§7. Charge Transfer in F^{2+} Ions Colliding with He Atoms Below keV Energies

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Recently HF molecules have been detected in interstellar medium, and the origin and formation mechanisms are sought [1]. From this observation, therefore, F^{q+} ions are expected to be present in interstellar environment, and to play a subtle role for astrochemistry. Also fluorine ions (F^{q+}) and atoms are known to be present in biological systems including the human-body, and the knowledge of its interaction with other atoms and molecules are needed for medical and biological study. Therefore, we conduct a theoretical investigation on charge transfer in collision of F^{q+} ions with He atoms based on a molecular state expansion method below 1 keV/u. The processes we are concerned with are:

(i) the ground-state ion impact:

$$F^{2+}\ (^4S) + He(^1S) \rightarrow F^+ + He^+ , \quad (1)$$

(ii) the excited-state ion impact:

$$F^{2+}\ (^2D) + He(^1S) \rightarrow F^+ + He^+ , \quad (2)$$

and their reverse processes. The energy defect between the ground F^{2+} (^4S) and the excited F^{2+} (^2D) states is approximately 4.3 eV. Therefore these two ions may be produced simultaneously through γ-ray- or ion-impact ionization in natural environment like the astrophysical environment, or laboratory plasma. Hence it is necessary to put together all information of the effect from these states when modeling scattering dynamics. The adiabatic potential curves of HeF^{2+} are obtained by employing the *ab initio* multireference single- and double-excitation configuration interaction (MRD-CI) method [2], with configuration selection at a threshold of 5.0 x 10^{-8} E_h. The two electrons in the first (lowest) molecular orbital (MO) are kept inactive in the present CI calculation. The coupling matrix elements are calculated using the resulting CI wave functions. A semiclassical MO expansion method with a straight-line trajectory of the incident ion was employed to study the collision dynamicsn [3]. Substituting the total wave function into the time-dependent Schrödinger equation, we obtain a set of first-order coupled equations in time t. By solving the coupled equations numerically, we obtain the scattering amplitudes for transitions, and hence the cross sections. The molecular states included in the dynamical calculations are the two sets of states, quartet and doublet states.

For both collision systems, the ground state and first excited states for the initial channel are considered. For F^{2+} + He collisions, the magnitude of the cross sections for charge transfer by ground-state ion impact is nearly similar to those by excited state ion impact. The ion-ion collision both for the dround and excited manifolds is found to be less effective in entire collision energies and corresponding cross sections are smaller by one to two orders of magnitude. This effect is due in part to the strong repulsion between two positively charged cores.

References

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