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Identification of gas phase DNA bases specific isomers via high accuracy single photon ionization and ab initio computations

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DNA/RNA bases and amino acids are building blocks of life. The spectroscopy and stability of their ionic forms are relevant to their survival rate under interstellar conditions, and to the field of radiation damage, where ionizing radiation can lead to DNA/RNA strand breaking and production of hazardous by-products through processes involving nucleobases.
Several experimental works at BESSY II, Advanced Light Source and synchrotron SOLEIL were devoted to unveil the structure and the spectroscopy of the cationic species of DNA bases and amino acids and analogues. Since they possess numerous tautomers and isomers that lie close in energy, the experimental characterization of a unique tautomer is challenging. For this purpose, we apply single photon VUV synchrotron based experiments combined with state-of-the-art ab initio computations.
Experimentally, we use the VUV light emitted by the DESIRS beamline of synchrotron SOLEIL coupled to the double imaging photoelectron photoion coincidence (i2PEPICO) spectrometer DELICIOUS3. [1] The coincidence scheme allows the photoelectron images to be filtered as a function of mass and ion kinetic energy in a multiplex manner. Treatment of such photoelectron images as a function of the photon energy leads to the threshold / slow photo electron spectra of the selected masses. [2] Theoretically, the structures and the energetics of neutral and cationic molecular systems are determined using post Hartree-Fock-density functional theory composite schemes. We also treat these species in their electronic excited states using configuration interaction methods.[3] Afterwards, we use the theoretical results to disentangle the complex features observed experimentally.
Our combined theoretical and experimental approach can be applied to several DNA bases and analogues presenting a dense pattern of electronic and/or isomeric and/or tautomeric forms in their spectra. In sum, we established a non-equivocal way to characterize the neutral DNA bases in gas phase prior to photoionization. Also, we derive a set of thermodynamical data of specific gas phase tautomers/isomers/rotamers produced in a molecular beam (e.g. adiabatic ionization energies, bond energies). Several examples will be presented. [4-9]
This work is a long term collaborative project involving colleagues from Synchrotron SOLEIL, CNRS, CEA, U. Paris Saclay, Sorbonne U., U. PE Créteil, U. Gustave Eiffel, King Saud U., City U. Hong Kong, and U. Tunis.

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