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

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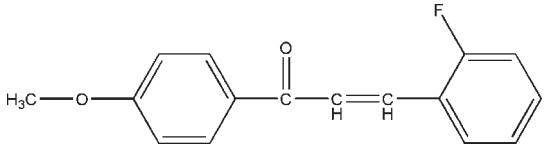
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.117; data-to-parameter ratio = 18.3.

The title compound, $C_{16}H_{13}FO_2$, was prepared from 4-methoxyhypnone and 2-fluorobenzophenone by a Claisen–Schmidt condensation reaction. The dihedral angle between the two benzene rings is 31.99 (2)°. In the crystal structure, molecules are linked by weak intermolecular C—H···O hydrogen bonds along [010].

Related literature

For the biological activity of chalcones, see: Hsieh *et al.* (1998); Anto *et al.* (1994); De Vincenzo *et al.* (2000); Dimmock *et al.* (1998). For related structures, see: Fun *et al.* (2008); Zhao *et al.* (2009).



Experimental

Crystal data

$C_{16}H_{13}FO_2$
M_r = 256.26
Orthorhombic, *Pbca*
a = 7.4511 (6) Å
b = 11.0541 (8) Å
c = 31.031 (3) Å
V = 2555.9 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
15509 measured reflections
3162 independent reflections
2162 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
S = 1.05
3162 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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	2.51	3.3679 (18)	153

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: LH2941).

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supplementary materials

Acta Cryst. (2009). E**65**, o3013 [**doi:10.1107/S1600536809045759**]

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

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Comment

Chalcones have been identified as interesting compounds having multiple biological activities which include antiinflammatory (Hsieh *et al.*,1998) and antioxidant (Anto *et al.*,1994). The effectiveness of chalcone compounds against 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 herein.

The molecular structure of (I) is shown in Fig.1. The dihedral angle between the two benzene rings (C1—C6 and C7—C12) is 31.99 (2)°. The bond lengths and bond angles are within normal ranges and comparable to those in a related structures (Fun *et al.*, 2008; Zhao *et al.*, 2009). In the crystal structure, molecules are linked by weak intermolecular C-H···O hydrogen bonds into one-dimensional chains along [010] (Fig. 2).

Experimental

A mixture of 4-methoxyhypnone (0.02 mol) and 2-fluorobenzophenone (0.02 mol) and 10% NaOH (10ml) was stirred in ethanol (30 ml) for 2 h to afford the title compound (yield 85%). Single crystals suitable for X-ray measurements were obtailed by recrystallization of an ethyl acetate solution of the title compound at room temperature.

Refinement

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

Figures

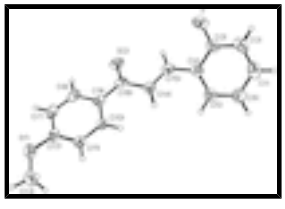

Fig. 1. The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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

Crystal data

$C_{16}H_{13}FO_2$	F_{000} = 1072
M_r = 256.26	D_x = 1.332 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation, λ = 0.71073 Å

