

Poster Presentation

CC.P26

Crystal structures of two isostructural thiosemicarbazones and DFT calculations

R. Meroño¹, S. Granda¹, K. Merz², R. Saravanan³, S. Seshadri⁴, S. Gunasekaran⁵

¹University of Oviedo, Department of Physical and Analytical Chemistry, Oviedo, Spain, ²Ruhr-University Bochum, Department of Inorganic Chemistry I, Bochum, Germany, ³AMET University, Department of Physics, Chennai, India, ⁴L.N. Govt. Arts College, Department of Physics, Thiruvallur, India, ⁵T. Peter's University, Department of Research & Development, Chennai, India

The families of thiosemicarbazone compounds have been extensively studied due to their wide range potential in medical applications [1]. Some studies with acetophenone derivatives and their coordination complexes [2] reveal that these compounds could be used as a new class of anti-trypanosomal drug candidate. In view of the importance of these compounds, two new thiosemicarbazones (I) and (II) have been synthesized (compound I substituted with Chloro atom and compound II substituted with Bromine atom), and their crystal structure features are presented here. The crystal structures are isostructural and the molecules crystallize in a P21/c space group. In the crystal packing the molecules are connected through N-H...S hydrogen bonds to form a centrosymmetric synthon. The optimized geometry of the compound (I) was calculated from the DFT-B3LYP gradient calculations employing 6-31G (d,p) basis set and calculated vibrational frequencies are evaluated via comparison with experimental values. Molecular stability has been analyzed using Natural Bond Orbital (NBO) and Natural Localized Molecular Orbital (NLMO) analysis and the limits of the molecular electrostatic potential calculated. The HOMO and LUMO energies shows the charge transfer occurs within the molecule. The results showed no significant geometrical differences (distances and angles), when the solid state crystal structure is compared with the optimized structure in the gas phase. Very good agreements have been found between principal vibrational frequencies calculated from the optimized structure and the experimental spectroscopic data [3]. We thank financial support from Spanish Ministerio de Economía y Competitividad (MAT2010-15094, Factoría de Cristalización- Consolider Ingenio 2010, ERDF funds and German Academic Exchange Service (DAAD)).

[1] O.M. Odenike, R.A. Larson, D. Gajria, M.E. Dolan, S.M. Delaney, T.G. Karrison, M.J. Ratain, W. Stock, *Invest New Drugs*, 2008, 26, 233-239, [2] A.P. Rebolledo, L.R. Teixeira, A.A. Batista, A.S. Mangrich, G. Aguirre, H. Cerecetto, M. González, P. Hernández, A.M. Ferreira, N.L. Speziali, H. Bernaldo, *Eur. J. Med*, 2008, 43, 939-948., [3] R.R. Saravanan, S. Seshadri, S. Gunasekaran, R. Mendoza-Meroño, S. Garcia-Granda, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2014, 121, 268-275

Keywords: thiosemicarbazone, single-crystal X-ray diffraction, DFT calculations