

## §20. Temperature Effect on Charge Transfer and Ionization in Collisions of $H^+$ Ions with Hydrocarbon Molecules

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In research on controlled thermonuclear fusion, charge transfer processes of slow  $H^+$  ions in collisions with impurity molecular gases such as 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 which employ carbon-coated or graphite walls as plasma facing materials. Particularly, these impurity hydrocarbons have been detected near the divertor region in many experimental fusion reactors. Although many experimental studies have been performed on electron capture of  $H^+$  ions in collisions with various gas atoms and molecules, these investigations were concerned with vibrationally ground-state molecules. But experimental as well as theoretical studies from vibrationally excited targets are nearly non-existence. However under the usual operational condition where various gases are put under the room-temperature, non-negligible amount of gases is known to be in vibrationally excited state. Although collision cross-section data from these vibrationally excited species are urgently needed, very few studies have been carried out so far.

For this reason, we have been undertaking a joint experimental and theoretical investigation and determined charge-transfer cross-sections of  $H^+$ ,  $C^+$  and  $O^+$  ions colliding with vibrationally excited hydrocarbons (high temperature

molecules) and others such as  $H_2$ ,  $D_2$ ,  $CH$ ,  $NH$ ,  $H_2O$ ,  $NH_3$ , and  $C_mH_n$  ( $m < 4$ ) 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 other molecules, 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 with both fully quantal and semiclassical formalisms.

We have observed strong evidence of *the temperature effect or vibrational effect*, in which the vibrational state of the target molecules significantly affects the charge transfer dynamics and cross sections in  $H^+ + C_mH_n$  collisions<sup>1,2)</sup>. The observed cross sections of the charge transfer processes show a gradual increase as the collision energy decreases for all the present collision systems [ $H^+ + C_mH_n$ ] investigated. The observed cross sections at the present collision energies appear to have a linear-relationship with the ionization energy of the target molecules. This relationship will be discussed in more systematic manner elsewhere<sup>2)</sup>.

### References

- 1) Suno, H., Buenker, R.J., Kimura, M. and Janev, R., Phys. Rev. A. 70 (2004) 032703.
- 2) Suzuki, R., Li, Y., Liebermann, H-P., Buenker, R.J., Pichl, P. and Kimura, M., Phys. Rev. A 71 (2005) 032710.