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Key indicators

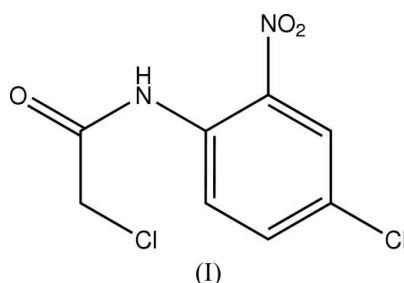
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.043
 wR factor = 0.106
Data-to-parameter ratio = 14.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2-Chloro-*N*-(4-chloro-2-nitrophenyl)acetamide

In the title compound, $\text{C}_8\text{H}_6\text{Cl}_2\text{N}_2\text{O}_3$, molecules are linked into infinite chains along the c axis by $\text{C}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds.

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Comment

2-Chloro-*N*-phenylacetamide is an important intermediate in organic synthesis, which can be used in the synthesis of many derivatives (Zhang *et al.*, 2006). As part of our ongoing studies, the title compound, (I), was synthesized and its structure is reported here.



In (I), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable with those in a related compound (Wen *et al.*, 2006). Ring *A* (atoms C1–C6) and the C6–C8/N1/O3 unit are planar, with a dihedral angle of $9.79(1)^\circ$ between them. There are three intramolecular hydrogen bonds, *viz.* N1–H1A \cdots Cl1, N1–H1A \cdots O1 and C1–H1B \cdots O3 (Table 1), forming a five- and two six-membered rings (Fig. 1), respectively.

In the crystal structure, the molecules are linked into infinite chains along the c axis by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1).

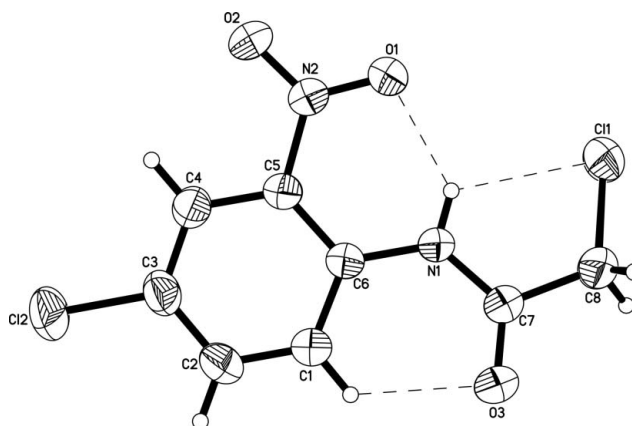


Figure 1

The molecular structure of the compound (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme. Dashed lines indicate hydrogen bonds.

Experimental

Chloroacetyl chloride (11.3 g, 0.1 mol) was added to a solution of 4-chloro-2-nitrophenylamine (17.3 g, 0.1 mol) and triethylamine (10.2 g, 0.1 mol) in benzene (60 ml) over a period of 30 min with cooling in an ice bath; the resulting mixture was stirred at room temperature for 4 h. After separation of the triethylamine hydrochloride by filtration, the organic phase was washed three times with water. The benzene layer was removed and evaporated. The title compound was obtained after drying the solid powder at room temperature for 48 h. Yellow single crystals were obtained by slow evaporation of an ethyl acetate solution over a period of 10 d.

Crystal data

$C_8H_6Cl_2N_2O_3$	$Z = 4$
$M_r = 249.05$	$D_x = 1.681 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 5.2652 (11) \text{ \AA}$	$\mu = 0.65 \text{ mm}^{-1}$
$b = 19.641 (6) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 9.5770 (19) \text{ \AA}$	Block, yellow
$\beta = 96.474 (7)^\circ$	$0.26 \times 0.16 \times 0.08 \text{ mm}$
$V = 984.1 (4) \text{ \AA}^3$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	5433 measured reflections
ω scans	1935 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1488 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.850$, $T_{\max} = 0.950$	$R_{\text{int}} = 0.028$
	$\theta_{\text{max}} = 26.1^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.2351P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.106$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.98$	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
1935 reflections	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
136 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots Cl1$	0.86	2.47	2.981 (2)	118
$N1-H1A\cdots O1$	0.86	1.99	2.632 (3)	131
$C1-H1B\cdots O3$	0.93	2.20	2.826 (3)	124
$C1-H1B\cdots O2^i$	0.93	2.50	3.239 (3)	137
$C4-H4A\cdots O3^{ii}$	0.93	2.45	3.342 (4)	160

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with $C-H = 0.93-0.97 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$; $N-H = 0.86 \text{ \AA}$, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

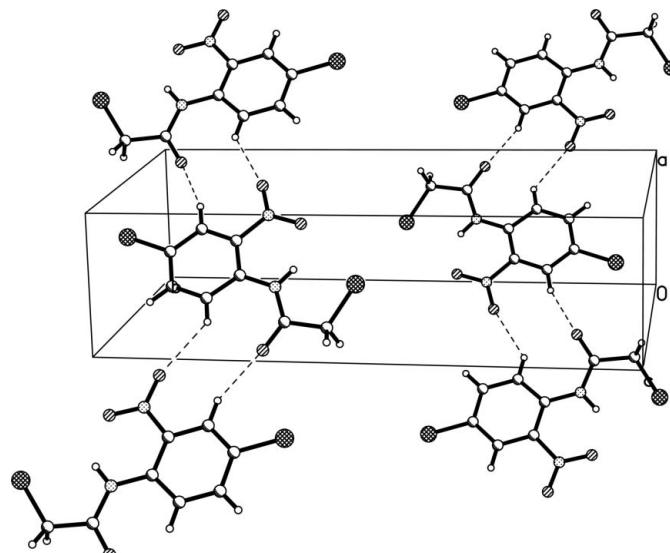


Figure 2

Packing diagram of (I), showing the intermolecular hydrogen bonds (dashed lines).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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