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Book of Abstracts

SELECTIVITY IN THE PHOTOFRAGMENTATION OF HALO-PYRIMIDINES

P. Bolognesi[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], L. Avaldi[1]

[1]CNR-Istituto di Struttura della Materia, Area della Ricerca di Roma1, Monterotondo Scalo, Italy
E-mail: paola.bolognesi@cnr.it
E-mail: lorenzo.avaldi@ism.cnr.it
[2]Department of Physics, University of Oulu, Finland
E-mail: ank@iki.fi
[3] Dipartimento di Chimica, Sapienza Università di Roma, Roma, Italy
E-mail: antonella.cartoni@uniroma1.it
[4] Elettra-Sincrotrone Trieste, Basovizza, Italy
E-mail: robert.richter@elettra.trieste.it
[5] Institute of Physics, University of Belgrade, Belgrade, Serbia
E-mail: seka@ipb.ac.rs
[6] CIMAP, CEA/CNRS/ENSICAEN, Université de Caen Basse-Normandie, Caen, France
E-mail: maclot@ganil.fr
E-mail: prousseau@ganil.fr
E-mail: delaunay@ganil.fr
E-mail: domaracka@ganil.fr

Pyrimidines are an important class of organic molecules because the pyrimidine ring forms the base structure of three nucleic acids (uracil, cytosine and thymine) and their halogenated substituted bases have found applications as radiosensitizers in radiotherapy. The observation of high relative biological effectiveness of soft X-ray in cells [1] has raised the question whether this is due to a specific physical/chemical effect or to the preferential localization of the ionizations in the DNA bases. In the former case this implies a fragmentation process induced by the radiation, while the latter implies that the bond breaks are due to the electron swarms produced following the absorption of the soft X-ray. To answer these questions we have undertaken an extensive study of the electron spectra from the inner shell ionized and excited molecules as well as their site selected fragmentation patterns.

In a series of works on pyrimidine [2] it has been observed that the resonant Auger spectrum shows a selective population of 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. Based on these previous results in this work we have studied the fragmentation of 2Br-, 2Cl- and 5Br-pyrimidine following direct valence shell photoionization as well as C and N 1s inner shell excitations. In the case of valence ionization the detection of the fragment ions in coincidence with energy selected photoelectrons allows a state selected study on the different cation states involved in the process. In the case of inner shell excitation the fragment ions are detected in coincidence with the resonant Auger electrons. In this way the selectivity on the site of the initial energy deposition is added, too.

In figure 1 an example of the fragmentation of the 2Cl-pyridime after valence photoionization is shown. The observation of the parent ion or its fragment ions strongly depends on the excited cationic state. The comparison with the fragmentation following the population of the same states via site-selective inner shell excitation indicates that the major role is played by the final

cationic state. Similarities and differences in the fragmentation as a function of the excitation site and halogenation will be presented in the poster.

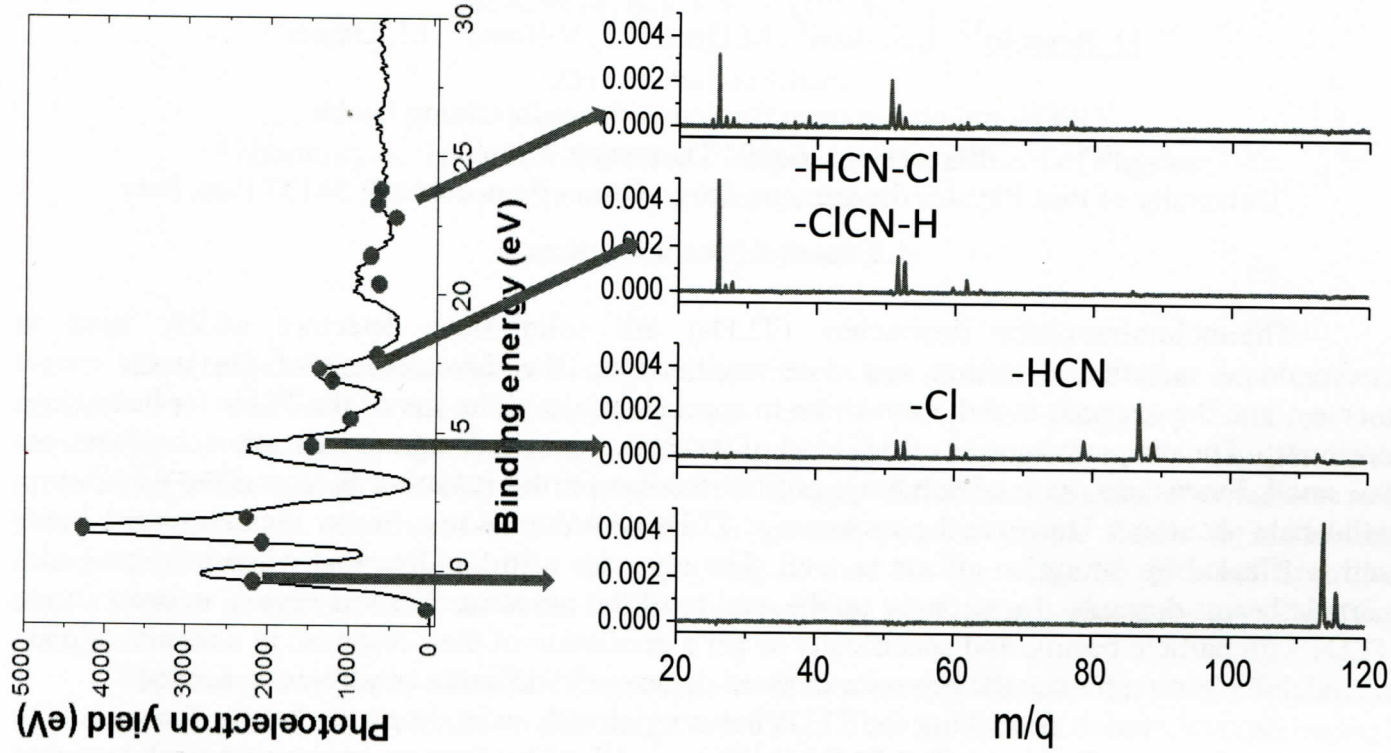

Figure 1: Photofragmentation of 2Cl-pyryimidine studied by a photoelectron-photoion coincidence experiment at 100 eV. On the left panel the photoelectron spectrum of the molecule is shown, while on the right panel some coincidence mass spectra at different binding energies are reported.

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