§3. Electron Capture in Collisions of H^+ and O^+ Ions with H_2, D_2 and Hydrocarbons and Other Fusion Relevant molecules below a Few-keV Regime

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In research on the controlled thermonuclear fusion, electron capture processes of H^+ and O^+ ions in collisions with H_2, D_2 and hydrocarbons and other fusion relevant molecules at low collision energies play a key role in low temperature edge plasmas of the current fusion devices with carbon-coated walls as plasma facing materials [1]. Although many experimental studies have been performed on electron capture of H^+ and O^+ ions in collisions with various gas 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 arising from multi-electron system as well as multi-center nature of target molecules accurately, except for some small-scale calculations.

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 H_2, D_2 and hydrocarbons in the energy range of 0.2 to 4.0 keV. All collision processes are exothermic with an appreciable energy difference. Vibrationally excited molecules in the initial channel reduce the exothermicity, significantly and hence, are expected to increase the electron capture cross section. On the other hand, vibrationally excited states in the product channel increase the exothermicity, which may lead to the smaller cross section. Hence, charge transfer to the vibrationally excited molecule needs to be considered carefully. In the present theory, the molecular - orbital expansion (MOCC) method is applied [2].

We have observed strong evidence that the isotope molecules significantly differ in the electron capture dynamics and cross sections between $H^+ + H_2$, and D_2 collisions. The cross section ratio between the two processes is found to be unity above a few keV, but gradually decrease to 0.7 at 0.2 keV. This is a surprising result because no marked isotope effect on charge transfer has been expected due to small energy differences in binding as well as vibrational levels. Our observation could require the reassessment of charge transfer cross section data previously published for H_2 and D_2 collisions.

We have also investigated charge transfer of O^+ collisions with H_2 below a few keV regime. There have been a few experimental investigations on this system past two decades, but two sets of experimental groups disagree drastically where one set shows a constant and larger cross sections below 1 keV with a value of 10^{-15} cm^2, while another set shows sharp decreasing trend reaching a value of 10^{-17} cm^2 at 0.1 keV. Our results agree well with the latter set of measurements, provide theoretical rationale to the discrepancy and resolve the controversies. In addition, our results give important data for charge transfer from fusion impurity ions.

References

[1] R. K. Janev, in *Atomic and Molecular Processes in Fusion Edge Plasmas*, edited by R. K. Janev, (Plenum, New York, 1995), pp.1-13.
[2] M. Kimura, Phys. Rev. A **32**, 802 (1985).
[3] T. Kusakabe, M. Kimura, L. Pichl, R. J. Buenker, and H. Tawara Phys. Rev A.68, Rapid Comm. R050701-R057014 (2003).
[4] L. Pichl, Y. Li, R. J. Buenker and M. Kimura, to be published in Phys. Rev. A. (2004).