Hall symbol: -P 2ac 2ab	Cell parameters from 2162 reflections
a = 7.4511 (6) Å	θ = 2.6–28.4º
b = 11.0541 (8) Å	μ = 0.10 mm^{-1}
c = 31.031 (3) Å	T = 298 K
V = 2555.9 (3) $Å^3$	Bar, yellow
Z = 8	0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer	2162 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.026
Monochromator: graphite	θ_{max} = 28.4º
T = 298 K	θ_{min} = 2.6º
φ and ω scans	$h = -8 \rightarrow 9$
Absorption correction: none	$k = -13 \rightarrow 14$
15509 measured reflections	$l = -39 \rightarrow 36$
3162 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.042	$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.3713P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.117	$(\Delta/\sigma)_{max} < 0.001$
S = 1.05	$\Delta\rho_{max}$ = 0.16 e $Å^{-3}$
3162 reflections	$\Delta\rho_{min}$ = −0.19 e $Å^{-3}$
173 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0083 (9)
Secondary atom site location: difference Fourier map	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C9	0.14251 (16)	0.07378 (11)	0.24089 (4)	0.0474 (3)
C16	0.16025 (17)	0.04544 (11)	0.19449 (5)	0.0530 (3)
O2	0.20708 (16)	−0.05586 (9)	0.18272 (3)	0.0723 (3)
C11	0.06705 (19)	0.20676 (12)	0.30007 (4)	0.0539 (3)
H11A	0.0271	0.2817	0.3097	0.065*
C10	0.08333 (18)	0.18431 (11)	0.25647 (4)	0.0507 (3)
H10A	0.0537	0.2451	0.2370	0.061*
C12	0.11063 (18)	0.11693 (12)	0.32916 (4)	0.0548 (3)
C15	0.0866 (2)	0.11137 (13)	0.12171 (5)	0.0598 (4)
H15A	0.1029	0.0307	0.1142	0.072*
C14	0.11574 (19)	0.13923 (12)	0.16225 (5)	0.0565 (4)
H14A	0.1082	0.2197	0.1709	0.068*
O1	0.09938 (16)	0.12870 (10)	0.37267 (3)	0.0747 (3)
C4	0.03134 (19)	0.19281 (13)	0.08723 (4)	0.0567 (4)
C8	0.1842 (2)	−0.01562 (12)	0.27107 (5)	0.0597 (4)
H8A	0.2232	−0.0909	0.2616	0.072*
F	−0.04947 (18)	0.02464 (10)	0.04543 (3)	0.1056 (4)
C7	0.1688 (2)	0.00549 (13)	0.31425 (5)	0.0656 (4)
H7A	0.1975	−0.0553	0.3338	0.079*
C5	0.0374 (2)	0.31898 (13)	0.09031 (5)	0.0638 (4)
H5A	0.0862	0.3546	0.1148	0.077*
C3	−0.0402 (2)	0.14689 (15)	0.04940 (5)	0.0698 (4)
C6	−0.0271 (3)	0.39113 (16)	0.05794 (5)	0.0783 (5)
H6A	−0.0227	0.4748	0.0608	0.094*
C13	0.0495 (2)	0.24277 (16)	0.39010 (5)	0.0743 (5)
H13A	0.0465	0.2376	0.4210	0.112*
H13B	−0.0671	0.2649	0.3796	0.112*
H13C	0.1354	0.3028	0.3815	0.112*
C2	−0.1052 (3)	0.21693 (19)	0.01653 (5)	0.0822 (5)
H2A	−0.1525	0.1818	−0.0082	0.099*
C1	−0.0987 (3)	0.3404 (2)	0.02105 (5)	0.0849 (5)
H1A	−0.1426	0.3900	−0.0008	0.102*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C9	0.0380 (6)	0.0385 (6)	0.0657 (8)	−0.0049 (5)	−0.0016 (5)	0.0041 (5)
C16	0.0447 (7)	0.0411 (7)	0.0731 (9)	−0.0071 (5)	0.0028 (6)	−0.0035 (6)
O2	0.0834 (8)	0.0458 (6)	0.0876 (8)	0.0051 (5)	0.0089 (6)	−0.0080 (5)
C11	0.0565 (8)	0.0436 (7)	0.0616 (8)	−0.0001 (6)	−0.0029 (6)	0.0026 (6)
C10	0.0531 (8)	0.0393 (6)	0.0597 (8)	−0.0011 (6)	−0.0050 (6)	0.0066 (5)
C12	0.0481 (7)	0.0579 (8)	0.0585 (8)	−0.0039 (6)	−0.0017 (6)	0.0110 (6)
C15	0.0627 (9)	0.0495 (7)	0.0672 (9)	−0.0063 (7)	0.0071 (7)	−0.0087 (6)
C14	0.0617 (9)	0.0461 (7)	0.0616 (8)	−0.0032 (6)	0.0036 (6)	−0.0055 (6)

