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(*E*)-2,4-Dichlorobenzaldehyde oxime

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.103
Data-to-parameter ratio = 13.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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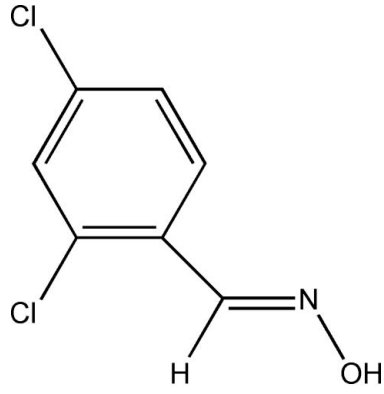
In the title molecule, $C_7H_5Cl_2NO$, which is an *E* isomer, all bond lengths and angles are normal. Intermolecular O—H···N hydrogen bonds link the molecules into centrosymmetric dimers. The crystal packing is further stabilized by van der Waals forces.

Comment

2,4-Dichlorobenzaldehyde oxime is an important intermediate for organic synthesis (Gholizadeh & Mohammadpoor, 2005). Two isomers are known for this compound (Sharghi & Sarvari, 2001), the Z and *E* isomers. We report here the crystal structure of the title compound, (I) (Fig. 1), which is the *E* isomer.



(I)

In (I), the bond lengths and angles (Table 1) are in agreement with the previously reported values (Li & Tian, 2006; Zhang *et al.*, 2006). Atoms N1 and O1 deviate from the mean plane of C1–C7/Cl1/Cl2 by 0.308 (2) and 0.209 (3) Å, respectively. Intermolecular O—H···N hydrogen bonds (Table 2) link the molecules into centrosymmetric dimers. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

Experimental

The title compound was synthesized by the reaction of 2,4-dichlorobenzaldehyde (0.01 mol) with hydroxylamine hydrochloride (0.01 mol) in the presence of sodium carbonate (0.01 mol) in an aqueous methanol (water:methanol *v*/*v* = 1:1) solution (20 ml) at room temperature (3 h). After diluting with water, the aqueous solution was extracted with dichloromethane and the organic phase was evaporated to afford the title product in 93% yield (1.77 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a hexane/dichloromethane (1:1 *v*/*v*) solution at room temperature over a period of one week.

Crystal data

$C_7H_5Cl_2NO$
M_r = 190.02
Monoclinic, $P2_1/c$
a = 3.8066 (15) Å
b = 14.275 (6) Å
c = 14.530 (6) Å
β = 94.150 (5)°
V = 787.5 (6) Å^3
Z = 4
D_x = 1.603 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.76 mm^{-1}
T = 298 (2) K
Plate, colourless
0.32 × 0.16 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.794, T_{max} = 0.956
3606 measured reflections
1390 independent reflections
1058 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.103
S = 1.02
1390 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C1	1.745 (3)	O1—N1	1.395 (3)
Cl2—C3	1.731 (3)	N1—C7	1.256 (4)
C7—N1—O1	112.1 (2)		
O1—N1—C7—C6	179.3 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···N1^{i}	0.82	2.09	2.822 (4)	148

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

All H atoms were placed in calculated positions, with C—H = 0.93 Å and O—H = 0.82 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O) for the hydroxyl H atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

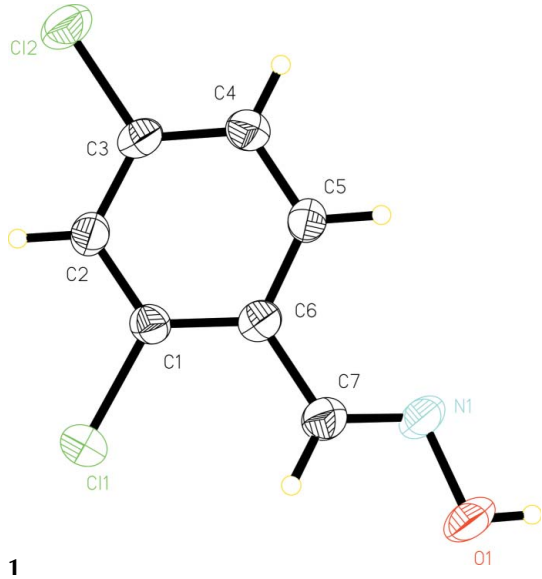


Figure 1
View of (I), with displacement ellipsoids drawn at the 40% probability level.

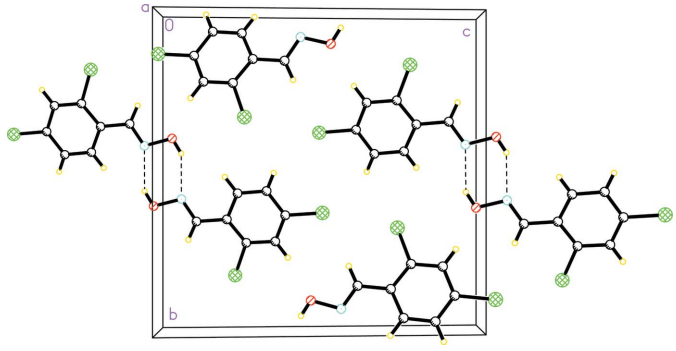


Figure 2
A packing diagram, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

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