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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-((4-((*E*)-(4-(benzyloxy) benzylidene) amino) phenyl) sulfonyl) phenyl)imino)-2-indolinone (**5**) ($C_{34}H_{25}N_3O_4S$) 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_o (esu), and hyperpolarizability, β (esu) are investigated. The thermal properties viz., thermal conductivity (K), viscosity (η_l), 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.

1. Introduction

Over the last forty years, special interest has been paid to the nonlinear optical (NLO) concept due to its extremely impactful applications in the realm of electronic, nonlinear optics, biomedicine devices, and many more [1,2]. The generated changes of optical characteristics in a molecular system due to contacting with strong laser light refer to NLO phenomena [3]. In organic NLO molecules, the electronic delocalization, intra-molecular charge transfer (ICT), and donor-π-acceptor configuration (D-π-A) are essential factors for promoting efficient NLO properties [4–6]. The recent publications have demonstrated that the increase of D-π-A property through the central π-electron bridge (aromatic molecules) exhibited a gradual enhancement in the measurement of first hyperpolarizability [7,8]. Meanwhile, an increase in aromatic units leads to increase the conjugation length in the entire π-conjugated system [9]. In addition, it has been reported that the structural alteration in the aromatic molecule skeleton in terms of the modifications of central bridging core is a considerable impact to modulate the NLO responses [10,11]. Therefore, significant attention and more investigations have been pushed to design aromatic architecture networks with more noteworthy NLO properties [12].

Schiff base compounds are verified from the fact that the compounds contain a CH=N chromophore, called an azomethine or imine linkage [13]. Schiff bases compounds are of interested subject due to their interesting properties that involve facile synthesis chemistry, easy workup of production, good solubility, high component economy, and optoelectronic characteristics [14]. In the optical field, various NLO activities have been characterized in Schiff base compounds as they can

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