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Synthesis, DFT study and optical nonlinear evaluations of a new 1,3,4-oxadiazole derivative

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ABSTRACT

The oxadiazole derivative (A5) is prepared by reacting the thiazolidine hydrazide with 3,4,5-trimethoxy-benzoic acid and $POCl_3$ solution. The prepared A5 compound is characterized via nuclear magnetic resonance (NMR) ^1H and ^{13}C, FT-IR and mass spectra. Density functional theory (DFT)/B3LYP via 6-311G (d,p) level has been used to calculate quantum chemical descriptors (QCDs) to investigate the optical nonlinear (ONL) properties theoretically. The comparison of results indicated that the A5 compound is the potential candidate for ONL material. The energy band gap of the sample is calculated based on the Tauc's expression and found to be equal to 2.54 eV. The A5 compound's ONL properties are studied under irradiation with a laser light beam of wavelength 473 nm via the diffraction patterns (DPs) and Z-scan. As high as 6.4654×10^{-7} cm^2/W of the nonlinear index of refractive (NLIR), n_2, via the DPs is estimated. The all-optical switching (AOS) of the A5 compound is obtained.

Conflict of Interest

1. Introduction

The seeking of media with large indexes of nonlinear refraction (IsNLR) and fast response times, irradiated with a continuous wave (CW) low power laser beam has led to extensive investigations of organic materials [1–5]. The optical nonlinear (ONL) materials development has led to their suitability for many applications in image processing, data storage devices, frequency conversion, optical computing and optical telecommunication, all-optical switching (AOS), modulation index of refractive, and optical limiting [6–12]. The IsNLR and coefficients of nonlinear absorption (CsNLA) of different materials can be calculated via a popular and well-known technique viz., the Z-scan pioneered in 1989–1990 [13,14]. The IsNLR can be estimated via diffraction patterns (DPs) [15,16]. Number of rings that resulted in a pattern at a proper power input can be used to estimate the IsNLR [17].

Heterocyclic compounds represent one of the classes of organic compounds that contain in their structure a heterogeneous atom, and the most prevalent atoms are nitrogen, oxygen, and sulfur. These compounds have aliphatic properties, such as thiazolidine or aromatic properties, such as oxadiazole and thiazole, and they play an effective role in biological applications [18–21]. Oxadiazole is a type of aromatic heterocyclic compound, that contains two nitrogen atoms and an oxygen atom and has unique properties [22,23]. Oxadiazole derivatives were used in many biological pharmacological functions and in the treatment of many diseases, including anti-fungal [24], anticancer [25], antiviral, antioxidant, antibacterial, anti-HIV [26–29], antimicrobial, many tumor cells, and other medicinal applications due to the distinctive stereoscopic structure that oxadiazole possesses [30,31]. Oxadiazole derivatives have been studied in many medical, industrial, and pharmaceutical applications [32–34]. Oxadiazole scaffolds are known for their electron-withdrawing nature, which enhances their ability to participate in charge-transfer interactions, making them valuable in electronic and optoelectronic applications. Additionally, the presence of heteroatoms in the oxadiazole ring contributes to hydrogen bonding and other intermolecular interactions, which play a crucial role in their pharmacological activities, including anticancer, antibacterial, and antiviral properties [34,35].

Furthermore, structural modifications such as substitutions at different positions of the oxadiazole ring have been reported to significantly alter their bioactivity and physicochemical properties. For example, electron-donating or withdrawing substituents can influence

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