XLIC
XUV/X-ray light and fast ions for ultrafast chemistry

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EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

Meeting of the XLIC Working Group 2

WG2 Expert Meeting on Biomolecules

27-30 April 2015, Fruška gora, Serbia

Institute of Physics Belgrade
University of Belgrade

Invited Lectures

Fragmentation of halopyrimidines and halouraciles by photoionization and ion impact

P. Bolognesi[1], M.C. Castrovilli[1], A. Kettunen[2], A. Cartoni[3], R. Richter[4], S. Tosic[5], S. Maclot[6], P. Rousseau[6],R. Delaunay[6], A. Domaracka[6],B. Huber[6] and L. Avaldi[1]

[1]*CNR-Istituto di Struttura della Materia, Area della Ricerca di Roma1, Monterotondo Scalo, Italy*
[2] *Department of Physics, University of Oulu, Finland*
[3] *Dipartimento di Chimica, Sapienza Università di Roma, Roma, Italy*
[4] *Elettra-Sincrotrone Trieste, Basovizza, Italy*
[5] *Institute of Physics, University of Belgrade, Belgrade, Serbia*
[6] *CIMAP, CEA/CNRS/ENSICAEN, Université de Caen Basse-Normandie, Caen, France*

In recent years we have focused our interest in processes induced in isolated molecules by soft X-ray and ion beams. By photon ionization the site and state of the energy deposition are well defined and the following chain of processes are characterized by coincidence techniques. In the fragmentation induced by low energy ions, the effects of the increasing complexity of the target and the role played by the 'environment' on the properties of the single molecule are addressed.
In the presentation two examples will be discussed. The first one is the photofragmentation of 2Cl-pyrimidine following inner shell excitation or direct valence ionization studied via electron-ion coincidence techniques. The experiments have been performed at the Gasphase photoemission beamline at Elettra, Trieste (Italy). The results show that the resonant Auger process following inner shell excitation selectively populates the final states of the singly charged ion and the site and state selected fragmentation patterns appear to depend only on the final state of the singly charged ion. The comparison with state selected photofragmentation after valence ionization confirms the role of the cationic state in the type of fragments produced.
In the second example the fragmentation of 5Br-uracil isolated molecules, homogeneous clusters and hydrated clusters by C^{4+} ions has been studied. The experiments have been performed at the ARIBE beamline of the GANIL facility,Caen (France). The observation of series of hydrated fragments provides the experimental evidence that a few water molecules attached to the 5Br-uracil can induce a tautomerisation process. This process can lead to mutagenesis and therefore to a different pairing in the DNA bases and can explain the radiosensitizing effect of compounds bases on 5Br-uracil.

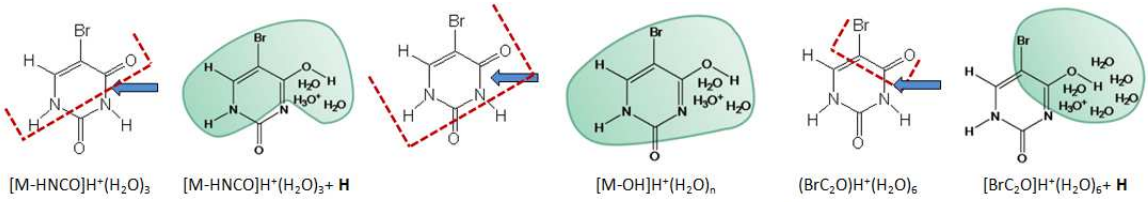

Fig.1. Schematic of the main fragments whose hydrated series are observed and assigned in the mass spectrum of hydrated clusters of 5Br-uracil. The blue arrows indicate the suggested site of hydration and the red dashed lines surround the charged (detected) fragment; M indicates the parent ion.The proposed tautomerisation processes mediated through the presence of a sufficient number of water moleculesis also shown.

PROGRAM SCHEDULE

COST XLIC WG2 Expert meeting on biomolecules

27-30 April 2015, CePTOR congress center, National park Fruška gora, Serbia

(Invited Lectures: 20 min + 10 min for discussion)

Monday 27th April 2015	
17:00-18:30	Registration
18:20-18:30	**Welcome to participants**
	***Session 1**, Chair: Manuel Alcami*
18:30-19:00	*Local control theory using TDDFT-based nonadiabatic dynamics* **Ivano Tavernelli,** EPFL, Switzerland
19:00-19:30	*Shedding light on molecular excited states with novel EUV sources* **Marcello Coreno,** CNR-ISM, Italy
19:30-20:00	*Obvious and nonobvious dissociation pathways of N-substituted glycine ions* **Jaroslaw Kočišek,** CIMAP - GANIL, France
20:00-21:30	Dinner
Tuesday 28th April 2015	
07:00-09:00	Breakfast
	***Session 2**, Chair: Aleksandar Milosavljević*
09:00-09:30	*Ion and photon interactions with superhydrogenated PAHs* **Thomas Schlathölter,** University of Groningen, The Netherlands
09:30-10:00	*Gas-phase spectroscopy of ferric heme nitrosyl cations* **Jean Wyer,** Aarhus University, Denmark
10:00-10:30	*DFT and TD-DFT of nanosolvated biomolecules* **Viktor Cerovski,** University of Belgrade, Serbia
10:30-11:00	Coffee break 1
	***Session 3**, Chair: Alicja Domaracka*
11:00-11:30	*On the role of fluoro-substituted nucleosides for radiosensitization in tumor radiation therapy* **Janina Kopyra,** Siedle University, Poland
11:30-12:00	*Low energy electron interactions with cyclic azines* **Jimena Gorfinkiel,** The Open University, UK
12:00-12:30	*Electron induced dissociation of biomolecules* **Andreas Mauracher,** University of Innsbruck, Austria
12:30-13:00	*Electron impact fragmentation of thymine and cytosine: partial ionization cross sections for positive fragments* **Peter van der Burgt,** National University of Ireland, Ireland
13:00-15:00	Lunch
	***Session 4**, Chair: Steen Broendsted Nielsen*
15:00-15:30	*Studies of biomolecules at the DESIREE facility* **Nathalie de Ruette,** Stockholm University, Sweden
15:30-16:00	*VUV photoionization study of gas phase biomolecules using aerosol thermodesorption* **Héloïse Dossmann,** Universite Pierre et Marie Curie, France
16:00-16:30	*Energy resolved photoelectron-ion-ion coincidence studies of DNA building blocks and amino acids* **Eero Itälä,** University of Turku, Finland

