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DFT structural and optical nonlinear investigations of a synthesized new azo β-diketone dye

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ABSTRACT

A new azo β-diketone (NA1) compound is synthesized by coupling reaction of 4-aminoantipyrine with acetylacetone. The NA1 compound is characterized via FTIR, Mass, ^{1}H NMR and ^{13}C NMR spectroscopies. The keto-enol tautomers of the compound electronic structures and energies are investigated using density functional theory (DFT) via B3LYP method/6-311G (d,p) level. The NA1 compound nonlinear optical (NLO) properties are studied via the diffraction patterns (DPs) and the Z-scan where the compound nonlinear index of refraction (NIR), the optical limiting (OLg) property using 473 nm visible, low power, continuous (cw) laser beam are used while the all-optical switching (AOS) property is studied using two laser beams of wavelengths 473 nm and 532 nm.

1. Introduction

Materials with high nonlinear indexes of refraction (NIR) and fast response being the subject of many researchers for different potential applications viz., optical limiting (OL) [1–4], modulation of the refractive index [5], all-optical switching (AOS) [6,7], data storage [8,9], phase conjugation [10], bi-stability [11,12] etc., so that in the past three decades many materials have been tested and/or synthesized for these characteristics [13–18].

To determine the nonlinear optical (NLO) properties of matters, two techniques have been initiated accidently viz., spatial self-phase modulation (SSPM) [19], and thermal lens [20] and a third one, Z-scan, was pioneered by S. Bahae et al. in 1990 [21]. Based on the 1st and 3rd techniques NIR, n_2, the nonlinear absorption coefficient (NAC), β , and their signs.

4- Aminoantipyrine and its derivatives have received attentions by the chemical society in different directions viz., biocidal, molar conductance, spectroscopic, studies of Pt(IV) and Au(III) etc. [22], antimicrobial activities [23,24], antibacterial properties [25,26], biologically active [27–29], cytotoxicity and DNA cleavage studies [30], scavenging activity against hydroxyl radical [31], insecticidal activities [32], corrosion inhibition [33], phersol sensing [34], spectral and nonlinear optical properties [35–38]. On the other hand acetylacetonate and its complexes and derivatives have received vast number of studies viz., new developments in the chemistry [39], molecular interaction study on binary mixtures [40], estimation of Fe(III) by substoichemetric isotope dilution analysis [41], thermal decomposition [42], composition and fluorescence of gadolinium [43], synthesis of some unsymmetrical dioxime esters [44], effect of titanium isopropoxide [45], synthesis, characterization and spectroscopic properties of azo dyes [46] and NLO optical properties [47–49], etc.

In the present work a new compound viz., (Z)-3-((1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-*1H*-pyrazol-4-yl)diazenyl)pentane-2,4-dione (NA1) was synthesized. The NLO properties of the NA1 compound solution such as refraction index (RI) total change, its NIR, its optical limiting (OLg) property are studied all at 473 nm with low power(1< Watt), Gaussian distribution and continuous wave, (cw) laser beam, studied using the SSPM, and the Z-scan techniques. All optical switching (AOS) property was studied using two, controlling, 473 nm, and controlled, 532 nm, laser beams, the first being the excitation beam with high input power as the control beam one and the second being the controlled beam of low input power. The first beam generate diffraction patterns based on the SSPM, while the weak beam generate diffraction patterns (DPs) based on the cross self-phase modulation (XSPM) [50].

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