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3-Chloromethyl-2-hydroxybenzaldehyde

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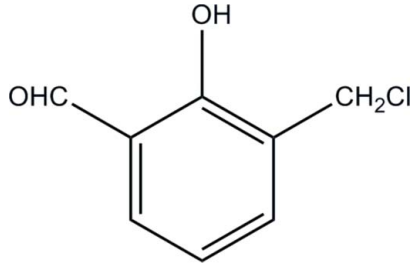
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.033; wR factor = 0.133; data-to-parameter ratio = 13.6.

In the title compound, $C_8H_7ClO_2$, the hydroxyl and aldehyde groups are co-planar with the benzene ring [maximum deviation 0.018 (3) Å], and the Cl—C—C plane is almost perpendicular to the benzene ring [dihedral angle 83.7 (2)°]. An intramolecular O—H···O hydrogen bond occurs between the hydroxyl and aldehyde groups.

Related literature

For related structures, see: Zondervan *et al.* (1997); Tang *et al.* (2010). For the synthesis, see: Song & Liu (2004).



Experimental

Crystal data

$C_8H_7ClO_2$
M_r = 170.59
Orthorhombic, $P2_12_12_1$
a = 4.483 (6) Å
b = 12.521 (18) Å
c = 13.71 (2) Å
V = 769.6 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 293 K
0.30 × 0.23 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.88, T_{max} = 0.92
3730 measured reflections
1369 independent reflections
1075 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.133
S = 0.98
1369 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 6571 Friedel pairs
Flack parameter: −0.06 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	1.91	2.628 (5)	146

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5608).

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supporting information

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S1. Comment

5-(Chloromethyl)-2-hydroxybenzaldehyde are well investigated just as it can be a precusor to an inhibitor-schiff bases for metal. However, just as we synthesize 5-(chloromethyl)-2-hydroxybenzaldehyde following one mehtod(Song & Liu, 2004) an unexpected byprodut 3-(chloromethyl)-2-hydroxybenzaldehyde was found and its cystal structure was determined.

S2. Experimental

Following a reference (Song *et al.* 2004), salicylaldehyde (30.5 g), paraformaldehyde (13.5 g) and conc. HCl (150 ml) were mixed and stirred at room temperature for 48 h. The precipitated benzylchloride derivatives which mostly are 5-(chloromethyl)-2-hydroxybenzaldehyde were filtered off then washed with 0.5% $NaHCO_3$ solution and water slightly. These humid precipitate were then dried in vac. for about 3 months. There are block colorless crystals appeared on the surface of precipitate.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model.

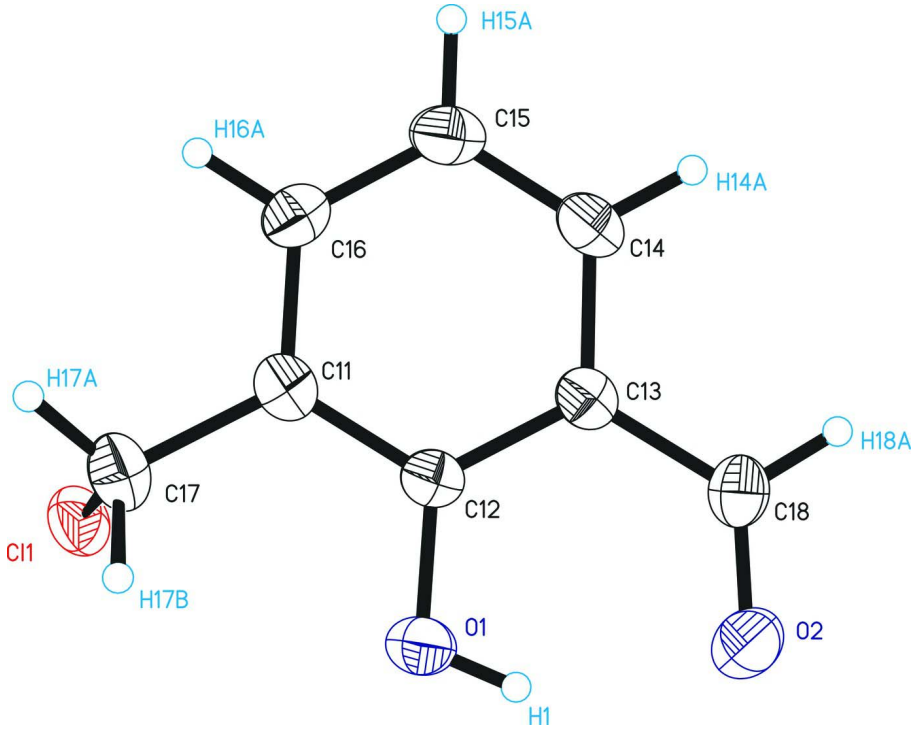

Figure 1

The molecular structure of title compound, with atom labels and 30% probability displacement ellipsoids for all atoms.

