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Formation and temporal evolution of diffraction ring patterns in a newly prepared dihydropyridone

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ABSTRACT

A dihydropyridone has been prepared from butylamine and curcumin. A theoretical DFT study was conducted to determine the most stable conformer of the studied molecule (among three conformers) using the B3LYP/6-311 + G(d,p) level of theory. This is assisted by the prediction of the ¹³C NMR chemical shifts of the conformers which then correlated with the observed ¹³C NMR chemical shifts. A TD-DFT study was conducted to analyze the electronic spectrum of the most stable conformer in order to determine the transitions responsible for the longer band in the electronic spectrum of the molecule. As well the frontier orbitals in the most stable conformer were analyzed to establish the density of donor and acceptor sites in the molecule that may be responsible for the nonlinear optical (NLO) properties of the studied molecule. Diffraction ring patterns were observed as a result of the use of visible, 473 nm, low power single mode laser beam traversed a thin cell containing solution of dihydropyridone. The nonlinear refractive index, n_2 , was determined based on the number of diffraction rings per a pattern observed and by the Z-scan technique and both results are compared. The upward convection heat effect appears to be responsible for the asymmetries observed in the diffraction ring patterns. The use of convergent and divergent laser beams has led to new types of diffraction ring patterns. Temporal evolution of each diffraction ring patterns was registered. The diffraction ring patterns experimentally obtained are numerically calculated using the Fresnel-Kirchhoff diffraction integral, with good qualitative and reasonable quantitative agreements.

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1. Introduction

The search for new nonlinear materials has not come into an end yet. Such materials can have various applications in the future in the field of photonic and electronic devices [1–12]. For these purposes two basic properties should these materials have viz., high nonlinear refractive index and short response time. The refractive indexes of all optical materials depend on the intensity of laser light. Many physical mechanisms can result in the intensity dependent contributions to the nonlinear refractive indexes. Orientation of anisotropic molecules results when a strong light field is used in liquids and the average refractive index is altered. In isotropic molecules in liquid, the nonlinearity may arise because of redistribution of molecules or by electronic polarizability that results by a distortion of electronic cloud [13]. Resonant effect such as saturation or two-photon absorption can change the refractive indexes

of the materials. Thermal effects have large contribution to the nonlinear refractive indexes.

The change in refractive index, Δn , of materials usually described by the relations

$$n = n_0 + \Delta n \quad (1)$$

$$n = n_0 + n_2 I \quad (2)$$

where n_0 is the linear refractive index of the material in the absence of laser beam, n_2 is nonlinear refractive index and I is the laser light intensity. Nonlinear refractive index coefficient is an important parameter that is responsible for many interesting nonlinear optical effects viz., self-focusing and self-defocusing [14,15], optical phase conjugation [16], optical data storage [17], optical-bi-stability [18], optical limiting [19–21], optical switching [22], soliton pulse-propagation [23], self-phase modulation (SPM) [24], laser induced grating [25], to name a few. SFM is a self-action phenomena occur as a result of interplay between nonlinear photo response of the medium and divergence of the laser beam. Diffraction ring patterns occur as a result of constructive and destructive interferences within the phase-modulated beam in

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