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2,6-Dichlorobenzaldehyde oxime

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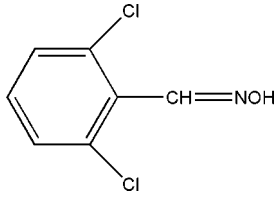
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.085; data-to-parameter ratio = 16.1.

In the title compound, $C_7H_5Cl_2NO$, there are two molecules in the asymmetric unit. The molecules are essentially identical. Each molecule is connected to a symmetry-related molecule through an inversion center by O—H···N hydrogen bonds, building an $R_2^2(6)$ graph-set motif.

Related literature

For related literature, see: Xu & Jin (1999). For graph-set notation, see: Etter *et al.* (1990); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_7H_5Cl_2NO$
M_r = 190.02
Triclinic, $P\overline{1}$
a = 3.8074 (1) Å
b = 14.3712 (2) Å
c = 14.3835 (3) Å
α = 89.108 (1)°
β = 88.545 (1)°
γ = 85.296 (1)°
V = 784.04 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.76 mm^{-1}
T = 296 (2) K
0.26 × 0.24 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.818, T_{max} = 0.884
11107 measured reflections
3235 independent reflections
2809 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.06
3235 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 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···N1^{i}	0.82	2.14	2.854 (2)	145
O2—H2···N2^{ii}	0.82	2.15	2.850 (2)	144

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2391).

References

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supporting information

Acta Cryst. (2008). E**64**, o2134 [doi:10.1107/S1600536808033217]

2,6-Dichlorobenzaldehyde oxime

Feng-Yu Bao

S1. Comment

2,6-Dichlorobenzaldehyde oxime, is an important intermediate for organic synthesis(Xu & Jin,1999). As part of our task, we have synthesized the title compound (I) .

In the title compound, $C_7H_6Cl_2NO$, there are two molecules in the asymmetric unit. Both molecules are roughly identical, the oxime fragment is twisted with respect to the dichlorobenzene ring by 53.83 (11)° and 42.99 (14)° respectively (Fig. 1).

Each molecule is connected to its symmetry related one through inversion center by O-H···N hydrogen bonds building a $R_2^2(6)$ graph-set motif (Etter *et al.*, 1990; Bernstein *et al.*, 1995) (Fig. 2 and Table 1).

S2. Experimental

2,6-dichlorobenzaldehyde (1 mmol) was dissolved in anhydrous methanol, hydroxylamine hydrochloride and sodium carbonate were added to this, the mixture was stirred for 3 h at room temperature. The product was isolated and recrystallized in dichloromethane, colourless single crystals of (I) was obtained after 5 d.

S3. Refinement

All H atoms were placed in calculated position and treated as riding on their parent atoms with C—H=0.93Å or O—H=0.82 Å with U_{iso}(H)=1.2U_{eq}(C) or 1.5U_{eq}(O) for the hydroxyl H atom.