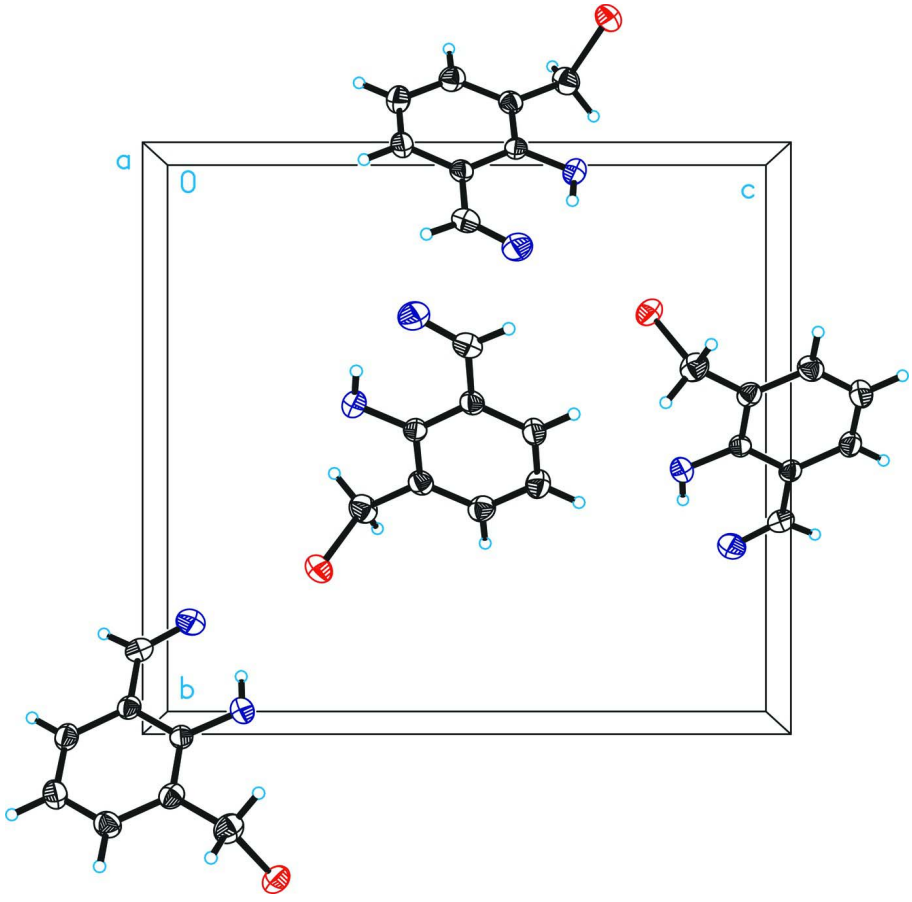

Figure 2

The cell packing diagram of title compound, viewed down the *a* axis.

3-Chloromethyl-2-hydroxybenzaldehyde

Crystal data

$C_8H_7ClO_2$
$M_r = 170.59$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.483$ (6) Å
$b = 12.521$ (18) Å
$c = 13.71$ (2) Å
$V = 769.6$ (19) Å^3
$Z = 4$
$F(000) = 352$
$D_x = 1.472$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1369 reflections
$\theta = 2.2$–$25.0°$
$\mu = 0.44$ mm^{-1}
$T = 293$ K
Block, colorless
0.30 × 0.23 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.88$, $T_{max} = 0.92$
3730 measured reflections
1369 independent reflections
1075 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 25.2°$, $\theta_{min} = 2.2°$
$h = -5 \rightarrow 5$
$k = -15 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.133$
$S = 0.98$
1369 reflections
101 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
$w = 1/[\sigma^2(F_o^2) + (0.P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Absolute structure: Flack (1983), 6571 Friedel pairs
Absolute structure parameter: −0.06 (13)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.5383 (2)	0.21212 (5)	0.21927 (5)	0.0606 (3)
O1	0.3758 (7)	−0.05428 (14)	0.16474 (16)	0.0558 (7)
H1	0.2636	−0.1057	0.1598	0.084*
O2	0.0222 (7)	−0.18989 (15)	0.07502 (19)	0.0640 (7)
C11	0.6216 (8)	0.07288 (19)	0.0685 (2)	0.0440 (7)
C12	0.4289 (7)	−0.01314 (17)	0.0756 (2)	0.0384 (7)
C13	0.2937 (8)	−0.05626 (17)	−0.0076 (2)	0.0403 (7)
C14	0.3593 (9)	−0.0101 (2)	−0.0985 (2)	0.0509 (9)
H14A	0.2719	−0.0378	−0.1546	0.061*
C15	0.5488 (10)	0.0745 (2)	−0.1057 (2)	0.0560 (9)
H15A	0.5907	0.1043	−0.1663	0.067*
C16	0.6779 (9)	0.1157 (2)	−0.0228 (3)	0.0507 (8)
H16A	0.8062	0.1738	−0.0282	0.061*
C17	0.7744 (9)	0.1173 (3)	0.1567 (3)	0.0572 (9)
H17A	0.9581	0.1522	0.1371	0.069*
H17B	0.8252	0.0594	0.2007	0.069*
C18	0.0905 (9)	−0.14473 (19)	−0.0012 (2)	0.0504 (9)
H18A	0.0050	−0.1695	−0.0587	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0771 (7)	0.0537 (4)	0.0510 (5)	−0.0025 (4)	−0.0076 (4)	−0.0126 (3)

