

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

N-(2-Chlorophenyl)acetamide

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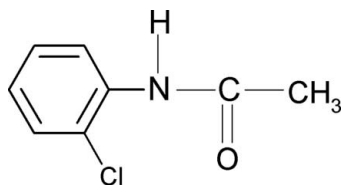
Received 12 June 2007; accepted 13 June 2007

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.032; wR factor = 0.081; data-to-parameter ratio = 14.1.

In the structure of the title compound, $\text{C}_8\text{H}_8\text{ClNO}$, the conformation of the N—H bond is *syn* to the *ortho*-chloro substituent, in contrast to the *anti* conformation observed for the *ortho*-methyl substituent in *N*-(2-methylphenyl)acetamide, although the geometric parameters of these two structures are similar. The molecules are linked into chains through N—H \cdots O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2003, 2007a, 2007b); Gowda, Kožíšek, Svoboda & Fuess (2007); Gowda, Kožíšek, Tokarčík & Fuess (2007).



Experimental

Crystal data

$\text{C}_8\text{H}_8\text{ClNO}$	$V = 808.92$ (15) Å ³
$M_r = 169.60$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 4.7468$ (4) Å	$\mu = 0.41$ mm ⁻¹
$b = 11.699$ (1) Å	$T = 100$ (2) K
$c = 14.640$ (2) Å	$0.40 \times 0.12 \times 0.04$ mm
$\beta = 95.74$ (2)°	

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	(Clark & Reid, 1995) $T_{\min} = 0.854$, $T_{\max} = 0.984$
Absorption correction: multi-scan (<i>CrysAlis RED</i> ; Oxford Diffraction, 2006) using a multifaceted crystal model	5681 measured reflections 1641 independent reflections 1204 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.081$	
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.29$ e Å ⁻³
1641 reflections	$\Delta\rho_{\text{min}} = -0.23$ e Å ⁻³
116 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

D—H \cdots A	D—H	H \cdots A	D \cdots A	D—H \cdots A
N1—H1 \cdots O1 ¹	0.813 (18)	2.079 (18)	2.8630 (19)	161.7 (17)

Symmetry code: (i) $x + 1, y, z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

BTG gratefully 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: BT2391).

References

- Clark, R. C. & Reid, J. S. (1995). *Acta Cryst.* **A51**, 887–897.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Gowda, B. T., Foro, S. & Fuess, H. (2007a). *Acta Cryst.* **E63**, o2341–o2342.
Gowda, B. T., Foro, S. & Fuess, H. (2007b). *Acta Cryst.* **E63**, o2631–o2632.
Gowda, B. T., Kožíšek, J., Svoboda, I. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**, 91–100.
Gowda, B. T., Kožíšek, J., Tokarčík, M. & Fuess, H. (2007). *Acta Cryst.* **E63**, o1977–o1978.
Gowda, B. T., Usha, K. M. & Jayalakshmi, K. L. (2003). *Z. Naturforsch. Teil A*, **58**, 801–806.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2007). E63, o3267 [doi:10.1107/S1600536807028991]

N-(2-Chlorophenyl)acetamide

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Comment

The structure of *N*-(2-chlorophenyl)-acetamide has been determined as part of a study on the systematization of the crystal structures of *N*-aromatic amides (Gowda *et al.*, 2007a, Gowda *et al.*, 2007b, Gowda, Kožíšek, Svoboda & Fuess 2007, Gowda, Kožíšek, Tokarčík & Fuess, 2007). The conformation of the N—H bond is *syn* to the *ortho*-chloro substituent (Fig. 1), in contrast to the anti conformation observed for the *ortho*-methyl substituent in *N*-(2-methylphenyl)-acetamide (Gowda, Kožíšek, Tokarčík & Fuess, 2007). The geometric parameters of these two structures and other acetanilides are similar (Gowda *et al.*, 2007a,b, Gowda, Kožíšek, Svoboda & Fuess 2007, Gowda, Kožíšek, Tokarčík & Fuess, 2007). The molecules are packed into chains through N—H···O hydrogen bonds (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 located in a difference map and their coordinates were refined with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{parent atom})$. The methyl group was refined using a riding model and was allowed to rotate but not to tip.

Figures

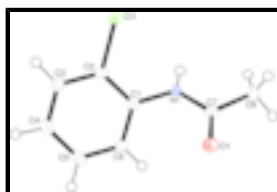


Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

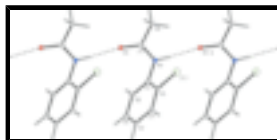


Fig. 2. Hydrogen bonding in the title compound. Hydrogen bonds are shown as dashed lines.

