Supporting Information

One-pot Synthesis of 1,3-Butadiene and 1,6-Hexandiol Derivatives from Cyclopentadiene (CPD) via Tandem Olefin Metathesis Reactions

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Contents

1. *In-situ* ^{1}H NMR investigation of the Diels Alder reaction of CPD with 3 in toluene

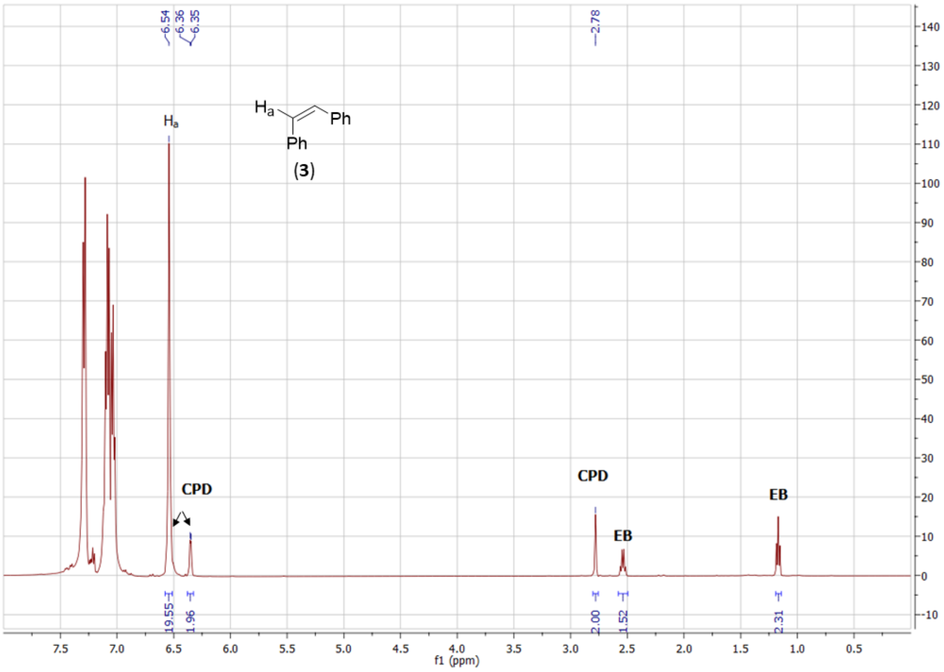

Figure S1. ^{1}H NMR spectrum of the mixture of **3** and **CPD** in toluene-d_8 after 6 hours using **EB** as internal standard.

2. Ring Opening Cross Metathesis (ROCM) of CPD with *cis*-stilbene (3)

Reaction of **CPD** with 1 equiv. of **3:**

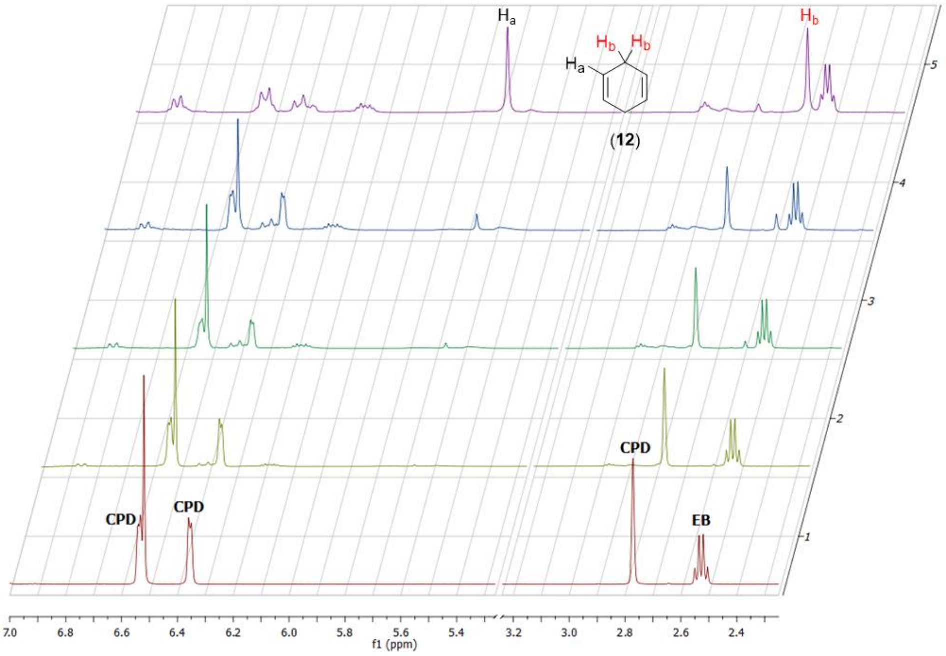

Figure S2. *In situ* stacked ^{1}H NMR spectrum of the reaction mixture of the metathesis of **CPD** and 1 equivalent of *cis*-stilbene (**3**) in toluene-d_8, formation of **12**.

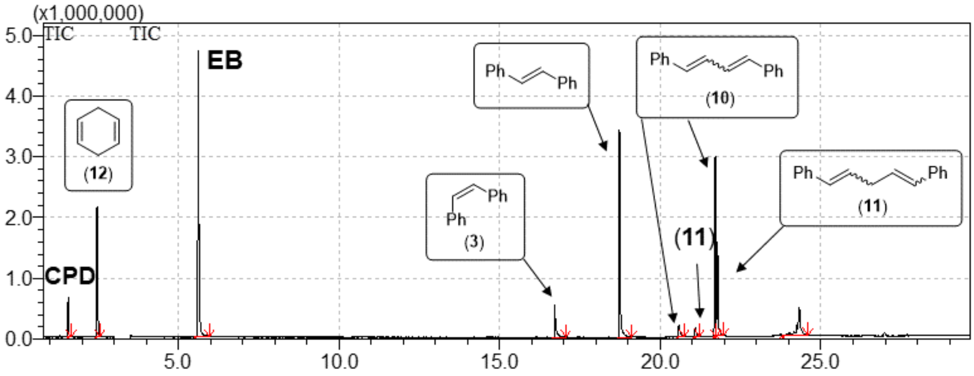

Figure S3. Total ion chromatogram of the reaction mixture of **CPD** and 1 equivalent of *cis*-stilbene (**3**) after 24 hours.

Table S1. Composition of the reaction mixture of the cross metathesis of **CPD** and 1 equivalent of **3** using **1-G3**.

T_R (min)	Area%	Name
1.58	2.07	**CPD**
2.47	9.27	1,4-Cyclohexadiene (**12**)
5.67	28.53	**EB**[a]
16.72	4.32	*cis*-Stilbene (**3**)
18.74	19.86	*trans*-Stilbene
20.59	1.87	Isomer of **10**
21.09	1.02	Isomer of **11**
21.70	16.25	Isomer of **10**
21.78	8.95	Isomer of **11**
24.32	7.86	Homologues of **10** and **11**

[a] Internal standard

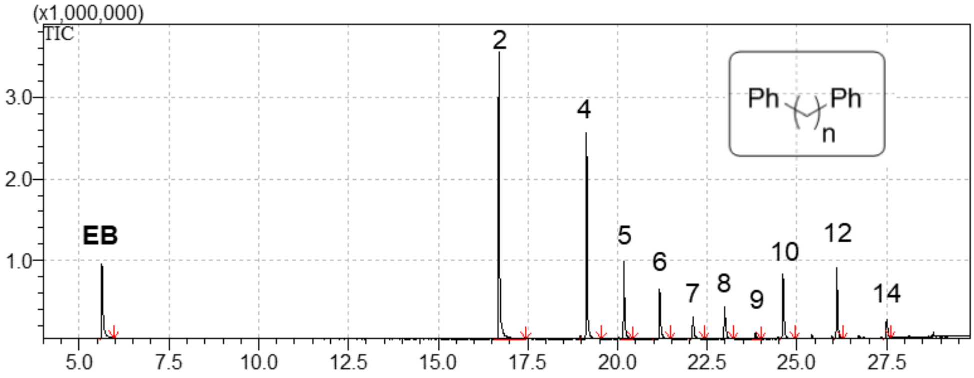

Figure S4. Total ion chromatogram of the hydrogenated reaction mixture of **CPD** and 1 equivalent of *cis*-stilbene (**3**) after 24 hours.

Table S2. Composition of the hydrogenated reaction mixture of the cross metathesis of **CPD** and 1 equivalent of **3** using **1-G3**.

T_R (min)	Area%	Name
5.63	10.08	**EB**[a]
16.70	30.79	1,2-Diphenylethane (n=2)[b]
19.14	19.74	1,4-Diphenylbutane (n=4)
20.18	9.00	1,5-Diphenylpentane (n=5)
21.18	5.96	1,6-Diphenylhexane (n=6)
22.10	2.84	1,7-Diphenylheptane (n=7)
22.99	4.04	1,8-Diphenyloctane (n=8)
23.84	0.96	1,9-Diphenylnonane (n=9)
24.62	7.20	1,10-Diphenyldecane (n=10)
26.11	7.25	1,11-Diphenyldodecane (n=12)
27.50	2.13	1,11-Diphenytetradecane (n=14)

[a]Internal standard, [b]Hydrogenated **3**

Reaction of **CPD** with 8 equiv. of **3**:

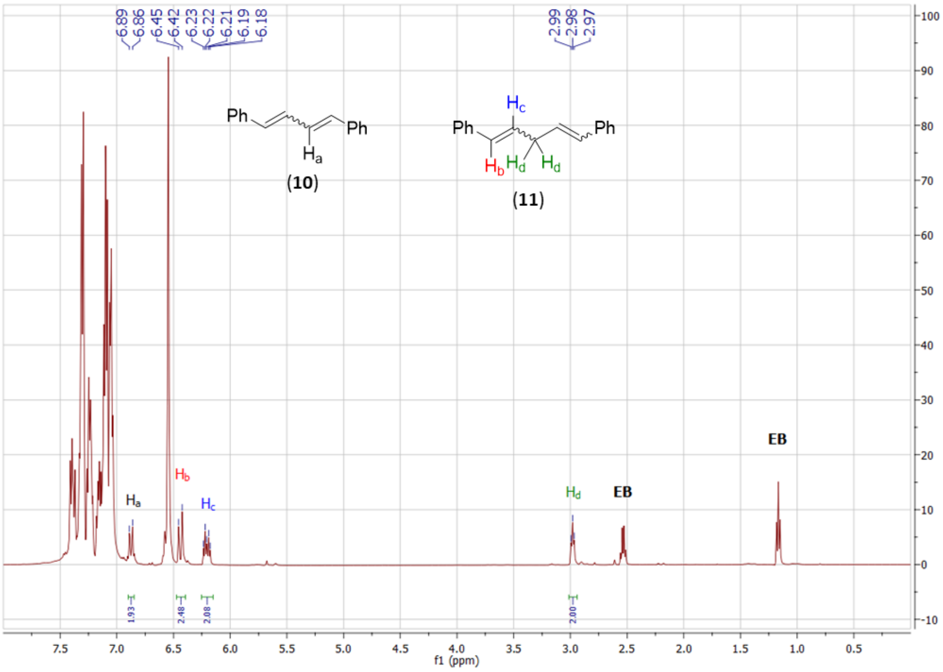

Figure S5. *In situ* ^{1}H NMR spectrum of the reaction mixture of **CPD** and 8 equivalents of *cis*-stilbene (**3**) after 6 hours in toluene-d_8.

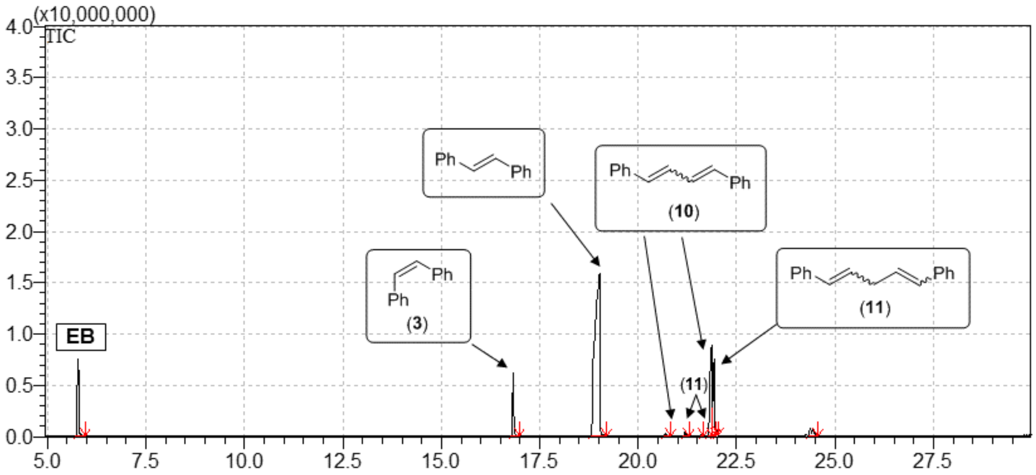

Figure S6. Total ion chromatogram of the reaction mixture of CPD and 8 equivalent of *cis*-stilbene (**3**) after 6 hours.

Table S3. Composition of the reaction mixture of the cross metathesis of **CPD** and 8 equivalent of **3** using **1-G3**.

T_R (min)	Area%	Name
5.77	8.14	**EB**[a]
18.82	5.91	*cis*-Stilbene (**3**)
19.02	60.55	*trans*-Stilbene
20.69	0.35	Isomer of **10**
21.18	0.46	Isomer of **11**
21.61	0.21	Isomer of **11**
21.86	14.97	Isomer of **10**
21.92	7.30	Isomer of **11**
24.36	1.79	Homologues of **10** and **11**

[a] Internal standard

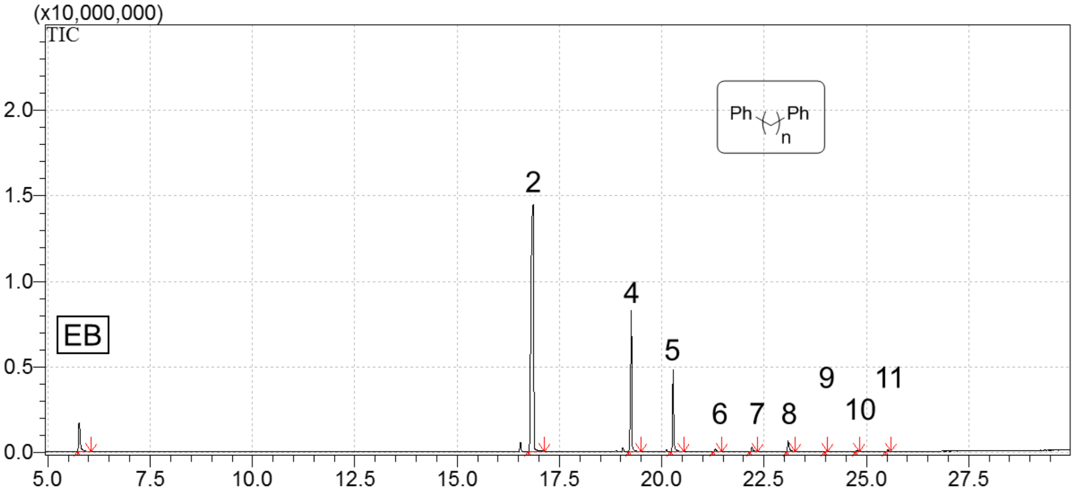

Figure S7. Total ion chromatogram of the hydrogenated reaction mixture of **CPD** and 8 equivalent of **3**.

Table S4. Composition of the hydrogenated reaction mixture of the cross metathesis of **CPD** and 8 equivalent of **3** using **1-G3**.

