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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

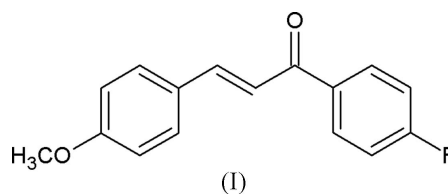
The planar molecules of the title compound, $\text{C}_{15}\text{H}_{13}\text{FO}_2$, are normal. The non-centrosymmetric crystal packing may be influenced by weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ interactions.

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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 $X = \text{NO}_2$

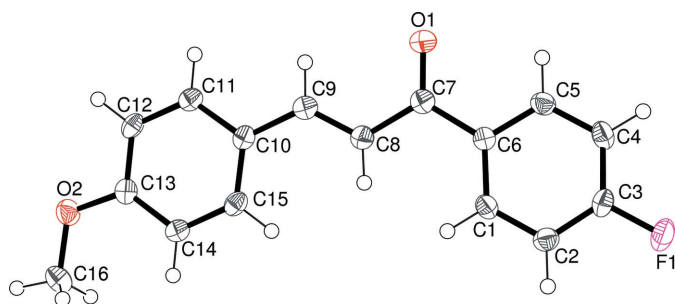


Figure 1
A view of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

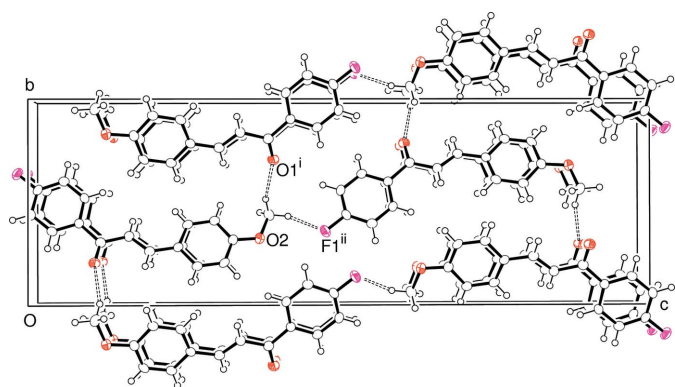


Figure 2
The packing in (I), viewed down [100], with C—H...O and C—H...F interactions indicated by dashed lines.

(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

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

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 (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
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 \AA) 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*.

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supporting information

Acta Cryst. (2006). E62, o3251–o3253 [https://doi.org/10.1107/S160053680602530X]

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

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Crystal data

$C_{16}H_{13}FO_2$	$F(000) = 536$
$M_r = 256.26$	$D_x = 1.384 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: P 2ac 2ab	Cell parameters from 1541 reflections
$a = 3.9148 (2) \text{ \AA}$	$\theta = 1.0\text{--}27.5^\circ$
$b = 10.1977 (5) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 30.8052 (14) \text{ \AA}$	$T = 120 \text{ K}$
$V = 1229.80 (10) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.65 \times 0.20 \times 0.15 \text{ mm}$

