Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(1-Naphthylmethyl)ammonium chloride

Ali R. Salimi,[a] Mahmood Azizpoor Fard,[b] Hossein Eshtiagh-Hosseini,[a] Mostafa M. Amini[b] and Hamid R. Khavasi[b]*

[a]Department of Chemistry, Ferdowsi University of Mashhad, Mashhad 917791436, Iran, and [b]Department of Chemistry, General Campus, Shahid Beheshti University, Tehran 1983963113, Iran
Correspondence e-mail: h-khavasi@sbu.ac.ir

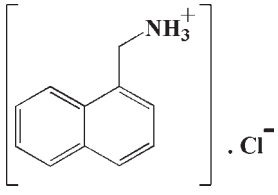
Received 4 January 2010; accepted 27 January 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.100; data-to-parameter ratio = 20.6.

The reaction of 1-naphthylmethylamine and hydrochloric acid in a 1:1 molar ratio resulted in the formation of the 1:1 proton-transfer compound, $C_{11}H_{12}N^+\cdot Cl^-$. In the crystal, the ions are linked by N—H···Cl hydrogen bonds into a sheet pattern in the *ab* plane such that each Cl^- ion is bonded to three NH groups from the naphthylmethylammonium ion.

Related literature

For 1-naphthylmethylammonium salts, see: Sada *et al.* (2004).



Experimental

Crystal data

$C_{11}H_{12}N^+\cdot Cl^-$
M_r = 193.67
Monoclinic, $P2_1$
a = 5.3395 (7) Å
b = 9.3355 (15) Å
c = 10.1432 (13) Å
β = 100.864 (10)°
V = 496.55 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 298 K
0.35 × 0.13 × 0.11 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: numerical (*X-RED* and *X-SHAPE*; Stoe & Cie, 2005)
T_{min} = 0.952, T_{max} = 0.968
5801 measured reflections
2677 independent reflections
2098 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.100
S = 1.19
2677 reflections
130 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 245 Friedel pairs
Flack parameter: 0.09 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1C···Cl1	0.86 (5)	2.37 (5)	3.226 (3)	172 (3)
N1—H1D···Cl1^{i}	0.94 (4)	2.27 (4)	3.187 (3)	164 (3)
N1—H1E···Cl1^{ii}	0.92 (4)	2.29 (4)	3.172 (3)	161 (3)

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

Data collection: *X-AREA*; cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors wish to acknowledge Shahid Beheshti University, GC, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2314).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sada, K., Inoue, K., Tanaka, T., Tanaka, A., Epergyes, A., Nagahama, S., Matsumoto, A. & Miyala, M. (2004). *J. Am. Chem. Soc.* **126**, 1764–1771.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2005). *X-AREA*, *X-RED* and *X-SHAPE*. Stoe & Cie, Darmstadt, Germany.

supporting information

Acta Cryst. (2010). E**66**, o509 [doi:10.1107/S160053681000334X]

(1-Naphthylmethyl)ammonium chloride

Ali R. Salimi, Mahmood Azizpoor Fard, Hossein Eshtiagh-Hosseini, Mostafa M. Amini and Hamid R. Khavasi

S1. Comment

1-naphthylmethylamine has been recognized as a suitable agent in the synthesis of proton-transfer systems (Sada *et al.*, 2004). We report here the synthesis and characterization of the title salt, 1-naphthylmethylammonium chloride. The structure shows the presence of a 1-naphthylmethylammonium species that arises from the protonation of the amine group (Fig. 1). Hydrogen bonds play a very important role in the structure. As it is clear from Figure 2, chloride atoms engage in three hydrogen bonds with the amine group in which the chloride is in the center of triangle from three H atoms from three different cations.

S2. Experimental

A solution of 2.5 ml of 2M hydrochloric acid was added to a solution of 5 mmol 1-naphthalenemethylamine (0.73 ml) in 30 ml pyridine. The resulting solution was stirred at 373 K for 5 h and at ambient temperature for 24 h. A pale brown solution resulted. After drying the remaining brown solid was dissolved in pure methanol. X-ray quality crystals were obtained by slow evaporation at room temperature.

S3. Refinement

All of the H atoms bonded to C were positioned geometrically with C—H = 0.93 and 0.97Å for aromatic ring and CH_2 hydrogen atoms respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. NH_3 hydrogens atoms were positioned from Fourier map and freely refined.