O1	0.078 (2)	0.0496 (10)	0.0400 (12)	−0.0038 (11)	−0.0019 (12)	0.0056 (7)
O2	0.074 (2)	0.0533 (9)	0.0649 (15)	−0.0091 (11)	0.0058 (15)	0.0042 (9)
C11	0.045 (2)	0.0425 (11)	0.0443 (16)	0.0089 (12)	−0.0040 (13)	−0.0039 (10)
C12	0.0424 (18)	0.0371 (9)	0.0358 (13)	0.0089 (11)	0.0027 (14)	0.0003 (9)
C13	0.042 (2)	0.0386 (10)	0.0398 (16)	0.0085 (12)	−0.0002 (13)	−0.0032 (9)
C14	0.067 (3)	0.0507 (12)	0.0353 (15)	0.0082 (14)	−0.0039 (16)	−0.0031 (10)
C15	0.067 (3)	0.0583 (14)	0.0427 (17)	0.0024 (16)	0.0070 (17)	0.0048 (11)
C16	0.050 (2)	0.0474 (12)	0.055 (2)	−0.0035 (14)	0.0055 (17)	0.0036 (12)
C17	0.054 (2)	0.0597 (14)	0.058 (2)	0.0024 (15)	−0.0145 (17)	−0.0069 (14)
C18	0.053 (2)	0.0412 (11)	0.057 (2)	0.0004 (12)	0.0011 (17)	−0.0076 (11)

Geometric parameters (Å, º)

Cl1—C17	1.808 (4)	C13—C18	1.437 (4)
O1—C12	1.348 (4)	C14—C15	1.362 (5)
O1—H1	0.8200	C14—H14A	0.9300
O2—C18	1.227 (4)	C15—C16	1.376 (5)
C11—C12	1.384 (4)	C15—H15A	0.9300
C11—C16	1.386 (5)	C16—H16A	0.9300
C11—C17	1.496 (5)	C17—H17A	0.9700
C12—C13	1.400 (4)	C17—H17B	0.9700
C13—C14	1.404 (4)	C18—H18A	0.9300
C12—O1—H1	109.5	C14—C15—H15A	120.2
C12—C11—C16	118.6 (3)	C16—C15—H15A	120.2
C12—C11—C17	121.2 (3)	C15—C16—C11	121.7 (3)
C16—C11—C17	120.2 (3)	C15—C16—H16A	119.2
O1—C12—C11	118.1 (3)	C11—C16—H16A	119.2
O1—C12—C13	121.0 (3)	C11—C17—Cl1	111.1 (3)
C11—C12—C13	120.9 (3)	C11—C17—H17A	109.4
C12—C13—C14	118.2 (3)	Cl1—C17—H17A	109.4
C12—C13—C18	121.5 (3)	C11—C17—H17B	109.4
C14—C13—C18	120.3 (3)	Cl1—C17—H17B	109.4
C15—C14—C13	121.0 (3)	H17A—C17—H17B	108.0
C15—C14—H14A	119.5	O2—C18—C13	124.5 (3)
C13—C14—H14A	119.5	O2—C18—H18A	117.8
C14—C15—C16	119.6 (3)	C13—C18—H18A	117.8
C16—C11—C12—O1	180.0 (3)	C18—C13—C14—C15	179.3 (3)
C17—C11—C12—O1	1.8 (4)	C13—C14—C15—C16	−0.1 (5)
C16—C11—C12—C13	0.1 (4)	C14—C15—C16—C11	0.4 (5)
C17—C11—C12—C13	−178.1 (3)	C12—C11—C16—C15	−0.4 (5)
O1—C12—C13—C14	−179.7 (3)	C17—C11—C16—C15	177.8 (3)
C11—C12—C13—C14	0.2 (4)	C12—C11—C17—Cl1	−84.7 (3)
O1—C12—C13—C18	0.9 (4)	C16—C11—C17—Cl1	97.2 (4)
C11—C12—C13—C18	−179.3 (3)	C12—C13—C18—O2	−0.9 (5)
C12—C13—C14—C15	−0.2 (5)	C14—C13—C18—O2	179.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.91	2.628 (5)	146