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4th XLIC General Meeting
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14 - 16 March 2017

Prague, Czech Republic

BOOK OF ABSTRACTS

The Czech Academy of Sciences

ÚFCH JH

4th XLIC GENERAL MEETING

14 – 16 March 2017

Organised by: J. Heyrovský Intitute of Physical Chemistry of the CAS, v.v.i.
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Photodissociation of hydrated peptide by synchrotron radiation in the VUV region

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Development of electrospray ionization along with already established synchrotron radiation and mass spectrometry techniques, made the studies of interaction of large biomolecules with energetic photons in the gas phase easily accessible. Combination of these techniques gave rise to action spectroscopy[1], a very powerful method, that can give more insights into fundamental physical and chemical properties of biologically relevant macromolecules such as nucleotides, amino acids, peptides[2] or proteins[3]. It is also very important to investigate the influence of the water surroundings or solvation effects on fundamental properties of these biomolecules in order to get more realistic picture of the radiation damage at molecular level.

We present the action spectroscopy results of protonated and hydrated Leucin-Enkephalin peptide, performed by coupling the VUV synchrotron radiation beamline (DESIRS, synchrotron SOLEIL) with the ion trap mass spectrometer. Results suggest that hydration with only three water molecules may have significant influence on the fragmentation pattern of this peptide, Figure 1.

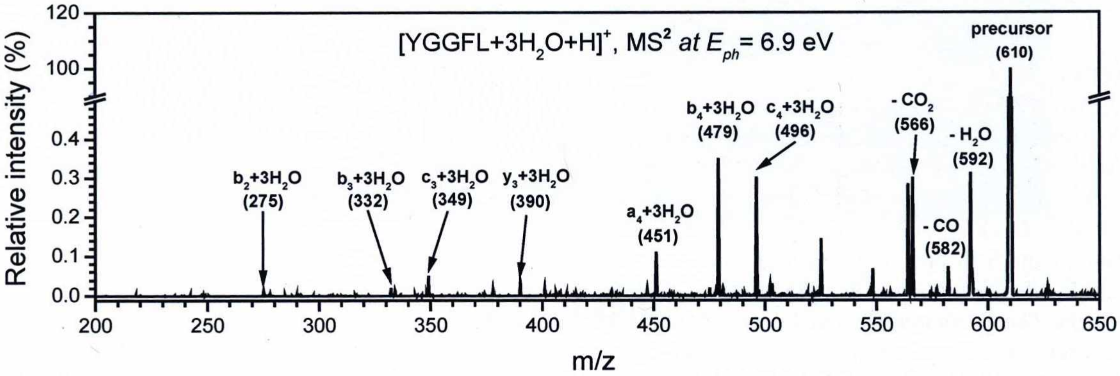

Figure 1. Tandem mass spectra (MS^2) recorded for Leucin-Enkephalin (YGGFL) peptide hydrated with three water molecules, obtained at photon energy of 6.9 eV.

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$K^{-2}V$ process in function of LEE energy distribution

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The study of atoms and molecules under extreme intensities of new light sources requires new theoretical models that can serve as guidance for experiments. These sources can be used for different purposes, and as a result atoms and molecules can be ionized and the photoelectrons produced. In the first step these electrons are removed from any atomic or molecular quantum level, but after that they can initiate further ionization or excitation processes. Our goal is to make a theoretical framework that enables *prediction* of the energy electrons distribution. Especially, main focus is on the low energy electrons (LEE), because they play significant role in bio damage. In order to achieve this, the channels of sequential, nonsequential ionization, and ionization with ionic core excitation (inelastic tunneling) have been taken into account, which is completely in accordance with nowadays researches on the simultaneous ionization and excitation processes of atomic and molecular systems. We started with $K^{-2}V$ process in helium like atoms.K-shell electrons experience two competing channels of simultaneous ionization-excitation processes with comparable intensities. The first one corresponds to direct shake-up of the remaining core electron after ionization and the second one to shake-off of the other core electron.

Our intention, in the further work, is not only to determine fundamental mechanisms that are involved in processes in biomolecules, but also, based on theoretical model, to find the control mechanisms of relevant parameters and, at the same time, induced effects.

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Wave-packet calculations of photoelectron momentum distributions at strong field ionization of sodium

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The momentum distribution of photoelectrons produced at strong field multiphoton ionization (MPI) of sodium are calculated using the wave-packet propagation technique (Ref. 1) and the single active electron approximation (Refs. 2 and 3). We considered the ionization by linearly polarized laser pulses of a few femtoseconds duration with the wavelengths in the near infrared domain and the peak intensities of a few TW/cm^2. Apart from the strong emission along the laser polarization the distribution shows maxima of the outgoing wave at specific directions, containing the information about contributions of the accessible emitted partial waves (Fig. 1). In addition, the obtained distribution patterns clearly show structures related to the above threshold ionization (ATI) as well as the resonantly enhanced multiphoton ionization (REMPI), observed in recently performed experiments with sodium (Ref. 4).