T_R (min)	Area%	Name
5.77	4.87	**EB**[a]
16.86	64.46	1,2-Diphenylethane (n=2)[b]
19.26	17.59	1,4-Diphenylbutane (n=4)
20.28	9.68	1,5-Diphenylpentane (n=5)
21.30	0.47	1,6-Diphenylhexane (n=6)
22.20	0.80	1,7-Diphenylheptane (n=7)
23.09	1.73	1,8-Diphenyloctane (n=8)
23.99	0.03	1,9-Diphenylnonane (n=9)
24.76	0.14	1,10-Diphenyldecane (n=10)
25.52	0.24	1,11-Diphenylundecane (n=11)

[a]Internal standard, [b]Hydrogenated **3**

3. Ring Opening Cross Metathesis (ROCM) of CPD with 8 equiv. of *cis*-butene diol diacetate (2)

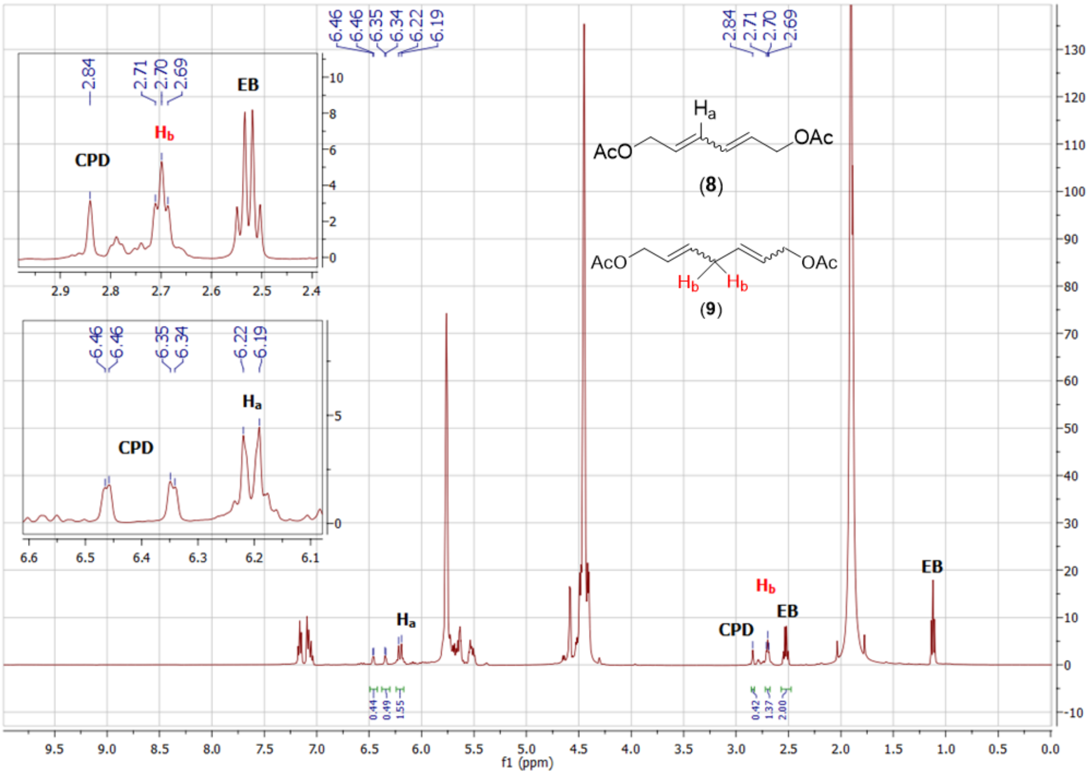

Figure S8. ^{1}H NMR spectrum of a typical metathesis reaction mixture of **CPD** and 8 equivalents of **2** in toluene-d_8.

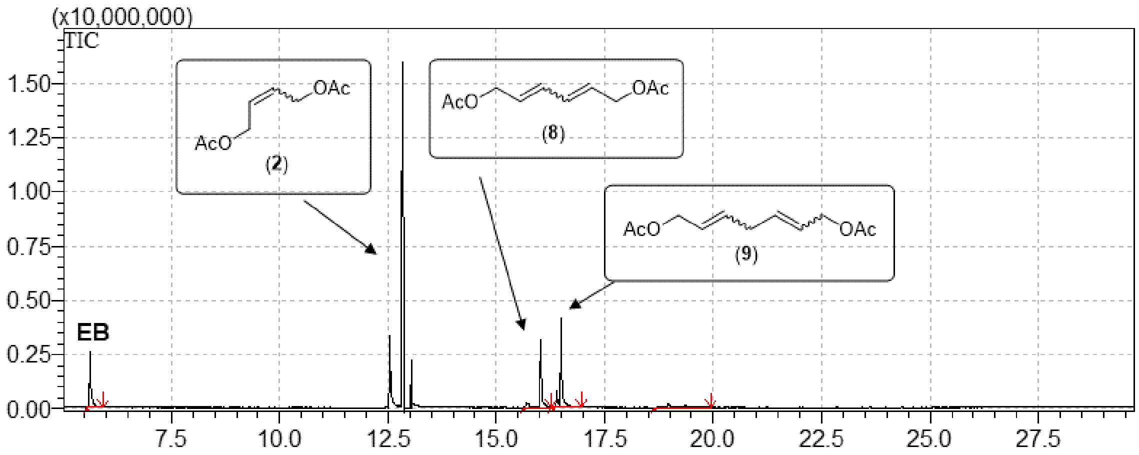

Figure S9. Total ion chromatogram of a reaction mixture of the metathesis of **CPD** and 8 equivalents of **2**.

Table S5. Composition of the reaction mixture of the metathesis of **CPD** and 8 equivalents of **2**.

T_R (min)	Area%	Name
1.57	0.30	**CPD**
5.63	24.51	**EB**[a]
16.02	28.69	Hexa-2,4-diene-1,6-diyl diacetate (**8**)
16.49	37.77	Hepta-2,5-diene-1,7-diyl diacetate (**9**)
18.95	8.72	Homologues of **8** and **9**

[a]Internal standard

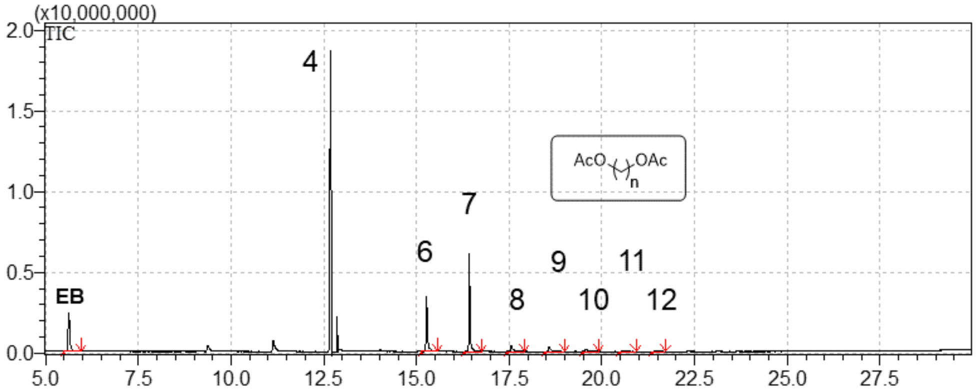

Figure S10. Total ion chromatogram of the hydrogenated reaction mixture of the metathesis of **CPD** and 8 equivalents of **2**.

Table S6. Composition of the typical hydrogenated reaction mixture of the ROCM of **CPD** and 8 equivalent of **2**.

T_R (min)	Area%	Name
5.63	22.85	**EB**[a]
15.27	25.58	1,6-Hexanediol diacetate (n=6)
16.43	37.76	1,7-Heptanediol diacetate (n=7)
17.55	5.09	1,8-Octanediol diacetate (n=8)
18.57	4.18	1,9-Nonanediol diacetate (n=9)
19.57	3.09	1,10-Decanediol diacetate (n=10)
20.56	0.95	1,11-Undecanediol diacetate (n=11)
21.45	0.50	1,12-Dodecanediol diacetate (n=12)

[a]Internal standard

4. Ethenolysis of CPD

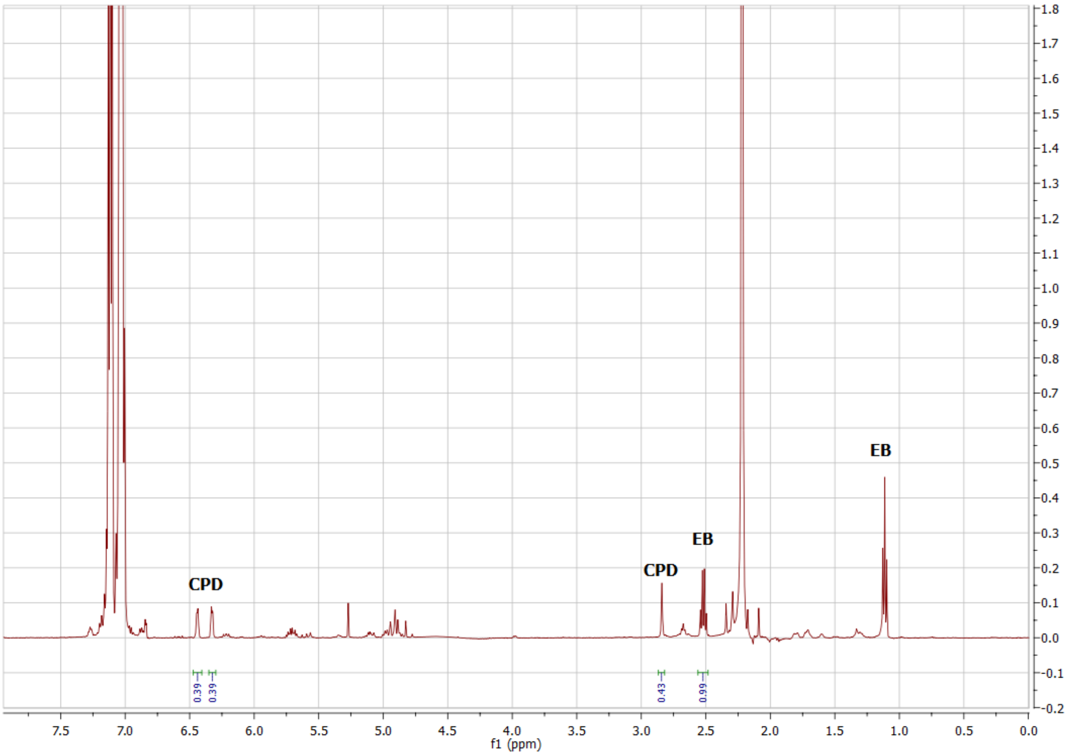

Figure S11. ^{1}H NMR spectrum of a typical ethenolysis reaction mixture in $CDCl_3$. A representative example for the determination of **CPD** conversion. (t_0 **CPD** (CH_2, 2.78 ppm)/**EB** (CH_2, 2.52 ppm) integral ratio is 1.53)

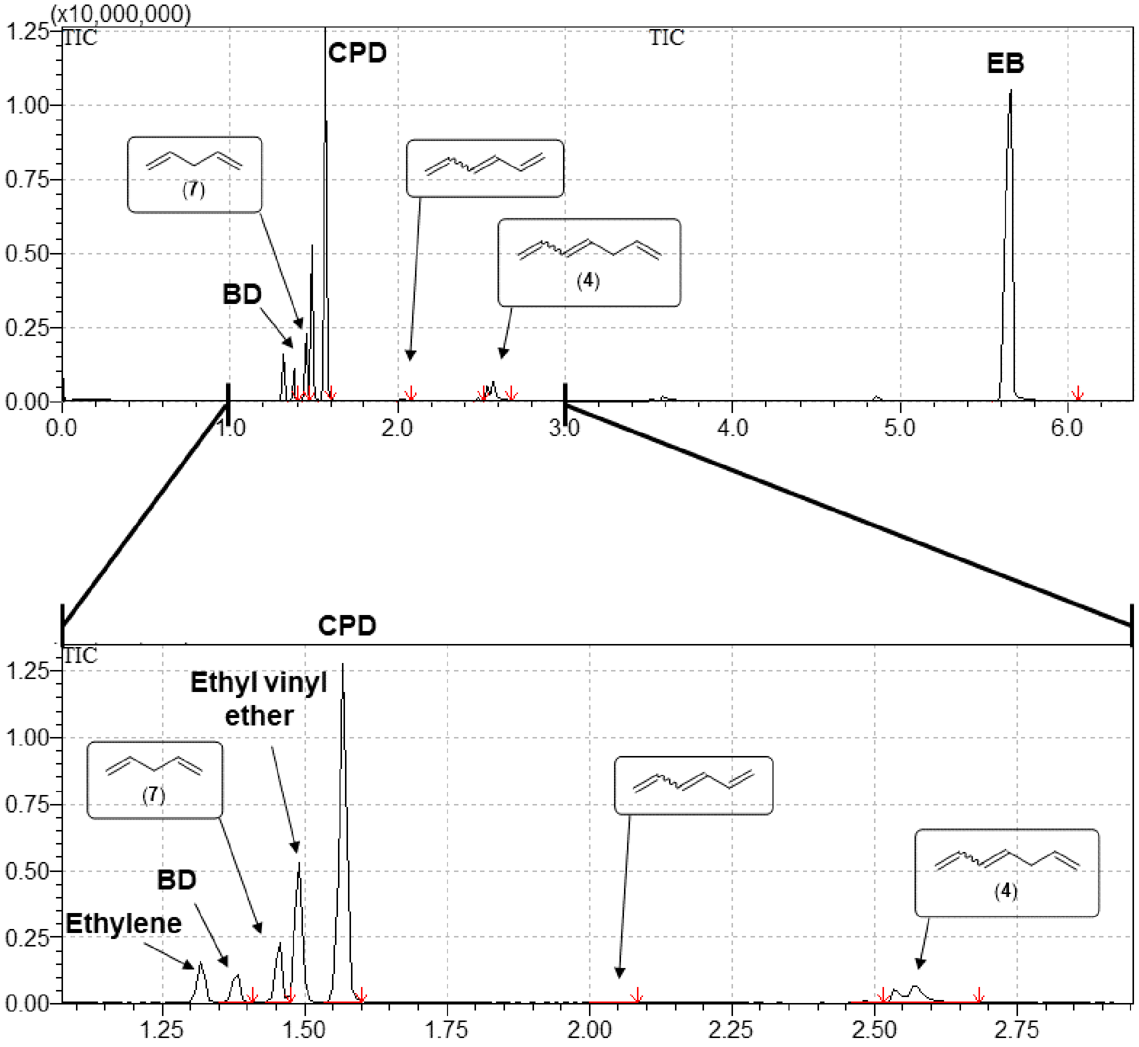

Figure S12. Total ion chromatogram of the liquid phase of the reaction mixture of the ethenolysis of **CPD**.

Table S7. Composition of the liquid reaction mixture of the cross metathesis of **CPD** and ethylene.

