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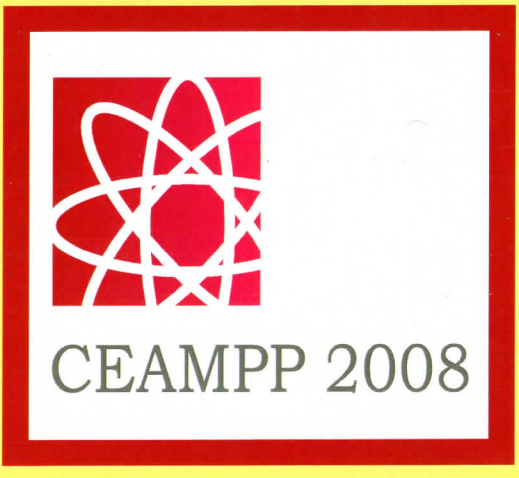

CONTRIBUTED PAPERS
&
ABSTRACTS OF INVITED LECTURES AND PROGRESS REPORTS

Editors:
Aleksandar R. Milosavljević
Dragutin Šević
Bratislav P. Marinković

Institute of Physics
Belgrade - Serbia

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Quantum-Chemical Calculations of the Products and Energies of Fragmentation Reactions

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Electron impact ionization has been studied using a crossed electron/molecule beam experiment built in Bratislava [1,2]. The products of collisions of low-energy electrons with molecules are analyzed using a quadrupole mass filter. Electron beam is produced with trochoidal electron monochromator (with resolution up to 150 meV). This allowed us to perform high resolution electron energy/ion yield dependency measurements.

Appearance energies determined from the experiment are analyzed with methods of quantum-chemistry. Theoretical treatment is used to perform conformational studies of parent molecule, to identify the stable fragmented products, both ionic and neutral (mostly radical), and finally to estimate the reaction energies that can be directly compared with our experimental observations.

Previously, both these treatments were successfully applied to several bio-molecules. Now we present our recent studies of electron impact ionization of 2-Furanmethanol, Tetrahydro- ($C_5H_{10}O_2$) and 3-Furanol, Tetrahydro- ($C_4H_8O_2$), both as important models for more complicated compounds like nucleic acids. Geometry optimizations on DFT level with B3LYP [3] functional are extended with G3MP2 [4] calculations, a set of higher-level ab initio methods empirically corrected to obtain more reliable results compared to experiment.

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Electron Energy-Loss Spectroscopy of Ag Atom

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Electron energy-loss spectroscopy (EELS) is based on measuring the energy which electron loses in inelastic electron-atom scattering. Since this energy is unique to both the energy state and the element in question, EELS technique is important in many applications ranging from various surface science researches to medical diagnosis. It is widely employed for the study of electronic structures, electronic correlation and elemental composition of different materials [1-3], as well as for analyzing biological structures and detection of a single atom contained in the macromolecule assembly [4].

Here we present the results of electron spectroscopy measurements of electron collisions with Ag atom at medium electron impact energies. Experimental measurements of electron impact excitation of the $4d^{10}5p\ ^2P_{1/2,\ 3/2}$ states of Ag have been made at incident electron energies E_0 = 10, 20, 40, 60, 80, and 100 eV. Data obtained include the energy-loss spectra of Ag recorded at different scattering angles using a crossed electron-atom beam technique in the electron spectrometer "ESMA" that operates in energy-loss mode. The experimental apparatus and procedure were described in detail elsewhere [5].

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