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5,7-Dichloroquinolin-8-ol

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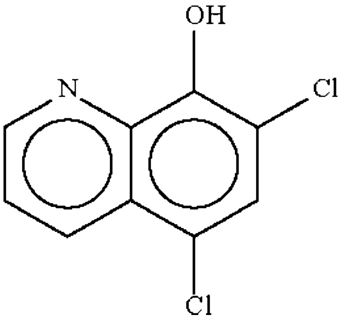
Key indicators: single-crystal X-ray study; *T* = 123 K; mean σ(C–C) = 0.003 Å; *R* factor = 0.040; *wR* factor = 0.112; data-to-parameter ratio = 15.7.

The molecule of the title compound, $C_9H_5Cl_2NO$, is essentially planar [give maximum or r.m.s. deviation] and the hydroxy group acts as a hydrogen-bond donor to the N atom of a symmetry-related molecule, generating a hydrogen-bonded dimer,which lies on a twofold rotation axis.

Related literature

Unlike quinolin-8-ol, which yields a large number of metal derivatives, 5,7-dichloroquinolin-8-ol forms only a small number of metal chelates. For their crystal structures, see: García-Granda *et al.* (1987); Artizzu *et al.* (2007, 2008); Day *et al.* (1980); González-Baró *et al.* (1998); Horton & Wendlandt (1963); Miyashita *et al.* (2005); Suganuma *et al.* (2001); Van Deun *et al.* (2004).



Experimental

Crystal data

$C_9H_5Cl_2NO$
M_r = 214.04
Monoclinic, *P*2/*c*
a = 15.5726 (3) Å
b = 3.8062 (1) Å
c = 16.1269 (3) Å
β = 118.029 (1)°
V = 843.76 (3) Å^3
Z = 4
Mo *K*α radiation
μ = 0.72 mm^{-1}
T = 123 K
0.36 × 0.09 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.782, T_{max} = 0.986
7279 measured reflections
1919 independent reflections
1644 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.05
1919 reflections
122 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^i	0.84 (1)	2.01 (2)	2.761 (2)	150 (3)

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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, 2009).

I thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2808).

References

Artizzu, F., Bernot, K., Caneschi, A., Coronado, E., Clemente-Juan, J. M., Marchiò, L., Mercuri, M. L., Pilia, L., Serpe, A. & Deplano, P. (2008). *Eur. J. Inorg. Chem.* pp. 3829–3826.
Artizzu, F., Marchiò, L., Mercuri, M. L., Pilia, L., Serpe, A., Quochi, F., Orrù, R., Cordella, F., Saba, M., Mura, A., Bongiovanni, G. & Deplano, P. (2007). *Adv. Func. Mater.* **17**, 2365–2376.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Day, R. O., Batschelet, W. H. & Archer, R. D. (1980). *Inorg. Chem.* **19**, 2113–2122.
García-Granda, S., Beurskens, P. T., Behm, H. J. J. & Gómez-Beltrán, F. (1987). *Acta Cryst.* C**43**, 39–41.
González-Baró, A. C., Piro, O. E., Parajón-Costa, B. S., Baran, E. J. & Castellano, E. E. (1998). *Monatsh. Chem.* **129**, 31–39.
Horton, G. R. & Wendlandt, W. W. (1963). *J. Inorg. Nucl. Chem.* **25**, 247–252.
Miyashita, Y., Ohashi, T., Imai, A., Amir, N., Fujisawa, K. & Okamoto, K.-I. (2005). *Sci. Technol. Adv. Mater.* **6** 660–666.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Suganuma, S., Tanada, A., Tomizawa, H., Tanaka, M. & Miki, E. (2001). *Inorg. Chim. Acta*, **320**, 22–30.
Van Deun, R., Fias, P., Nockemann, P., Schepers, A., Parac-Vogt, T. N., Van Hecke, K., Van Meervelt, L. & Binnemans, K. (2004). *Inorg. Chem.* **43**, 8461–8469.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

Acta Cryst. (2009). E**65**, o1131   [doi:10.1107/S1600536809014846]

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S1. Comment

A hydrogen-bonded dimer of the title compound is shown in Fig. 1.

S2. Experimental

The organic reactant was returned unchanged in an unsuccessful attempt at reacting it with a zinc salt in methanol.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 *U*(C). The hydroxy hydrogen 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.

