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

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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.

$$AB^+ + e^- \rightarrow AB^{*,**} \rightarrow \begin{cases} A + B \\ AB'^+ + e^- \\ A + B^+ + e^- \end{cases}, \quad (1)$$

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 H_2^+ [3], CO^+ [4], SH^+ [5], CH^+ [2,6], N_2^+ [7], ArH^+[8], $CH_2NH_2^+$[9]. Results for reactions similar to (1) but involving the neutral target CO_2 [10] will be also displayed. Comparisons with other existing theoretical and experimental results will be given.

References

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