N-(2-Chlorophenyl)acetamide

Crystal data

C_8H_8ClNO	$F_{000} = 352$
$M_r = 169.60$	$D_x = 1.393 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: $-P2_1n$	$\lambda = 0.71073 \text{ \AA}$
$a = 4.7468 (4) \text{ \AA}$	Cell parameters from 1844 reflections
$b = 11.699 (1) \text{ \AA}$	$\theta = 2.3\text{--}25.0^\circ$
$c = 14.640 (2) \text{ \AA}$	$\mu = 0.41 \text{ mm}^{-1}$
$\beta = 95.74 (2)^\circ$	$T = 100 (2) \text{ K}$
$V = 808.92 (15) \text{ \AA}^3$	Needle, colourless
$Z = 4$	$0.40 \times 0.12 \times 0.04 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	1641 independent reflections
Radiation source: Enhance (Mo) X-ray Source	1204 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.023$
Detector resolution: $8.4012 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 26.4^\circ$
$T = 100(2) \text{ K}$	$\theta_{\text{min}} = 2.8^\circ$
Rotation method data acquisition using ω and φ scans $h = -5 \rightarrow 5$	
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006) using a multifaceted crystal model (Clark & Reid, 1995)	$k = -14 \rightarrow 14$
$T_{\text{min}} = 0.854, T_{\text{max}} = 0.984$	$l = -18 \rightarrow 18$
5681 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.081$	$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2]$
$S = 1.07$	where $P = (F_o^2 + 2F_c^2)/3$
1641 reflections	$(\Delta/\sigma)_{\text{max}} = 0.008$
116 parameters	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
	Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ is used only for calculating 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	−0.0446 (3)	0.05702 (15)	0.35962 (11)	0.0146 (4)
C2	0.0451 (4)	0.01850 (15)	0.27730 (12)	0.0166 (4)
C3	−0.0388 (4)	−0.08698 (16)	0.24092 (13)	0.0200 (4)
H3	0.031 (4)	−0.1113 (15)	0.1851 (13)	0.024*
C4	−0.2228 (4)	−0.15359 (16)	0.28474 (13)	0.0216 (4)
H4	−0.278 (4)	−0.2266 (17)	0.2550 (13)	0.026*
C5	−0.3189 (4)	−0.11594 (16)	0.36608 (13)	0.0206 (4)
H5	−0.448 (4)	−0.1583 (16)	0.3943 (12)	0.025*
C6	−0.2289 (4)	−0.01185 (16)	0.40335 (13)	0.0166 (4)
H6	−0.288 (4)	0.0123 (15)	0.4588 (13)	0.020*
C7	−0.1093 (4)	0.23926 (15)	0.43748 (12)	0.0158 (4)
C8	0.0367 (4)	0.34568 (15)	0.47456 (13)	0.0219 (4)
H8A	−0.0056	0.4087	0.4313	0.026*
H8B	0.2417	0.3327	0.4828	0.026*
H8C	−0.0305	0.3651	0.5338	0.026*
N1	0.0540 (3)	0.16230 (13)	0.39826 (10)	0.0142 (3)
H1	0.221 (4)	0.1778 (16)	0.3978 (12)	0.017*
O1	−0.3652 (2)	0.22592 (11)	0.44072 (9)	0.0223 (3)
Cl1	0.27008 (9)	0.10385 (4)	0.21925 (3)	0.02233 (16)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0125 (9)	0.0149 (9)	0.0157 (9)	0.0015 (8)	−0.0020 (7)	0.0011 (8)
C2	0.0135 (9)	0.0195 (10)	0.0172 (9)	0.0006 (8)	0.0039 (7)	0.0035 (8)
C3	0.0178 (9)	0.0221 (11)	0.0197 (10)	0.0027 (8)	0.0005 (8)	−0.0041 (9)
C4	0.0209 (10)	0.0149 (10)	0.0279 (10)	−0.0010 (8)	−0.0036 (9)	−0.0036 (9)
C5	0.0189 (9)	0.0201 (11)	0.0226 (10)	−0.0050 (8)	0.0007 (8)	0.0050 (9)
C6	0.0171 (10)	0.0186 (10)	0.0140 (9)	0.0004 (8)	0.0015 (8)	0.0015 (8)
C7	0.0142 (9)	0.0185 (10)	0.0146 (9)	0.0004 (8)	0.0009 (7)	0.0019 (8)
C8	0.0214 (10)	0.0194 (10)	0.0253 (10)	0.0030 (8)	0.0049 (8)	−0.0035 (9)
N1	0.0083 (7)	0.0152 (8)	0.0193 (8)	−0.0033 (7)	0.0021 (6)	−0.0006 (7)

supplementary materials

O1	0.0124 (7)	0.0248 (7)	0.0302 (8)	-0.0008 (6)	0.0039 (6)	-0.0035 (6)
Cl1	0.0220 (3)	0.0250 (3)	0.0214 (2)	-0.0030 (2)	0.00937 (18)	-0.0004 (2)

Geometric parameters (Å, °)

