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

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Highlights

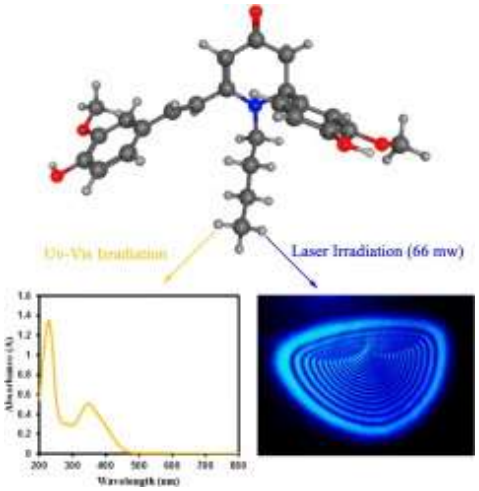
- A dihydropyridone has been prepared from butylamine and curcumin.
- The nonlinear optical properties of dihydropyridone are studied.
- Nonlinear refractive index of sample is determined using diffraction ring patterns and Z-scan techniques.
- Sample exhibits self-diffraction ring patterns due self-phase modulation.

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 ^{13}C NMR chemical shifts of the conformers which then correlated with the observed ^{13}C 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.

Graphical abstract



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Keywords

Self-phase modulation; Thermal nonlinearity; Nonlinear refractive index; Diffraction ring pattern; *Z*-scan technique

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