Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(3,4-Dimethoxyphenyl)(4-fluorophenyl)-methanone

Quanjian Lv* and Jianling Wang

Department of Quality Detection and Management, Zhengzhou College of Animal Husbandry Engineering, Zhengzhou 450011, People's Republic of China
Correspondence e-mail: jyzhang2004@126.com

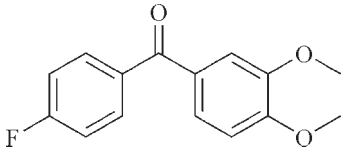
Received 22 May 2010; accepted 2 June 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.173; data-to-parameter ratio = 12.8.

In the title compound, $C_{15}H_{13}FO_3$, the dihedral angle between the two aromatic rings is 52.78 (8)°. In the crystal, intermolecular C—H···O hydrogen bonds link molecules into chains running parallel to the c axis.

Related literature

For applications of benzophenone and its derivatives, see: Riechers *et al.* (1996); Khanum *et al.* (2009); Schlecht *et al.* (2008).



Experimental

Crystal data

$C_{15}H_{13}FO_3$
M_r = 260.25
Monoclinic, $P2_1/c$
a = 10.8926 (9) Å
b = 11.3632 (11) Å
c = 10.8369 (10) Å
β = 108.285 (1)°
V = 1273.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.48 × 0.38 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.952, T_{max} = 0.985
6183 measured reflections
2227 independent reflections
1391 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.173
S = 1.00
2227 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.93	2.58	3.343 (3)	139

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

We gratefully acknowledge financial support from the National Natural Science Foundation of China (No. 20572103).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2456).

References

Khanum, S. A., Girish, V., Suparshwa, S. S., Khanum, N. F. (2009). *Bioorg. Med. Chem. Lett.* **19**, 1887–1891.
Riechers, H., Albrecht, H.-P. & Amberg, W. (1996). *J. Med. Chem.* **39**, 2123–2128..
Schlecht, C., Klammer, H., Frauendorf, H., Wuttke, W. & Jarry, H. (2008). *Toxicology*, **245**, 11–17.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supporting information

Acta Cryst. (2010). E**66**, o1585 [doi:10.1107/S1600536810021008]

(3,4-Dimethoxyphenyl)(4-fluorophenyl)methanone

Quanjian Lv and Jianling Wang

S1. Comment

Benzophenone derivatives are an important class of compounds having a broad spectrum of applications in the chemical and biochemical fields (Riechers *et al.*, 1996; Khanum *et al.*, 2009), and are widely used as UV-screens to protect industrial products from light induced damage (Schlecht *et al.*, 2008). In order to develop new applications for benzophenone and its derivatives, structural modifications of benzophenone have been extensively investigated. As a contribution to this field, we report here the crystal structure of the title compound.

The molecular structure of title compound is shown in Fig. 1. The dihedral angle formed by the benzene rings 52.78 (8)°. In the crystal packing (Fig. 2), intermolecular C—H···O hydrogen bonds (Table 1) link molecules into chains running parallel to the *c* axis.

S2. Experimental

To a solution of 1,2-dimethoxybenzene (138 g, 1.00 mol) in dichloromethane (2.00 l), $AlCl_3$ (199 g, 1.50 mol) was added. Then 4-fluorobenzoyl chloride (158 g, 2.00 mol) was added. The mixture was stirred at room temperature for 2 h, followed by filtration and purification by crystallization from ethyl acetate, giving the title compound as a colourless crystalline solid.

S3. Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms, with C—H = 0.93-0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms.

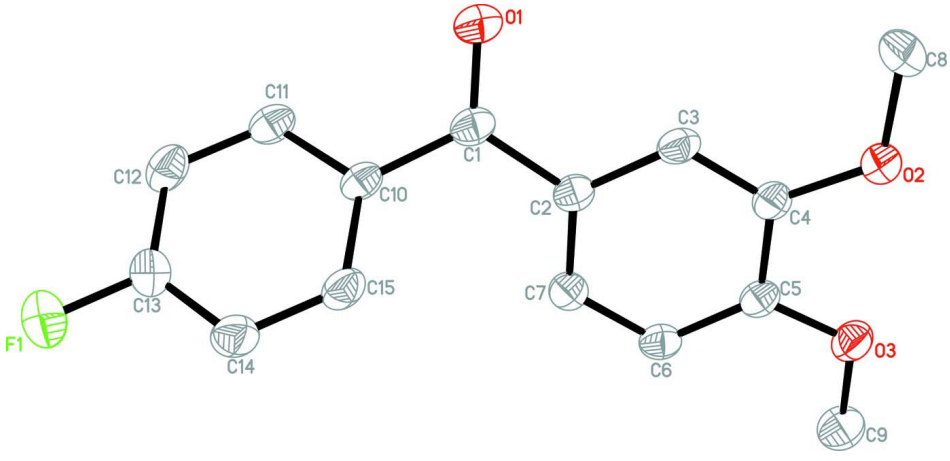


Figure 1

The molecular structure of the compound, with atom labels and 50% probability displacement ellipsoids. Hydrogen atoms are omitted.