T_R (min)	Area%	Name
1.38	2.25	1,3-Butadiene (**BD**)
1.46	4.43	1,4-Pentadiene (**7**)
1.57	25.46	**CPD**
2.02	0.26	1,3,5-Hexatriene
2.48	0.21	1,4-Cyclohexadiene (**12**)
2.57	3.79	1,3,6-Heptatriene (**4**)
5.56	63.61	**EB**[a]

[a] Internal standard

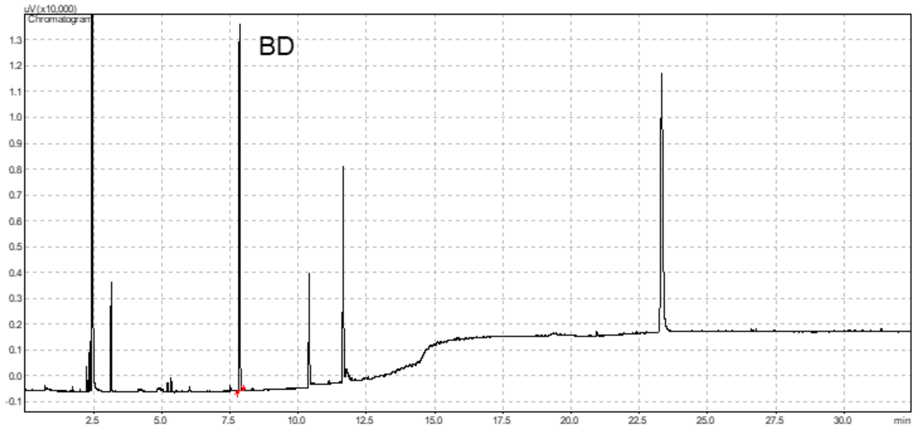

Figure S13. The gas chromatogram (FID) of the gas phase of the ethenolysis of **CPD**.

Table S8. BD quantity in the gas phase of the reaction mixture of the cross metathesis of **CPD** and ethylene.

T_R (min)	Area	Name
7.84	34268	1,3-Butadiene (**BD**)

5. ROCM of 1,3-cyclohexadiene (13) with 12 equiv. of 2

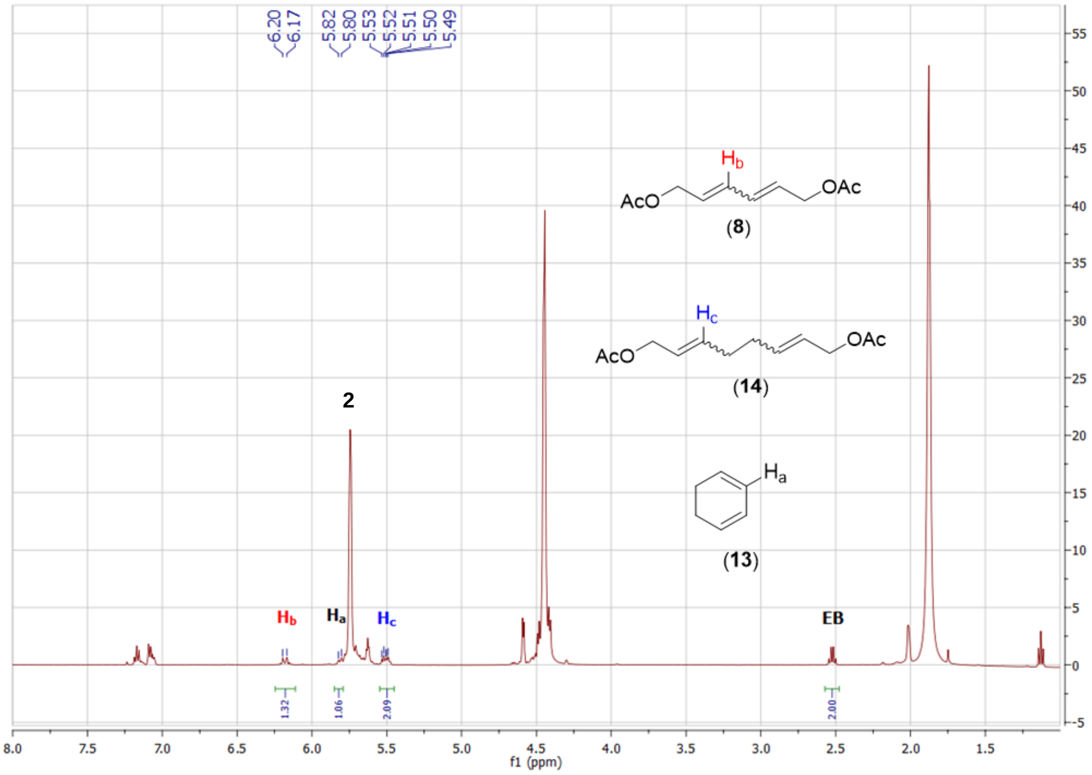

Figure S14. ^{1}H NMR spectrum of a typical metathesis reaction mixture of **13** and 8 equivalents of **2** in toluene-*d*$_8$.

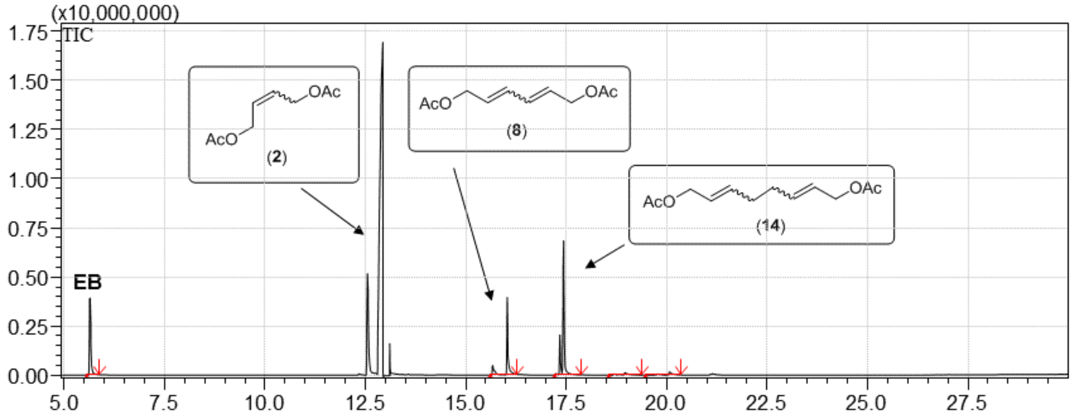

Figure S15. Total ion chromatogram of the reaction mixture of cross metathesis of **13** and 12 equivalents of **2**.

Table S9. Composition of the reaction mixture of the cross metathesis of **13** and 12 equivalents of **2**.

T_R (min)	Area%	Name
5.63	24.04	**EB**[a]
16.02	25.95	Hexa-2,4-diene-1,6-diyl diacetate (**8**)
17.42	43.98	Octa-2,6-diene-1,8-diyl diacetate (**14**)
18.95	2.67	Deca-2,6-diene-1,10-diyl diacetate
20.07	3.35	Other homologues of **8** and **14**

[a] Internal standard

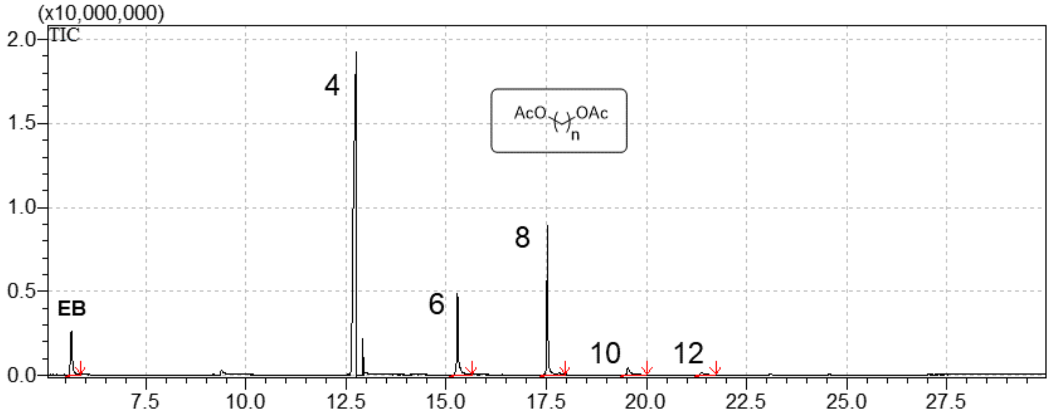

Figure S16. Total ion chromatogram of the hydrogenated reaction mixture of cross metathesis of **13** and 12 equivalents of **2**.

Table S10. Composition of the hydrogenated reaction mixture of the cross metathesis of **13** and **2**.

T_R (min)	Area%	Name
5.63	19.18	**EB**[a]
15.28	28.01	1,6-Hexanediol diacetate (n=6)
17.53	45.53	1,8-Octanediol diacetate (n=8)
19.53	5.25	1,10-Decanediol diacetate (n=10)
21.36	2.03	1,12-Dodecanediol diacetate (n=12)

[a] Internal standard

6. Solubility of ethylene

Solubility of ethylene in toluene-*d*8 was estimated based on the literature data for toluene (non-perdeuterated).[1] At 298K temperature and under 10 bar pressure, the solubility of **ethylene** expressed in mole fraction is: $x_{10\text{bar}} = 0.147$, respectively, which can be converted to approximate molar concentrations using the molar masses and the density of toluene-*d*8 ($943\text{g}/\text{dm}^3$).

$$c_{\text{solute}} = \frac{n_{\text{solute}}}{V_{solution}} = \frac{\frac{m_{\text{solute}}}{M_{\text{solute}}}}{\frac{m_{\text{solvent}} + m_{\text{solute}}}{\rho_{\text{solution}}}} = \frac{\rho_{\text{solution}} x_{\text{solute}}}{(1 - x_{\text{solute}}) M_{\text{solvent}} + x_{\text{solute}} M_{\text{solute}}} \approx \frac{\rho_{\textbf{solvent}} x_{\text{solute}}}{(1 - x_{\text{solute}}) M_{\text{solvent}} + x_{\text{solute}} M_{\text{solute}}} = 1.55M \tag{2}$$

7. Theoretical calculations

7.1. Tools

Electronic structure calculations were carried out using programs Gaussian 09 revC and Orca 4.0.1 (only for DLPNO-CCSD(T)).[2,3] Statistical thermodynamics calculations were done in Excel spreadsheets using standard formulae.

7.2. Finding lowest energy geometric conformers

All electronic structure calculations were done in the presence of an implicit toluene solvent. Multidimensional relaxed geometry scan calculations were carried out using PM6 semiempirical method[4] to locate all local minima for the compounds with internal hindered rotors. Geometry of all local minima found in the scans ~~dataset~~ were reoptimized at PM6 level, and the ones within 2kcal/mol of the lowest were reoptimized using density functional theory (DFT) with M06-2X hybrid meta functional[5], which was shown to provide reliable results for π-system thermochemistry (including π-system isomerization energies) and hydrocarbon thermochemistry[5]. ~~All electron, r~~Restricted calculations were carried out using the correlation consistent cc-pVDZ basis set proposed by Dunning[6]. Ultrafine grid was used and very tight SCF and geometry optimization convergence criteria were set. Singlet multiplicity was assumed for the ground state of the (neutral) ~~closed shell, neutral~~ molecules. Toluene ~~as~~ solvent was taken into account implicitly via the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM).[7,8]

7.3. Calculating energies of lowest energy conformers

The lowest energy conformer found at M06-2X/cc-pVDZ level was reoptimized at M06-2X/cc-pVTZ level for all compounds[5], and also with the G3, G4, CBS-APNO composite theories[9–11] for the species in synthesis path using **Ethylene** (**CPD**, **Ethylene**, **4**, **BD**, **7**, **12**, **15**). These composite methods were employed as P. Somers and J.M. Simmie[12] showed that the average of the G3, G4 and CBS-APNO results can predict formation enthalpies within chemical accuracy of the results of Active Thermochemical Tables (ATcT)[13].

Harmonic vibrational analysis was carried out and hindered rotor correction [14–16] was ~~were~~ determined at the geometry optimization level of the ~~corresponding~~ methods. Single point energy of all minimum-energy conformer obtained at M06-2X/cc-pVTZ level was also calculated with the linear-scaling domain-based local pair-natural orbital coupled cluster with perturbative triple excitation (DLPNO-CCSD(T)) method[17] with cc-pVTZ basis set (and cc-pVTZ for correlation fitting in the RI approximation) using frozen-core approximation, tight DLPNO threshold and SCF convergence criterion. These latter calculations were carried out with program ORCA and SMD implicit solvent model [új referencia] was used for toluene.

új referencia: A.V. Marenich, C.J. Cramer and D.G. Truhlar
J. Phys. Chem. B 2009, 113, 6378–6396.

7.4. Statistical thermodynamics calculation

Translational partition functions (per unit volume) were calculated using the standard formula[18]. Rotational partition functions were calculated based on the rigid rotor approximation[18] using the rotational constants of the minimum energy conformer. Vibrational partition functions were calculated using the harmonic oscillator approximation[18] at the minimum energy conformer with hindered rotor corrections proposed by McClurg and Flagan[14–16].

The calculated harmonic vibrational frequencies were scaled to correct for the systematic errors of the M06-2X/cc-pVTZ calculations to improve the accuracy of the vibrational zero-point energies and partition functions. Separate frequency scaling factors were used for vibrational zero-point energy (0.9735 for ZPE) and for the thermal contributions (determined at 298.15K) as proposed by Laury et al.[19]. Actually, they They ~~have~~ proposed separate scaling factors to correct entropy (1.0583) and enthalpy (1.0566) contributions to the free energy of formation at 298K, however, these factors ~~which~~ were differing only in the third significant digit, therefore their mean (1.0575) was used for direct calculation of the Helmholtz free energies of formation (*i.e.* $F = -RT\ \ln Q$). For the composite methods the default scaling factors were applied. **Ethylene** and **butadiene** are considered in a solvated form in the reactions, thus all considered reactions take place in solution. For such reactions the standard molar volume change of all reactions is negligible and the Helmholtz and Gibbs free energies of reactions ($\Delta_r F$, $\Delta_r G$) are equal.

7.5. Calculation of equilibrium constants

Ez a mondat szerepel később is.

~~Knowing the initial concentration of reactants and the equilibrium constants of all steps, one can predict equilibrium product compositions by solving Eq. (1) simultaneously for all steps.~~ From the standard free energy of reaction (at 298.15K and assuming $c^{\ominus} = 1M$ reference state), one can calculate the equilibrium constant expressed in molar concentrations (K_c) using the following formulae.

$$K_c = \exp\left(-\frac{\Delta_\mathrm{r} G^{\ominus}(T;c^{\ominus}=1\mathrm{M})}{RT}\right) = \prod_{i=1}^{n}\left(\frac{c_{i,eq}}{c^{\ominus}}\right)^{\nu_i} \tag{1}$$

Here, n is the number species involved in the reactions, and ν_i is their corresponding stoichiometric number. Knowing the initial concentration of reactants and the equilibrium constants of all steps one can predict equilibrium product compositions by solving Eq. (1) simultaneously for all steps.

