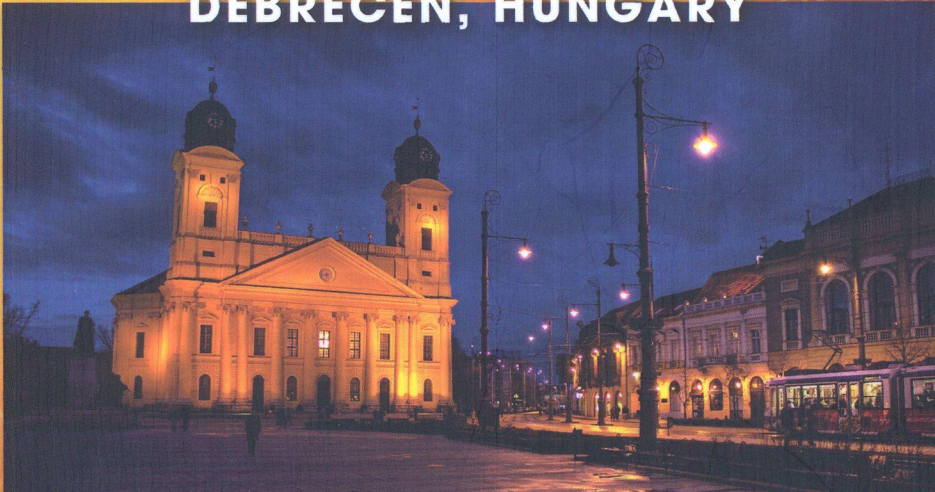


GENERAL MEETING

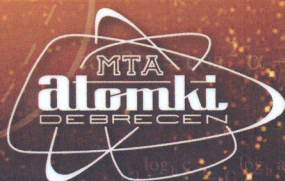
XLIC
XUV/X-ray light and fast
ions for ultrafast chemistry

(COST ACTION CM 1204)

**2-4 NOVEMBER 2015
DEBRECEN, HUNGARY**



**PROGRAMME AND
BOOK OF ABSTRACTS**



3rd XLIC GENERAL MEETING

2-4 NOVEMBER, 2015

Organised by: *ATOMKI / DE / ELFT*

Venue

Centrum Hotel, Debrecen, Hungary

The conference will be hosted at Centrum Hotel, Debrecen, Hungary. The hotel is located in the very heart of the city, at 4-8 Calvin square, next to the Reformed Great Church. All lectures, the poster sessions and the management committee meeting will be held here.

Book of Abstracts

This book contains the camera-ready copies of the abstracts as sent by the authors. In few cases only minor corrections were made.

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WELCOME

Welcome to the 3rd XLIC General Meeting XUV/X-ray light and fast ions for ultrafast chemistry (XLIC), organized in Debrecen (Hungary).

The workshop is an annual meeting of CM1204 action, which deals with physical and chemical phenomena induced by electromagnetic fields and charged particles. The meeting is planned for 2nd - 4th November, 2015. It will take place at Centrum Hotel, Debrecen, Hungary. There will be 24 talks given by invited speakers, 12 oral presentations by early stage scientists and 2 poster sessions.

The organization of this meeting and its funding with COST CM1204 budget was approved in the 3rd MC meeting, held in Gdansk (Poland) on October 10th, 2014.

The objectives of the workshop are to assess the state of the art in the current understanding of a variety of basic phenomena in the electron and atom dynamics such as charge-exchange processes collective as well as single-particle excitation and ionization, energy loss, and photon emission processes, collision induced physical, chemical and biological reactions radiation damage and materials modification.

The XLIC conference is held for the 3rd time. Previous conferences were organized in Madrid (Spain, 2013), Gdansk (Poland, 2014). It is a great honour for Debrecen to be the host of this prestigious event in 2015.

Debrecen is the second largest city of Hungary, one of the most important educational, research and cultural centres in Middle-Europe. Stadiums of Debrecen have given place to great sport events (like European Championship of Swimming, 2012) and the Carnival of Flowers attracts thousands of visitors from all over Europe every year. In addition, there are a lot of sights that must be seen, for instance the Great Church at the beautiful main square, Déri Museum, Reformed College and its unique library, the Great Forest and the main building of the University of Debrecen, but we could continue this list.

The 3rd XLIC conference is held at the Centrum Hotel. The hotel is located in the historic city centre of Debrecen, only 50 meters from the Great Reformed Church and the main square, the venue of many cultural events, in the close vicinity of the most important attractions, office buildings and institutions. It is one of the hotels of Eastern Hungary that provides ideal conditions for the work and recreation of business travellers, while also satisfying the needs of tourists in search of a lively atmosphere and vibrant experiences.

We hope that all participants will have a lively and successful meeting while enjoying the attractive surroundings in this beautiful region of Hungary. We hope, furthermore, we may offer exciting scientific programs in addition to various social and cultural programs, where you can enjoy the famous Hungarian dishes and wine, too. Organizers have been doing their best to guarantee pleasant experiences for everyone.

