.59449500
O -2.87095900 1.97675300 2.12514300
H -3.71165600 1.55045100 1.92534200
H 2.71282400 -1.15447400 -1.17010300
H -0.27369000 -2.60078100 -0.32485400
O 0.59809800 -3.03642400 -0.29729500
H 1.02532400 -2.48281100 0.38121000
Pd -0.03419100 0.44120700 0.37232300
N 1.25126900 2.03793900 0.45143400
C 2.39065800 1.70866600 -0.42373900
H 1.98143300 1.48723500 -1.41691200
C 3.22726300 0.56888200 0.08927500
C 2.70864200 -0.56711800 0.75948800
C 4.59374200 0.62742800 -0.18476200
C 3.62082600 -1.58271100 1.12440100
C 5.45609000 -0.38844500 0.16570300
H 4.99620000 1.49795800 -0.69387300
C 4.95915800 -1.50599000 0.82943100
H 3.21829100 -2.44656300 1.64379000
H 5.62832200 -2.31057600 1.11721400
O 1.44631000 -0.77323400 1.06870900
S 7.20532800 -0.30262200 -0.22184800
O 7.47187200 -1.44627100 -1.14040600
O 7.91688300 -0.44390800 1.08054900
O 7.42094300 1.02321800 -0.86392000
H 3.02464000 2.59623400 -0.53018400
H 1.59741200 2.16863800 1.39986300

54
RS_lambda_ID2_Ts1_chain_R, E(SCF) = -
2484.18033756, E(ZPE) = -2483.782165, E(G)
= -2483.852533 a.u.
C 0.48668300 3.24219900 -0.01156500
H 0.01615400 3.65364400 0.88448500
H 1.15660400 4.00281100 -0.42194400
C -0.57375000 2.84482700 -1.00744200
H -1.19758700 3.70233100 -1.27863900
H -0.12813900 2.45490000 -1.92727700
N -1.38778500 1.76887800 -0.40899100
C -2.30681400 1.10902300 -1.35469200
H -1.68434700 0.62863400 -2.11860400
C -3.18423400 0.12521200 -0.64941600
C -2.61860800 -0.94141900 0.08433600
C -4.56482700 0.25436400 -0.72338900
C -3.49393500 -1.85845700 0.69345100
C -5.40567700 -0.65399500 -0.10776100
H -4.99691200 1.08172500 -1.27755300
C -4.86080100 -1.72152600 0.59652900
H -3.05649000 -2.68037100 1.24994700
H -5.51382200 -2.44036600 1.08146400
O -1.32040800 -1.13088400 0.20953800
S -7.18869000 -0.50084400 -0.23310300
O -7.70031500 -0.50944000 1.16735100
O -7.64446800 -1.69000200 -1.00943100
O -7.44412300 0.78578900 -0.93822500
H -2.92083800 1.86720200 -1.85384500
H -1.93057900 2.12529700 0.39168500
O 2.14997700 -1.72600300 -2.25296200
H 1.59392700 -2.22804600 -1.62550400
H -2.34404100 1.68349600 2.70934600
O -2.83640600 2.22468300 2.08451400
H -3.68479700 1.77875400 1.99324500

H 2.71423900 -1.18758700 -1.68668100
H -0.27729200 -2.59500300 -0.28711900
O 0.59230400 -3.03531100 -0.25865900
H 1.02416400 -2.47877700 0.41431800
Pd -0.03411400 0.44736200 0.36983400
N 1.25562900 2.04242900 0.41410900
C 2.39098300 1.69412800 -0.45890200
H 1.97774800 1.45338900 -1.44580400
C 3.22763200 0.56355900 0.07474600
C 2.70854300 -0.55875300 0.76733100
C 4.59412900 0.61575500 -0.20067600
C 3.62013500 -1.56795800 1.15122100
C 5.45611500 -0.39333400 0.17002200
H 4.99707700 1.47586500 -0.72679500
C 4.95841900 -1.49787700 0.85470800
H 3.21689000 -2.42135500 1.68707100
H 5.62699900 -2.29736000 1.15774400
O 1.44663900 -0.75800300 1.08171400
S 7.20487700 -0.31720600 -0.20067600
O 7.42402500 1.00246300 -0.87522100
O 7.46572000 -1.46942900 -1.13119500
O 7.91834200 -0.45021700 1.08058600
H 3.02609400 2.57813900 -0.58585000
H 1.60603400 2.19003600 1.35849200

54
RS_lambda_ID2_Ts1_chain, E(SCF) = -
2484.15303047, E(ZPE) = -2483.754148, E(G)
= -2483.820209 a.u.
C 0.76815800 3.00020100 0.49813500
H 0.47666300 3.17934600 1.53513800
H 1.40739100 3.82652200 0.17853000
C -0.46845700 2.89201600 -0.35918500
H -1.09731700 3.78248700 -0.25382000
H -0.21538600 2.78007900 -1.41741000
N -1.19406300 1.68144700 0.06971400
C -2.41184100 1.39879800 -0.70125900
H -2.08117200 1.06248000 -1.69158400
C -3.35280000 0.39478800 -0.08950700
C -2.94467900 -0.71274600 0.70578700
C -4.69524600 0.53830200 -0.42372600
C -3.94893400 -1.64267800 1.06897500
C -5.65130700 -0.38236300 -0.04037800
H -5.00836100 1.39372600 -1.01556800
C -5.26651400 -1.48960500 0.70857600
H -3.63474000 -2.49552600 1.66349500
H -6.00597400 -2.22484900 1.01169800
O -1.72454800 -0.89332100 1.12825000
S -7.37595100 -0.16451100 -0.46720500
O -8.11362600 -0.07623500 0.82752900
O -7.76593200 -1.37222200 -1.25251300
O -7.45419200 1.09266800 -1.26376100
H -2.95017200 2.34358000 -0.85036000
H -1.41491700 1.75258100 1.07376000
O -0.83485000 -1.22253900 -1.58649000
H -0.77328900 -2.05968400 -1.07734100
H -1.44667600 0.26123400 2.44136000
O -1.31440200 1.12200300 2.89955900
H -2.03170000 1.19495300 3.53313200
H -0.19199500 -1.31415600 -2.29733800
H -0.89113200 -2.43930800 0.86454000
O -0.33896700 -3.10501100 0.39581200
H 0.54400900 -2.69811200 0.38292900
Pd 0.21667200 0.21016000 -0.04912100
N 1.52498900 1.71917800 0.47156800
C 2.63966300 1.65295500 -0.49905500
H 2.19763200 1.69290100 -1.50072900
C 3.49356600 0.43608500 -0.29239000
C 2.96686700 -0.86835300 -0.13552300
C 4.87419200 0.61484800 -0.28342600
C 3.88069900 -1.93218600 0.01316900
C 5.74767900 -0.44328700 -0.14379800
H 5.28051400 1.61541900 -0.39128900
C 5.23941000 -1.72970600 0.00388500
H 3.46843100 -2.92852500 0.13291000
H 5.91564600 -2.57096200 0.11923600
O 1.68795900 -1.17232100 -0.12282700

S 7.52260300 -0.19162700 -0.14698500
O 7.73127500 1.27621200 -0.28928800
O 8.04105700 -0.96939300 -1.30925500
O 8.01559000 -0.72659300 1.15500400
H 3.26288600 2.54642000 -0.38140900
H 1.90219100 1.53747700 1.39987200

56

RS_lambda_ID2_TS2-trigo_P, E(SCF) = -
2485.32763018, E(ZPE) = -2484.912577, E(G)
= -2484.985709 a.u.

C -0.07207800 -0.00881400 1.96495800
H 0.11613700 0.84901300 2.61357500
H -0.28086000 -0.87769000 2.59382600
C 1.11960100 -0.24027500 1.07880100
H 2.02071300 -0.39370900 1.68005800
H 0.99116400 -1.12166200 0.44270100
N 1.27700900 0.93947100 0.19774700
C 2.36113100 0.78779800 -0.81308600
H 2.47158500 1.77097200 -1.28161900
C 3.65629900 0.30050000 -0.24913500
C 4.38489800 1.13239600 0.64492300
C 4.12821900 -0.96071500 -0.58361100
C 5.60870100 0.61546900 1.13882000
C 5.32655000 -1.43508500 -0.08063800
H 3.55271000 -1.58853900 -1.25831500
C 6.06381900 -0.63443100 0.78917600
H 6.18078900 1.24243600 1.81582000
H 7.00615200 -1.00025500 1.18717600
O 3.95667100 2.29808800 0.99988200
S 5.93487600 -3.296360600 -0.50256600
O 5.97400500 -3.83777200 0.77375600
O 7.29894700 -2.86337100 -1.07513100
O 4.97051900 -3.62697100 -1.48999400
H 1.99624100 0.09086300 -1.57277500
H 1.48008400 1.75418200 0.79387300
O 0.46852400 4.28990300 -1.32516200
H 1.34625500 4.37580700 -0.89584000
H 2.61410900 2.74061900 2.04999100
O 1.70083300 3.01841200 2.28454200
H 1.61955600 3.86844000 1.83591600
H -0.16380000 4.60529900 -0.67430000
H 3.37755700 3.65629400 0.19825300
O 2.88538400 4.47843700 -0.04903900
H 3.53941200 5.12043100 -0.33239500
H -0.01382900 2.45921200 -1.77684100
H -0.12301700 1.74434000 -2.18111900
Pd -0.62586800 1.27073100 -0.56154100
N -1.26307700 0.32048100 1.13733600
C -2.07519200 -0.83306700 0.69307100
H -1.46449400 -1.41628800 -0.00559000
C -3.37968300 -0.40204900 0.09051300
C -3.49899600 0.68864800 -0.80209000
C -4.51398000 -1.14008100 0.41926900
C -4.77954200 0.97031200 -1.32420300
C -5.75237900 -0.84884800 -0.11140400
H -4.42545200 -1.97155200 1.11143000
C -5.88137400 0.22189500 -0.99065100
H -4.86373900 1.80899900 -2.00653800
H -6.85182300 0.46721500 -1.41070300
O -2.52333400 1.47957600 -1.19303300
S -7.20564600 -1.79953100 0.33538100
O -8.12403200 -0.84349600 1.01901000
O -6.72858900 -2.88869500 1.23202500
O -7.77081300 -2.30537000 -0.94850000
H -2.27339500 -1.47219700 1.55959000
H -1.86819200 0.95284200 1.65894600

54

RS_lambda_ID2_TS2-trigo_R_noH2, E(SCF) = -
2484.17029036, E(ZPE) = -2483.770079, E(G)
= -2483.838439 a.u.

