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Synthesis and study of nonlinear optical properties of an enaminone derived from dibenzoylmethane and N,N-diethylaminoaniline

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Abstract

The compound, (Z)-3-((4-(diethylamino)phenyl)amino)-1,3-diphenylprop-2-en-1-one, is synthesized by the reaction of dibenzoylmethane and 4-N,N-diethylaniline. The relative stabilities of the possible tautomers of the molecule are studied via the DFT B3LYP-D3BJ, CAM-B3LYP, M062X, and ωB97XD functionals in conjunction with the 6-311++G(d,p) basis set. The results showed that the enaminone tautomer with the intramolecularly hydrogen bonded chelated ring is the most stable. This is further confirmed by the Car–Parrinello MD calculations in the gas phase as well as the NCI analysis. The electronic spectrum is calculated by the TD DFT B3LYP/c-pVDZ level in ethanol, and the hole–electron analysis is carried out for the interpretation of the bands, which revealed that the longest one at 430 nm is of charge transfer origin while the others are of local transition origin. Atoms-in-molecules calculations in several media and levels of theory predicted that the ρBCP at the hydrogen bond in the gas phase to be 0.03791–0.04255 e/a_0^3 which is a characteristic of a medium strong hydrogen bond. Researchers investigated the enaminone's nonlinear optical (NLO) characteristics when it was exposed to a low power (<1 Watt), single fundamental transverse mode laser beam at 473 nm. By using diffraction patterns (DPs) and Z-scan methods, we calculated the nonlinear refractive index (NLRI) of the enaminone up to 4.597×10^{-11} $m^2 W^{-1}$ using DPs. The resulting DPs are numerically investigated using the Fraunhofer (F.) approximation and the Fresnel-Kirchhoff (F.K.) diffraction integral, showing excellent agreement with experimental findings. We successfully explored all-optical switching (AOS) in enaminone using two laser beams.

1. Introduction

Over the past thirty years, researchers have become increasingly interested in the potential uses of nonlinear optical (NLO) materials, particularly in the field of optical signal processing. These materials have been found to have applications in optical storage, all-optical modulation, optical delays, optical switching, optical limiting, optical computing, and optical susceptibility, among others [1–14]. For a material to be useful in any of these applications, it must possess certain important properties, viz., high nonlinear refractive indexes (NLRIs), nonlinear absorption coefficients (NLACs), and fast response times. Three experimental techniques have been widely used since 1967: spatial self-phase modulation (SSPM) based on diffraction patterns (DPs) [15–17], thermal lenses (TL) [18, 19], and Z-scans [20, 21]. SSPM and Z-scans have attracted popularity owing to their simplicity and ease of use.

In the past 20 years, enaminones have gained attention as a group of synthesized compounds due to their applications in both chemistry and biology. They serve as building blocks in drug development and exhibit