New insights in the low energy electron-driven reactivity of molecular cations

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Electron-impact dissociative recombination, ro-vibrational (de)excitation and dissociative excitation of molecular cations:

$$AB^+ + e^- \rightarrow AB^{*,**} \rightarrow \begin{cases} A + B \\ AB^{+*} + e^- \\ A + B^+ + e^- \end{cases}$$

are in the heart of the molecular reactivity in the cold ionized media[1], being major charged particles destruction reactions and producing often atomic species in metastable states, inaccessible through optical excitations. They involve super-excited molecular states undergoing predissociation and autoionization, having thus strong resonant character. Consequently, they are subject to beyond-Born-Oppenheimer theoretical approximations, and often require rather quasi-diabatic than adiabatic representations of the molecular states. In addition, they involve particularly sophisticated methods for modelling the collisional dynamics, able to manage the superposition of many continua and infinite series of Rydberg states.

We use the Multichannel Quantum Defect Theory[2], capable to account 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 the rotational effects. These features will be illustrated for several cations of high astrophysical[4] and cold plasma[5] physical relevance such as SH^+ and N_2^+, comparisons with other existing theoretical and experimental results being performed.

Advancement in the theoretical treatment - as the effect of the energy-dependence of the quantum defect on vibronic interactions for the benchmark cation H_2^+, the isotopic effects for diatomic[6] and polyatomic systems like H_2^+ and N_2H^+, etc. - will be presented.

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