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(*E*)-2-Chlorobenzaldehyde oxime

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Key indicators

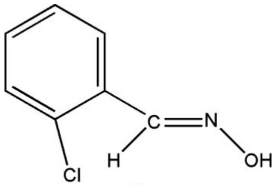
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.105
Data-to-parameter ratio = 13.8

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

In the title compound, C_7H_6ClNO, which exists as the *E* isomer, the crystal packing is stabilized by intermolecular O—H···N and C—H···O hydrogen bonds.

Comment

2-Chlorobenzaldehyde oxime, (I), is an important intermediate for organic synthesis (Xu & Jin, 1999), existing in two isomeric forms, *viz*. *Z* and *E* (Sharghi & Sarvari, 2001). We report here the crystal structure of (I) (Fig. 1), which is the *E* isomer.



(I)

In (I), the bond lengths and angles (Table 1) are in agreement with values reported previously (Jerslev, 1983; Jensen, 1970). Atoms N1 and O1 deviate from the mean plane of C1–C7/Cl1 by 0.278 (2) and 0.279 (3) Å, respectively. O—H···N hydrogen bonds (Table 2) link the molecules into centrosymmetric dimers. The crystal packing (Fig. 2) is further stabilized by weak intermolecular C—H···O interactions (Table 2).

Experimental

The title compound was synthesized by the reaction of 2-chlorobenzaldehyde (0.01 mol) with hydroxylamine hydrochloride (0.01 mol) in the presence of sodium carbonate (0.01 mol) in an aqueous methanol 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 90% isolated yield (1.41 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a solution in a hexane/dichloromethane mixture (1:1 *v*/*v*) at room temperature over a period of one week.

Crystal data

C_7H_6ClNO	D_x = 1.445 Mg m^{-3}
M_r = 155.58	Mo *K*α radiation
Monoclinic, $P2_1/c$	Cell parameters from 2273 reflections
a = 3.9231 (19) Å	θ = 2.3–26.3°
b = 14.160 (7) Å	μ = 0.46 mm^{-1}
c = 12.895 (6) Å	*T* = 298 (2) K
β = 93.544 (7)°	Block, colourless
V = 715.0 (6) Å^3	0.37 × 0.26 × 0.17 mm
Z = 4	

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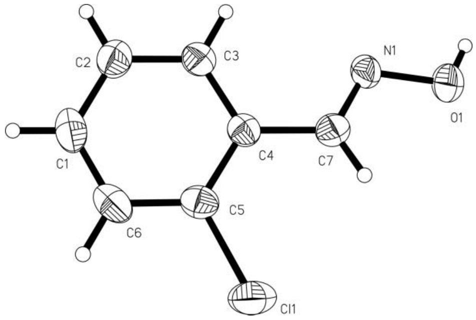

Figure 1
View of (I), with displacement ellipsoids drawn at the 40% probability level.

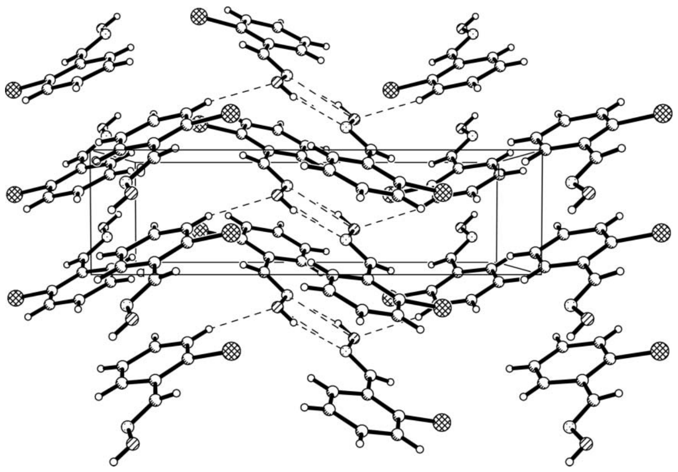

Figure 2
A perspective view of the packing along the *c* axis. Hydrogen bonds are indicated by dashed lines.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.871$, $T_{\max} = 0.918$
3621 measured reflections
1257 independent reflections
1146 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\max} = 25.0°$
$h = -4 \rightarrow 4$
$k = -16 \rightarrow 16$
$l = -12 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.105$
$S = 1.13$
1257 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 0.4106P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C5	1.744 (2)	N1—C7	1.266 (3)
O1—N1	1.402 (2)		
C7—N1—O1	111.71 (19)	N1—C7—C4	120.6 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N1$^{\rm i}$	0.82	2.14	2.855 (3)	146
C6—H6*A*···O1$^{\rm ii}$	0.93	2.55	3.451 (3)	162

Symmetry codes: (i) $-x-1, -y+2, -z$; (ii) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.

All H atoms were placed in calculated positions, with C—H = 0.93 Å and O—H = 0.82 Å, and included in the final cycles of refinement using a riding model, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for the C-bound H atoms and $1.5U_{\rm eq}({\rm O})$ for the hydroxyl H atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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