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CASPUR

CMP 2008

**Control Of Molecular Processes Induced by
Electrons and Photons:
Experiments and Interpretations
A Congress in Honour of Prof. Hotop**

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Control Of Molecular Processes Induced by Electrons and Photons: Experiments and Interpretations

The advent of several new experimental tools becoming available, either directly to many individual laboratories around the world or indirectly via large, shared international facilities, has allowed great progress to be achieved in our understanding of the variety of elementary mechanisms which drive the evolution of reactions at the molecular level.

As a consequence, the desire to be able to achieve the production of preselected outcomes has gained new force hence the field of molecular control of such processes has been steadily growing since its early beginnings only a decade ago.

The attention of the present meeting has therefore been focused on a small sub-area of controlling conditions: those induced by low-energy electrons and low energy photons as well as by cooling down the environment's thermal bath. By these means one can assess what can be gathered today from a rather broad range of experimental setups and findings.

The various sessions of the conference, therefore, describe different approaches to such molecular understanding by reporting on different findings in cases where electrons are used as probing tools and as possible "knobs" for controlling selected reactions. Photons and coincidence experiments with electrons are also considered, while the use of He droplets as highly quantum (and cold) environments in which to probe and control chemical properties, is presented in several other reports.

This gathering of scientists from nearly twenty different countries at the Lincei Academy in Rome would not have been possible without the financial support of the Academy itself (through its interdisciplinary centre "Beniamino Segre") and of various European Network and COST projects such as EIPAM and ECCL. In addition to all of these we also thank the Springer Publishing Company for the award of the EPJD Lectureship to be delivered during this conference. Naturally the generous involvement of all the members of the Scientific Committee and of the Local Organizing Committee has been essential for the felicitous completion of the many preparatory aspects of the meeting: to them go our most heartfelt thanks.

Before closing I should take this opportunity to say that it is a great joy for all of us to hereby celebrate the career and achievements of one of the most active members of our community: Professor Hartmut Hotop, to whom we wish many more years of activity in science.

F. A Gianturco
Chair, local and scientific committees

Electronic excitation of pyrimidine studied by VUV photoabsorption and electron energy loss spectroscopy methods

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It is already well known that a major part of the energy deposited by the primary radiation in cellular irradiation is channeled into the production of large number of secondary species such as low-energy electrons, which may further interact with the cellular matter, including DNA, via inelastic processes. We report preliminary results on electron energy loss (EEL) and VUV photoabsorption spectroscopy of pyrimidine. This molecule is akin to DNA and RNA basis – cytosine, thymine and uracil and is therefore considered as a good model compound to investigate electron interactions with constituents of DNA and RNA. Absolute vibrational and electronic cross sections for low-energy electron scattering from condensed pyrimidine have been published recently [1], where previous works on VUV and electron energy loss spectroscopy are also summarized. The present high-resolution VUV photoabsorption measurements were performed using the ASTRID – UV1 beam line at the Institute for Storage Ring Facilities (ISA), University of Aarhus, Denmark. A detailed description of the apparatus can be found elsewhere [2]. Briefly, a toroidal dispersion grating is used to select the synchrotron radiation with a FWHM wavelength resolution of approximately 0.075 nm. The synchrotron radiation passes through the static gas sample at room temperature. A photo-multiplier is used to detect the transmitted light. A LiF entrance window acts as an edge filter for higher order radiation restricting the photoabsorption measures to below 10.8 eV (115 nm). The grating itself provides a maximum wavelength (lower energy limit) of 320 nm (3.9 eV). The EEL measurements were performed using a cross-beam arrangement [3], with an electron gun, a double cylindrical mirror energy analyzer (fitted with cylindrical electrostatic zoom lenses), and a single channel electron multiplier as a detector. The best energy resolution was estimated to be ~ 0.5 eV. EEL spectra have been obtained for energy losses up to 15 eV, for different incident electron energies between 50 eV to 250 eV and at different scattering angles from 10° to 110°. The present VUV and EEL spectra agree very well, showing the most intensive band at about 7.6 eV, which is ascribed to ¹B₁ and ¹A₁ states [1] (dominant $\pi \rightarrow \pi^*$ transition). The spectra also show intensive excitations at about 4.3, 5.2 and 6.8 eV (the latter not being totally resolved in EEL due to the lower resolution). The high-resolution VUV spectrum reveals rich vibrational structure in all the absorption bands [4]. The present results are in a very good agreement with recent study performed for condensed pyrimidine [1].

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