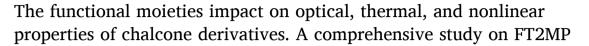
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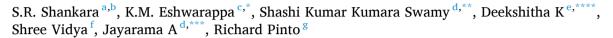
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ABSTRACT

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 $\Delta \phi = 0.95$, $n_2 = -9.605 \times 10^{-9}$ cm²/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.

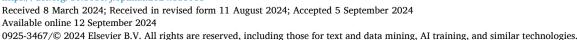
1. Introduction

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

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

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