

X-RAY ACTION SPECTROSCOPY OF GAS-PHASE BIOMOLECULAR IONS

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Abstract. Over the past decades, peptides and proteins have been investigated in the gas phase using state-of-art mass spectrometric techniques combined to electrospray ionization sources. In order to obtain new insights into the electronic and structural properties of such biomolecules, X-ray action spectroscopy experiments, which are based on the resonant photoexcitation of core electrons, have been carried out at synchrotron facilities, which offer a broad photon energy range and a high photon flux. It has been used successfully to unravel different aspects of the photodissociation of peptides and to probe conformational features of proteins. It is a current question to which extent the resonant photoabsorptions are sensitive toward effects of conformational isomerism, tautomerism, and intramolecular interactions in gas-phase peptides. Additionally, in the soft X-ray regime, the high degree of localization of the deposited energy allows getting a deeper understanding on the dissociation processes. However, identifying products of site-selective dissociation in large biomolecules is challenging at the carbon, nitrogen, and oxygen edges because of the high number of these atoms and related chemical groups. Probing the inner shells of a single sulfur atom within a biomolecule as the one and only excitation site is a promising way to overcome this obstacle. I will present here an overview of recent synchrotron-based experimental studies on the X-ray action spectroscopy of model peptides, carried across at the carbon, nitrogen, and oxygen K-edges^[1] as well as sulfur L-edge^[2].

References

- [1] Dörner S. *et al.*: 2021, *J. Am. Soc. Mass Spectrom.*, **32**, 3, 670-684
[2] L. Schwob L. *et al.*: 2020, *J. Phys. Chem. Lett.*, **11**, 1215-1221.