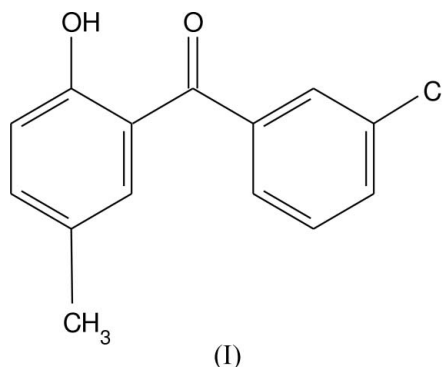


(3-Chlorophenyl)(2-hydroxy-5-methylphenyl)-methanone**S. A. Khanum,^a M. Mahendra,^b
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Mysore 570 006, IndiaCorrespondence e-mail:
mas@physics.uni-mysore.ac.in**Key indicators**Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.049
 wR factor = 0.151
Data-to-parameter ratio = 12.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.In the title compound, $\text{C}_{15}\text{H}_{14}\text{ClO}_2$, the dihedral angle
between the two benzene rings is 57.37 (12)°.Received 3 October 2005
Accepted 5 October 2005
Online 12 October 2005**Comment**The significance of benzophenone analogues in biological
systems, as well as in chemotherapy, is now well established
(Hsieh *et al.*, 2003; Revesz *et al.*, 2004). The chemistry of
hydroxybenzophenones constitutes a central and important
area of interest in synthetic organic, medicinal and pharma-
cological chemistry (Cuesta-Rubio *et al.*, 2002; Schlitzer *et al.*,
2002; Vidya *et al.*, 2003). Serving as attractive scaffolds for
drug design and conferring drug-like characteristics on
numerous structural motifs, halo-substituted hydroxy-
benzophenones are finding increasing applications in organic
and medicinal chemistry (Khanum *et al.*, 2005). Based on the
above observations, the title compound, (I), was synthesized
and its crystal structure is reported here.The molecule of (I) is non-planar (Fig. 1). The dihedral
angle between the two benzene rings is 57.37 (12)°, a value
much smaller than that of 75.2° observed for (2-chlorophenyl)
(3,4-dimethoxyphenyl)methanone, (II) (Mahendra *et al.*,
2003). The bond lengths and angles have normal values and
are comparable with those reported for (II). The crystal
packing is stabilized by intramolecular $\text{O9}-\text{H9}\cdots\text{O12}$ and
intermolecular $\text{C6}-\text{H6}\cdots\text{O12}$ hydrogen bonds (Table 2),
which link the molecules into chains (Fig. 2). A detailed study
of the biological activity of (I) is underway.**Experimental**A solution of anhydrous aluminium chloride (3.2 g, 0.02 mol) in dry
nitrobenzene (25 ml) was added to 4-methylphenyl chlorobenzoate
(5 g, 0.02 mol) dissolved in nitrobenzene (10 ml). The mixture was
protected from moisture by a calcium chloride guard tube and
refluxed with stirring for 30 min. At the end of this period, the
solution was cooled and treated with acidic ice-cold water. Nitro-

benzene was removed by steam distillation. The residual solid was crushed into a powder, extracted with 10% sodium hydroxide (150 ml), and the basic aqueous solution was neutralized with 10% hydrochloric acid. The product was extracted into diethyl ether and the ether layer washed well with a saturated sodium chloride solution. Evaporation of the ether after drying over anhydrous sodium sulfate followed by recrystallization from methanol gave (I) in 85% yield (m.p. 344–346 K). IR (Nujol): 1673 (C=O), 3550–3640 cm^{-1} (OH); ^1H NMR (CDCl_3): 2.2 (s, 3H, CH_3), 7.0–7.65 (m, 7H, Ar–H), 12.15 (bs, 1H, OH); MS (EI) m/z : 246 (M^+ , 88); Analysis calculated for $\text{C}_{14}\text{H}_{11}\text{ClO}_2$: C 68.15, H 4.46, Cl 14.40%; found: C 68.17, H 4.44, Cl 14.42%.

