

(4-Methoxyphenyl)(2-methylphenyl)methanone

M Mahendra,^a S. A. Khanum,^b
A. K. Singh,^b S. Shashikanth,^b
B. H. Doreswamy,^a
M. A. Sridhar^a and
J. Shashidhara Prasad^{a*}

^aDepartment of Studies in Physics,
Mansangotri, University of Mysore, Mysore
570 006, India, and ^bDepartment of Studies in
Chemistry, Mansangotri, University of
Mysore, Mysore 570 006, India

Correspondence e-mail:
mas@physics.uni-mysore.ac.in

In the title compound, C₁₅H₁₄O₂, the dihedral angle between the two benzene rings is 56.34 (7)°.

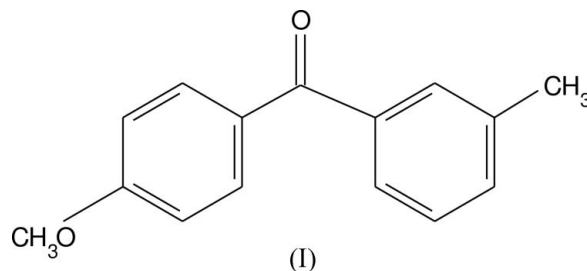
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Comment

Benzophenones play an important role in imparting anti-inflammatory (Khanum, Shashikanth *et al.*, 2004; Khanum, Venu *et al.*, 2004), anti-anaphylactic (Evans *et al.*, 1987), antimalarial (Wiesner *et al.*, 2001) and anticancer (Hsieh *et al.*, 2003) activities. The presence of different substituents on the benzophenone nucleus is crucial in determining the quantitative structure–activity relationships. Owing to the importance of various substituents on the nucleus, the title compound, (I), was synthesized and its crystal structure is reported here.



Key indicators

Single-crystal X-ray study

$T = 295\text{ K}$

Mean $\sigma(\text{C}–\text{C}) = 0.002\text{ \AA}$

R factor = 0.048

wR factor = 0.143

Data-to-parameter ratio = 13.5

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The molecule of (I) is non-planar (Fig. 1). The dihedral angle between the two benzene rings is 56.37 (3)°; this value is much smaller than the corresponding value of 75.2° observed in 3,4-dimethoxyphenyl(2-chlorophenyl)methanone [(II); Mahendra *et al.*, 2003]. Bond lengths and angles have normal values and are comparable with those reported for (II). The crystal packing is stabilized by intermolecular C15—H15A···O16ⁱ (symmetry code as in Table 2) hydrogen bonds, which link the molecules into chains (Fig. 2).

A detailed study of the biological activity of (I) is underway.

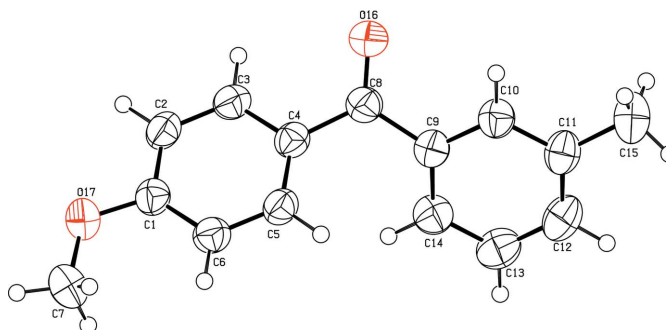


Figure 1
View of (I), with 50% probability displacement ellipsoids.

Experimental

To a mixture of anhydrous aluminium chloride (22 g, 9.2 mmol) in dry carbon disulfide (15 ml), 4-methoxy benzene (1 g, 9.2 mmol) and 3-methylbenzoic acid (1.25 g, 9.2 mmol) were added. The reaction mixture was protected from moisture by a calcium chloride guard tube and stirred for 30 min. At the end of this period, the solution was cooled and decomposed by acidified ice-cold water. The carbon disulfide was removed by distillation. The residual solid was crushed into a powder, extracted with diethyl ether (60 ml), and the ether layer was washed well with 10% sodium hydroxide solution (60 ml), followed by distilled water. Evaporation of the diethyl ether after drying over anhydrous sodium sulfate followed by recrystallization from ethyl alcohol gave the title compound (yield 85%; m.p. 329 K).

Crystal data

$C_{15}H_{14}O_2$	$D_x = 1.239 \text{ Mg m}^{-3}$
$M_r = 226.26$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4020 reflections
$a = 7.592 (4) \text{ \AA}$	$\theta = 2.3\text{--}25.0^\circ$
$b = 14.147 (7) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 11.342 (7) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 95.231 (2)^\circ$	Block, colourless
$V = 1213.1 (12) \text{ \AA}^3$	$0.3 \times 0.2 \times 0.2 \text{ mm}$
$Z = 4$	

Data collection

MacScience DIPLabo 32001 diffractometer	1882 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.019$
Absorption correction: none	$\theta_{\text{max}} = 25.0^\circ$
4020 measured reflections	$h = -9 \rightarrow 9$
2123 independent reflections	$k = -16 \rightarrow 16$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 0.1331P]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.143$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.19$	$\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$
2123 reflections	$\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$
157 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.22 (2)

Table 1

Selected geometric parameters (\AA , $^\circ$).

O17—C1	1.3593 (17)	C8—O16	1.2192 (18)
O17—C7	1.421 (2)	C8—C9	1.496 (2)
C4—C8	1.486 (2)		
C1—O17—C7	118.38 (12)	O17—C1—C2	115.50 (12)
O17—C1—C6	124.86 (13)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15—H15A \cdots O16 ⁱ	0.96	2.57	3.517 (3)	169

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

H atoms were placed at idealized positions and allowed to ride on their parent atoms, with C—H distances of 0.96 \AA and $U_{\text{iso}}(\text{H})$ values set equal to $xU_{\text{eq}}(\text{carrier atom})$, where $x = 1.5$ for methyl H atoms and

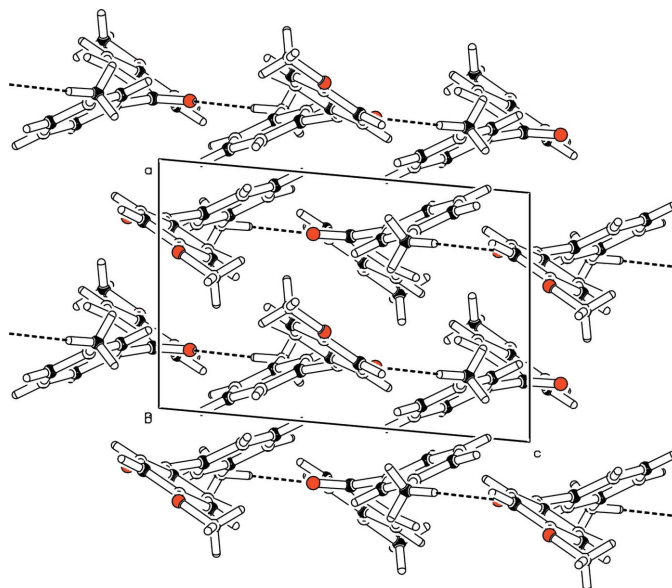


Figure 2

The packing of (I), viewed down the b axis. Dashed lines indicate hydrogen bonds.

1.2 for other H atoms. A rotating group refinement was used for the methyl groups.

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski and Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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