§8. Elastic and Inelastic Processes in $H^+ + C_2H_2$ Collision below 1.5 keV Regime

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Electron capture in collisions of ions with atoms in the low-keV energy regions has been one of the most active research areas, experimentally and theoretically, in atomic physics in the last two decades. This is because it provides information fundamental for atomic and molecular spectroscopy and many-body collision dynamics. Unlike the case for atomic targets, both experimental and theoretical studies of molecular targets are scarce because of the difficulties arising from the complexity of the non-spherical field of a molecule. We have carried out a rigorous theoretical investigation of elastic and electron capture processes in collision of H^+ ions with CH_4 (methane) in the region below a few keV earlier [1]. In the present note, we report the results for electron capture and direct elastic scattering in collisions of H^+ ions with C_2H_2 molecules for energies below 1.5 keV. Contribution from electron-capture accompanied with simultaneous target excitation is also examined. Hence, the processes studied are:

$H^+ + C_2H_2$ --------> $H + C_2H_2^+$ (1a)
(electron capture)
--------> $H + C_2H_2^{+*}$ (1b)
(electron-capture with simultaneous target excitation)
--------> $H^+ + C_2H_2^*$ (1c)
(target excitation)

Two molecular configurations are specifically considered to study the effects of molecular orientations on collision dynamics: (i) a proton approaches an H atom along the molecular axis of the C-C bond and (ii) it approaches perpendicularly toward the midpoint of the C-C bond in C_2H_2. The interference arising from different molecular orientations is investigated. The adiabatic potential energy curves are calculated by means of the multireference single- and double-excitation configuration interaction (MRD-CI) method [2]. The calculations are carried out in two different point groups, depending on the approach of a proton toward the acetylene molecule. In the practical calculations of eigenvalues and eigenfunctions, all coordinates within the C_2H_2 molecule were frozen at the equilibrium intramolecular distances of the linear geometry: $r_{C\text{-}C} = 1.208$ Å and $r_{C\text{-}H} = 1.058$ Å. Hence, only the internuclear distance (R) between the H^+ projectile and the midpoint of the C-C bond was varied. This approximation should be valid when the collision time is shorter than the vibrational period of the target molecule, as discussed in a previous study[1] of $(H + CH_4)^+$. A fully quantum mechanical representation of the MO expansion method was employed; that is, dynamical transitions were driven by nonadiabatic couplings [3]. The total wavefunction for scattering is described as a product of the electronic and nuclear wavefunctions. Substitution of the total scattering wave function into the stationary Schrödinger equation yields coupled, second-order differential equations for nuclear wave function. The coupled equations are solved numerically to obtain the scattering S^l matrix for each partial wave l [3]. The differential cross section is then obtained from the standard formula. Its integration over all angles gives the total cross section. In the present calculation, we have employed two- and three-state close-coupling treatments with molecular orbitals (MOs) corresponding to the initial $[H^+ + C_2H_2]$ and electron capture $[H + C_2H_2^+]$ channels. Adiabatic potential curves are displayed in Figs. 1a and 1b. The differential cross sections obtained are shown in Figs. 2a and 2b both for C_{2v} and C_{00v} symmetries, respectively, for scattering angles 0-180° at 1.5 keV. Both electron capture and direct elastic scattering are included. Collision dynamics for C_{2v} and C_{00v} symmetries were found to be effective in nearly the same small scattering-angle regions. Hence, the interference arising from these two molecular configurations occurs rather strongly at narrow regions of scattering angle, and unambiguous structures in differential cross sections arising from the interference are observed.

References

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1). M. Kimura, Y. Li, G. Hirsch and R. J. Buenker,Phys. Rev. A 52, 1196 (1995).
2). R. J. Buenker and S. D. Peyerimhoff, Theoret. Chim. Acta 35, 33 (1974); 39, 217 (1975); R. J. Buenker, Intern. J. Quantum Chem. 29, 435 (1986).
3). M. Kimura and N. F. Lane, Adv. At. Mol. Phys., Vol. 26, Eds. D. R. Bates and B. Bederson (Academic Press, NY, 1989) p. 79.