Károly Tőkési
Chair
3rd XLIC General Meeting

András Csehi
Co-Chair
3rd XLIC General Meeting

Search for the ‘molecular scissor’ via site- and state-selected molecular fragmentation studies

P. Bolognesi^{1*}, A. Kettunen², A. Cartoni^{3,1}, R. Richter⁴, S. Tosic⁵, S. Maclot⁶, P. Rousseau⁶, R. Delaunay⁶, P. Markus¹, H. Sa’adeh⁷, Maša Masič⁸, B. Marinkovic⁵, K. Prince⁴, L. Avaldi¹

¹CNR-Istituto di Struttura della Materia, Area della Ricerca di Roma1, Monterotondo Scalo, Italy

²Department of Physics, University of Oulu, Finland

³Dipartimento di Chimica, Sapienza Università di Roma, Roma, Italy

⁴Elettra-Sincrotrone Trieste, Basovizza, Italy

⁵Institute of Physics, University of Belgrade, Belgrade, Serbia

⁶CIMAP, CEA/CNRS/ENSICAEN, Université de Caen Basse-Normandie, Caen, France

⁷Department of Physics, The University of Jordan, Amman, Jordan

⁸Cardiff University, School of Chemistry, Cardiff, United Kingdom

*Corresponding author: paola.bolognesi@cnr.it

The search for ‘molecular knife/scissors’ i.e. the ability to selectively control molecular fragmentation, is attracting a lot of interest [1,2]. This idea implies the possibility that the localization of the energy deposition into specific atomic sites and/or molecular orbitals could be used to control and address the fate of the molecule following photon absorption, i.e. the molecular fragmentation. Indeed, mass spectra measured at photon energies across inner shell excitation thresholds display marked differences (see Figure 1), suggesting a site-selected fragmentation. In this work we consider the cases of halopyrimidines [3] and nitroimidazoles, two classes of radiosensitisers, to investigate and explain the mechanisms of site- and state-selective fragmentation via a combination of spectroscopic techniques (mass spectrometry, photoelectron, resonant Auger electron as well as electron-ion coincidence spectroscopy) and tunable synchrotron radiation from the Gas Phase beamline of Elettra.

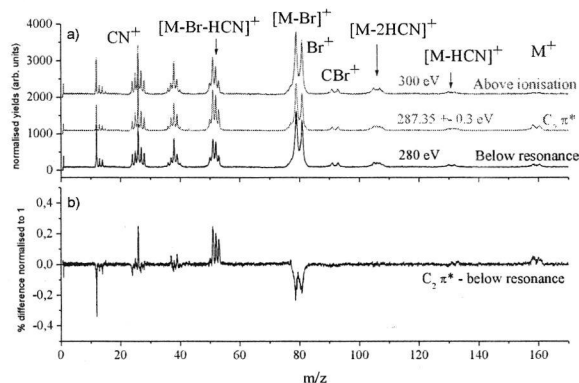


Figure 1: a) The fragmentation mass spectra of 2Br-pyrimidine measured at the $C_2(1s \rightarrow \pi^*)$ excitation (red spectrum) and in the ionization continuum below/above the inner shell resonances. b) The difference spectrum obtained by subtracting the direct ionization contribution from the resonance one.

Acknowledgments: Work partially supported by the XLIC COST Action, the Serbia – Italy Joint Research Project “Nanoscale Insight in the Radiation Damage”, the MIUR FIRB RBFR10SQZI project 2010, the ICTP TRIL Programme and project OII71020.

References

- [1] K. Tanaka *et al*, *Radiat. Phys. Chem.*, **75**, 2076-2079, (2006)
- [2] S. Nagaoka *et al*, *J Phys. Chem A*, **115**, 8822-8831, (2011)
- [3] P. Bolognesi *et al*, *Phys. Chem. Chem. Phys.*, DOI: 10.1039/C5CP02601F, (2015)

	MONDAY		TUESDAY	WEDNESDAY
8:00-9:00			Invited 8 Thomas Baumert	Invited 12 Piero Decleva
9:00-10:00	Registration		Invited 9 Luca Argenti	Invited 13 Daniela Ascenzi
10:00-11:00			Invited 10 Rebeca de Nalda	Invited 14 Daniel Dundas
11:00-12:00			Invited 11 Morten Forre	Invited 15 Ronnie Hoekstra
12:00-13:00			Coffee break	Coffee break
13:00-14:00			Young Scientist Forum I Sandra Gomez Mark Stockett Helena Levola András Csehi Aleksander Simonsen Morgane Vacher	Invited 16 Leticia Gonzalez
14:00-15:00	Lunch Opening (13:20)	Lunch	Invited 17 Nadja Doslic	
15:00-16:00	Invited 1 Thomas Weinacht	Conference Photo (14:20)	Invited 18 Matjaz Zitnik	
16:00-17:00	Invited 2 Franck Lepine	Young Scientist Forum II Rudy Delaunay Katrin Tanzer Michael Gatchell Vera Krizova Dmitrii Egorov Thomas Kierspel	Invited 19 Eva Lindroth	
17:00-18:00	Invited 3 Alicia Palacios		Invited 20 Jimena Gorfinkiel	
18:00-19:00	Coffee break		Invited 21 Sándor Borbély	
19:00-20:00	Invited 4 Benjamin Lasorne		Coffee break	
20:00-	Invited 5 Alexander Kuleff	Invited 22 Jan Petter Hansen	Invited 23 Marta Labuda	
	Invited 6 Attila G. Császár	Coffee break	Invited 24 Nikolay Shvetsov-Shilovskiy	
	Invited 7 Alejandro Saenz	Poster Session II	Dinner	
	Poster Session I			XLIC MC meeting
	Welcome dinner			