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

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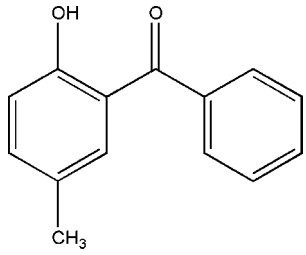
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.149; data-to-parameter ratio = 12.9.

In the title compound, $C_{14}H_{12}O_2$, the dihedral angle between the two aromatic rings is 60.02 (4)°. The crystal structure is stabilized by intramolecular O—H···O and intermolecular C—H···O hydrogen bonds.

Related literature

For related literature, see: Khanum *et al.* (2004).



Experimental

Crystal data

$C_{14}H_{12}O_2$
M_r = 212.24
Monoclinic, $P2_1/c$
a = 15.9176 (7) Å
b = 5.8509 (2) Å
c = 12.1429 (5) Å
β = 105.745 (2)°
V = 1088.46 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 273 (2) K
0.35 × 0.23 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.971, T_{max} = 0.990
11748 measured reflections
1913 independent reflections
1512 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.149
S = 1.00
1913 reflections
148 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	1.85	2.571 (1)	146
C13—H13···O2^{i}	0.93	2.72	3.532 (2)	147
C5—H5···O1^{ii}	0.93	2.56	3.449 (2)	159

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2217).

References

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Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.

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supplementary materials

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

J.-G. Chang, L.-L. Qiu, D.-F. Zhao and G.-F. He

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·As an extension of work on the structural characterization of Benzophenone derivatives,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 aromatic rings is 60.02 (4)°·The crystal structure is stabilized by intramolecular O—H···O and intermolecular C—H···O hydrogen bonds (Table 1, Fig. 2).

Experimental

Benzoyl chloride (7.02 g, 0.05 mol) was added dropwise to *p*-cresol (5.41 g,0.05 mol) and the mixture was reacted at room temperature for 1 h, then heated to 373 K for 2 h. After cooled to the ambient temperature, the chloroform diluted mixture was washed with sodium carbonate solution and water for several times. The organic layer was dried with anhydrous sodium sulfate, filtered, and the solvent was removed. Further purification was carried out by vacuum distillation, 4-methylphenyl benzoate was obtained (yield 85.3%). Then the mixture of 4-methylphenyl benzoate (9.05 g, 0.043 mol) and anhydrous aluminium chloride (17.20 g, 0.129 mol) gradually heated to 373 K in 0.5 h, then heated to 423 K and kept for 0.5 h. The reaction mixture was cooled to room temperature, hydrolyzed, and extracted with 60 ml chloroform. The organic layer washed with water, dried with anhydrous sodium sulfate. Filtered, chloroform was removed under reduced pressure. The residue was distilled under vacuum to obtain the title compound (yield 78.0%)·The compound was recrystallized from ethyl acetate to obtain colourless single crystals suitable for *x*-ray diffraction.

Refinement

All H atoms,were positioned geometrically and treated as riding on their parent atoms,with *C*—*H*(methyl) = 0.96 Å, C—H(aromatic) = 0.93 Å, O—H = 0.82 Å, and with U_{iso}(H) =1.5U_{eq}(C_{methyl},*O*) and 1.2U_{eq}($C_{aromatic}$).

Figures

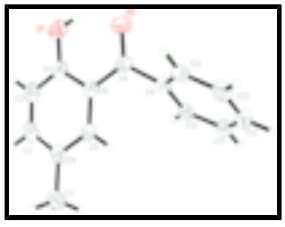

Fig. 1. The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

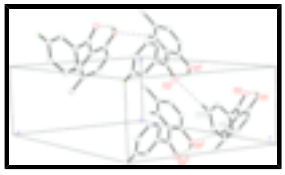

Fig. 2. Partial packing view of (I) showing intramolecular O—H···O and intermolecular C—H···O hydrogen bonds. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry code: (i) (i) *x*, 3/2 − *y*, 1/2 + *z*; (ii) *x*, 1/2 − *y*, 1/2 + *z*].