Data collection

Nonius KappaCCD area-detector diffractometer	8063 measured reflections
Radiation source: fine-focus sealed tube	1669 independent reflections
Graphite monochromator	1402 reflections with $I > 2\sigma(I)$
ω and ϕ scans	$R_{\text{int}} = 0.034$
Absorption correction: multi-scan	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.3^\circ$
SADABS (Bruker, 2003)	$h = -5 \rightarrow 4$
$T_{\text{min}} = 0.938$, $T_{\text{max}} = 0.985$	$k = -13 \rightarrow 13$
	$l = -40 \rightarrow 40$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.45P]$
$wR(F^2) = 0.083$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1669 reflections	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
174 parameters	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
0 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.017 (3)
Secondary atom site location: none	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3302 (6)	0.5221 (2)	0.08621 (6)	0.0249 (5)
H1	0.3789	0.5496	0.1150	0.030*
C2	0.4042 (7)	0.6047 (2)	0.05194 (6)	0.0271 (5)
H2	0.5029	0.6886	0.0568	0.033*
C3	0.3309 (6)	0.5622 (2)	0.01070 (6)	0.0259 (5)
C4	0.1873 (7)	0.4417 (2)	0.00202 (6)	0.0285 (6)
H4	0.1399	0.4153	-0.0269	0.034*
C5	0.1141 (7)	0.3604 (2)	0.03656 (6)	0.0265 (5)
H5	0.0140	0.2770	0.0313	0.032*
C6	0.1850 (6)	0.39877 (19)	0.07920 (6)	0.0216 (5)
C7	0.0968 (6)	0.3057 (2)	0.11487 (6)	0.0257 (5)
C8	0.2157 (6)	0.3353 (2)	0.15937 (6)	0.0265 (5)
H8	0.3639	0.4078	0.1639	0.032*
C9	0.1196 (6)	0.2625 (2)	0.19346 (6)	0.0249 (5)
H9	-0.0287	0.1909	0.1876	0.030*
C10	0.2193 (6)	0.2817 (2)	0.23866 (6)	0.0227 (5)
C11	0.1246 (6)	0.1895 (2)	0.26996 (6)	0.0242 (5)
H11	-0.0011	0.1142	0.2613	0.029*
C12	0.2094 (6)	0.2053 (2)	0.31321 (6)	0.0241 (5)
H12	0.1451	0.1406	0.3338	0.029*
C13	0.3895 (6)	0.3162 (2)	0.32649 (6)	0.0232 (5)
C14	0.4832 (6)	0.4105 (2)	0.29607 (6)	0.0236 (5)
H14	0.6024	0.4871	0.3049	0.028*
C15	0.4010 (6)	0.39162 (19)	0.25281 (6)	0.0245 (5)
H15	0.4704	0.4553	0.2321	0.029*
C16	0.6316 (7)	0.4400 (2)	0.38472 (7)	0.0323 (6)
H16A	0.6783	0.4321	0.4159	0.048*
H16B	0.4846	0.5162	0.3796	0.048*
H16C	0.8472	0.4512	0.3690	0.048*
O1	-0.0729 (5)	0.20711 (14)	0.10708 (5)	0.0344 (4)
O2	0.4625 (4)	0.32341 (14)	0.36970 (4)	0.0303 (4)
F1	0.4078 (4)	0.64183 (12)	-0.02341 (4)	0.0381 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0287 (14)	0.0251 (10)	0.0210 (9)	0.0020 (10)	-0.0018 (10)	-0.0029 (8)
C2	0.0290 (13)	0.0227 (10)	0.0296 (10)	-0.0013 (11)	0.0023 (10)	-0.0004 (8)
C3	0.0282 (14)	0.0268 (11)	0.0228 (9)	0.0060 (11)	0.0036 (10)	0.0061 (8)
C4	0.0358 (15)	0.0296 (12)	0.0200 (9)	0.0064 (12)	-0.0017 (10)	-0.0030 (8)

C5	0.0310 (13)	0.0214 (10)	0.0271 (10)	-0.0002 (11)	-0.0030 (11)	-0.0023 (8)
C6	0.0201 (12)	0.0226 (10)	0.0222 (9)	0.0022 (9)	0.0000 (9)	-0.0001 (8)
C7	0.0250 (12)	0.0248 (10)	0.0273 (10)	0.0021 (11)	0.0012 (10)	-0.0008 (8)
C8	0.0278 (13)	0.0266 (11)	0.0252 (10)	-0.0022 (11)	-0.0012 (10)	0.0012 (9)
C9	0.0230 (12)	0.0233 (10)	0.0285 (10)	0.0017 (11)	0.0004 (10)	0.0002 (8)
C10	0.0227 (12)	0.0214 (10)	0.0241 (9)	0.0049 (10)	0.0032 (9)	0.0026 (8)
C11	0.0232 (12)	0.0206 (10)	0.0289 (10)	0.0020 (11)	0.0031 (10)	0.0014 (8)
C12	0.0224 (12)	0.0232 (10)	0.0267 (10)	0.0033 (10)	0.0033 (9)	0.0077 (9)
C13	0.0189 (12)	0.0267 (10)	0.0240 (9)	0.0063 (11)	0.0005 (9)	0.0016 (8)
C14	0.0211 (12)	0.0210 (10)	0.0285 (10)	0.0013 (10)	0.0010 (10)	0.0012 (8)
C15	0.0243 (13)	0.0211 (10)	0.0282 (10)	0.0034 (10)	0.0054 (11)	0.0044 (8)
C16	0.0328 (14)	0.0349 (12)	0.0291 (10)	0.0033 (13)	-0.0056 (11)	-0.0064 (9)
O1	0.0414 (10)	0.0291 (8)	0.0327 (8)	-0.0111 (9)	-0.0038 (8)	0.0015 (6)
O2	0.0356 (10)	0.0309 (8)	0.0245 (7)	0.0013 (8)	-0.0037 (7)	0.0016 (6)
F1	0.0527 (10)	0.0345 (7)	0.0270 (6)	0.0042 (8)	0.0086 (7)	0.0092 (5)

Geometric parameters (Å, °)

