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Electronic reactive collisions in cold ionised media: from mechanisms to new state-to-state cross sections and rate coefficients

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Synopsis The major mechanisms governing the dynamics of electron-driven reactions of molecular cations will be illustrated.

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

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

are at the heart of molecular reactivity in the cold ionised media [1], being major molecular ion destruction reactions, 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. 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 and planetary relevance such as CO^+ [4], SH^+ [5], and CH^+ [6, 7], comparisons with other existing theoretical and experimental results being performed. A representative example is shown in figure 1. Advancement in the theoretical treatment - addressing the effect of spin-orbit coupling for HCl^+, polyatomic systems and predic

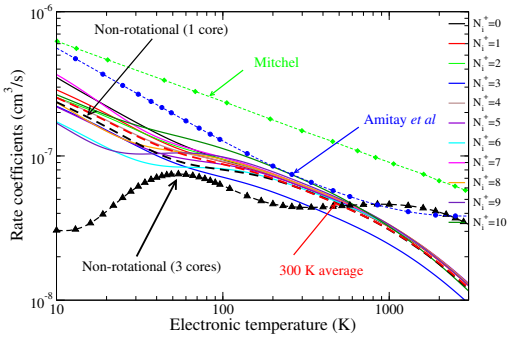

Figure 1. Maxwellian rate coefficients for dissociative recombination of vibrationally relaxed $CH^+(N_i^+)$ with electrons as functions of the kinetic temperature. Our results are compared with the experimental results of Amitay *et al.* [8] and of Mitchell [9].

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