Electron-molecular cation collisions in cold plasmas

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Dissociative recombination, ro-vibrational excitation and dissociative excitation [1]:

$$AB^+(N_i^+,v_i^+) + e^- \rightarrow AB^*, AB^{**} \rightarrow A+B,\ AB^+(N_f^+,v_f^+) + e^-,\ A + B^+ + e^-,$$

where N_i^+/ N_f^+ and v_i^+/v_f^+ are the rotational and vibrational quantum numbers of the initial/final state of the target, strongly drive the charged particles' kinetics in low-temperature plasmas, as well as the production of reactive atomic and molecular species. It occurs via super-excited molecular states singly (AB*) - or doubly- (AB**) - excited, embedded in the ionization continuum of the target ion. Quantum chemistry and R-matrix techniques are used to produce the relevant potential energy states and their mutual interactions. We use these molecular structure data in methods based on the Multichannel Quantum Defect Theory [2-4] and on the Configuration Interaction ("boomerang") method [5] for computing accurate state-to-state cross sections and rate coefficients, displaying a resonant character and a strong dependence on the target's initial state. We will illustrate these features for various cations - H_2^+, BeH^+, CH^+, BF^+, N_2^+, CO^+, SH^+, ArH^+ - which enter in the composition of several plasmas in interstellar space, comets, planetary ionospheres, boundary-layers in the entries of space-crafts and close to the walls of the magnetically controlled fusion devices.

References

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