Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,3-Dichlorobenzene-1,4-diol

Paul D. Ahn, Roger Bishop, Donald C. Craig and Marcia L. Scudder*

School of Chemistry, University of New South Wales, Sydney 2052, Australia
Correspondence e-mail: m.scudder@unsw.edu.au

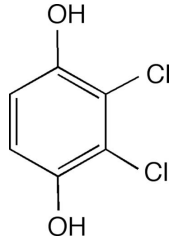
Received 3 March 2009; accepted 17 April 2009

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.050; data-to-parameter ratio = 14.0.

The achiral title compound, $C_6H_4Cl_2O_2$, crystallizes with O—H···O hydrogen bonding linking molecules into layers. Between layers there are chains of Cl···Cl···Cl interactions with alternating distances of 3.274 (2) and 3.742 (2) Å. Augmenting this arrangement there are also C—H···Cl (2.97 and 3.17 Å) and Cl···π (shortest distances 3.40 and 3.54 Å) interactions.

Related literature

For the structures of related dichloronaphthalenediols, see: Ahn *et al.* (1995, 1996). For the preparation of the title compound, see: Beddoes *et al.* (1981).



Experimental

Crystal data

$C_6H_4Cl_2O_2$
M_r = 179.0
Monoclinic, $P2_1/c$
a = 4.831 (1) Å
b = 11.347 (2) Å
c = 12.962 (3) Å
β = 105.94 (1)°
V = 683.2 (2) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 8.02 mm^{-1}
T = 294 K
0.15 × 0.15 × 0.06 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.33, T_{max} = 0.63
1449 measured reflections
1290 independent reflections
1187 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
1 standard reflections
frequency: 30 min
intensity decay: 21%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.050
S = 1.87
1290 reflections
92 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*1···O2^{i}	1.00	1.84	2.794 (2)	158
O2—H1*O*2···O1^{ii}	1.00	1.78	2.778 (2)	172

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

Data collection: *CAD-4 Manual* (Schagen *et al.*, 1989); cell refinement: *CAD-4 Manual*; data reduction: local program; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *RAELS* (Rae, 2000); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CrystalMaker* (CrystalMaker Software, 2005); software used to prepare material for publication: local programs.

This research was supported by the Australian Research Council.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2117).

References

Ahn, P. D., Bishop, R., Craig, D. C. & Scudder, M. L. (1995). *J. Incl. Phenom. Mol. Rec. Chem.* **20**, 267–276.
Ahn, P. D., Bishop, R., Craig, D. C. & Scudder, M. L. (1996). *J. Incl. Phenom. Mol. Rec. Chem.* **23**, 313–327.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Beddoes, R. L., Bruce, J. M., Finch, H., Heelam, L. M. J., Hunt, I. D. & Mills, O. S. (1981). *J. Chem. Soc. Perkin Trans. 1*, pp. 2670–2676.
CrystalMaker Software (2005). *CrystalMaker*. CrystalMaker Software, Yarnton, England. www.CrystalMaker.co.uk.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Meulenaer, J. de & Tompa, H. (1965). *Acta Cryst.* **19**, 1014–1018.
Rae, A. D. (2000). *RAELS*. Australian National University, Canberra, Australia.
Schagen, J. D., Straver, L., van Meurs, F. & Williams, G. (1989). *CAD-4 Manual*. Enraf–Nonius, Delft, The Netherlands.

supporting information

Acta Cryst. (2009). E**65**, o1103 [doi:10.1107/S1600536809014408]

2,3-Dichlorobenzene-1,4-diol

Paul D. Ahn, Roger Bishop, Donald C. Craig and Marcia L. Scudder

S1. Comment

Crystal structures of related dichloronaphthalenediols have been previously reported by us (Ahn *et al.*, 1995, 1996). In the title compound (Fig 1), each molecule participates in four hydrogen bonds, two as donor and two as acceptor, creating a layer structure in the *ac* plane with O1-H1O1···O2-H1O2···O1-H1O1··· chains parallel to *a* (Fig 2, Table 1). Aromatic offset face-face stacking at a distance of 3.5 Å takes place within the layer. Chains of Cl1···Cl1···Cl1 interactions (alternating distances 3.274 (2) and 3.742 (2) Å) which also run parallel to *a* link the layers into a three-dimensional array. In addition there are C5H···Cl2 and C6H···Cl2 (2.97 and 3.17 Å) and Cl2···π interactions (shortest distances 3.40 and 3.54 Å).

S2. Experimental

2,3-Dichlorobenzene-1,4-diol was prepared as described (Beddoes *et al.*, 1981). ^{1}H NMR (300 MHz, d_6-DMSO) δ 6.79 (s, 2H), 9.71 (s, 2H, –OH); ^{13}C NMR (75 MHz, d_6-DMSO) δ 115.1 (CH), 119.2 (C), 147.1 (C). X-ray quality solvent-free crystals were obtained from benzene solution.

S3. Refinement

H atoms attached to C were included at calculated positions (C—H = 1.0 Å). The hydroxy hydrogen atoms were located on a difference map, and were then fixed at a position along the OH vector with O—H = 1.0 Å. All hydrogen atoms were refined with isotropic thermal parameters equivalent to those of the atom to which they were bonded.