C1—C2	1.382 (3)	C9—H9	0.9500
C1—C6	1.397 (3)	C10—C11	1.397 (3)
C1—H1	0.9500	C10—C15	1.397 (3)
C2—C3	1.373 (3)	C11—C12	1.382 (3)
C2—H2	0.9500	C11—H11	0.9500
C3—F1	1.362 (2)	C12—C13	1.394 (3)
C3—C4	1.377 (3)	C12—H12	0.9500
C4—C5	1.379 (3)	C13—O2	1.363 (2)
C4—H4	0.9500	C13—C14	1.392 (3)
C5—C6	1.398 (3)	C14—C15	1.384 (3)
C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.493 (3)	C15—H15	0.9500
C7—O1	1.229 (3)	C16—O2	1.437 (3)
C7—C8	1.479 (3)	C16—H16A	0.9800
C8—C9	1.340 (3)	C16—H16B	0.9800
C8—H8	0.9500	C16—H16C	0.9800
C9—C10	1.460 (3)		
C2—C1—C6	121.08 (19)	C10—C9—H9	116.6
C2—C1—H1	119.5	C11—C10—C15	117.37 (18)
C6—C1—H1	119.5	C11—C10—C9	119.79 (19)
C3—C2—C1	118.06 (19)	C15—C10—C9	122.81 (18)
C3—C2—H2	121.0	C12—C11—C10	121.5 (2)
C1—C2—H2	121.0	C12—C11—H11	119.2
F1—C3—C2	118.63 (19)	C10—C11—H11	119.2
F1—C3—C4	118.20 (18)	C11—C12—C13	119.91 (19)
C2—C3—C4	123.16 (19)	C11—C12—H12	120.0
C3—C4—C5	118.11 (18)	C13—C12—H12	120.0
C3—C4—H4	120.9	O2—C13—C14	124.38 (19)
C5—C4—H4	120.9	O2—C13—C12	115.88 (18)

C4—C5—C6	121.03 (19)	C14—C13—C12	119.74 (18)
C4—C5—H5	119.5	C15—C14—C13	119.4 (2)
C6—C5—H5	119.5	C15—C14—H14	120.3
C1—C6—C5	118.56 (18)	C13—C14—H14	120.3
C1—C6—C7	123.56 (18)	C14—C15—C10	122.01 (19)
C5—C6—C7	117.88 (18)	C14—C15—H15	119.0
O1—C7—C8	121.24 (19)	C10—C15—H15	119.0
O1—C7—C6	120.10 (18)	O2—C16—H16A	109.5
C8—C7—C6	118.66 (19)	O2—C16—H16B	109.5
C9—C8—C7	121.6 (2)	H16A—C16—H16B	109.5
C9—C8—H8	119.2	O2—C16—H16C	109.5
C7—C8—H8	119.2	H16A—C16—H16C	109.5
C8—C9—C10	126.7 (2)	H16B—C16—H16C	109.5
C8—C9—H9	116.6	C13—O2—C16	117.11 (16)
C6—C1—C2—C3	0.0 (4)	C7—C8—C9—C10	180.0 (2)
C1—C2—C3—F1	-178.9 (2)	C8—C9—C10—C11	-173.7 (2)
C1—C2—C3—C4	0.2 (4)	C8—C9—C10—C15	8.0 (4)
F1—C3—C4—C5	179.1 (2)	C15—C10—C11—C12	-0.6 (3)
C2—C3—C4—C5	0.0 (4)	C9—C10—C11—C12	-179.0 (2)
C3—C4—C5—C6	-0.3 (4)	C10—C11—C12—C13	0.9 (3)
C2—C1—C6—C5	-0.2 (3)	C11—C12—C13—O2	-179.9 (2)
C2—C1—C6—C7	-179.5 (2)	C11—C12—C13—C14	-0.1 (3)
C4—C5—C6—C1	0.4 (3)	O2—C13—C14—C15	178.7 (2)
C4—C5—C6—C7	179.7 (2)	C12—C13—C14—C15	-1.1 (3)
C1—C6—C7—O1	169.8 (2)	C13—C14—C15—C10	1.5 (3)
C5—C6—C7—O1	-9.4 (3)	C11—C10—C15—C14	-0.6 (3)
C1—C6—C7—C8	-9.8 (3)	C9—C10—C15—C14	177.7 (2)
C5—C6—C7—C8	171.0 (2)	C14—C13—O2—C16	3.5 (3)
O1—C7—C8—C9	-5.8 (4)	C12—C13—O2—C16	-176.71 (19)
C6—C7—C8—C9	173.8 (2)		

Hydrogen-bond geometry (Å, °)

<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) $-x, y+1/2, -z+1/2$; (ii) $-x+3/2, -y+1, z+1/2$.