

The structure-property studies and mechanism of optical limiting action of methyl 4- benzoate crystal under continuous wave laser excitation

Abstract

This study focuses on the design of the new dye of donor- π -acceptor (D- π -A) system of methyl 4-((4-aminophenyl)ethynyl)benzoate (MAPEB) to highlight its structural-property relation through a combined experimental and quantum chemical calculation approaches for optical limiting applications. MAPEB was synthesized via aerobic condition palladium-catalysed Sonogashira cross-coupling reaction with good yield. This molecular structure was confirmed by single crystal X-ray crystallographic analysis and the crystal exhibits monoclinic non-centrosymmetric space group of Pc. The existence of intermolecular interactions was confirmed by Hirshfeld analysis, showing high contribution of C \cdots H contact which suggested the high nonlinear optical response of the compound. The experimental spectroscopic data including Fourier Transform Infrared (FT-IR), ^1H and ^{13}C Nuclear Magnetic Resonance, electronic absorption spectra, HOMO-LUMO energy gap were compared with Density Functional Theory (DFT) at 6-311++G (d,p) basis set. The experimental results complement the theoretical findings in supporting anticipated electronic properties of the molecule. Additionally, the z-scan analysis unveils an excellent value of χ^3 of MAPEB in the order of 10^{-6} esu which indicate good nonlinear optical material under 532 nm continuous wave laser. Low optical limiting action was measured at 110 kW/cm 2 which is suitable for various continuous wave laser applications. These findings prove that MAPEB has the potential to be employed as NLO materials for photonic applications.

Keywords

Acetylide; Crystal structure; D- π -A configuration; DFT; NLO material; Optical limiting