

Poster Presentations

[MS38-P02] **Experimental and DFT studies of 4-Methoxy-N-[(E)-(5nitrothiophen-2-yl)methylidene]aniline** Tufan Akbal^a, Ahmet Erdönmez^a, Ayşen Alaman Açar^b and Sümeyye Gümüş

^aDepartment of Physics, Ondokuz Mayıs University, Samsun, Turkey.

^bDepartment of Chemistry Ondokuz, Mayıs University, Samsun, Turkey
E-mail: erdonmez@omu.edu.tr

The title molecule, C₁₂H₁₀N₂O₃S, is nonplanar with an interplanar angle of 33.44(7)^o between the benzene and thiophene rings. In the crystal there exist only weak intermolecular C—H...O interactions, π interactions π ...between the benzene rings [centroid-centroid distance = 3.7465 (14) Å⁰] and X—Y... π interactions to the thiophene and benzene rings [N... centroid distances = 3.718(3)Å⁰ and 3.355(3) Å⁰, respectively]. Intermolecular C—H...O interactions link the molecules into chains parallel to the a axis (Fig.1). The length of the C11=N2 double bond is 1.268(3)Å⁰. This value agrees well with the analogous bond reported elsewhere. [1,2].

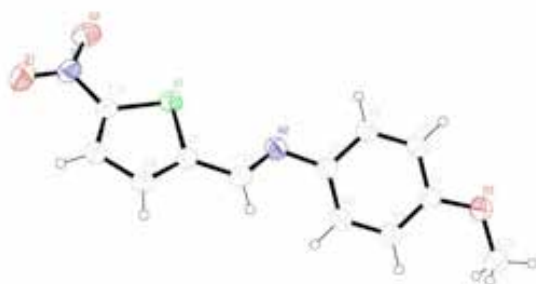


Fig.1 an ORTEP view of molecule

The theoretical calculations were performed with Gaussian03W software. In calculations, the stable structure geometries of the isolated molecules in the gas phase was investigated under the framework of Density Functional Theory (DFT). In order to find the stable molecular geometries, the global minimum scanning were performed on

the potential energy surfaces and some properties of molecules such as charge densities, dipole moments and frontier orbitals (HOMO and LUMO) from B3LYP/6-31G(d) calculations.

References:

- [1] Ceylan, •., Tanak, H., Gümüş,, S. & Açar, E. (2011). *Acta Cryst.* E67, o2004.
- [2] Özdemir Tarı, G. & Işık, Ş. (2012). *Acta Cryst.* E68, o415.

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