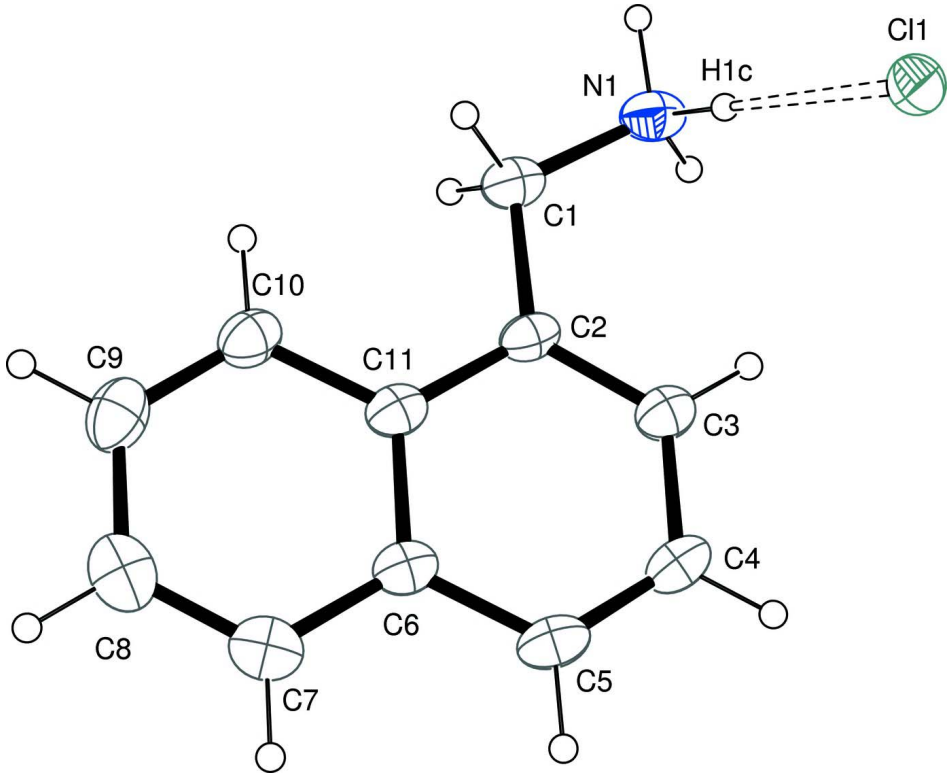


Figure 1

The molecular staucture with the atom-numbering scheme. Displacement ellipsoids are drawn at 30% probability level.

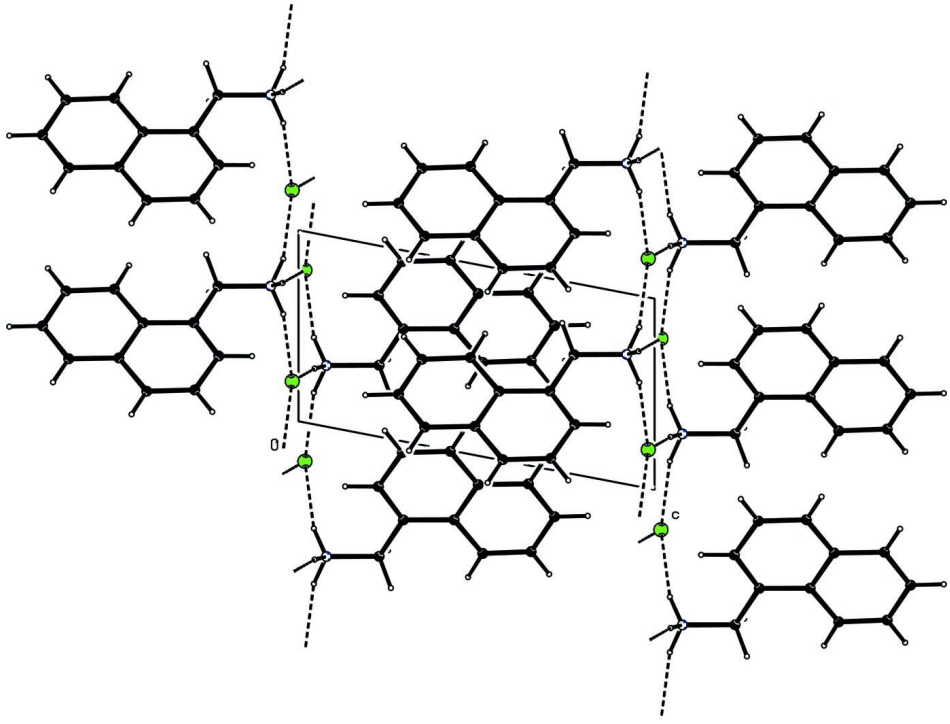


Figure 2

A packing diagram of the title compound in thr b-direction. Hydrogen bonds are shown as dashed lines.

