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PHOTOELECTRON SPECTROSCOPY OF SOLVATED BIOLOGICAL INTEREST MOLECULES IN LIQUID JET CONFIGURATION

M. FOURNIER[1,2], J. PALAUDOUX[2], R. DUPUY[2], F. PENENT[2] and C. NICOLAS[1]

[1]*Synchrotron SOLEIL, Saint-Aubin, France*
marine.fournier@synchrotron-soleil.fr

[2]*Laboratoire Chimie Physique – Matière et Rayonnement, Sorbonne Université, UMR 7614, Paris, France*

Uracil is a RNA nucleobase and 5-bromouracil, one of its haloderivatives and known for its radiosensitizer property in DeoxyriboNucleic Acid (DNA) (Zimbrick J D et al. 1969). Incorporated in DNA, it can both be responsible of mutagenic effect (Kavli B et al. 2007). The cause of this effect is largely studied, but doubts still subsist about the deprotonation site and the tautomer form present in liquid water. Probing the electronic structure gives information on the local environment, and consequently lets us to study the effect of solvation and chemical environment changes. This type of measurement is possible combining an electron spectrometer with an under-vacuum liquid jet device. With this configuration, it is possible to probe three molecular layers at the surface of the liquid-jet, enough to be in complete solvation condition. The measurements presented in this work have been done on PLEIADES beamline (Renault J-P et al. 2022), synchrotron SOLEIL. The C 1s and N 1s photoelectron spectra of each molecule has been measured at different pH conditions (6.5, 10.8, 12.6), far enough from the pKa value. Thus, we obtain photoelectron spectra of protonated form of uracil comparable to the ones measured in water-clusters (Mattioli G et al. 2022), which not reveal differences between micro-solvation and complete solvation. The increase of pH in solutions induces a shift of the photoelectron peaks to lower binding energies. Peak attribution is completed by theoretical calculations (team of Majdi Ochlaf, Université Marne la Vallée and the team of Petr Slavicek, University of chemistry and technology of Prague). Interestingly, the 5-bromouracil behaves differently compared to uracil at the higher pH condition whose the interpretation is still to be confirmed. We have extended our liquid XPS measurements to biggest biological molecule with solvated prototypical (DNA). These measurements are relevant to the study of radiation damage on DNA at the physical stage.

References

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