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(4-Pyridylmethyl)aminium chloride

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.090
Data-to-parameter ratio = 20.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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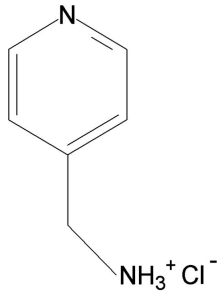
The crystal structure of the title compound, $C_6H_9N_2^+\cdot Cl^-$, is stabilized by extensive hydrogen bonding.

Comment

The aim of this work was to synthesize the neutral water-soluble *exo*-bidentate ligand ,*N*,*N*′-bispyridin-4-yl methyl glutaramide from the reaction of 4-aminomethylpyridine with glutaryl dichloride. The bidentate ligand is of interest owing to its biologically relevant functional groups, and as a supramolecular system that contains molecular cavities (Atwood *et al.*, 1998, 2000).



(I)

The title compound, (I), crystallizes in the space group $P2_1/c$ with the amine group protonated (Fig. 1). Each H atom on the ammonium cation is involved in intermolecular hydrogen bonding. Two of these H atoms are hydrogen-bonded to a Cl^- anion *via* a strong N—H···Cl hydrogen bond. These hydrogen bonds link the ions to form infinite chains that run parallel to the *c* axis (Fig. 2). The remaining ammonium H atom is

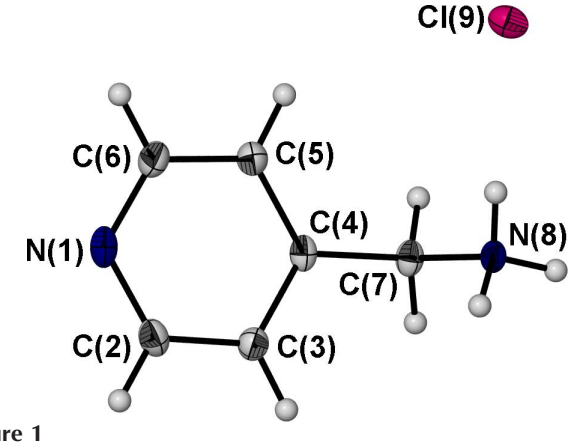


Figure 1
The molecular structure of (I), with the atom-labelling scheme and 50% probability displacement ellipsoids.

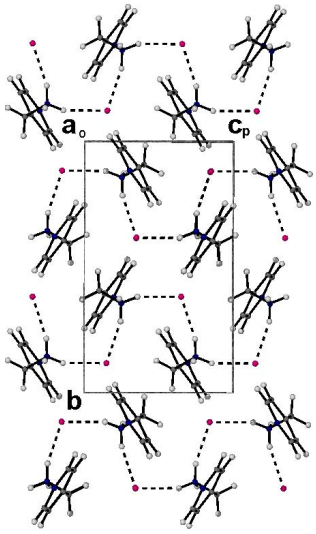


Figure 2
A crystal structure packing diagram for (I), viewed along [100]. Dashed lines indicate hydrogen bonds.

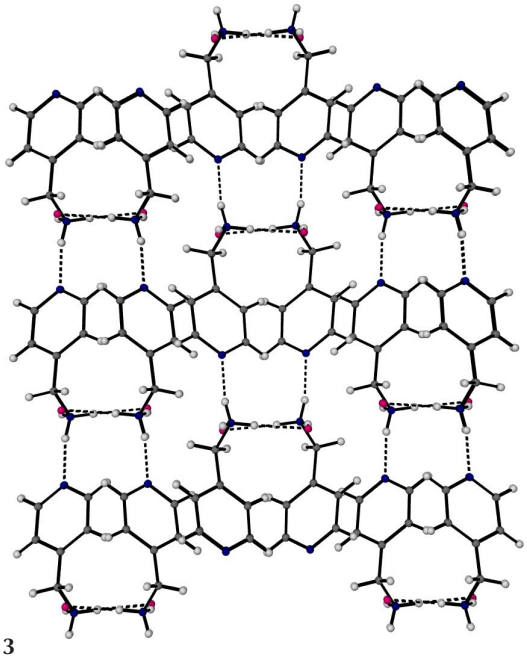


Figure 3
A crystal structure packing diagram for (I), viewed along [001]. Dashed lines indicate hydrogen bonds.

hydrogen-bonded to the heterocyclic amine *via* an N—H···N hydrogen bond (Fig. 3).

In addition to these hydrogen bonds, weak π–π interactions are observed between the pyridine aromatic rings [centroid-to-centroid distance of 3.83 (2) Å].

Experimental

The title compound was prepared by dissolving glutaryl dichloride (0.5875 ml, 4.6 mmol) and 4-aminomethylpyridine (0.9380 ml, 9.2 mmol) in distilled pyridine (10 ml). The reaction mixture was stirred for 2 h at room temperature. Water was added to stop the reaction and the combined solvent mixture was removed under reduced pressure. The residue was dissolved in ethanol and the solvent was allowed to evaporate. Colourless plate-like crystals formed after 2 d (43.2% yield).

Crystal data

$C_6H_9N_2^+\cdot Cl^-$
M_r = 144.60
Monoclinic, $P2_1/c$
a = 7.8401 (9) Å
b = 12.5177 (14) Å
c = 7.6177 (8) Å
β = 103.049 (2)°
V = 728.30 (14) Å^3
Z = 4
D_x = 1.319 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4476 reflections
θ = 2.7–28.2°
μ = 0.44 mm^{-1}
T = 100 (2) K
Plate, colourless
0.20 × 0.17 × 0.05 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997, Blessing, 1995)
T_{min} = 0.899, T_{max} = 0.979
4476 measured reflections
1687 independent reflections
1523 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.2°
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -9 \rightarrow 5$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.090
S = 1.08
1687 reflections
83 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 0.2493P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8A···Cl9^{i}	0.91	2.21	3.0899 (14)	163
N8—H8B···N1^{ii}	0.91	1.96	2.8551 (18)	169
N8—H8C···Cl9^{iii}	0.91	2.28	3.1523 (13)	160

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

The ammonium H atoms were located in difference Fourier maps and refined as part of a rigid rotor, with N—H = 0.91 Å and U_{iso}(H) = 1.5U_{eq}(N). All other H atoms were positioned geometrically and constrained to ride on their attached atoms, with C—H distances in the range 0.95–0.99 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *X-SEED*.

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