

# INTERNATIONAL CONFERENCE ON PHOTONIC ELECTRONIC AND ATOMIC COLLISIONS

26 JULY - 1 AUGUST 2017 | CAIRNS CONVENTION CENTRE | QUEENSLAND, AUSTRALIA

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WE-2	<b>Photoionization of neutral iron from ground and metastable states</b> <i>Oleg Zatsarinny, Luis Fernández-Menchero, Klaus Bartschat</i>
WE-3	<b>Low-energy outer-shell photodetachment of the negative ion of aluminum</b> <i>Oleg Zatsarinny, Klaus Bartschat, Elizabeth Nagy, Sergey Gedeon, Viktor Gedeon, Vladimir Lazur</i>
WE-4	<b>Photoexcitation of atoms by Laguerre-Gaussian beams</b> <i>Stephan Fritzsche, Anton Peshkov</i>
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WE-7	<b>Two-photon K-shell ionization cross sections for neutral atoms</b> <i>Stephan Fritzsche, Jiri Hofbrucker</i>
WE-8	<b>Atomic photoionisation calculated using the singularity-free convergent close-coupling method</b> <i>Alexander Bray, Anatoli Kheifets, Igor Bray</i>
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**TH-35 Spectator Auger decays of cis-1,1,2,2,3,4-hexafluorocyclobutane in the F 1s region***Kazumasa Okada, Takuma Kaneda, Hiroshi Iwayama, Eiji Shigemasa***TH-36 Multicoincidence Studies of Ionization of Chiral Molecules in Strong Laser Fields***Kilian Fehre, Maksim Kunitski, Lothar Ph. Schmidt, Christian Janke, Stefan Zeller, Martin Pitzer, Till Jahnke, Reinhard Dörner, Markus Schöffler***TH-37 A method to determine the energy-transfer distribution in ion-molecule collisions via PEPICO experiments: the case of glycine***Paola Bolognesi, Jacopo Chiarinelli, Alicja Domaracka, Patrick Rousseau, Robert Richter, Lorenzo Avaldi***TH-38 PLEIADES: an ultra-high resolution soft x-ray beamline for spectroscopy of dilute species***John Bozek, Christophe Nicolas, Aleksandar Milosavljevic, Emmanuel Robert, Jean-Marc Bizau, Catalin Miron***TH-39 X-ray absorption spectra of excited triplet states of organic molecules***Atsunari Hiraya, Haruka Inui, Sho Yamahira, Osamu Takahashi***TH-40 "Position" does matter : the photofragmentation of the nitroimidazole isomers***Jacopo Chiarinelli, Paola Bolognesi, Annarita Casavola, Antonella Cartoni, Mattea Castrovilli, Daniele Catone, Robert Richter, Stefano Borocci, Sanja Tosic, Hanan Sa'adeh, Masa Masic, Bratislav Marinkovic, Kevin Prince, Lorenzo Avaldi***TH-41 Photodetachment cross sections for molecular anions of astrophysical interest***Lorenzo Ugo Ancarani, Carlos Mario Granados-Castro, Miguel Lara, Thierry Stoecklin***TH-42 NOO peroxy isomer discovered in the velocity-map imaged photoelectron spectrum of NO<sub>2</sub><sup>-</sup>***Benjamin Laws, Steven Cavanagh, Brenton Lewis, Stephen Gibson***TH-43 Double Photoionization of tribromoborazine***Ralf Wehlitz, Mike MacDonald, Lucia Zuin, Antonio Santos, Narayan Appathurai*

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**6. LEPTON - MOLECULE****Abstract****Title/Authors****TH-45 Single and Double differential cross sections for ionization of water molecules in the liquid state by fast electrons.***Maria Laura De Sanctis, Marie-Françoise Politis, Rodolphe Vuilleumier, Carlos Raúl Stia, Omar Ariel Fojón*

# “Position” does matter : the photofragmentation of the nitroimidazole isomers

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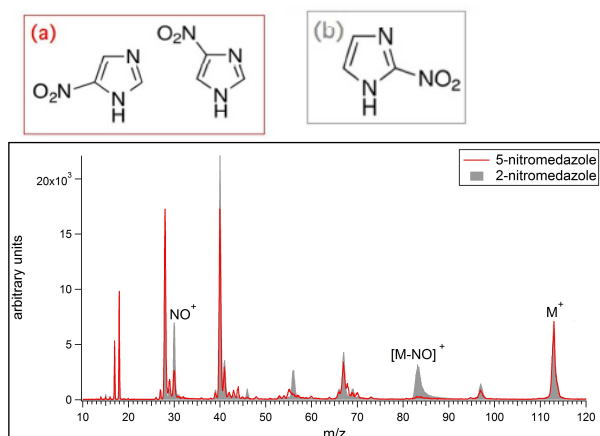
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**Synopsis** Experimental and theoretical spectroscopic methods have been combined to disentangle the fundamental mechanism of VUV induced fragmentation of the three isomers of nitroimidazole radiosensitizers.

Radiotherapy is one of main techniques used in cancer treatment and radiosensitizers are drugs used to selectively improve its effectiveness against tumour 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 photofragmentation of 2-nitroimidazole and 4(5)-nitroimidazole, which are the “building blocks” of Misonidazole and Nimorazole, respectively. To the purpose time of flight mass spectrometry has been used to investigate the fragmentation of these molecules. These measurements have been then extended via the determination of the Appearance Energies (AE) of the different fragments and by Photoelectrons-Photoions Coincidences (PEPICO) experiments using synchrotron radiation [1]. To interpret the results DFT calculations [1] have been also performed.

The mass spectra of the two molecules display many similar features and relative intensities, but also a few intriguing peculiarities. The most striking differences are the fragments at  $m/z$  55<sup>+</sup> and 56<sup>+</sup>, present exclusively in 4(5)NI and 2NI, respectively, and the fragment at  $m/z$  83<sup>+</sup>, which is one of the leading fragmentation channels in 2NI, but is almost absent in the 4(5)NI sample. The results of mass spectrometry are confirmed by the photoelectron-photoion coincidence measurements.

Based on DFT calculations, a model is proposed which fully explains such differences, and reveals the subtle fragmentation mechanisms leading to the release of neutral species like NO, CO and HCN. The present results



**Figure 1.** Mass Spectra of 4(5)-nitroimidazole (red line and scheme a) and 2-nitroimidazole (grey area and scheme b) molecules measured with a He lamp.

suggest that the products of decomposition of the different nitroimidazole isomers might play a role in determining their distinctive degrees of effectiveness in radiotherapy.

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## References

[1] P. Bolognesi et al. J Chem Phys Comm. 145, 191102 (2016)

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