Journal of Molecular Liquids 379 (2023) 121696

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

# Synthesis, two dimensional NMR analysis, DFT, and nonlinear optical investigations of a new cyclic imide

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ARTICLE INFO

*Article history:*
Received 30 January 2023
Revised 10 March 2023
Accepted 19 March 2023
Available online 22 March 2023

*Keywords:*
DFT
2D-NMR
DPs
Z-scan
All-optical switching

ABSTRACT

Diels Alder reaction is employed to prepare a new cyclic imide. The structure of synthesized cyclic imide (11aR)-2-(2-nitrophenyl)-2,3,5,6,11,11a-hexahydro-1H-6,11-[1,2] benzen-ebenzo [5,6] cyclohepta [1,2-c]pyridine-1,4(4aH)-dione (A3) is characterized by FTIR, Mass, 1D and 2D NMR spectra. Theoretical calculations are performed using density functional theory (DFT) to investigate the possibility of nonlinear optical (NLO) behavior. The NLO properties of the cyclic imide are studied via the calculation of the nonlinear refraction index (NLRI) using diffraction patterns (DPs) and Z-scan. The all-optical switching (AOS) of the prepared cyclic imide is studied using two laser beams.



## 1. Introduction

Materials having nonlinear refraction indexes (NLRIs) and short response times attracted endless attention during the last three decades due to the possibility of using in all-optical switching (AOS) [1–6], signal processing and computing [7–8], data storage [9–12], phase conjugation [13], and limiting [14–17]. For such reasons so many available materials have been tested [18–23], many other materials properties have been improved via the irradiation with γ-rays [24], and new materials have been synthesized for the same purposes [25 –35].

In 1967 it was recognized by Callen et al. [36], that the passing of a continuous wave (cw) laser beams through self-defocusing (SDF) media led to the production of diffraction patterns (DPs) and was recognized by Ogusu et al. [37], that the NLRI might be calculated using the total number of rings in DPs at the highest power input of laser beam. In 1990 a new technique have been introduced by Sheik Bahae et al. [38,39], named as Z-scan, where it can be used to measure the nonlinear (NL) susceptibility and the sign of its real part. The NLRI, $n_2$, and the nonlinear absorption coefficient (NLAC) can be obtained via the closed and open apertures Z-scans using single continuous wave (cw) laser beam.

When a laser beam traverses a material, an intensity dependent refractive index in the medium can be observed. Nonlinear optical properties of many media are currently being explored. An example of interest that has attracted a lot of attention is the light-induced optical property changes. There are two types of interaction viz., light-induced absorption changes usually described by the equation

$$\alpha = \alpha_o + \beta I \quad (1)$$

α is the absorption coefficient in the presence of laser light, $\alpha_o$ is the linear absorption coefficient, I is the incident laser beam intensity and β is the nonlinear absorption coefficient. The light-induced refractive index changes that usually described by the equation

$$n = n_o + n_2 I \quad (2)$$

n is the medium refractive index in the presence of laser beam, $n_o$ is the medium linear refractive index, and $n_2$ is the nonlinear refractive index coefficient. When a laser beam with Gaussian distribution traverses through a nonlinear medium, a large number of spatial effects viz., self-phase modulation, self-defocusing, and self-focusing can be observed.

The cyclic imides have always been known for their biological activity [40] and thus have played important role in pharmaceutical applications. There are many well-known drugs prepared from different cyclic imide derivatives [41].

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https://doi.org/10.1016/j.molliq.2023.121696
0167-7322/