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(*E*)-3-(4-Fluorophenyl)-1-(4-methylphenyl)prop-2-en-1-one

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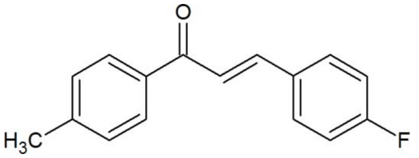
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.137; data-to-parameter ratio = 24.5.

In the title molecule, $C_{16}H_{13}FO$, the planar 4-fluorophenyl and 4-methylphenyl groups are twisted from the prop-2-en-1-one group by 23.6 (6) and 18.9 (2)°, respectively, and by 26.1 (6)° from each other. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between a 4-methylphenyl hydrogen and the prop-2-en-1-one group, which links the molecules into a chain along the *b* axis.

Related literature

For related structure, see: Yathirajan *et al.* (2006); Harrison *et al.* (2006); Butcher *et al.* (2006). For related literature, see: Goto *et al.* (1991); Indira *et al.* (2002); Lawrence *et al.* (2001); Pandey *et al.* (2005); Sarojini *et al.* (2006); Bhat *et al.* (2005); Dhar (1981); Di Carlo *et al.* (1999); Dimmock *et al.* (1999); Lin *et al.* (2002); Opletalova & Sedivy (1999).



Experimental

Crystal data

$C_{16}H_{13}FO$
M_r = 240.26
Monoclinic, $P2_1/c$
a = 11.0082 (7) Å
b = 10.7499 (6) Å
c = 11.5415 (7) Å
β = 117.122 (9)°
V = 1215.60 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 203 K
0.55 × 0.47 × 0.31 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.737, T_{max} = 1.000 (expected range = 0.716–0.972)
11487 measured reflections
4010 independent reflections
1699 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.137
S = 0.89
4010 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···O1^{i}	0.94	2.53	3.3598 (17)	148

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *WinGX*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2095).

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supplementary materials

Acta Cryst. (2007). E**63**, o3833 [**doi:10.1107/S160053680703989X**]

(*E*)-3-(4-Fluorophenyl)-1-(4-methylphenyl)prop-2-en-1-one

R. J. Butcher, J. P. Jasinski, H. S. Yathirajan, B. Narayana and **K. Veena**

Comment

Chalcones are one of the major classes of natural products with widespread distribution in fruits, vegetables, spices, tea and soy based foodstuff and have recently been subjects of great interest for their interesting pharmacological activities (Di Carlo *et al.*, 1999). A vast number of naturally occurring chalcones are polyhydroxylated in the aryl rings. The radical quenching properties of the phenolic groups present in many chalcones have raised interest in using these compounds or chalcone rich plant extracts as drugs or food preservatives (Dhar, 1981). Chalcones can be easily obtained from the aldol condensation of aromatic aldehydes and aromatic ketones. This class of compounds presents interesting biological properties such as cytotoxicity (Pandey *et al.*, 2005; Bhat *et al.*, 2005), antiherpes and antitumour activity and may be useful for the chemotherapy of leishmaniasis among others (Lawrence *et al.*, 2001). A review on the bioactivities of chalcones is described (Dimmock *et al.*, 1999). Chalcones and their heterocyclic analogs as potential antifungal chemotherapeutic agents (Opletalova & Sedivy, 1999) and chalcones and flavonoids as anti-tuberculosis agents have been published (Lin *et al.*, 2002). Several organic compounds of chalcone derivatives are reported to have non-linear optics (NLO) properties because of their excellent blue light transmittance and good crystallization ability (Goto *et al.*, 1991; Indira *et al.*, 2002; Sarojini *et al.*, 2006). The crystal structures of some fluorinated chalcones, *viz*., 1-(2,4-dichloro-5-fluorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Yathirajan *et al.*, 2006), 1-(4-fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (Harrison *et al.*, 2006) and 3-(3,4-dimethoxyphenyl)-1-(4-fluorophenyl)prop-2-en-1-one (Butcher *et al.*, 2005) have been reported. In continuation of our work on chalcones, a new chalcone, (I), $C_{16}H_{13}FO$ is synthesized and its crystal structure is reported.

The planar 4-fluorophenyl and 4-methylphenyl groups of the title molecule (Fig. 1) are twisted from the prop-2-en-1-one group by 23.6 (6) and 18.9 (2)°, respectively, and 26.1 (6)° from each other forming torsion angles of −12.7 (3)° [C9–C10–C11–C12] and 13.7 (2)° [C6–C1–C8–C9].

Intermolecular C—H···O hydrogen bonding interactions (Table 1) between H2A from the 4-methylphenyl group and the prop-2-en-1-one oxygen, which link the molecules into a chain along the *b* axis, stabilize crystal packing (Fig. 2).

