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3,5-Dichlorosalicylaldehyde

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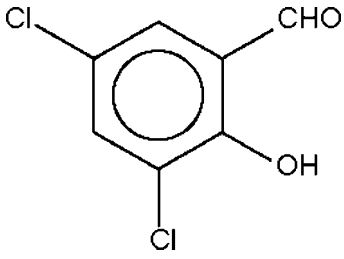
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 16.1.

The title compound (systematic name: 3,5-dichloro-2-hydroxybenzaldehyde), $C_7H_4Cl_2O_2$, crystallizes as discrete molecules, the conformation of which may be influenced by an intramolecular hydroxy–carbonyl O—H···O hydrogen bond.

Related literature

For the crystal structure of 3′,5′-dichloroacetophenone, see: Filarowski *et al.* (2004).



Experimental

Crystal data

$C_7H_4Cl_2O_2$
M_r = 191.00
Monoclinic, $P2_1/c$
a = 8.2823 (2) Å
b = 13.7412 (3) Å
c = 7.0973 (2) Å
β = 115.185 (2)°
V = 730.95 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.82 mm^{-1}
T = 100 (2) K
0.25 × 0.15 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.701, T_{max} = 0.960
8436 measured reflections
1672 independent reflections
1303 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.05
1672 reflections
104 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.84 (1)	1.87 (2)	2.628 (3)	149 (3)

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, 2008).

We thank the University of Malaya for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2606).

References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supporting information

Acta Cryst. (2008). E**64**, o917 [doi:10.1107/S1600536808011021]

3,5-Dichlorosalicylaldehyde

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S1. Comment

The intramolecular hydrogen bonds in small molecules such as *ortho*-hydroxyacetopheonone and its derivatives has been extensively studied, both theoretically and crystallographically. Such compounds can exist in a keto-enol equilibrium. For 3′,5′-dichloroacetophenone, geometry-optimization calculations suggest that the presence of two chlorine substituents raises the acidity of the hydroxyl proton and decreases the basicity of the carbonyl function. The O···O distance in the hydrogen bond is 2.567 (3) Å (Filarowski *et al.*, 2004).

The hydrogen bond in the title molecule (I) is longer with an O···O distance of 2.628 (3) Å. 3,5-Dichlorosalicylaldehyde (I) exists as a monomeric compound (Fig. 1); the molecule is flat and all bond dimensions are normal.

S2. Experimental

The compound was purchased from Aldrich Chemical Company; the chemical exists as colorless prismatic crystals. The bulk chemical has a yellow color.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C). The oxygen-bound H atom was located in a difference Fourier map, and was refined with a distance restraint of O–H 0.84±0.01 Å; its temperature factor was freely refined.

