

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

4-(Hydroxymethyl)phenol

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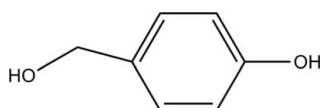
Received 15 May 2009; accepted 12 June 2009

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.035; wR factor = 0.076; data-to-parameter ratio = 16.8.

In the molecule of the title compound, $\text{C}_7\text{H}_8\text{O}_2$, the phenol O and hydroxymethyl C atoms lie in the ring plane [deviations of -0.015 (3) and 0.013 (3) Å, respectively]. In the crystal structure, intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds link molecules into a network. A weak $\text{C}-\text{H}\cdots\pi$ interaction is also found.

Related literature

For a related structure, see: Tale *et al.* (2003). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_7\text{H}_8\text{O}_2$
 $M_r = 124.13$
Orthorhombic, $Pna2_1$
 $a = 9.524$ (3) Å

$b = 11.006$ (4) Å
 $c = 5.942$ (2) Å
 $V = 622.9$ (4) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹

$T = 298$ K
 $0.65 \times 0.62 \times 0.55$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.940$, $T_{\max} = 0.949$

3751 measured reflections
1414 independent reflections
1200 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.076$
 $S = 1.00$
1414 reflections
84 parameters

1 restraint
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{O2}^{\text{i}}$	0.82	1.86	2.668 (3)	169
$\text{O2}-\text{H2}\cdots\text{O1}^{\text{ii}}$	0.82	2.01	2.817 (3)	167
$\text{C1}-\text{H1B}\cdots\text{Cg1}^{\text{iii}}$	0.97	2.77	3.694 (3)	159

Symmetry codes: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x + \frac{1}{2}, -y + \frac{1}{2}, z - 1$; (iii) $-x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$. Cg1 is the centroid of the C2-C7 ring.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* and *PLATON*.

The authors thank the National Natural Science Foundation of China (grant Nos. 20771048 and 20621091) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2691).

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supplementary materials

Acta Cryst. (2009). E65, o1689 [doi:10.1107/S1600536809022466]

4-(Hydroxymethyl)phenol

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Comment

The reduction of carboxylic acids to alcohols is a key synthetic transformation in organic chemistry. There are several ways to bring about this transformation. It is conventionally carried out using sodium borohydride as a reducing agent. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Ring A (C2-C7) is, of course, planar. Atoms O1, O2 and C1 are -0.015 (3), 1.279 (3) and 0.013 (3) Å away from the ring plane, respectively.

In the crystal structure, intermolecular O-H...O hydrogen bonds (Table 1) link the molecules into a network, in which they may be effective in the stabilization of the structure. There also exists a weak C—H... π interaction (Table 1).

Experimental

The title compound was prepared by reducing corresponding carboxylic acid using sodium borohydride in THF solution according to a literature method (Tale *et al.*, 2003). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate solution.

Refinement

H atoms were positioned geometrically, with O-H = 0.82 Å (for OH) and C-H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{O})$, where $x = 1.5$ for OH H and $x = 1.2$ for all other H atoms. The absolute structure could not be determined reliably, and 605 Friedel pairs were averaged before the last cycle of refinement.

Figures

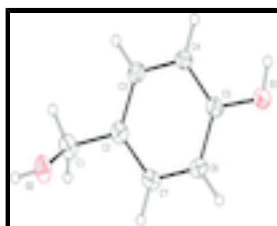


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

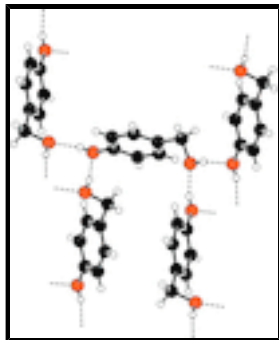


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

4-(Hydroxymethyl)phenol

Crystal data

$C_7H_8O_2$

$M_r = 124.13$

Orthorhombic, $Pna2_1$

Hall symbol: P 2c -2n

$a = 9.524 (3) \text{ \AA}$

$b = 11.006 (4) \text{ \AA}$

$c = 5.942 (2) \text{ \AA}$

$V = 622.9 (4) \text{ \AA}^3$

$Z = 4$

$F_{000} = 264$

$D_x = 1.324 \text{ Mg m}^{-3}$

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

Cell parameters from 1897 reflections

$\theta = 2.8\text{--}27.9^\circ$

$\mu = 0.10 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Block, colorless

