Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(5-Bromo-2-hydroxyphenyl)(phenyl)-methanone

Feng-Ke Yang,[a]* Yi-Ning Ding,[a] Wei Cheng[b] and Ke Xu[b]

[a]College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China, and [b]Key Laboratory of Advanced Materials, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China
Correspondence e-mail: minicocorain@163.com

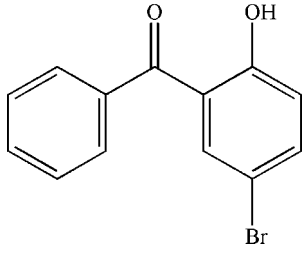
Received 26 August 2008; accepted 28 August 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.036; wR factor = 0.101; data-to-parameter ratio = 15.8.

In the title compound, $C_{13}H_9BrO_2$, the molecular conformation is stabilized by an intramolecular O—H···O hydrogen bond. In the crystal structure, weak intermolecular C—H···O hydrogen-bonding interactions link the molecules into chains along the c-axis direction.

Related literature

For related literature, see: Dale *et al.* (1999); Sridhar & Saravanan (2001); Wiktor *et al.* (2000); Hester *et al.* (2001); Idrees *et al.* (2001); Zhou (2006).



Experimental

Crystal data

$C_{13}H_9BrO_2$
M_r = 277.10
Monoclinic, $P2_1/c$
a = 15.938 (3) Å
b = 5.8929 (12) Å
c = 12.111 (2) Å
β = 106.15 (3)°
V = 1092.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.74 mm^{-1}
T = 295 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.417, T_{max} = 0.689
4878 measured reflections
2292 independent reflections
1767 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.08
2292 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1	0.82	1.85	2.570 (3)	146
C13—H13A···O2^{i}	0.93	2.59	3.475 (3)	160

Symmetry code: (i) $x, -y-\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

The authors thank the Natural Science Foundation of Shandong Province (No. Q2006B02).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2622).

References

Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dale, C. K., Leslie, A. D. & Stephen, D. F. (1999). *J. Phys. Chem. A*, **103**, 6420–6428.
Hester, J. B., Nidy, E. G., Perricone, S. C. & Poel, T. J. (2001). C07C257/00. WO Patent 0 144 188.
Idrees, M., Siddique, M., Patil, S. D., Doshi, A. G. & Raut, A. W. (2001). *Orient. J. Chem.* **17**, 131–133.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sridhar, S. K. & Saravanan, M. A. (2001). *J. Med. Chem.* **36**, 615–625.
Wiktor, Z., Danuta, M. & Therese, Z. H. (2000). *J. Phys. Chem. A*, **104**, 11685–11692.
Zhou, C. X. (2006). *J. Org. Chem.* **71**, 3551–3558.

supporting information

Acta Cryst. (2008). E**64**, o1873 [doi:10.1107/S1600536808027578]

(5-Bromo-2-hydroxyphenyl)(phenyl)methanone

Feng-Ke Yang, Yi-Ning Ding, Wei Cheng and Ke Xu

S1. Comment

Monocondensed Schiff bases are attractive because of their intermediates in the synthesis of unsymmetrical multidentate Schiff base ligands and metal complexes, which serve as potential chelating agents and catalyst in synthesis and pharmaceutical fields (Hester *et al.*, 2001). New examples are being tested for their antitumor, (Idrees *et al.*, 2001). antimicroial and antiviral activities (Sridhar & Saravanan, 2001). We describe the structure of the title compound is a precursor of monocondensed Schiff bases.

In the title compound, bond lengths are slightly different from those in similar compounds. The C—Br bond length [1.896 (3) Å] is longer than others reported [1.865 (1) (Dale *et al.*, 1999) and 1.884 (2)Å (Wiktor *et al.*, 2000)]. Molecular conformation is stabilized by an intramolecular O—H···O hydrogen bond. In the crystal structure, weak intermolecular C—H···O hydrogen bonding interactions (Table 1) link the molecules into chains along the b-direction.

S2. Experimental

5-Bromo-2-hydroxybenzophenone was prepared *via* the Fries rearrangement of *p*-bromophenyl benzoate at 433 K with $AlCl_3$ as the catalyst. The title compound was collected and washed with 10% diluted hydrochloric acid. Single crystals suitable for X-ray measurements were obtained by recrystallization from absolute ethanol and acetic ether (1:1,*v*/*v*) at room temperature.

