Observation of intermolecular Coulombic decay in water-tetrahydrofuran dimer induced by electron-impact

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Synopsis We report the direct observation of intermolecular Coulombic decay (ICD) in a hydrated tetrahydrofuran clusters induced by electron-impact using a multi-particle coincidence method in which the momentum vectors and the kinetic energies of final state particles are determined. ICD in water-tetrahydrofuran dimers is identified by kinetic energy release of two fragment ions and the scattered and ejected electron spectra supported by ionization potential calculations. This decay channel can be an efficient source of low-energy electrons that cause further radiation damage in biological matter.

Intermolecular Coulombic decay (ICD) [1] in clusters plays an important role for the production of highly active secondary species like low-energy electrons. ICD has been studied in numerous systems, e.g. in the Van-der-Waals clusters [2], hydrogen-bonding water dimers [3] and larger water clusters [4] as well as in the biochemically relevant systems associated with water [5].

Here, we investigate 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 an analog of the sugar ring in the DNA backbone linking the phosphate groups and the DNA bases. Experiments were carried out using a multi-particle imaging spectrometer (reaction microscope) [6, 7] in which the kinetic energies of final state electrons and ions are measured. The projectile electron energy of 66 eV is chosen to be in the range of the mean energy of secondary electrons which are produced in great numbers by any high-energy ionizing radiation. An artist view of the ICD process is shown in Fig. 1. The process is triggered by removing an inner-valence electron from the water molecule in the dimer. After that the $H_2O^+(2s^{-1})\cdot C_4H_8O$ dimer cation undergoes ICD, and a low-energy electron from the neighboring C_4H_8O will be ejected. Several signatures allow identification of ICD together with the ionization potential calculations. 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 [8]. Detailed results will be presented at the conference.

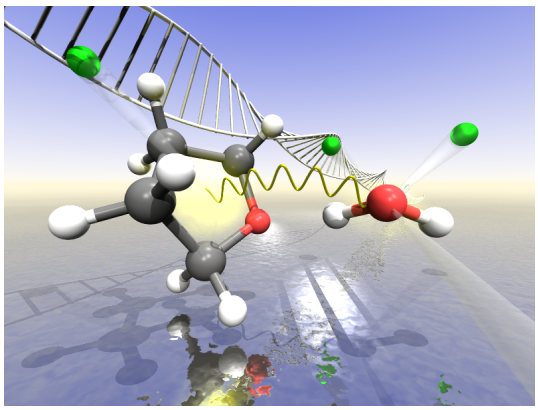

Figure 1. Artist view of ICD in a hydrated tetrahydrofuran clusters upon electron-impact.

References

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