$0.65 \times 0.62 \times 0.55 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298 \text{ K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.940$, $T_{\max} = 0.949$

3751 measured reflections

1414 independent reflections

1200 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 27.8^\circ$

$\theta_{\min} = 2.8^\circ$

$h = -12 \rightarrow 8$

$k = -14 \rightarrow 14$

$l = -7 \rightarrow 7$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.076$

$S = 1.00$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0125P)^2 + 0.2042P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

1414 reflections $\Delta\rho_{\max} = 0.15 \text{ e \AA}^{-3}$
 84 parameters $\Delta\rho_{\min} = -0.16 \text{ e \AA}^{-3}$
 1 restraint Extinction correction: none
 Primary atom site location: structure-invariant direct methods

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.65915 (14)	0.47478 (11)	0.5585 (2)	0.0477 (3)
H1	0.6206	0.5344	0.5036	0.072*
O2	0.99603 (14)	0.15137 (10)	-0.1224 (3)	0.0470 (3)
H2	1.0542	0.1183	-0.2037	0.071*
C1	1.05125 (18)	0.26412 (15)	-0.0417 (3)	0.0422 (4)
H1A	1.0696	0.3180	-0.1675	0.051*
H1B	1.1391	0.2500	0.0366	0.051*
C2	0.94754 (17)	0.32168 (14)	0.1149 (3)	0.0351 (4)
C3	0.87551 (17)	0.42678 (14)	0.0552 (3)	0.0367 (4)
H3	0.8929	0.4626	-0.0838	0.044*
C4	0.77818 (18)	0.47925 (15)	0.1993 (3)	0.0356 (4)
H4	0.7304	0.5492	0.1563	0.043*
C5	0.75251 (16)	0.42727 (13)	0.4065 (3)	0.0349 (4)
C6	0.82324 (18)	0.32200 (15)	0.4694 (3)	0.0406 (4)
H6	0.8058	0.2864	0.6086	0.049*
C7	0.91947 (18)	0.27084 (15)	0.3239 (3)	0.0411 (4)
H7	0.9666	0.2006	0.3668	0.049*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0571 (8)	0.0424 (7)	0.0437 (8)	0.0143 (6)	0.0121 (7)	0.0079 (6)
O2	0.0487 (7)	0.0391 (6)	0.0532 (8)	-0.0069 (6)	0.0148 (6)	-0.0085 (6)
C1	0.0361 (9)	0.0379 (8)	0.0526 (11)	-0.0041 (7)	0.0067 (8)	-0.0032 (9)
C2	0.0326 (8)	0.0322 (8)	0.0404 (10)	-0.0045 (7)	-0.0004 (7)	-0.0027 (7)
C3	0.0432 (9)	0.0326 (8)	0.0345 (9)	-0.0051 (7)	0.0014 (8)	0.0037 (8)
C4	0.0412 (9)	0.0277 (7)	0.0381 (10)	0.0003 (7)	-0.0028 (8)	0.0030 (7)

supplementary materials

C5	0.0365 (8)	0.0308 (7)	0.0374 (9)	0.0000 (6)	-0.0008 (7)	-0.0008 (7)
C6	0.0475 (10)	0.0382 (9)	0.0362 (9)	0.0035 (8)	0.0012 (8)	0.0088 (7)
C7	0.0425 (9)	0.0353 (8)	0.0454 (10)	0.0079 (7)	-0.0023 (8)	0.0035 (8)

Geometric parameters (Å, °)

