Optical Materials 149 (2024) 114983

Contents lists available at ScienceDirect

Optical Materials

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

Research Article

Isatin-indole hybrid molecule: A simple synthesis to design an efficient NLO material

Ghufran Salih Yaqoob [a], Qusay M.A. Hassan [b,*], Ahmed Majeed Jassem [a,**], H.A. Sultan [b], Adil Muala Dhumad [a], C.A. Emshary [b]

[a] Department of Chemistry, College of Education for Pure Sciences, University of Basrah, 61001, Iraq
[b] Department of Physics, College of Education for Pure Sciences, University of Basrah, Basrah, 61001, Iraq

ARTICLE INFO

Keywords:
Nonlinear optical properties
Diffraction patterns
Z-scan

ABSTRACT

The isatin-indole hybrid molecule, referred to as molecule **5**, (*Z*)-3-((4-((4-((*E*)-((1H-indol-3-yl)methylene) amino)phenyl)sulfonyl)phenyl)imino)indolin-2-one ($C_{29}H_{20}N_4O_3S$), is synthesized through a straightforward method and its structure confirmed using (^{1}H, ^{13}C) NMR, IR, Mass, and UV–vis. spectroscopic techniques. The molecular arrangement of molecule **5** is determined by employing Density Functional Theory (DFT) with the B3LYP functional to acquire its optimized geometry. Various theoretical parameters, including dipole moment (Debye), polarizability (α) in esu, hyperpolarizability (β) in esu, E_{HOMO} (eV), E_{LUMO} (eV), and Egap (eV), were computed using the DFT approach. These computed physiochemical attributes underscore the capability of both isatin and indole molecules to stabilize the optimized geometry of molecule **5** via interactions across the sulfonyl group. The outcomes indicated that hybrid molecule **5** exhibited superior nonlinear optical (NLO) efficiency, characterized by a small HOMO-LUMO energy gap and a substantial hyperpolarizability. Furthermore, an in-depth exploration of the theoretical UV–vis. spectrum using TD-DFT calculations provided detailed assignments for electronic transitions, demonstrating a noteworthy consistency with the experimental spectrum. This collective information reinforces the potential of the hybrid molecule **5** as an efficient candidate for optical and NLO applications.

1. Introduction

In recent decades, organic molecules, either commercially available or experimentally synthesized, have attracted much interest as an alternative to their inorganic counterparts [1]. The majority of organic molecules features push–pull phenomenon with raised values of polarizability and dipole moment [2]. Thus, the organic molecules are found to offer very notable nonlinear optical (NLO) properties with pronounced many applications [3–10]. Organic light-emitting diodes (OLEDs), effective transistors, white light sources, and photovoltaic devices are some of these applications [11]. Among these molecules, isatin or 1*H*-indole-2, 3-dione as a ring system consisting of benzene fused pyrrole ring, has two types of carbonyl groups (keto and lactam groups). Isatin and its derivatives are identified as a privileged precursor toward the synthesis and design of diverse drugs [12]. Also, several articles have reported that these molecules are important for acquiring compounds with promising optoelectronic properties. For instance, the polymerization and electrochemical study of an isatin molecule have been reported by Kasi et al. [13] and their study revealed that such modified molecules have good optoelectronic properties which are appropriate for optoelectronic applications. Thirumalaiselvam et al. [14] have introduced that an isatin molecule offers efficient 3rd-order nonlinear properties with a range of optical communication and information storage. The significance of isatin crystal resides in its contribution to the development of OLEDs, enabling efficient emission of red light for optimal power efficiency and a favorable external quantum yield [15]. The dielectric constant and dielectric loss of an isatin crystal were analyzed and found to be low at higher frequencies, indicating this crystal has an efficient ability to induce polarizability during the irradiation process with a powerful laser beam. Isatin and some of its Schiff bases have been discovered to be used as new red fluorescent materials for OLEDs. Sharbati et al. [16] have reported novel materials of red

* Corresponding author.
** Corresponding author.
E-mail address: qusayali64@yahoo.co.in (Q.M.A. Hassan).

https://doi.org/10.1016/j.optmat.2024.114983
Received 24 August 2023; Received in revised form 27 December 2023; Accepted 26 January 2024