§6. Electron Capture in Collisions of Protons with CO Molecules in the keV Region

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We have carried out theoretical investigations for electron capture resulting from proton collisions with CO molecules for collision energies less than 10 keV, and have intended to examine more specifically the steric effect on capture dynamics. The process is important in various applications. Specifically the process is important for modeling the interaction of the solar wind with comets [1]. Protons are the dominant species in the solar wind [2] while the coma is composed of about 15% CO. Charge transfer with the cometary neutrals may explain the loss of solar wind protons observed at comet Halley. The carbon monoxide (CO) molecule is also important for various applications in fusion research, plasma chemistry, and medical physics for cancer research. In recent years, various types of hydrocarbons including CO molecules have been detected near the divertor region in fusion reactors. Therefore it is extremely important and urgent to understand the role of these hydrocarbons in charge transfer processes. The processes we are concerned with are:

$H^+ + CO \rightarrow H + CO^+ - 3357\ cm^{-1}$ (1)
$\rightarrow H + CO^{+*} - 24090\ cm^{-1}$ (2)
$\rightarrow H^+ + CO^* - 48687\ cm^{-1}$ (3)

Because of the small energy defect, process (1) is expected to dominate in the energy region considered, while processes (2) and (3) are weaker channels with the energy defect larger than 3 eV. As for the orientation, we have considered three molecular configurations: (i) the H^+ approaches the center of mass of CO, (ii) H^+ approaches the C atom, in which CO lies along the collision trajectory, and (iii) the H^+ approaches toward the O atom. The investigation of these three molecular orientations should give significant insight into the details of the steric effect for electron capture, and is expected to provide a general guideline for further experimental research. The potential curves of the $(HCO)^+$ system are obtained by the multireference single- and double-excitation (MRD-CI) configuration interaction method [5]. In the CI calculations, the two lowest molecular orbitals (MOs) are always kept doubly occupied, whereas the two highest ones are discarded. A small selection threshold [3] of 0.32×10^{-6} hartree has been used in the present treatment. The radial coupling matrix elements are obtained using calculated MRD-CI wave functions. Scattering dynamics is studied on the basis of the fully quantum mechanical formulation of a molecular-orbital expansion [4]. Substitution of the total scattering wave function into the stationary Schrödinger equation yields coupled, second-order differential equations for the nuclear wave function. By soling the coupled equation numerically, one can obtain scattering S-matrix elements, and hence, differential and integrated cross sections.

Generally, the overall agreement with the present results and experimental measurements is found to be very good. The maximum of the cross section is found to occur around 250 eV/u with a value of 1.71×10^{-15} cm^2. The electron capture cross section is found to decrease slowly for higher energies, and is consistent with all of the measurements. At 1.5 keV/u, our result reaches a value of 1.3×10^{-15} cm^2, which compares favorably with one measurement reported the value of 1.48×10^{-15} cm^2. Another experiment reported the slightly smaller cross section with 1.0×10^{-15} cm^2 at 10 keV/u, but the present result lies well within their error bars.

The present differential cross sections are also in good agreement with the experiment for scattering angle from 0.01° to 1° at 1.5 keV/u, in which the theory can reproduce the oscillatory structures quite well. The steric effect is found to persist rather significantly in all energies. The present cross section data are considered to be useful for various applications.

References

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