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Pyrrolidinium chloride

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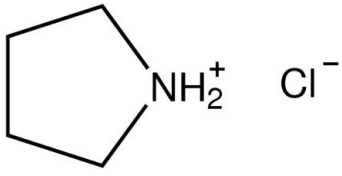
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.120; data-to-parameter ratio = 24.4.

The title compound, $C_4H_{10}N^+\cdot Cl^-$, was obtained as a decomposition product from 2,6-bis(pyrrolidinyl)pyridine. The anion lies on the same cristallographic mirror plane as the N atom of the cation, the complete cation being generated by mirror symmetry. The anions and cations are connected by $N^+—H\cdots Cl^-$ hydrogen bonds into chains along [100]. The pyrrolidinium cation is puckered in an envelope conformation E_{N1}.

Related literature

For details of the synthesis of 2,6-bis(pyrrolidinyl)pyridine, see: Folmer-Anderson *et al.* (2005). For related structures containing the pyrrolidinium cation, see: Kashino *et al.* (1978); Moritani *et al.* (1987); Jakubas *et al.* (2005). For a description of the E_{N1} conformation of the five-membered ring, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_4H_{10}N^+\cdot Cl^-$
M_r = 107.58
Orthorhombic, *Pnma*
a = 7.4429 (4) Å
b = 9.4104 (5) Å
c = 8.9021 (4) Å
V = 623.51 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 200 K
0.22 × 0.13 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
4239 measured reflections
756 independent reflections
608 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.120
S = 1.07
756 reflections
31 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H101···Cl1	0.92	2.17	3.091 (3)	180
N1—H102···Cl1^{i}	0.92	2.18	3.097 (2)	177

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

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2348).

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supporting information

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S1. Comment

The title compound was obtained as a decomposition product. The organic salt is composed of the pyrrolidinium cation and a chloride anion (Fig. 1). The crystal packing is shown in Fig. 2. In the crystal, both H atoms bonded to N1 of the pyrrolidinium cation are involved in hydrogen bonds with chloride as acceptor. Both can be described according to graph set analysis with a $D^1_1(2)$ descriptor on the unitary level. This bonding pattern leads to chains along [1 0 0] which, starting from chloride, can be described according to graph set analysis with a $C^2_1(4)$ descriptor on the binary level. The hydrogen bonding pattern is shown in Fig. 3.

The C_s symmetric five-membered pyrrolidinium ring can be described according to Cremer & Pople (1975) by the puckering parameters q_2 = 0.3061 Å and Φ_2 = 180.0000. The closest pucker descriptor is an envelope E_{N1}.

S2. Experimental

The title compound was obtained as decomposition product of 2,6-bis(pyrrolidinyl)pyridine, which was synthesized according to Folmer-Anderson *et al.* (2005), after 4 months at room temperature.

S3. Refinement

H atoms were placed in calculated positions (C—H = 0.99 Å, N—H = 0.92 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) = 1.2 U_{eq}(C/N).

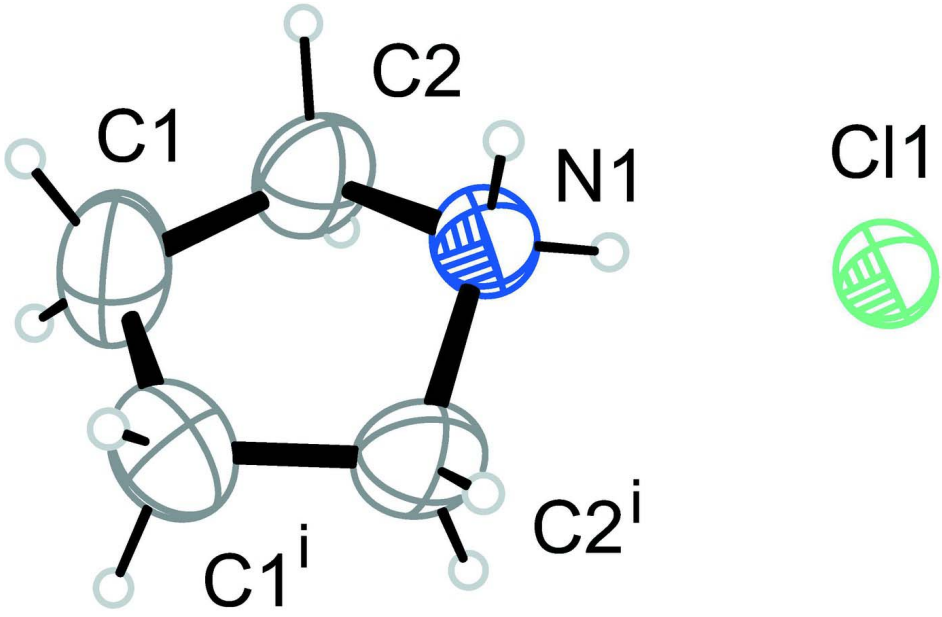

Figure 1

The molecular structure of the C_s symmetric title compound with anisotropic displacement ellipsoids drawn at 50% probability for non-H atoms. Symmetry code: (i) x, $-y + 1/2$, z.

