

SLOW PHOTOELECTRON SPECTROSCOPY AND STATE-SELECTED UNIMOLECULAR DECOMPOSITION OF IONIZED DNA BASES ANALOGUES

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We studied the single-photon ionization of gas-phase 2-Piperidone (DNA basis analogue) and of its dimer using vacuum-ultraviolet (VUV) synchrotron radiation coupled to a velocity map imaging electron/ion coincidence spectrometer^a. The slow photoelectron spectrum (SPES) of the monomer is dominated by the vibrational transitions to the ground state. These spectra are assigned with the help of theoretical calculations dealing with the equilibrium geometries, electronic-state patterns and evolutions, harmonic and anharmonic wavenumbers. After its formation, dimer is subject of intramolecular isomerization, H transfer and then unimolecular fragmentation processes.

The near threshold photofragmentation pattern of the cationic 2-Piperidone cation and its dimer has been recorded. The experimental method yields the fragment intensity as a function of the internal energy deposited into the parent cation. In parallel, ab initio studies on ionic and neutral fragmentation products have been performed with the aim of determining the isomers of the ionic products observed experimentally as well as of their neutral counterparts.

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