(2-hydroxy-5-methylphenyl)(phenyl)methanone

Crystal data

$C_{14}H_{12}O_2$	F_{000} = 448
M_r = 212.24	D_x = 1.295 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2709 reflections
a = 15.9176 (7) Å	θ = 2.7–24.2º
b = 5.8509 (2) Å	μ = 0.09 mm^{-1}
c = 12.1429 (5) Å	*T* = 273 (2) K
β = 105.745 (2)º	Plate, colourless
V = 1088.46 (8) Å^3	0.35 × 0.23 × 0.18 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	1913 independent reflections
Radiation source: fine-focus sealed tube	1512 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 273(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	*h* = −18→18
T_{min} = 0.971, T_{max} = 0.990	*k* = −6→6
11748 measured reflections	*l* = −13→14

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.13P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.149	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
1913 reflections	$\Delta\rho_{min}$ = −0.12 e Å^{-3}
148 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Extinction coefficient: 0.028 (5)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.71300 (9)	0.5107 (2)	−0.19822 (10)	0.0694 (5)
H1	0.7462	0.5893	−0.1494	0.104*
O2	0.80872 (9)	0.6108 (2)	0.00287 (11)	0.0677 (4)
C1	0.68806 (10)	0.3263 (3)	−0.14813 (14)	0.0523 (5)
C2	0.62578 (11)	0.1827 (4)	−0.21475 (15)	0.0643 (6)
H2	0.6047	0.2102	−0.2928	0.077*
C3	0.59494 (11)	0.0008 (4)	−0.16702 (17)	0.0658 (6)
H3	0.5532	−0.0938	−0.2137	0.079*
C4	0.62445 (10)	−0.0476 (3)	−0.04969 (15)	0.0536 (5)
C5	0.68934 (9)	0.0906 (3)	0.01512 (14)	0.0467 (4)
H5	0.7114	0.0591	0.0927	0.056*
C6	0.72332 (9)	0.2763 (3)	−0.03130 (13)	0.0445 (4)
C7	0.58701 (12)	−0.2407 (3)	0.00307 (18)	0.0705 (6)
H7A	0.6231	−0.2681	0.0792	0.106*
H7B	0.5848	−0.3761	−0.0423	0.106*
H7C	0.5291	−0.2016	0.0061	0.106*
C8	0.79057 (10)	0.4252 (3)	0.03944 (14)	0.0470 (4)
C9	0.83898 (9)	0.3586 (3)	0.15822 (13)	0.0426 (4)
C10	0.88182 (10)	0.1502 (3)	0.18194 (14)	0.0491 (4)
H10	0.8770	0.0428	0.1241	0.059*
C11	0.93172 (10)	0.1030 (3)	0.29179 (15)	0.0559 (5)
H11	0.9622	−0.0342	0.3074	0.067*
C12	0.93630 (11)	0.2590 (3)	0.37798 (15)	0.0606 (5)
H12	0.9692	0.2256	0.4520	0.073*
C13	0.89262 (12)	0.4636 (3)	0.35563 (15)	0.0602 (5)
H13	0.8950	0.5670	0.4146	0.072*
C14	0.84537 (10)	0.5149 (3)	0.24589 (14)	0.0514 (5)
H14	0.8175	0.6556	0.2303	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0801 (10)	0.0787 (10)	0.0484 (8)	0.0025 (7)	0.0159 (7)	0.0140 (7)
O2	0.0851 (9)	0.0528 (8)	0.0613 (9)	−0.0093 (6)	0.0130 (7)	0.0095 (6)
C1	0.0494 (9)	0.0640 (11)	0.0445 (10)	0.0117 (8)	0.0145 (7)	0.0014 (8)
C2	0.0523 (10)	0.0922 (15)	0.0435 (10)	0.0054 (10)	0.0049 (8)	−0.0046 (10)
C3	0.0473 (10)	0.0842 (14)	0.0597 (12)	−0.0042 (9)	0.0040 (8)	−0.0197 (10)
C4	0.0413 (8)	0.0578 (11)	0.0603 (11)	0.0026 (7)	0.0116 (8)	−0.0086 (8)
C5	0.0436 (8)	0.0504 (9)	0.0446 (9)	0.0073 (7)	0.0093 (7)	−0.0023 (7)
C6	0.0445 (8)	0.0493 (9)	0.0393 (9)	0.0080 (7)	0.0107 (7)	−0.0021 (7)
C7	0.0557 (10)	0.0633 (12)	0.0907 (15)	−0.0065 (9)	0.0167 (10)	−0.0058 (11)
C8	0.0510 (9)	0.0431 (9)	0.0477 (10)	0.0032 (7)	0.0148 (7)	0.0006 (7)
C9	0.0405 (8)	0.0420 (9)	0.0447 (9)	−0.0042 (6)	0.0108 (6)	−0.0030 (7)
C10	0.0493 (9)	0.0457 (9)	0.0515 (10)	−0.0018 (7)	0.0127 (7)	−0.0053 (7)
C11	0.0481 (9)	0.0537 (10)	0.0611 (11)	−0.0014 (7)	0.0066 (8)	0.0059 (9)
C12	0.0559 (10)	0.0701 (13)	0.0480 (10)	−0.0139 (9)	0.0006 (8)	0.0047 (9)
C13	0.0688 (11)	0.0623 (12)	0.0483 (11)	−0.0145 (9)	0.0139 (9)	−0.0133 (9)
C14	0.0556 (10)	0.0446 (9)	0.0541 (11)	−0.0038 (7)	0.0150 (8)	−0.0071 (8)

