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Preparation, DFT and optical nonlinear studies of a novel azo-(β)-diketone dye

Qusay M.A. Hassan [a,*], Nabeel A. Raheem [b], C.A. Emshary [a], Adil Muala Dhumad [b], H.A. Sultan [a], Tarek Fahad [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, Basrah 61001, Iraq

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ABSTRACT

New azo compound containing an antipyrine moiety is prepared via interaction of 4-aminoantipyrine with benzoylacetone. The coupling reaction of diazonium salt with benzoylacetone is employed to prepare the azo compound. The FTIR, ^{1}H NMR and mass spectroscopies are used for the characterization of the new azo compound. Density function theory DFT calculations are carried out to study the electronic structure and vibrational frequencies of the prepared azo compound. A linear correlation appeared between the Mulliken atomic charge of oxygen atoms and the values of calculated wavenumbers. The nonlinear optical NLO properties of the prepared compound solution are studied using 473 nm, continuous wave cw, single fundamental mode, low power laser beam via the diffraction ring patterns DRPs and the Z-scan techniques. The optical limiting OLg property of the compound solution is examined. The DRPs are simulated numerically using the Fresnel-Kirchhoff integral with reasonable accord compared to the experimental findings.

1. Introduction

During the last three decades, applications of the nonlinear optical NLO effects based on the optical field induced refractive indexes viz., self-phase modulation SPM, self-focusing SF and self-defocusing SDF, optical bistability etc., have attracted great deal of attention [1–17]. Such applications required materials with very high nonlinear refractive indexes, NRIs, and fast response times. So that hundreds of materials such as liquid crystals [18], curcumin [19–22], polymers [23–24], phthalocyanine [9,25], vegetable oils [26–28], nanoparticle materials [29–30], Schiff bases [31], azo dye [32–34] have been studied thoroughly to obtain their NRIs in the visible region of the electromagnetic spectrum using laser beams with Gaussian intensity distribution and low power (<1 Watt). To obtain the NRI, the nonlinear absorption coefficient NAC, the linear and nonlinear susceptibilities of these materials three techniques can be used viz., diffraction ring patterns DRPs [35], thermal lens TL [36] and Z-scan [37]. When a laser beam traverses a nonlinear medium, it acquires a phase shift that depends on the medium length and peak power of the Gaussian laser beam, a set of concentric DRPs resulted due to SPM. Based on the number of rings it is possible to calculate the NRI and the change in the medium refractive index based on the laser beam intensity, the sample thickness, the sample absorption coefficient, the laser beam spot size and wavelength. The Z-scan technique is based on the spatial distortion of a Gaussian laser beam traversing the NLO material, which is carried out via open and closed apertures so that it allows the determination of the NRI value and to assign its sign, (-ve) for SDF and (+ve) for SF and the NAC, the real and imaginary parts of the medium NLO susceptibility and the sign of the real part. Both techniques are rapid in the measurement of the NRI in the former and the NRI and NAC in the later.

4-aminoantipyrine and its derivatives have attracted intense attention by the chemical society in various directions viz., the evaluation of anthelmintic and insecticidal activities [38], antimicrobial activities of copper complexes derived from 4-aminoantipyrine [39], spectroscopic, molar conductance and biocidal studies [40], derivation of a novel Schiff bases [41], biological activities [42–43], phenol sensing [44], etc. 4-aminoantipyrine photo degradation property [45] , spectral [46] and NLO properties [47] via Z-scan was studied too. Benzoylacetone and its derivatives are another chemicals that have received much attention by the chemists viz., the toxicity [48], tautomery and acid based properties [49], synergetic extraction equilibrium of lanthanide(III) ions [50], spectroscopic study [51], symmetrical and non-symmetrical diimenes

* Corresponding author.
E-mail address: qusayali64@yahoo.co.in (Q.M.A. Hassan).

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