Cross Sections on the Processes Induced by Electron Collisions with H_2^+, HeH^+, and Their Isotopes

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The collision processes of molecular ions and electrons play an important role in the divertor plasma such as molecular assisted recombination. Besides the main process of dissociative recombination (DR), dissociative excitation (DE) and rotational-vibrational transition of molecular ion affect the distribution of molecular and atomic states in plasma. The cross sections (CSs) of those processes, in principle, strongly depend on the electronic, rotational, and vibrational states. Plasma simulation also requires the data on the electronic state distribution of dissociated products. Those CSs should be state-specific both for initial states and for final states.

Almost all of available experimental data are on the DR of which initial vibrational-rotational state are confined to the ground state or mixture. Theoretical calculation could give state specific CS for various states. Thus, the accuracy of calculated CS could be check by comparing with the experiment for some limited states of limited molecular species. Roughly speaking, recent calculation on the DR of H_2^+ and HD^+ agree with experiment within about 20% difference for the rotationally and vibrationally ground state ions at the collision energies below 0.2 eV. The isotope effect could be accurately estimated by theoretical calculations. That means the calculated CSs of D_2^+, HT^+, DT^+, and T_2^+ have accuracy equal to H_2^+ [1].

We need to investigate the physics to estimate the accuracy of calculations since the check by experiment is limited. The theoretical calculations of those processes are composed of two parts; one is (*a*) electron scattering by a fixed-nuclear molecular ion, the other is (*b*) dynamics including nuclear motion. The accuracy of part (*a*) depends how complete electronic basis functions are adopted in the variational or close coupling calculations like R-matrix method: the basis functions for (1) partial waves of incident electrons and for (2) excited states of collision complex. By investigating a convergence with various these two types of electronic basis functions, we could estimate the accuracy. A converged calculation of the low energy DR of HeH^+ could be achieved (collaboration with M. Tashiro). For the high energy, we should investigate the convergence on type (2) basis functions. On H_2^+, we need check the convergence both type (1) and type (2) even for low energy collisions. The accuracy for very high rotational and vibrational states could be secured if enough basis functions are adopted. Theoretical calculation shows that the rotational motion is not important at the collision energy higher than 1 eV. It is empirically known that the multichannel quantum defect theory (MQDT) for the dynamics (part (*b*)) gives more reliable cross sections than the perturbation theory. The MQDT, however, could not secure the accuracy quantitatively. The off-the-energy-shell contribution deeply affects the CS. The effect becomes about one order of magnitude (1000%) for the DR of H_2^+. This work was supported by the JAEA.

[1] H. Takagi and M. Tashiro, J. Phys. Conf. ser. 300 (2011) 012020