



Optical nonlinearity performance of a new isatin-thiazolidin-4-one hybrid molecule: synthesis, experimental, and DFT studies

C. A. Emshary¹ · Ahmed Majeed Jassem² · Qusay M. A. Hassan¹ · Adil Muala Dhumad² · H. A. Sultan¹ · Ayat Jawdat Kadhum² · Ayat Naji Hasan² · Noor Hamid Faisal² · Ruaa Qasim Ibrahim² · Nuha Ayad Mohammed² · Nuha Waleed Ali² · Faeza Abdul Kareem Almashal² · Fadhil A. Tuma¹

Received: 13 August 2024 / Accepted: 30 September 2024

© The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2024

Abstract

In this work, (Z)-2-((E)-(2-oxoindolin-3-ylidene)hydrazono)-3-phenylthiazolidin-4-one **7** (C₁₇H₁₂N₄O₂S) as a hybrid molecule is synthesized under an easy method and analytically ascertained by ¹HNMR, ¹³CNMR, IR, Mass, and UV–vis. spectroscopies. The optimized geometry of the synthesized hybrid molecule **7** is acquired using DFT-assisted calculations involving B3LYP equation with 6-31G(d,p) as a basis set level. At the same level, TD-DFT calculations are performed to collect the theoretical UV–vis. spectrum of the hybrid molecule **7**. The nonlinear optical (NLO) properties of the hybrid molecule **7** are studied under irradiation with a cw laser beam. The nonlinear refractive index (NLRI), n_2 , of the hybrid molecule **7** is estimated via diffraction patterns (DPs) and Z-scan. The all optical switching is tested for the hybrid molecule **7** using two, cw, laser beams. Both static and dynamic all-optical switching are studied.

Keywords Isatin-Thiazolidin-4-One hybrid · NLO properties · DPs · Z-Scan · All-Optical switching

1 Introduction

Recent articles into organic molecules have focused on clarifying and exploring the importance of these molecules compared to their inorganic counterparts (Papagiannouli et al. 2015). The majority of organic molecules are found to have push–pull phenomenon with efficient values of dipole moment and polarizability (Al-Hujaj et al. 2022). Organic molecules either naturally found or experimentally synthesized are abundant

✉ Ahmed Majeed Jassem
ahmed.majedd@uobasrah.edu.iq

¹ Department of Physics, College of Education for Pure Sciences, University of Basrah, Basrah 61001, Iraq

² Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah 61001, Iraq