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Molecular structure, second- and third-order nonlinear optical properties and DFT studies of a novel non-centrosymmetric chalcone derivative: (2E)-3-(4-fluorophenyl)-1-(4-[(1E)-(4-fluorophenyl)methylene]amino}phenyl)prop-2-en-1-one

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ABSTRACT

In the present work, the title chalcone, (2E)-3-(4-fluorophenyl)-1-(4-[(1E)-(4-fluorophenyl)methylene]amino}phenyl)prop-2-en-1-one (abbreviated as **FAMFC**), was synthesized and structurally characterized by single-crystal X-ray diffraction. The compound is crystallized in the monoclinic system with non-centrosymmetric space group $P2_1$ and hence is satisfied the essential condition for materials to exhibit second-order nonlinear optical properties. The molecular structure was further confirmed by using FT-IR and ^1H NMR spectroscopic techniques. The title crystal is transparent in the Vis-NIR region and has a direct band gap. The third-order nonlinear optical properties were investigated in solution (0.01 M) by Z-scan technique using a continuous wave (CW) DPSS laser at the wavelength of 532 nm. The title chalcone exhibited significant two-photon absorption ($\beta = 35.8 \times 10^{-5} \text{ cm W}^{-1}$), negative nonlinear refraction ($n_2 = -0.18 \times 10^{-8} \text{ cm}^2 \text{ W}^{-1}$) and optical limiting (OL threshold = 2.73 kJ cm^{-2}) under the CW regime. In support of the experimental results, a comprehensive theoretical study was carried out on the molecule of **FAMFC** using density functional theory (DFT). The

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