8. Results of the theoretical calculations

8.1. Results for the reactions with ethylene cross-coupling agent

Table S11. Theoretically calculated electronic energy (hartree) of the lowest energy conformers and reactions (kcal/mol) in toluene for ~~the~~ reactions (at 0K without zero-point energy) ~~when~~ with **ethylene** ~~used as a~~ cross-coupling agent. See further details in the theory section.

geometry + vibrations single-point energy	M062X	M062X DLPNO-CCSD(T)	G3	G4	CBS-APNO	G3, G4, CBS-APNO mean	 std
CPD (C_5H_6)	-194.079774	-193.735644	-194.023775	-194.061281	-194.094215		
Ethylene (C_2H_4)	-78.572682	-78.439531	-78.556876	-78.572654	-78.582733		
4^E (C_7H_{10})	-272.665430	-272.186500	-272.592792	-272.645850	-272.688208		
7 (C_5H_8)	-195.269524	-194.929625	-195.220392	-195.258774	-195.288076		
BD (C_4H_6)	-155.968663	-155.696461	-155.928714	-155.959238	-155.982438		
12 (cyc C_6H_8)	-233.390471	-232.977690	-233.325037	-233.370087	-233.409205		
15^E (lin C_6H_8)	-233.365820	-232.954531	-233.301926	-233.347196	-233.383543		
CPD + Ethylene ⇒ 4^E	-8.14	-7.11	-7.62	-7.48	-7.07	-7.39	0.29
4^E + Ethylene ⇒ 7 + BD	-0.05	-0.03	0.35	0.31	0.27	+0.31	0.04
CPD + 2 Ethylene ⇒ 7 + BD	-8.19	-7.14	-7.27	-7.17	-6.80	-7.08	0.25
7 ⇒ ½ 12 + Ethylene	1.01	0.78	0.63	0.68	0.46	+0.59	0.11
7 + 7 ⇒ 12 + 2 Ethylene	2.02	1.57	1.25	1.35	0.93	+1.18	0.22
BD ⇒ ½ 15^E + Ethylene	-0.37	-0.36	-0.43	-0.43	-0.44	-0.433	0.005
2 BD ⇒ 15^E + Ethylene	-0.74	-0.72	-0.86	-0.86	-0.88	-0.87	0.01

Table S12. Theoretically calculated standard free energies of formation (with separated electrons + nuclei reference; hartree) and standard free energies of reactions (at 298.15K for $c^{\ominus} = 1$M reference state; kcal/mol) in toluene for reactions with **ethylene** ~~as a~~ cross-coupling agent. See further details in the theory section. The values printed in red are presented in the manuscript (after rounding them to 2 significant digits).

geometry + vibrations single-point energy	M062X	M062X DLPNO-CCSD(T)	G3	G4	CBS-APNO	G3, G4, CBS-APNO mean	 std
CPD (C_5H_6)	-194.011888	-193.667758	-193.957601	-193.991896	-194.025879		
Ethylene (C_2H_4)	-78.540545	-78.407394	-78.525847	-78.539553	-78.550657		
4^E (C_7H_{10})	-272.552602	-272.073672	-272.483092	-272.530995	-272.575103		
7 (C_5H_8)	-195.184986	-194.845087	-195.138271	-195.172544	-195.203360		
BD (C_4H_6)	-155.907822	-155.635620	-155.869743	-155.896950	-155.921569		
12 (cyc C_6H_8)	-233.294726	-232.881944	-233.231655	-233.272552	-233.312936		
15^{EEE} (lin C_6H_8)	-233.275806	-232.864517	-233.214318	-233.255109	-233.293225		
CPD + Ethylene ⇒ 4^E	-0.11	0.93	0.22	0.28	0.90	**+0.47**	0.37
4^E + Ethylene ⇒ 7 + BD	0.21	0.23	0.58	0.66	0.52	**+0.59**	0.07
CPD + 2 Ethylene ⇒ 7 + BD	0.11	1.15	0.80	0.95	1.42	**+1.06**	0.32
7 ⇒ ½ 12 + Ethylene	-1.83	-2.06	-2.14	-2.06	-2.36	**-2.19**	0.16
7 + 7 ⇒ 12 + 2 Ethylene	-3.67	-4.12	-4.27	-4.12	-4.73	-4.37	0.31
BD ⇒ ½ 15^E + Ethylene	-0.22	-0.21	-0.21	-0.24	-0.23	**-0.23**	0.01
2 BD ⇒ 15^E + Ethylene	-0.44	-0.42	-0.43	-0.48	-0.47	-0.46	0.03

Table S13. Theoretically calculated equilibrium constants at 298.15K for $c^{\ominus} = 1$M reference state in toluene for reactions with **ethylene** ~~as a~~ cross-coupling agent. See further details in the theory section. The values printed in red are presented in the manuscript (after rounding them to 2 significant digits).

geometry + vibrations single-point energy	M062X	M062X DLPNO-CCSD(T)	G3	G4	CBS-APNO	G3, G2, CBS-APNO geom. mean	 uncertainty factor 1 std
CPD + Ethylene ⇒ 4^E	1.20	0.21	0.69	0.62	0.22	**0.45**	1.90
4^E + Ethylene ⇒ 7 + BD	0.70	0.68	0.38	0.33	0.41	**0.37**	1.12
CPD + 2 Ethylene ⇒ 7 + BD	0.83	0.14	0.26	0.20	0.091	**0.17**	1.73
7 ⇒ ½ 12 + Ethylene	22.1	32.2	36.8	32.4	54.0	**40**	1.30
7 + 7 ⇒ 12 + 2 Ethylene	488	1039	1351	1051	2913	**1605**	1.70
BD ⇒ ½ 15^E + Ethylene	1.45	1.43	1.43	1.50	1.48	**1.47**	1.023
2 BD ⇒ 15^E + Ethylene	2.11	2.04	2.05	2.24	2.20	**2.16**	1.047

8.2. Results for the reactions with *cis*-butene diol diacetate (2^Z) cross-coupling agent

Table S14. Theoretically calculated electronic energies (hartree) of the lowest energy conformers and reactions (at 0K without zero-point energy), standard free energies of species (hartree) and reactions (kcal/mol), and equilibrium constants of reactions at 298.15K with $c^{\ominus} = 1M$ reference state in toluene solvent for reactions with ***cis*-butene diol diacetate** (2^Z) ~~as a~~ cross-coupling agent. See further details in the theory section. The values printed in red are presented in the manuscript (after rounding them to 2 significant digits). The values for **CPD** and **12** are the same as in Tables S11-12.

	Electronic energy		Standard free energy ($c^{\ominus} = 1M$)		Equilibrium constant $K_c(c^{\ominus} = 1M)$	
geometry + vibrations single-point energy	**M062X**	**M062X DLPNO-CCSD(T)**	**M062X**	**M062X DLPNO-CCSD(T)**	**M062X**	**M062X DLPNO-CCSD(T)**
CPD (C_5H_6)	-194.079774	-193.735644	-194.011888	-193.667758		
2^Z ($C_8H_{12}O_4$)	-612.961164	-612.014927	-612.813635	-611.867398		
2^E ($C_8H_{12}O_4$)	-612.963576	-612.016677	-612.817496	-611.870597		
5^{EEE} ($C_{13}H_{18}O_4$)	-807.056425	-805.765762	-806.827029	-805.536366		
8^{EE} ($C_{10}H_{14}O_4$)	-690.359618	-689.274685	-690.184170	-689.099237		
9^{EE} ($C_{11}H_{16}O_4$)	-729.659811	-728.507158	-729.457851	-728.305198		
12 (cyc C_6H_8)	-233.390471	-232.977690	-233.294726	-232.881944		
CPD + $2^Z \Rightarrow 5^{EEE}$	-9.72	-9.53	-0.94	**-0.76**	4.9	**3.6**
5^{EEE}+ $2^Z \Rightarrow 8^{EE} + 9^{EE}$	-1.15	-0.72	-0.85	**-0.42**	4.2	**2.0**
CPD + $2^Z + 2^Z \Rightarrow 8^{EE} + 9^{EE}$	-10.87	-10.26	-1.80	**-1.18**	21	7.3
$9^{EE} \Rightarrow$ ½ 12 + 2^Z	2.14	2.12	-1.97	**-1.99**	28	**29**
$9^{EE} + 9^{EE} \Rightarrow$ 12 + $2^Z + 2^Z$	4.28	4.25	-3.95	-3.98	786	829
$9^{EE} \Rightarrow$ ½ 12 + 2^E	0.63	1.03	-4.40	**-4.00**	1673	**853**
$9^{EE} + 9^{EE} \Rightarrow$ 12 + $2^E + 2^E$	1.25	2.05	-8.80	-8.00	3347	1705

8.3. Results for the reactions with *cis*-stilbene (3^Z) cross-coupling agent

Table S15. Theoretically calculated electronic energies of the lowest energy conformers (hartree) and reactions (at 0K without zero-point energy), standard free energies of species (hartree) and reactions (kcal/mol), and equilibrium constants of reactions at 298.15K with $c^{\ominus} = 1M$ reference state in toluene solvent for reactions with ***cis*-stilbene** (3^Z) ~~as a~~ cross-coupling agent. See further details in the theory section. The values printed in red are presented in the manuscript (after rounding them to 2 significant digits). The values for **CPD** and **12** are the same as those appearing in Tables S11-12.

	Electronic energy		Standard free energy ($c^{\ominus} = 1M$)		Equilibrium constant $K_c(c^{\ominus} = 1M)$	
geometry + vibrations single-point energy	**M062X**	**M062X DLPNO-CCSD(T)**	**M062X**	**M062X DLPNO-CCSD(T)**	**M062X**	**M062X DLPNO-CCSD(T)**
CPD (C_5H_6)	-194.079774	-193.735644	-194.011888	-193.667758		
3^Z ($C_{14}H_{12}$)	-540.653902	-539.675210	-540.477380	-539.498688		
3^E ($C_{14}H_{12}$)	-540.659216	-539.680424	-540.483402	-539.504610		
6^{EEE} ($C_{19}H_{18}$)	-734.752076	-733.428017	-734.495484	-733.171425		
10^{EE} ($C_{16}H_{14}$)	-618.057141	-616.938973	-617.851892	-616.733723		
11^{EE} ($C_{17}H_{16}$)	-657.354832	-656.169772	-657.126524	-655.941464		
12 (cyc C_6H_8)	-233.390471	-232.977690	-233.294726	-232.881944		
CPD + $3^Z \Rightarrow 6^{EEE}$	-11.55	-10.77	-3.90	**-3.12**	723	**195**
6^{EEE}+ $3^Z \Rightarrow 10^{EE} + 11^{EE}$	-3.76	-3.46	-3.48	**-3.18**	358	**216**
CPD + $3^Z + 3^Z \Rightarrow 10^{EE} + 11^{EE}$	-15.31	-14.23	-7.38	**-6.31**	258419	42063
$11^{EE} \Rightarrow$ ½ 12 + 3^Z	3.57	3.59	1.12	**+1.13**	0.15	**0.15**
$11^{EE} + 11^{EE} \Rightarrow$ 12 + $3^Z + 3^Z$	7.15	7.17	2.23	+2.26	0.023	0.022
$11^{EE} \Rightarrow$ ½ 12 + 3^E	0.24	0.32	-2.66	**-2.58**	89	**78**
$11^{EE} + 11^{EE} \Rightarrow$ 12 + $3^E + 3^E$	0.48	0.63	-5.32	-5.17	7975	6145

9. Geometries, vibrational and rotational data

9.1. CPD (C_5H_6) – M06-2X/cc-pVTZ

```
*xyz 0 1
C  0.000000  1.173455 0.280263
C  0.000000  0.733920-0.985265
C  0.000000 -0.733920-0.985265
C  0.000000 -1.173455 0.280263
H  0.000000  2.202162 0.606278
H  0.000000  1.347309-1.874172
H  0.000000 -1.347309-1.874172
H  0.000000 -2.202162 0.606278
C  0.000000  0.000000 1.211814
H -0.875149  0.000000 1.869256
H  0.875149  0.000000 1.869256
*

Rotational symmetry number
2.

Rotational constants in GHz:
8.537960e+00 8.291310e+00 4.317360e+00

No hindered rotor corrections are necessary.

frequencies (cm-1)
344.7023   530.3732       685.2708       734.8416       815.5523       816.5912       921.9516
937.4717   978.2487       983.0768       987.2907       1020.3604      1109.8209      1129.8729
1130.9132  1272.2737      1325.5348      1399.6561      1416.4294      1587.4949      1669.7502
3054.7981  3084.2347      3224.8881      3234.2978      3252.6555      3258.9295
```

9.2. CPD (C_5H_6) – G3

```
*xyz 0 1 RHF\GTBas1
C  0.000000    1.174893    0.274754
C -0.000000    0.738600   -0.980700
C  0.000000   -0.738600   -0.980700
C  0.000000   -1.174893    0.274754
H  0.000000    2.198539    0.598571
H -0.000000    1.345165   -1.867308
H  0.000000   -1.345165   -1.867308
H -0.000000   -2.198539    0.598571
C  0.000000    0.000000    1.217708
H -0.873275    0.000000    1.868097
H  0.873275   -0.000000    1.868097
*

No hindered rotor corrections are necessary.

frequencies (cm-1)
380.0587   559.2828       750.7132       809.7231       865.2864       866.3984       983.2798
1033.5893  1037.8505      1066.7966      1074.9869      1083.0075      1214.2755      1229.9408
1252.5063  1411.9580      1453.3497      1532.2245      1578.7661      1738.2500      1814.8152
3195.2177  3222.1999      3380.7896      3389.9820      3408.0637      3416.4347

*xyz 0 1 RMP2-Full\GTBas1
C  0.000000    1.176393    0.285493
C -0.000000    0.731710   -0.992461
C  0.000000   -0.731710   -0.992461
C  0.000000   -1.176393    0.285493
H  0.000000    2.210096    0.613099
H -0.000000    1.348598   -1.885377
H -0.000000   -1.348598   -1.885377
H -0.000000   -2.210096    0.613099
C -0.000000    0.000000    1.214424
H -0.878913    0.000000    1.874302
H  0.878913   -0.000000    1.874302
*

Rotational symmetry number
2.

Rotational constants in GHz:
8.446477e+00 8.267058e+00 4.288301e+00
```

9.3. CPD (C_5H_6) – G4

```
*xyz 0 1
C     0.000000    1.179350    0.279965
C     0.000000    0.734449   -0.990565
C     0.000000   -0.734449   -0.990565
C     0.000000   -1.179350    0.279965
H     0.000000    2.209499    0.610041
H     0.000000    1.344851   -1.885237
H     0.000000   -1.344851   -1.885237
H     0.000000   -2.209499    0.610041
C     0.000000    0.000000    1.214743
H    -0.875178    0.000000    1.880692
H     0.875178    0.000000    1.880692
*

Rotational symmetry number
2.

Rotational constants in GHz:
8.465186e+00 8.236785e+00  4.283981e+00

No hindered rotor corrections are necessary.

frequencies (cm-1)
348.6191   524.4236      689.0860      720.3425      810.5881      810.9352      922.1997
925.4099   955.3536      962.0498      969.8223      1014.2406     1114.2872     1116.5288
1129.8486  1262.9642     1314.7235     1395.1785     1409.1752     1556.9983     1642.3874
3017.1796  3040.8038     3199.0211     3209.3509     3229.0939     3235.8283
```

9.4. CPD (C_5H_6) – CBS-APNO

```
*xyz 0 1 RHF\6-311G(d,p)
C -0.000000    1.174368    0.275215
C  0.000000    0.738815   -0.979869
C -0.000000   -0.738815   -0.979869
C -0.000000   -1.174368    0.275215
H -0.000000    2.198866    0.596969
H  0.000000    1.347098   -1.865411
H -0.000000   -1.347098   -1.865411
H  0.000000   -2.198866    0.596969
C -0.000000   -0.000000    1.217382
H -0.874472   -0.000000    1.866674
H  0.874472    0.000000    1.866674
*

No hindered rotor corrections are necessary.

frequencies (cm-1)
379.0516   559.5787      742.9919      806.7166      865.3330      866.9090      975.2722
1021.5991  1026.1000     1056.4589     1070.6852     1082.9833     1197.8256     1214.2772
1239.6853  1392.0535     1436.7117     1512.5903     1547.7014     1713.7376     1789.2086
3160.2858  3186.3857     3336.3322     3345.1574     3363.4862     3372.3654


*xyz 0 1 RQCISD-FC\6-311G(d,p)
C -0.000000    1.183003    0.282908
C  0.000000    0.740727   -0.994451
C -0.000000   -0.740727   -0.994451
C -0.000000   -1.183003    0.282908
H -0.000000    2.216947    0.611004
H  0.000000    1.356412   -1.888303
H  0.000000   -1.356412   -1.888303
H -0.000000   -2.216947    0.611004
C  0.000000    0.000000    1.224512
H -0.883702   -0.000000    1.878854
H  0.883702   -0.000000    1.878854
*

Rotational symmetry number
2.

Rotational constants in GHz:
8.387075e+00 8.158465e+00 4.244953e+00
```

