

2-Bromo-1-phenylethanone

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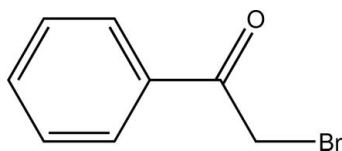
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Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.029; wR factor = 0.072; data-to-parameter ratio = 20.5.

The title compound, $\text{C}_8\text{H}_7\text{BrO}$, is a halogenated derivative of acetophenone. The molecule shows noncrystallographic C_s symmetry. The intracyclic C—C—C angles cover the range 118.8 (2)–120.4 (3)°. In the crystal structure, C—H...O contacts connect the molecules into undulating sheets perpendicular to the crystallographic c axis.

Related literature

For the crystal structure of α -chloro-acetophenone, see: Barrans & Maisseu (1966); Grossert *et al.* (1984). For the crystal structure of α -iodo-acetophenone, see: Lere-Porte *et al.* (1982). For the crystal structures of coordination compounds using the title compound as a ligand, see: Laube *et al.* (1991). For details of graph-set analysis of hydrogen bonds, see: Etter *et al.* (1990); Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_8\text{H}_7\text{BrO}$ $M_r = 199.05$ Orthorhombic, $P2_12_12_1$ $a = 4.1459$ (2) Å $b = 9.6731$ (5) Å $c = 18.8178$ (9) Å $V = 754.66$ (6) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 5.37$ mm⁻¹ $T = 200$ K $0.54 \times 0.43 \times 0.09$ mm

Data collection

Bruker APEXII CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Bruker, 2010)

 $T_{\min} = 0.588$, $T_{\max} = 1.000$

7436 measured reflections

1867 independent reflections

1692 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.037$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.029$ $wR(F^2) = 0.072$ $S = 1.08$

1867 reflections

91 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.42$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.66$ e Å⁻³

Absolute structure: Flack (1983),

with 736 Friedel pairs

Flack parameter: 0.015 (14)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C2}-\text{H21}\cdots\text{O1}^i$	0.99	2.46	3.317 (4)	145
$\text{C2}-\text{H22}\cdots\text{O1}^{ii}$	0.99	2.44	3.268 (4)	141
$\text{C8}-\text{H8}\cdots\text{O1}^i$	0.95	2.60	3.442 (3)	148

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

Data collection: APEX2 (Bruker, 2010); cell refinement: SAINT (Bruker, 2010); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

The authors thank Mr Benjamin Wilson for helpful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2008).

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supplementary materials

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2-Bromo-1-phenylethanone

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Comment

Derivatives of acetophenone are widely used in preparative organic chemistry. At the beginning of a comprehensive study about the effects of various substituents on benzo-annulated seven-membered ring systems, the molecular structure of the title compound was determined to enable comparisons with acetophenone-derived target compounds.

Intracyclic C—C—C angles span a range from 118–120°. The smallest angle is found on the C atom bearing the carbonylic substituent while the second smallest one is found on the C atom in *para*-position. The atoms of the aliphatic substituent are nearly coplanar with the aromatic system and its conjugated carbonyl group, the least-squares planes defined by their respective atoms intersect at an angle of only 4.18 (15)°.

In the crystal structure, C—H···O contacts can be observed which stem from both H atoms of the methylene group as well as one of the H atoms in *ortho*-position to the substituent on the phenyl ring. The carbonylic O atom serves as threefold acceptor (Fig. 2). Describing these contacts in terms of graph-set analysis necessitates a $C(4)C(4)C(5)$ descriptor on the unitary level. In total, the molecules are connected to waved sheets perpendicular to the crystallographic *c* axis. The shortest distance between the centroids of two π -systems was measured at 5.8289 (17) Å.

The packing of the compound in the crystal is shown in Fig. 3.

Experimental

The compound was obtained commercially (Schuchardt). Crystals suitable for the X-ray diffraction study were taken directly from the provided batch.

Refinement

Carbon-bound H atoms were placed in calculated positions (C—H 0.99 Å for the methylene group and C—H 0.95 Å for aromatic C atoms) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$.

Figures

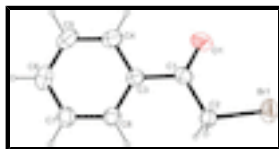


Fig. 1. The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level).

