Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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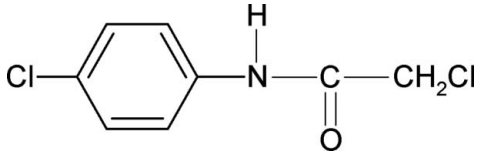
Received 24 October 2007; accepted 25 October 2007

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.125; data-to-parameter ratio = 14.3.

The structure of the title compound, $C_8H_7Cl_2NO$, resembles those of *N*-(4-chlorophenyl)acetamide, *N*-2-chloro-(4-methylphenyl)acetamide, *N*-2-chloro-(4-nitrophenyl)acetamide and other related amides, with similar bond parameters. Molecules are linked into chains through N—H···O hydrogen bonding.

Related literature

For related literature, see: Gowda *et al.* (2003, 2007*a*,*b*,*c*).



Experimental

Crystal data

$C_8H_7Cl_2NO$
M_r = 204.05
Monoclinic, $P2_1/n$
a = 4.4223 (9) Å
b = 22.469 (4) Å
c = 9.022 (2) Å
β = 99.89 (2)°
V = 883.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 299 (2) K
0.50 × 0.15 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.726, T_{max} = 0.967
1987 measured reflections
1575 independent reflections
1325 reflections with $I > 2s(I)$
R_{int} = 0.036
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.08
1575 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1^{i}	0.86	2.06	2.871 (2)	156

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

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2563).

References

Stoe & Cie (1987). *REDU4*. Version 6.2c. Stoe & Cie GmbH, Darmstadt, Germany.
Enraf–Nonius (1996). *CAD-4-PC Software*. Version 2.0. Enraf–Nonius, Delft, The Netherlands.
Gowda, B. T., Foro, S. & Fuess, H. (2007*a*). *Acta Cryst.* E**63**, o2333–o2334.
Gowda, B. T., Foro, S. & Fuess, H. (2007*b*). *Acta Cryst.* E**63**, o2335–o2336.
Gowda, B. T., Foro, S. & Fuess, H. (2007*c*). *Acta Cryst.* E**63**, o3392.
Gowda, B. T., Usha, K. M. & Jayalakshmi, K. L. (2003). *Z. Naturforsch. Teil A*, **58**, 801–806.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

  doi:10.1107/S1600536807053093

supplementary materials

Acta Cryst. (2007). E**63**, o4488 [**doi:10.1107/S1600536807053093**]

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

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Comment

The structure of *N*-(4-chlorophenyl)-2-chloroacetamide (4CP2CA) has been determined as part of a study on the systematization of the crystal structures of N-aromatic amides (Gowda *et al.*, 2007*a*, *b*, *c*). The structure of 4CP2CA (Fig. 1) is closely related to *N*-(4-chlorophenyl)-acetamide (Gowda *et al.*, 2007*c*), *N*-(4-methylphenyl)-2-chloroacetamide(Gowda *et al.*, 2007*a*), *N*-(4-nitrophenyl)-2-chloroacetamide(Gowda *et al.*, 2007*b*) and other related amides, with similar bond parameters. The molecules are linked into chains through N—H···O hydrogen bonding (Fig. 2 & Table 1).

Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2003). Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

Refinement

The H atoms were positioned with idealized geometry using a riding model with N—H = 0.86 Å and C—H = 0.93–0.97 Å. U_{iso}(H) values were set equal to 1.2U_{eq} of the parent atom.

Figures

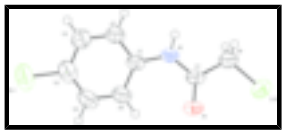

Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme and the displacement ellipsoids are drawn at the 50% probability level.

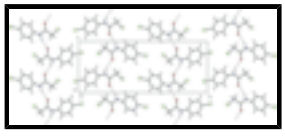

Fig. 2. Packing diagram of the title compounds with hydrogen bonding shown as dashed lines.

