# **Electron induced reactivity of molecular cations:** from mechanisms to new state-to-state cross sections and rate coefficients

J. Zs. Mezei[1,2], E. Djuissi[2], A. Abdoulanziz[2], F. Iacob[3], N. Pop[4], D. Talbi[5], V. Laporta[6],
M. Ayouz[7], V. Kokoouline[8] and I. F. Schneider[2]
[1]Institute for Nuclear Research, Hungarian Academy of Sciences, H-4001 Debrecen, Hungary
[2]LOMC, CNRS, Normandie Université, le Havre, 76056 Le Havre, France
[3]West University of Timisoara, 300223 Timisoara, Romania
[4]Politechnica University of Timisoara, 300223 Timisoara, Romania
[5]LUPM, Université Montpellier, CNRS, 34095 Montpellier, France
[6]P. Las.M. I. Lab. Nanotec, CNR, Univ. du Havre, 70126 Bari, Italy
[7]LGPM, CNRS, CentralSupelec Univ. Paris Saclay, 91190 Gif sur Yvette, France
[8]University of Central Florida, 32816 Orlando, Florida, USA

Electron-impact dissociative recombination, rovibrational (de)excitation and dissociative excitation of molecular cations are at the heart of molecular reactivity in the interstellar media and early Universe [1], being a major charge destruction path, and producing often atomic species in metastable states un-accessible through optical excitations.

These processes involve super-excited molecular states undergoing predissociation and autoionization, having thus strong resonant character. We use methods based on the Multichannel Quantum Defect Theory [2] and R-matrix theory [3], capable to account for 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 for rotational effects. These features will be illustrated and extensive data will be shown for several cations of high astrophysical and planetary relevance such as $H_2^+$ and $HD^+$[4], $CO^+$ [5], $SH^+$ [6], $CH^+$ [2,7], $N_2^+$ [8], $ArH^+$[9], and polyatomic systems like $HCO^+$, $N_2H^+$ [2], $CH_2NH_2^+$ [10] and $NH_2CH_2O^+$ [11]. Comparisons with other existing theoretical and experimental results will be given, and perspectives on the advancement in the theoretical treatment - addressing polyatomic systems, predicting branching ratios - will be outlined.

## References

[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**, 2376 (2019).
[3] J. Tennyson, *Phys. Rep.* **491**, 29 (2010).
[4] M. D. Epee Epee et al, *MNRAS* **455**, 276 (2016).
[5] Y. Moulane et al, *A&A* **615**, A53 (2018).
[6] J. Zs. Mezei et al, *J. Chem. Phys.* **146**, 204109 (2017).
[7] K. Chakrabarty et al, *J. Phys. B.* **51**, 104002 (2018).
[8] D. A. Little et al, *Phys. Rev. A* **90**, 052705 (2014).
[9] A. Abdoulanziz et al, *MNRAS* **479**, 2415 (2018).
[10] C. H. Yuen et al, *MNRAS* **484**, 659 (2019).
[11] M. A. Ayouz et al, *MNRAS* **490**, 1325 (2019).