

REACTIVE ELECTRON/MOLECULE COLLISIONS: FROM MECHANISMS TO NEW STATE-TO-STATE CROSS SECTIONS AND RATE COEFFICIENTS

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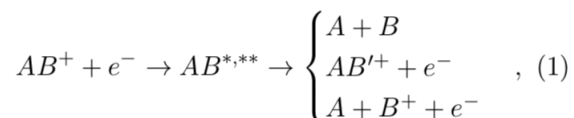
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Electron-impact dissociative recombination, ro-vibrational (de)excitation and dissociative excitation of molecular cations are at the heart of molecular reactivity in the cold ionised media [1], being major molecular ion destruction reactions, and producing often atomic species in metastable states, un-accessible through optical excitation.



These processes involve super-excited molecular states undergoing pre-dissociation and autoionization, having thus strong resonant character. We use methods based on Multichannel Quantum Defect Theory and R-Matrix Theory [2], capable to account for the strong mixing between ionization and dissociative channels, open - direct mechanism - and closed - indirect mechanism, via capture into prominent Rydberg resonances [3] correlating to the ground and excited ionic states, and for rotational effects. These features will be illustrated for several cations of high astrophysical and planetary relevance such as H₂⁺ [3], CO⁺ [4], SH⁺ [5], CH⁺ [2,6], N₂⁺ [7], ArH⁺ [8], CH₂NH₂⁺ [9]. Results for reactions similar to (1) but involving the neutral target CO₂ [10] will be also displayed. Comparisons with other existing theoretical and experimental results will be given.

References

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