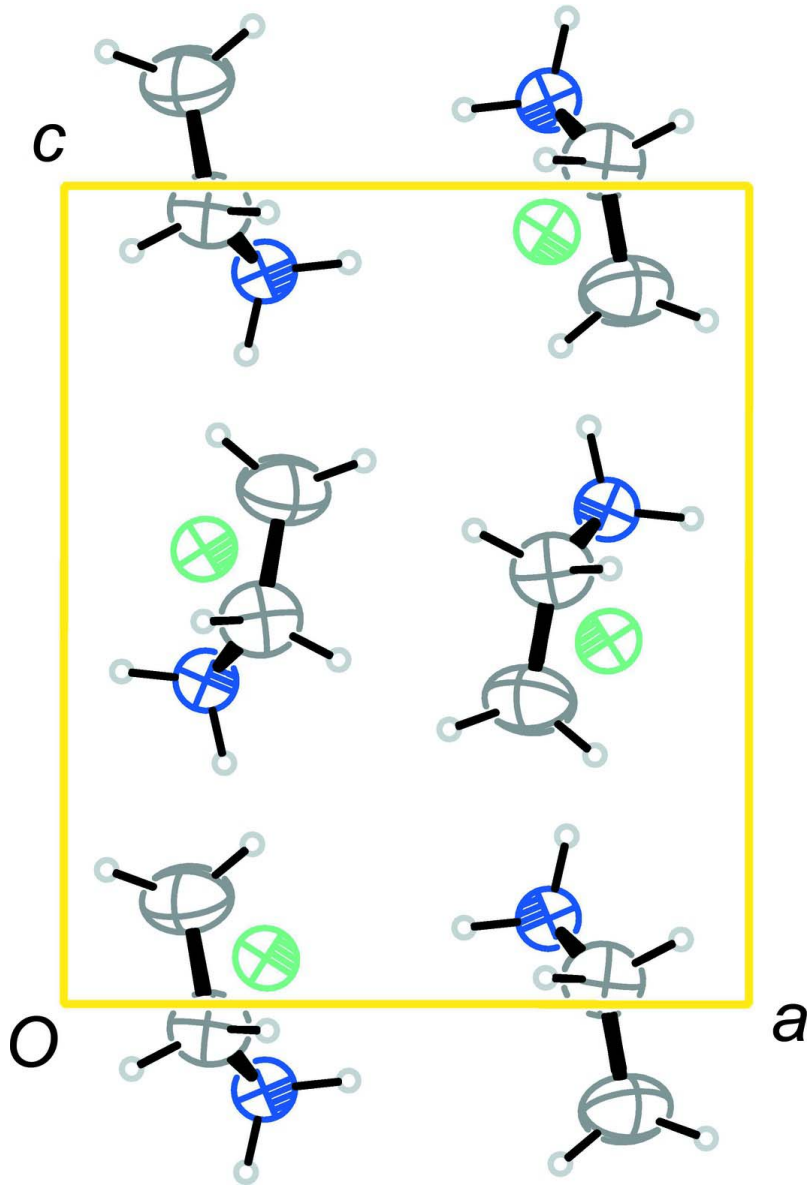

Figure 2

Packing of the title compound, viewed along [0 1 0].