C -0.05910900 -0.86353200 1.67374500
H 0.20741100 -0.27169300 2.55168900
H -0.29910600 -1.87759800 2.00231400
C 1.08248600 -0.85245000 0.69408400
H 2.00206600 -1.21552000 1.16492200

H 0.87459800 -1.48882800 -0.17169200
N 1.25896800 0.53296300 0.20611300
C 2.31124500 0.64554800 -0.83741900
H 2.21923200 1.63896600 -1.27873600
C 3.68905200 0.44192200 -0.29727900
C 4.25687100 1.46631900 0.51089400
C 4.40090500 -0.71473400 -0.57784800
C 5.56787200 1.23884000 0.99531900
C 5.68046800 -0.90444800 -0.08602100
H 3.95126200 -1.48787100 -1.19528300
C 6.26062600 0.08630700 0.70264600
H 6.01740600 2.01177700 1.61115700
H 7.26537000 -0.05502700 1.09059500
O 3.60888100 2.54928600 0.80488700
S 6.62088200 -2.37176900 -0.49161700
O 7.09922700 -2.93350400 0.80595800
O 7.75213200 -1.91917100 -1.35568700
O 5.68122500 -3.28294500 -1.20535700
H 2.07386100 -0.08577800 -1.01467400
H 1.51631600 1.11695800 1.01439300
O -0.05454000 2.57697200 -1.72588200
H 0.57115500 3.21375100 -1.27923500
H 2.58749000 2.29929100 2.19868700
O 1.87973800 1.89629900 2.75259100
H 1.30493400 2.62124100 3.00941900
H -0.84724400 3.06536900 -1.97887500
H 2.43619100 3.43872400 0.42787200
O 1.68891400 3.98360700 -0.33895100
H 2.08200700 4.79107100 -0.67717100
Pd -0.64352700 1.15120500 -0.30377800
N -1.25735500 -0.22376800 1.06362000
C -2.19831400 -1.13353300 0.37489100
H -1.68041100 -1.53321100 -0.50413700
C -3.48744900 -0.45065100 0.01748400
C -3.55386300 0.84314800 -0.55523900
C -4.66743400 -1.15761100 0.23426600
C -4.82830500 1.33998800 -0.90330900
C -5.90086700 -0.64668100 -0.11196300
H -4.62111800 -2.14232000 0.68904800
C -5.97533400 0.61446500 -0.69514900
H -4.87066300 2.32924200 -1.34592000
H -6.93850100 1.03032800 -0.97361000
O -2.53022400 1.63194700 -0.78947800
S -7.40375400 -1.58778000 0.15033100
O -8.32237800 -0.68860300 0.90623800
O -7.00551700 -2.79731300 0.92290600
O -7.92493500 -1.91250100 -1.20946700
H -2.41427900 -1.98009500 1.03533400
H -1.77434900 0.26425900 1.79345200

56

RS_lambda_ID2_TS2-trigo_R, E(SCF) = -
2485.34433995, E(ZPE) = -2484.927884, E(G)
= -2484.997354 a.u.

C -0.04728100 -0.79185900 1.74881300
H 0.22783200 -0.17686700 2.60813000
H -0.28610900 -1.79619800 2.10700900
C 1.08673600 -0.80978200 0.76021000
H 2.00879900 -1.16167600 1.23457600
H 0.87362800 -1.47048900 -0.08607500
N 1.26259100 0.56155500 0.23451100
C 2.29996700 0.64513400 -0.82655200
H 2.21029300 1.63141900 -1.28450100
C 3.68419200 0.43953100 -0.30414600
C 4.27910100 1.47857100 0.46494500
C 4.37581700 -0.73437300 -0.56379200
C 5.59724400 1.24872900 0.92923400
C 5.66184500 -0.92640000 -0.09085000
H 3.90535500 -1.51874600 -1.15083000
C 6.26940800 0.07918300 0.65739100
H 6.06843400 2.03328700 1.51336700
H 7.28010300 -0.06442300 1.02882700
O 3.64973100 2.57677400 0.74236700
S 6.57103900 -2.42377000 -0.45375700
O 7.00808800 -2.97529200 0.86277400
O 7.73093500 -2.01541900 -1.30120100
O 5.62225700 -3.32271300 -1.17094300

| | | | |
|----|-------------|-------------|-------------|
| H | 2.04405500 | -0.09829100 | -1.58656100 |
| H | 1.53460500 | 1.16218300 | 1.02526800 |
| O | -0.06210600 | 2.56917500 | -1.72773200 |
| H | 0.57711100 | 3.21124900 | -1.30873500 |
| H | 2.64323100 | 2.36732300 | 2.15555900 |
| O | 1.94065000 | 1.98498800 | 2.73016300 |
| H | 1.37656700 | 2.72163300 | 2.97726000 |
| H | -0.85347300 | 3.05933300 | -1.98161500 |
| H | 2.46621100 | 3.45535100 | -0.03340300 |
| O | 1.71392100 | 3.99341900 | -0.39995700 |
| H | 2.10100900 | 4.79758300 | -0.75257300 |
| H | -0.42877600 | -0.29501700 | -2.81305800 |
| H | -0.31360100 | -1.02939500 | -2.71355500 |
| Pd | -0.64290500 | 1.18211100 | -0.26272100 |
| N | -1.24995100 | -0.16691200 | 1.13242100 |
| C | -2.18616500 | -1.09357000 | 0.46172100 |
| H | -1.66288000 | -1.51502900 | -0.40365300 |
| C | -3.47561300 | -0.42598800 | 0.07574700 |
| C | -3.54915000 | 0.86151900 | -0.51010300 |
| C | -4.65012600 | -1.14689300 | 0.27739900 |
| C | -4.82431500 | 1.33844200 | -0.88318800 |
| C | -5.88383900 | -0.65612800 | -0.09507700 |
| H | -4.59878800 | -2.12720400 | 0.74113100 |
| C | -5.96517500 | 0.59991800 | -0.68838200 |
| H | -4.87196500 | 2.32362900 | -1.33423000 |
| H | -6.92887200 | 1.00074300 | -0.98636700 |
| O | -2.53334400 | 1.66394800 | -0.73286600 |
| S | -7.37896200 | -1.61365800 | 0.15144600 |
| O | -8.31333500 | -0.72589400 | 0.90158600 |
| O | -6.97505900 | -2.82097200 | 0.92451900 |
| O | -7.88493200 | -1.94000200 | -1.21366000 |
| H | -2.40432700 | -1.92352400 | 1.14223400 |
| H | -1.76684900 | 0.33205800 | 1.85478400 |

56

| | | | |
|--|-------------|-------------|-------------|
| RS_lambda_ID2_TS2-trigo, E(SCF) = - | | | |
| 2485.32076414, E(ZPE) = -2484.906105, E(G) | | | |
| = -2484.974593 a.u. | | | |
| C | -0.01870200 | -0.04931700 | 1.91879500 |
| H | 0.21056800 | 0.80336300 | 2.56094000 |
| H | -0.22668800 | -0.91663700 | 2.55019400 |
| C | 1.14272400 | -0.30204000 | 0.99728200 |
| H | 2.05890000 | -0.46595400 | 1.57350900 |
| H | 0.98401200 | -1.18156200 | 0.36546000 |
| N | 1.28777800 | 0.87498300 | 0.11254300 |
| C | 2.36676700 | 0.73635200 | -0.90118500 |
| H | 2.41473000 | 1.70036200 | -1.41788700 |
| C | 3.68863600 | 0.35405100 | -0.31925000 |
| C | 4.34334500 | 1.25351100 | 0.56581600 |
| C | 4.24553000 | -0.88186400 | -0.61214900 |
| C | 5.58614600 | 0.82774100 | 1.09695000 |
| C | 5.46168600 | -1.26637300 | -0.07574100 |
| H | 3.72306500 | -1.56224400 | -1.27876000 |
| C | 6.12628200 | -0.39996000 | 0.78979500 |
| H | 6.10262800 | 1.50451200 | 1.77066800 |
| H | 7.08009700 | -0.69496800 | 1.21773300 |
| O | 3.82888400 | 2.39603600 | 0.88279700 |
| S | 6.17299700 | -2.86768100 | -0.43610200 |
| O | 6.20846800 | -3.60958600 | 0.85942200 |
| O | 7.54360700 | -2.60630200 | -0.96675400 |
| O | 5.27567800 | -3.50576500 | -1.44140100 |
| H | 2.03947700 | -0.01830300 | -1.62181300 |
| H | 1.49976400 | 1.68459700 | 0.71021600 |
| O | -0.11475500 | 3.65630000 | -0.95473700 |
| H | 0.76862400 | 3.97837400 | -0.67272200 |
| H | 2.53666200 | 2.69653600 | 2.06024100 |
| O | 1.61975200 | 2.87436700 | 2.36381200 |
| H | 1.41747900 | 3.71908500 | 1.94524100 |
| H | -0.75567200 | 4.22313800 | -0.51860400 |
| H | 3.01519700 | 3.65259200 | 0.10530400 |
| O | 2.38311300 | 4.38446700 | -0.10432300 |
| H | 2.88305000 | 5.06686900 | -0.55651900 |
| H | -0.16747000 | 1.94163700 | -2.37958300 |
| H | -0.08100300 | 1.17466900 | -2.49348400 |
| Pd | -0.62052300 | 1.21801500 | -0.61119800 |
| N | -1.22797000 | 0.30749700 | 1.12921700 |
| C | -2.09086200 | -0.83021900 | 0.75279900 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.50639300 | -1.47783700 | 0.09023800 |
| C | -3.38551100 | -0.39886600 | 0.12760500 |
| C | -3.49958100 | 0.67756300 | -0.78342900 |
| C | -4.52136400 | -1.13785700 | 0.45052500 |
| C | -4.77550400 | 0.94289200 | -1.32680800 |
| C | -5.75426100 | -0.86332100 | -0.10117400 |
| H | -4.43753600 | -1.95917800 | -1.15538200 |
| C | -5.87805200 | 0.19458300 | -0.99667800 |
| H | -4.85497000 | 1.77099000 | -2.02253800 |
| H | -6.84378000 | 0.42811100 | -1.43392300 |
| O | -2.52716900 | 1.47351100 | -1.16797000 |
| S | -7.20765100 | -1.81446400 | 0.34358900 |
| O | -8.12844600 | -0.85893800 | 1.02505500 |
| O | -6.73210500 | -2.90283900 | 1.24215500 |
| O | -7.77024800 | -2.32174900 | -0.94091900 |
| H | -2.31000100 | -1.40889400 | 1.65721000 |
| H | -1.78877600 | 0.97173300 | 1.66046200 |

