World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

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

Authors : A. Didaoui, N. Benhalima, M. Elkeurti, A. Chouaih, F. Hamzaoui

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 xperimental X-ray data. The polarizability and first order hyperpolarizabilty 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) comportment with non-zero values.

Keywords : DFT, Gaussian 03, NLO, N-(2-Methylphenyl)-2-nitrobenzenesulfonamide
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020