Interference in fast bare ions colliding with diatomic molecules

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Synopsis Total as well as differential cross sections for electron capture in collisions of bare ions with diatomic molecules have been investigated at incident projectile energies ranging from 20 to 1000 keV/amu in the framework of distorted wave (DW) approximation. The present DW calculation is the simplest possible quantum calculation for this system. The present differential cross sections (DCS) are in good agreement with the shape of the observed angular dependence at forward angles.

Electron capture from molecular targets differs from capture from atoms because of the multi-center configuration of molecules, At high impact energies, a diatomic molecule may be regarded as a target where the incoming-projectile wave fronts scatter from both atomic centres providing interference patterns in the outgoing waves. This idea was recognized by Tuan and Gerjuoy [1] who first calculated electron-capture cross-sections from molecular hydrogen by protons at high collision velocities. In 2008, Schmidt et al [2] reported on strong interference effects in fast $H^+ + H_2$ collisions when only one electron is transferred to a fast H^+ ion to form a fast neutral H atom. Later, Misra et al investigated the first experimental observation of Young-type interference effects in a two electron transfer process in $He^{2+} + H_2$ collision at 1.2 and 2 MeV respectively. In the present theoretical investigation, we have focused our attention on single transfer of diatomic molecules by the impact of bare ions in the incident energy range 50-5000 keV. The differential cross-sections for electron capture, averaged over all orientations of the internuclear axis $\vec{\rho}$ of the hydrogen molecule is given in the DW approximation by

$$\frac{d\sigma_M}{d\Omega} = 2\left(\frac{\mu_i \mu_f}{4\pi^2}\frac{k_f}{k_i}\right)\frac{1}{4\pi}|T_{if}|^2 d\Omega_\rho .$$

he factor of 2 in the right hand side occurs because either of the two molecular electrons may be involved in the capture process. The transition amplitude is given by

$$T_{if} = \langle \psi_f^- | V_i | \psi_i \rangle .$$

The initial and final states are given by

$$\psi_i = e^{i\vec{k}_i \cdot \vec{r}_i} \phi_M(\vec{r}_1, \vec{r}_2, \vec{\rho}),$$

$$\psi_f^- = e^{i\vec{k}_f \cdot \vec{R}_f} \phi_I(\vec{r}_2, \vec{\rho}) \phi_{nlm}(\vec{s}) C_{t-e_1},$$

where $\vec{k}_i(\vec{k}_f)$ is the initial (final) momenta. ϕ_M, ϕ_I and ϕ_{nlm} are the wavefunction for H_2, H_2^+ and hydrogen like projectile respectively. Here C_{t-e_1} represent the interaction between the target ion and the captured electron. Here we consider the electron e_1 in any one of the atom in the molecule is active which is captured by the projectile and the other electron e_2 is passive in the other atom of the molecule (H_2^+). We will represent theoretical results for single capture cross sections for $H^+ - H_2/He^{2+} - H_2$ collisions in the intermediate to high energy range and will compared them with the available experimental dada.

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References

[1] T F Tuan and E Gerjuoy 1960 *Phys. Rev.* ***117*** 756

[2] H T Schmidt et al 2008 *Phys. Rev. Lett.* ***101*** 083201

[3] D Misra et al 2009 *J. Phys. Rev. Lett.* ***102*** 153201

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