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1-(2-Hydroxy-5-methylphenyl)-2-phenylethanone

Chun-Hong He,[a] Jian-Ping Zhang[b] and Jian-Guo Chang[b]*

[a]School of Chemical Engineering, Tianjin University, 300072 Tianjin, People's Republic of China, and [b]Department of Materials Science and Chemical Engineering, Taishan University, 271021 Taian, Shandong, People's Republic of China
Correspondence e-mail: tsucjg@163.com

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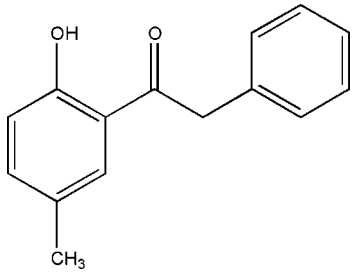
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.064; wR factor = 0.242; data-to-parameter ratio = 13.5.

In the title compound, $C_{15}H_{14}O_2$, the dihedral angle between the two aromatic rings is 87.98 (13)°. The primary interaction is an intramolecular O—H···O=C interaction [O···O = 2.559 (3) Å]. Intermolecular interactions/contacts are weak and are of the O—H···C, C—H···π(arene) and π–π(arene) types [$Cg\cdots Cg(-x+1,-y+1,-z+2)$ = 3.927 (1) Å; Cg is the centroid of the phenyl ring].

Related literature

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



Experimental

Crystal data

$C_{15}H_{14}O_2$
M_r = 226.26
Monoclinic, $P2_1/c$
a = 8.2951 (10) Å
b = 18.010 (2) Å
c = 8.9186 (10) Å
β = 114.103 (4)°
V = 1216.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 273 (2) K
0.35 × 0.24 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.975, T_{max} = 0.986
12849 measured reflections
2115 independent reflections
1303 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.242
S = 1.01
2115 reflections
157 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

Cg is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	1.85	2.559 (3)	144
O1—H1···C7^{i}	0.82	2.67	3.093 (4)	114
C9—H9B···Cg^{ii}	0.97	3.47	3.737 (2)	99

Symmetry code: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+2$.

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*.

This project was supported by Taishan University (grant No. Y05-2-09).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2032).

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.

  doi:10.1107/S1600536807039542

supplementary materials

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1-(2-Hydroxy-5-methylphenyl)-2-phenylethanone

C.-H. He, J.-P. Zhang and J.-G. Chang

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 87.98 (13)°. The crystal structure is stabilized by intramolecular O—H···O hydrogen bonds and intermolecular O—H···C contacts together with C—H···π(arene) contacts and π···π stacking interactions, (Table 1, Fig. 2).

Experimental

Phenylacetyl chloride (7.73 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 $CHCl_3$ 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 phenylacetate was obtained (yield 81.2%). Then the mixture of 4-methylphenyl phenylacetate (9.19 g, 0.041 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 30 min. The reaction mixture was cooled to room temperature, hydrolyzed, and extracted with 60 ml $CHCl_3$. The organic layer washed with water, dried with anhydrous sodium sulfate. Filtered, $CHCl_3$ was removed under reduced pressure. The residue was distilled under vacuum to obtain the title compound (I) (yield 76.1%)·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*(methylene) = 0.97 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}($C_{aromatic}$,$C_{methylene}$).

Figures

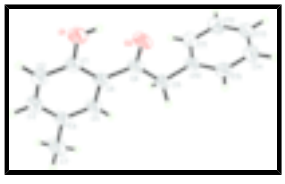

Fig. 1. The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

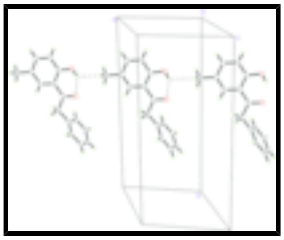

Fig. 2. Packing diagram of (I), showing intramolecular O—H···O and intermolecular O—H···C hydrogen bonds.(dashed lines).

