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

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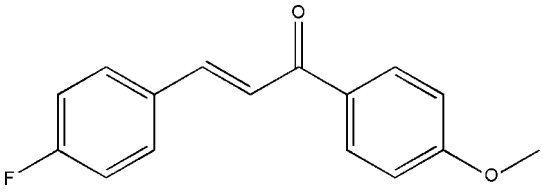
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.116; data-to-parameter ratio = 17.6.

The title compound, $C_{16}H_{13}FO_2$, was prepared from 4-methoxyhypnone and 4-fluorobenzophenone by Claisen–Schmidt condensation. All the bond lengths and bond angles are in normal ranges. The dihedral angle formed by the two benzene rings is 33.49 (2)°. The crystal packing is stabilized by intermolecular C—H···O hydrogen-bonding interactions.

Related literature

For the biological activity of chalcones, see: Hsieh *et al.* (1998); Anto *et al.* (1994). For the effectiveness of chalcones against cancer, see: De Vincenzo *et al.* (2000); Dimmock *et al.* (1998). For a related structure, see: Guo *et al.* (2008).



Experimental

Crystal data

$C_{16}H_{13}FO_2$
M_r = 256.26
Orthorhombic, *Pbca*
a = 7.457 (4) Å
b = 11.072 (6) Å
c = 31.063 (18) Å
V = 2565 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 273 K
0.13 × 0.12 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
14904 measured reflections
3050 independent reflections
2203 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.01
3050 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···O2^{i}	0.93	2.50	3.376 (2)	158

Symmetry code: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2773).

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supporting information

Acta Cryst. (2009). E**65**, o1402 [doi:10.1107/S1600536809018121]

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

Pu-Su Zhao, Xian Wang, Huan-Mei Guo and Fang-Fang Jian

S1. Comment

Among flavonoids, chalcones have been identified as interesting compounds having multiple biological actions which include antiinflammatory (Hsieh *et al.*, 1998) and antioxidant (Anto *et al.*, 1994). Of particular interest, the effectiveness of chalcones againist cancer has been investigated (De Vincenzo *et al.*, 2000; Dimmock *et al.*, 1998). As part of our search for new biologically active compounds we synthesized the title compound (I) and report its crystal structure here.

In the crystal structure of compound (I) (Fig. 1), the dihedral angle formed by the benzene rings (C1–C6) and (C7–C12) is 33.49 (2)°. All the bond lengths and bond angles are in normal ranges. (Guo *et al.*, 2008). There are intra- and intermolecular C—H···O hydrogen-bond interactions to stabilize the crystal structure (Table 1, Fig. 2).

S2. Experimental

A mixture of the 4-methoxyhypnone (0.02 mol), 4-fluorobenzophenone (0.02 mol) and 10% NaOH (10 ml) was stirred in ethanol (30 ml) for 3 h to afford the title compound (yield 83%). Single crystals suitable for X-ray measurements were obtailed by recrystallization from ethanol at room temperature.

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.96 Å, respectively, and with U_{iso}(H) = 1.2 or 1.5U_{eq} of the parent atoms.

