

X-ray photophysics and solvent-bond breaking of controlled gas-phase molecules and clusters

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The properties of atoms and molecules are strongly dependent on their environment and hydrogen bonds are of universal importance in chemistry and biochemistry. Therefore, it is highly desirable to bridge the gap between the accurate understanding of single, isolated molecules and the complexity of molecules in solvation.

We present results of a photofragmentation study of indole, the chromophore of the amino acid tryptophan, and indole-water₁ clusters, i.e., indole ‘solvated’ by a single water molecule. The indole-water₁ clusters were spatially separated from monomeric indole using the electric deflector [1,2]. Photofragmentation was induced by site specific 1s core hole ionization of the indole’s nitrogen or carbon atom leading to a relaxation of the highly excited molecules and clusters via an emission of electrons and/or photons and subsequent Coulomb explosion.

Photo and Auger electrons as well as ionic fragments were recorded in coincidence with a double-sided velocity map imaging (VMI) spectrometer. The photofragmentation of indole and indole-water was compared by means of (photoelectron-) photoion-photoion (PEPIPICO) coincidences. Charge, proton or hydrogen transfer to the hydrogen bonded water molecule, as well as different Coulomb explosion channels, due to further emission of electrons on the indole-side of the cluster, were observed. The results will be discussed based on the fragmentation channels of the different species, photoelectron and ion VMI images for different ionic fragments, and the 3D reconstruction of the molecule’s orientation.

Additionally, we present preliminary results on solvent-bond-breaking of indole-water in a pump-probe experimental scheme. Indole-water₁ was neutrally dissociated by a single UV photon, and the dissociation was probed by site specific 1s core hole ionization of the indole’s nitrogen or carbon. The experimental conditions were comparable to the static measurement of indole [3] and indole-water₁, but the detection was limited to an ion VMI spectrometer.

The experiments were carried out in a collaboration with DESY and Kansas State University. The experiments were conducted at the Variable Polarization XUV Beamline P04 of PETRA III at DESY and at the AMO beamline of the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory.

References

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