§ 10. Electron Capture and Ionization in Collisions of Slow H^+ Ions with Hydrocarbons and Other Fusion Relevant Molecules

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In research on the controlled thermonuclear fusion, electron capture processes of slow H^+ ions in collisions with hydrocarbons and other fusion relevant molecules below a few-keV energies play a key role in low temperature edge plasmas of the current fusion devices with carbon-coated or graphite-lined walls as plasma facing materials [1]. Although many experimental studies have been performed on electron capture of H^+ ions in collisions with various gas atoms and molecules, cross section data are still fragmentary and are not consistent with each other. This is particularly so for hydrocarbons, and other important molecules and hence, more systematic determination of electron capture cross sections is urgently required. Theoretical approaches applicable to slow ion – molecule collisions are also scarce because of the difficulty of treating the intrinsic multicenter nature of molecules accurately, although some small-scale exploratory studies have been carried out.

For these reasons, we have undertaken a joint experimental and theoretical investigation and determined electron capture cross sections of H^+ and O^+ ions colliding with the hydrocarbons and others such as H_2, D_2, CH, NH, H_2O, C_3H_4, C_2H_6, and C_3H_8 molecules in the energy range of 0.2 to 4.0 keV in collaboration with Prof. Buenker at U. Wuppertal. All collision processes which involve hydrocarbon molecules are exothermic with an appreciable energy difference, although it is relatively small for larger hydrocarbons. For some molecules, vibrationally excited molecules in the initial channel decrease the exothermicity, and hence, are expected to increase the electron capture cross section by an order of magnitude even when the target is in the first vibrational excited state. On the other hand, for others, vibrational excited states are found to increase the exothermicity, which may lead to the smaller cross section. Hence, dynamics of electron capture from the vibrationally excited molecule varies from system to system, and needs to be considered carefully and systematically. In the present theory, the molecular - orbital expansion (MOCC) method is applied [2 –3].

We have observed strong evidence that the vibrational state of the target molecules significantly affects the electron capture dynamics and cross sections in in $H^+ + C_mH_n$ collisions. The observed cross sections of the electron capture processes show a gradual increase as the collision energy decreases for all the present collision systems [$H^+ + C_mH_n$] investigated, except for C_2H_2, in the collision energy range between 0.2 and 20 keV. In this system, the vibrationally excited product states enforce the "accidental" resonance condition in the electron capture processes. The observed cross sections at the present collision energies tend to become large as the ionization energy of the target molecules becomes small, and there seems to be a systematic relationship with the number of electrons or atoms in the target molecules. This relationship will be discussed in more systematic manner elsewhere.

References

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