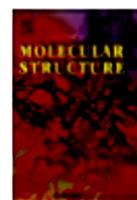




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Design, synthesis, structural characterization, and DFT approach of a new bis-Schiff base-derived sulfonyldianiline: Thermal and nonlinear optical performances in a fluid system

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ABSTRACT

The synthesis, structural elucidation, thermal calculations, and nonlinear optical (NLO) activity of a new bis-Schiff base-derived sulfonyldianiline, (Z)-3-((4-((E)-4-(benzyloxy) benzylidene) amino) phenyl) sulfonyl phenyl)imino)-2-indolinone (5) ($C_{34}H_{28}N_2O_4S$) using spectroscopic, thermal, and NLO techniques, are reported. The structure of the entitled compound (5) was deduced based on NMR, FT-IR, mass, and UV-visible spectra. The DFT-calculations in terms of the NLO descriptors such as mean polarizability, α_0 (esu), and hyperpolarizability, β (esu) are investigated. The thermal properties viz., thermal conductivity (K), viscosity (η), and specific heat capacity (c_p) with values of 0.21-0.27 W/mK, 1.3×10^{-3} Pa.sec at 27.7 °C, and 1631 J/Kg. K respectively, are obtained. Heat conduction in the sample studied using two-dimensional transient heat conduction model that is solved using Finite Difference Method (FDM). The NLO properties of bis-Schiff base chromophore (5) are studied via the passage of the laser beam (473 nm) based on the diffraction patterns (DPs) viz., beam power input, its wave front, and temporal evolution. The resulted diffraction patterns (DPs) are assessed numerically using Fresnel-Kirchhoff integral based on Fraunhofer approximation solved using MATLAB system. The numerically obtained results agree well with experimental findings. In addition, the all-optical switching (AOS) is evaluated using three laser beams. Overall, the results indicate that the target chromophore (5) is recommended for upcoming optical applications such as AOS viz., static and dynamic.