Poster Presentation

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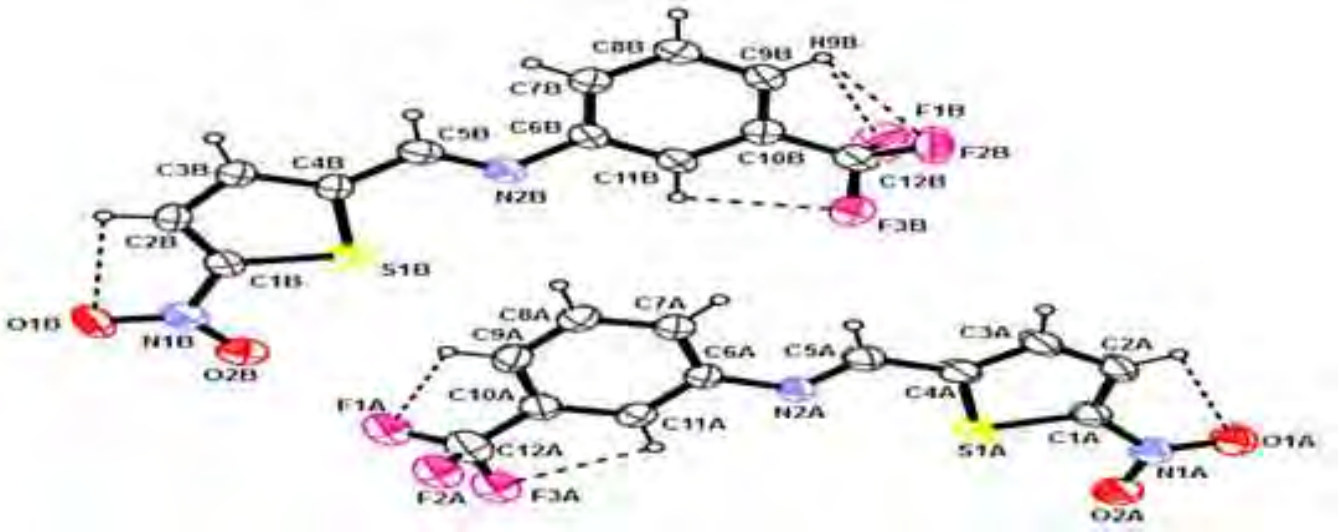
Structure of (E)-N-((5-Nitrothiophen-2-YL)Methylene)-3-(Trifluoromethyl)Aniline

Ö. Deveci[1], S. Gümüş[2], E. Ağar[2]

[1]Ondokuz Mayıs University, Department of Physics, Faculty of Arts and Sciences, Kurupelit, Turkey, [2]Ondokuz Mayıs University, Department of Chemistry, Faculty of Arts and Science, Kurupelit, Turkey

The Schiff base compound, C12H7N2O2F3S, has been synthesized and characterized by IR, UV-Vis, 1H-NMR, 13C-NMR and single-crystal X-ray diffraction (XRD) and elemental analysis. The compound, an Ortep-3 [1] view of which is shown in Fig. 1, crystallizes in the monoclinic space group P-1 with a= 7.5700(11) Å, b= 12.8280(16) Å, c= 13.0170(16) Å, α= 89.295(10)o, β= 88.691(11)o, γ= 82.246(11)o and Z=4 in the unit cell. The molecular structure is stabilized by C-H…O and C-H…F intramolecular hydrogen bonds and molecules are linked through intermolecular C-H…O and C-H…F type hydrogen bonds and C-H…Cg (π-ring) interaction. The molecular geometry from X-ray determination of the title compound in the ground state has been compared using the Hartre-Fock (HF) and density functional theory (DFT/B3LYP) [2] with 6-31G(d) [3] basis set. The results of the optimized molecular structure are exhibited and compared with the experimental X-ray diffraction. To determine conformational flexibility, molecular energy profile of the title compound was obtained by B3LYP with the 6-31G(d) basis set calculations with respect to selected degree of torsional freedom, which was varied from −180° to +180° in steps of 10°. In addition, molecular electrostatic potential (MEP) distribution and frontier molecular orbitals (FMOs) properties of the title molecule were investigated by theoretical calculations at the B3LYP/6-31G (d) level. Figure 1. Ortep 3 diagram of the title compound. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

[1] *L.J. Farrugia, J. Appl. Cryst. 1997, 30, 565.,* ***[2]*** *A.D. Becke, J. Chem. Phys. 1993, 98, 5648.,* ***[3]*** *R. Ditchfield, W.J. Hehre, and J.A. Pople, J. Chem. Phys. 1971, 54, 724.*



Keywords: X-ray diffraction, Hartree-Fock and DFT calculations, Schiff base