(1-Naphthylmethyl)ammonium chloride

Crystal data

$C_{11}H_{12}N^+\cdot Cl^-$
$M_r = 193.67$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 5.3395\ (7)$ Å
$b = 9.3355\ (15)$ Å
$c = 10.1432\ (13)$ Å
$\beta = 100.864\ (10)°$
$V = 496.55\ (12)$ Å^3
$Z = 2$
$F(000) = 204$
$D_x = 1.295$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1056 reflections
$\theta = 2.0–29.2°$
$\mu = 0.34$ mm^{-1}
$T = 298$ K
Prism, colorless
0.35 × 0.13 × 0.11 mm

Data collection

Stoe IPDS II diffractometer
rotation method scans
Absorption correction: numerical (*X-RED* and *X-SHAPE*; Stoe & Cie, 2005)
$T_{min} = 0.952$, $T_{max} = 0.968$
5801 measured reflections
2677 independent reflections
2098 reflections with $I > 2\sigma(I)$
$R_{int} = 0.065$
$\theta_{max} = 29.2°$, $\theta_{min} = 2.0°$
$h = -7\rightarrow6$
$k = -12\rightarrow12$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.100$
$S = 1.19$
2677 reflections
130 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0155P)^2 + 0.2107P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Absolute structure: Flack (1983), 1245 Friedel pairs
Absolute structure parameter: 0.09 (10)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6260 (6)	0.3230 (3)	0.7737 (3)	0.0472 (8)
H1A	0.5852	0.2242	0.7487	0.057*
H1B	0.7793	0.3481	0.7406	0.057*
C2	0.4110 (5)	0.4171 (3)	0.7057 (3)	0.0387 (6)
C3	0.2613 (6)	0.4950 (3)	0.7758 (3)	0.0442 (7)
H3	0.2941	0.4919	0.8691	0.053*

C4	0.0597 (6)	0.5793 (4)	0.7084 (4)	0.0505 (8)
H4	−0.0375	0.6326	0.7577	0.061*
C5	0.0047 (6)	0.5840 (3)	0.5736 (3)	0.0501 (8)
H5	−0.1313	0.6396	0.531	0.06*
C6	0.1509 (5)	0.5057 (3)	0.4954 (3)	0.0409 (7)
C7	0.0961 (7)	0.5081 (3)	0.3544 (4)	0.0529 (9)
H7	−0.0423	0.561	0.3104	0.063*
C8	0.2421 (8)	0.4342 (4)	0.2810 (4)	0.0591 (9)
H8	0.2043	0.4373	0.1877	0.071*
C9	0.4484 (7)	0.3540 (4)	0.3465 (4)	0.0571 (9)
H9	0.5481	0.3039	0.2962	0.069*
C10	0.5064 (6)	0.3476 (3)	0.4826 (4)	0.0486 (8)
H10	0.6454	0.2933	0.5238	0.058*
C11	0.3593 (5)	0.4221 (3)	0.5631 (3)	0.0395 (6)
N1	0.6799 (6)	0.3336 (3)	0.9219 (3)	0.0495 (7)
H1C	0.708 (8)	0.418 (5)	0.955 (4)	0.069 (12)*
H1D	0.835 (7)	0.288 (3)	0.957 (3)	0.046 (9)*
H1E	0.546 (8)	0.298 (4)	0.957 (4)	0.065 (12)*
Cl1	0.79683 (14)	0.66025 (10)	1.01767 (8)	0.04759 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0375 (17)	0.0408 (16)	0.062 (2)	0.0020 (14)	0.0058 (15)	0.0015 (15)
C2	0.0302 (14)	0.0284 (13)	0.0570 (18)	0.0001 (11)	0.0074 (13)	0.0007 (12)
C3	0.0404 (16)	0.0394 (15)	0.0531 (19)	0.0020 (13)	0.0096 (14)	0.0017 (13)
C4	0.0441 (18)	0.0429 (16)	0.067 (2)	0.0118 (14)	0.0171 (16)	0.0025 (16)
C5	0.0401 (17)	0.0416 (16)	0.068 (2)	0.0088 (14)	0.0095 (16)	0.0115 (15)
C6	0.0335 (16)	0.0328 (13)	0.056 (2)	−0.0042 (11)	0.0083 (13)	0.0032 (13)
C7	0.050 (2)	0.0468 (18)	0.060 (2)	−0.0081 (15)	0.0048 (16)	0.0078 (16)
C8	0.069 (2)	0.056 (2)	0.053 (2)	−0.0188 (19)	0.0126 (18)	−0.0009 (17)
C9	0.061 (2)	0.0467 (18)	0.069 (2)	−0.0062 (16)	0.0242 (19)	−0.0125 (17)
C10	0.0424 (18)	0.0398 (16)	0.064 (2)	0.0014 (13)	0.0104 (16)	−0.0065 (15)
C11	0.0308 (14)	0.0318 (13)	0.0561 (18)	−0.0066 (11)	0.0087 (13)	−0.0008 (13)
N1	0.0387 (16)	0.0421 (16)	0.0640 (19)	0.0032 (13)	0.0002 (14)	0.0029 (14)
Cl1	0.0426 (3)	0.0466 (3)	0.0527 (4)	−0.0046 (4)	0.0067 (3)	−0.0113 (4)