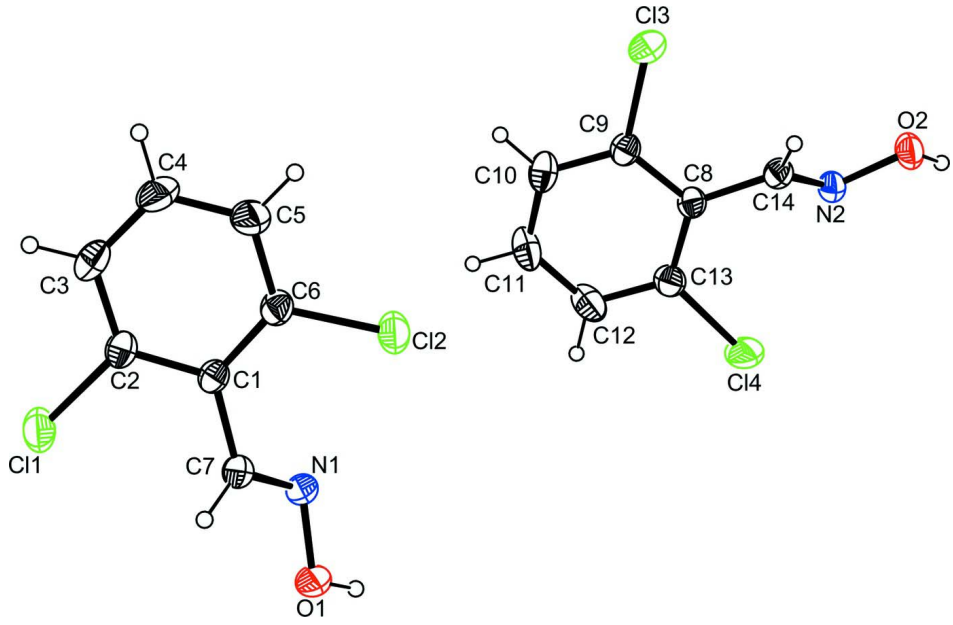

Figure 1

The asymmetric unit of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

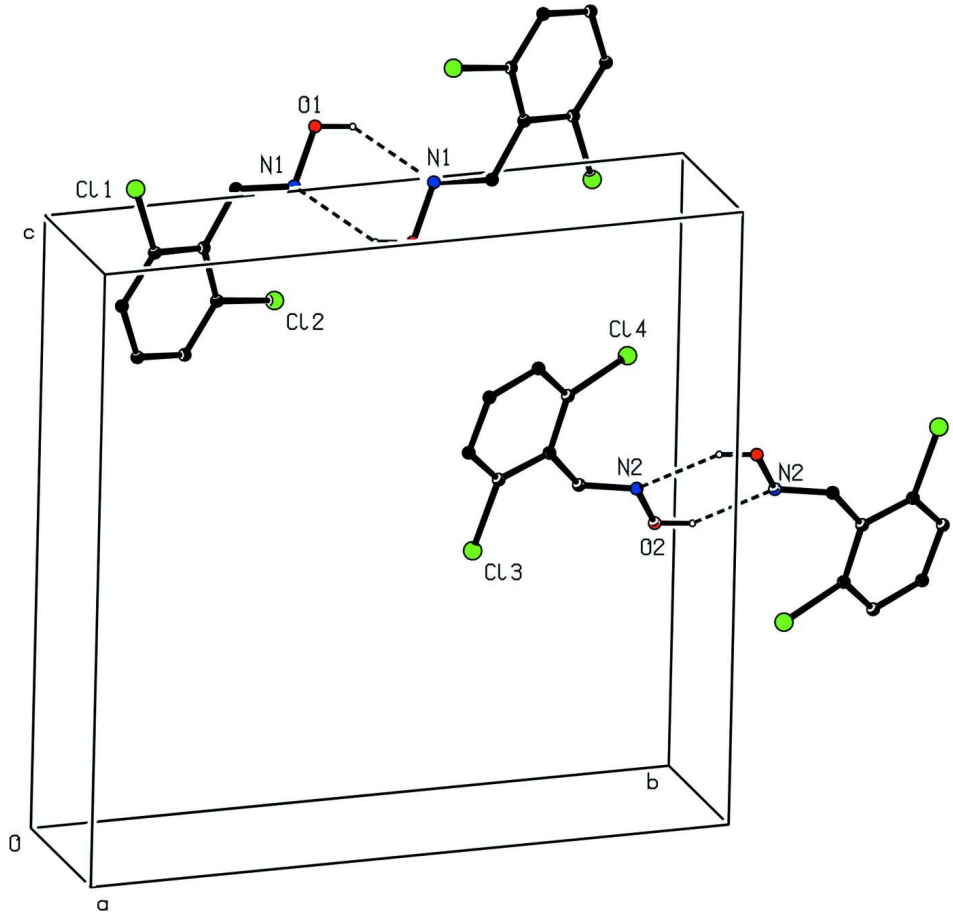

Figure 2

Partial packing view of compound (I), showing the formation of dimer through $R_2^2(6)$ graph set motif. H bonds are represented as dashed lines. H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (i) -x, -y+1, -z+2; (ii) -x+1 , -y+2, -z+1.]

