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2-Chloro-*N*-(4-nitrophenyl)acetamide

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Key indicators

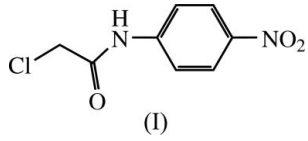
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.108
Data-to-parameter ratio = 14.1

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

In the molecule of the title compound, $C_8H_7ClN_2O_3$, an intramolecular C—H···O hydrogen bond forms a six-membered ring. In the crystal structure, the molecules are linked by intermolecular N—H···O hydrogen bonds, forming infinite chains along the *c* axis. The chains are further stabilized in ribbons by Cl···O short-contact interactions.

Comment

N-(Substituted phenyl)-2-chloroacetamides are important intermediates in organic synthesis. They can be used in the synthesis of many derivatives such as (quinolin-8-yl-oxy)acetamide (Zhang, Xu *et al.*, 2006), 2,5-piperazinedione (Wen *et al.*, 2006) and 2,2-(1,3,4-thiadiazolyl-2,5-dithio)diacetamide (Wen *et al.*, 2005). In our studies on *N*-(substituted phenyl)-2-chloroacetamide compounds (Zhang, Wen *et al.* 2006), the title compound, (I), was synthesized. In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987), and comparable to those of a related compound (Zhang, Wen *et al.*, 2006). Ring *A* (C1–C6) and the C6–C8/O3/N2 unit are planar and the dihedral angle between them is 7.8 (1)°. An intramolecular C1—H1*A*···O3 hydrogen bond (Table 2) forms a six-membered ring.



(I)

As can be seen from the packing diagram (Fig. 2), intermolecular N2—H2*A*···O3^{i} [symmetry code: (i) $\frac{1}{2}-x, -y, \frac{1}{2}+z$] hydrogen bonds (Table 2) link the molecules into infinite chains along the *c* axis. The chains are further stabilized in ribbons by Cl···O^{i} [3.191 (2) Å] short-contact interactions.

Experimental

Chloroacetyl chloride (5.65 g, 0.05 mol) was added to a solution of 4-nitrophenylamine (6.85 g, 0.05 mol) and triethylamine (5.1 g, 0.05 mol) in benzene (50 ml) over a period of 30 min, with cooling in an ice bath, and then the mixture was stirred at room remperature 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 colorless powder at room temperature for 48 h. Yellow single cystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution over a period of 10 d.

Crystal data

$C_8H_7ClN_2O_3$
M_r = 214.61
Orthorhombic, *Pbca*
a = 9.498 (2) Å
b = 9.457 (2) Å
c = 20.205 (5) Å
V = 1814.9 (7) Å^3
Z = 8
D_x = 1.571 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 293 (2) K
Needle, yellow
0.35 × 0.12 × 0.08 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.872, T_{max} = 0.969
9718 measured reflections
1787 independent reflections
1416 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
S = 1.05
1787 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.5597P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O3^{i}	0.86	2.04	2.840 (2)	154
C1—H1A···O3	0.93	2.27	2.869 (3)	121

Symmetry code: (i) $x-\frac{1}{2}, y, -z+\frac{5}{2}$.

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93, 0.97 and 0.96 Å for aromatic, methine and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N).

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

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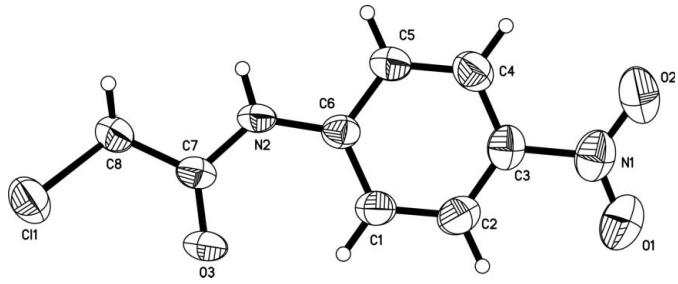

Figure 1
The molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

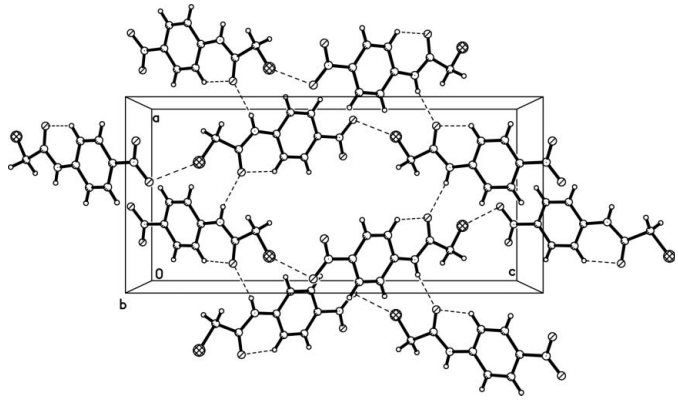

Figure 2
A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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