

Electron-driven reactivity of molecular cations in cold plasmas

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The cold plasmas produced in various contexts - hypersonic entry of spacecrafts in planetary atmospheres, at the wall of the magnetic fusion devices, industrial processes, discharge-assisted combustion - are the seat of a very rich physical chemistry, mainly due to the presence of electrons, photons and excited molecular species. The successful modelling of the kinetics of these environments - highly non-linear - relies in a critical manner on the accuracy of the rate coefficients for the governing collisional and/or radiative elementary processes.

Among them, electron impact recombination, (ro-)vibrational, electronic and dissociative excitation of molecular cations are in the heart of the molecular reactivity, being major destruction paths for the charged species and producing often atoms in metastable states, inaccessible through optical excitations. They involve superexcited molecular states undergoing predissociation and autoionization, having thus strong resonant character. They are subject to beyond-Born-Oppenheimer approximation modeling within the quasi-adiabatic representation, and they require special treatment due to the superposition of many continua and infinite series of Rydberg states.

The methods based on the Multichannel Quantum Defect Theory (MQDT) are the most suitable approaches for these processes, 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 effects.

New results on H_2^+ , N_2^+ , ArH^+ , NeH^+ , BeH^+ , BH^+ , N_2H^+ , C_2H^+ as well as advancement in the theoretical treatment - as the inclusion of new dissociative pathways, the isotopic effects, etc.... will be presented.