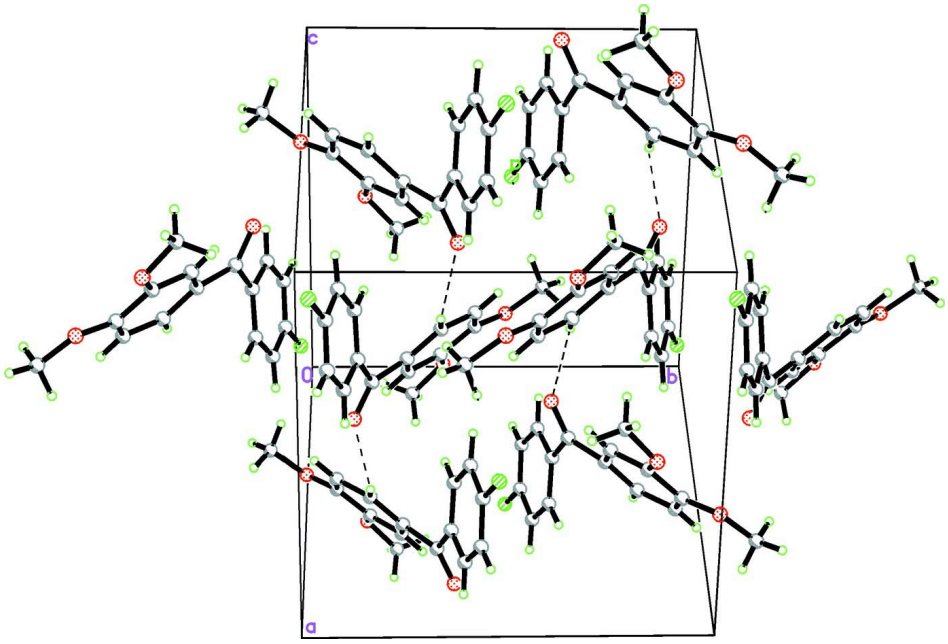


Figure 2

Crystal packing of the title compound. Intermolecular hydrogen bonds are shown as dashed lines.

(3,4-Dimethoxyphenyl)(4-fluorophenyl)methanone

Crystal data

$C_{15}H_{13}FO_3$
$M_r = 260.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.8926\ (9)$ Å
$b = 11.3632\ (11)$ Å
$c = 10.8369\ (10)$ Å
$\beta = 108.285\ (1)°$
$V = 1273.6\ (2)$ Å^3
$Z = 4$
$F(000) = 544$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1872 reflections
$\theta = 2.7–26.1°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Needle, colourless
0.48 × 0.38 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.952$, $T_{max} = 0.985$
6183 measured reflections
2227 independent reflections
1391 reflections with $I > 2\sigma(I)$
$R_{int} = 0.083$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -7\rightarrow12$
$k = -13\rightarrow13$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.173$
$S = 1.00$
2227 reflections
174 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0915P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.20$ e Å^{-3}
	$\Delta\rho_{min} = -0.32$ e Å^{-3}

