Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Chlorophenyl)acetamide

Dong-Sheng Ma,* Pei-Jiang Liu, Shuai Zhang and Guang-Feng Hou

College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: hgf1000@163.com

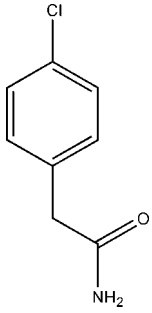
Received 1 November 2011; accepted 7 November 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.083; data-to-parameter ratio = 16.7.

In the title compound, C_8H_8ClNO, the acetamide group is twisted out the benzene plane with a dihedral angle of 83.08 (1)°. In the crystal, molecules are linked by N—H···O hydrogen bonds, forming layers parallel to the *ab* plane.

Related literature

For details of the nitrile hydrolysis of the same substrate (4-chlorobenzonitrile) by another method, see: Moorthy & Singhal (2005).



Experimental

Crystal data

C_8H_8ClNO
M_r = 169.60
Orthorhombic, $P2_12_12_1$
a = 4.917 (2) Å
b = 6.033 (4) Å
c = 26.680 (12) Å
V = 791.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 293 K
0.29 × 0.22 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.887, T_{max} = 0.970
7733 measured reflections
1807 independent reflections
1451 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.083
S = 1.05
1807 reflections
108 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 704 Friedel pairs
Flack parameter: −0.12 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H11···O1^{i}	0.88 (1)	2.05 (1)	2.911 (2)	165 (2)
N1—H12···O1^{ii}	0.89 (1)	2.22 (1)	3.064 (3)	157 (2)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors thank Heilongjiang University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5191).

References

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Moorthy, J. N. & Singhal, N. (2005). *J. Org. Chem.* **70**, 1926–1929.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o3261 [https://doi.org/10.1107/S1600536811046836]

2-(4-Chlorophenyl)acetamide

Dong-Sheng Ma, Pei-Jiang Liu, Shuai Zhang and Guang-Feng Hou

S1. Comment

The title compound is formed by hydrolysis of appropriate nitriles (Moorthy *et al.*, 2005), while the final product of hydrolysis of nitriles should be carboxylic acid. In this paper, we report the synthesis and the crystal structure of the title compound prepared from 4-cyanobenzylchloride under solvothermal condition.

In the title molecule (Fig.1), the acetamide group is twisted out the benzene plane with a dihedral angle of 83.08 (1) °. In the crystal packing, the molecules are linked by N—H···O hydrogen bonds to form layers parallel to *ab* plane (Fig. 2, Table 1).

S2. Experimental

A mixture of NaN_3 (0.39 g, 6 mmol), $CuCl_2{\cdot}2H_2O$ (0.684 g, 4 mmol), and 4-cyanobenzylchloride (0.606 g, 4 mmol) was sealed in a 15 ml teflon-lined reactor and heated in an oven at 150 ° C for 72 hrs and slowly cooled to room temperature. The resulting mixture was washed with water, and pale yellow blocklike crystals were collected (yeild 31%).

S3. Refinement

N-bound H atoms were located in a differece Fourier map and refined with restraint of N—H = 0.89 (1) Å. C-bound H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic); C —H = 0.97 Å (methylene), and with U_{iso}(H) = 1.2U_{eq}(C).

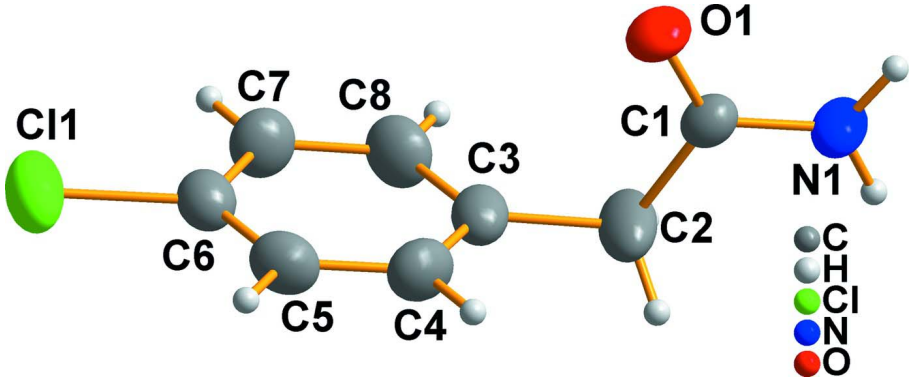


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level.

