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

J Zs Mezei¹*, A Orbán¹, K Chakrabarti², Y Moulane³, M D Epée Epée⁴,
O Motapon⁴, D Talbi⁵ and I F Schneider^{6,7}†

¹Institute for Nuclear Research, Hungarian Academy of Sciences, Debrecen, H-4001, Hungary

²Department of Mathematics, Scottish Church College, University of Calcutta, Calcutta, 700006, India

³High Energy Physics and Astrophysics Laboratory, Cadi Ayyad University, Marrakech, 40000, Morocco

⁴Dept. of Physics, Faculty of Sciences, University of Douala, Douala, 24157, Cameroon

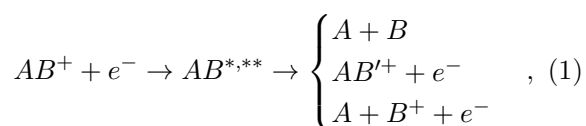
⁵LUPM CNRS-UMR5299, Univ. Montpellier, Montpellier, 34095, France

⁶LOMC CNRS-UMR6294, Univ. Normandie, Univ. du Havre, Le Havre, 76058, France

⁷LAC CNRS-UMR9188, Univ. Paris Sud, ENS Cachan, Univ. Paris-Saclay, Orsay, 91405, France

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



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 pre-

dic 1.

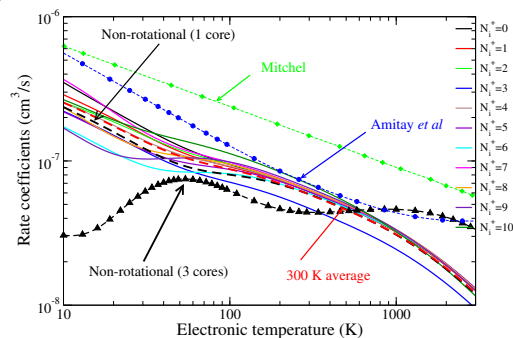


Figure 1. Maxwellian rate coefficients for dissociative recombination of vibrationally relaxed CH⁺(N_i⁺) with electrons as functions of the kinetic temperature. Our results are compared with the experimental results of Amitay *et al.* [8] and of Mitchell [9].

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*E-mail: mezei.zsolt@atomki.mta.hu

†E-mail: ioan.schneider@univ-lehavre.fr

