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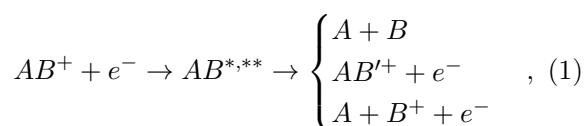
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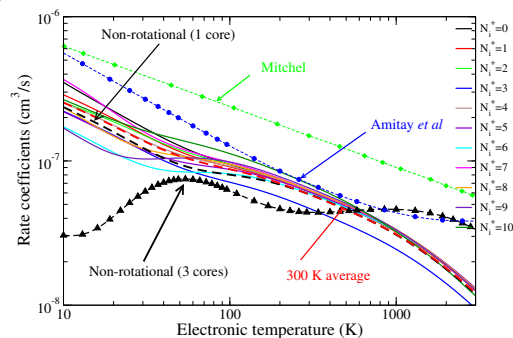
**Synopsis** The major mechanisms governing the dynamics of electron-driven reactions of molecular cations will be illustrated.

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



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<sup>+</sup> [4], SH<sup>+</sup> [5], and CH<sup>+</sup> [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<sup>+</sup>, polyatomic systems and pre-

dic 1.



**Figure 1.** Maxwellian rate coefficients for dissociative recombination of vibrationally relaxed CH<sup>+</sup>(N<sub>i</sub><sup>+</sup>) 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].

## References

- [1] I. F. Schneider, O. Dulieu, and J. Robert (editors) 2015 *Eur. Phys. J. Web of Conf.* **84**
- [2] Jungen Ch (editor), 1996 *Molecular Applications of Quantum Defect Theory*, (IoP Publish. Bristol)
- [3] Schneider I F *et al* 1991 *J. Phys. B* **24** L289
- [4] Moulane Y *et al* 2018 *A&A* **615** A53
- [5] Kashinski D O *et al* 2017 *J. Chem. Phys.* **146** 204109
- [6] Faure A *et al* 2017 *MNRAS* **469** 612
- [7] Chakrabarti K *et al* 2018 *J. Phys. B* **51** 104002
- [8] Amitay Z *et al* 1996 *Phys. Rev. A* **54** 4032
- [9] Mitchell J B A 1990 *Phys. Rep.* **186** 215

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