

1-(4-Fluorophenyl)-3-(4-methoxyphenyl)-
prop-2-en-1-oneWilliam T. A. Harrison,^{a*} H. S. Yathirajan,^b H. G. Anilkumar,^b B. K. Sarojini^c and B. Narayana^d^aDepartment of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland, ^bDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, ^cDepartment of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and ^dDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, IndiaCorrespondence e-mail:
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Key indicators

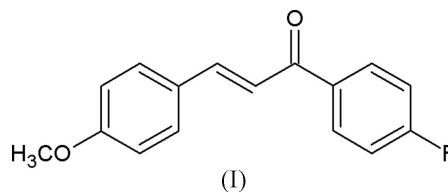
Single-crystal X-ray study
 $T = 120$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.036
 wR factor = 0.083
Data-to-parameter ratio = 9.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The planar molecules of the title compound, $\text{C}_{15}\text{H}_{13}\text{FO}_2$, are normal. The non-centrosymmetric crystal packing may be influenced by weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ interactions.

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Comment

Among the various organic compounds reported for their non-linear optical (NLO) properties, chalcone derivatives are notable for their excellent blue-light transmittance and good crystallizability (Uchida *et al.*, 1998). They provide a necessary molecular electronic configuration to show NLO effects, with two aromatic rings connected through a conjugated bridge (Goto *et al.*, 1991; Tam *et al.*, 1989; Indira *et al.*, 2002). Substitution on either of the benzene rings appears to increase the likelihood of non-centrosymmetric crystal packing, as well as enhancing the electronic properties of the molecule (Fichou *et al.*, 1988). As part of our ongoing studies in this area (Harrison *et al.*, 2005; Harrison, Yathirajan, Sarojini, Narayana & Vijaya Raj, 2006), we have prepared the title chalcone derivative, (I) (Fig. 1).



The geometric parameters for (I) are normal. The dihedral angle between the C1–C6 and C10–C15 benzene rings is $7.15(10)^\circ$. The C16 methyl C atom is displaced from the C10–C15 ring plane by $0.059(4)$ Å. The enone group is close to planar (r.m.s. deviation from the mean plane of C6–C10 + O1 = 0.028 Å). Overall, the molecule of (I) is approximately planar, which is different from the significantly more twisted conformation of the 4-chloro derivative (Harrison, Yathirajan, Sarojini, Narayana & Indira, 2006), where the dihedral angle between the benzene rings is $21.82(6)^\circ$.

The only possible non-van der Waals intermolecular interactions in (I) are $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ bonds arising from the methyl group (Table 2, Fig. 2). There are no $\pi-\pi$ stacking interactions in (I).

Compound (I) complements other chalcone derivatives with different substituents X at the 4-fluoro position (see scheme), including $X = \text{Cl}$ (Harrison, Yathirajan, Sarojini, Narayana & Indira, 2006), $X = \text{OH}$ (Sathiya Moorthi *et al.*, 2005), $X = \text{CH}_3$ (Wang *et al.*, 2005), $X = \text{H}$ (Rabinovich & Schmidt, 1970), $X = \text{OCH}_3$ (Zheng *et al.*, 1992) and $X = \text{NO}_2$

