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2-Chlorobenzamide oxime monohydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.072
wR factor = 0.191
Data-to-parameter ratio = 15.2

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

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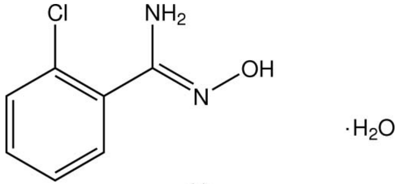
The title compound, $C_7H_7ClN_2O{\cdot}H_2O$, crystallizes with two organic molecules and two water molecules in the asymmetric unit. A network of O—H···N and O—H···O hydrogen bonds helps to consolidate the crystal packing.

Comment

As part of our onging studies of benzonitrile derivatives (Wang *et al.*, 2007), we report here the crystal structure of the title compound, (I), which crystallizes with two independent organic molecules and two water molecules in the asymmetric unit (Fig. 1).



(I)

The dihedral angle between the C1–C6 and C7/N1/N2/O1 mean planes is 71.0 (3)°. The equivalent angle for the C8–C13 and C14/N3/N4/O2 mean planes is 70.5 (2)°.

As well as intramolecular N—H···O hydrogen bonds in each organic molecule (Table 1), a network of intermolecular O—H···O and O—H···N hydrogen bonds involving both the organic and water molecules helps to establish the crystal packing in (I), resulting in (001) sheets.

Experimental

Three solutions were made up: (i) 2-chlorobenzonitrile (20 mmol) in ethanol (8 ml); (ii) hydroxylamine hydrochloride (20 mmol) in ethanol (6 ml); (iii) potassium carbonate (10 mmol) in water (10 ml). The three solutions were mixed, and the resulting solution was refluxed for 24 h. After cooling and filtration, the crude title compound was obtained and purified by recrystallizion from a mixture of ethanol (6 ml) and water (2 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_7H_7ClN_2O{\cdot}H_2O$
$M_r = 188.61$
Triclinic, $P\bar{1}$
$a = 4.5550\ (9)$ Å
$b = 6.8790\ (14)$ Å
$c = 28.715\ (6)$ Å
$\alpha = 91.37\ (3)^\circ$
$\beta = 90.58\ (3)^\circ$
$\gamma = 101.21\ (3)^\circ$
$V = 882.2\ (3)$ Å^3
$Z = 4$
$D_x = 1.420$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.39$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.40 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.858$, $T_{\max} = 0.962$
3672 measured reflections
3472 independent reflections
2517 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\max} = 26.0°$
3 standard reflections every 200 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.072$
$wR(F^2) = 0.191$
$S = 1.06$
3472 reflections
229 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 3P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.44$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O*W*2	0.82	1.92	2.686 (5)	155
N2—H2*A*···O1	0.86	2.23	2.540 (6)	101
N2—H2*A*···O*W*2$^{\rm i}$	0.86	2.27	3.112 (6)	167
O*W*1—H*W*1*B*···N4	0.85 (4)	2.02 (4)	2.859 (5)	172 (5)
O*W*1—H*W*1*A*···O2$^{\rm ii}$	0.85 (4)	2.02 (4)	2.854 (5)	170 (5)
O2—H2*D*···O*W*1$^{\rm iii}$	0.82	1.93	2.697 (5)	155
N3—H3*A*···O*W*1$^{\rm iv}$	0.86	2.27	3.117 (5)	168
N3—H3*A*···O2	0.86	2.24	2.546 (6)	101
O*W*2—H*W*2*A*···O1$^{\rm v}$	0.85 (4)	2.02 (4)	2.862 (5)	170 (5)
O*W*2—H*W*2*B*···N1$^{\rm vi}$	0.85 (4)	2.01 (3)	2.853 (5)	174 (6)

Symmetry codes: (i) $-x+2, -y+2, -z$; (ii) $-x+3, -y+2, -z+1$; (iii) $-x+4, -y+2, -z+1$; (iv) $x, y+1, z$; (v) $x+1, y, z$; (vi) $-x+2, -y+1, -z$.

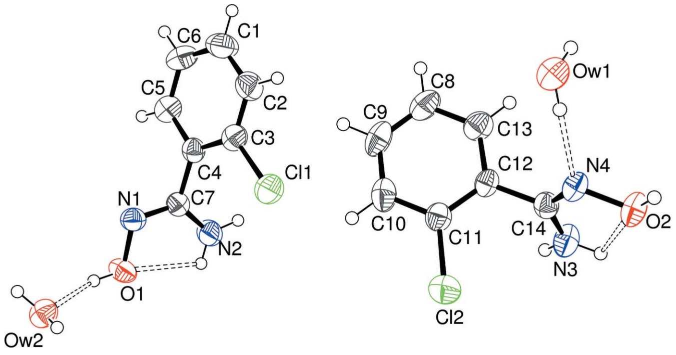


Figure 1
The asymmetric unit of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). Hydrogen bonds are indicated by double dashed lines.

The H atoms of the organic molecule were positioned geometrically (C—H = 0.93–0.97, O—H = 0.82 and N—H = 0.86 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2$ or $1.5U_{\rm eq}$ of the carrier atom. The water H atoms were located in a difference map and their positions were refined with the restraint O—H = 0.85 (1) Å and with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo,1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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