C1—C6	1.391 (2)	C5—H5	0.918 (18)
C1—C2	1.393 (2)	C6—H6	0.928 (18)
C1—N1	1.415 (2)	C7—O1	1.2305 (19)
C2—C3	1.387 (3)	C7—N1	1.353 (2)
C2—Cl1	1.7440 (18)	C7—C8	1.500 (2)
C3—C4	1.376 (3)	C8—H8A	0.9800
C3—H3	0.955 (19)	C8—H8B	0.9800
C4—C5	1.389 (3)	C8—H8C	0.9800
C4—H4	0.983 (19)	N1—H1	0.813 (18)
C5—C6	1.384 (3)		
C6—C1—C2	118.13 (16)	C5—C6—C1	120.76 (17)
C6—C1—N1	121.20 (15)	C5—C6—H6	120.3 (11)
C2—C1—N1	120.65 (15)	C1—C6—H6	119.0 (11)
C3—C2—C1	121.30 (17)	O1—C7—N1	122.80 (16)
C3—C2—Cl1	119.26 (14)	O1—C7—C8	120.91 (16)
C1—C2—Cl1	119.45 (14)	N1—C7—C8	116.25 (15)
C4—C3—C2	119.75 (18)	C7—C8—H8A	109.5
C4—C3—H3	121.3 (11)	C7—C8—H8B	109.5
C2—C3—H3	118.9 (11)	H8A—C8—H8B	109.5
C3—C4—C5	119.88 (18)	C7—C8—H8C	109.5
C3—C4—H4	116.1 (11)	H8A—C8—H8C	109.5
C5—C4—H4	124.0 (11)	H8B—C8—H8C	109.5
C6—C5—C4	120.14 (18)	C7—N1—C1	124.61 (14)
C6—C5—H5	119.4 (11)	C7—N1—H1	117.0 (13)
C4—C5—H5	120.4 (11)	C1—N1—H1	118.3 (13)
C6—C1—C2—C3	-2.0 (3)	C4—C5—C6—C1	0.8 (3)
N1—C1—C2—C3	176.81 (15)	C2—C1—C6—C5	0.3 (3)
C6—C1—C2—Cl1	178.65 (13)	N1—C1—C6—C5	-178.47 (15)
N1—C1—C2—Cl1	-2.6 (2)	O1—C7—N1—C1	-2.3 (3)
C1—C2—C3—C4	2.5 (3)	C8—C7—N1—C1	179.90 (15)
Cl1—C2—C3—C4	-178.12 (14)	C6—C1—N1—C7	-42.7 (2)
C2—C3—C4—C5	-1.3 (3)	C2—C1—N1—C7	138.56 (18)
C3—C4—C5—C6	-0.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H \cdots A	D—H	H \cdots A	D \cdots A	D—H \cdots A
N1—H1 \cdots O1 ⁱ	0.813 (18)	2.079 (18)	2.8630 (19)	161.7 (17)

Symmetry codes: (i) $x+1, y, z$.

Fig. 1

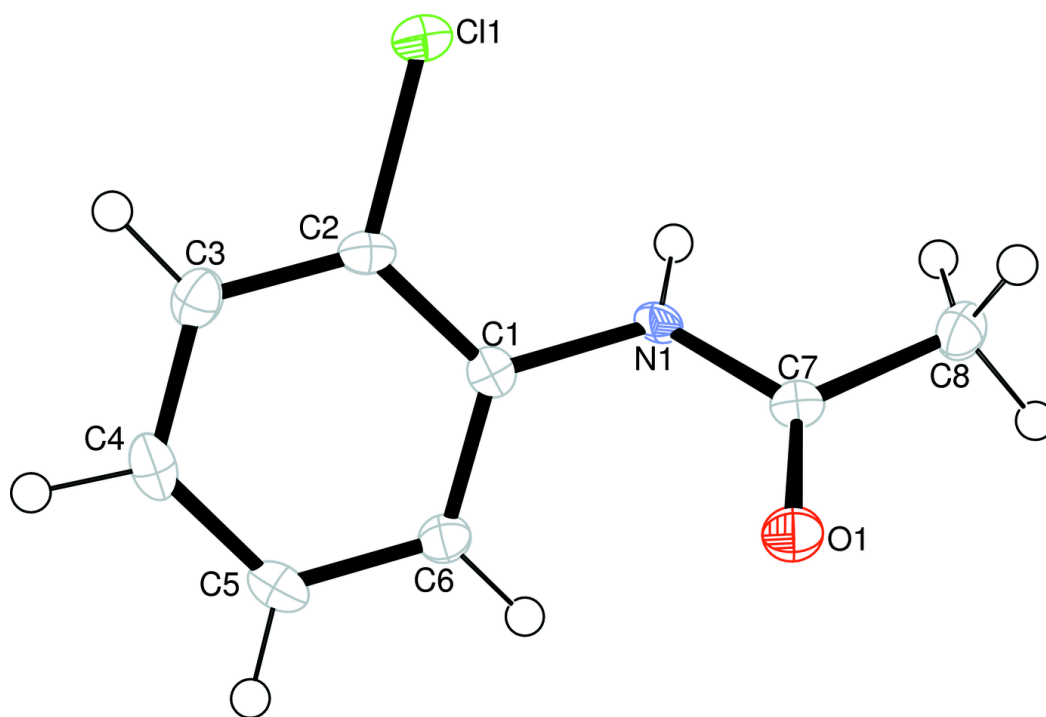


Fig. 2