O1	0.0864 (8)	0.0769 (7)	0.0608 (7)	0.0062 (6)	−0.0007 (5)	0.0141 (5)
C4	0.0545 (8)	0.0621 (8)	0.0535 (8)	−0.0062 (7)	0.0087 (6)	−0.0085 (6)
C8	0.0562 (8)	0.0419 (7)	0.0809 (10)	0.0065 (6)	0.0026 (7)	0.0073 (6)
F	0.1581 (12)	0.0820 (7)	0.0768 (7)	−0.0307 (7)	−0.0027 (6)	−0.0256 (5)
C7	0.0654 (9)	0.0541 (8)	0.0773 (10)	0.0088 (7)	−0.0005 (8)	0.0223 (7)
C5	0.0702 (10)	0.0624 (9)	0.0587 (8)	−0.0028 (8)	0.0039 (7)	−0.0065 (7)
C3	0.0782 (11)	0.0721 (10)	0.0592 (9)	−0.0144 (8)	0.0106 (8)	−0.0159 (8)
C6	0.0958 (13)	0.0692 (10)	0.0698 (10)	0.0077 (9)	0.0080 (9)	0.0008 (8)
C13	0.0755 (11)	0.0871 (12)	0.0604 (9)	−0.0049 (9)	−0.0012 (8)	0.0005 (8)
C2	0.0839 (12)	0.1103 (15)	0.0525 (9)	−0.0108 (11)	0.0016 (8)	−0.0104 (9)
C1	0.0877 (13)	0.1064 (15)	0.0607 (10)	0.0128 (11)	0.0051 (9)	0.0075 (10)

Geometric parameters (Å, °)

C9—C10	1.3859 (18)	C4—C5	1.399 (2)
C9—C8	1.3964 (18)	C8—C7	1.365 (2)
C9—C16	1.4794 (19)	C8—H8A	0.9300
C16—O2	1.2285 (15)	F—C3	1.3587 (19)
C16—C14	1.478 (2)	C7—H7A	0.9300
C11—C12	1.3807 (18)	C5—C6	1.370 (2)
C11—C10	1.3808 (19)	C5—H5A	0.9300
C11—H11A	0.9300	C3—C2	1.369 (2)
C10—H10A	0.9300	C6—C1	1.382 (2)
C12—O1	1.3591 (17)	C6—H6A	0.9300
C12—C7	1.385 (2)	C13—H13A	0.9600
C15—C14	1.3134 (19)	C13—H13B	0.9600
C15—C4	1.457 (2)	C13—H13C	0.9600
C15—H15A	0.9300	C2—C1	1.373 (3)
C14—H14A	0.9300	C2—H2A	0.9300
O1—C13	1.421 (2)	C1—H1A	0.9300
C4—C3	1.386 (2)		
C10—C9—C8	117.44 (13)	C7—C8—H8A	119.4
C10—C9—C16	123.68 (12)	C9—C8—H8A	119.4
C8—C9—C16	118.87 (12)	C8—C7—C12	120.40 (13)
O2—C16—C14	120.11 (13)	C8—C7—H7A	119.8
O2—C16—C9	120.52 (13)	C12—C7—H7A	119.8
C14—C16—C9	119.34 (11)	C6—C5—C4	121.29 (15)
C12—C11—C10	119.38 (13)	C6—C5—H5A	119.4
C12—C11—H11A	120.3	C4—C5—H5A	119.4
C10—C11—H11A	120.3	F—C3—C2	118.48 (15)
C11—C10—C9	121.88 (12)	F—C3—C4	117.44 (15)
C11—C10—H10A	119.1	C2—C3—C4	124.06 (16)
C9—C10—H10A	119.1	C5—C6—C1	120.44 (17)
O1—C12—C11	124.49 (13)	C5—C6—H6A	119.8
O1—C12—C7	115.86 (12)	C1—C6—H6A	119.8
C11—C12—C7	119.65 (13)	O1—C13—H13A	109.5
C14—C15—C4	127.23 (13)	O1—C13—H13B	109.5
C14—C15—H15A	116.4	H13A—C13—H13B	109.5
C4—C15—H15A	116.4	O1—C13—H13C	109.5

C15—C14—C16	121.39 (13)	H13A—C13—H13C	109.5
C15—C14—H14A	119.3	H13B—C13—H13C	109.5
C16—C14—H14A	119.3	C3—C2—C1	118.28 (16)
C12—O1—C13	118.62 (12)	C3—C2—H2A	120.9
C3—C4—C5	115.82 (14)	C1—C2—H2A	120.9
C3—C4—C15	120.28 (14)	C2—C1—C6	120.11 (17)
C5—C4—C15	123.83 (13)	C2—C1—H1A	119.9
C7—C8—C9	121.24 (13)	C6—C1—H1A	119.9

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11A···O2^{i}	0.93	2.51	3.3679 (18)	153

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

Fig. 1