

## Poster Presentation

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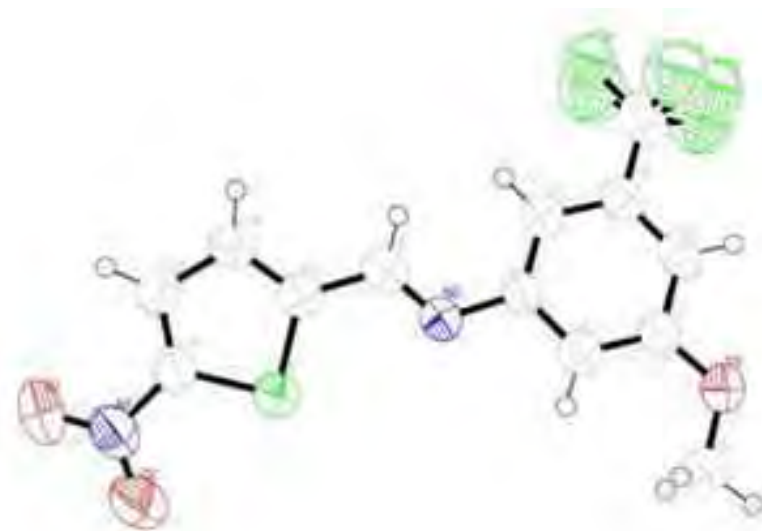
### Experimental and DFT studies of Mtpnm

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Experimental and DFT studies of (Z)-N-[3-Methoxy-5-(trifluoromethyl) phenyl]-1-(5-nitrothiophene-2-yl)methanamine Tufan Akbala, Erbil Ađarb, Sümeyye Gümüřb and Ahmet Erdönmeza aDepartment of Physics, Ondokuz Mayıs University, Samsun, Turkey . b Department of Chemistry Ondokuz Mayıs University, Samsun, Turkey E-mail: erdonmez@omu.edu.tr The title molecule, C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>F<sub>3</sub>S, is nonplanar with an interplanar angle of 23.94(23)° between the benzene and thiophene rings. In the crystal there exist only weak intermolecular C—H...O interactions and  $\pi$ ... $\pi$  interactions between the benzene rings and thiophene rings [centroid–centroid distance= 4.892(3) Å]. The length of the C=N double bond is 1.2534 Å. This value agrees well with the analogous bond reported elsewhere. [1,2]. 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] Akbal T., Ađar E., Erdönmez A., 2012. Acta Cryst. E68, 2673. [2] Aygün M., Iřık ř., Öcal N., Nawaz T.M., Kaban ř. & Büyükgüngör O., 1998. Acta Cryst. C54, 527-529. Keywords: tautomerism, crystal and molecular structure, density functional theory(DFT) studies

[1] Akbal T., Ađar E., Erdönmez A., 2012. Acta Cryst. E68, 2673, [2] Aygün M., Iřık ř., Öcal N., Nawaz T.M., Kaban ř. & Büyükgüngör O., 1998. Acta Cryst. C54, 527-529.



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