2,6-Dichlorobenzaldehyde oxime

Crystal data

$C_7H_5Cl_2NO$
$M_r = 190.02$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$\beta = 88.545\ (1)°$
$\gamma = 85.296\ (1)°$
$V = 784.04\ (3)$ Å^3
$Z = 4$
$F(000) = 384$
$D_x = 1.610$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5529 reflections
$\theta = 2.8–27.4°$
$\mu = 0.76$ mm^{-1}
$T = 296$ K
Block, colourless
0.26 × 0.24 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.818, T_{max} = 0.884
11107 measured reflections
3235 independent reflections
2809 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 26.5°, θ_{min} = 1.4°
$h = -4 \rightarrow 4$
$k = -17 \rightarrow 17$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.06
3235 reflections
201 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
$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 0.3155P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.16981 (16)	0.12516 (3)	1.04669 (4)	0.06328 (16)
Cl2	−0.28140 (15)	0.39071 (3)	0.79443 (4)	0.05813 (16)
N1	−0.0849 (4)	0.39836 (10)	0.99884 (10)	0.0430 (3)
O1	−0.2185 (4)	0.44211 (9)	1.07941 (9)	0.0574 (4)
H1	−0.1779	0.4973	1.0774	0.086*
C1	−0.0441 (4)	0.25470 (11)	0.91699 (11)	0.0371 (4)
C2	0.1056 (5)	0.16371 (12)	0.93282 (13)	0.0426 (4)
C3	0.2132 (6)	0.10360 (13)	0.86200 (16)	0.0551 (5)
H3	0.3128	0.0437	0.8752	0.066*
C4	0.1703 (7)	0.13390 (15)	0.77145 (16)	0.0653 (6)
H4	0.2431	0.0943	0.7229	0.078*
C5	0.0202 (6)	0.22243 (15)	0.75209 (14)	0.0599 (5)
H5	−0.0105	0.2422	0.6908	0.072*
C6	−0.0839 (5)	0.28136 (12)	0.82397 (13)	0.0434 (4)
C7	−0.1573 (5)	0.31429 (12)	0.99624 (12)	0.0416 (4)
H7	−0.2847	0.2895	1.0454	0.050*

Cl3	0.60840 (16)	0.62545 (3)	0.44764 (4)	0.06139 (16)
Cl4	0.35612 (19)	0.88605 (4)	0.71520 (4)	0.07117 (19)
N2	0.4237 (4)	0.89871 (10)	0.50330 (10)	0.0429 (3)
O2	0.2629 (4)	0.94385 (9)	0.42708 (9)	0.0538 (3)
H2	0.3079	0.9987	0.4256	0.081*
C8	0.5024 (4)	0.75283 (11)	0.58413 (11)	0.0384 (4)
C9	0.6303 (5)	0.66160 (12)	0.56212 (13)	0.0421 (4)
C10	0.7785 (5)	0.59945 (13)	0.62661 (16)	0.0546 (5)
H10	0.8605	0.5393	0.6093	0.065*
C11	0.8035 (6)	0.62748 (15)	0.71651 (16)	0.0618 (6)
H11	0.9070	0.5864	0.7604	0.074*
C12	0.6773 (6)	0.71567 (15)	0.74256 (14)	0.0612 (6)
H12	0.6931	0.7340	0.8039	0.073*
C13	0.5265 (5)	0.77725 (12)	0.67727 (13)	0.0477 (4)
C14	0.3507 (5)	0.81491 (11)	0.51094 (12)	0.0406 (4)
H14	0.1973	0.7919	0.4693	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0848 (4)	0.0441 (3)	0.0602 (3)	0.0013 (2)	−0.0151 (3)	0.0096 (2)
Cl2	0.0817 (4)	0.0398 (3)	0.0525 (3)	0.0009 (2)	−0.0155 (2)	0.0047 (2)
N1	0.0565 (9)	0.0348 (7)	0.0375 (8)	−0.0012 (6)	−0.0006 (6)	−0.0057 (6)
O1	0.0891 (11)	0.0393 (7)	0.0429 (7)	−0.0001 (7)	0.0089 (7)	−0.0099 (6)
C1	0.0395 (9)	0.0296 (8)	0.0428 (9)	−0.0062 (6)	−0.0018 (7)	−0.0032 (7)
C2	0.0440 (10)	0.0329 (8)	0.0514 (10)	−0.0052 (7)	−0.0040 (8)	−0.0010 (7)
C3	0.0587 (12)	0.0330 (9)	0.0729 (14)	0.0009 (8)	0.0011 (10)	−0.0095 (9)
C4	0.0859 (16)	0.0477 (12)	0.0617 (13)	−0.0014 (11)	0.0098 (12)	−0.0206 (10)
C5	0.0861 (16)	0.0497 (11)	0.0445 (11)	−0.0080 (10)	0.0018 (10)	−0.0081 (9)
C6	0.0516 (10)	0.0331 (8)	0.0462 (10)	−0.0065 (7)	−0.0038 (8)	−0.0026 (7)
C7	0.0480 (10)	0.0349 (9)	0.0417 (9)	−0.0035 (7)	0.0023 (7)	0.0002 (7)
Cl3	0.0811 (4)	0.0450 (3)	0.0574 (3)	0.0006 (2)	0.0000 (3)	−0.0139 (2)
Cl4	0.1140 (5)	0.0476 (3)	0.0511 (3)	−0.0031 (3)	0.0111 (3)	−0.0128 (2)
N2	0.0526 (9)	0.0351 (7)	0.0403 (8)	−0.0002 (6)	−0.0031 (6)	0.0031 (6)
O2	0.0744 (9)	0.0380 (7)	0.0486 (7)	0.0001 (6)	−0.0127 (7)	0.0071 (6)
C8	0.0419 (9)	0.0317 (8)	0.0422 (9)	−0.0069 (7)	0.0001 (7)	0.0022 (7)
C9	0.0444 (10)	0.0337 (8)	0.0488 (10)	−0.0068 (7)	−0.0008 (8)	−0.0002 (7)
C10	0.0569 (12)	0.0343 (9)	0.0728 (14)	−0.0048 (8)	−0.0082 (10)	0.0080 (9)
C11	0.0744 (15)	0.0481 (11)	0.0644 (13)	−0.0124 (10)	−0.0206 (11)	0.0208 (10)
C12	0.0871 (16)	0.0552 (12)	0.0443 (11)	−0.0219 (11)	−0.0113 (10)	0.0082 (9)
C13	0.0630 (12)	0.0371 (9)	0.0441 (10)	−0.0105 (8)	0.0017 (8)	−0.0001 (7)
C14	0.0451 (10)	0.0346 (9)	0.0422 (9)	−0.0027 (7)	−0.0020 (7)	−0.0020 (7)

