

The Spectroscopic, Molecular Structure and Electrostatic Potential, Polarizability, Hyperpolarizability, and HOMO-LUMO Analysis of Monomeric and Dimeric Structures of N-(2-Methylphenyl)-2-Nitrobenzenesulfonamide

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Abstract : The monomer and dimer structures of the title molecule have been obtained from density functional theory (DFT) B3LYP method with 6-31G(d,p) as basis set calculations. The optimized geometrical parameters obtained by B3LYP/6-31G(d,p) method show good agreement with experimental X-ray data. The polarizability and first order hyperpolarizability of the title molecule were calculated and interpreted. The intermolecular N-H...O hydrogen bonds are discussed in dimer structure of the molecule. The vibrational wave numbers and their assignments were examined theoretically using the Gaussian 03 set of quantum chemistry codes. The predicted frontier molecular orbital energies at B3LYP/6-31G(d,p) method set show that charge transfer occurs within the molecule. The frontier molecular orbital calculations clearly show the inverse relationship of HOMO-LUMO gap with the total static hyperpolarizability. The results also show that N-(2-Methylphenyl)-2-nitrobenzenesulfonamide molecule may have nonlinear optical (NLO) compartment with non-zero values.

Keywords : DFT, Gaussian 03, NLO, N-(2-Methylphenyl)-2-nitrobenzenesulfonamide, polarizability

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