

(1-Naphthylmethyl)ammonium chloride

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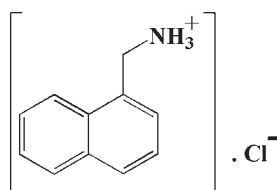
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.054; wR factor = 0.100; data-to-parameter ratio = 20.6.

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, $\text{C}_{11}\text{H}_{12}\text{N}^+\cdot\text{Cl}^-$. In the crystal, the ions are linked by $\text{N}-\text{H}\cdots\text{Cl}$ 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

 $\text{C}_{11}\text{H}_{12}\text{N}^+\cdot\text{Cl}^-$ $M_r = 193.67$ Monoclinic, $P2_1$ $a = 5.3395$ (7) Å $b = 9.3355$ (15) Å $c = 10.1432$ (13) Å $\beta = 100.864$ (10)° $V = 496.55$ (12) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 0.34$ mm⁻¹
 $T = 298$ K

0.35 × 0.13 × 0.11 mm

Data collection

Stoe IPDS II diffractometer

Absorption correction: numerical

 $(X\text{-RED}$ and $X\text{-SHAPE}$; Stoe & Cie, 2005) $T_{\min} = 0.952$, $T_{\max} = 0.968$

5801 measured reflections

2677 independent reflections

2098 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.065$

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, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1C}\cdots\text{Cl1}$	0.86 (5)	2.37 (5)	3.226 (3)	172 (3)
$\text{N1}-\text{H1D}\cdots\text{Cl1}^{\text{i}}$	0.94 (4)	2.27 (4)	3.187 (3)	164 (3)
$\text{N1}-\text{H1E}\cdots\text{Cl1}^{\text{ii}}$	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).

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

References

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supplementary materials

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(1-Naphthylmethyl)ammonium chloride

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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.

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.

Refinement

All of the H atoms bonded to C were positioned geometrically with C—H = 0.93 and 0.97 Å for aromatic ring and CH₂ hydrogen atoms respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. NH₃ hydrogen atoms were positioned from Fourier map and freely refined.

Figures

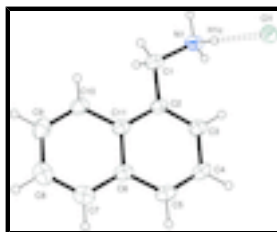


Fig. 1. The molecular structure with the atom-numbering scheme. Displacement ellipsoids are drawn at 30% probability level.

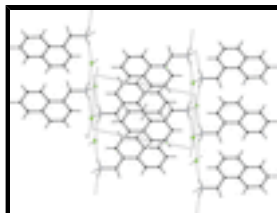


Fig. 2. A packing diagram of the title compound in the b-direction. Hydrogen bonds are shown as dashed lines.

(1-Naphthylmethyl)ammonium chloride

Crystal data

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

Data collection

Stoe IPDS II diffractometer	2098 reflections with $I > 2\sigma(I)$
rotation method scans	$R_{\text{int}} = 0.065$
Absorption correction: numerical (XRED and XSHAPE; Stoe & Cie, 2005)	$\theta_{\text{max}} = 29.2^\circ$, $\theta_{\text{min}} = 2.0^\circ$
$T_{\text{min}} = 0.952$, $T_{\text{max}} = 0.968$	$h = -7 \rightarrow 6$
5801 measured reflections	$k = -12 \rightarrow 12$
2677 independent reflections	$l = -13 \rightarrow 13$

Refinement

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	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)

supplementary materials

Geometric parameters (Å, °)

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, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
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) $-x+2, y-1/2, -z+2$; (ii) $-x+1, y-1/2, -z+2$.

Fig. 1

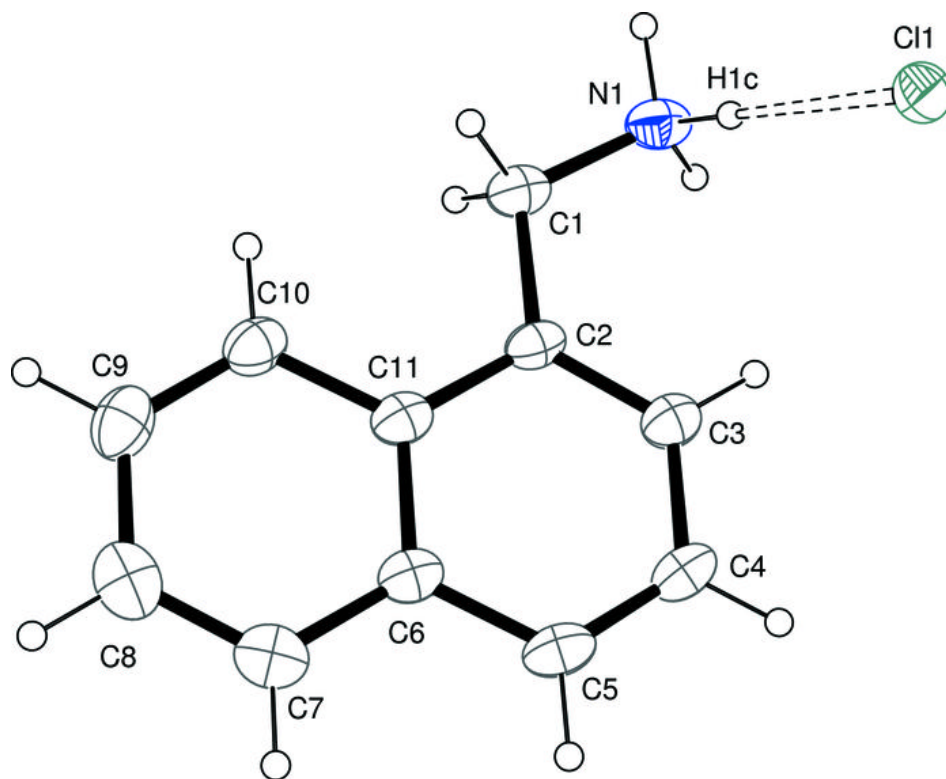


Fig. 2