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}
F1	0.13858 (16)	0.52452 (18)	−0.33034 (17)	0.0864 (7)
O1	0.46324 (18)	0.62209 (18)	0.24672 (19)	0.0638 (6)
O2	0.88706 (15)	0.85244 (17)	0.40525 (17)	0.0555 (6)
O3	0.86314 (15)	1.01546 (15)	0.23481 (17)	0.0512 (5)
C1	0.4782 (2)	0.6672 (2)	0.1495 (3)	0.0433 (6)
C2	0.5825 (2)	0.7552 (2)	0.1622 (2)	0.0384 (6)
C3	0.6868 (2)	0.7580 (2)	0.2777 (2)	0.0420 (6)
H3	0.6928	0.7015	0.3414	0.050*
C4	0.7801 (2)	0.8432 (2)	0.2976 (2)	0.0405 (6)
C5	0.7682 (2)	0.9316 (2)	0.2037 (2)	0.0392 (6)
C6	0.6666 (2)	0.9291 (2)	0.0898 (2)	0.0416 (6)
H6	0.6597	0.9865	0.0269	0.050*
C7	0.5739 (2)	0.8405 (2)	0.0688 (2)	0.0399 (6)
H7	0.5057	0.8387	−0.0086	0.048*
C8	0.8996 (3)	0.7711 (3)	0.5078 (3)	0.0682 (9)
H8A	0.8272	0.7790	0.5397	0.102*
H8B	0.9782	0.7867	0.5768	0.102*
H8C	0.9020	0.6925	0.4761	0.102*
C9	0.8510 (3)	1.1108 (3)	0.1468 (3)	0.0664 (9)
H9A	0.8506	1.0811	0.0637	0.100*
H9B	0.9225	1.1637	0.1798	0.100*
H9C	0.7715	1.1519	0.1374	0.100*
C10	0.3889 (2)	0.6332 (2)	0.0193 (2)	0.0396 (6)
C11	0.2630 (2)	0.6010 (2)	0.0084 (3)	0.0475 (7)
H11	0.2355	0.6042	0.0813	0.057*
C12	0.1782 (3)	0.5644 (2)	−0.1084 (3)	0.0545 (7)
H12	0.0938	0.5431	−0.1154	0.065*
C13	0.2215 (3)	0.5604 (3)	−0.2141 (3)	0.0554 (8)
C14	0.3456 (3)	0.5881 (3)	−0.2083 (3)	0.0559 (8)
H14	0.3728	0.5816	−0.2812	0.067*

C15	0.4290 (2)	0.6260 (2)	−0.0911 (3)	0.0462 (7)
H15	0.5131	0.6470	−0.0854	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0788 (12)	0.1100 (15)	0.0628 (12)	−0.0321 (12)	0.0113 (9)	−0.0168 (10)
O1	0.0677 (13)	0.0799 (14)	0.0502 (12)	−0.0215 (11)	0.0274 (10)	0.0033 (10)
O2	0.0450 (11)	0.0706 (13)	0.0473 (11)	−0.0113 (9)	0.0094 (9)	0.0127 (9)
O3	0.0463 (11)	0.0513 (11)	0.0573 (12)	−0.0076 (9)	0.0183 (8)	0.0060 (9)
C1	0.0400 (14)	0.0476 (15)	0.0491 (16)	0.0021 (12)	0.0239 (12)	0.0029 (12)
C2	0.0338 (13)	0.0456 (14)	0.0422 (14)	0.0041 (11)	0.0210 (10)	−0.0028 (11)
C3	0.0398 (14)	0.0480 (15)	0.0446 (15)	0.0002 (12)	0.0223 (11)	0.0055 (12)
C4	0.0317 (13)	0.0504 (15)	0.0427 (15)	0.0043 (12)	0.0165 (11)	0.0016 (12)
C5	0.0366 (13)	0.0412 (14)	0.0457 (15)	0.0032 (12)	0.0215 (11)	−0.0022 (11)
C6	0.0440 (14)	0.0427 (14)	0.0433 (14)	0.0050 (12)	0.0210 (11)	0.0036 (11)
C7	0.0353 (13)	0.0463 (14)	0.0402 (14)	0.0060 (12)	0.0148 (10)	−0.0010 (11)
C8	0.0643 (19)	0.080 (2)	0.0492 (17)	−0.0084 (17)	0.0021 (14)	0.0185 (16)
C9	0.076 (2)	0.0543 (17)	0.069 (2)	−0.0170 (16)	0.0224 (16)	0.0105 (15)
C10	0.0358 (13)	0.0402 (14)	0.0490 (16)	−0.0007 (11)	0.0225 (11)	0.0006 (11)
C11	0.0426 (14)	0.0522 (16)	0.0568 (17)	−0.0010 (13)	0.0286 (12)	0.0019 (13)
C12	0.0389 (14)	0.0595 (18)	0.0688 (19)	−0.0084 (14)	0.0223 (13)	−0.0028 (15)
C13	0.0566 (17)	0.0554 (18)	0.0515 (17)	−0.0119 (15)	0.0132 (13)	−0.0072 (14)
C14	0.0630 (18)	0.0610 (18)	0.0541 (18)	−0.0105 (15)	0.0332 (14)	−0.0102 (14)
C15	0.0396 (14)	0.0513 (15)	0.0560 (17)	−0.0068 (13)	0.0267 (12)	−0.0057 (13)

Geometric parameters (Å, º)