56

| | | | |
|--|-------------|-------------|-------------|
| RS_lambda_ID2_TS3-trigo_P, E(SCF) = - | | | |
| 2485.35829832, E(ZPE) = -2484.941043, E(G) | | | |
| = -2485.011888 a.u. | | | |
| C | -0.06798300 | -0.49458700 | 1.73336100 |
| H | 0.15493600 | 0.17926400 | 2.56393100 |
| H | -0.22053100 | -1.49690700 | 2.14932100 |
| C | 1.10431700 | -0.50088500 | 0.78151500 |
| H | 2.01089500 | -0.79756300 | 1.32050100 |
| H | 0.95553800 | -1.21489600 | -0.03495800 |
| N | 1.26928800 | 0.84434100 | 0.17990500 |
| C | 2.36894900 | 0.90146900 | -0.81858000 |
| H | 2.41329400 | 1.93151400 | -1.17588100 |
| C | 3.69566300 | 0.43144100 | -0.29506300 |
| C | 4.48928000 | 1.22452800 | 0.53842800 |
| C | 4.14294600 | -0.85108600 | -0.60360300 |
| C | 5.66974200 | 0.71739600 | 1.07455200 |
| C | 5.32087300 | -1.34590100 | -0.08186400 |
| H | 3.54780500 | -1.48157900 | -1.25689500 |
| C | 6.08536400 | -0.56130900 | 0.77048900 |
| H | 6.25616400 | 1.35777600 | 1.72318800 |
| H | 7.00913400 | -0.94963200 | 1.18610300 |
| O | 4.14322000 | 2.48586300 | 0.90748000 |
| S | 5.89604100 | -3.00038400 | -0.49939000 |
| O | 6.07716300 | -3.69767300 | 0.80363900 |
| O | 7.18039500 | -2.80098300 | -1.22680600 |
| O | 4.83057300 | -3.60181000 | -1.34508700 |
| H | 2.06624400 | 0.28146600 | -1.66565800 |
| H | 1.47356300 | 1.49349000 | 0.95158800 |
| O | 0.49190900 | 4.43009400 | -0.21185500 |
| H | 2.20159500 | 4.40915600 | -0.63978300 |
| H | 2.87300600 | 2.45266100 | 2.31133800 |
| O | 2.04092200 | 2.13408600 | 2.69990300 |
| H | 1.64947600 | 2.89375600 | 3.13781000 |
| H | 0.27496900 | 4.43529400 | 0.72505700 |
| H | 3.76165100 | 3.03024500 | 0.17335500 |
| O | 3.15961800 | 4.27166200 | -0.80291500 |
| H | 3.28404000 | 4.29832000 | -1.75444700 |
| H | 0.09592200 | 3.60596300 | -0.55495500 |
| H | -0.11148700 | 2.14137200 | -1.74360400 |
| Pd | -0.64097600 | 1.29721600 | -0.52782200 |
| N | -1.29075100 | 0.00231900 | 1.07888400 |
| C | -2.11193500 | -1.00592900 | 0.38951900 |
| H | -1.52931200 | -1.38343800 | -0.46036100 |
| C | -3.42784600 | -0.43399800 | -0.05351400 |
| C | -3.53898300 | 0.76388800 | -0.81130600 |
| C | -4.58021600 | -1.13980100 | 0.27908600 |
| C | -4.84121700 | 1.15906900 | -1.20067100 |
| C | -5.83692300 | -0.72742300 | -0.11614800 |
| H | -4.49220800 | -2.04646700 | 0.86979300 |
| C | -5.96078400 | 0.43582800 | -0.86989100 |
| H | -4.92490500 | 2.07009500 | -1.78412200 |
| H | -6.94170600 | 0.77558800 | -1.18864600 |
| O | -2.55319100 | 1.53236700 | -1.19443100 |
| S | -7.30324600 | -1.66338200 | 0.30503900 |
| O | -8.21038600 | -0.71327200 | 1.01342400 |
| O | -6.84821500 | -2.78650800 | 1.17254800 |
| O | -7.88139400 | -2.13012300 | -0.98972600 |
| H | -2.29606800 | -1.86044100 | 1.05305400 |

H -1.87399000 0.47202700 1.76490900

56
RS_lambda_ID2_TS3-trigo, E(SCF) = -
2485.32012581, E(ZPE) = -2484.907540, E(G)
= -2484.977515 a.u.

| | | | |
|----|-------------|-------------|--------------|
| C | -0.05888200 | -0.49535200 | 1.79862400 |
| H | 0.16317200 | 0.21591300 | 2.59781100 |
| H | -0.25238500 | -1.47072000 | 2.25394200 |
| C | 1.10940500 | -0.55529000 | 0.85128300 |
| H | 2.02022200 | -0.83949700 | 1.38764200 |
| H | 0.95068300 | -1.29005300 | 0.05527300 |
| N | 1.26906400 | 0.77349100 | 0.21961100 |
| C | 2.36168300 | 0.81429100 | -0.79121600 |
| H | 2.39773700 | 1.84138300 | -1.16179200 |
| C | 3.68889900 | 0.38387300 | -0.25512500 |
| C | 4.40911600 | 1.24851300 | 0.61392300 |
| C | 4.19805000 | -0.86513400 | -0.58460300 |
| C | 5.64915500 | 0.76961900 | 1.10342800 |
| C | 5.41217700 | -1.30190100 | -0.08775200 |
| H | 3.63300500 | -1.51610000 | -1.24605600 |
| C | 6.13592900 | -0.47160200 | 0.76530000 |
| H | 6.21184600 | 1.42144600 | 1.76454300 |
| H | 7.09074100 | -0.80738500 | 1.15979600 |
| O | 3.96749800 | 2.41908700 | 0.95352600 |
| S | 6.06809000 | -2.91200800 | -0.51137900 |
| O | 6.21221100 | -3.65321200 | 0.77649500 |
| O | 7.38743900 | -2.66590000 | -1.16519100 |
| O | 5.07561500 | -3.53881500 | -1.43024600 |
| H | 2.05287600 | 0.17115800 | -1.62015900 |
| H | 1.47014500 | 1.45582800 | 0.96538200 |
| O | 0.35630400 | 4.17395900 | -0.97333300 |
| H | 1.34400400 | 4.24130300 | -0.76623900 |
| H | 2.66205200 | 2.60121000 | 2.06166900 |
| O | 1.77175600 | 2.55568400 | 2.48424500 |
| H | 1.40594500 | 3.44080300 | 2.41352900 |
| H | -0.12991100 | 4.41931000 | -0.17669200 |
| H | 3.33487900 | 3.58306000 | 0.00769800 |
| O | 2.89053200 | 4.34373700 | -0.46267400 |
| H | 3.45775500 | 4.58705200 | -1.19760100 |
| H | 0.04138600 | 2.97370900 | -1.28310300 |
| H | -0.11810800 | 2.11262100 | -1.77348400 |
| Pd | -0.63613500 | 1.25459600 | -0.44143300 |
| N | -1.26669500 | 0.00150100 | 1.09653400 |
| C | -2.11895500 | -1.02682500 | 0.46662100 |
| H | -1.54787500 | -1.46691600 | -0.35940800 |
| C | -3.42897500 | -0.45459500 | 0.00883300 |
| C | -3.53527900 | 0.76427500 | -0.70745000 |
| C | -4.58204900 | -1.18223000 | 0.29081500 |
| C | -4.82713900 | 1.16619900 | -1.11571200 |
| C | -5.83040400 | -0.76574500 | -0.12217700 |
| H | -4.50114800 | -2.10663100 | 0.85426200 |
| C | -5.94715200 | 0.42266500 | -0.83677900 |
| H | -4.90374400 | 2.09730100 | -1.66695500 |
| H | -6.92308400 | 0.76575900 | -1.16617000 |
| O | -2.54587800 | 1.56136100 | -1.103348600 |
| S | -7.30209900 | -1.71954200 | 0.24306000 |
| O | -8.21931500 | -0.79379300 | 0.96914900 |
| O | -6.85676800 | -2.87043800 | 1.07755300 |
| O | -7.85614800 | -2.13966400 | -1.07710000 |
| H | -2.30880900 | -1.82813700 | 1.18926100 |
| H | -1.84105100 | 0.52541300 | 1.75327300 |

48
RR_W-inside_R, E(SCF) = -2331.30511471,
E(ZPE) = -2330.956236, E(G) = -2331.017637
a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.38165000 | 1.85961000 | 0.08571800 |
| N | -1.38157000 | 1.85960400 | -0.08535900 |
| C | 2.47534900 | 1.52644200 | 1.02075100 |
| H | 3.10554300 | 2.40933800 | 1.17374900 |
| C | -2.47517900 | 1.52640200 | -1.02047500 |
| H | -2.00124900 | 1.28639300 | -1.97886300 |
| C | 3.30737700 | 0.39712200 | 0.49929500 |
| C | 2.72627600 | -0.83386900 | 0.11441800 |
| C | 4.68660500 | 0.55622700 | 0.42708600 |
| C | 3.59211400 | -1.86278100 | -0.30772000 |

| | | | |
|----|-------------|-------------|-------------|
| C | 5.51335600 | -0.46881200 | 0.01227300 |
| H | 5.13034300 | 1.50387700 | 0.71594300 |
| C | 4.95525100 | -1.68846000 | -0.35563000 |
| H | 3.14426000 | -2.80659800 | -0.60213400 |
| H | 5.59572300 | -2.50059500 | -0.68538400 |
| C | -3.30729500 | 0.39710600 | -0.49909600 |
| C | -2.72627400 | -0.83388500 | -0.11406600 |
| C | -4.68653900 | 0.55620900 | -0.42724000 |
| C | -3.59225700 | -1.86282800 | 0.30772900 |
| C | -5.51341700 | -0.46884700 | -0.01271200 |
| H | -5.13017100 | 1.50388100 | -0.71618700 |
| C | -4.95540600 | -1.68851600 | 0.35525900 |
| H | -3.14449600 | -2.80665900 | 0.60223900 |
| H | -5.59596100 | -2.50068800 | 0.68476000 |
| O | 1.43774300 | -1.09194900 | 0.14730500 |
| O | -1.43774400 | -1.09196300 | -0.14646600 |
| S | 7.28925100 | -0.24609600 | -0.09245700 |
| S | -7.28931500 | -0.24605100 | 0.09170400 |
| O | -7.88617600 | -1.34177900 | -0.72477300 |
| O | -7.56783700 | 1.10939400 | -0.45932400 |
| O | 7.56787900 | 1.10949400 | 0.45815500 |
| O | 7.63259300 | -0.36804100 | -1.53898300 |
| O | 7.88619200 | -1.34161100 | 0.72424900 |
| H | 1.77680600 | 1.94716500 | -0.85193000 |
| H | 2.00151500 | 1.28651000 | 1.97920500 |
| H | -1.77679300 | 1.94718700 | 0.85226000 |
| H | -3.10534200 | 2.40929800 | -1.17359300 |
| Pd | 0.00002000 | 0.34689100 | 0.00027400 |
| C | -0.63426800 | 3.09605100 | -0.40768400 |
| C | 0.63435500 | 3.09606000 | 0.40802400 |
| H | 1.24446600 | 3.98135900 | 0.21114800 |
| H | 0.40557400 | 3.07196200 | 1.47728100 |
| H | -0.40548000 | 3.07191400 | -1.47693800 |
| H | -1.24438600 | 3.98135000 | -0.21084000 |
| O | 0.00008300 | -3.47561300 | 0.00081900 |
| H | -0.73032800 | -2.84392100 | -0.11038000 |
| H | 0.73024300 | -2.84354300 | 0.11168400 |

