

Theoretical and Experimental Electrostatic Parameters Determination of 4-Methyl-N-[(5- Nitrothiophen-2-Ylmethylidene)] Aniline Compound

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Abstract : We present the electron density analysis of organic compound 4-methyl-N-[(5- nitrothiophen-2-ylmethylidene)] aniline with chemical formula $C_{12}H_{10}N_2O_2S$. Indeed, determining the electrostatic properties of nonlinear optical organic compounds requires knowledge of the distribution of the electron density with high precision. On the other hand, a structural analysis is performed. Two methods are used to obtain the structure, X-ray diffraction and theoretical calculation with density functional theory (DFT). The electron density study is performed using the Mopro program1503 based on the multipolar model of Hansen and Coppens. Electron density analysis allows determination of the value and orientation of the dipole moment. The net atomic charges, electrostatic potential and the molecular dipole moment have been determined in order to understand the nature of inter- and intramolecular charge transfer. The study reveals the nature of intermolecular interactions including charge transfer and hydrogen bonds in the title compound. Crystallographic data: monoclinic system - space group $P2_1/n$. Cell parameters: $a = 4.7606(4) \text{ \AA}$, $b = 22.415(2) \text{ \AA}$, $c = 10.7008(15) \text{ \AA}$, $\beta = 92.566(13)^\circ$, $V = 1140.7(2) \text{ \AA}^3$, $Z = 4$, $R = 0.0034$ for 2693 observed reflections.

Keywords : electron density, dipole moment, electrostatic potential, DFT, Mopro

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