§6. Charge Transfer in Collisions of H$^+$ Ions with CH$_4$ and C$_2$H$_2$ Molecules below 2 keV

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Charge transfer 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, because it provides fundamental information for atomic and molecular spectroscopy and many-body collision dynamics. Unlike studies of atomic targets, both experimental and theoretical studies of molecular targets are scarce, although molecular targets are as important as atomic counterparts. The complexity in theoretical approaches for treating molecules prevents further active involvement of theoreticians.

In this paper, we report charge transfer resulting from collisions of H$^+$ ions with CH$_4$ and C$_2$H$_2$ molecules below 2 keV based on our experimental and theoretical studies. Three and two molecular configurations for CH$_4$ and for C$_2$H$_2$, respectively, are specifically considered to study the effects of molecular orientations on collision dynamics; For CH$_4$, (i) a proton approaches the H atom in a C-H bond, (ii) it comes along the same line as in (I) but in the opposite direction, passing through the center of an H$_3$ triangle, and (iii) a proton approaches along the bisector of an H-C-H bong angle, and for C$_2$H$_2$, (i) a proton approaches a 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$_2$H$_2$.

The adiabatic potential-energy curves are calculated by using the multireference single- and double-excitation configuration-interaction method. In the practical calculation of eigenvalues and eigenfunctions, all coordinates within the CH$_4$ and C$_2$H$_2$ were frozen at the equilibrium intramolecular distances of the tetrahedral and linear geometries, respectively,: for CH$_4$, $r_{C-H} = 1.094$ Å and $\theta_{H-C-H} = 109.47°$, and for C$_2$H$_2$, $r_{C-C} = 1.208$ Å and $r_{C-H} = 1.058$ Å. Hence, only the internuclear distance between the H$^+$ projectile and the target CH$_4$ and

C$_2$H$_2$ was varied. Collision dynamics are studied on the basis of the fully quantum-mechanical formulation of a molecular-orbital expansion method in which dynamical transitions are driven by nonadiabatic couplings. By solving the coupled equations numerically, one can yield the scattering S-matrix element and hence, transition probabilities.

The present theoretical differential cross sections for CH$_4$ and C$_2$H$_2$ averaged over the molecular configuration are shown in Fig. 1 (at 1.5 keV) and Fig. 2 (at 1.0 keV), respectively. For CH$_4$, the present theory agrees reasonably well with the measurement.
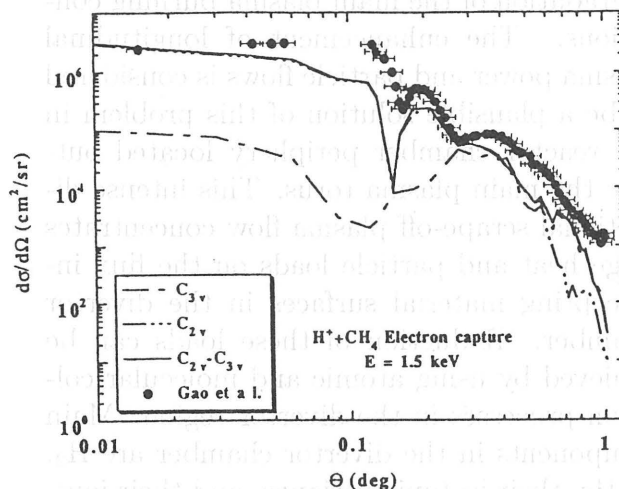

Fig. 1 Differential cross section for CH$_4$ at 1.5 keV. The symbols represent the experimental data of Gao et al. [1].
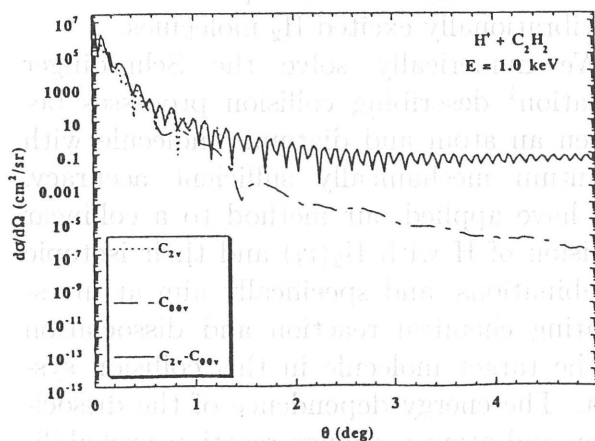

Fig. 2 Differential cross section for C$_2$H$_2$ at 1.0 keV.

Reference:

[1] R. S. Gao, L. Johnson, K. Smith and R. Stebbings, Phys. Rev. A53, 1212 (1993).