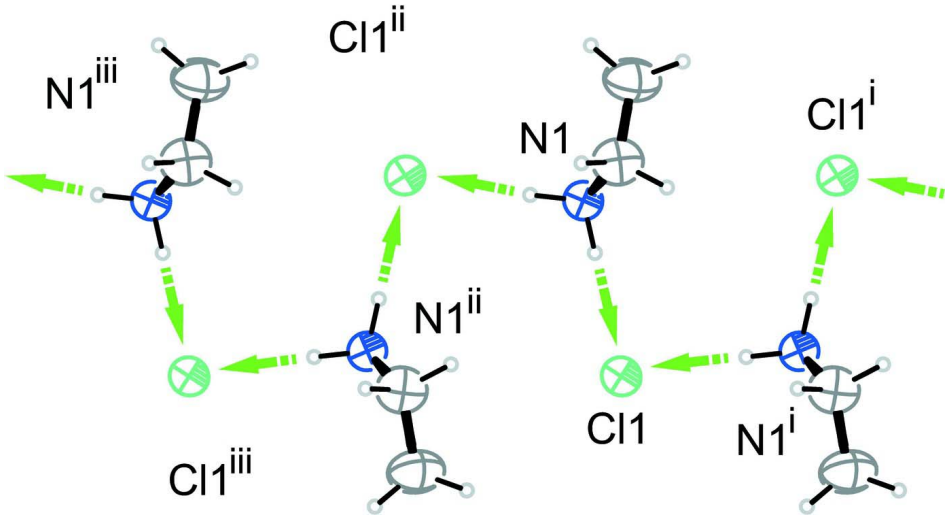

Figure 3

N—H···Cl hydrogen bonds lead to chain-like structures in the crystal structure along [1 0 0], shown here normal to [0 1 0]. Symmetry codes: (i) *x* + 1/2, -*y* + 1/2, -*z* + 1/2; (ii) *x* - 1/2, -*y* + 1/2, -*z* + 1/2; (iii) *x* - 1, *y*, *z*.

Pyrrolidinium chloride

Crystal data

$C_4H_{10}N^+\cdot Cl^-$
$M_r = 107.58$
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
$a = 7.4429\ (4)$ Å
$b = 9.4104\ (5)$ Å
$c = 8.9021\ (4)$ Å
$V = 623.51\ (5)$ Å^3
$Z = 4$
$F(000) = 232$
$D_x = 1.146$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2321 reflections
$\theta = 3.1$–$27.5°$
$\mu = 0.48$ mm^{-1}
$T = 200$ K
Block, colourless
0.22 × 0.13 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: rotating anode
MONTEL, graded multilayered X-ray optics monochromator
φ and ω scans
4239 measured reflections
756 independent reflections
608 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -8 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -11 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.120$
$S = 1.07$
756 reflections
31 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 0.1854P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Refinement. Hydrogen atoms were placed in calculated positions (C–H 0.99 Å for methylene C atoms and N–H 0.92 Å for N atoms) and were included in the refinement in the riding model approximation with U(H) set to 1.2 U_{eq}(C) for C atoms and 1.2 U_{eq}(N) for N atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.2072 (3)	0.2500	0.3955 (3)	0.0473 (6)
H101	0.2341	0.2500	0.2946	0.057*
H102	0.0843	0.2500	0.4065	0.057*
C1	0.3204 (4)	0.1712 (3)	0.6283 (3)	0.0781 (8)
H11	0.2249	0.1348	0.6954	0.094*
H12	0.4376	0.1348	0.6641	0.094*
C2	0.2871 (3)	0.1242 (2)	0.4702 (3)	0.0623 (6)
H21	0.4009	0.0963	0.4208	0.075*
H22	0.2032	0.0427	0.4677	0.075*
Cl1	0.29515 (8)	0.2500	0.05610 (7)	0.0488 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0466 (12)	0.0500 (13)	0.0452 (12)	0.000	−0.0007 (10)	0.000
C1	0.102 (2)	0.0775 (16)	0.0553 (14)	0.0109 (14)	−0.0060 (13)	0.0106 (12)
C2	0.0803 (16)	0.0411 (11)	0.0657 (14)	0.0045 (10)	0.0013 (11)	0.0050 (9)
Cl1	0.0477 (4)	0.0528 (4)	0.0459 (4)	0.000	−0.0020 (3)	0.000

Geometric parameters (Å, º)

N1—C2^{i}	1.482 (3)	C1—C2	1.495 (4)
N1—C2	1.482 (2)	C1—H11	0.9900
N1—H101	0.9200	C1—H12	0.9900
N1—H102	0.9200	C2—H21	0.9900
C1—C1^{i}	1.482 (5)	C2—H22	0.9900
C2^{i}—N1—C2	105.9 (2)	C1^{i}—C1—H12	110.3
C2^{i}—N1—H101	110.5	C2—C1—H12	110.3
C2—N1—H101	110.5	H11—C1—H12	108.5
C2^{i}—N1—H102	110.5	N1—C2—C1	104.64 (19)
C2—N1—H102	110.5	N1—C2—H21	110.8
H101—N1—H102	108.7	C1—C2—H21	110.8
C1^{i}—C1—C2	107.20 (13)	N1—C2—H22	110.8
C1^{i}—C1—H11	110.3	C1—C2—H22	110.8
C2—C1—H11	110.3	H21—C2—H22	108.9
C2^{i}—N1—C2—C1	31.4 (3)	C1^{i}—C1—C2—N1	−19.16 (18)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H101···Cl1	0.92	2.17	3.091 (3)	180
N1—H102···Cl1^{ii}	0.92	2.18	3.097 (2)	177

Symmetry code: (ii) $x-1/2, y, -z+1/2$.