

Electron capture and dissociation in collision of H_2^+ with He

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Synopsis The quantum-mechanical molecular orbital close-coupling (QMOCC) method is employed to calculate the collision-induced dissociation (CID), electron capture (EC) and dissociative capture (DC) processes in H_2^+ +He collision.

The dissociation of 2-50keV H_2^+ ions colliding with He target has been measured by Williams and Dunbar [1] through detecting the H^+ formation. Suzuki *et al.* [2] measured the dissociated fragments, neutral particles and ionized target atoms in the energy range of 4-16keV. The energy dependency of their CID results is different with that of Williams and Dunbar [1], in which the H^+ formation cross sections decrease monotonously with decreasing energy. At energies below 1 keV, no experimental results are available for integral cross sections. On the theoretical side, Furlan and Russek [3] have investigated the EC, CID and excitation processes in the few keV energy region. Their calculations are performed by the straight-line trajectory method based on the *ab initio* molecular structure. A three-state approximation is employed in their calculations. Their CID cross sections are several times smaller than the experimental results, and the EC results are almost one order larger than the experimental measurements. We present the QMOCC calculations [4, 5] for the CID, EC and DC processes of the H_2^+ + He collision.

The *ab initio* molecular structure is calculated by the multireference single- and double-excitation configuration interaction (MRD-CI) method [6, 7]. The vibrational and rotational motions of the molecular ion are neglected in the calculation. With the fixed internuclear distance and orientation of the incident molecule, the cross sections can be calculated the same as the QMOCC treatment in ion-atom collisions.

The CID, EC and DC cross sections in H_2^+ +He collision are present in figure 1 in the energy range of 0.03-10 keV/u. The present results are compared with the experimental measurements of Suzuki *et al.* [2]. The CID process is the main process in the collision. The present CID results are smaller than those in Ref. [2].

The CID cross sections sensitively depend on the molecular alignment at energies below 1 keV/u. It is easier to dissociation when the molecular axis is perpendicular to the collision trajectory.

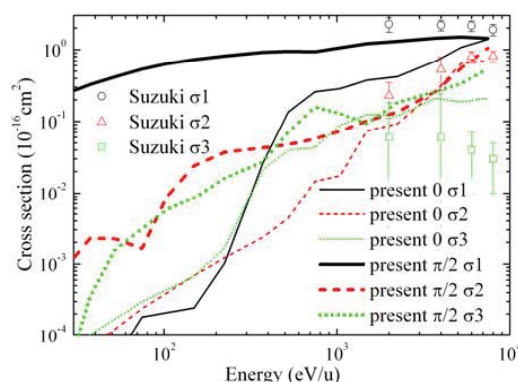


Figure 1. The CID (σ_1), EC (σ_2) and DC (σ_3) cross sections for H_2^+ + He($1s^2$) collision. Experimental results are from Suzuki *et al.* [2].

References

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