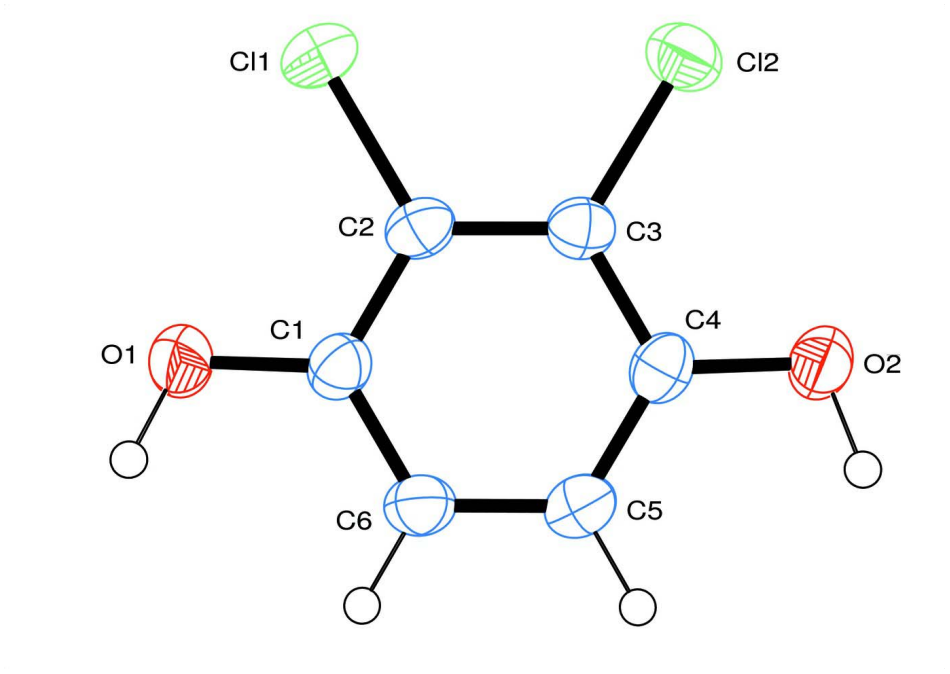


Figure 1

A molecule of the title compound, showing atom labelling. Thermal ellipsoids are drawn at the 50% level.

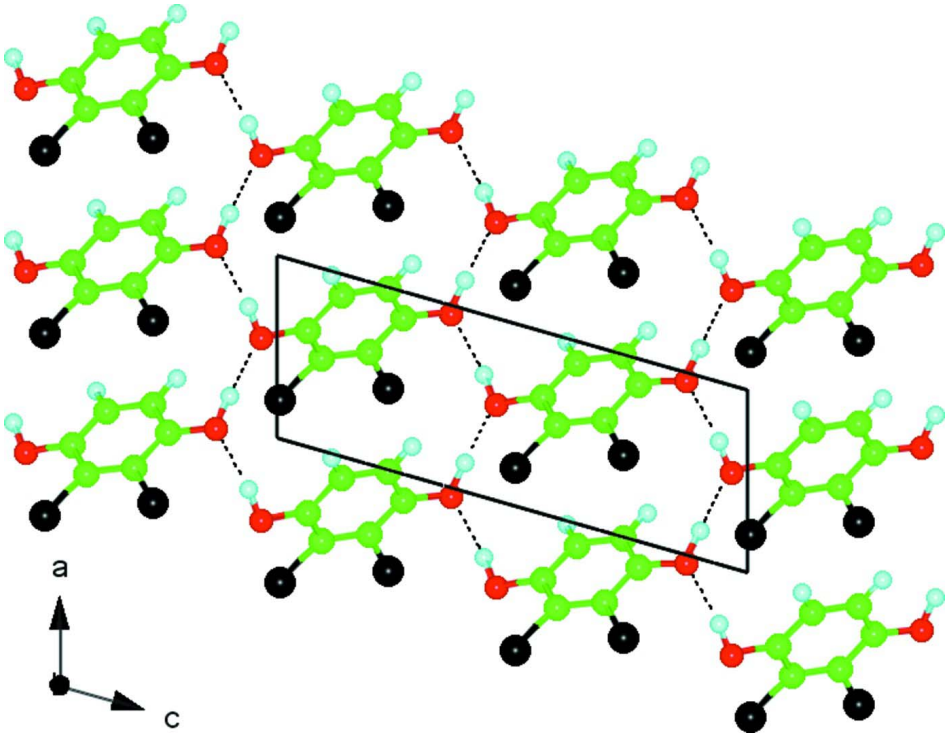


Figure 2

A hydrogen bonded layer. Each molecule participates in two donor and two acceptor hydrogen bonds which are represented as dashed lines.

