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4-(4-Hydroxybenzoyl)phenol monohydrate

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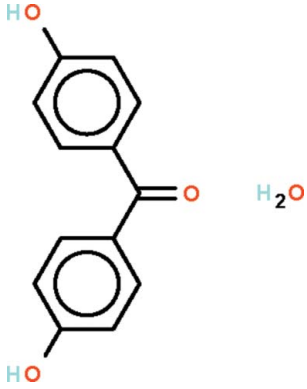
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.123; data-to-parameter ratio = 15.1.

The aromatic rings of the title compound, $C_{13}H_{10}O_3\cdot H_2O$, are aligned at dihedral angles of 20.6 (1) and 40.8 (1)° with respect to the triangular C_{aryl}–C(=O)–C_{aryl} fragment. The hydroxy groups are each hydrogen-bond donors to separate water molecules, the water molecule itself being hydrogen-bonded to one hydroxy group and one carbonyl group. The water molecule exists in an unusual four-coordinate environment in the resulting layer structure.

Related literature

For the crystal structure of anhydrous 4,4′-dihydroxybenzophenone, see: Ferguson & Glidewell (1996).



Experimental

Crystal data

$C_{13}H_{10}O_3\cdot H_2O$
M_r = 232.23
Monoclinic, $P2_1/c$
a = 4.9398 (1) Å
b = 9.8273 (2) Å
c = 23.1446 (4) Å
β = 94.520 (1)°
V = 1120.06 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.45 × 0.30 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
8356 measured reflections
2572 independent reflections
2016 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.123
S = 1.05
2572 reflections
170 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1w^{i}	0.85 (1)	1.95 (1)	2.774 (2)	164 (2)
O3—H3···O1w^{ii}	0.85 (1)	1.95 (1)	2.773 (2)	164 (2)
O1w—H11···O2	0.84 (1)	1.93 (1)	2.762 (2)	168 (2)
O1w—H12···O1^{iii}	0.84 (1)	2.18 (2)	2.898 (2)	143 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2075).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ferguson, G. & Glidewell, C. (1996). *Acta Cryst.* C**52**, 3057–3062.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2010). E**66**, o2867 [https://doi.org/10.1107/S1600536810041425]

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S1. Comment

4,4′-Dihydroxbenzophenone exists as a *O*–*H*···$O_{hydroxy}$ hydrogen-bonded chains that are linked by *O*–*H*···$O_{carbonyl}$ hydrogen bonds into sheets. The first set of hydrogen bonds [2.785 (4), 2.791 (4) Å] is longer than the second set [2.624 (4), 2.627 (4) Å] (Ferguson & Glidewell, 1996). The monohydrated title compound $C_{13}H_{10}O_3{\cdot}H_2O$ (Scheme I, Fig. 1) also adopts a hydrogen-bonded sheet motif. The aromatic rings are aligned at 20.6 (1) and 40.8 (1) ° with respect to the triangular-shaped C_{aryl}–C(═*O*)–C_{aryl} fragment. The hydroxy groups are each hydrogen-bond donors to separate water molecules which also act as hydrogen-bond donors to an hydroxy group and a carbonyl group (Table 1). There are no hydroxy···carbonyl interactions, unlike those found in the anhydrous compound. The water molecule exists in an unusual four-coordinate environment in the resulting two-dimensional layer structure (Fig. 2).

S2. Experimental

Anhydrous 4,4′-dihydroxybenzophenone (0.25 mmol, 0.054 g) and boric acid (0.50 mmol, 0.031 g) were dissolved in a water-ethanol mixture (50 ml/100 ml *v*/*v*). Trimethylamine (33% aqueous solution) was added until the solution registered a neutral pH. The mixture was then set aside for a few days after which yellow crystal blocks of the title compound were isolated.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H = 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C). The hydroxy and water H-atoms were located in a difference Fourier map, and were included in the refinement with a distance restraint of O–H = 0.84±0.01 Å and with their isotropic displacement parameters refined.