9.5. Ethylene (C_2H_4) – M06-2X/cc-pVTZ

```
*xyz 0 1
C -0.660910 1.966902  0.01495600
H -1.227729 2.888861  0.02785500
```

```
C  0.660911 1.966901 -0.01495400
H  1.227731 2.888859 -0.02785500
H -1.227730 1.044945  0.02785400
H  1.227730 1.044943 -0.02785600
*

Rotational symmetry number
4.

Rotational constants in GHz:
1.474856e+02 3.050290e+01 2.527544e+01

No hindered rotor corrections are necessary.

frequencies (cm-1)
827.8550
990.2005
1005.4723
1071.9505
1240.4563
1383.0548
1471.4773
1714.3515
3157.5245
3173.6008
3233.9762
3259.7418
```

9.6. Ethylene (C_2H_4) – G3

```
*xyz 0 1 RHF\GTBas1
 C  -0.658596    1.966902    0.014943
 H  -1.225584    2.881479    0.027796
 C   0.658596    1.966901   -0.014943
 H   1.225585    2.881478   -0.027795
 H  -1.225585    1.052326    0.027795
 H   1.225584    1.052325   -0.027796
*

No hindered rotor corrections are necessary.

frequencies (cm-1)
896.0364
1094.8638
1101.9980
1156.1755
1349.9065
1492.4349
1607.8633
1852.1033
3318.9754
3342.5595
3393.6045
3418.6769

*xyz 0 1 RMP2-Full\GTBas1
 C  -0.667504    1.966902    0.015146
 H  -1.237471    2.890027    0.028065
 C   0.667504    1.966901   -0.015146
 H   1.237473    2.890025   -0.028064
 H  -1.237473    1.043779    0.028065
 H   1.237472    1.043777   -0.028065
*
Rotational symmetry number
4.

Rotational constants in GHz:
1.471133e+02 2.994761e+01 2.488235e+01
```

9.7. Ethylene (C_2H_4) – G4

```
*xyz 0 1
 C    -0.663799    1.966902    0.015070
 H    -1.237482    2.888627    0.028064
 C     0.663800    1.966901   -0.015069
 H     1.237484    2.888626   -0.028062
 H    -1.237484    1.045178    0.028063
 H     1.237483    1.045177   -0.028063
*
```

```
Rotational symmetry number
4.

Rotational constants in GHz:
1.475604e+02 3.015906e+01 2.504105e+01

No hindered rotor corrections are necessary.

frequencies (cm-1)
822.7260
970.1280
981.3813
1072.7949
1234.5690
1381.3389
1469.4805
1694.3943
3137.7459
3154.3413
3210.6099
3237.5628
```

9.8. Ethylene (C_2H_4) – CBS-APNO

```
*xyz 0 1 RHF\6-311G(d,p)
C -0.658500    1.966902    0.014938
H -1.223653    2.883274    0.027753
C  0.658500    1.966901   -0.014938
H  1.223655    2.883273   -0.027752
H -1.223654    1.050531    0.027752
H  1.223654    1.050529   -0.027753
*

No hindered rotor corrections are necessary.

frequencies (cm-1)
888.4214
1079.8721
1097.9721
1144.8140
1334.4006
1468.6027
1581.2037
1817.6752
3268.2805
3291.3596
3344.9964
3372.1145

*xyz 0 1 RQCISD-FC\6-311G(d,p)
C -0.669346    1.966902    0.015183
H -1.238427    2.893349    0.028088
C  0.669346    1.966901   -0.015183
H  1.238428    2.893348   -0.028087
H -1.238428    1.040456    0.028087
H  1.238427    1.040454   -0.028088
*

Rotational symmetry number
4.

Rotational constants in GHz:
1.460599e+02 2.982625e+01 2.476840e+01
```

9.9. 4^E (C_7H_{10}) – M06-2X/cc-pVTZ

```
*xyz 0 1
C  3.344417 -0.375672 -0.491504
H  3.471900  0.410889 -1.225493
C  2.197122 -0.522131  0.165081
H  2.093547 -1.318058  0.896240
C  1.033116  0.331624 -0.029960
H  1.130838  1.131183 -0.759691
C -0.113943  0.181520  0.629040
H -0.201944 -0.628248  1.349066
C -1.319647  1.046106  0.453808
C -2.538116  0.318849 -0.050995
H -3.459899  0.891303 -0.029940
C -2.560185 -0.923151 -0.509861
H -1.662747 -1.527472 -0.557148
```

```
H -1.576671  1.508555  1.412624
H -1.090475  1.872852 -0.224157
H -3.478998 -1.372774 -0.860715
H  4.185200 -1.032143 -0.317422
*

Rotational symmetry number
1.

Rotational constants in GHz:
7.628310e+00 1.085650e+00 1.007740e+00

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                   7.251

frequencies (cm-1)
56.6207       127.7155      152.6867      169.1391      227.4099      326.8693      442.3936
456.7592      564.8595      596.2255      686.6619      863.7996      923.9653      939.7332
963.2407      970.2818      982.8197      1005.9805     1039.6448     1057.8559     1060.0840
1127.2203     1178.1618     1234.2304     1298.1102     1325.2551     1330.5735     1332.2707
1365.3650     1447.6957     1456.3633     1467.2244     1700.5055     1731.9062     1759.8153
3038.6293     3075.2771     3151.8113     3155.4487     3161.4865     3162.3140     3170.1821
3172.9033     3251.6001     3254.1342
```

9.10. 4^E (C_7H_{10}) – G3

```
*xyz 0 1 RHF\GTBas1
C  3.370105   -0.363765   -0.476079
H  3.506506    0.408668   -1.213726
C  2.225879   -0.514783    0.171391
H  2.131211   -1.301516    0.902797
C  1.042474    0.328429   -0.033997
H  1.136985    1.116676   -0.764651
C -0.099842    0.171563    0.617700
H -0.185022   -0.622789    1.343403
C -1.318089    1.034141    0.442585
C -2.553601    0.309448   -0.041960
H -3.463102    0.887192    0.013277
C -2.610724   -0.918896   -0.519311
H -1.739633   -1.543416   -0.608910
H -1.558681    1.503007    1.396074
H -1.099126    1.850975   -0.241402
H -3.542973   -1.344361   -0.846438
H  4.211149   -1.007337   -0.291779
*

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)  McClurg
 Total                  7.342

frequencies (cm-1)
59.7628       127.0980      154.9657      170.3016      236.3194      332.2006      465.6018
483.2401      603.5408      640.9470      734.5763      924.0102      983.5280      1014.2242
1053.6584     1063.4578     1075.6479     1105.7572     1125.5901     1152.9009     1155.3594
1207.1139     1269.3854     1340.2998     1420.0038     1443.8944     1447.3233     1454.1396
1505.6047     1584.6435     1590.0781     1617.3190     1832.5167     1871.3195     1908.8056
3178.1263     3214.2326     3320.9868     3323.2062     3324.8854     3331.7846     3340.0472
3341.1124     3411.4899     3412.3448

*xyz 0 1  RMP2-Full\GTBas1
C  3.327563   -0.400300   -0.517203
H  3.442502    0.357107   -1.287581
C  2.185060   -0.523349    0.179075
H  2.105093   -1.294882    0.944955
C  1.019080    0.322246   -0.023352
H  1.097107    1.095816   -0.789226
C -0.124356    0.201113    0.675605
H -0.199411   -0.578565    1.435259
C -1.331841    1.061661    0.481925
C -2.534625    0.318510   -0.043956
H -3.479305    0.860260   -0.004240
C -2.514990   -0.917252   -0.554952
H -1.597104   -1.491572   -0.626797
H -1.605208    1.529256    1.438502
H -1.092337    1.891248   -0.197471
H -3.420717   -1.387658   -0.923083
H  4.177006   -1.050404   -0.338488
*

Rotational symmetry number
```

```
1.

Rotational constants in GHz:
7.334874e+00 1.095614e+00 1.014535e+00
```

9.11. 4^E (C_7H_{10}) – G4

```
*xyz 0 1
C  3.388414 -0.356792 -0.476407
H  3.535468  0.436456 -1.203804
C  2.223135 -0.514106  0.160532
H  2.115895 -1.322036  0.883426
C  1.053594  0.325861 -0.035426
H  1.154333  1.136434 -0.757447
C -0.108929  0.166094  0.609860
H -0.204113 -0.649472  1.326456
C -1.320092  1.032272  0.437954
C -2.561232  0.317994 -0.046308
H -3.470597  0.916300 -0.008317
C -2.623521 -0.929564 -0.501605
H -1.743391 -1.561814 -0.566191
H -1.563575  1.509720  1.400327
H -1.094443  1.862838 -0.245487
H -3.559863 -1.364689 -0.834600
H  4.232432 -1.012260 -0.293988
*

Rotational symmetry number
1.

Rotational constants in GHz:
7.751733e+00 1.058396e+00 9.849025e-01

 Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)     McClurg
 Total                      7.407

frequencies (cm-1)
55.4187       123.0009      144.8910      173.2181      222.1855      312.8442      434.0439
448.7018      559.0309      590.6637      680.5841      851.7699      914.0762      922.6249
933.1310      948.1749      975.8099      1001.0729     1035.7571     1049.9141     1060.7259
1117.3371     1170.7684     1228.5427     1295.1547     1319.0067     1327.0366     1331.9707
1357.4366     1443.7061     1453.7914     1461.7695     1672.3846     1711.4409     1721.9216
2985.4369     3025.6371     3127.0881     3132.1242     3134.7106     3139.8768     3147.5721
3150.7814     3228.4274     3232.4881
```

9.12. 4^E (C_7H_{10}) – CBS-APNO

```
*xyz 0 1 RHF\6-311G(d,p)
C  3.370319   -0.360420   -0.476097
H  3.503572    0.413753   -1.213437
C  2.226897   -0.513634    0.170859
H  2.133470   -1.301167    0.902215
C  1.042870    0.328266   -0.035208
H  1.135385    1.116991   -0.766298
C -0.097695    0.169276    0.616942
H -0.179175   -0.626466    1.342613
C -1.316028    1.030408    0.442760
C -2.551565    0.310425   -0.046397
H -3.458035    0.895217   -0.002253
C -2.614968   -0.919822   -0.516191
H -1.746856   -1.551048   -0.594465
H -1.558520    1.493382    1.398897
H -1.097239    1.849810   -0.237995
H -3.550074   -1.337189   -0.847198
H  4.211158   -1.004549   -0.289773
*

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.) McClurg
 Total                  7.290

frequencies (cm-1)
60.6012       129.2014      155.0105      171.4480      237.4998      332.0328      463.2573
482.2074      603.6005      638.6941      732.8743      918.2353      974.1805      1008.8577
1043.9430     1053.3206     1066.8993     1094.0157     1114.1920     1143.0075     1144.2824
1195.9157     1256.0187     1326.5686     1404.0741     1426.7870     1429.3724     1437.5460
1486.8352     1560.9071     1566.1570     1590.0053     1805.4232     1841.6949     1884.0726
3146.4406     3183.0407     3274.3904     3277.0709     3280.4766     3287.8066     3292.1497
3297.2881     3364.5186     3365.6017
```

```
*xyz 0 1 RQCISD-FC\6-311G(d,p)
C  3.359735   -0.388272   -0.508104
H  3.475968    0.382581   -1.267553
C  2.210496   -0.525396    0.176844
H  2.122399   -1.306988    0.932418
C  1.031195    0.326986   -0.025902
H  1.115540    1.111066   -0.780825
C -0.117363    0.189907    0.660677
H -0.196358   -0.600488    1.409937
C -1.333634    1.058095    0.471752
C -2.553312    0.320071   -0.047014
H -3.487911    0.881650   -0.013305
C -2.558971   -0.924833   -0.542770
H -1.651323   -1.519875   -0.607114
H -1.596948    1.523594    1.433612
H -1.096937    1.884840   -0.213204
H -3.478584   -1.379085   -0.902361
H  4.209525   -1.040619   -0.328114
*

Rotational symmetry number
1.

Rotational constants in GHz:
7.386982e+00 1.074769e+00 9.970749e-01
```

9.13. 7 (C_5H_8) – M06-2X/cc-pVTZ

```
*xyz 0 1
C -1.795557  0.103437  0.239869
H -1.122113  0.003231 -0.602234
C -1.394577  0.615751  1.393398
H -2.106973  0.705330  2.207260
C -0.006153  1.111560  1.697318
C  1.010402  0.777394  0.651096
H  1.176248 -0.280851  0.471452
C  1.693118  1.669845 -0.048962
H  1.545003  2.733083  0.099858
H -0.037803  2.193645  1.852378
H  0.305051  0.680521  2.654447
H -2.815951 -0.226160  0.099550
H  2.422197  1.371738 -0.790277
*

Rotational symmetry number
2.

Rotational constants in GHz:
1.122220e+01 3.176190e+00 2.703950e+00

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                   4.772

frequencies (cm-1)
90.9708       154.8041      264.7847      419.5925      502.7768      576.5476      688.3419
898.0078      925.8920      969.3062      974.9747      975.8838      1046.6785     1051.0670
1084.3738     1144.9029     1253.8275     1318.7248     1329.1909     1354.4386     1445.5985
1454.0912     1473.6531     1731.1047     1740.0620     3040.1537     3075.3532     3153.6402
3161.6817     3163.0398     3173.1261     3243.8790     3251.6076
```

9.14. 7 (C_5H_8) – G3

```
*xyz 0 1  RHF\GTBas1
C -1.826351    0.103084    0.242398
H -1.189347    0.012149   -0.619450
C -1.399935    0.601500    1.386893
H -2.092660    0.673728    2.210869
C -0.009587    1.113641    1.686440
C  1.028148    0.784941    0.647892
H  1.208800   -0.265526    0.481526
C  1.717950    1.672878   -0.041195
H  1.570610    2.732033    0.087180
H -0.055154    2.190101    1.835570
H  0.303106    0.694395    2.641953
H -2.842630   -0.229807    0.126160
H  2.459942    1.375406   -0.761082
```

```
*

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                    4.797

frequencies (cm-1)
95.8910        148.9858       268.7784       441.6909       536.1226       620.0213       732.5202
948.1822       1009.8157      1032.3647      1074.0232      1076.3550      1141.4376      1147.8631
1182.3808      1239.1849      1367.9612      1436.6735      1444.9615      1492.5584      1583.8908
1592.6050      1621.3964      1870.8670      1876.8739      3180.3071      3214.6895      3320.4417
3320.9463      3334.9439      3341.0442      3403.4677      3411.4237

*xyz 0 1  RMP2-Full\GTBas1
C -1.790754    0.132732    0.219886
H -1.119161    0.075013   -0.630342
C -1.389084    0.604878    1.404980
H -2.105600    0.653801    2.224435
C -0.002710    1.108174    1.717138
C  1.019063    0.760888    0.678362
H  1.220300   -0.300643    0.537358
C  1.673519    1.657486   -0.067626
H  1.494705    2.723740    0.039833
H -0.034013    2.197498    1.855635
H  0.307290    0.692735    2.686114
H -2.810102   -0.205262    0.065767
H  2.409438    1.357483   -0.806386
*

Rotational symmetry number
2.

Rotational constants in GHz:
1.083565e+01 3.207914e+00 2.714948e+00
```

