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# Curcumin analogue: Synthesis, DFT and nonlinear optical studies

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## ABSTRACT

The synthesis of a new curcumin analogue dye via 3-chloro-2,4-pentanedion condensing with an aromatic aldehyde is considered. Following that, the synthesized compound is diagnosed utilizing spectroscopic methods, including FTIR, mass, <sup>1</sup>H NMR, and <sup>13</sup>CNMR. The curcumin analogue geometric optimization and theoretical studies are conducted on thermodynamic properties using DFT. The B3LYP techniques, which are hybrid functional with a 6–311+G(d) as the basis set, are adopted to compute the HOMO, LUMO, and Mullikan atom charges of the studied compound. The curcumin analogue dye nonlinear optical (NLO) properties are examined under excitation with a 473 nm, low power, cw and TEM<sub>00</sub> mode laser beam. The index of nonlinear refraction (INLR) and coefficient of nonlinear absorption (CNLA) are estimated using diffraction patterns for the former and Z-scan for the latter. The INLR reaches a value as high as  $6.86 \times 10^{-11} \text{ m}^2/\text{W}$ , while the CNLA reaches  $2.23 \times 10^{-3} \text{ cm/W}$ . All-optical switching (AOS) is tested in the novel curcumin analogue dye using two methods: static AOS and dynamic AOS.

## 1. Introduction

Laser beam self-interaction in a medium occurs due to the changes in the medium optical properties created via incident radiation. During the last three decades, considerable interest has been paid to problems concerning the nonlinear interaction of a Gaussian laser beam with a nonlinear medium (NLM) such as self-defocusing (SDF), self-phase modulation (SPM) and self-focusing (SF) can be observed. For example, a ring intensity distribution patterns can be induced. The technique known as the diffraction patterns (DPs) can be used in determining, the index of nonlinear refraction, INLR [1]. Self-phase modulation (SPM) effect is attributed to the refractive index dependent on intensity. Such effect was observed in a number of systems [2–5]. When a laser beam transverses an NLM, the beam spot size varies in area based on SF or SDF, so when drawing the beam power transmitted through a narrow iris against the sample position relative to the lens focus ( $\pm z$ ), a peak then a valley resulted when the medium showed SDF, and a valley then a peak resulted when the system showed SF. Such a technique is known as Z-scan, discovered by Sheik-Bahae et al., in 1989–1990 [6,7], where it can be used to estimate the coefficient of nonlinear absorption (CNLA) as well as the INLR.

Organic dyes and organic compounds offer unique applications in the areas of optical computing, harmonic creation, optical power limiting, optical switching, optical communications, and optical storage, because they show nonlinear optical (NLO) features [8–12].

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