Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl *N*-(4-chlorophenyl)carbamate

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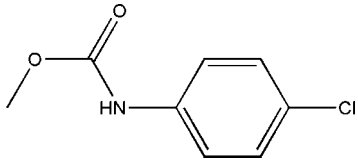
Received 30 August 2011; accepted 13 September 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.159; data-to-parameter ratio = 18.2.

In the title compound, $C_8H_8ClNO_2$, the dihedral angle between the chlorobenzene ring and the side chain is 8.79 (11)°. In the crystal, molecules are linked by N—H···O hydrogen bonds into a $C(4)$ chain propagating in the b-axis direction.

Related literature

For related structures, see: Li (2011*a*,*b*).



Experimental

Crystal data

$C_8H_8ClNO_2$
M_r = 185.60
Monoclinic, $P2_1/c$
a = 11.126 (2) Å
b = 9.833 (2) Å
c = 8.0076 (16) Å
β = 99.34 (3)°
V = 864.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 293 K
0.23 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
8281 measured reflections
1987 independent reflections
1011 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.159
S = 1.06
1987 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.86	2.22	3.069 (2)	168

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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: *SHELXTL*.

This study was supported by the Natural Science Foundation of Shandong Province (no. ZR2010BL025).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6394).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, Y.-F. (2011*a*). *Acta Cryst.* E**67**, o1796.
Li, Y.-F. (2011*b*). *Acta Cryst.* E**67**, o2492.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2011). E**67**, o2750 [**doi:10.1107/S1600536811037123**]

Methyl *N*-(4-chlorophenyl)carbamate

Y.-F. Li

Experimental

A mixture of methanol (0.06 mol), and (4-chlorophenyl)carbamic chloride (0.06 mol) was stirred in refluxing ethanol (15 ml) for 4 h to afford the title compound (0.05 mol, yield 83%). Colourless blocks of the title compound were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93–0.97 Å; N—H = 0.86Å and with U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(C_{methyl}).

Figures

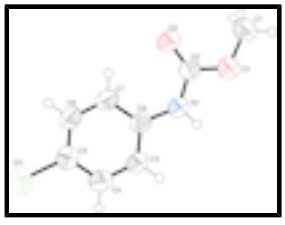


Fig. 1. The molecular structure of the title compound showing 50% probability displacement ellipsoids.

Methyl *N*-(4-chlorophenyl)carbamate

Crystal data

$C_8H_8ClNO_2$	$F(000)$ = 384
M_r = 185.60	D_x = 1.426 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1987 reflections
a = 11.126 (2) Å	θ = 3.0–27.2°
b = 9.833 (2) Å	μ = 0.40 mm^{-1}
c = 8.0076 (16) Å	T = 293 K
β = 99.34 (3)°	Block, colorless
V = 864.5 (3) Å^3	0.23 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	1011 reflections with $I > 2\sigma(I)$

Radiation source: fine-focus sealed tube	$R_{int} = 0.036$
graphite	$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
φ and ω scans	$h = -14 \rightarrow 13$
8281 measured reflections	$k = -12 \rightarrow 12$
1987 independent reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.159$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.081P)^2 + 0.0499P]$ where $P = (F_o^2 + 2F_c^2)/3$
1987 reflections	$(\Delta/\sigma)_{max} < 0.001$
109 parameters	$\Delta\rho_{max} = 0.18$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.26$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.51185 (8)	0.66723 (9)	0.21431 (13)	0.1092 (4)
N1	0.95328 (17)	0.52547 (19)	0.6982 (3)	0.0611 (5)
H1A	0.9543	0.4420	0.7304	0.073*
O2	1.06775 (16)	0.71949 (15)	0.7364 (2)	0.0699 (5)
C8	0.8511 (2)	0.56561 (19)	0.5821 (3)	0.0527 (6)
O1	1.12660 (16)	0.52441 (16)	0.8735 (2)	0.0749 (5)
C2	1.0498 (2)	0.6012 (2)	0.7656 (3)	0.0570 (6)
C7	0.8409 (2)	0.6894 (2)	0.4978 (3)	0.0628 (6)
H7A	0.9042	0.7521	0.5166	0.075*
C6	0.7360 (2)	0.7191 (2)	0.3855 (3)	0.0660 (7)
H6A	0.7294	0.8021	0.3290	0.079*
C5	0.6422 (2)	0.6283 (2)	0.3568 (3)	0.0665 (7)
C4	0.6513 (2)	0.5048 (2)	0.4395 (3)	0.0715 (7)