S3. Refinement

All H atoms were placed at calculated positions and allowed to ride on their attached atoms, with C—H distance = 0.93 Å and O—H = 0.82 Å, and with U_{iso} =1.2 U_{eq} (C) and U_{iso} =1.5 U_{eq} (O).

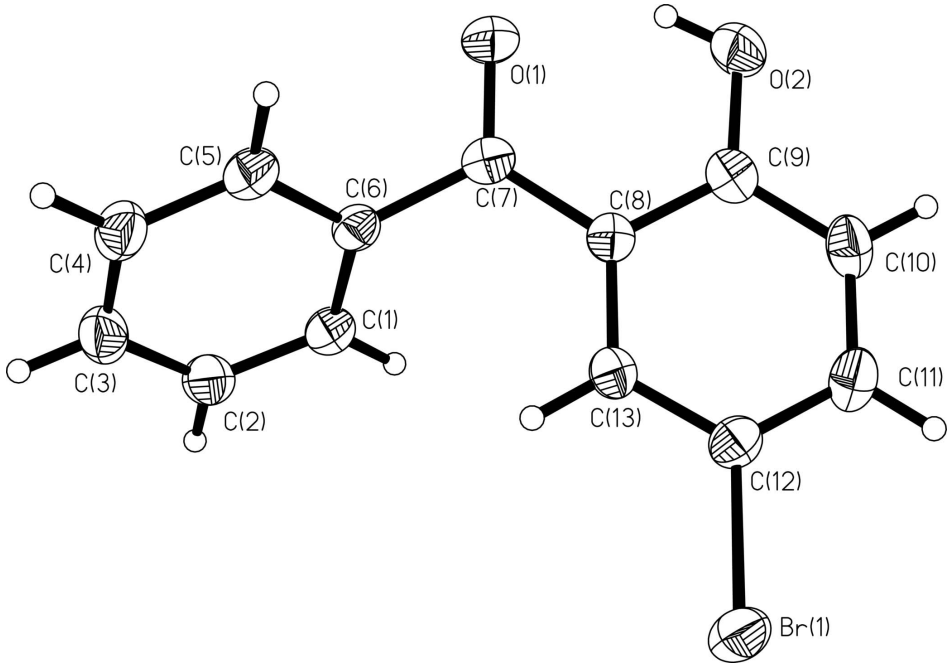


Figure 1

The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

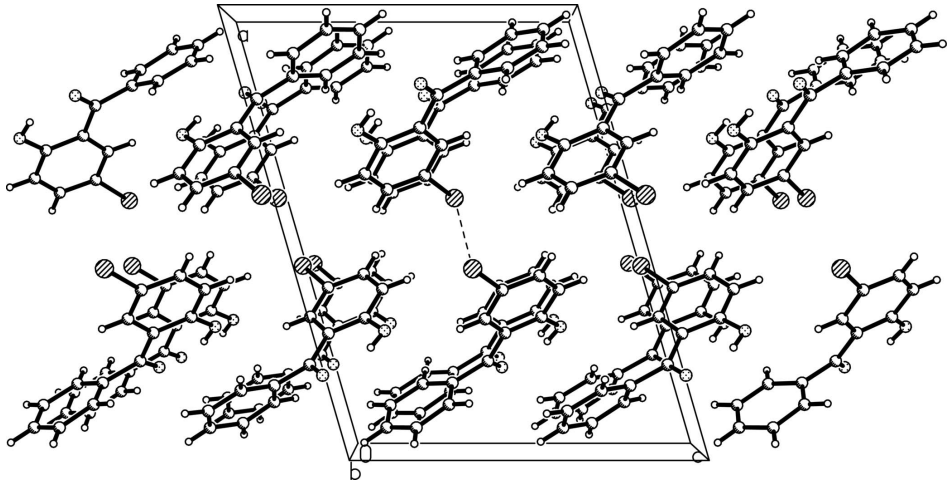


Figure 2

The packing of (I), viewed down the *b* axis.

(5-Bromo-2-hydroxyphenyl)(phenyl)methanone

Crystal data

$C_{13}H_9BrO_2$
M_r = 277.10
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.938 (3) Å
b = 5.8929 (12) Å
c = 12.111 (2) Å
β = 106.15 (3)°
V = 1092.6 (4) Å^3
Z = 4
F(000) = 552
D_x = 1.685 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1025 reflections
θ = 1.3–27.0°
μ = 3.74 mm^{-1}

T = 295 K
Block, yellow

0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Thin–slice ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.417, T_{max} = 0.689

4878 measured reflections
2292 independent reflections
1767 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 26.7°, θ_{min} = 1.3°
h = −19→19
k = −7→6
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.08
2292 reflections
145 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.0875P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 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.

