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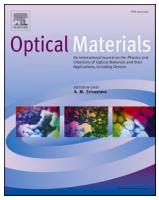

Research Article

Synthesis, spectral, and NLO studies of indol derivative bearing 1, 2, 4-triazole-3-thiol group

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ABSTRACT

The indol-3- triazole derivative, is synthesized from indol-3-carbohydrazide, (indol- 3 –DMT) and characterized using spectroscopic methods such as FTIR and ^{1}H NMR, ^{13}CNMR, and Mass spectra. The thermodynamic properties and optimized geometry of the compound are theoretically examined using DFT. The hybrid functional B3LYP and CAM-B3LYP techniques are used to estimate the HOMO, LUMO, electronic spectrum, and Mullikan atom charges of examined indol-3-DMT molecule. The nonlinear optical (NLO) properties of the indol-3-DMT are studied under illumination with cw, visible, low power laser beam where nonlinear refractive index (NLRI) is obtained via the diffraction patterns (DPs) and the Z-scan. As high as 5.98×10^{-11} m^2/W is obtained for the NLRI. The all-optical switching (AOS) is studied via static and dynamic AOS.

1. Introduction

Since 1990, much interest have been paid for the search of nonlinear materials having high nonlinear refractive indexes (NLRIs) and short response time to be used in many applications viz., refractive index modulation, light-controlled phase, all – optical switching, optical data storage, optical communication, phase conjugation, frequency conversion, optical limiting [1–14] etc. Changes of the materials refractive index (RI) induced by high coherent optical fields can leads to variety of nonlinear phenomena. The interplay between the nonlinear optical (NLO) property of the medium, and divergence of the light, in the spatial domain, can elicit to phase trapping, spontaneous pattern due to modulation instability and soliton formation [15–17].

NLO substances have captured significant interest in various uses such as integrated photonics and optical rectification [18–20]. NLO materials possess an exceptional nature. These materials have the ability to generate an altered field when exposed to an externally applied field [21–24]. The usage of NLO materials in various industries has been noted since 1961, when the first instance of SHG was observed in single crystal quartz [25]. Since that time, numerous studies have been directed towards the creation and development of organic/inorganic NLO materials that exhibit enhanced polarizability [26].The existence of π electrons delocalization in organic systems [27–30], which involve alternating single and double bonds for the formation of molecular structure, is the most suitable contender to demonstrate NLO capability. It is widely recognized that a substance demonstrating NLO capability must be noncentrosymmetric [31,32]. In recent times, there has been a rise in research conducted on indole compounds and their derivatives. The advantage of indole derivatives lies in their ability to exhibit various optical properties, such as fluorescence, extinction coefficient, absorption, transition energy, excited state dipole moment, and HOMO–LUMO energy gap, which are crucial in the development of future molecules. Strong electron donors and massive conjugated structures have been shown to significantly enhance NLO characteristics. This gives an understanding of the NLO response of conjugated and donor molecules on 3-substituted indole [33–35]. We have conducted a study on the indole bearing a 1,2,4-triazole derivative that was synthesized from indole carbohydrazide.

The Z-scan technique [36,37] offers simplicity and sensitivity for measuring the nonlinear refractive index (NLRI) and nonlinear absorption coefficient (NLAC). The generation of diffraction patterns (DPs) [38,39] can be used in the calculation of NLRI based on the number of rings obtained at the maximum power input.

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