Quantum-mechanical calculations of rovibrationally resolved cross sections for the charge transfer and excitation in H\(^+\)+H\(_2\) and H+H\(_2^+\) collisions

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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 (QMOCC) approach within the coupled states (CS) approximation [1,2]. Denoting by \(\rho\) the diatomic internuclear distance, by \(R\) the distance from the center of mass of the molecule to the projectile nucleus and by \(\gamma\) the angle between \(\rho\) and \(R\), the Schrödinger equation for nuclear motion in the body-fixed frame is given by

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

where \(T_N\) is the kinetic-energy operator, \(\Psi\) is the state vector. In the two-electronic surfaces case, the diabatic potential matrix \(W\) has the form

\[
W = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}
\]

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\(_2^+\). 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\(_2^+\) at fixed \(\gamma=90\).

References