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Crystal data

$C_{15}H_{14}O_2$	F_{000} = 480
M_r = 226.26	D_x = 1.236 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3447 reflections
a = 8.2951 (10) Å	θ = 2.3–25.1º
b = 18.010 (2) Å	μ = 0.08 mm^{-1}
c = 8.9186 (10) Å	T = 273 (2) K
β = 114.103 (4)º	Plate, colourless
V = 1216.2 (2) Å^3	0.35 × 0.24 × 0.18 mm
Z = 4	

Data collection

Bruker APEX II CCD diffractometer	2115 independent reflections
Radiation source: fine-focus sealed tube	1303 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.053
T = 273(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −9→9
T_{min} = 0.975, T_{max} = 0.986	k = −21→21
12849 measured reflections	l = −10→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.064	H-atom parameters constrained
$wR(F^2)$ = 0.242	$w = 1/[\sigma^2(F_o^2) + (0.12P)^2 + 0.7798P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
2115 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}

157 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
1 restraint	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.010 (4)

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	0.7193 (3)	0.17283 (14)	1.0078 (4)	0.0955 (10)
H1	0.6678	0.2127	0.9949	0.143*
O2	0.6970 (3)	0.31456 (13)	0.9929 (4)	0.0975 (11)
C1	0.8678 (4)	0.18261 (17)	1.0027 (5)	0.0675 (10)
C2	0.9580 (5)	0.12019 (19)	1.0045 (5)	0.0812 (11)
H2	0.9105	0.0737	1.0069	0.097*
C3	1.1103 (5)	0.1267 (2)	1.0029 (5)	0.0811 (11)
H3	1.1754	0.0844	1.0044	0.097*
C4	1.1785 (4)	0.1956 (2)	0.9990 (5)	0.0738 (11)
C5	1.0873 (4)	0.25743 (18)	0.9949 (5)	0.0677 (10)
H5	1.1355	0.3036	0.9909	0.081*
C6	0.9320 (4)	0.25309 (16)	0.9965 (4)	0.0578 (8)
C7	1.3490 (5)	0.2031 (3)	1.0001 (7)	0.1133 (18)
H7A	1.4366	0.1904	1.1068	0.170*
H7B	1.3663	0.2535	0.9749	0.170*
H7C	1.3596	0.1706	0.9194	0.170*
C8	0.8332 (4)	0.31987 (17)	0.9903 (5)	0.0662 (10)
C9	0.9037 (4)	0.39513 (18)	0.9815 (5)	0.0758 (11)
H9A	1.0025	0.4045	1.0857	0.091*
H9B	0.9504	0.3937	0.8980	0.091*
C10	0.7835 (4)	0.45875 (17)	0.9461 (5)	0.0658 (10)
C11	0.6748 (5)	0.4736 (2)	0.7773 (6)	0.0851 (12)
H11	0.6796	0.4434	0.6947	0.102*
C12	0.5657 (6)	0.5323 (2)	0.7409 (6)	0.0960 (13)
H12	0.4928	0.5438	0.6326	0.115*
C13	0.5649 (5)	0.5762 (2)	0.8734 (6)	0.0826 (12)
H13	0.4887	0.6167	0.8477	0.099*
C14	0.6721 (5)	0.5627 (2)	1.0419 (6)	0.0808 (12)