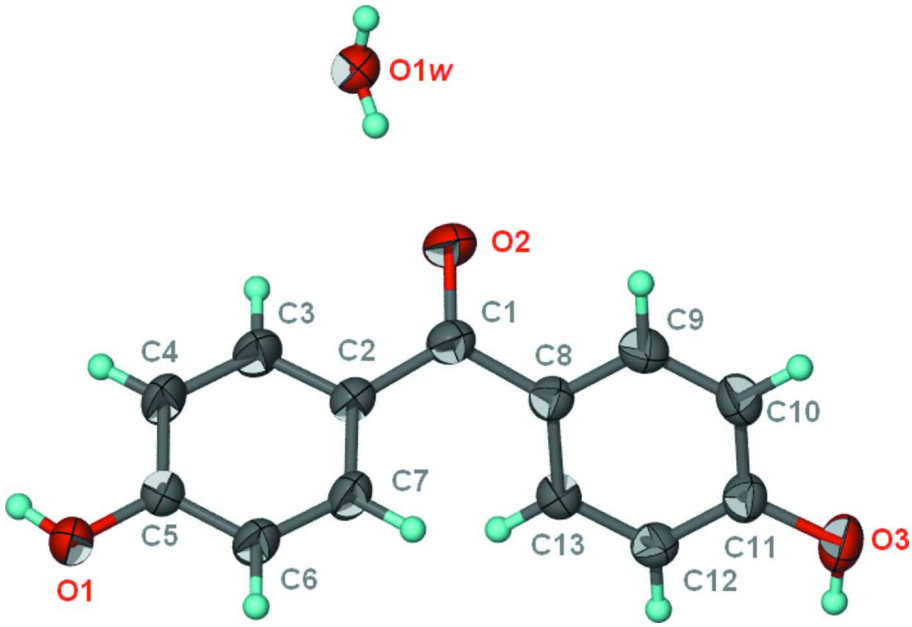

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{13}H_{10}O_3 \cdot H_2O$ at the 50% probability level.

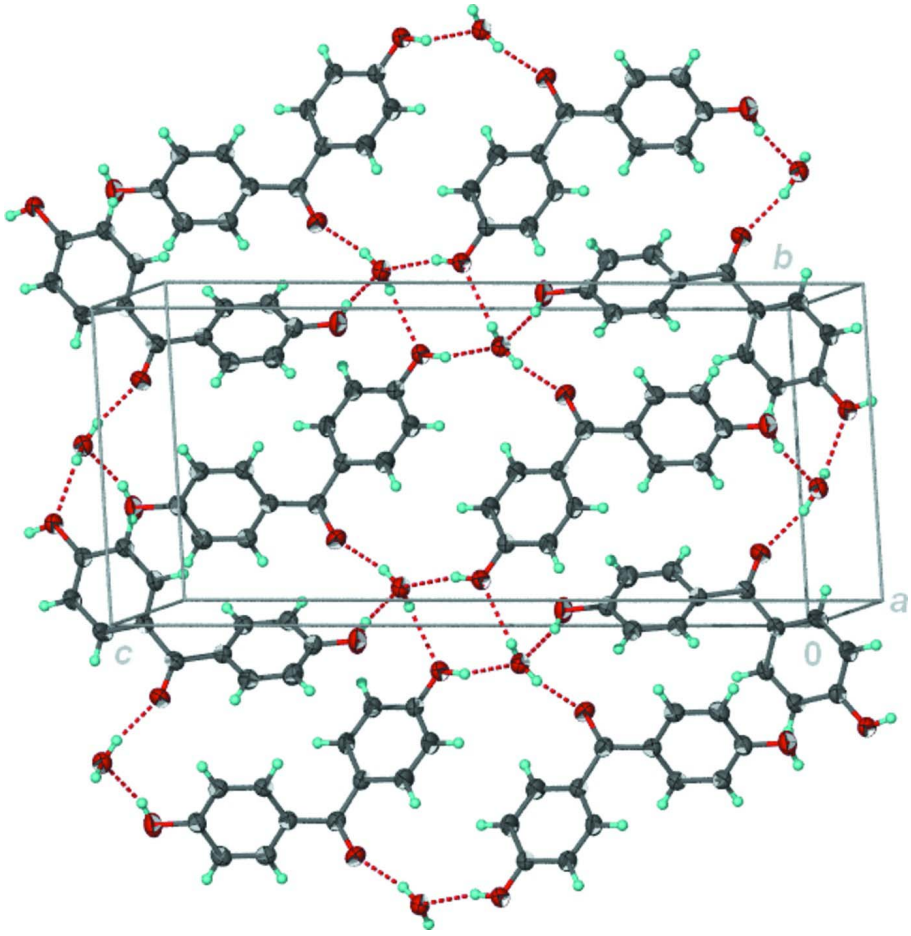

Figure 2

The layer structure of the title compound with hydrogen-bonding interactions shown as dashed lines.