48
RR_W-inside_TS, E(SCF) = -2331.24736196,
E(ZPE) = -2330.900493, E(G) = -2330.962279
a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | 1.25034100 | 1.82803500 | -0.16004500 |
| N | -1.78431200 | 2.09658800 | -0.22545800 |
| C | 2.48727900 | 1.60543300 | 0.58933700 |
| H | 3.10423900 | 2.51236800 | 0.55929100 |
| C | -2.37070000 | 1.21907500 | -1.25916000 |
| H | -1.55415500 | 0.84004600 | -1.88273400 |
| C | 3.27826300 | 0.44822000 | 0.03653900 |
| C | 2.72581300 | -0.59731700 | -0.74488200 |
| C | 4.63712900 | 0.42520500 | 0.33835600 |
| C | 3.60059800 | -1.62020900 | -1.17404000 |
| C | 5.46661000 | -0.58799900 | -0.09229900 |
| H | 5.06076300 | 1.23056900 | 0.93109500 |
| C | 4.93846500 | -1.61722300 | -0.86574300 |
| H | 3.17123000 | -2.41775100 | -1.77063000 |
| H | 5.57965900 | -2.42008000 | -1.21602400 |
| C | -3.13913900 | 0.08760300 | -0.63085000 |
| C | -2.52767400 | -1.08826400 | -0.10957800 |
| C | -4.52108900 | 0.22480400 | -0.54191000 |
| C | -3.37852200 | -2.06677200 | 0.45029200 |
| C | -5.32671100 | -0.74802300 | 0.01740400 |
| H | -4.98737300 | 1.12204900 | -0.93911000 |
| C | -4.74265900 | -1.90733200 | 0.51435800 |
| H | -2.90899000 | -2.96513900 | 0.83715100 |
| H | -5.36077600 | -2.68383500 | 0.95431800 |
| O | 1.47325600 | -0.69512000 | -1.14949300 |
| O | -1.24154100 | -1.36234700 | -0.12979500 |
| S | 7.21705800 | -0.58669900 | 0.29602800 |
| S | -7.09968700 | -0.52233800 | 0.15043200 |
| O | -7.38955800 | -0.41193500 | 1.61019700 |
| O | -7.71559800 | -1.73749700 | -0.45652800 |
| O | -7.41621300 | 0.72614200 | -0.59793900 |
| O | 7.44578900 | 0.59454600 | 1.17390900 |
| O | 7.92498100 | -0.48485800 | -1.01294600 |
| O | 7.48324900 | -1.88368700 | 0.98250100 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.48186800 | 1.85601700 | -1.15411800 |
| H | 2.20496300 | 1.44443100 | 1.63669200 |
| H | -2.55030700 | 2.56118900 | 0.25426700 |
| H | -3.04163500 | 1.78004700 | -1.92360200 |
| Pd | 0.05691700 | 0.18914700 | -0.00043700 |
| C | -0.79884500 | 3.10070300 | -0.65459300 |
| C | 0.48270200 | 3.04657100 | 0.16447200 |
| H | 1.10346900 | 3.92640400 | -0.03846100 |
| H | 0.26088400 | 3.02896500 | 1.23455800 |
| H | -0.55808300 | 2.94591100 | -1.71272000 |
| H | -1.21208100 | 4.10985400 | -0.58068400 |
| O | -0.88045600 | 0.74412300 | 2.08719600 |
| H | -1.57091100 | 1.27084200 | 1.65206100 |
| H | -1.32145900 | -0.03221600 | 2.45090200 |

48

RR_W-inside, E(SCF) = -2331.25219152,
E(ZPE) = -2330.902981, E(G) = -2330.962377
a.u.

| | | | |
|----|-------------|-------------|-------------|
| N | 1.17830300 | 1.76969700 | -0.11925800 |
| N | -1.93402100 | 2.22805800 | -0.28714900 |
| C | 2.51331200 | 1.68624700 | 0.47832200 |
| H | 3.08615400 | 2.58719100 | 0.22253800 |
| C | -2.19642000 | 1.06460600 | -1.17760000 |
| H | -1.23261000 | 0.66538600 | -1.50739700 |
| C | 3.26541700 | 0.46959300 | 0.00376100 |
| C | 2.66577200 | -0.65219700 | -0.61852400 |
| C | 4.64319000 | 0.47945800 | 0.20124500 |
| C | 3.51171500 | -1.71033700 | -1.01242500 |
| C | 5.44499900 | -0.57249800 | -0.18673900 |
| H | 5.10485200 | 1.34181700 | 0.67362200 |
| C | 4.86974300 | -1.67466100 | -0.81106700 |
| H | 3.04379000 | -2.56447500 | -1.48979800 |
| H | 5.49040700 | -2.50691900 | -1.12768400 |
| C | -3.02708300 | -0.00529900 | -0.51425300 |
| C | -2.50346900 | -1.14492400 | 0.16988400 |
| C | -4.40764000 | 0.15110100 | -0.60032600 |
| C | -3.44149100 | -2.05092300 | 0.71489700 |
| C | -5.29660800 | -0.75728800 | -0.05935000 |
| H | -4.80281000 | 1.01056500 | -1.13612200 |
| C | -4.79996600 | -1.86966200 | 0.60896700 |
| H | -3.04118800 | -2.91797300 | 1.22981300 |
| H | -5.48443700 | -2.59612300 | 1.03486600 |
| O | 1.38015900 | -0.78829200 | -0.90448200 |
| O | -1.23617900 | -1.46331600 | 0.31159900 |
| S | 7.22080300 | -0.52671200 | 0.06020100 |
| S | -7.06252200 | -0.46895000 | -0.13239800 |
| O | -7.43727800 | 0.13205700 | 1.18211800 |
| O | -7.68853100 | -1.80549400 | -0.34263600 |
| O | -7.28264100 | 0.46471400 | -1.27269100 |
| O | 7.50249200 | 0.73209500 | 0.80428400 |
| O | 7.82173200 | -0.54215500 | -1.30476000 |
| O | 7.55643900 | -1.75281000 | 0.83942200 |
| H | 1.28536500 | 1.64845700 | -1.12779400 |
| H | 2.38644800 | 1.68537100 | 1.56711800 |
| H | -2.79275600 | 2.76288900 | -0.21599000 |
| H | -2.71060400 | 1.40581000 | -2.08482700 |
| Pd | 0.09783100 | 0.07925200 | 0.36754100 |
| C | -0.84339800 | 3.12119400 | -0.71574600 |
| C | 0.44641400 | 3.03096700 | 0.09597600 |
| H | 1.09392500 | 3.86383900 | -0.20288800 |
| H | 0.25481300 | 3.14464100 | 1.16566200 |
| H | -0.61202200 | 2.96268700 | -1.77778900 |
| H | -1.18596900 | 4.15415600 | -0.63331400 |
| O | -1.16583400 | 0.93012600 | 1.84666900 |
| H | -0.68522200 | 1.40661800 | 2.53205900 |
| H | -1.61060000 | 1.59913100 | 1.23272200 |

41

PdSS, E(SCF) = -2252.46131607, E(ZPE) = -
2252.186577, E(G) = -2252.243364 a.u.

| | | | |
|---|-------------|------------|-------------|
| N | -1.30842900 | 1.77758800 | -0.17445500 |
| N | 1.30843000 | 1.77758100 | 0.17444800 |
| C | -2.58277300 | 1.64011800 | -0.19335100 |
| H | -3.18593700 | 2.54643200 | -0.29318200 |
| C | 2.58277300 | 1.64009900 | 0.19341200 |
| C | -3.30715700 | 0.40971400 | -0.10257500 |

| | | | |
|----|-------------|-------------|-------------|
| C | -2.69594400 | -0.88427800 | -0.07417200 |
| C | -4.71250700 | 0.51256100 | -0.07160000 |
| C | -3.56888100 | -2.00308800 | -0.00180400 |
| C | -5.51395400 | -0.59108700 | -0.00084300 |
| H | -5.17000000 | 1.49654400 | -0.10364400 |
| C | -4.92665000 | -1.86475400 | 0.03305000 |
| H | -3.10758700 | -2.98394200 | 0.02134400 |
| H | -5.55996400 | -2.74483100 | 0.08710600 |
| C | 3.30715100 | 0.40969700 | 0.10258600 |
| C | 2.69593700 | -0.88429000 | 0.07409500 |
| C | 4.71250400 | 0.51253900 | 0.07164700 |
| C | 3.56887400 | -2.00309900 | 0.00168300 |
| C | 5.51395300 | -0.59110400 | 0.00086500 |
| H | 5.16999900 | 1.49651800 | 0.10378700 |
| C | 4.92664400 | -1.86476800 | -0.03313200 |
| H | 3.10757600 | -2.98394900 | -0.02155300 |
| H | 5.55995200 | -2.74484800 | -0.08721700 |
| O | -1.43016000 | -1.12814300 | -0.11636000 |
| O | 1.43015000 | -1.12815400 | 0.11623300 |
| S | -7.30129900 | -0.45221500 | 0.04052600 |
| S | 7.30130000 | -0.45221400 | -0.04041400 |
| O | 7.72395500 | -1.07717900 | -1.32613600 |
| O | 7.78940500 | -1.21074100 | -1.14617200 |
| O | 7.60188500 | 1.00351000 | 0.02974300 |
| O | -7.60192000 | 1.00351100 | -0.02948600 |
| O | -7.72385400 | -1.07730800 | 1.32622100 |
| O | -7.78945100 | -1.21076500 | -1.14608900 |
| H | 3.18594000 | 2.54640400 | 0.29330500 |
| Pd | 0.00000000 | 0.30435300 | -0.00005000 |
| C | 0.64970100 | 3.06729500 | 0.38696000 |
| C | -0.64969100 | -3.06728100 | -0.38707200 |
| H | -1.29731200 | 3.89282900 | -0.08120600 |
| H | -0.44319800 | 3.16735900 | -1.45729900 |
| H | 0.44319800 | 3.16744800 | 1.45717900 |
| H | 1.29733500 | 3.89281600 | 0.08105000 |