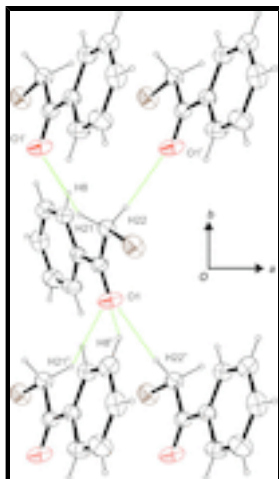


Fig. 2. Intermolecular contacts, viewed along $[001]$. Symmetry operators: ⁱ $-x + 1, y + 1/2, -z + 1/2$; ⁱⁱ $-x + 2, y + 1/2, -z + 1/2$; ⁱⁱⁱ $-x + 1, y - 1/2, -z + 1/2$; ^{iv} $-x + 2, y - 1/2, -z + 1/2$.

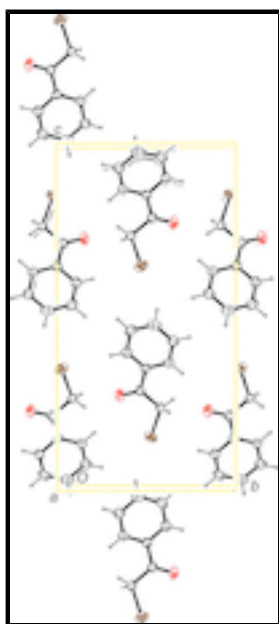


Fig. 3. Molecular packing of the title compound, viewed along $[100]$ (anisotropic displacement ellipsoids drawn at 50% probability level).

2-Bromo-1-phenylethanone

Crystal data

C_8H_7BrO

$M_r = 199.05$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 4.1459 (2) \text{ \AA}$

$b = 9.6731 (5) \text{ \AA}$

$c = 18.8178 (9) \text{ \AA}$

$V = 754.66 (6) \text{ \AA}^3$

$Z = 4$

$F(000) = 392$

$D_x = 1.752 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 5571 reflections

$\theta = 2.4\text{--}28.2^\circ$

$\mu = 5.37 \text{ mm}^{-1}$

$T = 200 \text{ K}$

Platelet, colourless

$0.54 \times 0.43 \times 0.09 \text{ mm}$

Data collection

Bruker APEXII CCD diffractometer	1867 independent reflections
Radiation source: fine-focus sealed tube graphite	1692 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.037$
Absorption correction: multi-scan (SADABS; Bruker, 2010)	$\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 3.9^\circ$
$T_{\text{min}} = 0.588$, $T_{\text{max}} = 1.000$	$h = -4 \rightarrow 5$
7436 measured reflections	$k = -12 \rightarrow 12$
	$l = -25 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.072$	$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 0.0956P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
1867 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
91 parameters	$\Delta\rho_{\text{max}} = 0.42 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.66 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 736 Friedel pairs
	Flack parameter: 0.015 (14)

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.94179 (9)	0.02569 (3)	0.353315 (15)	0.04357 (12)
O1	0.7669 (6)	-0.1520 (2)	0.22942 (12)	0.0462 (6)
C1	0.6825 (7)	-0.0344 (3)	0.21549 (14)	0.0288 (5)
C2	0.7424 (7)	0.0837 (3)	0.26609 (14)	0.0302 (6)
H21	0.5345	0.1292	0.2771	0.036*
H22	0.8828	0.1527	0.2426	0.036*
C3	0.5113 (6)	-0.0030 (2)	0.14809 (12)	0.0269 (5)
C4	0.4564 (9)	-0.1109 (3)	0.10021 (14)	0.0361 (6)
H4	0.5303	-0.2014	0.1111	0.043*
C5	0.2955 (9)	-0.0866 (3)	0.03729 (16)	0.0416 (7)
H5	0.2609	-0.1604	0.0049	0.050*
C6	0.1839 (9)	0.0449 (4)	0.02105 (16)	0.0400 (7)
H6	0.0712	0.0610	-0.0221	0.048*
C7	0.2374 (8)	0.1525 (3)	0.06797 (14)	0.0355 (7)
H7	0.1621	0.2426	0.0569	0.043*
C8	0.4002 (7)	0.1294 (3)	0.13102 (14)	0.0303 (6)

