World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:10, No:03, 2016

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 C12H10N2O2S. 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 P21 / n. Celle parameters: a = 4.7606 (4) Å, b = 22.415 (2) Å, c = 10.7008 (15) Å, β = 92.566 (13) 0, V = 1140.7 (2) Å3, Z = 4, R = 0.0034 for 2693 observed reflections.

Keywords : electron density, dipole moment, electrostatic potential, DFT, Mopro
Conference Title : ICCME 2016 : International Conference on Chemical and Molecular Engineering
Conference Location : Paris, France
Conference Dates : March 14-15, 2016