



Synthesis, 2D-NMR analysis, DFT, and optical nonlinear studies of a new cyclic imide

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ABSTRACT

The synthesis of (11R,15S)-13-(3-hydroxyphenyl)-9,10-dihydro-9,10-[3,4]epipy-rroloanthracene-12,14-dione, cyclic imide compound **B3**, via three path ways as a new compound is detailed. The new cyclic imide compound **B3** is characterized by FTIR, Mass, 1 and 2D NMR (HSQC) and UV-vis. spectra. The cyclic imide compound **B3** structure is studied using B3LYP method with the 6-311G* basis set level to carry out the density functional theory (DFT) calculations. The nonlinear optical(NLO(properties of the synthesized compound are studied using low power, continuous wave (cw), visible laser beam of wavelength 473 nm via two techniques viz., diffraction patterns (DPs) and Z-scan. Nonlinear refractive index (NLRI) of the compound **B3** is calculated using both techniques where as high as $7.7 \times 10^{-7} \text{ cm}^2/\text{W}$ at input power of 57 mW is obtained due to DPs technique. The all-optical switching (AOS) of the synthesized cyclic imide compound **B3** is successfully examined using visible laser beams of wavelength 473 nm as controlling beam and 532 nm as the controlled beam based on the cross-passing technique.

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1. Introduction

Nonlinear optical (NLO) materials have attracted vast number of researchers in the recent years owe to the potential use in applications such as optical limiting [1–4], image processing [5], phase conjugation [6], bi-stability [7–10], all-optical switching (AOS) [11–14], and data storage [15]. Variation of materials index of refraction (IR) can be induced via moderate optical field which can be supplied by laser devices. Spatially, the interplay between the NLO response of the medium and the propagating beam divergence lead to range of self-action behaviors such as spontaneous pattern formation, optical self-trapping, etc. The important parameters that are basic requirement for nonlinear materials are the sign and amplitude of the nonlinear refractive index (NLRI) and the nonlinear absorption coefficient (NLAC) that are related to the imaginary and real parts of the third order NLO susceptibility, χ^3 . These parameters can be partly obtained by the diffraction patterns (DPs) technique that was discovered in 1967 [16] and the Z-scan [17,18]. DP_s is based on a branch of NLO effect named spatial self-phase modulation (SSPM) where at high laser beam intensity incident on a homogeneous medium, DPs are observed on a screen in the far

field, where its phase modulated by its own intensity. Based on the generated rings number at maximum power input (or intensity), one can determine the total change of the medium IR, Δn , and the NLRI, n_2 .

The Z-scan is another technique pioneered by M. S. Bahae [17,18] works on the spatial beam distortion principle that offers sensitivity and simplicity. It is used in the measurements of both the NLRI and NLAC. This technique have been implemented and applied to many materials using single laser beam each time [19–25].

Cyclic imides are present in composition of many pharmaceutical substances and interesting part as building blocks in the natural products, drug and polymers [26–29]. They are prepared by heating dicarboxylic acid or their anhydrides and ammonia or primary amines.

The cyclic imides are known for their wide applications in the medical and pharmaceutical fields. Numerous studies have proven their effectiveness as antibiotics against different types of bacteria and fungi. This is why cyclic imides have been widely used in the preparation of various pharmaceutical drugs such as anti-inflammatories, antidepressants, and others [30–32].

The researchers worked to prepare and study several classes of compounds with optical and NLO properties, because of their great importance in NLO applications and devices. The linear op-

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