Geometric parameters (Å, º)

C1—N1	1.480 (5)	C6—C11	1.425 (4)
C1—C2	1.506 (4)	C7—C8	1.363 (5)
C1—H1A	0.97	C7—H7	0.93
C1—H1B	0.97	C8—C9	1.393 (5)
C2—C3	1.374 (4)	C8—H8	0.93
C2—C11	1.421 (4)	C9—C10	1.357 (5)
C3—C4	1.402 (4)	C9—H9	0.93
C3—H3	0.93	C10—C11	1.418 (4)
C4—C5	1.344 (5)	C10—H10	0.93

C4—H4	0.93	N1—H1C	0.86 (4)
C5—C6	1.416 (4)	N1—H1D	0.94 (3)
C5—H5	0.93	N1—H1E	0.92 (4)
C6—C7	1.405 (5)		

N1—C1—C2	114.3 (3)	C8—C7—C6	121.1 (3)
N1—C1—H1A	108.7	C8—C7—H7	119.4
C2—C1—H1A	108.7	C6—C7—H7	119.4
N1—C1—H1B	108.7	C7—C8—C9	119.6 (3)
C2—C1—H1B	108.7	C7—C8—H8	120.2
H1A—C1—H1B	107.6	C9—C8—H8	120.2
C3—C2—C11	119.2 (3)	C10—C9—C8	121.2 (3)
C3—C2—C1	122.7 (3)	C10—C9—H9	119.4
C11—C2—C1	118.1 (3)	C8—C9—H9	119.4
C2—C3—C4	120.9 (3)	C9—C10—C11	121.3 (3)
C2—C3—H3	119.6	C9—C10—H10	119.4
C4—C3—H3	119.6	C11—C10—H10	119.4
C5—C4—C3	121.0 (3)	C10—C11—C2	123.2 (3)
C5—C4—H4	119.5	C10—C11—C6	117.3 (3)
C3—C4—H4	119.5	C2—C11—C6	119.5 (3)
C4—C5—C6	121.0 (3)	C1—N1—H1C	116 (3)
C4—C5—H5	119.5	C1—N1—H1D	110.2 (19)
C6—C5—H5	119.5	H1C—N1—H1D	101 (3)
C7—C6—C5	122.0 (3)	C1—N1—H1E	111 (2)
C7—C6—C11	119.5 (3)	H1C—N1—H1E	106 (4)
C5—C6—C11	118.4 (3)	H1D—N1—H1E	113 (3)

N1—C1—C2—C3	−6.2 (4)	C8—C9—C10—C11	0.1 (5)
N1—C1—C2—C11	175.2 (3)	C9—C10—C11—C2	179.2 (3)
C11—C2—C3—C4	−0.1 (5)	C9—C10—C11—C6	−1.0 (5)
C1—C2—C3—C4	−178.8 (3)	C3—C2—C11—C10	178.7 (3)
C2—C3—C4—C5	1.2 (5)	C1—C2—C11—C10	−2.6 (4)
C3—C4—C5—C6	−0.9 (5)	C3—C2—C11—C6	−1.1 (4)
C4—C5—C6—C7	179.5 (3)	C1—C2—C11—C6	177.6 (3)
C4—C5—C6—C11	−0.4 (5)	C7—C6—C11—C10	1.6 (4)
C5—C6—C7—C8	178.7 (3)	C5—C6—C11—C10	−178.5 (3)
C11—C6—C7—C8	−1.4 (4)	C7—C6—C11—C2	−178.5 (3)
C6—C7—C8—C9	0.4 (5)	C5—C6—C11—C2	1.4 (4)
C7—C8—C9—C10	0.2 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···Cl1	0.86 (5)	2.37 (5)	3.226 (3)	172 (3)
N1—H1*D*···Cl1^{i}	0.94 (4)	2.27 (4)	3.187 (3)	164 (3)
N1—H1*E*···Cl1^{ii}	0.92 (4)	2.29 (4)	3.172 (3)	161 (3)

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