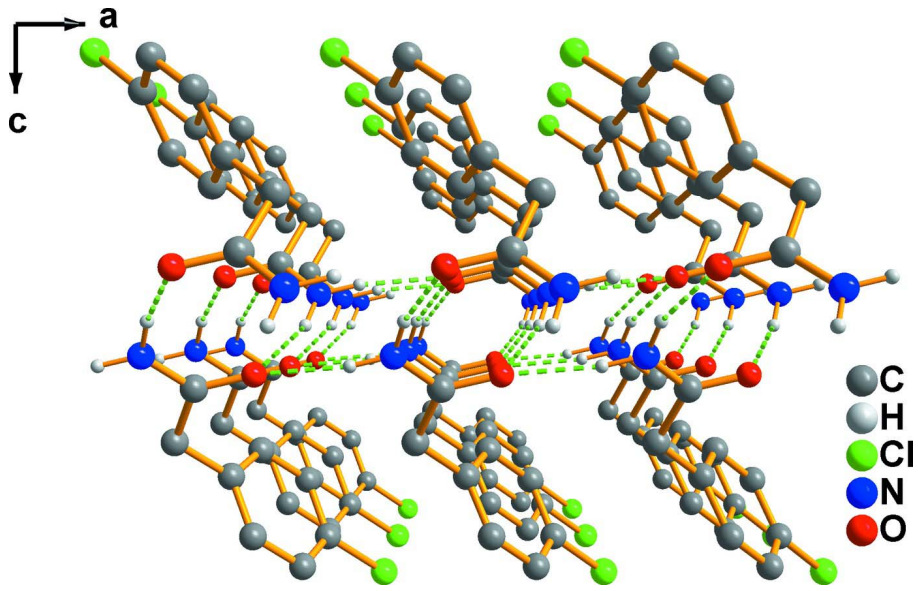


Figure 2

A portion of the crystal packing, showing a two-dimensional structure formed by N—H···O hydrogen bonds (dashed lines).

2-(4-Chlorophenyl)acetamide

Crystal data

C_8H_8ClNO
$M_r = 169.60$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.917$ (2) Å
$b = 6.033$ (4) Å
$c = 26.680$ (12) Å
$V = 791.5$ (7) Å^3
$Z = 4$
$F(000) = 352$
$D_x = 1.423$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5994 reflections
$\theta = 3.1$–$27.4°$
$\mu = 0.42$ mm^{-1}
$T = 293$ K
Block, colorless
0.29 × 0.22 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.887$, $T_{max} = 0.970$
7733 measured reflections
1807 independent reflections
1451 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.1°$
$h = -6 \rightarrow 6$
$k = -7 \rightarrow 7$
$l = -34 \rightarrow 33$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.083$
$S = 1.05$
1807 reflections
108 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.1017P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Absolute structure: Flack (1983), 704 Friedel pairs
Absolute structure parameter: −0.12 (8)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3632 (4)	0.5073 (3)	0.79843 (7)	0.0335 (4)
C2	0.2527 (4)	0.3677 (5)	0.84087 (10)	0.0603 (7)
H2A	0.1560	0.4638	0.8639	0.072*
H2B	0.1222	0.2633	0.8272	0.072*
C3	0.4640 (4)	0.2408 (4)	0.86973 (8)	0.0429 (5)
C4	0.5575 (5)	0.0374 (4)	0.85279 (8)	0.0487 (6)
H4	0.4907	−0.0195	0.8228	0.058*
C5	0.7475 (5)	−0.0822 (3)	0.87944 (8)	0.0451 (5)
H5	0.8079	−0.2185	0.8676	0.054*
C6	0.8470 (4)	0.0017 (4)	0.92375 (8)	0.0410 (5)
C7	0.7620 (5)	0.2049 (4)	0.94146 (8)	0.0472 (6)
H7	0.8324	0.2622	0.9711	0.057*
C8	0.5697 (5)	0.3221 (4)	0.91430 (8)	0.0487 (5)
H8	0.5100	0.4586	0.9262	0.058*
Cl1	1.08553 (13)	−0.14906 (11)	0.95804 (2)	0.0605 (2)
N1	0.1788 (3)	0.6234 (4)	0.77353 (7)	0.0441 (4)
H11	0.004 (2)	0.613 (4)	0.7811 (8)	0.046 (6)*
H12	0.225 (5)	0.714 (4)	0.7485 (7)	0.064 (8)*
O1	0.6073 (3)	0.5149 (3)	0.78808 (5)	0.0435 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0263 (9)	0.0376 (11)	0.0367 (10)	−0.0005 (9)	0.0007 (8)	−0.0027 (8)
C2	0.0291 (11)	0.0819 (19)	0.0699 (15)	0.0050 (12)	0.0050 (11)	0.0347 (15)
C3	0.0310 (11)	0.0528 (13)	0.0449 (11)	0.0000 (9)	0.0035 (9)	0.0145 (9)
C4	0.0493 (13)	0.0554 (14)	0.0416 (11)	−0.0093 (12)	−0.0077 (11)	−0.0001 (10)
C5	0.0511 (13)	0.0368 (12)	0.0475 (12)	0.0016 (9)	0.0072 (11)	−0.0041 (9)
C6	0.0381 (11)	0.0444 (12)	0.0406 (10)	0.0018 (10)	0.0046 (9)	0.0071 (9)
C7	0.0514 (13)	0.0514 (14)	0.0387 (11)	0.0009 (10)	−0.0027 (10)	−0.0056 (10)
C8	0.0503 (13)	0.0433 (13)	0.0525 (12)	0.0118 (12)	0.0069 (12)	−0.0003 (10)

