

Electron-Collision Induced Ionization and Fragmentation in Hydrated Biomolecule Clusters

Xueguang Ren¹, Alexander Dorn²

Max Planck Institute for Nuclear Physics, 69117 Heidelberg, Germany

Synopsis We study the ionization and fragmentation of tetrahydrofuran (THF) and water-THF mixed clusters induced by low-energy ($E_0 = 65$ eV) electron-collision using an (e, 2e + ion) triple coincidence method. The momentum vectors and, consequently, the kinetic energies for all three final-state charged particles are determined. The ionic fragments are identified from the measured ion time-of-flight spectra which are significantly different between monomers and water-mixed clusters. The influence of the water environment on the biomolecule is investigated by comparing the triple-differential cross sections and binding energy spectra between monomers and water-mixed clusters.

Electron-impact ionization of atoms and molecules is a fundamental process which is relevant to understand and interpret a wide range of scientific phenomenon and technological applications, including the physics and chemistry of planetary atmospheres, reactive plasmas, and more recently even radiation tumor therapy [1, 2]. An important role in this respect plays water which is ubiquitous on earth and surrounds all biological matter. Water and hydrated biomolecule (water-mixed) clusters have been the subjects of intense studies due to their importance in life and environmental sciences [3].

In the present work, we report an experimental study on the electron-collision induced ionization and fragmentation processes in clusters consisting of water and bio-relevant molecules like DNA constituents. We use the multi-particle coincidence technique (reaction microscope) [4, 5] in which the momentum vectors and, consequently, the kinetic energies of all final state particles (electrons and ions) are measured in coincidence. 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. Figure 1 presents the measured fragment ion time-of-flight (TOF) spectra for both THF and hydrated THF clusters induced by electron ionization (65 eV). Compared to the fragmentation of isolated THF molecules where the most abundant fragment ion is identified as $C_3H_6^+$ [3], the observed major species for THF cluster fragmentation are $(C_4H_8O)H^+$, $(C_4H_8O)C_2H_4O^+$ and $(C_4H_8O)_2H^+$. For the hydrated THF clusters we find $(C_2H_4O)H_2O^+$, $(C_4H_8O)(H_2O)H^+$, $(C_4H_8O)(H_2O)_2H^+$ and $(C_4H_8O)(H_2O)_3H^+$ species. Therefore, we observe that the fragmentation processes are modified by the presence of the water molecule. From the measured kinetic energies of two

outgoing electrons and one fragment cluster ion, the binding energy ($BE = E_0 - E_1 - E_2$) for each fragmentation channel is obtained. In addition, the triple-differential cross sections related to each fragmentation channel are also measured in the experiment. Thus, by comparing the triple-differential cross sections and the correlation spectra of binding energy and fragment species between clusters and the isolated molecule, we can investigate in detail the role of the neighbor for the modification of the biomolecular fragmentation. Detailed results will be presented at the conference.

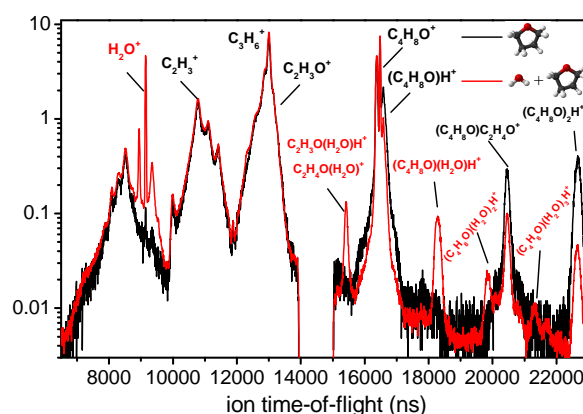


Figure 1. Measured fragment ion time-of-flight spectra of THF and hydrated THF clusters induced by electron-impact ($E_0 = 65$ eV) ionization.

References

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¹E-mail: ren@mpi-hd.mpg.de

²E-mail: Alexander.Dorn@mpi-hd.mpg.de