Optik
Volume 311, September 2024, 171917

Original research article

Synthesis of a new cyclic amide derivative: Study its optical nonlinear properties and molecular docking

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https://doi.org/10.1016/j.ijleo.2024.171917

Abstract

2-(1,3-dioxoisoindolin-2-yl)-N-(pyrimidin-2-yl) acetamide is synthesized as a new cyclic amide derivative. The structure of this derivative has been characterized by NMR, FTIR, and Mass spectra. The molecular docking calculations of the prepared cyclic amide against (PDB ID: 3PP0) receptor are performed. The prepared compound has the potential to inhibit breast cancer cells, according to molecular docking results. The DFT/B3LYP via 6−311 G(d,p) level was performed to optimize the geometrical structure and the global and local reactivity descriptors of this compound. The calculated values of polarizability and hyperpolarizability of the prepared cyclic amide equal 30.774 $\times 10^{-24}$ esu and 114.678 $\times 10^{-32}$ esu, respectively. The nonlinear optical (NLO) properties of the prepared compound are studied under

compound is studied using the same laser beam. An optical limiting threshold of 15 mW is obtained.

Introduction

Researchers have been actively seeking new materials with strong and rapid nonlinearities at low-intensity laser beams for applications in light-controlled phase manipulation, optical limiting, optical switching, and refractive index modulation over the past four decades [1], [2], [3], [4]. During the past years, we have been studying the nonlinear properties of many available materials [5], [6], [7], [8], [9], [10], improving some materials properties by the use of γ-ray [11], [12], or by adding number of materials [13], [14], [15] or by the synthesize of new materials [16], [17], [18], [19], [20]. The measurements of the nonlinear refractive indexes (NLRIs) is the main task for the researchers together with nonlinear absorption coefficients (NLAC), β. The NLRI, n_2, can be easily estimated using a technique known as the spatial self-phase modulation (SSPM) [21] that leads to the generation of diffraction patterns (DPs) at a cw laser beam with low input power. Based on the laser beam of low power input that leads to the DPs with the maximum number of rings, N, n_2 can be estimated. The standard Z-scan technique offers a way to easily obtain n_2 and β. This method relies on the principle of phase transformation, which causes distortions in the beam amplitude while the beam propagates through a nonlinear medium [22], [23].

One of the subjects that has attracted substantial attention is light-induced alterations in optical properties, which can be classified into two categories: light-induced changes in absorption and light-induced changes in refractive index (RI). The former, α, is described by the following equation:$\alpha = \alpha_o + \beta I$

When α is the medium absorption coefficient, α_o is its linear absorption coefficient, β is the NLAC and I is the light beam intensity. The later is described by the following equation: $n = n_o + n_2 I$where n is the medium RI, n_o is the linear RI, n_2 is the NLRI, and I is the light beam intensity. β contains nonlinear optical effects, viz, two photon absorption (TPA) [24], reverse saturation absorption (RSA) [25] and saturation absorption (SA) [26]. n_2 is an effective parameter that contains laser induced grating [27], self-diffraction [28], soliton pulse propagation [29], optical switching [30], self-optical limiting [31], optical bistability [32], self-focusing (SF) [33], and self-defocusing (SDF) [34] and self-phase modulation [35].

Cyclic amides are a class of organic compounds that contain a nitrogen atom bonded to two carbon atoms and a carbonyl group (C═O). They can be synthesized in a variety of ways, including the condensation of carboxylic acids and amines, the Michael addition of amines to carbonyl compounds, and the cyclization of amides [36]. Cyclic amides have demonstrated a broad spectrum of potential applications in biological evaluation, including antimicrobial agents, anti-inflammatory drugs, and cancer chemotherapeutics. They were shown to have neuroprotective and anti-diabetic properties [37].

NLO materials exhibit changes in their RI when exposed to an intense electromagnetic field. Cyclic amides have been shown to exhibit promising NLO properties due to their high second-order hyperpolarizability. This property makes them prime candidates for groundbreaking optical switching, data storage, and laser devices applications [38]. Here are some specific examples of cyclic amides that were studied for their NLO and biological properties: Anisomycin is a cyclic amide antibiotic that is active against a variety of bacteria. It is also known to have anti-inflammatory and anti-cancer properties [39]. Pyrrole-2-carboxylic acid amide is a cyclic amide NLO material that has been shown to exhibit high second-order hyperpolarizability [40], [41]. NLO materials are fundamental to advancements in numerous fields, serving as key enablers of innovation, including energy storage devices, telecommunications, high-resolution spectroscopy, solid-state lasers, photodynamic therapy, optoelectronics, optical fibers, photonics, and optical switching [42]. Research on cyclic amides is ongoing, and new applications for these compounds are being discovered all the time. They are applied in a variety of fields, ranging from medicine to materials science [38].

In this study, a new cyclic amide was prepared and characterized using NMR, FTIR and mass spectroscopy. The nonlinear optical (NLO) properties of the sample were studied under irradiation with cw visible laser beam, where the nonlinear refractive index (NLRI) of the sample was obtained via the diffraction patterns (DPs) and the Z-scan under irradiation. DPs were numerically obtained using a theoretical model. The optical limiting (OL) property of the prepared sample is tested.

Section snippets

Apparatus

The FT-IR 8400 S spectrometer from Shimadzu was used with KBr disc to recorded spectrum of FT-IR. ^{1}HNMR spectrum recorded by Bruker 400 spectrometer. The mass spectrum was recorded with (EI, 70 eV) using Agilent Technologies-5975 C....

Materials and methods

Commercially obtained starting materials were used directly without further purification. Melting points (m.p.) were determined using open glass capillaries in a Fisher–Johns