Geometric parameters (Å, º)

Cl1—C2	1.7376 (19)	Cl3—C9	1.7403 (19)
Cl2—C6	1.7370 (18)	Cl4—C13	1.7336 (19)
N1—C7	1.262 (2)	N2—C14	1.261 (2)

N1—O1	1.3919 (19)	N2—O2	1.3945 (18)
O1—H1	0.8200	O2—H2	0.8200
C1—C6	1.394 (2)	C8—C13	1.397 (2)
C1—C2	1.401 (2)	C8—C9	1.399 (2)
C1—C7	1.471 (2)	C8—C14	1.468 (2)
C2—C3	1.378 (3)	C9—C10	1.377 (3)
C3—C4	1.376 (3)	C10—C11	1.368 (3)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.379 (3)	C11—C12	1.372 (3)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.376 (3)	C12—C13	1.383 (3)
C5—H5	0.9300	C12—H12	0.9300
C7—H7	0.9300	C14—H14	0.9300
C7—N1—O1	111.93 (15)	C14—N2—O2	111.98 (15)
N1—O1—H1	109.5	N2—O2—H2	109.5
C6—C1—C2	115.78 (16)	C13—C8—C9	115.73 (16)
C6—C1—C7	124.33 (15)	C13—C8—C14	124.76 (16)
C2—C1—C7	119.86 (15)	C9—C8—C14	119.50 (15)
C3—C2—C1	123.02 (18)	C10—C9—C8	122.98 (18)
C3—C2—Cl1	118.10 (15)	C10—C9—Cl3	118.38 (15)
C1—C2—Cl1	118.86 (14)	C8—C9—Cl3	118.63 (14)
C4—C3—C2	118.71 (18)	C11—C10—C9	119.02 (19)
C4—C3—H3	120.6	C11—C10—H10	120.5
C2—C3—H3	120.6	C9—C10—H10	120.5
C3—C4—C5	120.56 (19)	C10—C11—C12	120.62 (19)
C3—C4—H4	119.7	C10—C11—H11	119.7
C5—C4—H4	119.7	C12—C11—H11	119.7
C6—C5—C4	119.7 (2)	C11—C12—C13	119.8 (2)
C6—C5—H5	120.2	C11—C12—H12	120.1
C4—C5—H5	120.2	C13—C12—H12	120.1
C5—C6—C1	122.23 (17)	C12—C13—C8	121.80 (18)
C5—C6—Cl2	117.14 (15)	C12—C13—Cl4	117.71 (16)
C1—C6—Cl2	120.61 (13)	C8—C13—Cl4	120.46 (14)
N1—C7—C1	121.30 (16)	N2—C14—C8	121.45 (16)
N1—C7—H7	119.4	N2—C14—H14	119.3
C1—C7—H7	119.4	C8—C14—H14	119.3

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	2.14	2.854 (2)	145
O2—H2···N2^{ii}	0.82	2.15	2.850 (2)	144

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