Poster Presentation

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Theoretical and X-ray diffraction studies of organic photovoltaic compounds

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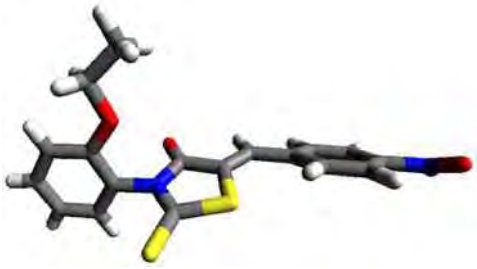
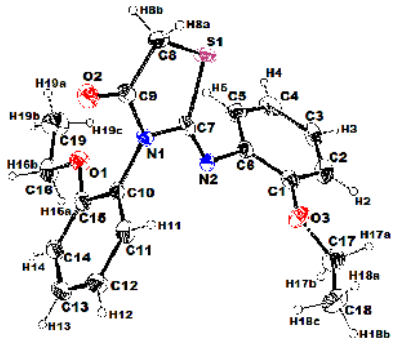
The electronic and structural properties of thiazolic ring derivatives were studied using density functional theory (DFT) and X-ray diffraction in terms of their application as organic semiconductor materials in photovoltaic devices. The B3LYP hybrid functional in combination with Pople type 6-31G(d) basis set with a polarization function was used in order to determine the optimized geometries and the electronic properties of the ground state, while transition energies and excited state properties were obtained from DFT with B3LYP/6-31G(d) calculation. The investigation of thiazolic derivatives formed by the arrangement of several monomeric units revealed that three-dimensional (3D) conjugated architectures present the best geometric and electronic characteristics for use as an organic semiconductor material. The highest occupied molecular orbital (HOMO) . lowest unoccupied molecular orbital (LUMO) energy gap was decreased in 3D structures that extend the absorption spectrum toward longer wavelengths, revealing a feasible intramolecular charge transfer process in these systems. All calculations in this work were performed using the Gaussian 03 W software package.

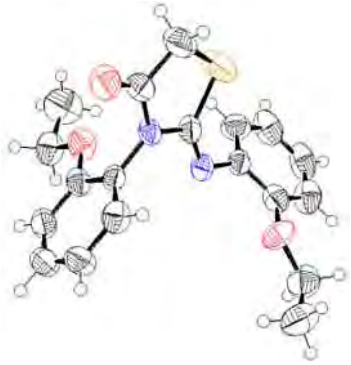
[1] *N. Benhalima, K. Toubal, A. Chouaih, G. Chita, S. Maggi, A. Djafri, F. Hamzaoui, Journal of Chemical Crystallography, November 2011, Volume 41, Issue 11, pp 1729-1736,* ***[2]*** *Shokol TV, Gorbulenko NV, Turov AV, Khilya VP (2013) Chemistry of Heterocyclic Compounds, Vol. 49, No. 2:325*



Compound I



Compound II



Compound III

Keywords: Structure, Thiazole, Dipole moment