Phd Title : Kinematical Analysis of Ionization and Fragmentation of Molecules
Scholar Name : Koushik Saha
Institute : Physical Research Laboratory, Ahmedabad
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Present Position:Post Doctoral Fellow at Weizmann Institute of Science, Israel

Synopsis :

The thesis is concerned with the study of molecular fragmentation due to various electron loss and decay mechanisms. Molecules are quantum mechanical systems in which the electrons and nuclei are in a dynamic equilibrium. Loss of electrons through ionization due to perturbation such as charged particle impact or photoabsorption, disturbs the equilibrium of the molecular system and the molecule attains excited state. De-excitation inevitably follows, often leading to dissociation of the molecule.

The energy supplied to a molecule upon projectile impact is shared among its electronic and nuclear degrees of freedom. Since there is a priori no fixed pattern in which the energy transferred to the molecule is shared between the electrons and nuclei, the question that immediately arise is, will this energy sharing affect the kinematics of dissociation? And if so, how? What kind of kinematical differences are induced due to various energy sharing mechanisms? To address these questions, the fragmentation of molecules is studied in the light of the kinematical differences between various electron loss and decay processes. Systematic analysis of the electron decay mechanisms and their subsequent effect on the kinematics of molecular dissociation, has been carried out and presented in this thesis.

To carry out these studies, a combined electron ion spectrometer was built which is capable of analyzing both the electrons and ions simultaneous in a dissociation event. The instrument is a combination of an electrostatic cylindrical mirror analyzer to identify the electronic decay process by analyzing the energy of the ejected electron from a molecule and a recoil ion momentum spectrometer to reveal the corresponding dissociation kinematics by analyzing the fragment ions for their charge state, mass, as well as momentum and detect them in a time ordered sequence, simultaneously. The studies were limited to simple di- and tri-atomic molecules such as CO, OCS and CS_2. Dissociative ionization of molecules was effected in our experiments using photon beams of specific energies. Experiments were performed at Reflectivity beamline at Indus-1 synchrotron facility at RRCAT, Indore. Analysis of the fragmentation processes for valence and core ionized molecules were carried out.

Our study reveals that molecular dissociation is highly dependent on the electronic decay mechanisms, to the extent that for the same ionizing perturbation the stability of the molecular ion is governed by which electronic decays follow the primary perturbation. The kinematics of the dissociation is also found to be dependent on the electron loss processes. The dependence can be understood in terms of the energy sharing between the electrons and nuclei of the molecule. It is also found that bent conformations of the triatomic molecular ions are accessed in course of the dissociation and the fragment kinetic energies are found to depend on the geometry of the transient molecular ion. These observations will aid theoretical computations of the dissociative ionization processes, as the observations provide clues to the coupling between electronic and nuclear degrees of freedom in excited molecular ion states. They also provide clues as to which molecular ion conformations are relevant to dissociation.