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H8 0.4366 0.2039 0.1629 0.036*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04576 (18)	0.04907 (17)	0.03589 (16)	-0.00752 (13)	-0.01195 (14)	0.01138 (12)
O1	0.0662 (17)	0.0267 (9)	0.0455 (12)	0.0095 (11)	-0.0047 (13)	0.0036 (8)
C1	0.0309 (13)	0.0263 (11)	0.0293 (13)	0.0013 (11)	0.0051 (11)	0.0042 (10)
C2	0.0328 (15)	0.0308 (12)	0.0270 (12)	-0.0025 (12)	-0.0040 (12)	0.0023 (11)
C3	0.0288 (13)	0.0273 (12)	0.0246 (11)	-0.0022 (8)	0.0046 (12)	0.0001 (9)
C4	0.0474 (17)	0.0269 (11)	0.0341 (14)	-0.0029 (13)	0.0083 (15)	-0.0029 (9)
C5	0.052 (2)	0.0408 (15)	0.0325 (15)	-0.0080 (16)	0.0017 (16)	-0.0121 (13)
C6	0.0385 (16)	0.0567 (19)	0.0247 (13)	-0.0042 (14)	-0.0012 (13)	0.0008 (12)
C7	0.0393 (18)	0.0386 (14)	0.0286 (14)	0.0046 (13)	0.0011 (14)	0.0028 (11)
C8	0.0360 (16)	0.0288 (12)	0.0262 (13)	-0.0008 (11)	0.0026 (12)	-0.0005 (9)

Geometric parameters (\AA , $^\circ$)

Br1—C2	1.922 (3)	C4—H4	0.9500
O1—C1	1.219 (3)	C5—C6	1.388 (5)
C1—C3	1.485 (4)	C5—H5	0.9500
C1—C2	1.508 (4)	C6—C7	1.382 (4)
C2—H21	0.9900	C6—H6	0.9500
C2—H22	0.9900	C7—C8	1.383 (4)
C3—C4	1.397 (3)	C7—H7	0.9500
C3—C8	1.399 (3)	C8—H8	0.9500
C4—C5	1.379 (4)		
O1—C1—C3	120.8 (2)	C3—C4—H4	119.8
O1—C1—C2	121.6 (3)	C4—C5—C6	120.4 (3)
C3—C1—C2	117.6 (2)	C4—C5—H5	119.8
C1—C2—Br1	112.88 (19)	C6—C5—H5	119.8
C1—C2—H21	109.0	C7—C6—C5	119.7 (3)
Br1—C2—H21	109.0	C7—C6—H6	120.1
C1—C2—H22	109.0	C5—C6—H6	120.1
Br1—C2—H22	109.0	C6—C7—C8	120.3 (3)
H21—C2—H22	107.8	C6—C7—H7	119.8
C4—C3—C8	118.8 (2)	C8—C7—H7	119.8
C4—C3—C1	118.4 (2)	C7—C8—C3	120.4 (2)
C8—C3—C1	122.8 (2)	C7—C8—H8	119.8
C5—C4—C3	120.4 (3)	C3—C8—H8	119.8
C5—C4—H4	119.8		
O1—C1—C2—Br1	-2.6 (4)	C1—C3—C4—C5	179.4 (3)
C3—C1—C2—Br1	176.40 (19)	C3—C4—C5—C6	-0.5 (5)
O1—C1—C3—C4	-1.6 (4)	C4—C5—C6—C7	0.7 (5)
C2—C1—C3—C4	179.4 (3)	C5—C6—C7—C8	-0.3 (5)
O1—C1—C3—C8	177.7 (3)	C6—C7—C8—C3	-0.2 (4)
C2—C1—C3—C8	-1.3 (4)	C4—C3—C8—C7	0.3 (4)
C8—C3—C4—C5	0.0 (4)	C1—C3—C8—C7	-179.0 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C2—H21···O1 ⁱ	0.99	2.46	3.317 (4)	145
C2—H22···O1 ⁱⁱ	0.99	2.44	3.268 (4)	141
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Fig. 1