49

PdSS_D1_REF, E(SCF) = -2406.51489657,
E(ZPE) = -2406.175532, E(G) = -2406.241147
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.65133200 | 3.23622400 | 0.37159500 |
| H | 0.42435300 | 3.32352600 | 1.43849800 |
| H | 1.30319400 | 4.06503700 | 0.08568500 |
| C | -0.63112200 | 3.23827800 | -0.42776200 |
| H | -1.28337900 | 4.06495000 | -0.13654700 |
| H | -0.40526200 | 3.33199800 | -1.49427200 |
| N | -1.29676600 | 1.94987200 | -0.22237500 |
| N | 1.31847200 | 1.94942200 | 0.15994100 |
| C | -2.57047300 | 1.82121500 | -0.24290100 |
| H | -3.16565100 | 2.73208500 | -0.34568400 |
| C | 2.59192900 | 1.82063800 | 0.19212300 |
| C | -3.31025100 | 0.59693300 | -0.14723000 |
| C | -2.72141900 | -0.69922500 | -0.11409600 |
| C | -4.71263900 | 0.71595500 | -0.10397200 |
| C | -3.59245300 | -1.80884100 | -0.02148400 |
| C | -5.52394000 | -0.38075700 | -0.01565000 |
| H | -5.16037600 | 1.70394300 | -0.13939700 |
| C | -4.95146500 | -1.65740800 | 0.02581800 |
| H | -5.59191400 | -2.53088300 | 0.09488700 |
| C | 3.33241000 | 0.59704200 | 0.10010000 |
| C | 2.74399400 | -0.69880600 | 0.05746300 |
| C | 4.73547600 | 0.71564400 | 0.08062100 |
| C | 3.61665800 | -1.80891800 | -0.01601500 |
| C | 5.54795300 | -0.38113500 | 0.00727300 |
| H | 5.18303800 | 1.70343000 | 0.12316500 |
| C | 4.97600700 | -1.65811500 | -0.04018600 |
| H | 5.61738300 | -2.53194300 | -0.09526200 |
| O | -1.44404100 | -0.95032700 | -0.16559400 |
| O | 1.46642000 | -0.95062400 | 0.08797700 |
| S | -7.31248800 | -0.22242700 | 0.03467500 |
| S | 7.33671100 | -0.22157900 | -0.01955200 |
| O | 7.77228500 | -0.83128400 | -1.30724000 |
| O | 7.82039100 | -0.98416500 | 1.16504100 |
| O | 7.61645000 | 1.23684000 | 0.06465900 |
| O | -7.59413600 | 1.23632200 | -0.03422600 |
| O | -7.73172300 | -0.84335100 | 1.32227600 |
| O | -7.80942800 | -0.97571900 | -1.15039100 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.18578400 | 2.73116200 | 0.30512300 |
| Pd | 0.01226800 | 0.47764900 | -0.03592400 |
| H | -3.14013200 | -2.79505300 | 0.00283000 |
| H | 3.16387900 | -2.79482500 | -0.04671100 |
| H | -0.80753200 | -2.32113200 | 1.14462600 |
| H | -1.78803100 | 0.12182000 | 3.11592400 |
| H | -1.66285700 | -0.20397400 | 2.45238500 |
| O | -0.09948400 | -2.75194700 | 1.64614100 |
| H | 0.67744100 | -2.30969600 | 1.27141600 |
| H | -0.64856400 | -2.26111700 | -1.41230400 |
| O | 0.13644600 | -2.66510500 | -1.81155700 |
| H | 0.83734500 | -2.24963900 | -1.28764500 |

49

PdSS_D1_TS1_P, E(SCF) = -2406.47286044,
E(ZPE) = -2406.131550, E(G) = -2406.196903
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.58160200 | 3.13763600 | 0.09617800 |
| H | -0.32996600 | 3.51694700 | -0.89860400 |
| H | -1.20320400 | 3.87888400 | 0.60406900 |
| C | 0.66720400 | 2.83440300 | 0.87998700 |
| H | 1.36238100 | 3.67786600 | 0.86910600 |
| H | 0.39964500 | 2.62395300 | 1.92071000 |
| N | 1.31175300 | 1.62470600 | 0.34259500 |
| N | -1.30811200 | 1.88266100 | -0.07157900 |
| C | 2.57941400 | 1.48521800 | 0.51755900 |
| H | 3.10585200 | 2.38966000 | 0.84464600 |
| C | -2.58411900 | 1.78404200 | -0.03116500 |
| C | 3.41292800 | 0.32596000 | 0.37751500 |
| C | 2.96937100 | -1.00850000 | 0.67844600 |
| C | 4.77302900 | 0.56904800 | 0.10645200 |
| C | 3.95657600 | -2.03284300 | 0.57959600 |
| C | 5.67963200 | -0.45079900 | 0.01644100 |
| H | 5.10852100 | 1.58903800 | -0.05630400 |
| C | 5.25609700 | -1.76859000 | 0.25259000 |
| H | 3.63126000 | -3.04692700 | 0.78635800 |
| H | 5.97564400 | -2.57930300 | 0.18557700 |
| C | -3.35883100 | 0.61188300 | -0.29546400 |
| C | -2.81935300 | -0.58991800 | -0.83512300 |
| C | -4.74009700 | 0.69196700 | -0.02906500 |
| C | -3.71222300 | -1.66354900 | -1.05676100 |
| C | -5.57123600 | -0.36879300 | -0.25139300 |
| H | -5.15038800 | 1.61424100 | 0.36977300 |
| C | -5.04571600 | -1.55841200 | -0.77145100 |
| H | -3.29772000 | -2.57905500 | -1.46388000 |
| H | -5.70468200 | -2.40234500 | -0.94842800 |
| O | 1.77521800 | -1.28559200 | 1.03156200 |
| O | -1.57326500 | -0.78653100 | -1.15824400 |
| S | 7.40061300 | -0.14226000 | -0.37464900 |
| S | -7.32928700 | -0.27528300 | 0.10562800 |
| O | -7.58769900 | -1.35510800 | 1.09770300 |
| O | -8.01057900 | -0.51893400 | -1.19586300 |
| O | -7.56236200 | 1.09023300 | 0.64612400 |
| O | 7.53516900 | 1.33459800 | -0.50893700 |
| O | 7.66151500 | -0.87106800 | -1.64913400 |
| O | 8.18269500 | -0.70026000 | 0.76568200 |
| H | 0.34836400 | -2.50488300 | 0.83378400 |
| H | 1.02740800 | -0.63380900 | -1.51602300 |
| H | 1.09894700 | -0.96777100 | -0.77957300 |
| O | -0.57578500 | -2.81250000 | 0.77978700 |
| H | -0.93879800 | -2.33547400 | 0.01847100 |
| H | 0.43097500 | -0.51148200 | 2.18889500 |
| O | -0.44025700 | -0.52777200 | 2.62226400 |
| H | -0.84474700 | -1.29412500 | 2.18797400 |
| H | -3.14425000 | 2.68507400 | 0.23002300 |
| Pd | -0.07751300 | 0.40173000 | -0.51789000 |

49

PdSS_D1_TS1_R, E(SCF) = -2406.51414633,
E(ZPE) = -2406.174159, E(G) = -2406.240802
a.u.

| | | | |
|---|-------------|------------|-------------|
| C | -0.68710200 | 3.28623600 | -0.31687900 |
| H | -0.46363600 | 3.40005900 | -1.38209700 |
| H | -1.34131600 | 4.10580300 | -0.00997600 |
| C | 0.59835500 | 3.27585500 | 0.47882200 |
| H | 1.24803200 | 4.10942300 | 0.20153800 |
| H | 0.37454800 | 3.34942600 | 1.54734900 |

| | | | |
|----|-------------|-------------|-------------|
| N | 1.26604700 | 1.99299700 | 0.24911100 |
| N | -1.34764700 | 1.99258600 | -0.13296600 |
| C | 2.53979600 | 1.86638000 | 0.26045800 |
| H | 3.13528800 | 2.77582400 | 0.37414200 |
| C | -2.62151700 | 1.85798700 | -0.14817700 |
| C | 3.27890800 | 0.64298500 | 0.14450300 |
| C | 2.69034800 | -0.65358500 | 0.10566700 |
| C | 4.68097500 | 0.76358100 | 0.09638000 |
| C | 3.56359100 | -1.76140000 | 0.00072800 |
| C | 5.49348300 | -0.33126500 | -0.00392600 |
| H | 5.12751500 | 1.75193200 | 0.13707700 |
| C | 4.92226000 | -1.60826200 | -0.04978000 |
| H | 3.11314700 | -2.74848600 | -0.02195900 |
| H | 5.56328400 | -2.48061300 | -0.12727000 |
| C | -3.35109200 | 0.62728900 | -0.03039000 |
| C | -2.74842100 | -0.66535600 | -0.10586100 |
| C | -4.75494900 | 0.73218800 | -0.03637000 |
| C | -3.61424900 | -1.78536800 | -0.07125900 |
| C | -5.55700400 | -0.37362600 | 0.00076700 |
| H | -5.21122400 | 1.71707700 | -0.02623800 |
| C | -4.97334900 | -1.64720900 | -0.02283900 |
| H | -3.15360200 | -2.76758400 | -0.08373000 |
| H | -5.60675800 | -2.52828600 | 0.00372000 |
| O | 1.41381700 | -0.90816500 | 0.16127200 |
| O | -1.47449100 | -0.90230000 | -0.16574500 |
| S | 7.28154100 | -0.17096800 | -0.05782600 |
| S | -7.34590800 | -0.23021300 | 0.04110000 |
| O | -7.78176500 | -0.99808200 | 1.24083000 |
| O | -7.82362200 | -0.84147100 | -1.23133400 |
| O | -7.63593200 | 1.22578100 | 0.13701800 |
| O | 7.56213000 | 1.28806300 | 0.01075000 |
| O | 7.69928100 | -0.79131900 | -1.34626600 |
| O | 7.78190100 | -0.92383000 | 1.12618300 |
| H | 0.77338500 | -2.40991400 | -1.06936300 |
| H | 1.47646900 | 0.08536200 | -3.02965400 |
| H | 1.66741900 | -0.42396600 | -2.51476100 |
| O | 0.01308300 | -2.97653700 | -1.26981100 |
| H | -0.71748300 | -2.38953800 | -1.00255800 |
| O | 0.89561900 | -2.41538100 | 1.38710600 |
| O | 0.57692800 | -3.31298100 | 1.56519800 |
| H | 0.26070700 | -3.57293000 | 0.68674700 |
| H | -3.22216500 | 2.76792700 | -0.22473900 |
| Pd | -0.03758700 | 0.52090900 | 0.02807500 |

49

PdSS_D1_TS1, E(SCF) = -2406.47268424,
E(ZPE) = -2406.133243, E(G) = -2406.197578
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.59524400 | 3.18709800 | 0.05828300 |
| H | -0.37335400 | 3.55624900 | -0.94726400 |
| H | -1.21986800 | 3.92344900 | 0.56958300 |
| C | 0.67596600 | 2.91843600 | 0.81780600 |
| H | 1.36116100 | 3.76866000 | 0.76937000 |
| H | 0.43641500 | 2.73260300 | 1.86989600 |
| N | 1.31837300 | 1.70362900 | 0.29127300 |
| N | -1.30279500 | 1.91730500 | -0.07755700 |
| C | 2.58324100 | 1.55205800 | 0.47362000 |
| H | 3.12125700 | 2.44951900 | 0.79945300 |
| C | -2.57701800 | 1.80198900 | -0.02708200 |
| C | 3.39179200 | 0.37720900 | 0.34182100 |
| C | 2.89273000 | -0.94658300 | 0.59452900 |
| C | 4.76704800 | 0.58089600 | 0.12200400 |
| C | 3.84641000 | -2.00285200 | 0.50872700 |
| C | 5.64097500 | -0.46795400 | 0.04241400 |
| H | 5.14171800 | 1.59176300 | -0.00886400 |
| C | 5.16523300 | -1.77510200 | 0.23472700 |
| H | 3.47975300 | -3.00947700 | 0.67989200 |
| H | 5.85938100 | -2.60842200 | 0.17504600 |
| C | -3.33980000 | 0.61977000 | -0.28155900 |
| C | -2.79022400 | -0.57316900 | -0.83086300 |
| C | -4.71886100 | 0.68181900 | -0.00114000 |
| C | -3.67278200 | -1.65561500 | -1.05107900 |
| C | -5.53947400 | -0.38792400 | -0.22068300 |
| H | -5.13635700 | 1.59737300 | 0.40559000 |
| C | -5.00486300 | -1.56793600 | -0.75294600 |
| H | -3.25251400 | -2.56356800 | -1.46923400 |
| H | -5.65553500 | -2.41821400 | -0.93014900 |