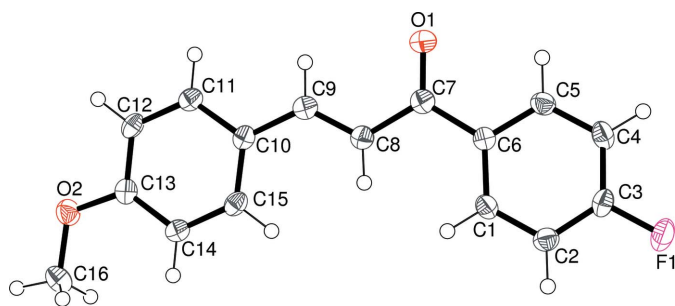


Figure 1
A view of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

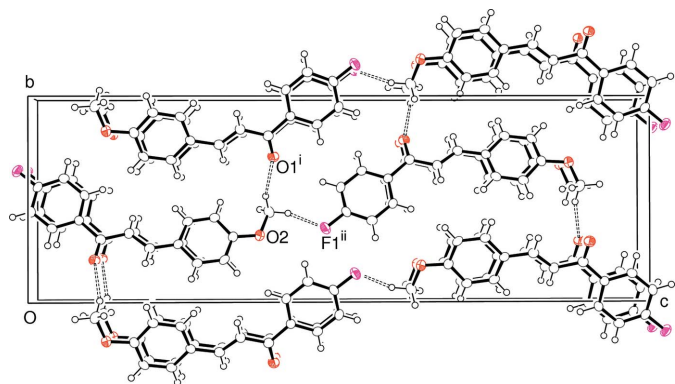


Figure 2
The packing in (I), viewed down [100], with C–H...O and C–H...F interactions indicated by dashed lines.

(Patil *et al.*, 2006). All of these compounds crystallize with different structures.

Experimental

4-Fluoroacetophenone (1.38 g, 0.01 mol) in ethanol (25 ml) was mixed with 4-methoxy-benzaldehyde (1.36 g, 0.01 mol) in ethanol (25 ml) and the mixture was treated with an aqueous solution (20 ml) of potassium hydroxide (20 ml, 5%). The resulting mixture was stirred well and left for 24 h, and the solid product was collected by filtration and dried. Crystals of (I) were recrystallized from ethanol (yield 90%; m.p. 371 K). Analysis, found (calculated) for $C_{16}H_{13}FO_2$: C 74.29 (74.92%), H 5.72 (5.07%).

Crystal data

$C_{16}H_{13}FO_2$
 $M_r = 256.26$
 Orthorhombic, $P2_12_12_1$
 $a = 3.9148$ (2) Å
 $b = 10.1977$ (5) Å
 $c = 30.8052$ (14) Å
 $V = 1229.80$ (10) Å³
 $Z = 4$
 $D_x = 1.384$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 120$ (2) K
 Block, colourless
 $0.65 \times 0.20 \times 0.15$ mm

Data collection

Nonius KappaCCD area-detector diffractometer
 ω and φ scans
 Absorption correction: multi-scan *SADABS* (Bruker, 2003)
 $T_{min} = 0.938$, $T_{max} = 0.985$
 8063 measured reflections
 1669 independent reflections
 1402 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.034$
 $\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.083$
 $S = 1.09$
 1669 reflections
 174 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.45P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.21$ e Å⁻³
 $\Delta\rho_{min} = -0.17$ e Å⁻³
 Extinction correction: *SHELXL97* (Sheldrick, 1997)
 Extinction coefficient: 0.017 (3)

Table 1

Selected torsion angles ($^\circ$).

| | | | |
|-------------|----------|-------------|----------|
| C5–C6–C7–O1 | –9.4 (3) | O1–C7–C8–C9 | –5.8 (4) |
|-------------|----------|-------------|----------|

Table 2

Hydrogen-bond geometry (Å, $^\circ$).

| <i>D</i> –H... <i>A</i> | <i>D</i> –H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> –H... <i>A</i> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| C16–H16B...O1 ⁱ | 0.98 | 2.56 | 3.502 (3) | 161 |
| C16–H16A...F1 ⁱⁱ | 0.98 | 2.59 | 3.458 (3) | 148 |

Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}, -y + 1, z + \frac{1}{2}$.

In the absence of significant anomalous scattering effects, Friedel pairs were averaged and the absolute structure of the crystal studied is indeterminate. The H atoms were placed in idealized locations (C–H = 0.95–0.98 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(\text{methyl C})$. The methyl group was rotated to fit the electron density.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*, *DENZO* (Otwinowski & Minor, 1997), and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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