9.15. 7 (C_5H_8) – G4

```
*xyz 0 1
C  -1.825068    0.095462    0.239963
H  -1.169529    0.002098   -0.620179
C  -1.402966    0.605456    1.393056
H  -2.101364    0.686870    2.224942
C  -0.010782    1.112695    1.688266
C   1.021327    0.784915    0.647341
H   1.188700   -0.277246    0.472563
C   1.720920    1.676899   -0.047053
H   1.581263    2.745674    0.092460
H  -0.049824    2.199507    1.847458
H   0.304093    0.690243    2.655002
H  -2.847932   -0.242139    0.110513
H   2.464053    1.378091   -0.779177
*

Rotational symmetry number
2.

Rotational constants in GHz:
1.127895e+01 3.098534e+00 2.648355e+00

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)    McClurg
 Total                     4.808

 frequencies (cm-1)
89.3238        151.6044       249.3298       408.5717       495.2849       571.9891       680.0527
884.0558       922.6913       949.1085       953.2801       960.8475       1043.8411      1048.0387
1078.5929      1136.3151      1245.3348      1317.1524      1325.2729      1348.0189      1441.7487
1452.0344      1468.8443      1711.8057      1716.7345      2991.6519      3026.5186      3133.9698
3134.9294      3143.7352      3151.4795      3221.5984      3229.2325
```

9.16. 7 (C_5H_8) – CBS-APNO

```
*xyz 0 1 RHF\6-311G(d,p)
C -1.828648    0.098456    0.244450
H -1.189712   -0.004165   -0.615430
C -1.400499    0.604580    1.384118
H -2.095076    0.688368    2.206409
C -0.009001    1.111920    1.682878
C  1.029199    0.786423    0.645063
H  1.211638   -0.263779    0.473935
```

```
C  1.720071    1.676587   -0.038747
H  1.570760    2.735564    0.094789
H -0.054319    2.187748    1.836123
H  0.302914    0.686315    2.636103
H -2.847996   -0.228366    0.133305
H  2.463558    1.378873   -0.757843
*

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                    4.762

frequencies (cm-1)
98.0368        152.5332       268.3664       440.3144       535.4114       618.7808       729.5837
939.4257       1000.8406      1023.3285      1065.6880      1067.3386      1131.6710      1137.7879
1170.3578      1227.4006      1354.7312      1419.7910      1428.7959      1472.9761      1560.1252
1568.0736      1594.2097      1841.4333      1847.9383      3148.4104      3182.7129      3270.8467
3274.2720      3287.0965      3292.3220      3355.7764      3364.3682

*xyz 0 1 RQCISD-FC\6-311G(d,p)
C -1.810337    0.115927    0.224585
H -1.140259    0.037091   -0.627857
C -1.400244    0.606326    1.402283
H -2.113948    0.674801    2.224387
C -0.003588    1.109695    1.711198
C  1.027251    0.766130    0.665364
H  1.220535   -0.296603    0.512110
C  1.696871    1.669822   -0.062307
H  1.524127    2.737444    0.061843
H -0.038630    2.199358    1.852681
H  0.309573    0.685337    2.676951
H -2.835341   -0.217108    0.084044
H  2.436882    1.370305   -0.800129
*

Rotational symmetry number
2.

Rotational constants in GHz:
1.090724e+01 3.141327e+00 2.670684e+00
```

9.17. 12 (cyc C_6H_8) – M06-2X/cc-pVTZ

```
*xyz 0 1
C -1.55662600  0.36487200  0.04621100
C -0.23105400  0.36473900  0.03181100
C -0.23092000  2.86179800  0.02110600
C -1.55649100  2.86193200  0.03550500
H -2.09001500 -0.57861500  0.05608100
H  0.30223100 -0.57885700  0.03003500
H  0.30246900  3.80528600  0.01123600
H -2.08977700  3.80552700  0.03728100
C  0.59968500  1.61318600  0.01748000
H  1.25935600  1.60941500 -0.85698900
H  1.27796600  1.61681900  0.87760300
C -2.38723100  1.61348500  0.04983600
H -3.04690200  1.61725500  0.92430300
H -3.06551100  1.60985200 -0.81028800
*

Rotational symmetry number
4.

Rotational constants in GHz:
5.197810e+00 4.941200e+00 2.612560e+00

frequencies (cm-1)
116.5114       388.6884       415.2863       541.0343       580.7061       634.4087       730.8251
872.9545       904.3035       960.2257       967.6437       973.6654       992.6965       1023.2166
1044.1560      1049.5355      1175.3129      1226.1093      1228.1020      1228.4281      1366.1665
1392.4577      1417.0896      1442.2015      1469.4119      1473.2342      1735.4824      1782.0028
3030.5076      3032.2133      3045.7288      3047.0650      3171.3949      3171.8333      3192.9131
3195.1786
```

9.18. 12 (cyc C_6H_8) – G3

```
*xyz 0 1 RHF\GTBas1
C -0.659714    1.252169   -0.000001
C  0.659714    1.252169    0.000001
C  0.659714   -1.252169    0.000001
```

```
C -0.659714   -1.252169   -0.000001
H -1.193100    2.188648   -0.000002
H  1.193100    2.188648    0.000003
H  1.193100   -2.188648    0.000001
H -1.193100   -2.188648   -0.000004
C  1.495145    0.000000    0.000000
H  2.157969   -0.000001    0.865205
H  2.157963    0.000000   -0.865210
C -1.495145    0.000000    0.000001
H -2.157970    0.000001   -0.865203
H -2.157962    0.000000    0.865211
*

No hindered rotor corrections are necessary.

frequencies (cm-1)
140.7757       416.4100       438.5101       577.4501       617.3902       698.8869       798.6293
908.6309       950.8034       1011.8070      1051.5701      1060.8426      1100.0611      1116.5842
1120.7233      1145.5980      1280.2336      1328.4187      1335.6635      1338.7591      1494.8347
1526.7704      1548.5970      1568.8887      1623.8670      1625.4062      1872.2149      1920.5256
3169.6224      3169.6586      3182.6589      3182.9292      3326.9326      3327.4225      3351.0606
3354.7774

*xyz 0 1 RMP2-Full\GTBas1
C -0.669546    1.248675    0.000000
C  0.669546    1.248675    0.000000
C  0.669546   -1.248675    0.000000
C -0.669546   -1.248675    0.000000
H -1.203706    2.197421    0.000000
H  1.203706    2.197421    0.000000
H  1.203706   -2.197421    0.000000
H -1.203706   -2.197421    0.000000
C  1.500704    0.000000    0.000000
H  2.173237    0.000000    0.870857
H  2.173238    0.000000   -0.870856
C -1.500704    0.000000    0.000000
H -2.173237    0.000000   -0.870856
H -2.173237    0.000000    0.870856
*

Rotational symmetry number
4.

Rotational constants in GHz:
5.190606e+00 4.882575e+00 2.594931e+00
```

9.19. 12 (cyc C_6H_8) – G4

```
*xyz 0 1
C -1.559434    0.360246    0.046227
C -0.228248    0.360111    0.031830
C -0.228112    2.866425    0.021089
C -1.559297    2.866559    0.035486
H -2.100420   -0.583085    0.056121
H  0.312636   -0.583329    0.030023
H  0.312875    3.809756    0.011195
H -2.100181    3.809999    0.037293
C  0.604317    1.613185    0.017456
H  1.273275    1.609395   -0.858154
H  1.292057    1.616837    0.878393
C -2.391862    1.613486    0.049860
H -3.060821    1.617275    0.925469
H -3.079602    1.609834   -0.811078
*

Rotational symmetry number
4.

Rotational constants in GHz:
5.163733e+00 4.899804e+00 2.592560e+00

No hindered rotor corrections are necessary.

frequencies (cm-1)
125.1698       384.8332       412.8969       537.9669       576.6230       635.7791       729.3474
859.4570       891.7568       946.8562       968.4039       970.5195       995.0700       1006.4550
1022.8955      1041.8016      1169.3599      1207.0740      1216.2227      1223.9847      1359.7902
1382.9422      1394.3200      1437.1908      1462.9750      1466.6603      1712.6945      1756.6149
2977.3156      2978.1659      2983.2473      2984.5073      3141.4264      3141.8262      3163.7387
3166.7198
```

9.20. 12 (cyc C_6H_8) – CBS-APNO

```
*xyz 0 1 RHF\6-311G(d,p)
C -0.659239    1.252079    0.000000
C  0.659239    1.252079    0.000000
C  0.659239   -1.252079    0.000000
C -0.659239   -1.252079    0.000000
H -1.191630    2.189566    0.000000
H  1.191630    2.189566    0.000000
H  1.191630   -2.189566    0.000000
H -1.191630   -2.189566   -0.000001
C  1.493869    0.000000    0.000000
H  2.155186    0.000000    0.866337
H  2.155185    0.000000   -0.866337
C -1.493869    0.000000    0.000000
H -2.155186    0.000000   -0.866336
H -2.155185    0.000000    0.866338
*

No hindered rotor corrections are necessary.

frequencies (cm-1)
139.5110       417.2127       435.6174       576.6335       615.0152       693.5409       795.4995
900.6954       941.7395       1002.1114      1046.9813      1050.7181      1088.9766      1104.0138
1115.6299      1139.1626      1265.5173      1312.5159      1323.4977      1324.9037      1475.8815
1507.3722      1533.3018      1550.9069      1594.3264      1595.9278      1846.0778      1895.7129
3138.9466      3139.0580      3150.1343      3150.4956      3284.0193      3284.5396      3309.0137
3312.6170

*xyz 0 1 RQCISD-FC\6-311G(d,p)
C  0.000000    0.670256    1.257906
C  0.000000   -0.670256    1.257906
C  0.000000   -0.670256   -1.257906
C  0.000000    0.670256   -1.257906
H  0.000007    1.206776    2.206099
H  0.000007   -1.206775    2.206099
H  0.000007   -1.206775   -2.206099
H  0.000007    1.206776   -2.206099
C -0.000001   -1.506924    0.000000
H -0.875499   -2.174341    0.000000
H  0.875493   -2.174346    0.000000
C -0.000001    1.506924    0.000000
H  0.875493    2.174346    0.000000
H -0.875500    2.174340    0.000000
*

Rotational symmetry number
4.

Rotational constants in GHz:
5.122354e+00 4.855531e+00 2.571057e+00
```

9.21. 15^{EEE} (lin C_6H_8) – M06-2X/cc-pVTZ

```
*xyz 0 1
C -0.19686200 -3.05062500 0.00000000
H  0.36696900 -3.97262000 0.00000000
H -1.27731700 -3.12865400 0.00000000
C  0.40602100 -1.86367200 0.00000000
H  1.49026600 -1.81101200 0.00000000
C -0.30298700 -0.59663700 0.00000000
H -1.38868300 -0.64108100 0.00000000
C  0.30298700  0.59663700 0.00000000
H  1.38868300  0.64108100 0.00000000
C -0.40602100  1.86367200 0.00000000
H -1.49026600  1.81101200 0.00000000
C  0.19686200  3.05062500 0.00000000
H -0.36696900  3.97262000 0.00000000
H  1.27731700  3.12865400 0.00000000
*

Rotational symmetry number
2.

Rotational constants in GHz:
2.659680e+01 1.350390e+00 1.285140e+00

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                    1.038
```

```
frequencies (cm-1)
95.7816        146.6965       215.4760       258.0056       353.5803       448.0567       545.0039
625.1698       722.4716       925.5027       947.2344       959.4376       965.7922       979.5719
991.8469       1040.4076      1066.0287      1161.9663      1222.2951      1279.0580      1319.6479
1329.1529      1332.0053      1438.3124      1465.5380      1670.0306      1720.7111      1740.3556
3157.0897      3159.0314      3164.8321      3165.8252      3172.4738      3172.9542      3258.2227
3258.2364
```

9.22. 15^{EEE} (lin C_6H_8) – G3

```
*xyz 0 1  RHF\GTBas1
C  1.209098    2.811245    0.000000
H  2.124510    3.374224    0.000000
H  0.293522    3.377721    0.000000
C  1.209098    1.487146    0.000000
H  2.147943    0.956745    0.000000
C -0.001996    0.664749    0.000000
H -0.942795    1.192813    0.000000
C  0.001996   -0.664749    0.000000
H  0.942795   -1.192813    0.000000
C -1.209098   -1.487146    0.000000
H -2.147943   -0.956745    0.000000
C -1.209098   -2.811245    0.000000
H -2.124510   -3.374224    0.000000
H -0.293522   -3.377721    0.000000
*

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.) McClurg
 Total                  1.043

frequencies (cm-1)
96.7797        157.9431       210.5837       267.3838       375.7407       469.9703       580.6840
669.6373       777.2695       1001.6689      1018.7247      1044.2809      1063.0915      1067.0136
1092.5582      1137.4006      1161.9604      1229.0628      1311.9695      1398.4767      1434.9039
1446.6155      1455.9290      1568.1606      1600.8124      1802.0486      1862.5822      1899.8493
3323.6817      3326.8161      3330.7363      3334.6278      3341.4282      3341.5239      3415.6629
3415.6783

*xyz 0 1  RMP2-Full\GTBas1
C  1.206079    2.826998    0.000000
H  2.128955    3.396743    0.000000
H  0.278830    3.393385    0.000000
C  1.206079    1.482158    0.000000
H  2.155953    0.947282    0.000000
C  0.000680    0.676142    0.000000
H -0.952198    1.208382    0.000000
C -0.000680   -0.676142    0.000000
H  0.952198   -1.208382    0.000000
C -1.206079   -1.482158    0.000000
H -2.155953   -0.947282    0.000000
C -1.206079   -2.826998    0.000000
H -2.128955   -3.396743    0.000000
H -0.278830   -3.393385    0.000000
*

Rotational symmetry number
2.

Rotational constants in GHz:
2.636018e+01 1.337481e+00 1.272896e+00
```

9.23. 15^{EEE} (lin C_6H_8) – G4

```
*xyz 0 1
C -0.199779   -3.068047    0.000000
H  0.370197   -3.989995    0.000000
H -1.281840   -3.162639    0.000000
C  0.397412   -1.869235    0.000000
H  1.485399   -1.816565    0.000000
C -0.302365   -0.602522    0.000000
H -1.391337   -0.645986    0.000000
C  0.302365    0.602522    0.000000
H  1.391337    0.645986    0.000000
C -0.397412    1.869235    0.000000
H -1.485399    1.816565    0.000000
C  0.199779    3.068047    0.000000
H -0.370197    3.989995    0.000000
H  1.281840    3.162639    0.000000
*
```

```
Rotational symmetry number
2.

Rotational constants in GHz:
2.679938e+01 1.336116e+00 1.272666e+00

 Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.) McClurg
 Total                  1.034

frequencies (cm-1)
99.8121        145.4500       227.5879       257.5935       348.0942       444.6881       539.0953
624.5116       716.8391       909.5522       930.1265       934.7288       942.7894       979.2298
984.0779       1037.4703      1068.7814      1157.0877      1218.9178      1281.8991      1312.9513
1327.9332      1331.7799      1437.2691      1467.0123      1641.6353      1690.7823      1695.5727
3130.6050      3130.7731      3139.1032      3143.7226      3148.9341      3149.0790      3235.2736
3235.2781
```