O 1.67593900 -1.18687900 0.89329600
O -1.54466200 -0.75082300 -1.16520700
S 7.38308000 -0.21104400 -0.28730500
S -7.29500100 -0.31716400 0.15327200
O -7.53112700 -1.40385300 1.14340200
O -7.98568400 -0.56397700 -1.14272800
O -7.53961200 1.04337600 0.70134500
O 7.56958300 1.26253900 -0.38972100
O 7.66156400 -0.92567200 -1.56596500
O 8.10789700 -0.81512000 0.86705900
H 0.37337500 -2.49180400 0.69467400
H 1.05507000 -0.50626100 -1.76702700
H 1.15744100 -0.91536600 -1.10078500
O -0.52861300 -2.85928400 0.62209700
H -0.92020200 -2.35301900 -0.10545400
H 0.34598900 -0.57520800 2.16175200
O -0.51048900 -0.68654100 2.60870600
H -0.86533300 -1.45300800 2.13303900
H -3.14566000 2.69837200 0.23191100
Pd -0.05717800 0.45039200 -0.52744900

49

PdSS_D1_TS2_P, E(SCF) = -2406.49887737,
E(ZPE) = -2406.155529, E(G) = -2406.221469
a.u.

C -0.50216200 0.16065500 2.97187900
H -0.09133100 1.16578600 3.11755300
H -1.14230100 -0.07100900 3.82925600
C 0.62804400 -0.84091900 2.86676400
H 1.29817100 -0.77602900 3.72828600
H 0.21778000 -1.85425800 2.81687600
N 1.37722100 -0.64007000 1.61221900
N -1.23430900 0.13647100 1.72081900
C 2.64796800 -0.69711300 1.65839900
H 3.12051100 -0.78012400 2.64290900
C -2.48571000 0.36250400 1.64106500
C 3.55767900 -0.63226100 0.51653500
C 3.52234600 -1.52836900 -0.56298000
C 4.57497100 0.32459300 0.57494500
C 4.47169200 -1.39031800 -1.58098900
C 5.49180700 0.45339300 -0.44160500
H 4.63067300 0.99052500 1.42964600
C 5.43776600 -0.41436900 -1.52852000
H 4.42880400 -2.08870100 -2.40859100
H 6.16370600 -0.32462600 -2.32968800
C -3.25812900 0.38830800 0.42366300
C -2.73679600 0.19977300 -0.89195500
C -4.63799400 0.60998600 0.58712100
C -3.66661400 0.23214100 -1.96161600
C -5.50218100 0.64129700 -0.47343500
H -5.02979600 0.75888400 1.58866500
C -5.00367300 0.44429500 -1.76567000
H -3.26837600 0.07860600 -2.95879400
H -5.68126000 0.46095100 -2.61358700
O 2.69454900 -2.56913100 -0.68510200
O -1.49244200 -0.00354300 -1.22119700
S 6.78079200 1.70632600 -0.37962000
S -7.25759800 0.92890000 -0.24421900
O -7.93805900 -0.26587800 -0.81938000
O -7.56302800 0.217563300 -1.00170900
O -7.46291200 1.07037200 1.22313300
O 6.56989700 2.55325000 -1.58644000
O 8.06572400 0.95471800 -0.42538600
O 6.57395100 2.44064200 0.89705400
H -1.13564800 -3.13001200 -2.46343100
H 1.02248400 -0.52148400 -1.07244100
H 1.93213100 -2.60897600 -0.06550200
O -1.37390900 -2.81591800 -1.58761600
H -1.35886000 -1.84200300 -1.64521600
O 0.45013500 -4.36768600 0.62278800
O 0.39148100 -3.411308200 0.53110300
H -0.24414100 -3.25832700 -0.19767800
H -3.05023700 0.55284800 2.56136500
Pd 0.03065200 -0.25914900 0.11458300

49

PdSS_D1_TS2_R, E(SCF) = -2406.47286018,
E(ZPE) = -2406.131560, E(G) = -2406.196912
a.u.

C -0.58140500 3.13782900 0.09567100
H -0.32964600 3.51728800 -0.89902500
H -1.20295600 3.87904900 0.60365900
C 0.66731800 2.83428500 0.87952100
H 1.36261700 3.67765100 0.86874300
H 0.39965800 2.62380300 1.92020800
N 1.31174700 1.62451100 0.34210000
N -1.30805000 1.88298000 -0.07237600
C 2.57933400 1.48480200 0.51744000
H 3.10580600 2.38913300 0.84479500
C -2.58403400 1.78429400 -0.03145500
C 3.41284500 0.32551800 0.37748100
C 2.96919600 -1.00910100 0.67751000
C 4.77308100 0.56871400 0.10715900
C 3.95628800 -2.03345400 0.57829700
C 5.67967500 -0.45113000 0.01694900
H 5.10874200 1.58877200 -0.05483000
C 5.25598100 -1.76905800 0.25204000
H 3.63083500 -3.04765000 0.78428700
H 5.97549600 -2.57976500 0.18466700
C -3.35874400 0.61211700 -0.29574800
C -2.81942700 -0.58944600 -0.83610500
C -4.73986900 0.69194300 -0.02852700
C -3.71230900 -1.66310200 -1.05758200
C -5.57099300 -0.36887000 -0.25064500
H -5.15003400 1.61402900 0.37087200
C -5.04564500 -1.55824600 -0.77144500
H -3.29795300 -2.57840900 -1.46530200
H -5.70460200 -2.40221600 -0.94826500
O 1.77486100 -1.28627900 1.03016100
O -1.57350600 -0.78579900 -1.16005600
S 7.40089800 -0.14240800 -0.37299200
S -7.32888200 -0.27565800 0.10722900
O -7.58675800 -1.35601500 1.09885400
O -8.01071200 -0.51868200 -1.19409800
O -7.56177900 1.08957300 0.64852600
O 7.66278100 -0.87110800 -1.64733400
O 8.18227500 -0.70035200 0.76783000
O 7.53537100 1.33447900 -0.50708000
H 0.34730200 -2.50547800 0.83207200
H 1.02741100 -0.63384000 -1.51613500
H 1.09886000 -0.96727700 -0.77935800
O -0.57768200 -2.81074800 0.77914200
H -0.93917500 -2.33628500 0.01549800
H 0.43081800 -0.51047100 2.18860100
O -0.44088400 -0.52769300 2.62090200
H -0.84438100 -1.29369100 2.18493900
H -3.14413000 2.68520200 0.23022700
Pd -0.07765800 0.40206900 -0.51912300

49

PdSS_D1_TS2, E(SCF) = -2406.47133592,
E(ZPE) = -2406.131223, E(G) = -2406.196668
a.u.

C -0.57320800 2.93009800 0.56221800
H -0.28719000 3.39204700 -0.38776700
H -1.17533300 3.64589700 1.12776600
C 0.65380400 2.51926600 1.33373800
H 1.35699400 3.34968800 1.43766300
H 0.36076900 2.18981200 2.33585600
N 1.30107800 1.37032900 0.67773000
N -1.33767700 1.72217000 0.26974900
C 2.58304900 1.30187000 0.71171300
H 3.08981700 2.20687700 1.06617700
C -2.61546900 1.70289600 0.19224500
C 3.48774600 0.22505900 0.38116700
C 3.22125700 -1.16396400 0.58461300
C 4.78240900 0.62975800 0.00671100
C 4.28480600 -2.06528400 0.34094300
C 5.77588800 -0.27820400 -0.24472100
H 5.00036700 1.68844500 -0.09746900
C 5.52032600 -1.64271200 -0.07042600
H 4.07929600 -3.11930800 0.49252100
H 6.30964900 -2.36491300 -0.25474500

C -3.43205600 0.58949500 -0.18239000
C -2.92551200 -0.66216800 -0.63497700
C -4.82578200 0.78007100 -0.09905800
C -3.86765500 -1.66645300 -0.95992500
C -5.70520200 -0.21279200 -0.42455100
H -5.20847200 1.73840200 0.23724800
C -5.21404400 -1.45097000 -0.85862200
H -3.47806700 -2.61987900 -1.29845400
H -5.90986500 -2.24273900 -1.11735500
O 2.07369700 -1.61421500 0.98639500
O -1.66989000 -0.96654000 -0.79184600
S 7.40699300 0.24516800 -0.77916600
S -7.48063000 0.03763900 -0.32271900
O -7.97522500 -1.00466800 0.61900700
O -7.98910500 -0.15794500 -1.70914100
O -7.66769200 1.42389700 0.18258700
O 7.58688000 -0.33711500 -2.13915800
O 8.35835500 -0.32711700 0.21429000
O 7.38055900 1.73286800 -0.77776900
H 0.40705100 -2.95029200 0.84885200
H 0.84547200 -1.00925900 -0.86828800
H 1.15795400 -1.16091900 -0.05354600
O -0.54326000 -3.06639000 0.99281200
H -0.96623200 -2.51923100 0.31123700
H 0.98252300 -1.11191200 2.52248500
O 0.19951200 -1.18556500 3.09325900
H -0.34157800 -1.81081500 2.58683000
H -3.14728100 2.62646000 0.43566600
Pd -0.14291900 0.18925600 -0.16353100

49

PdSS_EI_D1_TS1_P, E(SCF) = -2406.47849245,
E(ZPE) = -2406.137169, E(G) = -2406.203286
a.u.

