Optical Materials 157 (2024) 116083

Contents lists available at ScienceDirect

Optical Materials

journal homepage: www.elsevier.com/locate/optmat

Research Article

The functional moieties impact on optical, thermal, and nonlinear properties of chalcone derivatives. A comprehensive study on FT2MP

S.R. Shankara [a,b], K.M. Eshwarappa [c,*], Shashi Kumar Kumara Swamy [d,**], Deekshitha K [e,****], Shree Vidya [f], Jayarama A [d,***], Richard Pinto [g]

[a] Research and Development Centre, Bharathiar University, Coimbatore, 641040, India
[b] Department of Physics, BGS Institute of Technology, Adichunchanagiri University, B.G Nagara, 571448, India
[c] Department of Studies in Physics, Davangere University, Shivagangothri, Davanagere, 577007, Karnataka, India
[d] Department of Physics, Alva's Institute of Engineering and Technology, Moodabidri, 574225, India
[e] Department of Civil Engineering, NMAM Institute of Technology, Nitte, Affiliated to Nitte (Deemed to be University), Udupi, India
[f] Department of PG Studies and Research in Physics, Sri Dharmasthala Manjunatheshwara College (Autonomous), Ujire, 574240, India
[g] Department of Electronics and Communication Engineering, Alva's Institute of Engineering and Technology, Moodabidri, 574225, India

ARTICLE INFO

Keywords:
Chalcones
FT2MP
Z-scan
Nonlinear refraction
2-Acetyl furan
SHG
Nonlinear optical

ABSTRACT

This study explains the intricate interplay between functional groups and the single crystal structure of the compound 1-(furan-2-yl)-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one (FT2MP) using Density Functional Theory (DFT) calculations. Notably, geometry optimization at B3LYP using 6-311G+(2d,p) closely aligned with experimental distances from X-ray diffraction (XRD) upon comparison. A Q-switched, frequency-doubled pulsed Nd. YAG laser (532 nm, 7 ns pulses), a 25 cm focal length lens, and a 0.001 mol/L FT2MP solution in Dimethylformamide was used to measure third-order nonlinear optical (NLO) parameters and subsequently the origin of second/third harmonic generation efficiency is discussed. The third-order nonlinear parameters of FT2MP were found to be $\Delta\phi = 0.95$, $n_2 = -9.605 \times 10^{-9}$ cm^2/W, $\beta = 2.74 \times 10^{-6}$ cm/W, and $\chi^{(3)} = 5.58 \times 10^{-7}$ esu. Information about the electronic structure and reactivity of the molecule is provided via the addition of Global Chemical Reactivity Descriptors (GCRD), molecular electrostatic potential (MEP) and Frontier Molecular Orbitals (FMOs) for electronic structure and reactivity insights. Hirshfeld surface analysis was used to study intermolecular interactions. This investigation indicates the potential of FT2MP for third harmonic generation, providing a comprehensive understanding of its molecular structure, reactivity, and intermolecular interactions.

1. Introduction

Nonlinear optical (NLO) materials, important for cutting-edge innovative and high-technological applications such as quantum computing, optical communications, signal processing, and laser technology, are the prioritized areas of our research [1–3] Although a variety of materials show NLO properties, organic NLO materials have gained importance due to their improved processability, extensive nonlinear coefficients, and molecular design flexibility, present advantages over traditional inorganic equivalents [4,5]. Integrating efficient donor-pi-acceptor (D-π-A) molecular systems enhances the intramolecular charge transfer, which is a vital tactic for increasing the NLO properties of chalcone systems. This tactic leverages the molecular framework's electron transport principles to improve charge transfer and enables efficient modulation of electronic properties as well as overall nonlinear optical (NLO) responses [6]. Since organic molecules have got importance due to its facile synthesis, cost-effectiveness and may be easily modified to tailor structurally to produce unique nonlinearities and faster response times, the study of nonlinear optical materials has experienced rapid expansion [7–9]. The present study is

* Corresponding author.
** Corresponding author.
*** Corresponding author.
**** Corresponding author.
E-mail addresses: km.eshwarappa@gmail.com (K.M. Eshwarappa), kushana007@gmail.com (S.K. Kumara Swamy), deekshithapattori@gmail.com (D. K), jrmarasalike@gmail.com (J. A).

https://doi.org/10.1016/j.optmat.2024.116083
Received 8 March 2024; Received in revised form 11 August 2024; Accepted 5 September 2024
Available online 12 September 2024

H.O.D
Dept. Of Physics
Alva's Institute of Engg. & Technology
Mijar, MOODBIDRI - 574 225