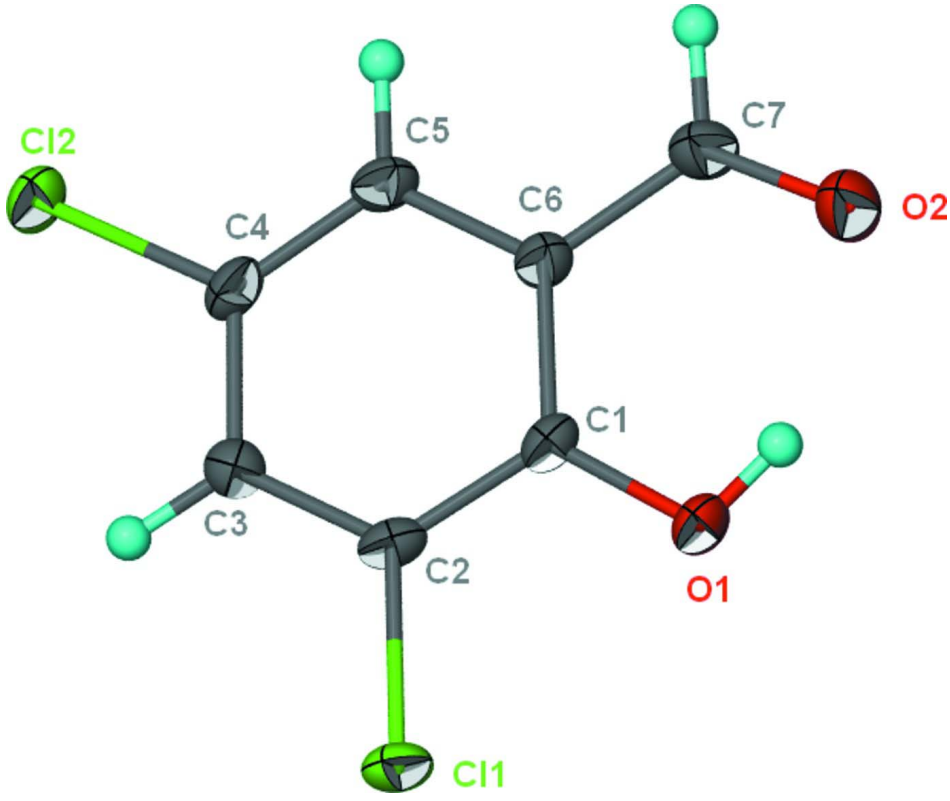

Figure 1

70% Probability thermal ellipsoid plot of 3,5-dichlorosalicylaldehyde. Hydrogen atoms are drawn as spheres of arbitrary radius.

3,5-dichloro-2-hydroxybenzaldehyde

Crystal data

$C_7H_4Cl_2O_2$
$M_r = 191.00$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.2823$ (2) Å
$b = 13.7412$ (3) Å
$c = 7.0973$ (2) Å
$\beta = 115.185$ (2)°
$V = 730.95$ (3) Å^3
$Z = 4$
$F(000) = 384$
$D_x = 1.736$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3128 reflections
$\theta = 3.0$–$28.2°$
$\mu = 0.82$ mm^{-1}
$T = 100$ K
Block, colorless
0.25 × 0.15 × 0.05 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.701$, $T_{max} = 0.960$
8436 measured reflections
1672 independent reflections
1303 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.7°$
$h = -10 \rightarrow 10$
$k = -17 \rightarrow 17$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.101$
$S = 1.05$
1672 reflections
104 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 0.8939P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.17794 (9)	0.14230 (4)	0.48280 (10)	0.01972 (18)
Cl2	0.15345 (9)	0.53148 (4)	0.39904 (11)	0.02166 (19)
O1	0.5328 (3)	0.17615 (13)	0.8080 (3)	0.0200 (4)
H1	0.631 (3)	0.192 (3)	0.905 (4)	0.038 (10)*
O2	0.7916 (3)	0.28892 (14)	1.0580 (3)	0.0252 (4)
C1	0.4488 (3)	0.25960 (17)	0.7232 (4)	0.0155 (5)
C2	0.2766 (3)	0.25497 (17)	0.5629 (4)	0.0164 (5)
C3	0.1851 (4)	0.33804 (17)	0.4659 (4)	0.0168 (5)
H3	0.0680	0.3339	0.3572	0.020*
C4	0.2680 (4)	0.42815 (17)	0.5306 (4)	0.0177 (5)
C5	0.4355 (4)	0.43592 (17)	0.6906 (4)	0.0179 (5)
H5	0.4890	0.4980	0.7336	0.021*
C6	0.5266 (3)	0.35155 (17)	0.7897 (4)	0.0160 (5)
C7	0.7028 (4)	0.35892 (18)	0.9634 (4)	0.0206 (6)
H7	0.7517	0.4220	1.0058	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0225 (3)	0.0110 (3)	0.0228 (3)	−0.0036 (2)	0.0068 (3)	−0.0026 (2)
Cl2	0.0204 (3)	0.0122 (3)	0.0276 (4)	0.0029 (2)	0.0056 (3)	0.0051 (2)
O1	0.0193 (10)	0.0111 (8)	0.0243 (11)	0.0025 (7)	0.0042 (9)	0.0025 (7)
O2	0.0211 (10)	0.0197 (9)	0.0272 (11)	0.0004 (8)	0.0030 (9)	0.0033 (8)
C1	0.0182 (13)	0.0111 (10)	0.0180 (12)	0.0028 (9)	0.0083 (11)	0.0016 (9)
C2	0.0216 (13)	0.0106 (10)	0.0186 (12)	−0.0017 (9)	0.0100 (11)	−0.0016 (9)
C3	0.0163 (13)	0.0162 (12)	0.0172 (13)	−0.0004 (9)	0.0063 (11)	−0.0007 (9)
C4	0.0201 (14)	0.0114 (11)	0.0213 (13)	0.0038 (9)	0.0086 (12)	0.0032 (9)
C5	0.0202 (14)	0.0108 (11)	0.0228 (14)	−0.0024 (9)	0.0093 (12)	0.0000 (9)
C6	0.0151 (13)	0.0123 (11)	0.0195 (13)	−0.0004 (9)	0.0064 (11)	0.0003 (9)
C7	0.0212 (14)	0.0149 (12)	0.0229 (14)	−0.0029 (10)	0.0068 (12)	−0.0003 (10)