C -0.53642900 2.83317000 0.85863900
H -1.15311600 3.73458200 0.86117200
H -0.26464500 2.58803200 1.89056500
C 0.71131500 3.00412000 0.02666900
H 0.44516800 3.34533600 -0.97836200
H 1.39295900 3.72938400 0.47730200
N 1.34093700 1.68529100 -0.07789000
N -1.28239900 1.70407700 0.29831300
C 2.60268500 1.55462400 0.14099000
H 3.14089200 2.49441600 0.30483100
C -2.55512100 1.59746500 0.40514900
C 3.43395600 0.38973700 0.18558400
C 2.96788700 -0.93896200 0.47512600
C 4.81408200 0.62571300 0.02260400
C 3.95736000 -1.96655800 0.47576600
C 5.72422200 -0.39409400 0.03614600
H 5.16347700 1.64070700 -0.14226500
C 5.28025800 -1.70787000 0.26019300
H 3.61263300 -2.97625800 0.67247000
H 6.00159400 -2.51966500 0.27012300
C -3.37794800 0.52145300 -0.04779400
C -2.88476300 -0.64979900 -0.68897800
C -4.76290300 0.65029700 0.18326900
C -3.82675200 -1.63598900 -1.06375700
C -5.64270200 -0.32344300 -0.19247100
H -5.13737600 1.54365100 0.67258800
C -5.16313200 -1.48086500 -0.82034300
H -3.44558900 -2.52710400 -1.54925500
H -5.86091800 -2.25709200 -1.11805300
O 1.75106400 -1.20906800 0.73779100
O -1.63728400 -0.89539700 -0.96061400
S 7.47094100 -0.09420800 -0.22287400
S -7.40813900 -0.15207600 0.09082700
O -7.79444900 -1.33408900 0.90963800
O -8.02730600 -0.16787300 -1.26364500
O -7.58234900 1.14181600 0.80283900
O 7.62161100 1.38136600 -0.35364300
O 7.82730100 -0.83070800 -1.46960500
O 8.15938500 -0.64896800 0.97761400
H 0.49227300 -2.57278200 0.62193200
H 0.85227500 -0.52225700 -1.87843000
H 1.05074200 -0.91327700 -1.20416300
O -0.39346600 -2.98309500 0.62415200

H -0.89412500 -2.44812900 -0.01143600
O 0.52200000 -0.71233700 2.14078200
O -0.28132800 -0.87583300 2.66389100
H -0.64112800 -1.64925300 2.20390600
H -3.07802400 2.42078500 0.89790800
Pd -0.11328700 0.36341400 -0.57499800

49

PdSS_EI_D1_TS1_R, E(SCF) = -2406.51353337,
E(ZPE) = -2406.173575, E(G) = -2406.239291
a.u.

C -0.69436800 3.19142400 0.67074700
H -1.34896900 4.03752600 0.44898500
H -0.47649000 3.19140200 1.74304900
C 0.59344000 3.26690500 -0.11491400
H 0.37422000 3.44867400 -1.17254800
H 1.24034000 4.06934500 0.24746500
N 1.26390000 1.96931100 -0.01516900
N -1.35106000 1.92415200 0.34306200
C 2.53780900 1.85148000 -0.06543700
H 3.12733700 2.77155800 -0.09020100
C -2.62489600 1.79013300 0.34780900
C 3.28302300 0.62863000 -0.10242000
C 2.69852900 -0.66765200 -0.19331000
C 4.68561000 0.75181700 -0.06927000
C 3.57975000 -1.77451900 -0.23293300
C 5.50391200 -0.34195800 -0.10888400
H 5.12764000 1.74102800 -0.00628800
C 4.93803600 -1.61995300 -0.19165500
H 3.13479400 -2.76238200 -0.28935200
H 5.58339300 -2.49217800 -0.22062300
C -3.36009800 0.58115400 0.13284100
C -2.76474700 -0.70401600 -0.03377900
C -4.76340400 0.70154700 0.11193600
C -1.79982100 -1.79982100 -0.23217300
C -5.57440900 -0.38113600 -0.07949300
H -5.21113400 1.68075300 0.24948700
C -4.99883300 -1.64608100 -0.25419800
H -3.19352200 -2.77938800 -0.36211300
H -5.63786800 -2.51008200 -0.40605100
O 1.42334600 -0.92183100 -0.24445100
O -1.49205400 -0.95358100 -0.00923700
S 7.29147100 -0.17509300 -0.07534900
S -7.36135400 -0.21874000 -0.12780700
O -7.87484400 -1.15237900 0.91301800
O -7.76110000 -0.62445700 -1.50454300
O -7.65026300 1.20996800 0.16930500
O 7.56131800 1.28113300 0.06395400
O 7.76911000 -0.74085600 -1.36833700
O 7.74363400 -0.97322300 1.09801700
H 0.66507700 -2.73113700 -0.72902300
H 0.82296900 1.38079400 -3.12934100
H 1.10790100 0.76906900 -2.80440700
O -0.09048600 -3.30313800 -0.52502600
H -0.77276900 -2.62778900 -0.35440200
H 1.11667400 -1.84950500 1.65262800
O 0.88975600 -2.66868700 2.11244400
H 0.50506500 -3.18675000 1.38691200
H -3.22204900 2.68604300 0.53627700
Pd -0.03813800 0.47866900 0.02401000

49

PdSS_EI_D1_TS1, E(SCF) = -2406.47817460,
E(ZPE) = -2406.138272, E(G) = -2406.202345
a.u.

C -0.51035000 2.88705600 0.78256300
H -1.12852600 3.78738900 0.79872500
H -0.22259500 2.63570800 1.80889700
C 0.72564900 3.06409800 -0.06629400
H 0.44670000 3.41668500 -1.06366800
H 1.41670400 3.78167600 0.38242900
N 1.34718400 1.74403400 -0.19342900
N -1.26333200 1.75781000 0.23037000
C 2.60191400 1.58757200 0.04510900
H 3.15471100 2.51274200 0.23825800
C -2.52961700 1.63388300 0.37901000
C 3.40403600 0.40370400 0.08792700

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 2.89116700 | -0.92256500 | 0.29380300 | O | -7.63038900 | 1.25146600 | 0.52799700 |
| C | 4.79701200 | 0.61268900 | 0.03052900 | O | 7.63651300 | -0.93284600 | -1.80686200 |
| C | 3.85556500 | -1.97256900 | 0.33115700 | O | 8.35302100 | -0.34577500 | -0.49253200 |
| C | 5.68235900 | -0.42700800 | 0.08056400 | O | 7.48191900 | 1.42194600 | -1.02439000 |
| H | 5.17776200 | 1.62416800 | -0.07439800 | H | -0.09908700 | -3.51506100 | 0.10889400 |
| C | 5.19628500 | -1.73635300 | 0.23003400 | H | 0.95119200 | -0.65826400 | -1.13017500 |
| H | 3.47610200 | -2.97983700 | 0.46694400 | H | 1.30862000 | -0.70037400 | 1.01440000 |
| H | 5.89866200 | -2.56375500 | 0.26966500 | O | -0.92206600 | -3.13026700 | 0.42074000 |
| C | -3.35177400 | 0.54619200 | -0.04905700 | H | -1.12044700 | -2.40649000 | -0.20689200 |
| C | -2.86395900 | -0.61258900 | -0.71730300 | H | 0.33254200 | -1.52200200 | 2.91154100 |
| C | -4.72726400 | 0.64642900 | 0.24170600 | O | -0.61603100 | -1.55477400 | 2.75639000 |
| C | -3.80255700 | -1.61517500 | -1.05578200 | H | -0.70958100 | -2.13418200 | 1.97596100 |
| C | -5.60382200 | -0.34400400 | -0.09798600 | H | -3.16188200 | 2.42942000 | 0.99744700 |
| H | -5.09765000 | 1.52983900 | 0.75174700 | Pd | -0.05575300 | 0.30914000 | -0.40101400 |
| C | -5.12997900 | -1.48830400 | -0.75311200 | | | | |
| H | -3.42607100 | -2.49654500 | -1.56277700 | | | | |
| H | -5.82371600 | -2.27824600 | -1.02270100 | | | | |
| O | 1.65291900 | -1.17607900 | 0.45935300 | | | | |
| O | -1.62575900 | -0.83154900 | -1.04552700 | | | | |
| S | 7.45135400 | -0.15603200 | 0.00464000 | | | | |
| S | -7.35810000 | -0.20348500 | 0.26101700 | | | | |
| O | -7.70110500 | -1.41682300 | 1.05298900 | | | | |
| O | -8.03165100 | -0.17864100 | -1.06718800 | | | | |
| O | -7.51521000 | 1.06295100 | 1.02475200 | | | | |
| O | 7.63658000 | 1.31441000 | -0.13770700 | | | | |
| O | 7.92994900 | -0.92470800 | -1.17990500 | | | | |
| O | 7.99627900 | -0.62832000 | 1.28445200 | | | | |
| H | 0.46263000 | -2.59277500 | 0.35862900 | | | | |
| H | 0.85163900 | -0.31576500 | -2.19590700 | | | | |
| H | 1.04931900 | -0.83307800 | -1.64302300 | | | | |
| O | -0.41256600 | -3.02522500 | 0.34572000 | | | | |
| H | -0.92194600 | -2.46299900 | -0.25877500 | | | | |
| H | 0.45888100 | -0.77943200 | 1.92898800 | | | | |
| O | -0.33738100 | -0.96528200 | 2.45478400 | | | | |
| H | -0.70442500 | -1.71752300 | 1.96636100 | | | | |
| H | -3.04654500 | 2.44799600 | 0.89325400 | | | | |
| Pd | -0.10098000 | 0.42641300 | -0.66658200 | | | | |

49
PdSS_EI_D1_TS2_P, E(SCF) = -2406.49892886,
E(ZPE) = -2406.155489, E(G) = -2406.220135
a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.57127300 | 2.74117600 | 1.15612900 |
| H | -1.13817400 | 3.67644500 | 1.19530400 |
| H | -0.33489400 | 2.44018100 | 2.18304900 |
| C | 0.71526200 | 2.92491500 | 0.37621700 |
| H | 0.48519100 | 3.29353600 | -0.62775200 |
| H | 1.37750000 | 3.64031600 | 0.86988700 |
| N | 1.38239100 | 1.61746900 | 0.22420800 |
| N | -1.32390600 | 1.67302500 | 0.52315500 |
| C | 2.64244500 | 1.55844200 | 0.42413400 |
| H | 3.15400000 | 2.50159700 | 0.64011400 |
| C | -2.59706400 | 1.62000900 | 0.52139700 |
| C | 3.52503000 | 0.40239600 | 0.39205900 |
| C | 3.21680900 | -0.88048300 | 0.87710500 |
| C | 4.83555200 | 0.65235500 | -0.03995600 |
| C | 4.20272400 | -1.86560500 | 0.89066200 |
| C | 5.78827000 | -0.33615300 | -0.04960500 |
| H | 5.10137000 | 1.64704500 | -0.38236500 |
| C | 5.47040000 | -1.60486900 | 0.42589900 |
| H | 3.93689400 | -2.84253700 | 1.27637600 |
| H | 6.22358200 | -2.38533800 | 0.43392400 |
| C | -3.39105300 | 0.56386500 | -0.05412500 |
| C | -2.87620300 | -0.58582700 | -0.72400200 |
| C | -4.78353600 | 0.70082100 | 0.09585000 |
| C | -3.81705100 | -1.53886700 | -1.18448700 |
| C | -5.66142300 | -0.23821000 | -0.37213400 |
| H | -5.17247900 | 1.57958400 | 0.60099800 |
| C | -5.16495600 | -1.37750600 | -1.01410500 |
| H | -3.42098000 | -2.41739000 | -1.68257900 |
| H | -5.85355000 | -2.13134400 | -1.38279800 |
| O | 2.03337700 | -1.21780000 | 1.42075400 |
| O | -1.62255400 | -0.85536100 | -0.96646600 |
| S | 7.45670800 | -0.01598400 | -0.64859200 |
| S | -7.43432100 | -0.04710200 | -0.17169300 |
| O | -7.87560600 | -1.22076700 | 0.63330000 |
| O | -7.99648000 | -0.06062800 | -1.55173300 |