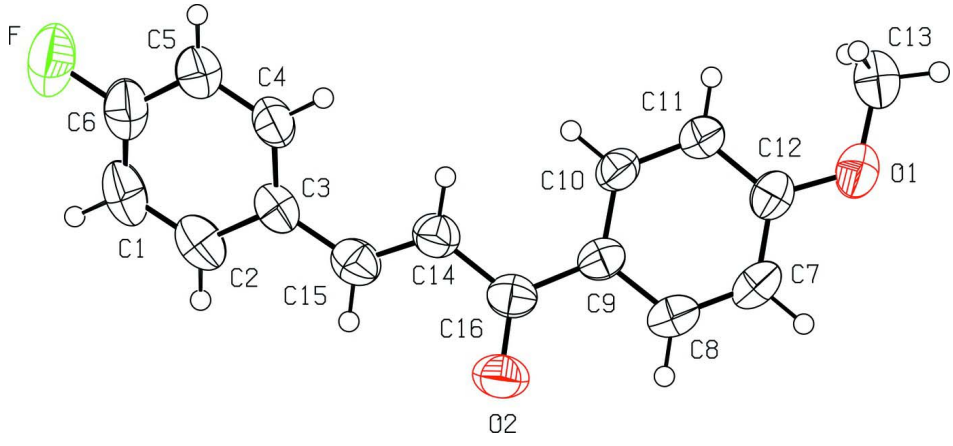

Figure 1

The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

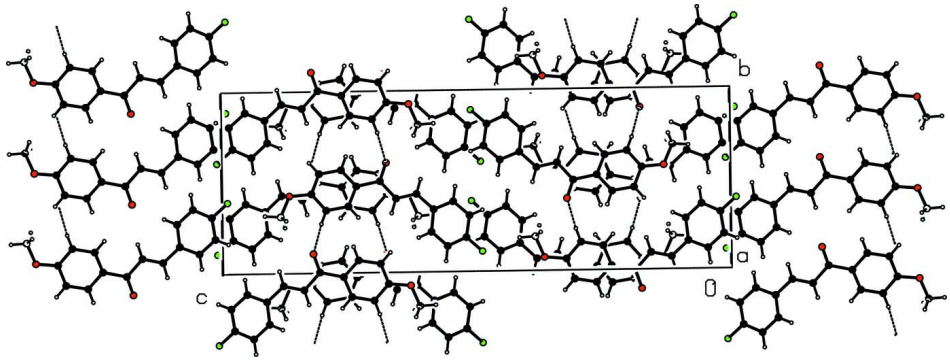

Figure 2

The packing and the hydrogen bonding interactions of (I),viewed down a axis.