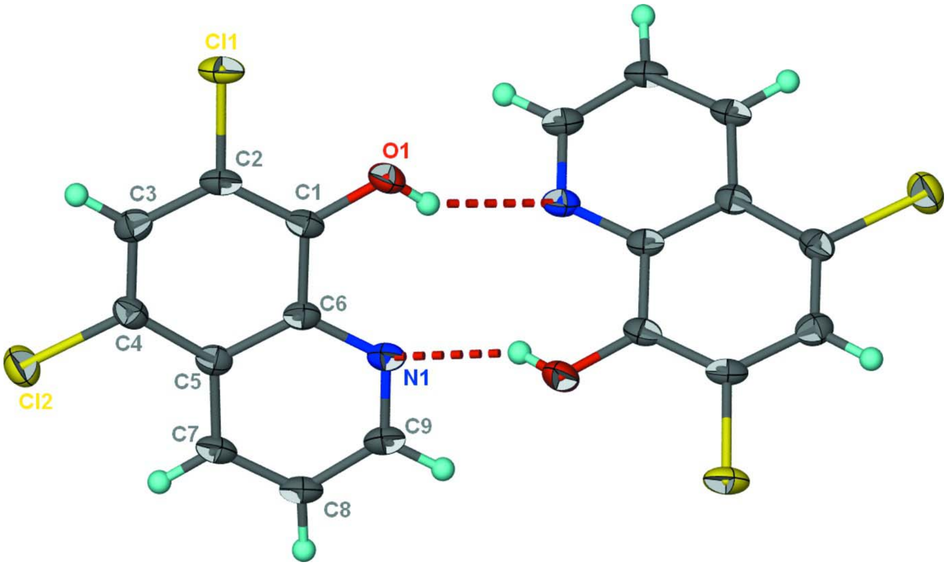

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of a hydrogen-bonded dimer of the title compound; ellipsoids are drawn at the 70% probability level and H atoms of arbitrary radius. The unlabeled molecule is related by the symmetry operator -x, y, -z+1/2

5,7-Dichloroquinolin-8-ol

Crystal data

$C_9H_5Cl_2NO$	Monoclinic, *P*2/*c*
M_r = 214.04	Hall symbol: -P 2yc

a = 15.5726 (3) Å
b = 3.8062 (1) Å
c = 16.1269 (3) Å
β = 118.029 (1)°
V = 843.76 (3) Å^3
Z = 4
F(000) = 432
D_x = 1.685 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3573 reflections
θ = 2.5–28.3°
μ = 0.72 mm^{-1}
T = 123 K
Plate, colorless
0.36 × 0.09 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.782, T_{max} = 0.986

7279 measured reflections
1919 independent reflections
1644 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 1.5°
$h = -20 \rightarrow 20$
$k = -4 \rightarrow 4$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.05
1919 reflections
122 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
$w = 1/[\sigma^2(F_o^2) + (0.0684P)^2 + 0.4949P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.29367 (4)	0.38966 (13)	0.24587 (3)	0.02310 (17)
Cl2	0.44255 (4)	0.89258 (14)	0.59720 (3)	0.02635 (18)
O1	0.10638 (11)	0.6233 (4)	0.22642 (10)	0.0223 (3)
N1	0.07459 (12)	0.9357 (4)	0.36439 (11)	0.0186 (4)
H1	0.0565 (14)	0.729 (7)	0.220 (2)	0.051 (9)*
C1	0.18119 (14)	0.6852 (5)	0.31223 (13)	0.0176 (4)
C2	0.27416 (15)	0.5885 (5)	0.33230 (13)	0.0184 (4)
C3	0.35486 (14)	0.6504 (5)	0.42003 (14)	0.0193 (4)
H3	0.4180	0.5794	0.4316	0.023*
C4	0.34192 (14)	0.8134 (5)	0.48869 (13)	0.0183 (4)
C5	0.24865 (14)	0.9212 (5)	0.47354 (13)	0.0168 (4)
C6	0.16747 (14)	0.8502 (5)	0.38470 (13)	0.0170 (4)