Crystal data

$\text{C}_{14}\text{H}_{11}\text{ClO}_2$
 $M_r = 246.68$
 Monoclinic, $P2_1/c$
 $a = 10.485$ (9) Å
 $b = 7.823$ (4) Å
 $c = 16.297$ (13) Å
 $\beta = 116.949$ (2)°
 $V = 1191.59$ (15) Å³
 $Z = 4$

$D_x = 1.375$ Mg m^{-3}
 Mo $K\alpha$ radiation
 Cell parameters from 3643 reflections
 $\theta = 2.3$ – 25.0°
 $\mu = 0.31$ mm^{-1}
 $T = 295$ (2) K
 Block, pale yellow
 $0.3 \times 0.2 \times 0.2$ mm

Data collection

MacScience DIPLabo 32001 diffractometer
 ω scans
 Absorption correction: none
 3643 measured reflections
 1945 independent reflections

1690 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -12 \rightarrow 12$
 $k = -8 \rightarrow 7$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.151$
 $S = 1.09$
 1945 reflections
 156 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.089P)^2 + 0.3587P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.56$ e \AA^{-3}
 $\Delta\rho_{\text{min}} = -0.33$ e \AA^{-3}
 Extinction correction: SHELXL97
 Extinction coefficient: 0.069 (8)

Table 1 Selected geometric parameters (Å, °).

C11–C15	1.747 (3)	O12–C11	1.234 (3)
O9–C8	1.351 (3)		
O9–C8–C7	117.9 (2)	O12–C11–C10	121.2 (2)
O9–C8–C10	123.05 (19)	C11–C15–C16	119.5 (3)
O12–C11–C13	118.0 (2)	C11–C15–C14	118.72 (19)

Table 2 Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O9–H9 \cdots O12	0.82	1.87	2.585 (3)	145
C6–H6 \cdots O12 ⁱ	0.93	2.54	3.408 (3)	156

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

Difficulties with processing some strong reflections led to their omission from the data set, limiting the completeness of data used in this determination. H atoms were placed at idealized positions and allowed to ride on their parent atoms, with C–H distances of 0.96 Å and $U_{\text{iso}}(\text{H})$ values set equal to $xU_{\text{eq}}(\text{carrier atom})$, where $x = 1.5$ for

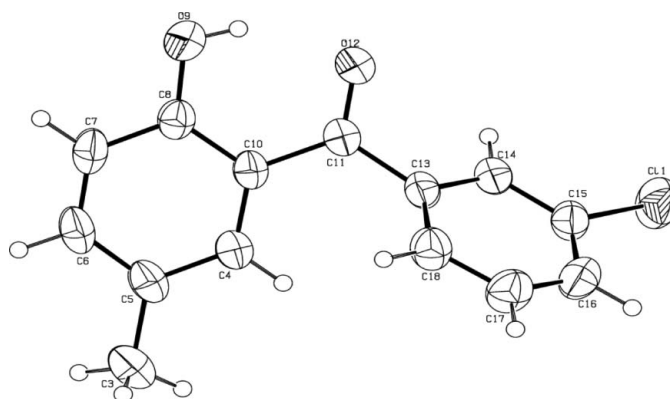


Figure 1 View of (I), shown with 50% probability displacement ellipsoids.

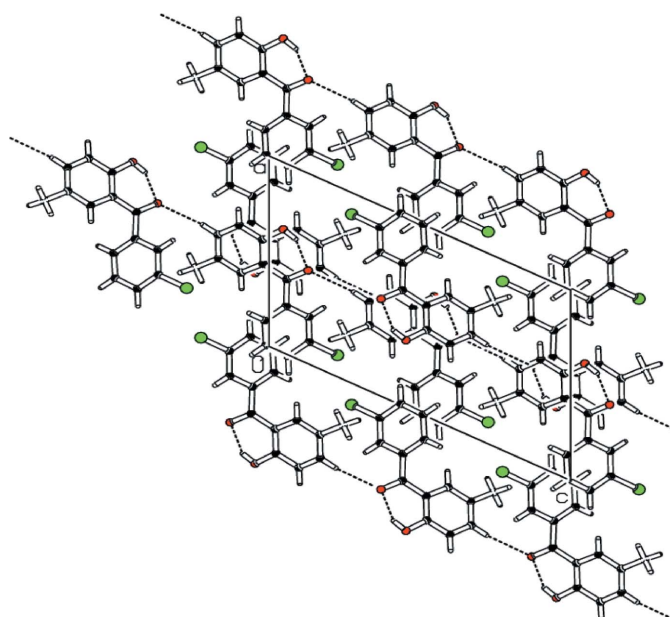


Figure 2 The crystal packing in (I), viewed down the b axis. Dashed lines indicate hydrogen bonds.

methyl and hydroxyl H atoms and 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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