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

Crystal data

$C_{16}H_{13}FO_2$
$M_r = 256.26$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 7.457$ (4) Å
$b = 11.072$ (6) Å
$c = 31.063$ (18) Å
$V = 2565$ (3) Å^3
$Z = 8$
$F(000) = 1072$
$D_x = 1.327$ Mg m^{-3}
$D_m = 1.327$ Mg m^{-3}
D_m measured by not measured
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4576 reflections
$\theta = 2.6$–$27.2°$
$\mu = 0.10$ mm^{-1}
$T = 273$ K
Bar, yellow
0.13 × 0.12 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
14904 measured reflections
3050 independent reflections
2203 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 28.1°$, $\theta_{min} = 2.6°$
$h = -8 \rightarrow 9$
$k = -14 \rightarrow 14$
$l = -31 \rightarrow 40$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.116$
$S = 1.01$
3050 reflections
173 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.3952P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0151 (14)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.19197 (16)	0.39463 (9)	0.32285 (3)	0.0679 (3)
O1	0.09858 (15)	0.57395 (10)	0.13185 (3)	0.0674 (3)
C16	0.15026 (17)	0.49647 (12)	0.31027 (4)	0.0497 (3)
C9	0.13654 (16)	0.52293 (11)	0.26375 (4)	0.0447 (3)
C15	0.06589 (19)	0.56911 (13)	0.38189 (5)	0.0567 (4)
H15A	0.0689	0.4883	0.3900	0.068*
C10	0.07845 (18)	0.63325 (11)	0.24765 (4)	0.0484 (3)
H10A	0.0485	0.6945	0.2668	0.058*
C12	0.10839 (18)	0.56345 (12)	0.17528 (4)	0.0504 (3)
F	−0.15021 (16)	0.89082 (12)	0.50973 (3)	0.1015 (4)
C14	0.10856 (19)	0.59300 (12)	0.34157 (4)	0.0535 (3)
H14A	0.1125	0.6731	0.3326	0.064*
C11	0.06382 (18)	0.65460 (12)	0.20395 (4)	0.0498 (3)
H11A	0.0246	0.7292	0.1939	0.060*
C4	0.0339 (2)	0.77956 (13)	0.41030 (4)	0.0578 (4)
H4A	0.0854	0.8098	0.3852	0.069*
C8	0.17978 (19)	0.43239 (12)	0.23404 (5)	0.0550 (4)
H8A	0.2185	0.3575	0.2439	0.066*
C7	0.1660 (2)	0.45230 (13)	0.19088 (5)	0.0600 (4)
H7A	0.1953	0.3910	0.1717	0.072*
C3	0.01471 (18)	0.65509 (13)	0.41510 (4)	0.0533 (3)
C5	−0.0214 (2)	0.85891 (16)	0.44174 (5)	0.0668 (4)
H5A	−0.0084	0.9418	0.4381	0.080*
C6	−0.0961 (2)	0.81261 (18)	0.47852 (5)	0.0702 (4)
C2	−0.0617 (2)	0.61339 (16)	0.45340 (5)	0.0682 (4)
H2A	−0.0753	0.5307	0.4576	0.082*
C13	0.0497 (2)	0.68788 (15)	0.11415 (5)	0.0679 (4)
H13A	0.0469	0.6822	0.0833	0.102*
H13B	0.1360	0.7477	0.1226	0.102*
H13C	−0.0667	0.7106	0.1246	0.102*
C1	−0.1175 (2)	0.69190 (19)	0.48511 (5)	0.0755 (5)
H1A	−0.1686	0.6631	0.5104	0.091*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0827 (8)	0.0466 (6)	0.0744 (7)	0.0011 (5)	−0.0083 (6)	0.0087 (5)
O1	0.0825 (8)	0.0703 (7)	0.0494 (6)	0.0061 (6)	−0.0002 (5)	−0.0128 (5)
C16	0.0457 (7)	0.0435 (7)	0.0600 (8)	−0.0068 (5)	−0.0021 (6)	0.0038 (6)
C9	0.0386 (6)	0.0389 (6)	0.0567 (7)	−0.0051 (5)	0.0001 (5)	−0.0038 (5)
C15	0.0590 (8)	0.0532 (8)	0.0578 (8)	−0.0064 (6)	−0.0015 (6)	0.0086 (6)
C10	0.0546 (7)	0.0400 (6)	0.0504 (7)	−0.0005 (5)	0.0041 (6)	−0.0071 (5)
C12	0.0474 (7)	0.0532 (8)	0.0508 (7)	−0.0031 (6)	0.0009 (6)	−0.0102 (6)
F	0.1113 (9)	0.1308 (10)	0.0624 (6)	0.0123 (7)	0.0144 (6)	−0.0209 (6)
C14	0.0613 (8)	0.0466 (7)	0.0525 (8)	−0.0033 (6)	−0.0038 (6)	0.0037 (6)
C11	0.0551 (8)	0.0425 (7)	0.0516 (7)	0.0011 (6)	0.0011 (6)	−0.0035 (5)
C4	0.0687 (9)	0.0642 (9)	0.0407 (7)	−0.0032 (7)	−0.0014 (6)	0.0075 (6)
C8	0.0549 (8)	0.0407 (7)	0.0693 (9)	0.0032 (6)	−0.0018 (6)	−0.0069 (6)
C7	0.0638 (9)	0.0497 (8)	0.0665 (9)	0.0064 (6)	0.0020 (7)	−0.0202 (7)
C3	0.0531 (7)	0.0624 (9)	0.0443 (7)	−0.0044 (6)	−0.0045 (6)	0.0098 (6)
C5	0.0815 (11)	0.0689 (10)	0.0501 (8)	0.0018 (8)	−0.0055 (7)	0.0013 (7)
C6	0.0671 (10)	0.0968 (13)	0.0467 (8)	0.0076 (9)	−0.0016 (7)	−0.0049 (8)
C2	0.0699 (10)	0.0777 (10)	0.0571 (9)	−0.0075 (8)	0.0018 (7)	0.0184 (8)
C13	0.0723 (10)	0.0804 (11)	0.0508 (8)	−0.0039 (8)	0.0007 (7)	−0.0011 (7)
C1	0.0704 (10)	0.1107 (15)	0.0454 (8)	−0.0035 (10)	0.0081 (7)	0.0135 (9)

