

Quantum-mechanical calculations of rovibrationally resolved cross sections for the charge transfer and excitation in H^+H_2 and $\text{H}+\text{H}_2^+$ collisions

Fuyang Zhou^{*1}, Yong Wu^{*2}, Jianguo Wang^{*} and Predrag Krstić[#]

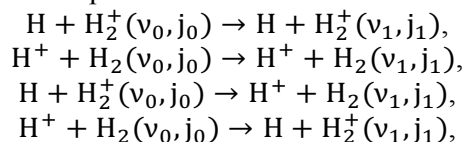
^{*} Institute of Applied Physics and Computational Mathematics, Beijing 100088, China

[#] Institute for Advanced Computational Science, Stony Brook University, NY, 11794, US

We present a quantum-mechanical study of slow collisions of H^+H with rovibrationally excited H_2/H_2^+ . Cross sections for charge transfer and excitation are calculated using molecular-orbital close coupling approach. A detailed picture of the inelastic processes that involve two lowest potential energy surfaces of the H_3^+ molecule is presented.

Collisions between ion and molecule are of great importance in the study of plasma and astrophysics. The collisions play an important role in the energy and particle transport in the plasmas with low electron density. There are abundant hydrogen atoms and molecules as well as their ions exist in the interplanetary atmosphere environment and the divertor plasmas area in magnetic confinement fusion device, and the slow collisions between these particles are of great importance for the simulation of relevant plasma evolution. However, the rovibrational processes of molecules have been usually ignored in the relevant astrophysics and fusion research, mainly because of the lack of state-to-state-resolved cross sections. Besides its relevance in astrophysics and fusion research, the H^+H_2 and $\text{H}+\text{H}_2^+$ collisions are fundamental few-body systems which constitutes the benchmark for the theoretical description of all ion-molecule collisions.

The purpose of the present study is to calculate the rovibrationally resolved cross sections for charge transfer and excitation in H^+H_2 and $\text{H}+\text{H}_2^+$ collisions. The following processes are studied in the present work:



where ν and j are vibrational and rotational quantum numbers, respectively.

In this work, cross sections for charge transfer and excitation are calculated using molecular-orbital close coupling (QMOCC) approach within the coupled states (CS) approximation [1,2]. Denoting by ρ the diatomic internuclear distance, by R the distance from the center of mass of the molecule to the projectile nucleus and by γ the angle between ρ and R , the Schrödinger

equation for nuclear motion in the body-fixed frame is given by

$$[\mathbf{W}(R, \rho, \gamma) + (T_N - E)\mathbf{I}]\Psi = 0,$$

where T_N is the kinetic-energy operator, Ψ is the state vector. In the two-electronic surfaces case, the diabatic potential matrix \mathbf{W} has the form

$$\mathbf{W} = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}.$$

One critical point in the calculation is the appropriate description of the conical intersection between the ground and first potential energy surfaces (PESs) of H_3^+ . In this work, both the two lowest diabatic PESs and the relevant electronic matrix elements are constructed with the diatom-in-molecule (DIM) method [3] using the potential curves for the diatomic fragments (ground state of H_2 and H_2^+). The two lowest diabatic PESs are shown for an example of $\gamma=90$ in Figure 1.

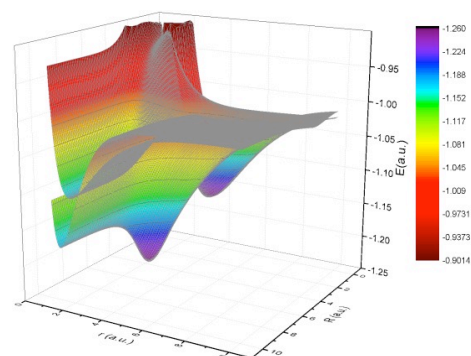


Figure 1. The two lowest adiabatic potential surface of H_3^+ at fixed $\gamma=90$.

References

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¹E-mail: zhoufy91@163.com

²E-mail: wu_vong@iapcm.ac.cn