Observation of Intermolecular Coulombic Decay in Water-Tetrahydrofuran Dimers Induced by Electron-Impact Ionization

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Synopsis We report the direct observation of intermolecular Coulombic decay (ICD) in a hydrated tetrahydrofuran clusters induced by electron-impact ionization (E_0 = 67 eV). The experiment was performed using a multi-particle coincidence method in which the momentum vectors and consequently, the kinetic energies of final state electrons and ions are determined. ICD in water-tetrahydrofuran dimer is identified by the measurement of kinetic energy release of two fragment ions and the scattered and ejected electron spectra. The observed decay channel can be an efficient source of low-energy electrons that contribute to cause radiation damage in biological matter.

It is well-known that low-energy electrons are of great importance in radiation damage to living cells [1]. In recent years it became apparent that for the transition from isolated molecules to clusters or the condensed matter, a wealth of new energy and charge transfer phenomena emerge which are absent for isolated molecules. One example is the intermolecular Coulombic decay (ICD) [2] in which the system decays by releasing low-energy electrons. Experimentally ICD has been identified in numerous systems, e.g. in the Van-der-Waals clusters [3], in the hydrogen-bonding water dimer [4] and in larger water clusters [5]. ICD in biochemically relevant systems, i.e. a biomolecule associated with water, has been recently predicted by theory [6], but so far the process has not been observed.

Here, we study ICD in mixed clusters consisting of water and bio-relevant molecules. The biomolecule employed here is tetrahydrofuran (THF, C_4H_8O) which is often regarded as being the simplest molecular analog of deoxyribose, part of the DNA backbone linking the phosphate groups and the DNA bases. Experiments were carried out using a multi-particle imaging spectrometer (reaction microscope) [7, 8] with a heatable supersonic molecular jet and an implemented low energy electron beam. The kinetic energies of final state electrons and ions are obtained in our experiment. The projectile electron energy of 67 eV is chosen in the range of the mean energy of secondary electrons which are produced in great numbers by high-energy ionizing radiation in matter. The ICD process is shown schematically in Fig. 1. The process is triggered by removing an inner-valence electron from the water molecule in the water-THF dimer, i.e. an electron is ionized from the oxygen (O) 2s-type orbital of water by electron-impact [Fig. 1(a)]. After that the $H_2O^+(2s^{-1})\cdots C_4H_8O$ dimer cation undergoes ICD, an electron from higher lying orbital of H_2O^+ will fill the O-2s vacancy, and a low-energy electron from the neighboring C_4H_8O will be ejected [Fig. 1(b)]. The repulsion between the two positive charges produced by the ICD process on the two hydrogen-bonded species will lead to a Coulomb explosion of the system [Fig. 1(c)]. Several signatures allow identification of ICD. There is the kinetic energy release by the fragment ions. The coincident projectile energy loss spectrum which reveals a O-2s vacancy, and the low-energy electron spectrum showing increased intensity due to ICD electrons. Detailed results will be presented at the conference.

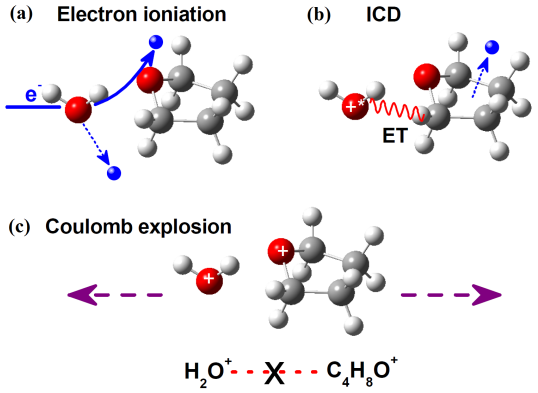

Figure 1. Schematic of ICD of an inner-valence vacancy in a hydrogen-bonded water-tedrahydrofuran dimer induced by electron-impact ionization.

References

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