O1—H1	0.8200	C3—H3	0.9300
O2—H2	0.8200	C4—C5	1.380 (2)
C1—O2	1.430 (2)	C4—H4	0.9300
C1—C2	1.498 (2)	C5—O1	1.371 (2)
C1—H1A	0.9700	C5—C6	1.391 (2)
C1—H1B	0.9700	C6—C7	1.380 (3)
C2—C7	1.388 (3)	C6—H6	0.9300
C2—C3	1.391 (2)	C7—H7	0.9300
C3—C4	1.388 (2)		
C5—O1—H1	109.5	C2—C3—H3	119.4
C1—O2—H2	109.5	C5—C4—C3	119.76 (15)
O2—C1—C2	109.44 (13)	C5—C4—H4	120.1
O2—C1—H1A	109.8	C3—C4—H4	120.1
C2—C1—H1A	109.8	O1—C5—C4	123.00 (14)
O2—C1—H1B	109.8	O1—C5—C6	117.03 (16)
C2—C1—H1B	109.8	C4—C5—C6	119.96 (16)
H1A—C1—H1B	108.2	C7—C6—C5	119.52 (17)
C7—C2—C3	117.92 (16)	C7—C6—H6	120.2
C7—C2—C1	120.83 (15)	C5—C6—H6	120.2
C3—C2—C1	121.25 (16)	C6—C7—C2	121.61 (16)
C4—C3—C2	121.22 (17)	C6—C7—H7	119.2
C4—C3—H3	119.4	C2—C7—H7	119.2
O2—C1—C2—C7	68.9 (2)	C3—C4—C5—C6	-0.6 (2)
O2—C1—C2—C3	-110.49 (18)	O1—C5—C6—C7	-179.38 (16)
C7—C2—C3—C4	-0.2 (2)	C4—C5—C6—C7	0.4 (3)
C1—C2—C3—C4	179.21 (16)	C5—C6—C7—C2	-0.2 (3)
C2—C3—C4—C5	0.5 (2)	C3—C2—C7—C6	0.1 (3)
C3—C4—C5—O1	179.21 (15)	C1—C2—C7—C6	-179.37 (16)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots O2 ⁱ	0.82	1.86	2.668 (3)	169
O2—H2 \cdots O1 ⁱⁱ	0.82	2.01	2.817 (3)	167
C1—H1B \cdots Cg1 ⁱⁱⁱ	0.97	2.77	3.694 (3)	159

Symmetry codes: (i) $-x+3/2, y+1/2, z+1/2$; (ii) $x+1/2, -y+1/2, z-1$; (iii) $-x+1/2, y+1/2, z+1/2$.

Fig. 1

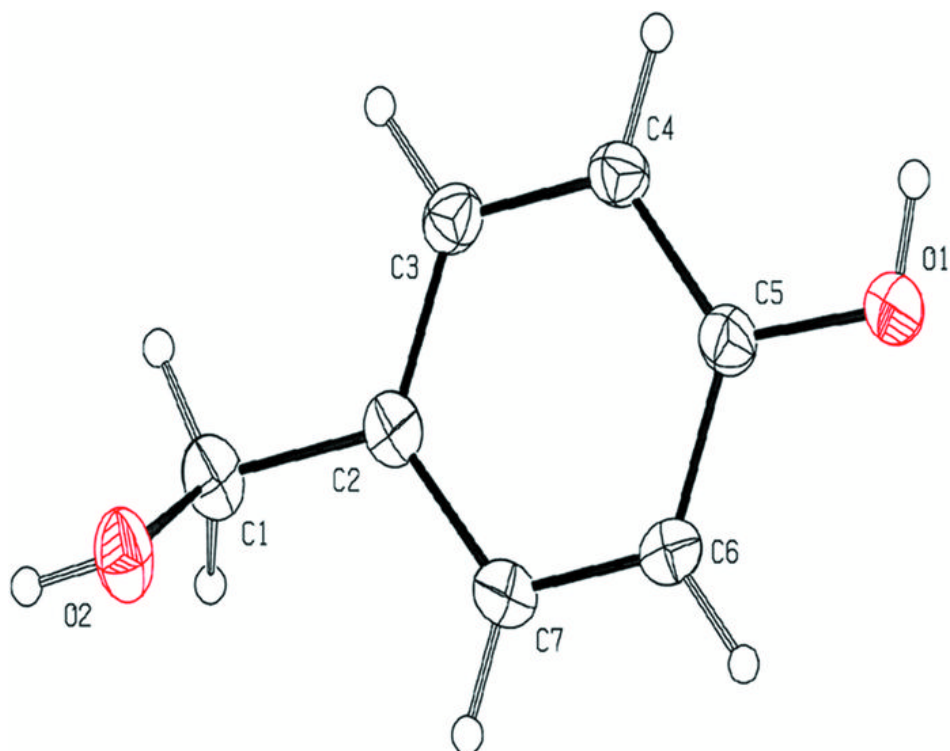


Fig. 2

