



## PAPER

RECEIVED  
28 May 2024REVISED  
29 October 2024ACCEPTED FOR PUBLICATION  
25 November 2024PUBLISHED  
4 December 2024

## Design, DFT, experimental, and NLO studies of a new hybrid containing 1,3,4-oxadiazole and indole moieties

Sabreen Mahdi Hassan<sup>1</sup>, Ahmed Majeed Jassem<sup>1</sup> , Qusay M A Hassan<sup>2</sup> , H A Sultan<sup>2</sup>, Adil Muala Dhumad<sup>1</sup> and C A Emshary<sup>2</sup><sup>1</sup> Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah 61001, Iraq<sup>2</sup> Department of Physics, College of Education for Pure Sciences, University of Basrah, Basrah 61001, IraqE-mail: [ahmed.majedd@uobasrah.edu.iq](mailto:ahmed.majedd@uobasrah.edu.iq)

Keywords: hybrid molecule, DFT, nonlinear optical properties, diffraction patterns, Z-scan

Supplementary material for this article is available [online](#)

## Abstract

In this article, design and nonlinear optical (NLO) response studies of a new synthesized hybrid molecule (HM 6) containing 1, 3, 4-oxadiazole and indole moieties are introduced. The spatial structure of the target hybrid is analytically determined using <sup>1</sup>HNMR, <sup>13</sup>CNMR, FT-IR, UV-vis., and Mass spectra. Efficiency of the fully optimized geometry of the synthesized HM (6) is elucidated via energy gap ( $E_{\text{HOMO}}-E_{\text{LUMO}}$ ), potential ionization, and electron affinity. The small energy gap leads to efficient NLO response. The cooperation of 1, 3, 4-oxadiazol moiety as a good acceptor and indole as a good donor in the HM (6) enhances long  $\pi$ -conjugation system, led to large hyperpolarizability ( $\beta = 2.79 \times 10^{-28}$  esu). Density functional theory and TD-DFT-assisted calculations proved high potential intramolecular charge transfer and effective  $\beta$  value verify NLO activities. The NLO activities of the HM (6) are examined under the excitation with 473 nm, single transverse, low power laser beam via diffraction patterns (DPs), and Z-scan techniques. As high as  $5.49 \times 10^{-11}$  m<sup>2</sup>/W of nonlinear refractive index due to the DPs technique has been obtained. Both the nonlinear refractive index and nonlinear absorption coefficient are estimated via the standard Z-scan methods. The all-optical switching, both static and dynamic, prove to occur in the HM (6) using two visible laser beams.

## 1. Introduction

In recent years, organic molecules showing effective nonlinear optical (NLO) responses have become an unique scope of advanced researches due to their fascinating applications in the optical fields of storage [1, 2], integrated laser medicine [3], telecommunications [4], fluorescence imaging [5], high density optical materials [6], integrated photonics [7], second harmonic generation (SHG) [8], and optical rectification [9], etc. Ease of handling, low cost, high thermal stability, strong electronic mobility, enhancing of modification under external field, composing of non-centro symmetric, and high electro-optic activities are inherent advantages of the organic NLO materials [10–12]. These materials constitute push–pull chromophore groups which normally contain  $\pi$ -conjugated bridge (D- $\pi$ -A). The D- $\pi$ -A presence acts to create a suitable route for the rapid delocalization of electronic charges in the external applied field [13]. Such  $\pi$ -conjugated system is conducted as an efficient way to minimize the band gap since their HOMO and LUMO levels can be adjusted via the overlapping effect of molecular orbitals due to the high induced effect generated from charge transfer phenomenon between donor and acceptor groups [14]. Thus, a strong electronic acceptor and short spacers help to increase D–A interactions, while a weak electronic acceptor and long spacers act to decrease the D–A interactions [15]. It was found that the addition of an extra electronic donating atom into the donor part or electronic accepting atom into the acceptor part can significantly enhance the NLO responses [16].

Among the organic heterocyclic molecules, indole or benzopyrrole is an interesting electron donating molecule in the  $\pi$ -conjugated system to offer electronic and optoelectronic properties [17]. Examples of optoelectronic applications of compounds containing an indole based chromophores include high NLO