4-(4-Hydroxybenzoyl)phenol monohydrate

Crystal data

$C_{13}H_{10}O_3 \cdot H_2O$
$M_r = 232.23$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 4.9398$ (1) Å
$b = 9.8273$ (2) Å
$c = 23.1446$ (4) Å
$\beta = 94.520$ (1)°
$V = 1120.06$ (4) Å^3
$Z = 4$

$F(000) = 488$
$D_x = 1.377$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3494 reflections
$\theta = 2.7$–$27.2°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Block, yellow
0.45 × 0.30 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans

8356 measured reflections
2572 independent reflections
2016 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$

$h = -6 \rightarrow 6$
$k = -11 \rightarrow 12$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.123$
$S = 1.05$
2572 reflections
170 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 0.2426P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.2714 (2)	0.12226 (11)	0.49586 (5)	0.0570 (3)
O2	0.5003 (3)	0.68859 (12)	0.38317 (5)	0.0671 (4)
O3	1.0143 (3)	0.54977 (14)	0.15066 (5)	0.0634 (3)
O1W	0.1638 (3)	0.86726 (12)	0.43550 (5)	0.0554 (3)
C1	0.5324 (3)	0.57501 (15)	0.36223 (6)	0.0465 (3)
C2	0.4542 (3)	0.45204 (15)	0.39381 (6)	0.0442 (3)
C3	0.2632 (4)	0.46347 (17)	0.43426 (8)	0.0676 (5)
H3A	0.1772	0.5466	0.4387	0.081*
C4	0.1979 (4)	0.35531 (17)	0.46788 (8)	0.0668 (5)
H4	0.0674	0.3653	0.4944	0.080*
C5	0.3249 (3)	0.23209 (15)	0.46244 (6)	0.0454 (3)
C6	0.5141 (3)	0.21717 (16)	0.42219 (7)	0.0536 (4)
H6	0.5993	0.1338	0.4180	0.064*
C7	0.5768 (3)	0.32592 (16)	0.38821 (6)	0.0508 (4)
H7	0.7037	0.3148	0.3610	0.061*
C8	0.6547 (3)	0.56332 (14)	0.30623 (6)	0.0426 (3)
C9	0.8488 (3)	0.65824 (16)	0.29241 (7)	0.0509 (4)
H9	0.8994	0.7271	0.3186	0.061*
C10	0.9667 (3)	0.65163 (17)	0.24064 (7)	0.0552 (4)
H10	1.1004	0.7139	0.2326	0.066*
C11	0.8866 (3)	0.55235 (15)	0.20044 (6)	0.0459 (3)
C12	0.6853 (3)	0.46052 (15)	0.21229 (6)	0.0457 (3)
H12A	0.6253	0.3962	0.1847	0.055*
C13	0.5745 (3)	0.46505 (14)	0.26519 (6)	0.0451 (3)
H13	0.4440	0.4013	0.2735	0.054*

H1	0.147 (4)	0.141 (2)	0.5179 (8)	0.091 (7)*
H3	0.946 (5)	0.4859 (19)	0.1296 (9)	0.103 (9)*
H11	0.260 (4)	0.8047 (19)	0.4233 (10)	0.101 (8)*
H12	0.262 (5)	0.921 (2)	0.4565 (10)	0.111 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0723 (7)	0.0453 (6)	0.0572 (7)	−0.0005 (5)	0.0286 (6)	0.0009 (5)
O2	0.1019 (10)	0.0421 (6)	0.0609 (7)	0.0052 (6)	0.0298 (7)	−0.0063 (5)
O3	0.0714 (8)	0.0729 (8)	0.0487 (6)	−0.0131 (6)	0.0223 (6)	−0.0028 (6)
O1W	0.0679 (7)	0.0496 (7)	0.0508 (6)	−0.0027 (6)	0.0174 (6)	−0.0040 (5)
C1	0.0537 (8)	0.0424 (8)	0.0440 (7)	0.0039 (6)	0.0080 (6)	−0.0038 (6)
C2	0.0493 (8)	0.0432 (8)	0.0413 (7)	0.0013 (6)	0.0103 (6)	−0.0042 (6)
C3	0.0859 (12)	0.0445 (9)	0.0784 (12)	0.0133 (8)	0.0452 (10)	−0.0004 (8)
C4	0.0808 (12)	0.0522 (9)	0.0741 (11)	0.0072 (8)	0.0478 (10)	−0.0008 (8)
C5	0.0519 (8)	0.0429 (8)	0.0429 (7)	−0.0032 (6)	0.0118 (6)	−0.0021 (6)
C6	0.0650 (9)	0.0450 (8)	0.0539 (9)	0.0108 (7)	0.0234 (7)	0.0010 (7)
C7	0.0582 (9)	0.0501 (8)	0.0470 (8)	0.0083 (7)	0.0223 (7)	0.0007 (6)
C8	0.0485 (7)	0.0388 (7)	0.0411 (7)	0.0031 (6)	0.0074 (6)	0.0012 (6)
C9	0.0605 (9)	0.0439 (8)	0.0486 (8)	−0.0085 (7)	0.0064 (7)	−0.0056 (6)
C10	0.0595 (9)	0.0514 (9)	0.0559 (9)	−0.0154 (7)	0.0123 (7)	−0.0002 (7)
C11	0.0505 (8)	0.0468 (8)	0.0413 (7)	0.0020 (6)	0.0089 (6)	0.0052 (6)
C12	0.0539 (8)	0.0426 (8)	0.0408 (7)	−0.0022 (6)	0.0045 (6)	−0.0030 (6)
C13	0.0497 (8)	0.0407 (7)	0.0458 (7)	−0.0041 (6)	0.0088 (6)	−0.0001 (6)

