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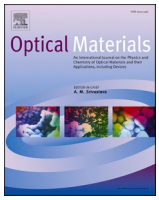

Research Article

Synthesis, characterization, theoretical and experimental studies of nonlinear optical properties of a new 3-cyano-2-oxa- pyridine derivative

Qusay M.A. Hassan [a,*], Sarah Arif Kamil [b], C.A. Emshary [a], Zainab Al Shuhaib [b], H.A. Sultan [a], Sadiq M.H. Ismael [b], Kawkab Ali Hussein [b]

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

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ABSTRACT

3-cyano-2-oxa-pyridine (Z5) compound is synthesized by mixing 4-aminoacetophenone and 2,4-dimethoxy benzaldehyde with ethyl cyanoacetate and extra ammonium acetate in ethanol. The newly synthesized substance has been analyzed using ^{1}H, ^{13}C NMR spectroscopies, and mass spectrometry. To accomplish geometry optimization, the 6-311+G(d,p) basis set and the B3LYP functional have been used. Using the same functional and basis set as for geometry optimization, excited states are computed using the time-dependent density functional theory (TD-DFT) approach. Through the computation of quantum chemical descriptors, nonlinear optical (NLO) properties are examined. Based on theoretical findings, the 3-cyano-2-oxa-pyridine compound showed considerable NLO's response characteristics depending on significant linear polarizability, α (306.511u) magnitude. Diffraction patterns (DPs) resulted when the laser beam of wavelength 473 nm, and continuous wave (CW) traverses the 3-cyano-2-oxa-pyridine compound. The nonlinear refractive index (NLRI) of the sample is found equal to 6.105×10^{-7} cm^2/W. With the same beam, the Z-scan open and closed aperture are employed to find the compound NLRI, which is equal to 0.19×10^{-7} cm^2/W. This value of the NLRI is considered high compared to the values of compounds known to have high values of the NLRI, which makes it a candidate for use in photonic applications. It is found that the sample have no nonlinear absorption coefficient (NLAC). Two laser beams at 473 nm (controlling) and the one is 532 nm (for controlled), are utilized to investigate the all-optical switching (AOS) method.

1. Introduction

During the past 30 years, the nonlinear optical (NLO) materials have been studied extensively. These substances can be utilized in many ways, such as image processing, all-optical switching, and phase coupling [1–7]. As the laser beam passes through a substance, its refractive index (RI) changes due to the strength of the beam. NLO properties of vast number of media are currently explored for the possible employment in optical devices, viz., sensors and optical limiters [8–12]. To determine the nonlinear refractive index (NLRI), several techniques have been developed since the birth of the first laser device in 1960 by Maiman [13]. The simplest techniques are the diffraction patterns (DPs) that are utilized to determine the NLRI and the change of the sample RI [14], and the single beam Z-scan due to Sheik-Bahae et al. [15,16] to measure the sample's nonlinear susceptibility.

Pyridine is a heterocyclic chemical compound that is structurally identical to benzene but lacks the CH group in favor of one nitrogen atom [17]. As an essential component, a solvent, and an organic synthesis reagent, it is significant in industrial organic chemistry [18]. Furthermore, in many biological systems, pyridine derivatives are crucial parts of proteins, nucleic acids, vitamins, and enzymes [19]. Pyridine derivatives play a significant role in therapeutic chemistry. A prominent group of these compounds with anticancer properties includes several examples [20]. 2-Amino-3-cyanopyridines have been shown to have cardiotonic, analgesic, anti-inflammatory, antibacterial, antimicrobial, and antifungal effects [21–24]. The main reason these compounds are helpful in biology is that they form hydrogen bonds between the target and lone pair electrons in the sp2 hybrid orbital of a nitrogen atom [25]. Pharmaceuticals commonly use pyridine moieties due to their fundamental characteristics, stability, ability to form hydrogen bonds, water solubility, and small molecular size [26].

The aim of the current study is to find a new material with high NLO

* Corresponding author.
E-mail address: qusayali1964@gmail.com (Q.M.A. Hassan).

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