

MS30-P2 Theoretical and Experimental Investigation of (E)-2-([3,4-dimethylphenyl]imino)methyl)-3-methoxyphenol

Orhan Büyükgüngör¹, Zeynep Demircioğlu¹, Çiğdem Albayrak²

1. Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Samsun, Turkey

2. Department of Chemistry, Faculty of Arts and Science, Sinop University, Sinop, Turkey

email: orhanb@omu.edu.tr

The molecular structure and spectroscopic properties of the title compound were investigated by X-ray diffraction, FT-IR and UV-vis spectroscopy. The x-ray structure analysis showed that the molecule has O–H...N intramolecular hydrogen bonding and it adopts the enol-imine tautomeric form. This is also confirmed by the calculations made using density functional theory (DFT) method with B3LYP applying 6-31G(d,p) basis set, for both O–H...N interactions in enol-imine form and N–H...O interactions in keto-amine form.

The harmonic vibrational frequencies (FT-IR) were calculated and compared with the experimental values. The study of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) analysis has been used to elucidate information regarding charge transfer within the molecule. Moreover, the calculation of Mulliken Population analysis and Natural Population analysis were provided to estimate partial atomic charges. Stability of the molecule arising from hyper-conjugative interactions and charge delocalization has been analyzed by using Natural Bond Orbital (NBO) analysis. The results of nonlinear optical (NLO) properties of the molecule showed that it exhibits good nonlinear optical (NLO) activity and so can be used as an effective optical material.

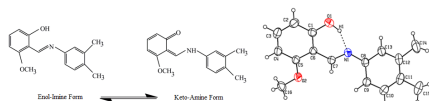


Figure 1. Enol-imine and keto-amine tautomeric forms (left) and the molecular structure (right) of the title compound.

Keywords: X-ray Diffraction, Density Functional Theory (DFT), Natural Population Analysis (NPA), Natural Bond Analysis (NBO), Chemical activity.

MS30-P3 Charge density analysis of intermolecular interactions in the crystal structures of two molecular complexes of p-hydroxybenzoic acid

Maciej Kubicki¹, Agata Owczarzak¹

1. Faculty of Chemistry, Adam Mickiewicz University, Poznan, Poland

email: mkubicki@amu.edu.pl

Experimental charge density analysis, based on high-resolution diffraction data, has its own and high technical demands, but it gives - in return - an opportunity of deeper insight into the details of charge density distribution in the crystal, in particular into both, intra- and intermolecular interactions. It has been shown that this method can be very important for the hydrogen bond analysis, allowing for instance for the building of the hierarchy of the interactions.

We have performed high resolution diffraction studies of two molecular complexes: N-methyl piperidine betaine with p-hydroxybenzoic acid and trygonelline hydrate with p-hydroxybenzoic acid (Fig. 1). The charge density analysis of these structures together with the Atoms-In-Molecules description of the interactions will be presented.

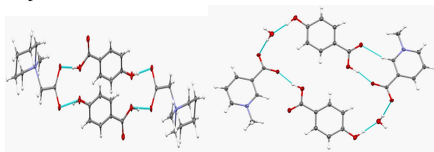


Figure 1. Main hydrogen bonding motifs in the structures of 1 (left) and 2 (right)

Keywords: charge density, hydrogen bonds, atoms-in-molecules