C7	0.23008 (15)	1.0924 (5)	0.54108 (13)	0.0191 (4)
H7	0.2822	1.1462	0.6013	0.023*
C8	0.13659 (15)	1.1807 (5)	0.51946 (14)	0.0201 (4)
H8	0.1230	1.2970	0.5641	0.024*
C9	0.06103 (15)	1.0957 (5)	0.42978 (14)	0.0204 (4)
H9	−0.0036	1.1574	0.4155	0.024*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0336 (3)	0.0238 (3)	0.0188 (3)	0.00576 (19)	0.0180 (2)	0.00172 (18)
Cl2	0.0229 (3)	0.0305 (3)	0.0203 (3)	0.0002 (2)	0.0057 (2)	−0.00406 (19)
O1	0.0229 (7)	0.0304 (8)	0.0137 (6)	0.0030 (6)	0.0086 (6)	−0.0021 (5)
N1	0.0230 (8)	0.0202 (9)	0.0157 (7)	0.0008 (6)	0.0117 (6)	0.0020 (6)
C1	0.0242 (10)	0.0166 (9)	0.0139 (8)	−0.0012 (7)	0.0105 (7)	0.0016 (7)
C2	0.0280 (10)	0.0158 (10)	0.0171 (9)	0.0009 (7)	0.0154 (8)	0.0016 (7)
C3	0.0223 (9)	0.0173 (10)	0.0215 (9)	0.0015 (7)	0.0130 (8)	0.0025 (8)
C4	0.0211 (9)	0.0182 (10)	0.0145 (8)	−0.0019 (7)	0.0074 (7)	0.0014 (7)
C5	0.0216 (9)	0.0142 (9)	0.0164 (9)	−0.0012 (7)	0.0104 (7)	0.0021 (7)
C6	0.0220 (9)	0.0161 (9)	0.0162 (9)	−0.0010 (7)	0.0117 (7)	0.0010 (7)
C7	0.0276 (10)	0.0183 (10)	0.0143 (8)	−0.0029 (8)	0.0122 (8)	−0.0001 (7)
C8	0.0297 (10)	0.0187 (10)	0.0181 (9)	−0.0013 (8)	0.0164 (8)	−0.0007 (7)
C9	0.0263 (10)	0.0210 (10)	0.0200 (9)	0.0004 (8)	0.0160 (8)	0.0019 (7)

Geometric parameters (Å, º)

Cl1—C2	1.7337 (19)	C3—H3	0.9500
Cl2—C4	1.7412 (19)	C4—C5	1.416 (3)
O1—C1	1.346 (2)	C5—C7	1.411 (3)
O1—H1	0.835 (10)	C5—C6	1.422 (3)
N1—C9	1.318 (2)	C7—C8	1.370 (3)
N1—C6	1.364 (2)	C7—H7	0.9500
C1—C2	1.377 (3)	C8—C9	1.408 (3)
C1—C6	1.428 (3)	C8—H8	0.9500
C2—C3	1.402 (3)	C9—H9	0.9500
C3—C4	1.364 (3)		
C1—O1—H1	111 (2)	C7—C5—C6	117.26 (17)
C9—N1—C6	117.95 (17)	C4—C5—C6	118.24 (17)
O1—C1—C2	120.07 (17)	N1—C6—C5	122.49 (17)
O1—C1—C6	121.87 (17)	N1—C6—C1	117.25 (17)
C2—C1—C6	118.05 (17)	C5—C6—C1	120.26 (17)
C1—C2—C3	122.49 (18)	C8—C7—C5	119.71 (18)
C1—C2—Cl1	119.33 (15)	C8—C7—H7	120.1
C3—C2—Cl1	118.17 (15)	C5—C7—H7	120.1
C4—C3—C2	119.43 (18)	C7—C8—C9	118.71 (17)
C4—C3—H3	120.3	C7—C8—H8	120.6
C2—C3—H3	120.3	C9—C8—H8	120.6

C3—C4—C5	121.50 (18)	N1—C9—C8	123.88 (18)
C3—C4—Cl2	119.21 (15)	N1—C9—H9	118.1
C5—C4—Cl2	119.28 (14)	C8—C9—H9	118.1
C7—C5—C4	124.50 (18)		

O1—C1—C2—C3	179.21 (17)	C7—C5—C6—N1	−1.1 (3)
C6—C1—C2—C3	−0.9 (3)	C4—C5—C6—N1	178.25 (17)
O1—C1—C2—Cl1	0.4 (3)	C7—C5—C6—C1	178.50 (17)
C6—C1—C2—Cl1	−179.66 (14)	C4—C5—C6—C1	−2.1 (3)
C1—C2—C3—C4	−0.2 (3)	O1—C1—C6—N1	1.6 (3)
Cl1—C2—C3—C4	178.56 (15)	C2—C1—C6—N1	−178.29 (17)
C2—C3—C4—C5	0.2 (3)	O1—C1—C6—C5	−178.02 (17)
C2—C3—C4—Cl2	−179.52 (14)	C2—C1—C6—C5	2.1 (3)
C3—C4—C5—C7	−179.67 (18)	C4—C5—C7—C8	−179.00 (19)
Cl2—C4—C5—C7	0.0 (3)	C6—C5—C7—C8	0.3 (3)
C3—C4—C5—C6	1.0 (3)	C5—C7—C8—C9	0.3 (3)
Cl2—C4—C5—C6	−179.31 (14)	C6—N1—C9—C8	−0.6 (3)
C9—N1—C6—C5	1.2 (3)	C7—C8—C9—N1	−0.2 (3)
C9—N1—C6—C1	−178.39 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.84 (1)	2.01 (2)	2.761 (2)	150 (3)

Symmetry code: (i) $-x, y, -z+1/2$.