Geometric parameters (Å, º)

O2—C16	1.2334 (17)	C4—C5	1.377 (2)
O1—C12	1.3561 (18)	C4—C3	1.394 (2)
O1—C13	1.424 (2)	C4—H4A	0.9300
C16—C9	1.478 (2)	C8—C7	1.363 (2)
C16—C14	1.478 (2)	C8—H8A	0.9300
C9—C10	1.3892 (19)	C7—H7A	0.9300
C9—C8	1.4002 (19)	C3—C2	1.398 (2)
C15—C14	1.319 (2)	C5—C6	1.371 (2)
C15—C3	1.455 (2)	C5—H5A	0.9300
C15—H15A	0.9300	C6—C1	1.362 (3)
C10—C11	1.382 (2)	C2—C1	1.378 (3)
C10—H10A	0.9300	C2—H2A	0.9300
C12—C11	1.3864 (19)	C13—H13A	0.9600
C12—C7	1.391 (2)	C13—H13B	0.9600
F—C6	1.361 (2)	C13—H13C	0.9600
C14—H14A	0.9300	C1—H1A	0.9300
C11—H11A	0.9300		
C12—O1—C13	118.30 (11)	C7—C8—H8A	119.5
O2—C16—C9	120.57 (12)	C9—C8—H8A	119.5
O2—C16—C14	120.38 (13)	C8—C7—C12	120.62 (12)
C9—C16—C14	119.03 (12)	C8—C7—H7A	119.7
C10—C9—C8	117.65 (13)	C12—C7—H7A	119.7

C10—C9—C16	123.23 (12)	C4—C3—C2	117.37 (14)
C8—C9—C16	119.11 (12)	C4—C3—C15	122.98 (12)
C14—C15—C3	127.26 (14)	C2—C3—C15	119.63 (14)
C14—C15—H15A	116.4	C6—C5—C4	118.32 (16)
C3—C15—H15A	116.4	C6—C5—H5A	120.8
C11—C10—C9	121.91 (12)	C4—C5—H5A	120.8
C11—C10—H10A	119.0	F—C6—C1	118.87 (15)
C9—C10—H10A	119.0	F—C6—C5	118.44 (18)
O1—C12—C11	124.31 (13)	C1—C6—C5	122.70 (16)
O1—C12—C7	116.05 (12)	C1—C2—C3	121.55 (16)
C11—C12—C7	119.64 (13)	C1—C2—H2A	119.2
C15—C14—C16	122.03 (13)	C3—C2—H2A	119.2
C15—C14—H14A	119.0	O1—C13—H13A	109.5
C16—C14—H14A	119.0	O1—C13—H13B	109.5
C10—C11—C12	119.17 (13)	H13A—C13—H13B	109.5
C10—C11—H11A	120.4	O1—C13—H13C	109.5
C12—C11—H11A	120.4	H13A—C13—H13C	109.5
C5—C4—C3	121.62 (14)	H13B—C13—H13C	109.5
C5—C4—H4A	119.2	C6—C1—C2	118.45 (15)
C3—C4—H4A	119.2	C6—C1—H1A	120.8
C7—C8—C9	121.01 (13)	C2—C1—H1A	120.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···O2^{i}	0.93	2.50	3.376 (2)	158
C15—H15*A*···O2	0.93	2.50	2.825 (2)	101

Symmetry code: (i) −*x*, *y*+1/2, −*z*+1/2.