

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

J. Zs. Mezei^{(*)1,2}, A. Abdoulanziz², E. Djuissi², F. Iacob³, N. Pop⁴, K. Chakrabarti⁵,
V. Laporta⁶, M. Ayouz⁷, V. Kokoouline⁸, I. F. Schneider^{2,9}

¹ Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary

² LOMC, Université Le Havre Normandie, 76600 Le Havre, France

³ Department of Physics, West University of Timisoara, 300223 Timisoara, Romania

⁴ Fundamentals of Physics for Engineers Department, Politehnica University Timisoara, 300223 Timisoara, Romania

⁵ Department of Mathematics, Scottish Church College, 700006 Kolkata, India

⁶ Istituto per la Scienza e Tecnologia dei Plasmi, CNR, 70126 Bari, Italy

⁷ LGPM, CentraleSupélec, Université Paris-Saclay, F-91190 Gif-sur-Yvette, France

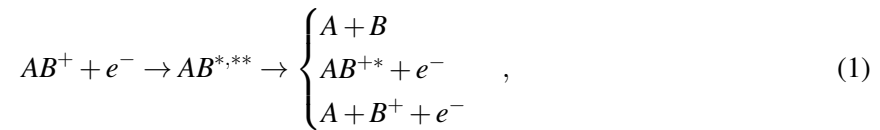
⁸ Department of Physics, University of Central Florida, Orlando, Florida 32816, United States

⁹ LAC, Université Paris-Saclay, 91405 Orsay, France

(*) mezei.zsolt@atomki.mta.hu

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 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. 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 correlating to the ground and excited ionic states, and the rotational structure and interactions.

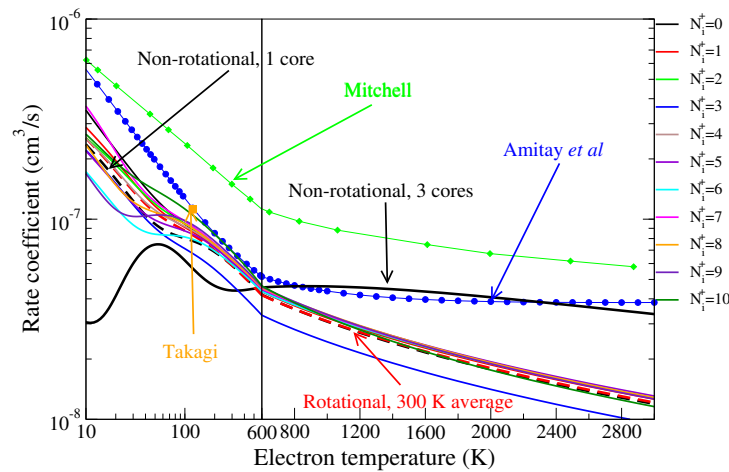


Fig. 1: Maxwellian rate coefficients for dissociative recombination of vibrationally relaxed $CH^+(N_i^+)$ with electrons as functions of the kinetic temperature. Our results are compared with the experimental results of Amitay *et al.* [3] and of Mitchell [4].

These features will be illustrated for several cations of highly relevance for cold laboratory plasmas such as ArH^+ [5], N_2^+ [6], BF_n^+ [7, 8], BeH^+ and its isotopologues [9] and CH^+ [2], 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 couplings, polyatomic systems and prediction of branching ratios - will be outlined.

- [1] I. F. Schneider, O. Dulieu, and J. Robert (editors) *Eur. Phys. J. Web of Conf.* **84** (2015).
- [2] J. Zs. Mezei et al, *ACS Earth Space Chem.* **3** (2019) 2376-2389.
- [3] Z. Amitay et al, *Phys. Rev. A* **54** (1996) 4032-4050.
- [4] J. B. A. Mitchell *Phys. Rep.* **186** (1990) 215-248.
- [5] A. Abdoulanziz et al, *MNRAS* **479** (2018) 2415-2420.
- [6] D. A. Little et al, *Phys. Rev. A* **90** (2014) 052705 (14pp).
- [7] J. Zs. Mezei et al, *PSST* **25** (2016) 055022 (12pp).
- [8] V. Kokoouline et al, *PSST* **27** (2018) 115007 (6pp).
- [9] S. Niyonzima et al, *PSST* **27** (2018) 025015 (10pp).