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PII: S1386-1425(17)30382-7
DOI: doi: 10.1016/j.saa.2017.05.015
Reference: SAA 15157

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received date: 21 October 2016
Revised date: 6 May 2017
Accepted date: 8 May 2017

Please cite this article as: Shivaraj R. Maidur, Parutagouda Shankaragouda Patil, Anusha Ekbote, Tze Shyang Chia, Ching Kheng Quah , 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, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2016), doi: 10.1016/j.saa.2017.05.015

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ABSTRACT

In the present work, the title chalcone, (2*E*)-3-(4-fluorophenyl)-1-(4-{[(1*E*)-(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 ^{1}H 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 ($\beta = 35.8 \times 10^{-5}$ cm W^{-1}), negative nonlinear refraction ($n_2 = -0.18 \times 10^{-8}$ cm^2 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