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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 = 9.6

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

1-(4-Fluorophenyl)-3-(4-methoxyphenyl)-prop-2-en-1-one

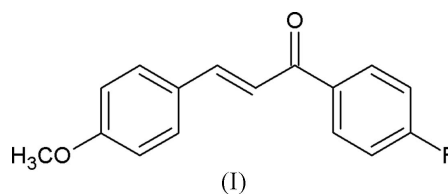
The planar molecules of the title compound, $\text{C}_{15}\text{H}_{13}\text{FO}_2$, are normal. The non-centrosymmetric crystal packing may be influenced by weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ interactions.

Received 27 June 2006

Accepted 30 June 2006

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 $X = \text{NO}_2$

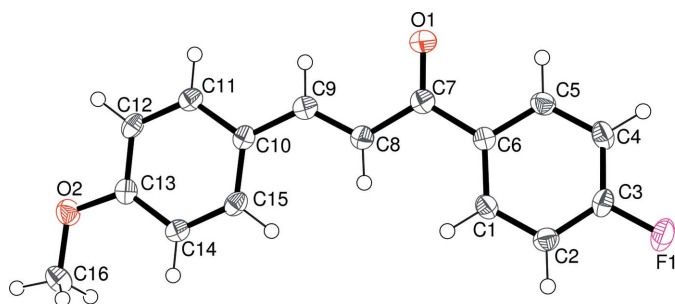


Figure 1
A view of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

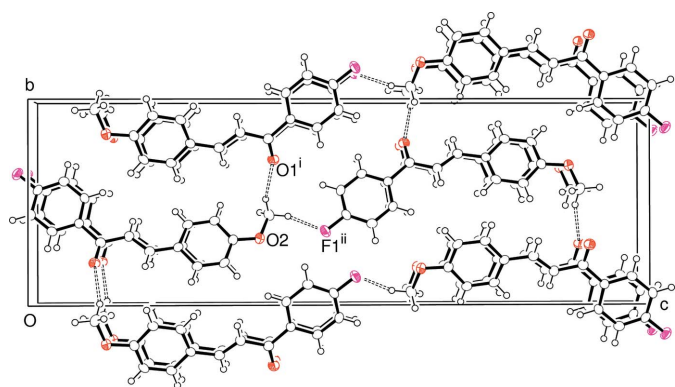


Figure 2
The packing in (I), viewed down [100], with C–H...O and C–H...F interactions indicated by dashed lines.

(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

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

Data collection

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

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.45P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.083$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
1669 reflections	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
174 parameters	Extinction correction: <i>SHELXL97</i> (Sheldrick, 1997)
H-atom parameters constrained	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)
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Table 2

Hydrogen-bond geometry (Å, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. 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*.

The authors thank the EPSRC National Crystallography Service (University of Southampton) for data collection. HGS thanks the University of Mysore for provision of research facilities. BKS thanks AICTE, Government of India, New Delhi, for financial assistance under the Career Award for Young Teachers (CAYT) scheme.

References

- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
 Bruker (2003). *SADABS*, Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *Jpn J. Appl. Phys.* **27**, 429–430.
 Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
 Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Anilkumar, H. G. (2005). *Acta Cryst.* **C61**, o728–o730.
 Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Indira, J. (2006). *Acta Cryst.* **E62**, o1647–o1649.
 Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Vijaya Raj, K. K. (2006). *Acta Cryst.* **E62**, o1578–o1579.

- Indira, J., Karat, P. P. & Sarojini, B. K. (2002). *J. Cryst. Growth*, **242**, 209–214.
- Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Patil, P. S., Teh, J. B.-J., Fun, H.-K., Razak, I. A. & Dharmaprasath, S. M. (2006). *Acta Cryst.* **E62**, o896–o898.
- Rabinovich, D. & Schmidt, G. M. J. (1970). *J. Chem. Soc. B*, pp. 6–9.
- Sathya Moorthi, S., Chinnakali, K., Nanjundan, S., Radhika, R., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* **E61**, o480–o482.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Tam, W., Guerin, B., Calabrese, J. C. & Stevenson, S. H. (1989). *Chem. Phys. Lett.* **154**, 93–96.
- Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abduryim, A. & Watanabe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **315**, 135–140.
- Wang, L., Lu, C.-R., Zhang, Y. & Zhang, D.-C. (2005). *Jiegou Huaxue (Chin. J. Struct. Chem.)*, **24**, 191–195. (In Chinese).
- Zheng, J., Zhang, D., Sheng, P., Wang, H. & Yao, X. (1992). *Yingyong Huaxue (Chin. J. Appl. Chem.)*, **9**, 66–69. (In Chinese).