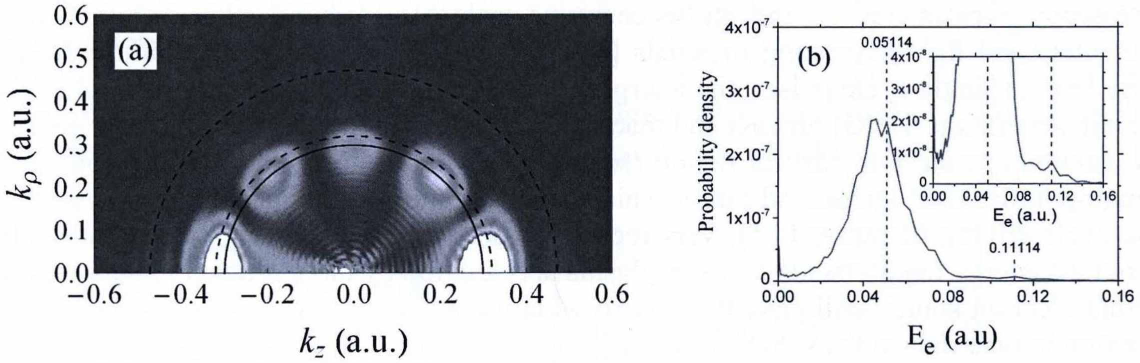

Figure 1: (a) The probability density in the momentum space of the photoelectrons emitted from the sodium atom irradiated by the 10 fs laser pulse with the wavelength of 760 nm and the peak intensity of 1.72 10^{12} W/cm^2. Dashed semicircles denote the expected values of the momentum for the four-photon (MPI) and five-photon (ATI) processes. Four and five minima along the semicircles indicate that in these two processes the g and the h partial waves, respectively, are dominant. (b) The corresponding excess energy distribution of photoelectrons. Substructures in the threshold peak as well as in the ATI area can be related to the REMPI.

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"Position" does matter: The photofragmentation of the nitroimidazole isomers

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Radiotherapy is one of main techniques used in cancer treatment and radiosesitizers are drugs used to selectively improve its effectiveness against tumor cells. Misonidazole and Nimorazole are two radiosensitizers with similar chemical structure. However clinical trials have shown that they have different efficiency in the tumor treatment. In order to understand why this happens we have studied the photo-fragmentation of 2-nitroimidazole and 4(5)-nitroimidazole, which are the "building blocks" of Misonidazole and Nimorazole, respectively. Time of Flight Mass spectrometry (fig 1) shows important differences in their fragmentation, which can be linked with medical applications. To have a better knowledge of these processes we have also measured Appearance Energy (AE) and Photoelectron-Photoion Coincidences (PEPICO) with Synchrotron Light (Elettra, Trieste), and performed theoretical calculations Ref. 1.

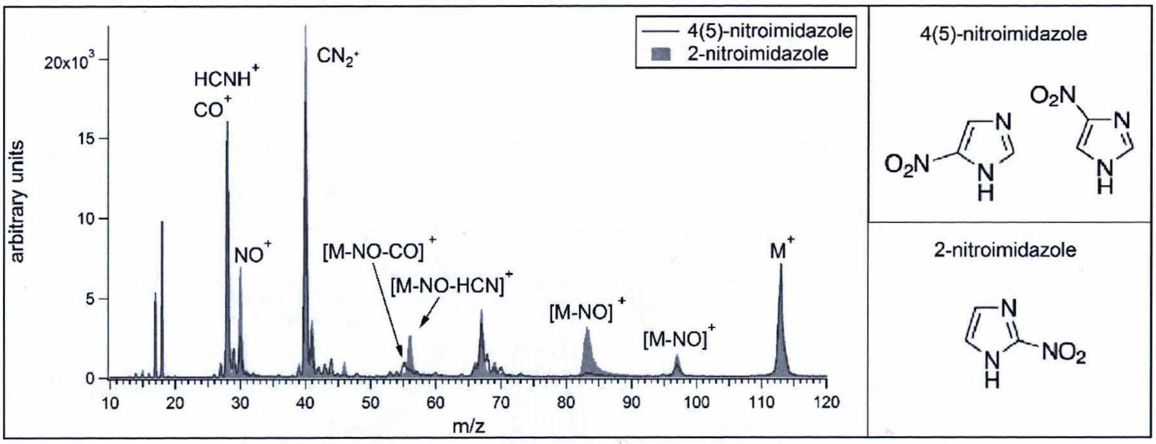

Figure 1: Time of Flight Mass Spectrum (TOF-MS).

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Oxygen K-edge action spectroscopy of isolated nanosolvated Substance P: Resolving the excitation of the peptide and the attached water network

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The study of isolated biomolecules solvated on an atomic level is important to understand the hydrogen bonding network of water molecules and their interaction with the biomolecule that overall defines its structure and functionality [1]. Here we report preliminary results of a pioneering study of inner-shell excitation of an isolated nanosolvated peptide.

We have performed O K-edge inner-shell action spectroscopy of both bare and hydrated Substance P peptide ions isolated in the gas phase, by coupling a commercial linear quadrupole ion trap mass spectrometer (LTQ XL) to the PLEIADES soft X-ray beamline at the SOLEIL synchrotron, as previously described [2,3]. For the first time, we recorded O K-edge ion yield spectra for isolated doubly charged Substance P peptide, as well as for the same system hydrated with 11 water molecules. The present results suggest that processes upon excitation of the peptide and the attached water cluster could be resolved. We are presently performing high-level DFT calculations in order to understand the structure and the excitation processes of the solvated peptide.

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