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(2-Hydroxy-5-methylphenyl)(4-methylphenyl)methanone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.051
wR factor = 0.145
Data-to-parameter ratio = 12.1

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

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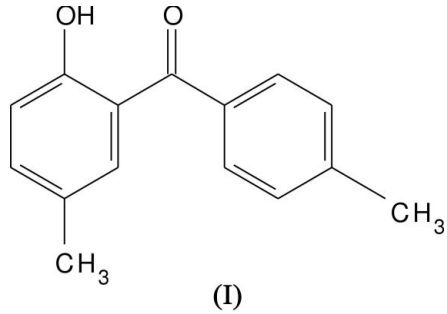
In the title compound, $C_{15}H_{14}O_2$, the dihedral angle between the two aromatic rings is 52.75 (7)°.

Comment

The competence of benzophenones as chemotherapeutic agents, especially as inhibitors of HIV-1 reverse transcriptase RT, cancer and inflammation, is well established and their chemistry has been studied extensively. In addition, methyl-substituted benzophenones exhibit chemotherapeutical activity against fungi. Due 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 52.75 (7)°; this compares with a corresponding value of 56.37 (3)° observed for (4-methoxyphenyl)(2-methylphenyl)methanone, (II) (Mahendra *et al.*, 2005). The C4—C5—C7—O16 and O16—C7—C8—C9 torsion angles are 12.9 (2) and 41.1 (2)°, respectively, indicating that the carbonyl group lies nearly in the 2-hydroxy-5-methylphenyl plane but is rather more displaced out of the 4-methylphenyl plane. Bond lengths and angles have normal values and are comparable with those reported for (II). The molecular conformation is stabilized by a strong intramolecular O—H···O hydrogen bond (Table 2). A detailed study of the biological activity of (I) is underway.

Experimental

4-Methylphenyl-4-methylbenzoate (0.022 mol, 5 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 ether. Finally, the product was isolated and recrystallized from ethanol to afford the title compound (yield: 90%; m.p. 359 K). Analysis calculated: C 79.69, H 6.25, O 14%.

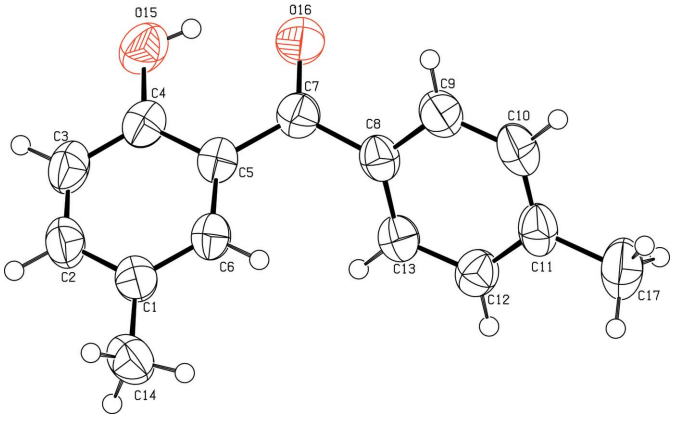


Figure 1
View of (I), with 50% probability displacement ellipsoids.

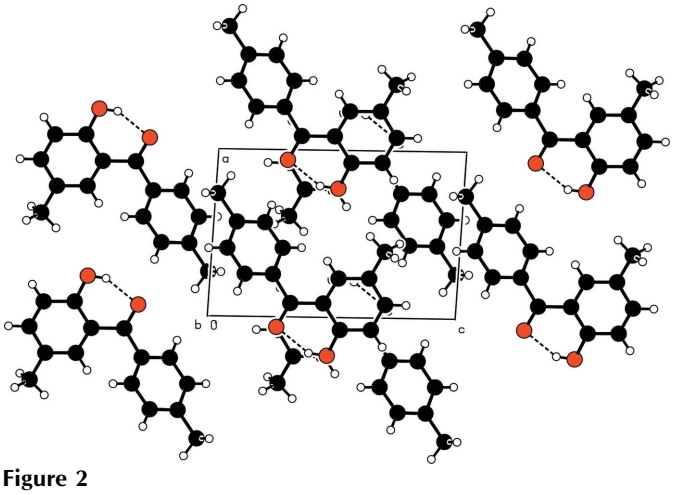


Figure 2
The crystal packing in (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

Crystal data

$C_{15}H_{14}O_2$
M_r = 226.26
Triclinic, $P\overline{1}$
a = 7.427 (5) Å
b = 7.484 (9) Å
c = 10.940 (13) Å
α = 88.155 (3)°
β = 86.638 (7)°
γ = 82.765 (8)°
V = 602.0 (11) Å^3
Z = 2
D_x = 1.248 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3046 reflections
θ = 2.8–25.0°
μ = 0.08 mm^{-1}
T = 295 (2) K
Block, white
0.25 × 0.2 × 0.2 mm

Data collection

MacScience DIPLabo 32001 diffractometer
ω scans
Absorption correction: none
3046 measured reflections
1905 independent reflections
1666 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.0°
$h = -8 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.145
S = 1.09
1905 reflections
157 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0809P)^2 + 0.0862P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.27 (3)

Table 1
Selected geometric parameters (Å, °).

O15—C4	1.354 (2)	O16—C7	1.237 (2)
O15—C4—C3	118.06 (14)	O16—C7—C8	118.28 (14)
O15—C4—C5	122.84 (14)	O16—C7—C5	120.61 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
O15—H15···O16	0.82	1.87	2.580 (4)	145

H atoms were placed at idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.92–0.97 Å and O—H = 0.82 Å; U_{iso}(H) values were set equal to 1.2U_{eq}(carrier atom).

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski and 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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