IOP Publishing Phys. Scr. 99 (2024) 105915 https://doi.org/10.1088/1402-4896/ad720c

Physica Scripta

PAPER

RECEIVED
28 May 2024

REVISED
13 August 2024

ACCEPTED FOR PUBLICATION
21 August 2024

PUBLISHED
3 September 2024

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

Rita S Elias[1], **Qusay M A Hassan**[2], **Bahjat A Saeed**[3], **H A Sultan**[2], **Poul Erik Hansen**[4] and **C A Emshary**[2]

[1] Department of Pharmaceutical Chemistry, College of Pharmacy, University of Basrah, Basrah 61001, Iraq
[2] Department of Physics, College of Education for Pure Sciences, University of Basrah, Basrah 61001, Iraq
[3] Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah 61001, Iraq
[4] Department of Science and Environment, Roskilde University, Roskilde, Denmark

E-mail: qusayali64@yahoo.co.in

Keywords: Nonlinear optical properties, diffraction patterns, Z-scan

Supplementary material for this article is available online

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.