16:30-17:00	Coffee break 2
17:00-18:00	*Round table discussions 1*
18:00-20:00	***Poster session***
20:00-21:30	Dinner
Wednesday 29th April 2015	
07:00-09:00	Breakfast
	***Session 5**, Chair: Thomas Schlathölter*
09:00-09:30	*Fragmentation of halopyrimidines and halouraciles by photoionization and ion impact* **Lorenzo Avaldi,** CNR, Italy
09:30-10:00	*UV and electron induced dynamics in biomolecules and clusters* **Samuel Eden,** The Open University, UK
10:00-10:30	*Plasma interaction with biomolecules* **Nevena Puač,** University of Belgrade, Serbia
10:30-11:00	Coffee break 3
	***Session 6**, Chair: Paola Bolognesi*
11:00-11:30	*Ultrafast non-reactive deactivation induced by excited state hole transfer from retinal chromophore to counterion* **Nadja Došlić,** Rudjer Boškovic Institute, Croatia
11:30-12:00	*Pure electron dynamics in biomolecules initiated by XUV attosecond pulses* **Andrea Trabattoni,** Politecnico di Milano, Italy
12:00-12:30	*Ultrafast electron dynamics in amino acids initiated by attosecond pulses* **Alicia Palacios,** Universidad Autónoma de Madrid, Spain
12:30-13:00	*Photo-induced ultrafast nuclear dynamics in (deeply) core-excited molecules* **Oksana Travnikova,** CNRS, France
13:00-15:00	Lunch
15:00-19:30	***Excursion***
20:00-22:00	**Dinner**
Thursday 30th April 2015	
07:00-09:00	Breakfast (***Departure to Belgrade airport***)
09:00-09:15	**Closing remarks**
09:15-11:00	*Round table discussions 2*
11:00-11:30	Coffee break 4 (***Departure to Belgrade airport***)
11:30-13:00	*Round table discussions 3*
13:00	***Departure to Belgrade airport***

This Book of Abstracts is supported by COST CM 1204 (XLIC) Action

This Book of Abstracts may be cited as:
COST Action Cm1204 - Book of Abstract - WG2 Expert Meeting on Biomolecules, April, 2015

WG2 Expert Meeting on Biomolecules is organized in the framework of the COST Action CM1204 ('XUV/X-ray Light and fast Ions for ultrafast Chemistry', XLIC). The project aims to better understand, to monitor and to control the complex ultrafast electronic and nuclear dynamics that occur in medium-sized and large molecules. Furthermore, new control strategies of reactions and a new generation of ultrafast spectroscopies combining attosecond temporal and sub-Angstrom spatial resolutions will be developed.

The WG2 Expert Meeting on Biomolecules will take place in Fruška gora (Serbia) from April 27th to April 30th, 2015. This meeting brings together experts from different disciplines (physics, chemistry), experiments and theory to discuss aspects on photon, ion and electron interaction with biomolecules, as well as properties of biomolecules, stability of highly excited and highly charged biological molecules in the gas phase and their reactivity.

We hope that this meeting will initiate new projects and collaborations, inspire new scientific achievements and help promotion of young researchers. We would like to thank the members of the Scientific Committee and Local Organizing Committee for their collaboration and the excellent work.

Paola Bolognesi and AleksandarMilosavljević
The Meeting Chairs

Committee

Meeting chairs

Aleksandar Milosavljević *(Institute of Physics Belgrade, University of Belgrade, Serbia)*

Paola Bolognesi *(CNR-Istituto di Struttura della Materia, Roma, Italy)*

Scientific Committee

Paola Bolognesi *(CNR-Istituto di Struttura della Materia, Roma, Italy)*

Alicja Domaracka *(CIMAP, Caen, France)*

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Local Organising Committee *(IPB, Belgrade, Serbia)*

Aleksandar Milosavljević

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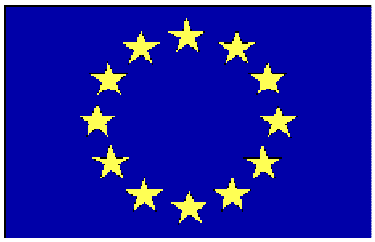

COST is supported by the EU Framework Programme Horizon 2020