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ORIGINAL PAPER

Synthesis and study of nonlinear optical properties of an enaminothione derived from enaminone and Lawesson's reagent

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Abstract: Lawesson's reagent is used with β-enaminone to synthesize the compound (Z)-1,3-diphenyl-3-(phenylamino) prop-2-ene-1-thione. The 6–311 + + G(d,p) basis set is employed to evaluate the stability of the molecule's probable tautomers via DFT with the functionals ωB97XD, M062X, B3LYP, and CAM-B3LYP. The ρBCP value for the hydrogen bond in the gas phase ranges from 0.035962 to 0.038105 e/a03. The intramolecular hydrogen bonding is relatively weak, as evidenced by atoms in molecules (AIM) computations conducted across several media and theoretical models. We examine the nonlinear optical (NLO) properties of enaminothione after illuminating with two continuous wave (CW) laser beams. We employ diffraction patterns (DPs) and the closed aperture (CA) Z-scan techniques to determine the nonlinear refractive index (NLRI) of enaminothione. The NLRI is equal 4.996×10^{-7} cm^2/W at the wavelength 473 nm. The application of 473 nm and 532 nm laser beams on enaminothione has demonstrated its ability to transition between all-optical switching (AOS).

Keywords: Enaminothione; DFT; NCI; AIM; Nonlinear optics

1. Introduction

There has been enormous need for nonlinear optical (NLO) materials that finds use with low-intensity laser beams in many applications such as optical limiting, phase conjugation, optical switching, signal processing, sensors, etc. [1–14]. When a laser beam propagates along a nonlinear absorbing medium, intensity-dependent phenomena in the medium can be observed, such as the thermal effect, reverse saturable absorption (RSA), or other effects [15–17].

Among the practical methods used to investigate the nonlinear properties that are in use, the most popular and informative is the Z-scan, closed and open technique, which leads to the determination of both nonlinear refraction index (NLRI) value and sign using a single beam. The second most popular one is the diffraction patterns (DPs). It is a direct consequence of the spatial distribution of the refraction index (RI) or thermal effect. The self-DPs formed due to the interference of light beams emanating from each point on the wave front based on the phase diffractions, the beam suffers. In this technique, the change of the medium RI and the NLRI can be obtained based on the number of rings at the highest power input.

Over the past three decades, the NLO properties of various materials, both liquid and solid, have been studied extensively [18–28]. These studies have investigated numerous parameters affecting NLO properties, such as solvent and concentration, among others. Most of these materials, in both liquid and solid forms, have demonstrated high NLO properties. Organic materials that exhibit large NLO properties have emerged as an important class of electronic materials with interesting characteristics for photonic applications [29]. Enaminones are chemical substances that present a conjugated system of the type N–C=C–C=O with different geometric forms. Enaminones serve as structural components in drug development and exhibit antibacterial, biological, anti-inflammatory, pharmacological, and cytotoxic effects [30–39]. Enaminones

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