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 $F^2 > \sigma(F^2)$ 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}
Br1	0.42247 (2)	0.27571 (6)	0.49704 (3)	0.06162 (16)
O1	0.18993 (15)	−0.6147 (4)	0.49901 (19)	0.0609 (6)
O2	0.28487 (15)	−0.5189 (4)	0.70244 (19)	0.0613 (6)
H2A	0.2498	−0.5930	0.6532	0.092*
C1	0.11815 (19)	−0.1537 (5)	0.3198 (3)	0.0457 (7)
H1A	0.1235	−0.0469	0.3779	0.055*
C2	0.06832 (19)	−0.1057 (5)	0.2101 (3)	0.0518 (7)
H2B	0.0378	0.0305	0.1950	0.062*
C3	0.0635 (2)	−0.2590 (5)	0.1225 (3)	0.0580 (9)
H3A	0.0308	−0.2246	0.0480	0.070*
C4	0.1071 (2)	−0.4629 (5)	0.1454 (3)	0.0560 (8)
H4A	0.1049	−0.5649	0.0861	0.067*
C5	0.1541 (2)	−0.5160 (5)	0.2561 (3)	0.0484 (7)
H5A	0.1816	−0.6563	0.2718	0.058*

C6	0.16053 (17)	−0.3611 (5)	0.3442 (2)	0.0398 (6)
C7	0.20826 (18)	−0.4302 (5)	0.4640 (3)	0.0432 (6)
C8	0.27492 (18)	−0.2824 (4)	0.5359 (3)	0.0387 (6)
C9	0.30999 (19)	−0.3350 (5)	0.6535 (3)	0.0469 (7)
C10	0.3733 (2)	−0.1974 (6)	0.7230 (3)	0.0554 (8)
H10A	0.3943	−0.2292	0.8011	0.066*
C11	0.4053 (2)	−0.0134 (6)	0.6774 (3)	0.0564 (8)
H11A	0.4476	0.0795	0.7245	0.068*
C12	0.37446 (18)	0.0319 (5)	0.5617 (3)	0.0453 (7)
C13	0.30905 (17)	−0.0964 (5)	0.4910 (2)	0.0408 (6)
H13A	0.2876	−0.0595	0.4136	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0542 (2)	0.0546 (2)	0.0743 (3)	−0.01334 (14)	0.01486 (18)	0.00225 (16)
O1	0.0721 (15)	0.0486 (12)	0.0597 (14)	−0.0165 (11)	0.0143 (12)	0.0081 (10)
O2	0.0680 (15)	0.0658 (14)	0.0489 (13)	−0.0075 (11)	0.0140 (11)	0.0156 (11)
C1	0.0468 (16)	0.0418 (14)	0.0496 (18)	−0.0017 (13)	0.0151 (14)	−0.0040 (13)
C2	0.0443 (17)	0.0504 (17)	0.057 (2)	0.0004 (13)	0.0087 (14)	0.0051 (15)
C3	0.0526 (19)	0.072 (2)	0.0452 (18)	−0.0139 (16)	0.0063 (15)	0.0036 (16)
C4	0.065 (2)	0.0589 (19)	0.0454 (18)	−0.0105 (16)	0.0173 (16)	−0.0108 (15)
C5	0.0524 (18)	0.0421 (15)	0.0526 (18)	−0.0039 (13)	0.0174 (15)	−0.0071 (13)
C6	0.0377 (14)	0.0398 (14)	0.0428 (16)	−0.0044 (11)	0.0128 (12)	−0.0016 (12)
C7	0.0458 (16)	0.0391 (14)	0.0484 (17)	−0.0014 (12)	0.0194 (13)	−0.0020 (12)
C8	0.0360 (14)	0.0399 (14)	0.0414 (16)	0.0049 (11)	0.0126 (12)	−0.0018 (11)
C9	0.0442 (16)	0.0540 (16)	0.0450 (18)	0.0055 (13)	0.0165 (13)	0.0029 (13)
C10	0.0492 (18)	0.077 (2)	0.0365 (17)	0.0005 (16)	0.0067 (14)	0.0010 (15)
C11	0.0470 (18)	0.072 (2)	0.0476 (19)	−0.0087 (15)	0.0084 (14)	−0.0105 (16)
C12	0.0402 (15)	0.0461 (15)	0.0516 (18)	−0.0020 (12)	0.0160 (13)	−0.0031 (13)
C13	0.0392 (15)	0.0443 (15)	0.0387 (16)	0.0046 (11)	0.0105 (12)	−0.0001 (12)