Experimental

4-Fluorobenzaldehyde (1.5 ml, 0.01 mol) in ethanol (50 ml) was mixed with 1-(4-methyl phenyl) ethanone (1.34 ml, 0.01 mol) and the mixture was treated with 10 ml of 10% KOH. The reaction mixture was then kept for constant stirring. The solid precipitate obtained was filtered, washed with alcohol and dried. The crystal growth was carried out in acetone by the slow evaporation technique (m.p.: 400 K). Analysis found: C 79.89, H 5.36%; $C_{16}H_{13}FO$ requires: C 79.98, H 5.45%.

Refinement

The H atoms, were refined using a riding model with C—H = 0.94–0.97 Å, and with $U_{iso}(H) = 1.18–1.50U_{eq}(C)$.

Figures

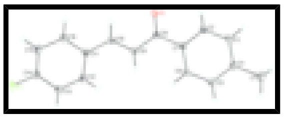

Fig. 1. Molecular structure of the title compound, showing atom labelling and 50% probability displacement ellipsoids.

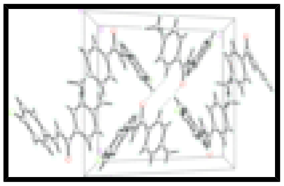

Fig. 2. Packing diagram of the title compound, viewed down the *a* axis. Dashed lines indicate C—H···O hydrogen bonds.

(*E*)-3-(4-Fluorophenyl)-1-(4-methylphenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{13}FO$

M_r = 240.26

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

a = 11.0082 (7) Å

b = 10.7499 (6) Å

c = 11.5415 (7) Å

β = 117.122 (9)°

V = 1215.60 (13) Å^3

Z = 4

F_{000} = 504

D_x = 1.313 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71073 Å

Cell parameters from 3092 reflections

θ = 5.1–32.5°

μ = 0.09 mm^{-1}

T = 203 K

Prism, colorless

0.55 × 0.47 × 0.31 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 10.5081 pixels mm^{-1}

T = 203 K

φ and ω scans

Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)

T_{min} = 0.737, T_{max} = 1.000

11487 measured reflections

4010 independent reflections

1699 reflections with $I > 2\sigma(I)$

R_{int} = 0.045

θ_{max} = 32.5°

θ_{min} = 5.1°

$h = -16 \rightarrow 16$

$k = -13 \rightarrow 15$

$l = -17 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.050

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.137$	$w = 1/[\sigma^2(F_o^2) + (0.0694P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.89$	$(\Delta/\sigma)_{max} = 0.001$
4010 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
164 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	1.05207 (9)	0.89421 (9)	0.09765 (9)	0.0545 (3)
O1	0.52636 (11)	0.57091 (10)	0.35150 (10)	0.0447 (3)
C1	0.43320 (13)	0.75350 (13)	0.39312 (12)	0.0319 (3)
C2	0.38265 (14)	0.68882 (13)	0.46662 (13)	0.0346 (3)
H2A	0.4031	0.6039	0.4844	0.042*
C3	0.30284 (14)	0.74811 (15)	0.51359 (13)	0.0392 (4)
H3A	0.2703	0.7028	0.5634	0.047*
C4	0.26944 (14)	0.87354 (14)	0.48879 (13)	0.0382 (4)
C5	0.32190 (15)	0.93751 (15)	0.41701 (15)	0.0421 (4)
H5A	0.3024	1.0227	0.4003	0.050*
C6	0.40182 (15)	0.87941 (14)	0.36952 (15)	0.0393 (4)
H6A	0.4354	0.9252	0.3208	0.047*
C7	0.18030 (18)	0.93690 (17)	0.53779 (17)	0.0580 (5)
H7A	0.1745	1.0249	0.5174	0.087*
H7B	0.2191	0.9261	0.6313	0.087*
H7C	0.0897	0.9006	0.4963	0.087*
C8	0.52024 (14)	0.68530 (14)	0.34601 (13)	0.0330 (3)
C9	0.60209 (14)	0.75656 (14)	0.29695 (13)	0.0355 (3)
H9A	0.5780	0.8391	0.2689	0.043*
C10	0.70932 (14)	0.70500 (13)	0.29217 (14)	0.0356 (3)
H10A	0.7300	0.6231	0.3237	0.043*
C11	0.79915 (13)	0.75967 (13)	0.24395 (13)	0.0324 (3)
C12	0.76801 (14)	0.86948 (14)	0.17171 (13)	0.0354 (4)
H12A	0.6879	0.9130	0.1560	0.042*
C13	0.85251 (15)	0.91552 (14)	0.12290 (14)	0.0395 (4)

