

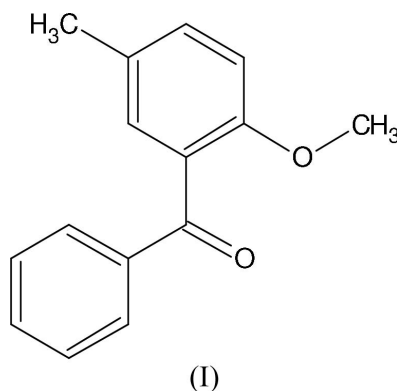
2-Methoxy-5-methylphenyl phenyl ketone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(C-C)$ = 0.004 Å
R factor = 0.073
wR factor = 0.187
Data-to-parameter ratio = 17.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.In the title compound, C₁₅H₁₄O₂, the aromatic rings are
twisted by 67.18 (8)° with respect to each other. Inter-
molecular C—H···O hydrogen bonds form *C*(7) chains along the
b axis.Received 14 February 2005
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Comment

Phenylmethanone derivatives show many pharmacological
properties. 4-Aminobenzophenones have anti-inflammatory
activity (Ottosen *et al.*, 2003), a benzophenylcyanone deriva-
tive acts as a vasorelaxant (Duncan *et al.*, 2004), and the
piperidinyl derivative produces analgesia (Colpaert *et al.*,
2004). Some aminothiophenes of phenylmethanone act as
regulators of the human A1 adenosine receptor (Figler *et al.*,
2003) and biphenyl derivatives show activity against *Myco-*
bacterium tuberculosis (de Souza *et al.*, 1999). These features
prompted us to carry out the crystal structure determination
of the title compound, (I).The two benzene rings are planar and twisted by 67.18 (8)°
with respect to each other. Atom O8 is displaced by
0.962 (4) Å from the plane of the C1–C6 benzene ring and by
0.357 (4) Å from the plane of the C9–C14 benzene ring. The
C2–C1–C7–O8 [−124.9 (3)°] and O8–C7–C9–C14
[−160.4 (3)°] torsion angles deviate significantly from the
corresponding values [28.8 (4) and −139.2 (3)°, respectively]
observed in *N*-(2-benzoyl-4-chlorophenyl)-2-chloroacetamide
(Malathy Sony *et al.*, 2005). These variations are due to
different substituents at the C2 position. In the chloroacet-
amide derivative, the C=O group is rotated about the C1–C7
bond, to form an intramolecular N–H···O hydrogen bond
with the amide N atom, whereas in the methoxy derivative it is
rotated away from the methoxy O atom due to steric repulsion
(Fig. 1). This clearly demonstrates the substitution-induced
conformational changes in both structures.

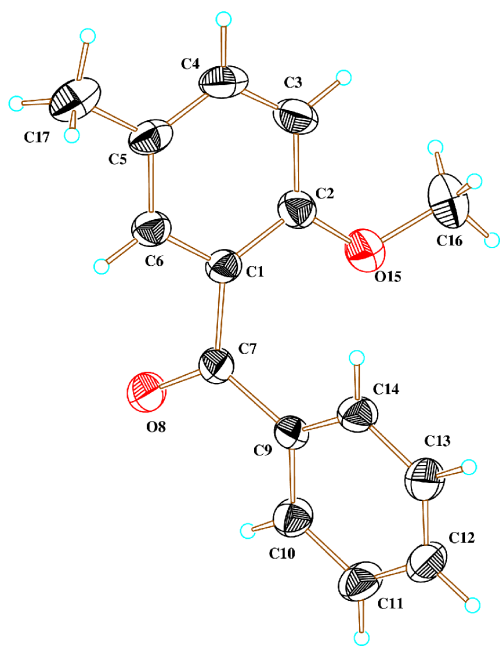


Figure 1
ZORTEP plot (Zsolnai, 1998) of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

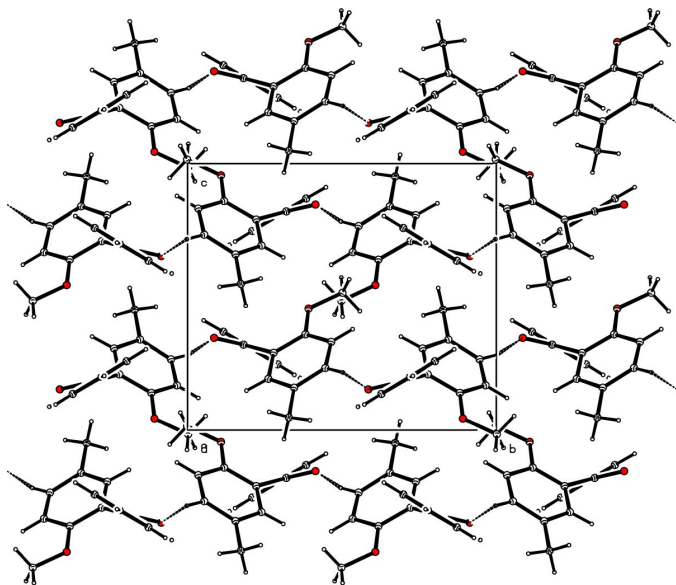


Figure 2
The packing of (I), viewed down the *a* axis. Dashed lines represent hydrogen bonds.

In this methoxy derivative, comparatively few hydrogen-bonding interactions are found. A one-dimensional C—H···O hydrogen-bonded chain of pattern type *C*(7) involving atoms C4 and O8 ($-x, \frac{1}{2} + y, \frac{1}{2} - z$) [$D \cdots A = 3.493$ (4) Å, $H \cdots A = 2.62$ Å and $D-H \cdots A = 157^\circ$] is found in the crystal structure. These zigzag chains run along the *b* axis (Fig. 2).

Experimental

Benzoyl chloride (0.01 *M*) and 4-methoxytoluene (0.01 *M*) were placed in a dry vessel. Finely powdered anhydrous AlCl₃ was added

to the reaction mixture, which was then stirred vigorously for 10 min. The reaction mixture was placed on a water bath and refluxed for 3 h until HCl was no longer evolved; it was then poured on to crushed ice. Concentrated HCl (100 ml) was added to the mixture, which was then washed with aqueous NaOH solution. The product was separated and recrystallized by slow evaporation of a solution in benzene.

Crystal data

C ₁₅ H ₁₄ O ₂	$D_x = 1.225 \text{ Mg m}^{-3}$
$M_r = 226.26$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4798 reflections
$a = 10.5883$ (18) Å	$\theta = 1.9\text{--}28.0^\circ$
$b = 11.5887$ (18) Å	$\mu = 0.08 \text{ mm}^{-1}$
$c = 10.0140$ (17) Å	$T = 293$ (2) K
$\beta = 92.904$ (3)°	Block, colourless
$V = 1227.2$ (4) Å ³	$0.27 \times 0.25 \times 0.22 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	1589 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.024$
Absorption correction: none	$\theta_{\text{max}} = 28.0^\circ$
4798 measured reflections	$h = -12 \rightarrow 13$
2759 independent reflections	$k = -7 \rightarrow 14$
	$l = -7 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0796P)^2 + 0.2394P]$
$R[F^2 > 2\sigma(F^2)] = 0.073$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.187$	$(\Delta/\sigma)_{\text{max}} = 0.028$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
2759 reflections	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$
156 parameters	
H-atom parameters constrained	

H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms [$U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 times $U_{\text{eq}}(\text{parent atom})$].

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003), ORTEP-3 (Farrugia, 1997) and ZORTEP (Zsolnai, 1998); software used to prepare material for publication: PLATON.

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