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A simple synthesis and DFT approach of a new unsymmetrical dithizone as an efficient NLO substance: Thermal and experimental studies in a fluid medium

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ABSTRACT

The objective of the present work is to synthesize a new unsymmetrical dithizone chromophore **8** namely, (*E*)-5-(4-nitrophenyl)-1-phenylthiocarbazone ($C_{13}H_{11}N_5O_2S$) using simple chemistry reactions. Upon identifying its chemical structure, the extensive computational, thermal, and experimental studies are devoted to investigate its nonlinear optical (NLO) activity. The theoretical outcomes disclosed that the target chromophore **8** showed high linear polarizability, α (esu), and first hyperpolarizability, β (esu), owing to the ability of aromatic rings to extent electron density across π–conjugation in a direction towards the NO_2 substituent as a potent acceptor group. The molecular electrostatic potential (MEP) diagram, time-dependent density-functional theory (TD-DFT), Mulliken charges, and natural bond orbital (NBO) investigations are addressed theoretically. The thermal properties of the target chromophore **8** are studied through the assessment of its thermal conductivity (K), viscosity (η), and specific heat capacity (c_p) in addition to simulation of its thermal diffusion using a Finite difference method through solving the 2D transient heat conduction equation. By irradiating the target sample with continuous wave (CW) laser beams (473 and 532 nm), its NLO response is improved *via* the generation of diffraction patterns (DPs). The simulation results of DPs *via* the use of Fresnel–Kirchhoff integral are obtained with good accord compare to experimental results. For the target chromophore **8**, the properties related to its all-optical switching (AOS) are studied utilizing two CW visible laser beams. To have efficient materials for use in optoelectronic devices, the work findings strongly encourage to conduct this chromophore for further experimental investigations in order to reach this goal.

1. Introduction

Due to impactful and fascinating applications that featured by nonlinear optical (NLO) materials in the sophisticated electronic and optoelectronic systems, lot of interest has been paid to design or develop these materials with pronounced various applications [1,2]. Potential applications in terms of optoelectronic scope have spurred extensive investigations on new potential optical molecules involving exploitation of organic molecules [3,4]. By comparing with their inorganic counterparts, the structural alterations or modifications in the organic molecules can be achieved through feasible chemical synthesis with inexpensive cost for production [5,6]. In principles, essential factors offered by the organic materials make them as qualified materials for significant NLO properties [7]. Electronic delocalized conjugation, extending π-conjugated bridge, and induced dipole moment are some important factors that featured by organic NLO materials [8–10]. The enhancement of these factors in the potential NLO organic materials is significantly affected by an alteration in their molecular structures. These alterations might lead to improve their high NLO properties with short response times [11,12]. Logically, the presence of donor-π-acceptor system (D-π-A) and conjugated π-bridge nature in the organic candidate chromophores plays an important role in the NLO magnitudes involving polarizability (α) and hyperpolarizability (β) [13,14]. Providing strong auxiliary π-electronic bridges in the D-π-A

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