H14	0.6672	0.5932	1.1241	0.097*
C15	0.7813 (4)	0.50376 (19)	1.0775 (5)	0.0755 (11)
H15	0.8542	0.4924	1.1859	0.091*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0523 (14)	0.0696 (16)	0.172 (3)	−0.0098 (11)	0.0535 (18)	0.0088 (17)
O2	0.0493 (14)	0.0712 (16)	0.189 (3)	0.0004 (11)	0.0659 (18)	0.0089 (16)
C1	0.0467 (17)	0.0606 (19)	0.094 (3)	−0.0052 (14)	0.0273 (17)	0.0027 (17)
C2	0.063 (2)	0.057 (2)	0.126 (3)	−0.0018 (16)	0.040 (2)	0.0014 (19)
C3	0.061 (2)	0.064 (2)	0.120 (3)	0.0118 (16)	0.038 (2)	0.000 (2)
C4	0.0425 (17)	0.075 (2)	0.108 (3)	0.0081 (15)	0.0350 (19)	0.0017 (19)
C5	0.0421 (17)	0.0597 (19)	0.103 (3)	−0.0007 (13)	0.0312 (18)	0.0020 (17)
C6	0.0377 (15)	0.0555 (18)	0.081 (2)	−0.0021 (12)	0.0249 (15)	0.0018 (15)
C7	0.052 (2)	0.103 (3)	0.197 (5)	0.012 (2)	0.063 (3)	0.002 (3)
C8	0.0439 (17)	0.0604 (19)	0.099 (3)	−0.0028 (13)	0.0338 (18)	0.0030 (17)
C9	0.0464 (17)	0.060 (2)	0.125 (3)	0.0004 (14)	0.0383 (19)	0.0051 (19)
C10	0.0431 (16)	0.0513 (17)	0.104 (3)	−0.0018 (13)	0.0312 (18)	0.0016 (17)
C11	0.080 (3)	0.074 (2)	0.102 (3)	0.0155 (19)	0.038 (2)	−0.007 (2)
C12	0.083 (3)	0.083 (3)	0.106 (3)	0.024 (2)	0.022 (2)	0.003 (2)
C13	0.060 (2)	0.060 (2)	0.132 (4)	0.0069 (15)	0.044 (2)	0.005 (2)
C14	0.078 (3)	0.066 (2)	0.112 (3)	−0.0015 (18)	0.052 (3)	−0.010 (2)
C15	0.059 (2)	0.069 (2)	0.095 (3)	0.0006 (16)	0.0286 (19)	0.003 (2)

Geometric parameters (Å, °)

O1—C1	1.263 (4)	C7—H7C	0.9600
O1—H1	0.8200	C8—C9	1.491 (4)
O2—C8	1.144 (4)	C9—C10	1.466 (4)
C1—C2	1.347 (5)	C9—H9A	0.9700
C1—C6	1.386 (4)	C9—H9B	0.9700
C2—C3	1.274 (5)	C10—C11	1.429 (5)
C2—H2	0.9300	C10—C15	1.431 (5)
C3—C4	1.371 (5)	C11—C12	1.342 (5)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.338 (4)	C12—C13	1.425 (6)
C4—C7	1.417 (5)	C12—H12	0.9300
C5—C6	1.297 (4)	C13—C14	1.420 (6)
C5—H5	0.9300	C13—H13	0.9300
C6—C8	1.443 (4)	C14—C15	1.346 (5)
C7—H7A	0.9600	C14—H14	0.9300
C7—H7B	0.9600	C15—H15	0.9300
C1—O1—H1	109.5	O2—C8—C9	119.3 (3)
O1—C1—C2	115.4 (3)	C6—C8—C9	122.1 (3)
O1—C1—C6	121.7 (3)	C10—C9—C8	118.4 (3)
C2—C1—C6	123.0 (3)	C10—C9—H9A	107.7
C3—C2—C1	118.2 (3)	C8—C9—H9A	107.7