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

Crystal data

$C_8H_7Cl_2NO$	F_{000} = 416
M_r = 204.05	D_x = 1.535 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: -P 2yn
a = 4.4223 (9) Å
b = 22.469 (4) Å
c = 9.022 (2) Å
β = 99.89 (2)º
V = 883.1 (3) Å^3
Z = 4

Cell parameters from 25 reflections
θ = 3.9–21.1º
μ = 0.68 mm^{-1}
T = 299 (2) K
Rod, colourless
0.50 × 0.15 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 299(2) K
ω/2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.726, T_{max} = 0.967
1987 measured reflections
1575 independent reflections
1325 reflections with $I > 2s(I)$

R_{int} = 0.036
θ_{max} = 25.1º
θ_{min} = 1.8º
h = −5→1
k = −26→0
l = −10→10
3 standard reflections
every 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.08
1575 reflections
110 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2 + 0.2824P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.055 (6)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.5699 (2)	−0.02471 (3)	0.21899 (10)	0.0885 (4)
Cl2	−0.51248 (17)	0.34111 (3)	0.26538 (8)	0.0663 (3)
O1	−0.2283 (4)	0.23829 (8)	0.14574 (16)	0.0619 (5)
N1	0.0322 (4)	0.20364 (8)	0.36674 (19)	0.0453 (5)
H1N	0.0775	0.2123	0.4608	0.054*
C1	0.1604 (5)	0.15047 (10)	0.3229 (2)	0.0443 (5)
C2	0.3877 (6)	0.12376 (11)	0.4262 (3)	0.0525 (6)
H2	0.4557	0.1423	0.5181	0.063*
C3	0.5145 (7)	0.07017 (12)	0.3951 (3)	0.0625 (7)
H3	0.6650	0.0522	0.4656	0.075*
C4	0.4146 (7)	0.04365 (12)	0.2578 (3)	0.0619 (7)
C5	0.1925 (7)	0.06973 (12)	0.1538 (3)	0.0643 (7)
H5	0.1277	0.0513	0.0615	0.077*
C6	0.0649 (7)	0.12291 (12)	0.1849 (3)	0.0554 (6)
H6	−0.0855	0.1405	0.1138	0.067*
C7	−0.1506 (5)	0.24245 (11)	0.2818 (2)	0.0440 (5)
C8	−0.2504 (6)	0.29315 (12)	0.3730 (3)	0.0557 (6)
H8A	−0.0709	0.3157	0.4178	0.067*
H8B	−0.3432	0.2768	0.4540	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1344 (8)	0.0529 (4)	0.0908 (6)	0.0109 (4)	0.0547 (6)	−0.0021 (4)
Cl2	0.0744 (5)	0.0662 (5)	0.0552 (4)	0.0144 (3)	0.0024 (3)	0.0104 (3)
O1	0.0878 (13)	0.0658 (11)	0.0268 (8)	0.0072 (10)	−0.0055 (8)	0.0001 (7)
N1	0.0602 (11)	0.0495 (11)	0.0243 (8)	−0.0041 (9)	0.0017 (8)	−0.0003 (7)
C1	0.0587 (14)	0.0443 (11)	0.0310 (10)	−0.0098 (10)	0.0106 (9)	0.0021 (8)
C2	0.0630 (14)	0.0545 (13)	0.0387 (12)	−0.0037 (11)	0.0055 (10)	0.0002 (10)
C3	0.0736 (17)	0.0588 (15)	0.0565 (15)	0.0037 (13)	0.0151 (13)	0.0057 (12)
C4	0.0866 (19)	0.0474 (14)	0.0597 (15)	−0.0076 (13)	0.0353 (14)	0.0008 (12)
C5	0.095 (2)	0.0556 (15)	0.0451 (13)	−0.0148 (14)	0.0192 (14)	−0.0096 (12)
C6	0.0736 (16)	0.0541 (14)	0.0377 (12)	−0.0093 (12)	0.0068 (11)	−0.0034 (10)
C7	0.0486 (12)	0.0532 (12)	0.0286 (10)	−0.0082 (10)	0.0022 (8)	0.0024 (9)
C8	0.0585 (14)	0.0692 (16)	0.0373 (12)	0.0090 (12)	0.0025 (11)	0.0000 (11)