Geometric parameters (Å, °)

O1—C1	1.350 (2)	C7—H7B	0.9600
O1—H1	0.8200	C7—H7C	0.9600
O2—C8	1.237 (2)	C8—C9	1.491 (2)
C1—C2	1.381 (2)	C9—C14	1.386 (2)
C1—C6	1.407 (2)	C9—C10	1.388 (2)
C2—C3	1.366 (3)	C10—C11	1.383 (2)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.403 (3)	C11—C12	1.376 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.378 (2)	C12—C13	1.374 (3)
C4—C7	1.500 (2)	C12—H12	0.9300
C5—C6	1.399 (2)	C13—C14	1.374 (2)
C5—H5	0.9300	C13—H13	0.9300
C6—C8	1.464 (2)	C14—H14	0.9300
C7—H7A	0.9600		
C1—O1—H1	109.5	H7A—C7—H7C	109.5
O1—C1—C2	118.30 (16)	H7B—C7—H7C	109.5
O1—C1—C6	122.32 (15)	O2—C8—C6	121.11 (15)
C2—C1—C6	119.37 (17)	O2—C8—C9	117.85 (14)
C3—C2—C1	120.60 (17)	C6—C8—C9	121.04 (14)
C3—C2—H2	119.7	C14—C9—C10	119.37 (15)
C1—C2—H2	119.7	C14—C9—C8	118.79 (14)
C2—C3—C4	121.92 (17)	C10—C9—C8	121.74 (14)
C2—C3—H3	119.0	C11—C10—C9	119.80 (16)
C4—C3—H3	119.0	C11—C10—H10	120.1