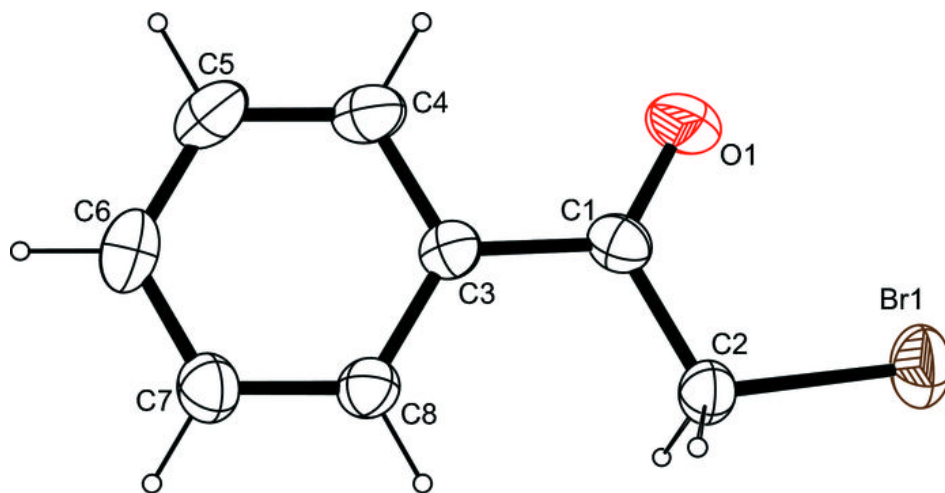


Fig. 2

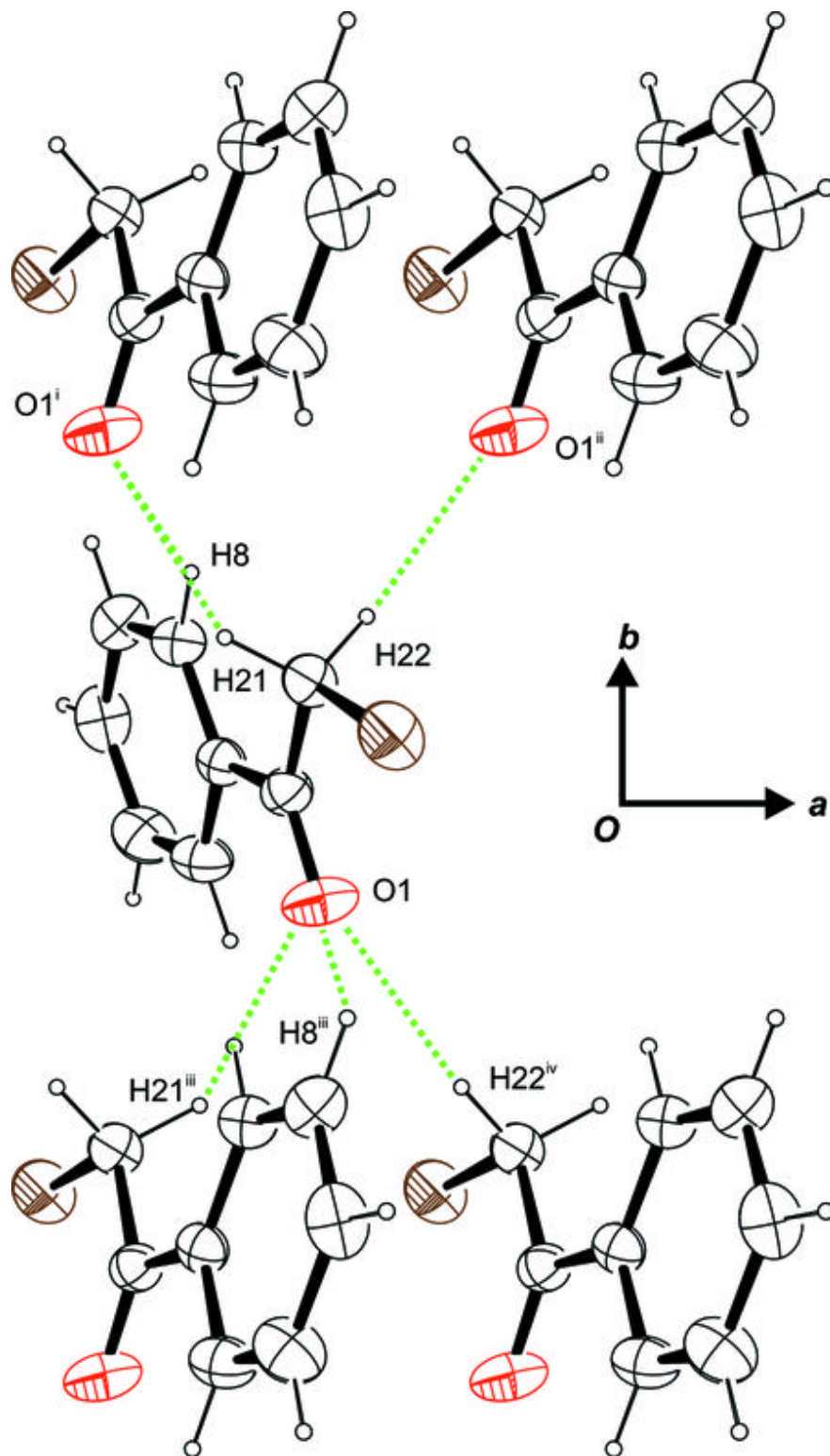


Fig. 3