49
PdSS_EI_D1_TS2_R, E(SCF) = -2406.47849336,
E(ZPE) = -2406.137151, E(G) = -2406.203289
a.u.

| | | | |
|----|-------------|-------------|-------------|
| C | -0.53700600 | 2.83344200 | 0.85899300 |
| H | -1.15372800 | 3.73482600 | 0.86072500 |
| H | -0.26591100 | 2.58875100 | 1.89120000 |
| C | 0.71127600 | 3.00411600 | 0.02777700 |
| H | 0.44573800 | 3.34492900 | -0.97755900 |
| H | 1.39259300 | 3.72959400 | 0.47854600 |
| N | 1.34105400 | 1.68529100 | -0.07596100 |
| N | -1.28259800 | 1.70408900 | 0.29860700 |
| C | 2.60284800 | 1.55493600 | 0.14278100 |
| H | 3.14095600 | 2.49486200 | 0.30619400 |
| C | -2.55533900 | 1.59731600 | 0.40511300 |
| C | 3.43414100 | 0.39004800 | 0.18759700 |
| C | 2.96812900 | -0.93836300 | 0.47857200 |
| C | 4.81407900 | 0.62575600 | 0.02285600 |
| C | 3.95750700 | -1.96608300 | 0.47884500 |
| C | 5.72408900 | -0.39418500 | 0.03594700 |
| H | 5.16336600 | 1.64060300 | -0.14314100 |
| C | 5.28016500 | -1.70774800 | 0.26138000 |
| H | 3.61287400 | -2.97559900 | 0.67668600 |
| H | 6.00140500 | -2.51963500 | 0.27101200 |
| C | -3.37792100 | 0.52124800 | -0.04808600 |
| C | -2.88446700 | -0.64964900 | -0.68974600 |
| C | -4.76294800 | 0.64990300 | 0.18264400 |
| C | -3.82633000 | -1.63559600 | -1.06548200 |
| C | -5.64258800 | -0.32367900 | -0.19386500 |
| H | -5.13761100 | 1.54296900 | 0.67234700 |
| C | -5.16278600 | -1.48067200 | -0.82235200 |
| H | -3.44501800 | -2.52639300 | -1.55143900 |
| H | -5.86045600 | -2.25672800 | -1.12078500 |
| O | 1.75158000 | -1.20805300 | 0.74278200 |
| O | -1.63690000 | -0.89510800 | -0.96098900 |
| S | 7.47048100 | -0.09482000 | -0.22593300 |
| S | -7.40810100 | -0.15265300 | 0.08915600 |
| O | -7.79431600 | -1.33475900 | 0.90787500 |
| O | -8.02708600 | -0.16850700 | -1.26540000 |
| O | -7.58265300 | 1.14116900 | 0.80121300 |
| O | 7.82480500 | -0.83300100 | -1.47223600 |
| O | 8.16071500 | -0.64806300 | 0.97424200 |
| O | 7.62111600 | 1.38058200 | -0.35880100 |
| H | 0.49249800 | -2.57208300 | 0.62623100 |
| H | 0.85407800 | -0.52260400 | -1.87498000 |
| H | 1.05088300 | -0.91400400 | -1.20027000 |
| O | -0.39342600 | -2.98198800 | 0.62748700 |
| H | -0.89273000 | -2.44786100 | -0.00981500 |
| H | 0.52139500 | -0.71123400 | -1.43068000 |
| O | -0.28228000 | -0.87349000 | 2.66611400 |
| H | -0.64259400 | -1.64695600 | 2.20664100 |
| H | -3.07847400 | 2.42060000 | 0.89768200 |
| Pd | -0.11295700 | 0.36336700 | -0.57388200 |

49
PdSS_EI_D1_TS2, E(SCF) = -2406.47556174,
E(ZPE) = -2406.135564, E(G) = -2406.202494
a.u.

| | | | |
|---|-------------|------------|------------|
| C | -0.52966300 | 2.70104300 | 0.88682400 |
| H | -1.09481600 | 3.63599500 | 0.90488000 |
| H | -0.24930800 | 2.44084800 | 1.91320700 |
| C | 0.71100700 | 2.82052800 | 0.03319100 |

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 0.43660600 | 3.16003100 | -0.97030200 | O | 7.74109800 | -1.26984800 | 1.19896900 |
| H | 1.41853000 | 3.53384400 | 0.46293100 | O | 7.60195000 | 0.94891400 | 0.08439300 |
| N | 1.31657100 | 1.48659300 | -0.08453100 | O | -7.60195000 | 0.94891300 | -0.08439500 |
| N | -1.33534300 | 1.61363900 | 0.34042500 | O | -7.73172200 | -1.12956000 | 1.27385400 |
| C | 2.58971700 | 1.37834000 | 0.05811100 | O | -7.74110300 | -1.26985400 | -1.19896000 |
| H | 3.10962800 | 2.32850800 | 0.21919200 | H | 3.21412600 | 2.54772100 | 0.00704900 |
| C | -2.61101000 | 1.57567900 | 0.44011300 | Pd | 0.00000000 | 0.35294200 | -0.00000100 |
| C | 3.49714500 | 0.25684100 | 0.03973600 | C | 0.76395500 | 3.17966500 | -0.00064400 |
| C | 3.17542500 | -1.12498000 | 0.20613800 | C | -0.76395500 | 3.17966500 | 0.00064600 |
| C | 4.85459400 | 0.62892800 | -0.05396800 | H | -1.13952800 | 3.70802800 | 0.88005600 |
| C | 4.24781000 | -2.04665200 | 0.21823500 | H | -1.14131900 | 3.70478800 | -0.87995500 |
| C | 5.86395400 | -0.29411700 | -0.04559700 | H | 1.14131800 | 3.70478500 | 0.87995900 |
| H | 5.11061800 | 1.68004300 | -0.14485800 | H | 1.13952900 | 3.70803100 | -0.88005300 |
| C | 5.55217600 | -1.65005700 | 0.09734100 | | | | |
| H | 3.99260900 | -3.09352000 | 0.33887200 | | | | |
| H | 6.34959600 | -2.38647600 | 0.11260300 | | | | |
| C | -3.47490500 | 0.52395000 | -0.00234600 | | | | |
| C | -3.02644700 | -0.69605400 | -0.58411100 | | | | |
| C | -4.85562500 | 0.72863800 | 0.19167500 | | | | |
| C | -4.01076800 | -1.64900100 | -0.93775400 | | | | |
| C | -5.77735900 | -0.21318000 | -0.16758300 | | | | |
| H | -5.19430600 | 1.65856700 | 0.63727000 | | | | |
| C | -5.34321400 | -1.41811300 | -0.73492400 | | | | |
| H | -3.66499500 | -2.57846100 | -1.37551000 | | | | |
| H | -6.07220400 | -2.17061900 | -1.01837600 | | | | |
| O | 1.96458600 | -1.56106400 | 0.37035900 | | | | |
| O | -1.78800700 | -1.01826600 | -0.81988300 | | | | |
| S | 7.58601800 | 0.19832800 | -0.17155000 | | | | |
| S | -7.53653900 | 0.05774700 | 0.07019000 | | | | |
| O | -7.99405500 | -1.04968200 | 0.95494600 | | | | |
| O | -8.13502800 | -0.01511100 | -1.29196500 | | | | |
| O | -7.66157200 | 1.40145800 | 0.69563400 | | | | |
| O | 8.11512400 | -0.50430500 | -1.37425100 | | | | |
| O | 8.22631200 | -0.27036900 | 1.08937900 | | | | |
| O | 7.57950700 | 1.67934200 | -0.31211000 | | | | |
| H | 0.46770500 | -2.90408100 | 0.48776800 | | | | |
| H | 0.71976100 | -0.88415000 | -1.45885500 | | | | |
| H | 1.13020900 | -1.09458600 | -0.67782300 | | | | |
| O | -0.45789700 | -3.12132100 | 0.67718400 | | | | |
| H | -0.96998800 | -2.54306700 | 0.08730600 | | | | |
| H | 0.95563700 | -1.00200700 | 2.02462000 | | | | |
| O | 0.23604100 | -1.12564500 | 2.66318700 | | | | |
| H | -0.27169800 | -1.82888500 | 2.22814700 | | | | |
| H | -3.10378800 | 2.42839300 | 0.91465100 | | | | |
| Pd | -0.20841600 | 0.20369000 | -0.52055500 | | | | |

41

PdSS_EI_TS, E(SCF) = -2252.45471012, E(ZPE)
= -2252.180630, E(G) = -2252.240340 a.u.

| | | | |
|---|-------------|-------------|-------------|
| N | -1.31890200 | 1.81704400 | 0.00352600 |
| N | 1.31890200 | 1.81704400 | -0.00352700 |
| C | -2.59164200 | 1.64846200 | -0.00139000 |
| H | -3.21412600 | 2.54772100 | -0.00705400 |
| C | 2.59164200 | 1.64846200 | 0.00138600 |
| C | -3.30235600 | 0.40794200 | 0.00090700 |
| C | -2.67819800 | -0.87875500 | 0.01376500 |
| C | -4.70971400 | 0.49294200 | -0.00825500 |
| C | -3.53686300 | -2.01059700 | 0.02223300 |
| C | -5.49818800 | -0.62222600 | -0.00411400 |
| H | -5.17987500 | 1.47150000 | -0.02082400 |
| C | -4.89653500 | -1.88978300 | 0.01445300 |
| H | -3.06344000 | -2.98580900 | 0.03390800 |
| H | -5.52006100 | -2.77848100 | 0.01925600 |
| C | 3.30235600 | 0.40794300 | -0.00091100 |
| C | 2.67819800 | -0.87875500 | -0.01376800 |
| C | 4.70971400 | 0.49294200 | 0.00825200 |
| C | 3.53686300 | -2.01059700 | -0.02223700 |
| C | 5.49818800 | -0.62222500 | 0.00411300 |
| H | 5.17987500 | 1.47150000 | 0.02082200 |
| C | 4.89653500 | -1.88978300 | -0.01445500 |
| H | 3.06344000 | -2.98580900 | -0.03391300 |
| H | 5.52006100 | -2.77848100 | -0.01925800 |
| O | -1.40907300 | -1.10152100 | 0.01798100 |
| O | 1.40907300 | -1.10152100 | -0.01798400 |
| S | -7.28743100 | -0.50340300 | -0.00403900 |
| S | 7.28743100 | -0.50340300 | 0.00404300 |
| O | 7.73172600 | -1.12956700 | -1.27384600 |