Geometric parameters (Å, °)

Cl1—C4	1.742 (3)	C3—C4	1.377 (4)
Cl2—C8	1.749 (3)	C3—H3	0.9300
O1—C7	1.221 (2)	C4—C5	1.369 (4)
N1—C7	1.337 (3)	C5—C6	1.371 (4)

N1—C1	1.408 (3)	C5—H5	0.9300
N1—H1N	0.8600	C6—H6	0.9300
C1—C2	1.385 (3)	C7—C8	1.514 (3)
C1—C6	1.389 (3)	C8—H8A	0.9700
C2—C3	1.377 (4)	C8—H8B	0.9700
C2—H2	0.9300		
C7—N1—C1	128.72 (18)	C4—C5—C6	120.3 (2)
C7—N1—H1N	115.6	C4—C5—H5	119.8
C1—N1—H1N	115.6	C6—C5—H5	119.8
C2—C1—C6	118.9 (2)	C5—C6—C1	120.0 (3)
C2—C1—N1	117.3 (2)	C5—C6—H6	120.0
C6—C1—N1	123.7 (2)	C1—C6—H6	120.0
C3—C2—C1	121.0 (2)	O1—C7—N1	124.4 (2)
C3—C2—H2	119.5	O1—C7—C8	123.1 (2)
C1—C2—H2	119.5	N1—C7—C8	112.56 (18)
C4—C3—C2	118.9 (3)	C7—C8—Cl2	112.92 (16)
C4—C3—H3	120.6	C7—C8—H8A	109.0
C2—C3—H3	120.6	Cl2—C8—H8A	109.0
C5—C4—C3	120.9 (3)	C7—C8—H8B	109.0
C5—C4—Cl1	120.1 (2)	Cl2—C8—H8B	109.0
C3—C4—Cl1	119.1 (2)	H8A—C8—H8B	107.8
C7—N1—C1—C2	168.2 (2)	Cl1—C4—C5—C6	178.6 (2)
C7—N1—C1—C6	−13.8 (4)	C4—C5—C6—C1	−0.2 (4)
C6—C1—C2—C3	−1.2 (4)	C2—C1—C6—C5	0.9 (4)
N1—C1—C2—C3	176.8 (2)	N1—C1—C6—C5	−177.0 (2)
C1—C2—C3—C4	0.9 (4)	C1—N1—C7—O1	−2.9 (4)
C2—C3—C4—C5	−0.2 (4)	C1—N1—C7—C8	177.7 (2)
C2—C3—C4—Cl1	−179.0 (2)	O1—C7—C8—Cl2	5.1 (3)
C3—C4—C5—C6	−0.1 (4)	N1—C7—C8—Cl2	−175.47 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O1^{i}	0.86	2.06	2.871 (2)	156

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2.

Fig. 1

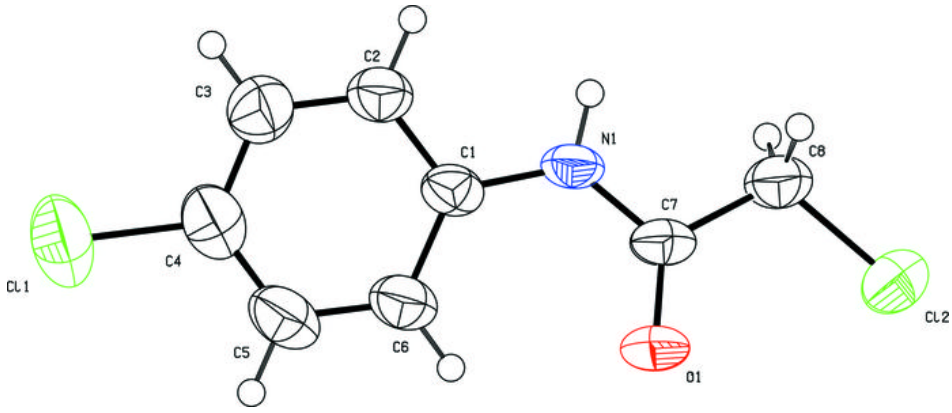

Fig. 2