Geometric parameters (Å, º)

O1—C5	1.3659 (17)	C5—C6	1.3784 (19)
O1—H1	0.847 (10)	C6—C7	1.377 (2)
O2—C1	1.2322 (18)	C6—H6	0.9300
O3—C11	1.3566 (17)	C7—H7	0.9300
O3—H3	0.847 (10)	C8—C13	1.390 (2)
O1W—H11	0.841 (10)	C8—C9	1.393 (2)
O1W—H12	0.844 (10)	C9—C10	1.375 (2)
C1—C8	1.4771 (19)	C9—H9	0.9300
C1—C2	1.479 (2)	C10—C11	1.384 (2)
C2—C3	1.385 (2)	C10—H10	0.9300
C2—C7	1.390 (2)	C11—C12	1.386 (2)
C3—C4	1.371 (2)	C12—C13	1.3810 (19)
C3—H3A	0.9300	C12—H12A	0.9300
C4—C5	1.374 (2)	C13—H13	0.9300
C4—H4	0.9300		
C5—O1—H1	110.4 (16)	C6—C7—C2	121.32 (13)
C11—O3—H3	108.2 (17)	C6—C7—H7	119.3
H11—O1W—H12	110 (2)	C2—C7—H7	119.3
O2—C1—C8	119.34 (13)	C13—C8—C9	118.22 (13)

O2—C1—C2	119.92 (13)	C13—C8—C1	122.62 (13)
C8—C1—C2	120.73 (12)	C9—C8—C1	119.08 (13)
C3—C2—C7	117.41 (14)	C10—C9—C8	121.01 (14)
C3—C2—C1	119.09 (13)	C10—C9—H9	119.5
C7—C2—C1	123.34 (12)	C8—C9—H9	119.5
C4—C3—C2	121.61 (15)	C9—C10—C11	120.05 (14)
C4—C3—H3A	119.2	C9—C10—H10	120.0
C2—C3—H3A	119.2	C11—C10—H10	120.0
C3—C4—C5	120.11 (14)	O3—C11—C10	117.16 (13)
C3—C4—H4	119.9	O3—C11—C12	122.99 (14)
C5—C4—H4	119.9	C10—C11—C12	119.84 (13)
O1—C5—C4	122.29 (12)	C13—C12—C11	119.68 (13)
O1—C5—C6	118.08 (13)	C13—C12—H12A	120.2
C4—C5—C6	119.64 (14)	C11—C12—H12A	120.2
C7—C6—C5	119.90 (14)	C12—C13—C8	121.10 (13)
C7—C6—H6	120.1	C12—C13—H13	119.5
C5—C6—H6	120.1	C8—C13—H13	119.5

O2—C1—C2—C3	22.9 (2)	O2—C1—C8—C13	−144.18 (16)
C8—C1—C2—C3	−158.45 (16)	C2—C1—C8—C13	37.2 (2)
O2—C1—C2—C7	−152.26 (16)	O2—C1—C8—C9	32.5 (2)
C8—C1—C2—C7	26.4 (2)	C2—C1—C8—C9	−146.10 (15)
C7—C2—C3—C4	0.4 (3)	C13—C8—C9—C10	−2.8 (2)
C1—C2—C3—C4	−175.06 (18)	C1—C8—C9—C10	−179.63 (15)
C2—C3—C4—C5	0.8 (3)	C8—C9—C10—C11	2.2 (3)
C3—C4—C5—O1	178.47 (18)	C9—C10—C11—O3	−178.83 (15)
C3—C4—C5—C6	−1.3 (3)	C9—C10—C11—C12	0.6 (2)
O1—C5—C6—C7	−179.09 (15)	O3—C11—C12—C13	176.64 (14)
C4—C5—C6—C7	0.7 (3)	C10—C11—C12—C13	−2.8 (2)
C5—C6—C7—C2	0.5 (3)	C11—C12—C13—C8	2.2 (2)
C3—C2—C7—C6	−1.0 (3)	C9—C8—C13—C12	0.6 (2)
C1—C2—C7—C6	174.23 (15)	C1—C8—C13—C12	177.31 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1w^{i}	0.85 (1)	1.95 (1)	2.774 (2)	164 (2)
O3—H3···O1w^{ii}	0.85 (1)	1.95 (1)	2.773 (2)	164 (2)
O1w—H11···O2	0.84 (1)	1.93 (1)	2.762 (2)	168 (2)
O1w—H12···O1^{iii}	0.84 (1)	2.18 (2)	2.898 (2)	143 (2)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) *x*, *y*+1, *z*.