9.24. 15^{EEE} (lin C_6H_8) – CBS-APNO

```
*xyz 0 1 RHF\6-311G(d,p)
C  1.209813    2.808281    0.000000
H  2.127376    3.368783    0.000000
H  0.292554    3.373262    0.000000
C  1.209813    1.484887    0.000000
H  2.148902    0.954082    0.000000
C -0.002142    0.664197    0.000000
H -0.943374    1.192280    0.000000
C  0.002142   -0.664197    0.000000
H  0.943374   -1.192280    0.000000
C -1.209813   -1.484887    0.000000
H -2.148902   -0.954082    0.000000
C -1.209813   -2.808281    0.000000
H -2.127376   -3.368783    0.000000
H -0.292554   -3.373262    0.000000
*

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.) McClurg
 Total                  1.042

frequencies (cm-1)
97.3991        157.5943       212.0164       267.9300       375.3825       467.5605       579.3345
669.2663       774.8116       998.6804       1008.7223      1034.2634      1052.2402      1058.0504
1082.2587      1127.0578      1150.3756      1215.5814      1297.5740      1382.5118      1417.0878
1427.5329      1439.3808      1544.4531      1576.7865      1775.2066      1835.0709      1875.5988
3278.4257      3279.4602      3289.6556      3289.7860      3297.7985      3300.1484      3368.9064
3368.9379

*xyz 0 1 RQCISD-FC\6-311G(d,p)
C  1.219520    2.835033    0.000000
H  2.145778    3.402592    0.000000
H  0.289202    3.399842    0.000000
C  1.219520    1.489389    0.000000
H  2.167083    0.949542    0.000000
C  0.000503    0.675418    0.000000
H -0.950686    1.210700    0.000000
C -0.000503   -0.675418    0.000000
H  0.950686   -1.210700    0.000000
C -1.219520   -1.489389    0.000000
H -2.167083   -0.949542    0.000000
C -1.219520   -2.835033    0.000000
H -2.145778   -3.402592    0.000000
H -0.289202   -3.399842    0.000000
*

Rotational symmetry number
2.

Rotational constants in GHz:
2.616632e+01 1.325402e+00 1.261503e+00
```

9.25. 2^{Z} ($C_8H_{12}O_4$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C    -1.26570500   -0.49434500    3.19257900
 C     0.65302600    1.46158400    0.85825300
 H     0.55586300    2.38300400    1.42101100
 C     1.06408200    1.52248700   -0.40058900
```

```
 H     1.29078300    2.49185300   -0.82963900
 C     0.95019500   -0.16495400   -3.57806300
 O     0.76705600    0.73361800   -2.59826600
 O     1.51345900   -1.21313900   -3.40706800
 C     0.36840700    0.31442700   -4.87413200
 H    -0.69438500    0.51164400   -4.74487300
 H     0.84529100    1.24998700   -5.16182300
 H     0.52212100   -0.43713300   -5.64044900
 C     1.29595200    0.36741600   -1.31544300
 H     0.81635700   -0.54996000   -0.97889300
 H     2.36200100    0.15954200   -1.42664100
 C    -2.51489200   -0.11459700    3.92972900
 H    -2.32721200    0.77645800    4.52660300
 H    -3.30006500    0.12602400    3.21511200
 H    -2.82354600   -0.93571400    4.56704800
 C     0.33460100    0.22509800    1.62928300
 H     1.13499200   -0.02014500    2.33019000
 H     0.17409900   -0.64625800    0.99693000
 O    -0.86044200    0.49189500    2.37771900
 O    -0.67998500   -1.53902200    3.29643700
*

Rotational symmetry number
2.

Rotational constants in GHz:
2.104390e+00 2.879800e-01 2.778300e-01

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                   29.066

frequencies (cm-1)
19.9625       29.2566       37.7756       62.9684       65.1056       76.4629       133.1373
146.2863      174.1861      182.2710      240.2016      320.9800      321.7792      395.3537
454.7383      495.6935      613.1351      615.5982      617.1367      649.7009      668.3014
723.6152      927.0285      952.2971      986.4753      992.0214      1012.5270     1013.7993
1041.4816     1053.3312     1073.8104     1074.1453     1096.1960     1105.5874     1152.3754
1262.8290     1273.9639     1288.0990     1296.8952     1303.5959     1364.7114     1396.8332
1407.2398     1425.4952     1462.9555     1469.8059     1470.5616     1475.5926     1475.8368
1499.7724     1507.7896     1776.0291     1839.6722     1842.3451     3074.8392     3076.7128
3089.2644     3089.4192     3127.1776     3139.1598     3157.9970     3158.1445     3177.4149
3196.6720     3200.7226     3201.4946
```

9.26. 2^E ($C_8H_{12}O_4$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C                -2.87217700    1.38525400    2.67253400
 C                -0.14431000    2.59379700    0.64944000
 H                 0.64963100    2.55085600    1.38868800
 C                 0.14862800    2.65864100   -0.63954200
 H                -0.64558100    2.68682200   -1.37917500
 C                 2.88011500    1.65897300   -2.76863700
 O                 1.69366800    1.69495400   -2.14330100
 O                 3.76839600    2.43386100   -2.53187900
 C                 2.93518800    0.54633100   -3.77227600
 H                 2.75415600   -0.40355300   -3.27217000
 H                 2.14846500    0.68519800   -4.51198600
 H                 3.90698500    0.54004300   -4.25315000
 C                 1.54143900    2.73356600   -1.16355900
 H                 2.27702000    2.59870100   -0.37106300
 H                 1.73587700    3.69320800   -1.64555700
 C                -2.92436700    0.18144200    3.56497500
 H                -2.76415600   -0.71671000    2.97071200
 H                -2.12386200    0.23769700    4.30058000
 H                -3.88867900    0.13815200    4.05890200
 C                -1.53757300    2.61191500    1.17735200
 H                -2.27238800    2.54793700    0.37527000
 H                -1.73716200    3.52118400    1.74697700
 O                -1.68502400    1.48553900    2.05553800
 O                -3.76372000    2.17503100    2.50815000
*

Rotational symmetry number
2.

Rotational constants in GHz:
2.884730e+00 2.437700e-01 2.355100e-01

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)    McClurg
```

```
 Total                   151.947

frequencies (cm-1)
26.7672        35.6571        36.5640        62.4608        74.4931        91.0455        93.7250
163.9261       174.2037       179.9783       225.3921       278.0679       291.9953       393.6950
470.6275       479.6277       527.7916       615.5306       617.6048       653.6757       666.9465
825.0830       916.3699       953.1468       984.1216       994.7191       1005.2493      1021.8707
1029.0862      1073.6902      1074.9998      1083.2165      1096.4113      1138.2539      1172.9261
1251.2786      1278.6946      1286.9315      1300.4403      1320.8719      1330.7546      1393.7517
1398.8739      1420.8087      1437.0157      1469.5022      1470.3950      1476.3619      1476.5820
1505.7175      1507.2517      1784.4553      1839.4959      1841.3520      3075.1634      3076.0026
3089.4944      3089.5000      3125.4186      3126.6353      3158.0810      3158.1514      3170.3573
3174.5627      3201.7888      3201.8476
```

9.27. 5^{EEE} ($C_{13}H_{18}O_4$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C    2.57487500    8.62323100   -0.84066400
 C    2.90392100    5.23525900    0.35228800
 H    3.97856000    5.10724700    0.26871000
 C    2.11026100    4.16935200    0.42482400
 H    1.03552100    4.31051100    0.50125100
 C    2.58909200    2.79555700    0.41341400
 H    3.66299000    2.65148000    0.33207900
 C    1.78885000    1.73443200    0.49806800
 H    0.71556100    1.88695700    0.57464900
 C    2.25278800    0.30776700    0.46975400
 C    1.69712100   -0.42177500   -0.72042500
 H    2.00041600   -0.04600400   -1.69404600
 C    0.85774300   -1.44471300   -0.65418300
 H    0.54513100   -1.83213600    0.31082300
 C    0.08094700   -4.27304000   -2.75507400
 H    3.34433800    0.28687200    0.43962400
 H    1.93525600   -0.20486100    1.38086600
 C    0.46570200   -5.71265000   -2.58340100
 H    1.55073000   -5.80085100   -2.57630300
 H    0.09899800   -6.07452900   -1.62421200
 H    0.04501900   -6.29956400   -3.39232900
 C    3.12521700    9.24335000   -2.09060000
 H    4.20803200    9.13100900   -2.10580100
 H    2.72727700    8.72258100   -2.95989100
 H    2.85502300   10.29294100   -2.12390000
 O    0.59554500   -3.51003300   -1.78059900
 O    2.88433600    7.32125900   -0.76411600
 C    2.40521700    6.63628200    0.40690100
 H    2.77946000    7.16397700    1.28602700
 H    1.31636400    6.67513500    0.42835300
 C    0.27530300   -2.10957400   -1.85360900
 H    0.67708200   -1.69469800   -2.77768500
 H   -0.81088200   -2.00988300   -1.88201700
 O    1.93385100    9.19618400    0.00041000
 O   -0.59954600   -3.83245300   -3.64356000
*

Rotational symmetry number
1.

Rotational constants in GHz:
1.310240e+00 7.828000e-02 7.531000e-02

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)    McClurg
 Total                   143.900

frequencies (cm-1)
12.6460        19.6360        31.3962        40.7191        42.6427        64.7121        70.1446
74.7345        79.8595        103.7239       121.7008       158.8884       173.4269       176.9564
197.2348       225.0760       262.7737       285.0421       311.3009       335.6621       340.4457
419.8641       450.2991       495.0724       520.3778       546.1371       564.4130       616.7953
616.9835       658.9318       660.3543       811.7268       831.2160       898.3279       914.4843
936.6411       947.5607       991.8076       994.4005       995.2536       1011.3299      1015.5182
1018.1042      1039.6833      1066.9067      1073.7662      1074.0043      1082.0719      1085.5633
1119.0581      1137.9145      1145.7989      1185.9011      1216.3788      1249.4876      1267.6426
1282.0810      1294.0324      1294.9105      1307.4076      1328.0453      1331.9642      1339.0556
1345.7989      1367.2922      1397.1746      1398.4697      1429.0985      1429.8877      1470.0058
1470.6082      1473.2454      1476.2821      1476.3833      1506.0319      1507.3475      1722.1059
1763.6576      1772.3387      1837.4852      1837.7284      3054.6464      3072.1395      3076.6219
3088.2930      3089.3753      3100.0428      3123.9539      3125.8506      3156.0203      3156.6021
3157.2556      3157.9824      3157.9904      3164.6006      3168.2665      3175.0298      3199.5430
3201.2005
```

9.28. 8^{EE} ($C_{10}H_{14}O_4$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C    3.28530300    0.77980800    4.73472600
 H    2.23079400    0.52253800    4.73205400
 C    4.20498000   -0.18068100    4.69139900
 H    5.25780800    0.08688900    4.68798100
 C    3.88886800   -1.60018800    4.64896000
 H    2.83599600   -1.86758300    4.64461300
 C    4.80875500   -2.56094500    4.61785500
 H    5.86323100   -2.30351400    4.61588200
 C    3.61324300    2.22931900    4.81667000
 H    3.26843100    2.66645100    5.75562600
 H    4.68577700    2.40472600    4.73670200
 C    4.48170700   -4.01295400    4.61463100
 H    4.83271300   -4.50546600    5.52336700
 H    3.40867100   -4.18378700    4.53133100
 C    5.75654500   -6.46562100    2.18537800
 H    5.38096900   -5.98225900    1.28510600
 H    6.81345600   -6.22018400    2.27520000
 H    5.62384700   -7.53979600    2.11982500
 C    2.33056400    4.82117400    2.54069500
 H    2.70020900    4.39142700    1.61120300
 H    1.27408900    4.57124900    2.62248400
 H    2.46388600    5.89725300    2.53728400
 O    2.93708000    2.89343100    3.73582800
 O    5.15062200   -4.61094700    3.49160800
 O    4.37949800   -6.60267300    4.15534600
 O    3.72645800    4.84077400    4.50213700
 C    5.01779700   -5.94089100    3.38035900
 C    3.07688000    4.22674300    3.69777100
*

Rotational symmetry number
2.

Rotational constants in GHz:
2.524030e+00 1.385900e-01 1.353900e-01

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)    McClurg
 Total                   167.871

frequencies (cm-1)
20.7982        30.2844        35.8831        57.1014        60.9947        74.8395        76.4844
111.8388       145.3816       159.5280       169.0431       207.1779       209.1469       272.5907
309.1491       330.8587       371.7667       461.8083       492.7789       529.7118       548.4444
616.6547       616.9897       659.5889       662.7646       815.1802       896.8768       933.0491
939.3845       990.3052       995.9548       996.6195       1008.7541      1023.4600      1038.4708
1074.0701      1074.1273      1084.9389      1086.4399      1126.7919      1151.4950      1196.8941
1238.1292      1267.9048      1286.0032      1295.8878      1296.1733      1327.5165      1336.6078
1351.3674      1391.9116      1400.8026      1422.1969      1436.0429      1470.2790      1470.5371
1476.4581      1476.7515      1505.3491      1505.9951      1731.5351      1773.2336      1838.6054
189.5319       3071.9271      3072.3970      3089.4413      3089.6047      3123.5919      3123.8886
3158.0547      3158.1754      3159.7712      3165.9546      3175.1634      3176.0788      3201.3748
3202.2452
```

9.29. 9^{EE} ($C_{11}H_{16}O_4$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C   -2.01966400    0.31125500    5.95534300
 C   -1.08570900    0.97944000    2.53450600
 H   -1.56511600    1.94122200    2.38048200
 C   -0.09340800    0.59631800    1.74571100
 H    0.37377900   -0.37038700    1.91672000
 C    0.43991200    1.39766800    0.59375700
 C    0.31614500    0.65121300   -0.70302900
 H    0.79800800   -0.32247900   -0.74555600
 C   -0.33197900    1.09510700   -1.76912200
 H   -0.82993000    2.05949300   -1.74304000
 C   -2.04055900   -0.44547200   -4.54851300
 H   -0.07992500    2.35368100    0.52740700
 H    1.49843700    1.60991700    0.77652200
 C   -1.87310200    1.18787000    7.16372600
 H   -0.82090100    1.42068100    7.31831100
 H   -2.39785700    2.12714200    6.99716900
 H   -2.27790000    0.67958200    8.03180800
 C   -1.62393200    0.14151600    3.64272400
 H   -1.06540400   -0.78786200    3.75103700
 H   -2.67363100   -0.11066800    3.48444200
```

```
 C   -0.40514400    0.34725800   -3.05571700
 H    0.07009800    0.89661100   -3.87000500
 H    0.07493600   -0.62813100   -2.98081600
 C   -3.51394300   -0.57365100   -4.79862700
 H   -3.67873400   -1.07066300   -5.74815700
 H   -3.97081600   -1.14212400   -3.99026300
 H   -3.96939600    0.41516800   -4.80503700
 O   -1.79435000    0.17116400   -3.38433500
 O   -1.52362400    0.90245800    4.85968100
 O   -2.51321900   -0.78556500    5.94345100
 O   -1.17047800   -0.83852700   -5.28016800
*

Rotational symmetry number
2.