H13A	0.8311	0.9896	0.0744	0.047*
C14	0.96921 (14)	0.84977 (15)	0.14727 (14)	0.0380 (4)
C15	1.00536 (14)	0.74242 (15)	0.21885 (14)	0.0423 (4)
H15A	1.0866	0.7004	0.2354	0.051*
C16	0.91890 (15)	0.69798 (14)	0.26577 (14)	0.0411 (4)
H16A	0.9414	0.6237	0.3140	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0518 (6)	0.0635 (7)	0.0638 (6)	−0.0022 (4)	0.0398 (5)	0.0037 (5)
O1	0.0561 (7)	0.0299 (6)	0.0578 (7)	0.0011 (5)	0.0344 (6)	0.0029 (5)
C1	0.0322 (7)	0.0314 (8)	0.0338 (7)	−0.0024 (6)	0.0165 (6)	0.0000 (6)
C2	0.0347 (8)	0.0310 (8)	0.0382 (8)	−0.0015 (6)	0.0167 (7)	0.0033 (6)
C3	0.0392 (8)	0.0469 (10)	0.0376 (8)	−0.0066 (7)	0.0227 (7)	0.0015 (7)
C4	0.0370 (8)	0.0401 (9)	0.0403 (8)	0.0001 (7)	0.0202 (7)	−0.0032 (7)
C5	0.0484 (9)	0.0317 (8)	0.0517 (9)	0.0029 (7)	0.0277 (8)	0.0024 (7)
C6	0.0446 (8)	0.0342 (9)	0.0492 (9)	0.0008 (7)	0.0302 (8)	0.0072 (7)
C7	0.0650 (11)	0.0567 (12)	0.0707 (11)	0.0037 (9)	0.0471 (10)	−0.0056 (9)
C8	0.0311 (7)	0.0334 (9)	0.0345 (7)	0.0002 (6)	0.0149 (6)	0.0020 (6)
C9	0.0400 (8)	0.0294 (8)	0.0410 (8)	0.0013 (6)	0.0220 (7)	0.0019 (6)
C10	0.0399 (8)	0.0292 (8)	0.0415 (8)	0.0014 (6)	0.0219 (7)	0.0017 (6)
C11	0.0334 (7)	0.0308 (8)	0.0352 (7)	0.0001 (6)	0.0177 (6)	−0.0023 (6)
C12	0.0321 (7)	0.0339 (9)	0.0405 (8)	0.0029 (6)	0.0168 (7)	−0.0003 (6)
C13	0.0399 (8)	0.0372 (9)	0.0429 (8)	0.0019 (7)	0.0202 (7)	0.0049 (7)
C14	0.0361 (8)	0.0442 (10)	0.0396 (8)	−0.0048 (7)	0.0224 (7)	−0.0057 (7)
C15	0.0333 (7)	0.0501 (10)	0.0458 (9)	0.0087 (7)	0.0201 (7)	0.0011 (8)
C16	0.0439 (9)	0.0375 (9)	0.0461 (9)	0.0079 (7)	0.0241 (8)	0.0056 (7)

Geometric parameters (Å, °)

F1—C14	1.3655 (15)	C7—H7C	0.9700
O1—C8	1.2316 (16)	C8—C9	1.4779 (19)
C1—C6	1.393 (2)	C9—C10	1.3278 (19)
C1—C2	1.3940 (18)	C9—H9A	0.9400
C1—C8	1.4920 (18)	C10—C11	1.4610 (18)
C2—C3	1.3806 (19)	C10—H10A	0.9400
C2—H2A	0.9400	C11—C16	1.3921 (19)
C3—C4	1.393 (2)	C11—C12	1.395 (2)
C3—H3A	0.9400	C12—C13	1.3804 (19)
C4—C5	1.389 (2)	C12—H12A	0.9400
C4—C7	1.501 (2)	C13—C14	1.378 (2)
C5—C6	1.380 (2)	C13—H13A	0.9400
C5—H5A	0.9400	C14—C15	1.368 (2)
C6—H6A	0.9400	C15—C16	1.3775 (19)
C7—H7A	0.9700	C15—H15A	0.9400
C7—H7B	0.9700	C16—H16A	0.9400
C6—C1—C2	118.13 (12)	C9—C8—C1	119.33 (12)

