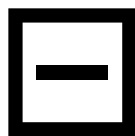


2-thioxo- 3N-(2-methoxyphenyl) –5 [4'-methyl -3'N -(2'-methoxyphenyl) thiazol-2'(3'H)-ylidene] thiazolidin-4-one: Synthesis, characterization, X-ray single crystal structure investigation and quantum chemical calculations

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Highlights

- Synthesis and characterization of the title compound have been reported.
- X-ray single crystal and molecular structures were determined.
- Hydrogen bonds were examined using Hirshfeld surface analysis.
- HOMO, LUMO and MEP were investigated.
- Molecular NLO properties were calculated.

Abstract

We report here the synthesis and a combined experimental and theoretical study on molecular structure of 2-thioxo- 3N-(2-methoxyphenyl) -5 [4'-methyl -3'N -(2'-methoxyphenyl) thiazol-2'(3'H)-ylidene] thiazolidin-4-one. The **crystal structure** has been determined by X-ray diffraction. Crystallographic data revealed that the compound crystallizes in a **monoclinic system** with a **space group** of $P2_1/c$, with crystal cell parameters: $a = 10.618 (3)$, $b = 13.180 (5)$, $c = 15.101 (3) \text{ \AA}$, $\beta = 97.766 (16)$, $V = 2093.9(11) \text{ \AA}^3$ and $Z = 4$. The final R-value was 0.0405 based on 4801 observed reflections. From the **dihedral angle** values, the structure was found to be significantly non planar. Density functional theory (DFT) calculation were carried out to obtain the ground state optimized geometry of the molecule using B3LYP and HSEH1PBE methods with 6-311G(d,p) basis set. The optimized geometry of the title compound was found to be consistent with the structure determined by X-ray diffraction. The stability of the title compound is due to the presence of a good number of potential donor and acceptor groups establishing **intermolecular interactions** like C—H \cdots O, C—H \cdots S and π - π stacking linking the molecules into dimers with $C(6)$, $R_2^2(18)$ and $R_2^2(24)$ graph sets. In addition, the **solid state** behaviors of molecules in the crystal were studied using 3D Hirshfeld **surface analysis** and associated 2D fingerprint plots. Calculated frontier **molecular orbitals**(FMOs) energies and **chemical reactivity** parameters indicated that the molecule under investigation exhibits high first **hyperpolarizability**, typical of a NLO material.

Graphical abstract