C3—C2—H2	120.9	C10—C9—H9B	107.7
C1—C2—H2	120.9	C8—C9—H9B	107.7
C2—C3—C4	120.3 (3)	H9A—C9—H9B	107.1
C2—C3—H3	119.9	C11—C10—C15	122.9 (3)
C4—C3—H3	119.9	C11—C10—C9	117.0 (3)
C5—C4—C3	121.3 (3)	C15—C10—C9	120.1 (3)
C5—C4—C7	118.2 (3)	C12—C11—C10	118.4 (4)
C3—C4—C7	120.5 (3)	C12—C11—H11	120.8
C6—C5—C4	120.2 (3)	C10—C11—H11	120.8
C6—C5—H5	119.9	C11—C12—C13	117.9 (4)
C4—C5—H5	119.9	C11—C12—H12	121.0
C5—C6—C1	117.1 (3)	C13—C12—H12	121.0
C5—C6—C8	120.0 (3)	C14—C13—C12	124.7 (3)
C1—C6—C8	122.9 (3)	C14—C13—H13	117.6
C4—C7—H7A	109.5	C12—C13—H13	117.6
C4—C7—H7B	109.5	C15—C14—C13	117.0 (4)
H7A—C7—H7B	109.5	C15—C14—H14	121.5
C4—C7—H7C	109.5	C13—C14—H14	121.5
H7A—C7—H7C	109.5	C14—C15—C10	119.1 (4)
H7B—C7—H7C	109.5	C14—C15—H15	120.5
O2—C8—C6	118.6 (3)	C10—C15—H15	120.5
O1—C1—C2—C3	−178.7 (4)	C5—C6—C8—C9	0.1 (6)
C6—C1—C2—C3	1.1 (7)	C1—C6—C8—C9	−179.2 (3)
C1—C2—C3—C4	−0.2 (7)	O2—C8—C9—C10	−11.1 (6)
C2—C3—C4—C5	−0.8 (7)	C6—C8—C9—C10	169.2 (3)
C2—C3—C4—C7	178.9 (4)	C8—C9—C10—C11	−83.9 (4)
C3—C4—C5—C6	0.8 (6)	C8—C9—C10—C15	97.4 (4)
C7—C4—C5—C6	−178.9 (4)	C15—C10—C11—C12	−0.2 (6)
C4—C5—C6—C1	0.1 (6)	C9—C10—C11—C12	−178.9 (4)
C4—C5—C6—C8	−179.3 (4)	C10—C11—C12—C13	0.0 (6)
O1—C1—C6—C5	178.7 (4)	C11—C12—C13—C14	0.3 (7)
C2—C1—C6—C5	−1.1 (6)	C12—C13—C14—C15	−0.3 (6)
O1—C1—C6—C8	−1.9 (6)	C13—C14—C15—C10	0.1 (5)
C2—C1—C6—C8	178.3 (4)	C11—C10—C15—C14	0.2 (5)
C5—C6—C8—O2	−179.5 (4)	C9—C10—C15—C14	178.8 (3)
C1—C6—C8—O2	1.1 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.85	2.559 (3)	144
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Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

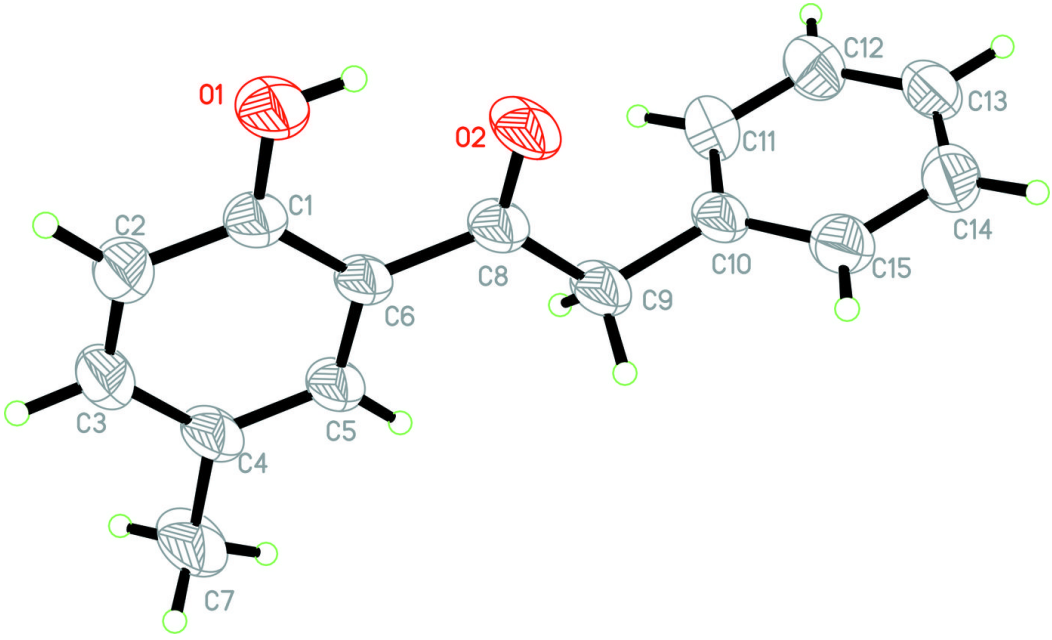

Fig. 2