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Data Article

Structural analysis of chalcone derivative: 2-{4-[(2E)-3-(4-fluorophenyl)prop-2-enoyl]phenoxy}acetic acid hydrate

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ABSTRACT

The crystal structure of the title compound has been determined from X-ray diffraction studies. The compound crystallizes from methanol in the monoclinic system with space group $P2_1/c$ with unit cell parameters: a = 10.647 (8), b = 8.494 (6), c = 16.743 (12) Å, β = 92.731 (13)°, Z = 4, V = 1512.4(19) Å^3. The structure was determined by direct methods and refined to a final R-factor of 0.06. The two six-membered rings, A and B are planar with RMS deviation of fitted atoms is 0.0041 Å and the structure is stabilized by strong O–H..O, weak C–H…O, and C–H…F interactions.

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Specifications table

Subject area	Organic Chemistry, Spectroscopy, Computational Chemistry, Physical Chemistry, Chemical crystallography.
Compounds	2-{4-[(2E)-3-(4-fluorophenyl)prop-2-enoyl]phenoxy}acetic acid hydrate
Data category	Crystallographic data
Data acquisition format	Single crystal X-ray diffraction.
Data type	Analyzed
Procedure	The compound has been synthesized by a known method for which single crystal X-ray diffraction studies have been carried out.
Data accessibility	Data can accessed using CCDC no 1507783.

1. Rationale

Chalcones and their derivatives possess various biological activities like antimicrobial, anticancer and anti-inflammatory properties [1–5]. These compounds also have a significant interest in the area of nonlinear optics as second and third-order NLO materials [6,7]. We have been working in this area for the last several years developing various chalcone derivatives incorporating structural variations at benzene rings chalcone moiety [8,9]. We also have investigated the molecules that incorporate thiophene ring. Chalcones are the vastly explored NLO material because of its easy synthetic procedure, simple isolation from the reaction mixture and having the ability to manipulate structure by substituents around benzene ring [10–12]. We have been working on synthesis and characterization of several chalcone derivatives and studying their structure-property relationships as antimicrobial agents as wells as in nonlinear optics. These materials also can serve as intermediates to generate several heterocyclic moieties like pyrazoles and pyrimidines [13]. We generally observed that many a time's incorporations of polar substituent give centrosymmetric crystal. In continuation of our work on the synthesis and investigation of antimicrobial and optical material application of chalcone derivatives, we herein report a novel molecular structure containing chalcone moiety as well as aryloxy acid group as a substituent. The presence of fluorine substituent is an additional feature which is expected to impart hydrogen bonding in the molecular structure. This class of compounds can also serve as an intermediate in the design of newer compounds as they possess reactive functional group in them. In this paper, we report the crystal structure analysis of the title compound (Fig. 1).

2. Procedure

The synthesis of the compound and its spectral data have been reported by us in our earlier publication [4]. The compound was crystallized by slow evaporation from methanol water mixture (9:1). A yellow colored crystal of size $0.23 \times 0.21 \times 0.19$ mm was used for intensity data collection at room temperature (293 K) on a Rigaku Saturn 72 + diffractometer using graphite monochromatized Mo$K\alpha$ radiation ($\lambda = 0.71075$). A complete data set was processed using *CrystalClear* [14]. Of the 6331 reflections measured, 2745 are independent and 1457 for which $I > 2\sigma$ were used in the structure analysis.

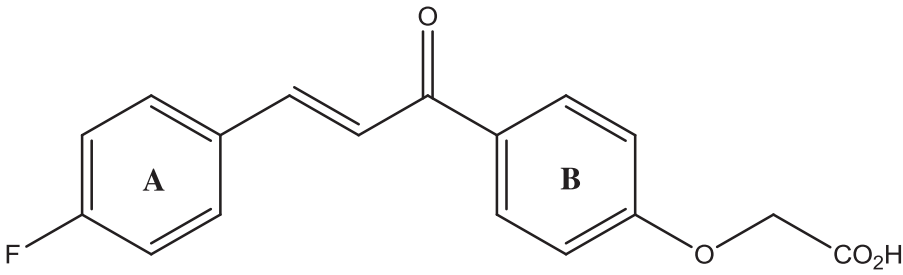

Fig. 1. Chemical structure of 2{4-[(2E)−3(4- fluorophenyl)prop-2- enoyl]phenoxy}acetic acid [FPAH].