Cl1	0.0520 (3)	0.0695 (4)	0.0598 (3)	0.0147 (3)	−0.0015 (3)	0.0194 (3)
N1	0.0243 (8)	0.0587 (12)	0.0494 (10)	−0.0006 (8)	0.0013 (8)	0.0149 (10)
O1	0.0237 (6)	0.0529 (9)	0.0538 (8)	−0.0038 (7)	0.0051 (7)	0.0046 (7)

Geometric parameters (Å, º)

C1—O1	1.232 (2)	C5—C6	1.376 (3)
C1—N1	1.324 (3)	C5—H5	0.9300
C1—C2	1.512 (3)	C6—C7	1.379 (3)
C2—C3	1.503 (3)	C6—Cl1	1.744 (2)
C2—H2A	0.9700	C7—C8	1.386 (3)
C2—H2B	0.9700	C7—H7	0.9300
C3—C4	1.386 (3)	C8—H8	0.9300
C3—C8	1.387 (3)	N1—H11	0.883 (10)
C4—C5	1.378 (3)	N1—H12	0.892 (10)
C4—H4	0.9300		
O1—C1—N1	122.34 (19)	C6—C5—C4	119.5 (2)
O1—C1—C2	122.57 (18)	C6—C5—H5	120.3
N1—C1—C2	115.08 (17)	C4—C5—H5	120.3
C3—C2—C1	114.78 (17)	C5—C6—C7	120.9 (2)
C3—C2—H2A	108.6	C5—C6—Cl1	119.88 (18)
C1—C2—H2A	108.6	C7—C6—Cl1	119.21 (17)
C3—C2—H2B	108.6	C6—C7—C8	118.8 (2)
C1—C2—H2B	108.6	C6—C7—H7	120.6
H2A—C2—H2B	107.5	C8—C7—H7	120.6
C4—C3—C8	117.9 (2)	C7—C8—C3	121.6 (2)
C4—C3—C2	120.9 (2)	C7—C8—H8	119.2
C8—C3—C2	121.2 (2)	C3—C8—H8	119.2
C5—C4—C3	121.3 (2)	C1—N1—H11	120.9 (16)
C5—C4—H4	119.3	C1—N1—H12	121.7 (18)
C3—C4—H4	119.3	H11—N1—H12	117 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H11···O1^{i}	0.88 (1)	2.05 (1)	2.911 (2)	165 (2)
N1—H12···O1^{ii}	0.89 (1)	2.22 (1)	3.064 (3)	157 (2)

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+1, *y*+1/2, −*z*+3/2.