Geometric parameters (Å, º)

Br1—C12	1.896 (3)	C5—C6	1.386 (4)
O1—C7	1.231 (3)	C5—H5A	0.9300
O2—C9	1.348 (4)	C6—C7	1.495 (4)
O2—H2A	0.8200	C7—C8	1.460 (4)
C1—C2	1.374 (4)	C8—C13	1.400 (4)
C1—C6	1.388 (4)	C8—C9	1.412 (4)
C1—H1A	0.9300	C9—C10	1.383 (4)
C2—C3	1.379 (5)	C10—C11	1.378 (4)
C2—H2B	0.9300	C10—H10A	0.9300
C3—C4	1.378 (4)	C11—C12	1.377 (4)
C3—H3A	0.9300	C11—H11A	0.9300
C4—C5	1.377 (4)	C12—C13	1.376 (4)
C4—H4A	0.9300	C13—H13A	0.9300

C9—O2—H2A	109.5	O1—C7—C6	118.0 (3)
C2—C1—C6	120.2 (3)	C8—C7—C6	120.4 (2)
C2—C1—H1A	119.9	C13—C8—C9	118.5 (3)
C6—C1—H1A	119.9	C13—C8—C7	122.2 (3)
C1—C2—C3	120.2 (3)	C9—C8—C7	119.3 (3)
C1—C2—H2B	119.9	O2—C9—C10	117.3 (3)
C3—C2—H2B	119.9	O2—C9—C8	122.5 (3)
C4—C3—C2	120.0 (3)	C10—C9—C8	120.2 (3)
C4—C3—H3A	120.0	C11—C10—C9	120.4 (3)
C2—C3—H3A	120.0	C11—C10—H10A	119.8
C5—C4—C3	120.1 (3)	C9—C10—H10A	119.8
C5—C4—H4A	120.0	C12—C11—C10	119.6 (3)
C3—C4—H4A	120.0	C12—C11—H11A	120.2
C4—C5—C6	120.2 (3)	C10—C11—H11A	120.2
C4—C5—H5A	119.9	C13—C12—C11	121.4 (3)
C6—C5—H5A	119.9	C13—C12—Br1	118.8 (2)
C5—C6—C1	119.2 (3)	C11—C12—Br1	119.8 (2)
C5—C6—C7	118.5 (3)	C12—C13—C8	119.8 (3)
C1—C6—C7	122.2 (3)	C12—C13—H13A	120.1
O1—C7—C8	121.6 (3)	C8—C13—H13A	120.1

C6—C1—C2—C3	−3.1 (5)	C6—C7—C8—C9	170.9 (2)
C1—C2—C3—C4	1.4 (5)	C13—C8—C9—O2	−175.9 (3)
C2—C3—C4—C5	1.4 (5)	C7—C8—C9—O2	0.6 (4)
C3—C4—C5—C6	−2.5 (5)	C13—C8—C9—C10	3.4 (4)
C4—C5—C6—C1	0.9 (4)	C7—C8—C9—C10	179.9 (3)
C4—C5—C6—C7	176.9 (3)	O2—C9—C10—C11	176.6 (3)
C2—C1—C6—C5	1.9 (4)	C8—C9—C10—C11	−2.8 (5)
C2—C1—C6—C7	−173.9 (3)	C9—C10—C11—C12	−0.5 (5)
C5—C6—C7—O1	−48.6 (4)	C10—C11—C12—C13	3.1 (5)
C1—C6—C7—O1	127.3 (3)	C10—C11—C12—Br1	−176.9 (2)
C5—C6—C7—C8	130.9 (3)	C11—C12—C13—C8	−2.4 (4)
C1—C6—C7—C8	−53.2 (4)	Br1—C12—C13—C8	177.60 (19)
O1—C7—C8—C13	166.7 (3)	C9—C8—C13—C12	−0.9 (4)
C6—C7—C8—C13	−12.8 (4)	C7—C8—C13—C12	−177.2 (2)
O1—C7—C8—C9	−9.6 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O1	0.82	1.85	2.570 (3)	146
C13—H13*A*···O2^{i}	0.93	2.59	3.475 (3)	160

Symmetry code: (i) *x*, −*y*−1/2, *z*−1/2.