Geometric parameters (Å, º)

Cl1—C2	1.730 (2)	C3—C4	1.395 (3)
Cl2—C4	1.742 (2)	C3—H3	0.9500
O1—C1	1.343 (3)	C4—C5	1.373 (4)
O1—H1	0.840 (10)	C5—C6	1.399 (3)
O2—C7	1.223 (3)	C5—H5	0.9500
C1—C2	1.397 (4)	C6—C7	1.459 (4)
C1—C6	1.406 (3)	C7—H7	0.9500
C2—C3	1.381 (3)		
C1—O1—H1	107 (3)	C5—C4—Cl2	120.53 (19)
O1—C1—C2	118.7 (2)	C3—C4—Cl2	117.9 (2)
O1—C1—C6	122.7 (2)	C4—C5—C6	119.4 (2)
C2—C1—C6	118.5 (2)	C4—C5—H5	120.3
C3—C2—C1	121.5 (2)	C6—C5—H5	120.3
C3—C2—Cl1	119.6 (2)	C5—C6—C1	120.3 (2)
C1—C2—Cl1	118.96 (18)	C5—C6—C7	119.9 (2)
C2—C3—C4	118.7 (2)	C1—C6—C7	119.8 (2)
C2—C3—H3	120.6	O2—C7—C6	124.1 (2)
C4—C3—H3	120.6	O2—C7—H7	118.0
C5—C4—C3	121.6 (2)	C6—C7—H7	118.0
O1—C1—C2—C3	−178.3 (2)	Cl2—C4—C5—C6	−178.17 (19)
C6—C1—C2—C3	2.0 (4)	C4—C5—C6—C1	1.3 (4)
O1—C1—C2—Cl1	0.8 (3)	C4—C5—C6—C7	−178.4 (2)
C6—C1—C2—Cl1	−178.90 (18)	O1—C1—C6—C5	177.7 (2)
C1—C2—C3—C4	0.1 (4)	C2—C1—C6—C5	−2.7 (4)
Cl1—C2—C3—C4	−179.03 (19)	O1—C1—C6—C7	−2.6 (4)
C2—C3—C4—C5	−1.5 (4)	C2—C1—C6—C7	177.1 (2)
C2—C3—C4—Cl2	177.52 (18)	C5—C6—C7—O2	−179.8 (3)
C3—C4—C5—C6	0.9 (4)	C1—C6—C7—O2	0.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.84 (1)	1.87 (2)	2.628 (3)	149 (3)