F1—C13	1.362 (3)	C8—H8A	0.9600
O1—C1	1.227 (3)	C8—H8B	0.9600
O2—C4	1.370 (3)	C8—H8C	0.9600
O2—C8	1.419 (3)	C9—H9A	0.9600
O3—C5	1.368 (3)	C9—H9B	0.9600
O3—C9	1.422 (3)	C9—H9C	0.9600
C1—C2	1.488 (3)	C10—C11	1.388 (3)
C1—C10	1.493 (3)	C10—C15	1.399 (3)
C2—C7	1.383 (3)	C11—C12	1.377 (4)
C2—C3	1.402 (3)	C11—H11	0.9300
C3—C4	1.370 (3)	C12—C13	1.370 (4)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.407 (4)	C13—C14	1.370 (4)
C5—C6	1.376 (3)	C14—C15	1.378 (4)
C6—C7	1.393 (3)	C14—H14	0.9300
C6—H6	0.9300	C15—H15	0.9300
C7—H7	0.9300		
C4—O2—C8	117.6 (2)	H8A—C8—H8C	109.5
C5—O3—C9	117.5 (2)	H8B—C8—H8C	109.5

O1—C1—C2	120.3 (2)	O3—C9—H9A	109.5
O1—C1—C10	118.7 (2)	O3—C9—H9B	109.5
C2—C1—C10	120.9 (2)	H9A—C9—H9B	109.5
C7—C2—C3	119.2 (2)	O3—C9—H9C	109.5
C7—C2—C1	121.9 (2)	H9A—C9—H9C	109.5
C3—C2—C1	118.6 (2)	H9B—C9—H9C	109.5
C4—C3—C2	120.6 (2)	C11—C10—C15	118.5 (2)
C4—C3—H3	119.7	C11—C10—C1	118.8 (2)
C2—C3—H3	119.7	C15—C10—C1	122.6 (2)
C3—C4—O2	125.4 (2)	C12—C11—C10	121.2 (2)
C3—C4—C5	119.7 (2)	C12—C11—H11	119.4
O2—C4—C5	114.9 (2)	C10—C11—H11	119.4
O3—C5—C6	124.7 (2)	C13—C12—C11	118.1 (2)
O3—C5—C4	115.4 (2)	C13—C12—H12	121.0
C6—C5—C4	119.9 (2)	C11—C12—H12	121.0
C5—C6—C7	120.0 (2)	F1—C13—C12	118.7 (2)
C5—C6—H6	120.0	F1—C13—C14	118.0 (3)
C7—C6—H6	120.0	C12—C13—C14	123.2 (3)
C2—C7—C6	120.5 (2)	C13—C14—C15	118.0 (3)
C2—C7—H7	119.8	C13—C14—H14	121.0
C6—C7—H7	119.8	C15—C14—H14	121.0
O2—C8—H8A	109.5	C14—C15—C10	120.9 (2)
O2—C8—H8B	109.5	C14—C15—H15	119.5
H8A—C8—H8B	109.5	C10—C15—H15	119.5
O2—C8—H8C	109.5		

O1—C1—C2—C7	−153.7 (3)	C3—C2—C7—C6	−0.9 (3)
C10—C1—C2—C7	25.5 (3)	C1—C2—C7—C6	173.2 (2)
O1—C1—C2—C3	20.4 (3)	C5—C6—C7—C2	0.5 (3)
C10—C1—C2—C3	−160.4 (2)	O1—C1—C10—C11	30.4 (3)
C7—C2—C3—C4	−0.7 (4)	C2—C1—C10—C11	−148.8 (2)
C1—C2—C3—C4	−175.1 (2)	O1—C1—C10—C15	−145.9 (3)
C2—C3—C4—O2	−178.5 (2)	C2—C1—C10—C15	34.9 (3)
C2—C3—C4—C5	2.7 (4)	C15—C10—C11—C12	−1.0 (4)
C8—O2—C4—C3	−3.3 (4)	C1—C10—C11—C12	−177.4 (2)
C8—O2—C4—C5	175.4 (2)	C10—C11—C12—C13	0.2 (4)
C9—O3—C5—C6	4.3 (3)	C11—C12—C13—F1	−179.9 (2)
C9—O3—C5—C4	−176.1 (2)	C11—C12—C13—C14	1.6 (5)
C3—C4—C5—O3	177.30 (19)	F1—C13—C14—C15	179.1 (2)
O2—C4—C5—O3	−1.6 (3)	C12—C13—C14—C15	−2.4 (5)
C3—C4—C5—C6	−3.1 (4)	C13—C14—C15—C10	1.5 (4)
O2—C4—C5—C6	178.1 (2)	C11—C10—C15—C14	0.2 (4)
O3—C5—C6—C7	−179.0 (2)	C1—C10—C15—C14	176.5 (2)
C4—C5—C6—C7	1.4 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.93	2.58	3.343 (3)	139

Symmetry code: (i) *x*, −*y*+3/2, *z*−1/2.