Rotational constants in GHz:
1.388720e+00 1.304100e-01 1.225000e-01

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                   23.528

frequencies (cm-1)
15.4876       22.9916       34.7610       46.1772       57.6915       63.4247       73.0230 81.1726
90.4503       150.5261      168.1351      178.5470      205.1887      236.3297      256.0532
282.0057      307.0609      342.4071      421.4656      467.9958      481.4836      523.9362
555.1876      616.3029      616.4274      657.5784      662.6098      796.9270      828.3689
926.6807      935.6784      956.0540      993.7261      996.6071      1002.4127     1015.2041
1016.0006     1023.2749     1067.3819     1073.1890     1074.1560     1078.8839     1084.2912
1107.8997     1140.5787     1176.7514     1211.6333     1268.1952     1269.7194     1288.8609
1296.5278     1298.5318     1322.0256     1329.8919     1344.4862     1364.1376     1396.5707
1398.9764     1428.5662     1432.4319     1470.2956     1470.4295     1472.5124     1475.7418
1476.2725     1508.1326     1509.0317     1769.6185     1777.2295     1837.2992     1837.7984
3040.2311     3075.2157     3076.7715     3088.7297     3089.1737     3110.7554     3125.2145
3126.0306     3150.4260     3154.7356     3157.2812     3157.7245     3171.2102     3171.5398
3200.7627     3200.9911
```

9.30. 3^Z ($C_{14}H_{12}$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C   -3.68863400   -0.25800600   -0.53819600
 C   -2.79246400    0.79888300   -0.60267300
 C   -1.58516500    0.75838200    0.09517200
 C   -1.31421000   -0.35450700    0.89400200
 C   -2.21246800   -1.40649800    0.96659700
 C   -3.39958200   -1.36637900    0.24492300
 H   -4.61527500   -0.21237800   -1.09419500
 H   -3.02390000    1.66725400   -1.20704200
 H   -0.39617900   -0.38680600    1.46523300
 H   -1.98914200   -2.25903500    1.59374700
 H   -4.09895500   -2.18920500    0.30267300
 C   -0.66739600    1.90987900    0.01574700
 H   -1.15796200    2.87753200   -0.00771200
 C    0.66739700    1.90987900   -0.01574800
 H    1.15796300    2.87753200    0.00771100
 C    1.58516500    0.75838200   -0.09517200
 C    1.31420900   -0.35450900   -0.89400000
 C    2.79246500    0.79888300    0.60267000
 C    2.21246700   -1.40650000   -0.96659400
 H    0.39617700   -0.38680900   -1.46523000
 C    3.68863500   -0.25800500    0.53819400
 H    3.02390200    1.66725500    1.20703700
 C    3.39958200   -1.36638000   -0.24492200
 H    1.98914000   -2.25903800   -1.59374300
 H    4.61527700   -0.21237700    1.09419200
 H    4.09895500   -2.18920600   -0.30267200
*

Rotational symmetry number
2.

Rotational constants in GHz:
1.531220e+00 4.207500e-01 3.653000e-01

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                    1.045

frequencies (cm-1)
33.2424       36.9236       78.3302       155.5044      167.7918      258.9405      264.6424
```

```
414.7856       419.6120       424.0719       455.4857       511.9580       529.1633       584.9496
631.9136       633.4571       701.2533       722.8513       723.3455       757.0689       777.6922
800.8300       812.2797       879.2370       879.6538       887.4095       957.8911       969.6614
1014.5490      1015.6734      1021.2842      1021.6172      1024.9973      1034.3943      1034.7932
1062.6476      1063.6300      1111.7557      1114.5493      1175.6700      1176.2525      1186.7401
1205.0751      1206.0598      1236.3427      1261.9839      1313.0558      1332.6107      1355.2825
1358.2901      1439.3743      1489.1234      1493.7061      1538.8568      1545.1134      1646.2659
1648.9350      1673.9774      1676.8278      1727.9036      3158.6765      3178.8812      3192.9339
3192.9492      3200.7379      3200.9275      3210.1799      3210.1971      3217.4812      3217.4966
3226.2261      3226.3637
```

9.31. 3^E ($C_{14}H_{12}$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C    2.56772600    3.46873000   -0.13437600
 C    1.38070100    2.75192400   -0.11639400
 C    1.37499400    1.36607000    0.05533000
 C    2.60311000    0.71799600    0.22294700
 C    3.78836100    1.43166000    0.20512200
 C    3.77801500    2.81059800    0.02443900
 H    2.54619700    4.54136500   -0.27151400
 H    0.43757200    3.26948100   -0.24096600
 H    2.63411200   -0.35161200    0.37900400
 H    4.72762300    0.91185800    0.33783200
 H    4.70643900    3.36475200    0.01285000
 C    0.08878800    0.66155800    0.05344700
 H   -0.77977700    1.31122000    0.03552700
 C   -0.08882900   -0.66171000    0.04776200
 H    0.77976300   -1.31121400    0.02596500
 C   -1.37502800   -1.36620200    0.04137600
 C   -1.38043000   -2.75048000   -0.14264400
 C   -2.60341500   -0.71964600    0.21278200
 C   -2.56741800   -3.46708600   -0.16903200
 H   -0.43708400   -3.26690100   -0.27023500
 C   -3.78863400   -1.43311900    0.18660300
 H   -2.63467900    0.34851100    0.37840500
 C   -3.77797200   -2.81038200   -0.00639300
 H   -2.54564400   -4.53845000   -0.31571200
 H   -4.72811700   -0.91452300    0.32242600
 H   -4.70637500   -3.36439700   -0.02454900
*

Rotational symmetry number
2.

Rotational constants in GHz:
2.739690e+00 2.647800e-01 2.423100e-01

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                    1.144

frequencies (cm-1)
23.6125        58.3957        62.7054        96.0292        206.4855       224.4000       277.9878
308.6693       414.4925       415.3632       463.0943       487.1234       548.0152       551.4692
631.0266       634.4771       652.9726       715.4340       717.7761       767.3699       798.1812
842.5960       872.2994       872.6607       888.9589       905.0458       952.7808       963.3301
1011.9487      1013.2759      1013.7845      1019.6595      1020.2751      1032.8452      1035.2458
1063.7755      1065.8910      1113.1770      1117.0124      1176.3332      1176.6814      1206.4404
1210.4397      1228.4477      1255.0468      1298.6840      1323.6727      1347.9432      1351.9670
1370.0918      1371.6830      1491.1740      1497.7769      1539.9326      1549.1388      1646.7292
1651.5101      1672.2247      1677.9604      1732.2728      3173.3283      3180.2531      3193.2929
3193.4262      3202.2337      3202.4056      3211.6515      3211.8615      3220.2459      3220.3271
3227.8977      3228.0764
```

9.32. 6^{EEE} ($C_{19}H_{18}$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C   -6.90786200   -1.33176300    0.39680100
 C   -5.73226000   -0.87798700    0.97579600
 C   -4.48707400   -1.19296600    0.42736800
 C   -4.45679200   -1.98119200   -0.72797100
 C   -5.62877400   -2.43452600   -1.30692900
 C   -6.86114700   -2.11293400   -0.74811000
 H   -7.86004900   -1.07456100    0.84070500
 H   -5.77292100   -0.26803400    1.86976400
 H   -3.50982600   -2.24190600   -1.18043400
 H   -5.58355100   -3.04255200   -2.20043000
 H   -7.77478500   -2.46907300   -1.20379800
 C   -3.27872600   -0.68628300    1.08260400
```

```
 H   -3.45412400   -0.07310500    1.96206600
 C   -2.01143400   -0.90140500    0.71316900
 H   -1.78740000   -1.50949700   -0.15715500
 C   -0.87050800   -0.35687900    1.42504100
 H   -1.08440600    0.25608000    2.29680200
 C    0.39790100   -0.57028900    1.07266600
 H    0.60827900   -1.17805100    0.19671500
 C    1.59082800   -0.00228000    1.78421800
 C    2.36783300    0.92158600    0.88992200
 H    1.83300700    1.80317500    0.55108600
 C    3.61994900    0.70386000    0.49757700
 H    4.12805800   -0.18134700    0.87083500
 C    4.42613800    1.55809200   -0.38722300
 C    5.79352400    1.30638500   -0.50493000
 C    3.88386300    2.61543700   -1.12303100
 C    6.60033300    2.09067900   -1.31650600
 H    6.22689100    0.48542100    0.05292000
 C    4.68695900    3.39921100   -1.93343800
 H    2.82303900    2.81996700   -1.07155900
 C    6.05001700    3.14279800   -2.03284000
 H    7.65834600    1.87807500   -1.38951200
 H    4.24804800    4.21173000   -2.49673000
 H    6.67403900    3.75579400   -2.66857400
 H    1.25256500    0.53612400    2.67279500
 H    2.24647000   -0.81085900    2.11659800
*

Rotational symmetry number
1.

Rotational constants in GHz:
1.138970e+00 8.320000e-02 8.041000e-02

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                    6.112

frequencies (cm-1)
10.3898       16.3399       22.2992       50.5521       62.8889       81.4853       100.4585
145.1483      164.1433      200.9615      210.2859      265.6030      289.9203      329.9349
351.3216      375.7870      414.8239      415.7729      421.0853      480.5800      521.1186
529.9336      566.0757      623.5817      629.7442      632.9602      633.5793      716.8701
719.0957      775.9804      780.5680      828.6717      854.8475      860.0710      872.7367
874.3853      885.5285      921.9903      940.4742      958.6430      958.9894      986.7932
1012.5956     1013.1313     1013.2544     1019.7860     1020.4123     1031.3143     1035.1321
1040.3227     1059.7399     1064.1558     1067.6150     1109.2100     1113.3560     1120.1868
1166.5710     1176.7112     1178.0164     1201.0749     1206.1008     1208.5883     1242.4349
1250.9876     1264.0285     1296.7803     1315.4948     1323.2974     1332.6812     1337.0763
1345.8874     1354.8166     1362.6835     1372.7359     1382.9281     1471.3396     1494.1582
1494.2832     1542.9633     1543.4353     1648.5478     1650.7955     1674.0610     1675.1943
1709.5542     1737.8879     1748.2869     3049.7494     3094.4120     3152.8048     3153.1709
3158.6772     3159.9729     3171.8100     3177.7660     3192.5212     3194.3894     3200.7556
3202.9082     3210.4383     3212.2954     3219.1821     3220.9808     3226.2536     3228.4786
```

9.33. 10^{EE} ($C_{16}H_{14}$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C     3.386622     4.394078     0.113247
 C     2.188794     3.695859     0.097530
 C     2.164703     2.303109    -0.007771
 C     3.386622     1.628385    -0.105199
 C     4.582413     2.323902    -0.090286
 C     4.589784     3.710370     0.020183
 H     3.379542     5.472339     0.197525
 H     1.251243     4.232924     0.170775
 H     3.403722     0.551218    -0.199004
 H     5.516403     1.783848    -0.167951
 H     5.526642     4.250152     0.030900
 C     0.871199     1.618507    -0.011951
 H     0.003137     2.271508    -0.001044
 C     0.659440     0.295932    -0.018022
 H     1.496602    -0.394421    -0.017603
 C    -0.659440    -0.295932    -0.018022
 H    -1.496602     0.394421    -0.017603
 C    -0.871199    -1.618507    -0.011951
 H    -0.003137    -2.271508    -0.001044
 C    -2.164703    -2.303109    -0.007771
 C    -2.188794    -3.695859     0.097530
 C    -3.386622    -1.628385    -0.105199
 C    -3.386622    -4.394078     0.113247
 H    -1.251243    -4.232924     0.170775
```

```
 C    -4.582413    -2.323902    -0.090286
 H    -3.403722    -0.551218    -0.199004
 C    -4.589784    -3.710370     0.020183
 H    -3.379542    -5.472339     0.197525
 H    -5.516403    -1.783848    -0.167951
 H    -5.526642    -4.250152     0.030900
*

Rotational symmetry number
2.

Rotational constants in GHz:
2.601700e+00 1.461000e-01 1.384300e-01

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                    1.176

frequencies (cm-1)
21.9286       37.5861       44.7510       53.8908       139.8896      161.4871      169.7032
229.1172      304.7063      305.2280      332.5462      414.0999      414.4050      463.0831
477.0860      508.2425      539.5255      619.6549      631.6670      633.4450      647.6485
715.0955      716.7665      773.4703      789.8564      845.4868      869.5571      873.1227
879.1769      882.2088      931.2460      956.9548      959.8080      986.2008      1013.3063
1013.4456     1019.3523     1019.5073     1030.0844     1033.5908     1041.8822     1064.1806
1064.8005     1113.6581     1114.1085     1171.0797     1176.7385     1182.4989     1206.6101
1208.0495     1235.9773     1259.9353     1262.1973     1317.0341     1325.5180     1337.0591
1348.9287     1358.8073     1369.0094     1386.3581     1492.2627     1497.1103     1542.5217
1545.3170     1646.3393     1649.2484     1672.3305     1674.7143     1708.7746     1725.5720
3158.9402     3160.0023     3172.8547     3180.9130     3192.9376     3192.9389     3201.5486
3201.6244     3211.7431     3211.7635     3220.5455     3220.6418     3227.8325     3227.9188
```

9.34. 11^{EE} ($C_{17}H_{16}$) – M06-2X/cc-pVTZ

```
*xyz 0 1
 C   -5.74653000   -1.06268600    0.27860200
 C   -4.66238100   -0.32377500    0.72968500
 C   -3.35397200   -0.76618400    0.53151400
 C   -3.16150000   -1.97373900   -0.14563400
 C   -4.24153400   -2.71265100   -0.59638400
 C   -5.54020600   -2.26227800   -0.38544100
 H   -6.75164900   -0.69973200    0.44574400
 H   -4.82761200    0.61275600    1.24793600
 H   -2.15917800   -2.33554500   -0.33047100
 H   -4.07159600   -3.64399200   -1.11969500
 H   -6.38137400   -2.84156500   -0.74064500
 C   -2.24385800    0.05393800    1.03895200
 H   -2.53408000    1.02271900    1.43689800
 C   -0.95586400   -0.27654500    1.07171500
 H   -0.62585900   -1.23841300    0.69244400
 C    0.13175700    0.61994500    1.59113900
 C    1.09593700    0.99145300    0.50083800
 H    0.67380900    1.56006500   -0.32164500
 C    2.38151400    0.65025100    0.49230300
 H    2.76883900    0.09100200    1.33986200
 C    3.37195700    0.96813600   -0.54711000
 C    4.71799200    0.69609300   -0.29988300
 C    3.02831700    1.53170000   -1.77917400
 C    5.69411500    0.98687800   -1.24185300
 H    4.99928400    0.25328800    0.64763100
 C    4.00044300    1.82266300   -2.72043000
 H    1.99136100    1.73589000   -2.00893700
 C    5.33902500    1.55378000   -2.45645200
 H    6.73144300    0.76912700   -1.02625800
 H    3.71393700    2.25735800   -3.66863200
 H    6.09555200    1.78102100   -3.19491900
 H   -0.31990100    1.52152900    2.01179800
 H    0.67731100    0.11697500    2.39309800
*

Rotational symmetry number
2.

Rotational constants in GHz:
1.389860e+00 1.310000e-01 1.261900e-01

Hindered rotor correction factor for Qvib
 Q(hin.)/Q(harm. osc.)   McClurg
 Total                    4.541

frequencies (cm-1)
```

```
15.9564        20.0509        23.5864        74.1987        78.4960        109.6133       137.8758
171.2839       230.4752       266.5893       301.0983       349.4235       394.7761       415.6062
415.7218       416.4003       473.2164       517.3830       551.8947       612.1436       632.4790
632.9350       635.9515       718.3950       719.4762       773.7621       781.5739       822.1371
852.1450       870.3914       873.3989       881.7155       890.4558       949.9948       958.1534
960.4064       1012.0026      1012.9172      1013.4281      1014.9073      1020.4845      1020.5433
1034.4626      1035.2013      1059.2260      1065.4400      1068.9276      1107.9818      1113.5110
1125.1340      1175.6280      1176.2704      1199.1150      1206.8816      1209.8646      1243.2764
1244.9976      1285.0759      1315.0853      1316.7546      1331.7369      1340.3007      1355.1101
1358.0596      1373.4335      1375.4319      1472.2471      1493.6883      1494.3150      1543.8185
1544.0332      1650.3723      1650.8689      1676.0210      1676.4141      1737.1187      1750.7891
3050.8020      3095.7723      3152.9235      3153.8968      3171.2346      3171.6540      3192.9138
3193.4526      3201.6378      3202.0618      3210.6590      3210.8484      3218.9163      3218.9843
3226.9498      3227.3653
```

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