

4 - 12 Collision Induced Dissociation in $\text{H}_2^+ + \text{He}$ Collisions*

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The collision induced dissociation (CID) of H_2^+ ion colliding with He target has been measured by Williams and Dunbar^[1] and Suzuki et al.^[2] in the keV energy region. In Ref. [1], the CID cross sections decrease monotonously with decreasing energy. But the energy dependency of the CID results in Ref. [2] is different with that in Ref. [1]. 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 electron capture (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. We present the quantum-mechanical molecular orbital close coupling (QMOCC) calculations^[4] for the CID process of the $\text{H}_2^+ + \text{He}$ collision.

In our work, the *ab initio* molecular structures are calculated by the multireference single- and double-excitation configuration interaction (MRDCI) method. The vibrational and rotational motions of the molecular ion are neglected in the calculation.

With the fixed internuclear distance and orientation of the incident molecular ion, the cross sections can be calculated similarly with the treatment in ion-atom collisions.

The CID cross sections in $\text{H}_2^+ + \text{He}$ collision are shown in Fig. 1 in the energy range of 0.02~10 keV/u. The present results are compared with the experimental measurements of Refs. [1, 2] and the calculations of Ref. [3]. Our results are close to the experimental results of Williams and Dunbar^[1], but are smaller than those in Ref. [2]. The CID cross sections sensitively depend on the molecular alignment at energies below 3 keV/u. The dissociation is strongly favored when the molecular ion is aligned perpendicular to the collision velocity direction.

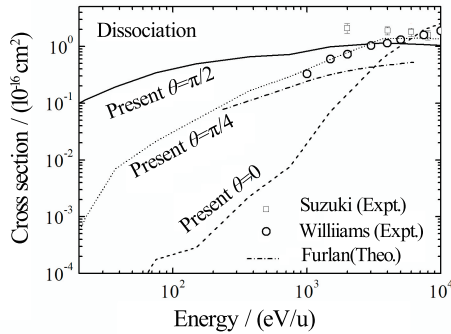


Fig. 1 The CID cross sections for $\text{H}_2^+ + \text{He}$ collision. The present results are compared with the experimental data of Williams and Dunbar^[1] and Suzuki et al.^[2], as well as the calculations of Furlan and Russek^[3].

References

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