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XRD, FT-IR, Electronic and Fluorescence Spectroscopic Studies of Benzothiophenesulfone-2-methanol

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Abstract

*The structural, vibrational and quantum mechanical properties of Benzothiophene sulfone-2-methanol have been studied on the optimized structure by applying experimental techniques (XRD, FT-IR,UV & Fluorescence) and density functional theory (DFT) employing B3LYP interchange interrelation with the 6-311++G** basis set. Single crystals of the title compound have been prepared with methanol as a solvent and developed by slow evaporation technique. The XRD crystal data is obtained and compared with the experimental data by which a good agreement is achieved. The FT-IR spectrum of the compound was recorded in the region 4000-400 cm^{-1} and simulations were performed with the theoretical data. Normal coordinate analysis was carried out to the compound using DFT force field revised by a recommended set of scaling factors producing fairly good agreement between the observed and computed frequencies. The total electron density in the molecule and three dimensional molecular electrostatic potential maps of the titled molecule was built by using B3LYP/6-311++G** basis set to visualize electrostatic potential (e^- + nuclei) distribution, nucleophilic and electrophilic substitution within the molecule. HOMO, LUMO orbitals along with their energies were calculated and explained. Stability of the titled compound originating from hyper conjugative interactions and charge transfer within the molecule has been examined by applying natural bond orbital (NBO) analysis. Dipole moment (D), polarizability (α), hyperpolarizability (β), global softness, energy gap (ΔE) ,Ionization Potential (I), chemical potential (μ) were calculated to examine the NLO application of our title compound. The Fluorescence spectra at different excitation wavelengths were recorded, analysed and presented.*

Keywords: Benzothiophenesulfone-2-methanol (BS2M), FT-IR, XRD, UV-Vis spectra, fluorescence spectra.

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