2,3-Dichlorobenzene-1,4-diol

Crystal data

$C_6H_4Cl_2O_2$
$M_r = 179.0$
Monoclinic, $P2_1/c$
$a = 4.831$ (1) Å
$b = 11.347$ (2) Å
$c = 12.962$ (3) Å
$\beta = 105.94$ (1)°
$V = 683.2$ (2) Å^3
$Z = 4$
$F(000) = 360.0$
$D_x = 1.74$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 10 reflections
$\theta = 25$–30°
$\mu = 8.02$ mm^{-1}
$T = 294$ K
Tabular, colourless
0.15 × 0.15 × 0.06 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
$T_{min} = 0.33$, $T_{max} = 0.63$
1449 measured reflections
1290 independent reflections
1187 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 70°$
$h = -5\rightarrow0$
$k = -13\rightarrow0$
$l = -15\rightarrow15$
1 standard reflections every 30 min
intensity decay: 21%

Refinement

Refinement on F
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.050$
$S = 1.87$
1290 reflections
92 parameters
0 restraints
H-atom parameters not refined
$w = 1/[\sigma^2(F) + 0.0004F^2]$
$(\Delta/\sigma)_{max} = 0.008$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.78228 (10)	0.11149 (4)	0.49607 (4)	0.0444 (2)
Cl2	0.54566 (11)	0.00422 (4)	0.26478 (4)	0.0439 (2)
O1	0.4715 (3)	0.3170 (1)	0.5364 (1)	0.0463 (4)
O2	0.0408 (3)	0.1224 (1)	0.1331 (1)	0.0404 (4)
C1	0.3548 (4)	0.2698 (2)	0.4364 (2)	0.0340 (4)
C2	0.4868 (4)	0.1726 (2)	0.4063 (1)	0.0328 (4)
C3	0.3797 (4)	0.1238 (2)	0.3049 (2)	0.0319 (4)
C4	0.1366 (4)	0.1719 (2)	0.2334 (1)	0.0334 (4)
C5	0.0028 (4)	0.2679 (2)	0.2647 (2)	0.0363 (4)
C6	0.1126 (4)	0.3174 (2)	0.3651 (2)	0.0363 (4)
H1O1	0.3196	0.3578	0.5622	0.046
H1O2	−0.1619	0.1499	0.1026	0.040
HC5	−0.1745	0.3018	0.2143	0.036
HC6	0.0168	0.3879	0.3864	0.036

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0340 (3)	0.0503 (3)	0.0427 (3)	0.0103 (2)	−0.0001 (2)	0.0039 (2)
Cl2	0.0407 (3)	0.0389 (3)	0.0521 (4)	0.0050 (2)	0.0128 (2)	−0.0066 (2)
O1	0.0360 (8)	0.0620 (9)	0.0367 (7)	0.0060 (6)	0.0030 (6)	−0.0131 (7)
O2	0.0365 (7)	0.0492 (8)	0.0324 (7)	−0.0001 (6)	0.0044 (6)	−0.0040 (6)
C1	0.0291 (9)	0.0403 (9)	0.0316 (9)	−0.0004 (7)	0.0068 (7)	−0.0004 (7)
C2	0.0251 (8)	0.0374 (9)	0.0352 (9)	0.0018 (7)	0.0072 (7)	0.0040 (7)
C3	0.0281 (9)	0.0318 (8)	0.037 (1)	0.0001 (6)	0.0101 (7)	0.0009 (7)
C4	0.0302 (9)	0.0386 (9)	0.0306 (9)	−0.0049 (7)	0.0070 (7)	0.0018 (7)
C5	0.0314 (9)	0.040 (1)	0.036 (1)	0.0038 (7)	0.0061 (7)	0.0051 (8)
C6	0.031 (1)	0.039 (1)	0.039 (1)	0.0056 (7)	0.0097 (8)	0.0020 (8)

Geometric parameters (Å, º)

Cl1—C2	1.721 (2)	C1—C6	1.386 (2)
Cl2—C3	1.727 (2)	C2—C3	1.389 (3)
O1—C1	1.372 (2)	C3—C4	1.392 (3)
O1—H1O1	1.000	C4—C5	1.383 (3)
O2—C4	1.374 (2)	C5—C6	1.383 (3)
O2—H1O2	1.000	C5—HC5	1.000
C1—C2	1.383 (3)	C6—HC6	1.000
C1—O1—H1O1	110.4	C2—C3—C4	120.1 (2)
C4—O2—H1O2	106.6	O2—C4—C3	118.2 (2)
O1—C1—C2	118.4 (2)	O2—C4—C5	122.4 (2)
O1—C1—C6	122.1 (2)	C3—C4—C5	119.4 (2)
C2—C1—C6	119.5 (2)	C4—C5—C6	120.4 (2)
Cl1—C2—C1	119.5 (1)	C4—C5—HC5	119.8
Cl1—C2—C3	120.3 (1)	C6—C5—HC5	119.8
C1—C2—C3	120.3 (2)	C1—C6—C5	120.3 (2)
Cl2—C3—C2	121.0 (1)	C1—C6—HC6	119.8
Cl2—C3—C4	118.9 (1)	C5—C6—HC6	119.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*1···O2^{i}	1.00	1.84	2.794 (2)	158
O2—H1*O*2···O1^{ii}	1.00	1.78	2.778 (2)	172

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) *x*−1, −*y*+1/2, *z*−1/2.