C6—C1—C8	123.33 (12)	C10—C9—C8	120.56 (14)
C2—C1—C8	118.53 (13)	C10—C9—H9A	119.7
C3—C2—C1	120.72 (13)	C8—C9—H9A	119.7
C3—C2—H2A	119.6	C9—C10—C11	128.09 (14)
C1—C2—H2A	119.6	C9—C10—H10A	116.0
C2—C3—C4	121.46 (13)	C11—C10—H10A	116.0
C2—C3—H3A	119.3	C16—C11—C12	117.75 (13)
C4—C3—H3A	119.3	C16—C11—C10	119.28 (13)
C5—C4—C3	117.35 (13)	C12—C11—C10	122.92 (12)
C5—C4—C7	121.40 (14)	C13—C12—C11	121.31 (13)
C3—C4—C7	121.24 (14)	C13—C12—H12A	119.3
C6—C5—C4	121.78 (14)	C11—C12—H12A	119.3
C6—C5—H5A	119.1	C14—C13—C12	118.14 (14)
C4—C5—H5A	119.1	C14—C13—H13A	120.9
C5—C6—C1	120.55 (13)	C12—C13—H13A	120.9
C5—C6—H6A	119.7	F1—C14—C15	118.83 (13)
C1—C6—H6A	119.7	F1—C14—C13	118.27 (14)
C4—C7—H7A	109.5	C15—C14—C13	122.90 (14)
C4—C7—H7B	109.5	C14—C15—C16	117.83 (14)
H7A—C7—H7B	109.5	C14—C15—H15A	121.1
C4—C7—H7C	109.5	C16—C15—H15A	121.1
H7A—C7—H7C	109.5	C15—C16—C11	122.06 (14)
H7B—C7—H7C	109.5	C15—C16—H16A	119.0
O1—C8—C9	120.57 (12)	C11—C16—H16A	119.0
O1—C8—C1	120.07 (12)		

C6—C1—C2—C3	0.52 (19)	C1—C8—C9—C10	159.24 (13)
C8—C1—C2—C3	179.32 (12)	C8—C9—C10—C11	178.29 (12)
C1—C2—C3—C4	0.4 (2)	C9—C10—C11—C16	169.98 (15)
C2—C3—C4—C5	−1.3 (2)	C9—C10—C11—C12	−12.7 (2)
C2—C3—C4—C7	178.75 (14)	C16—C11—C12—C13	0.2 (2)
C3—C4—C5—C6	1.2 (2)	C10—C11—C12—C13	−177.13 (13)
C7—C4—C5—C6	−178.76 (14)	C11—C12—C13—C14	0.1 (2)
C4—C5—C6—C1	−0.4 (2)	C12—C13—C14—F1	179.15 (12)
C2—C1—C6—C5	−0.5 (2)	C12—C13—C14—C15	−0.9 (2)
C8—C1—C6—C5	−179.28 (13)	F1—C14—C15—C16	−178.74 (12)
C6—C1—C8—O1	−168.27 (14)	C13—C14—C15—C16	1.3 (2)
C2—C1—C8—O1	12.99 (19)	C14—C15—C16—C11	−0.9 (2)
C6—C1—C8—C9	13.7 (2)	C12—C11—C16—C15	0.2 (2)
C2—C1—C8—C9	−165.02 (12)	C10—C11—C16—C15	177.66 (13)
O1—C8—C9—C10	−18.8 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···O1^{i}	0.94	2.53	3.3598 (17)	148

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1

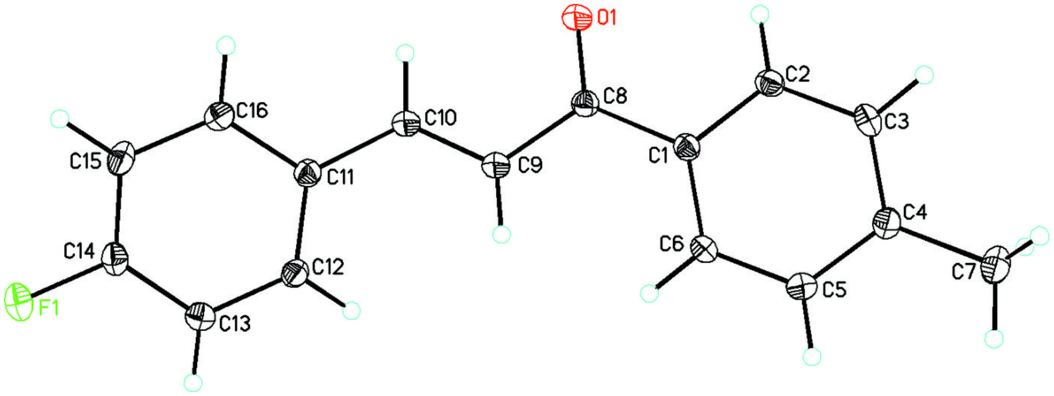

Fig. 2