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(4-Chlorophenyl)(2-hydroxy-5-methylphenyl)-methanone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.153
Data-to-parameter ratio = 12.2

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

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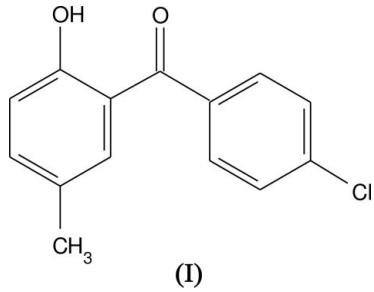
In the title compound, $C_{14}H_{11}ClO_2$, the dihedral angle between the two aromatic rings is 51.98 (11)°. The molecular conformation is stabilized by a strong intramolecular O—H···O hydrogen bond.

Comment

Benzophenones and related compounds have a wide variety of applications, in particular as biologically active compounds, which exhibit anti-inflammatory (Khanum *et al.*, 2004), antifungal, antibacterial and anticancer activities. They are also used as core steroid sulfatase (STS) inhibitors with IC50 values between 5 and 7 μ*M*. They are extensively used as sunscreen lotions for UVA protection. Owing to the importance of various substituents on the benzophenone nucleus, the title compound, (I), was synthesized and its crystal structure is reported here.



(I)

The molecule of (I) is non-planar (Fig. 1). The dihedral angle between the two aromatic rings is 51.98 (11)°; this compares with the corresponding value of 57.37 (12)° observed for (3-chlorophenyl)(2-hydroxy-5-methylphenyl)-methanone, (II) (Khanum *et al.*, 2005). The C4—C5—C7—O16 and O16—C7—C8—C9 torsion angles are −12.1 (3) and −40.8 (3)°, respectively, indicating that the carbonyl group is almost coplanar with the 2-hydroxy-5-methylphenyl plane but is considerably more displaced from the 4-chlorophenyl plane. Bond lengths and angles have normal values and are comparable to those reported for (II). The molecular conformation is stabilized by a strong intramolecular O—H···O hydrogen bond (Table 1). A detailed study of the biological activity of (I) is underway.

Experimental

4-Chlorophenyl-4-chlorobenzoate (0.039 mol, 10 g) was thoroughly mixed with montmorillonite K-10 clay in the solid state, using a vortex mixer and subjected to microwave irradiation at 40% power for 5 min. The completion of the reaction was monitored by thin layer chromatography and the product was extracted into dichloro-

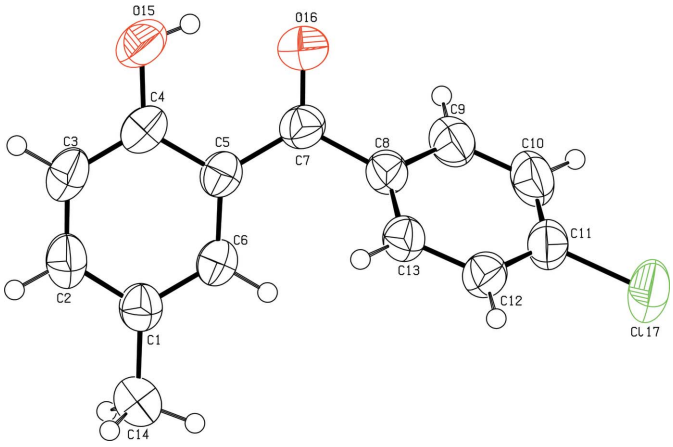


Figure 1
View of (I), with 50% probability displacement ellipsoids.

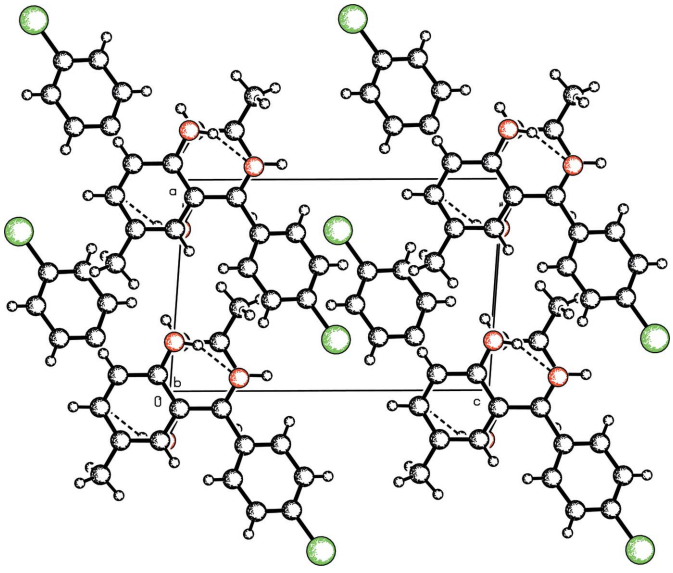


Figure 2
The crystal packing in (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

methane. The organic layer was dried over anhydrous sodium sulfate and evaporated to dryness, giving a crude solid, which, on recrystallization with ethanol, gave yellow crystals (yield 87%; m.p. 359 K).

Crystal data

$C_{14}H_{11}ClO_2$
M_r = 246.68
Triclinic, $P\overline{1}$
a = 7.362 (8) Å
b = 7.440 (10) Å
c = 11.001 (14) Å
α = 88.144 (5)°
β = 85.622 (9)°
γ = 82.831 (8)°
V = 596.0 (13) Å^3
Z = 2
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 295 (2) K
Block, pale yellow
0.25 × 0.20 × 0.20 mm

Data collection

MacScience DIPLabo 32001 diffractometer
ω scans
Absorption correction: none
3083 measured reflections
1898 independent reflections
1610 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.153
S = 1.08
1898 reflections
156 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0905P)^2 + 0.1264P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.14 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O15—H15···O16	0.82	1.85	2.569 (4)	145

H atoms were placed at idealized positions and allowed to ride on their parent atoms with C—H distances in the range 0.93–0.96 Å and O—H = 0.82 Å; U_{iso}(H) values were set equal to 1.2U_{eq}(C), or 1.5U_{eq}(C,O) for methyl and OH groups.

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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