H4A	0.5878	0.4423	0.4195	0.086*
C3	0.7548 (2)	0.4750 (2)	0.5514 (3)	0.0644 (6)
H3A	0.7604	0.3920	0.6079	0.077*
C1	1.2359 (3)	0.5899 (3)	0.9546 (4)	0.0819 (8)
H1B	1.2841	0.5264	1.0282	0.123*
H1C	1.2151	0.6659	1.0196	0.123*
H1D	1.2817	0.6212	0.8703	0.123*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0837 (6)	0.1053 (7)	0.1253 (8)	−0.0005 (4)	−0.0225 (5)	0.0310 (5)
N1	0.0645 (12)	0.0440 (10)	0.0726 (14)	−0.0029 (8)	0.0044 (10)	0.0032 (8)
O2	0.0731 (11)	0.0436 (9)	0.0893 (13)	−0.0026 (7)	0.0018 (9)	−0.0033 (8)
C8	0.0568 (13)	0.0435 (11)	0.0582 (14)	0.0003 (9)	0.0104 (11)	−0.0046 (9)
O1	0.0764 (12)	0.0545 (9)	0.0866 (13)	−0.0024 (8)	−0.0085 (10)	0.0031 (8)
C2	0.0626 (14)	0.0463 (12)	0.0608 (15)	0.0040 (10)	0.0063 (11)	−0.0061 (10)
C7	0.0694 (16)	0.0509 (12)	0.0679 (16)	−0.0083 (10)	0.0106 (13)	0.0044 (10)
C6	0.0761 (17)	0.0530 (13)	0.0683 (17)	−0.0025 (11)	0.0105 (13)	0.0114 (11)
C5	0.0677 (16)	0.0597 (13)	0.0713 (17)	0.0040 (12)	0.0086 (13)	0.0046 (11)
C4	0.0665 (16)	0.0555 (13)	0.0897 (19)	−0.0079 (11)	0.0045 (14)	0.0013 (13)
C3	0.0683 (15)	0.0418 (11)	0.0811 (17)	−0.0030 (10)	0.0059 (13)	0.0041 (10)
C1	0.0753 (19)	0.0700 (16)	0.091 (2)	−0.0008 (13)	−0.0140 (15)	−0.0020 (14)

Geometric parameters (Å, °)

Cl1—C5	1.736 (3)	C7—H7A	0.9300
N1—C2	1.345 (3)	C6—C5	1.364 (4)
N1—C8	1.404 (3)	C6—H6A	0.9300
N1—H1A	0.8600	C5—C4	1.379 (3)
O2—C2	1.209 (3)	C4—C3	1.371 (3)
C8—C3	1.385 (3)	C4—H4A	0.9300
C8—C7	1.388 (3)	C3—H3A	0.9300
O1—C2	1.345 (3)	C1—H1B	0.9600
O1—C1	1.435 (3)	C1—H1C	0.9600
C7—C6	1.384 (4)	C1—H1D	0.9600
C2—N1—C8	128.2 (2)	C6—C5—C4	120.1 (2)
C2—N1—H1A	115.9	C6—C5—Cl1	120.07 (19)
C8—N1—H1A	115.9	C4—C5—Cl1	119.9 (2)
C3—C8—C7	118.6 (2)	C3—C4—C5	119.4 (2)
C3—C8—N1	117.20 (19)	C3—C4—H4A	120.3
C7—C8—N1	124.2 (2)	C5—C4—H4A	120.3
C2—O1—C1	116.3 (2)	C4—C3—C8	121.5 (2)
O2—C2—O1	123.8 (2)	C4—C3—H3A	119.3
O2—C2—N1	126.9 (2)	C8—C3—H3A	119.3
O1—C2—N1	109.2 (2)	O1—C1—H1B	109.5
C6—C7—C8	119.7 (2)	O1—C1—H1C	109.5
C6—C7—H7A	120.2	H1B—C1—H1C	109.5

C8—C7—H7A	120.2	O1—C1—H1D	109.5
C5—C6—C7	120.8 (2)	H1B—C1—H1D	109.5
C5—C6—H6A	119.6	H1C—C1—H1D	109.5
C7—C6—H6A	119.6		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{i}	0.86	2.22	3.069 (2)	168

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

Fig. 1