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Photodissociation of protonated Leucine-Enkephalin peptide in the VUV range

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Synopsis We present results of VUV action spectroscopy of gas-phase protonated Leucine-Enkephalin peptide. The experiment has been performed by coupling a linear quadrupole ion trap with a synchrotron radiation VUV beamline.

Recent development of experimental methods that use electrospray ion source (ESI) to bring macromolecules into gas phase and collect the ions in an ion trap, which is coupled to bright synchrotron radiation sources, has allowed the investigation of large biopolymers (proteins and nucleotides) under well-defined conditions. These studies can provide more detailed insight into fundamental properties of biopolymers and their interaction with high energy photons.

We present the results of VUV photon action spectroscopy of Leucine-Enkephalin (Leu-Enk) peptide in 5-15 eV energy domain. This peptide has been studied with wide range of spectrometry techniques and has become a standard biomolecular target [1].

The experiment has been performed at the beamline DESIRS [2] of the synchrotron radiation facility SOLEIL near Paris, France. More details about the experimental setup can be found in recent publications [3, 4]. Briefly, precursor ions $[\text{Leu-Enk}+\text{H}]^+$ were produced by ESI and injected into the ion trap from the front side. Ions were irradiated with monochromatized VUV photon beam, during 500 ms from the back side of the ion trap. After irradiation all ion fragment species were ejected from the ion trap and tandem mass spectra (MS^2) as a function of the photon energies were recorded. Leu-Enk molecules were provided from Sigma Aldrich and dissolved in water/acetonitrile at 10 μM .

Photodissociation ion yields were extracted from the MS^2 and normalized to the total ion current and the photon flux. The ion yields show spectroscopic structure allowing the studying of absorption-like bands of the peptide.

Figure 1 shows the relative ion yield of one of the backbone fragments. The present experimental results are in good agreement with our time dependent density functional theory (TD DFT) calculations.

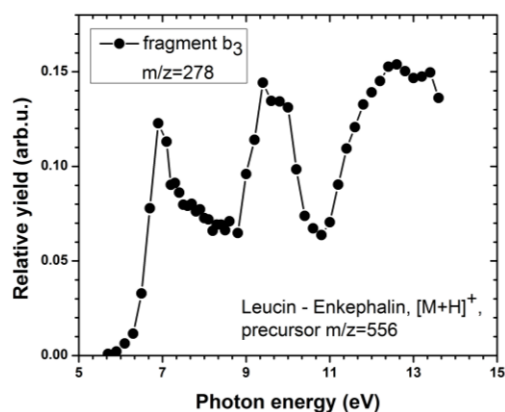


Figure 1. Relative ion yield of fragment b_3 from the photodissociation of precursor $[\text{Leu-Enk}+\text{H}]^+$.

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