C5—C4—C3	117.01 (17)	C9—C10—H10	120.1
C5—C4—C7	121.41 (17)	C12—C11—C10	119.95 (17)
C3—C4—C7	121.57 (17)	C12—C11—H11	120.0
C4—C5—C6	122.52 (16)	C10—C11—H11	120.0
C4—C5—H5	118.7	C13—C12—C11	120.56 (17)
C6—C5—H5	118.7	C13—C12—H12	119.7
C5—C6—C1	118.40 (15)	C11—C12—H12	119.7
C5—C6—C8	121.80 (14)	C14—C13—C12	119.76 (17)
C1—C6—C8	119.72 (15)	C14—C13—H13	120.1
C4—C7—H7A	109.5	C12—C13—H13	120.1
C4—C7—H7B	109.5	C13—C14—C9	120.51 (16)
H7A—C7—H7B	109.5	C13—C14—H14	119.7
C4—C7—H7C	109.5	C9—C14—H14	119.7
O1—C1—C2—C3	−176.52 (16)	C5—C6—C8—C9	12.9 (2)
C6—C1—C2—C3	3.6 (3)	C1—C6—C8—C9	−170.48 (13)
C1—C2—C3—C4	0.2 (3)	O2—C8—C9—C14	49.4 (2)
C2—C3—C4—C5	−3.0 (3)	C6—C8—C9—C14	−130.18 (16)
C2—C3—C4—C7	176.88 (16)	O2—C8—C9—C10	−126.78 (17)
C3—C4—C5—C6	2.0 (2)	C6—C8—C9—C10	53.6 (2)
C7—C4—C5—C6	−177.84 (15)	C14—C9—C10—C11	−1.4 (2)
C4—C5—C6—C1	1.6 (2)	C8—C9—C10—C11	174.81 (14)
C4—C5—C6—C8	178.26 (14)	C9—C10—C11—C12	2.3 (2)
O1—C1—C6—C5	175.68 (14)	C10—C11—C12—C13	−0.9 (3)
C2—C1—C6—C5	−4.4 (2)	C11—C12—C13—C14	−1.3 (3)
O1—C1—C6—C8	−1.1 (2)	C12—C13—C14—C9	2.2 (3)
C2—C1—C6—C8	178.85 (15)	C10—C9—C14—C13	−0.9 (2)
C5—C6—C8—O2	−166.70 (15)	C8—C9—C14—C13	−177.17 (15)
C1—C6—C8—O2	9.9 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.85	2.571 (1)	146
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Fig. 1

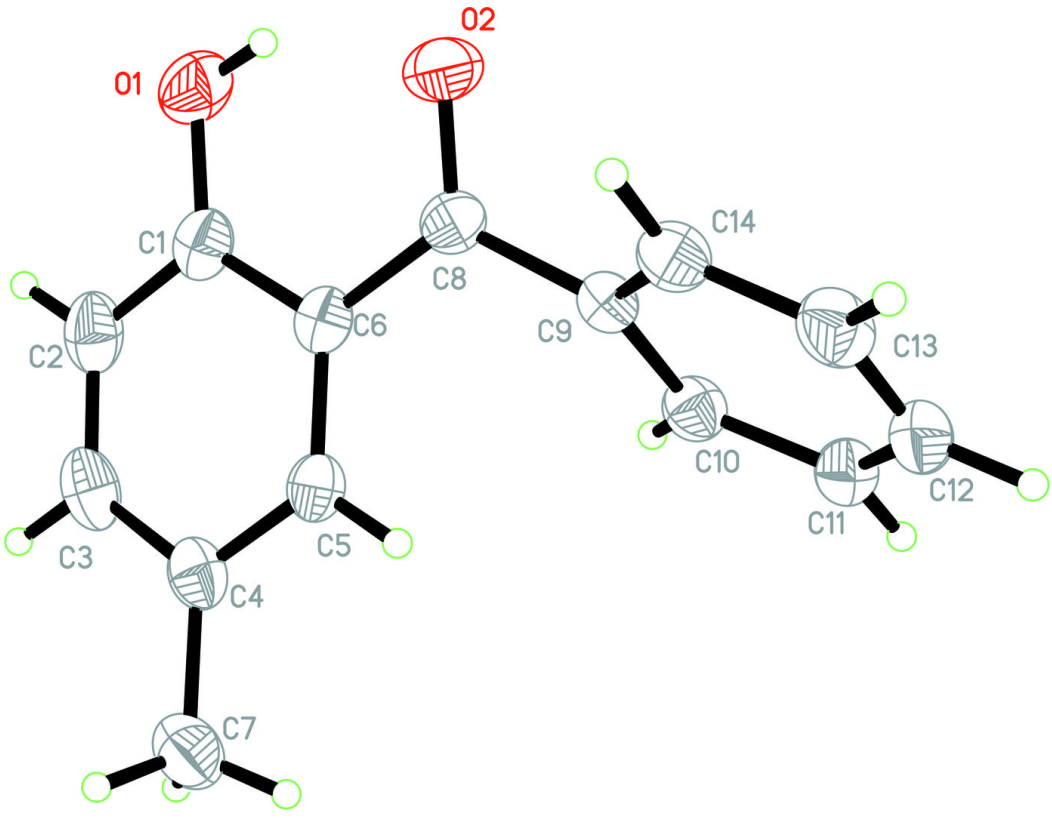

Fig. 2