§6. Charge Transfer in Collisions H^+ Ions with Ground State Mg Atom at Low keV Collision Energies

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Charge transfer cross sections of the process Mg + H^+ -> Mg^+ + H were measured for the range of 1 - 2 keV collision energies[1-3]. Most of the theoretical work were performed by using either classical approximations or semi-empirical approaches[4-5], and the results thus obtained were qualitative and hence, the agreement with experiment was found to be not satisfactory. The only quantum mechanical *ab-initio* calculation at keV energies was performed by Olson and Liu[6]. They calculated charge transfer cross sections by using a molecular orbital (MO) expansion method within a semiclassical framework and by employing straight-line trajectories. They obtained a good agreement with experiments around the maximum of the cross section at ~ 8 keV, but at the lower energies their calculated values appear to overestimate the electron capture, and thus they conjectured that higher MO states that populate the excited Mg states would be important for further convergence of the cross section. Therefore, it seems appropriate at this time to carry out an *ab-initio* calculation of charge transfer cross sections by the semi-classical impact parameter method, which was applied successfully to study many collision processes in the past, and by taking couplings to more MO states than previous calculations into account. In this report, we considered only the single-charge transfer cross sections in low keV collision energies, but coupled up to fourteen molecular states. In this energy region, it was shown experimentally that single charge transfer dominates other processes[2].

We have employed the semi-classical impact parameter method based on a MO expansion[7]. The $(MgH)^+$ molecule is treated as a quasi two-electron system by representing the $Mg^{++}(1s^22s^22p^6)$ ion core by a Gaussian-type pseudopotential. The configuration interaction (CI) method with linear combinations of Slater determinants consisting of Slater-type orbitals is used to obtain Born-Oppenheimer MO's and eigenenergies of the system. The level of accuracy of the present molecular structure calculation is found to be within 0.4 % in all states compared with experimental spectroscopic data. Total wavefunction is expanded in terms of the products of a molecular state and atomic-type electron translation factors (ETF's). Substituting the total wavefunction into the time-dependent Schroedinger equation, we obtain a set of first-order coupled equations in time. By solving the coupled equations numerically, we obtain the scattering amplitudes for transitions, and the square of the amplitude gives the transition probability. Integration of the probability over the impact parameter gives the cross section for the process concerned.

The adiabatic potential energies of the lowest fourteen states of the $(MgH)^+$ system were obtained by the method described above as a function of the internuclear separation R. Overall the present potential curves agree well with those obtained by Olson and Liu[6]. The total single-charge transfer cross sections were calculated by inclusion of the lowest fourteen MO's, together with some other theoretical results and experimental data. Our calculated charge transfer cross sections are in fairly good agreement above E ~ 3 keV with most of experimental data. At lower collision energies, however, the calculated cross sections become larger by 30% than measurements, although ours are smaller than the values by Olson and Liu. At lower energies, these measurements were carried out by using D^+ or He^+ ions instead of H^+ ions. Therefore, if the claim that when H^+ ions are used, the cross sections obtained become uniformly larger than those by D^+ and He^+ at low energies still holds and is taken into account, then we would expect that the discrepancy between the calculated cross sections and measurements should be somewhat reduced. More experimental efforts are desirable in this energy region (E < 3 keV) in order to verify the theoretical results. We consider that the total charge transfer cross sections obtained by our fourteen state calculations are reasonably converged in the energy range covered in this study.

References

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