Collisions réactives entre électrons et cations d'hydrures : approches théoriques et applications dans les milieux ionisés hors-équilibre

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Abstract

Electron-impact collisions of molecules are present in cold ionized media such as interstellar clouds, planetary atmospheres and cold plasma. With enough energy to move about and escape from capture, electrons collide and react with other species in their environment forming precursors of more complex molecules and destroying species, allowing for redistribution of energy and material. Experimental and theoretical researchers are working hand-in-hand to continuously improve their respective ability to probe and to describe the kinetic of such media. Experimental devices such as storage-rings (e.g. CSR) are now able to produce measurements with state-to-state resolution. On the other hand, theoretical studies are not restricted by physical (e.g. finance) or chemical (e.g. toxicity) limitations while still being time-consuming. This work is about two theoretical approaches and their applications to investigate different processes for three diatomic molecular cations. Firstly, we extend our group previous dissociative recombination study of SH+ by accounting for more dissociative states (coming from the 4Π neutral symmetry), by producing branching ratios and by calculating vibrational excitation cross sections and rate coefficients (using the SW-MQDT approach). While the rotational structure of the molecule is neglected and should be investigated in a future work, good agreement is found with the storage-ring measurements for the yields from the dissociative recombination process. Secondly, we also extend our group previous low energy study BeH+ to high energy including the dissociative excitation process through discretized ionization continua and by accounting for higher-lying dissociative states, allowing the production of cross sections and rate coefficients for the dissociative recombination, dissociative excitation and vibrational transitions (using the SW-MQDT approach). Finally, we investigate the dissociative recombination of CF+ using a different approach called RMT-MQDT, where electronic couplings and neutral dissociative states do not need to be explicitly calculated, based on R-matrix theory to calculate the electronic fixed-geometry scattering matrix and based also on MQDT theory --- for the treatment of the nuclear motion (frame transformation) and accounting for the Rydberg series of states (quantum defect with CCEP). Good agreement is found with the storage-ring experiment when accounting for the rotational structure of the molecule.