

## 2-Pyridiniohydrazinium dichloride

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## Key indicators

Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.026  
 $wR$  factor = 0.068  
Data-to-parameter ratio = 16.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

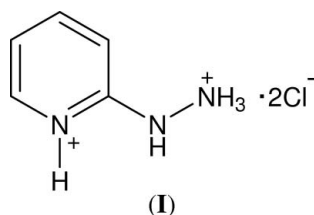
The crystal structure of the title compound,  $\text{C}_5\text{H}_9\text{N}_3^{2+} \cdot 2\text{Cl}^-$ , is stabilized by  $\text{N}-\text{H} \cdots \text{Cl}$  hydrogen bonds, forming a three-dimensional network. Each chloride anion forms three hydrogen bonds with N atoms, and the hydrazine unit forms  $R_2^1(5)$  motifs with one of the  $\text{Cl}^-$  anions. The aromatic ring is almost coplanar with both the N atoms of the hydrazine substituent and with one of the  $\text{Cl}^-$  anions.

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## Comment

Hydrogen bonding plays a key role in molecular recognition and the engineering of organic solids (Desiraju, 1989; Melendez & Hamilton, 1998). The design of highly specific solid-state compounds is of considerable significance in organic chemistry, due to the important applications of these compounds in the development of new optical, magnetic and electronic systems (Lehn, 1992). We present here the crystal structure of the title compound, (I).

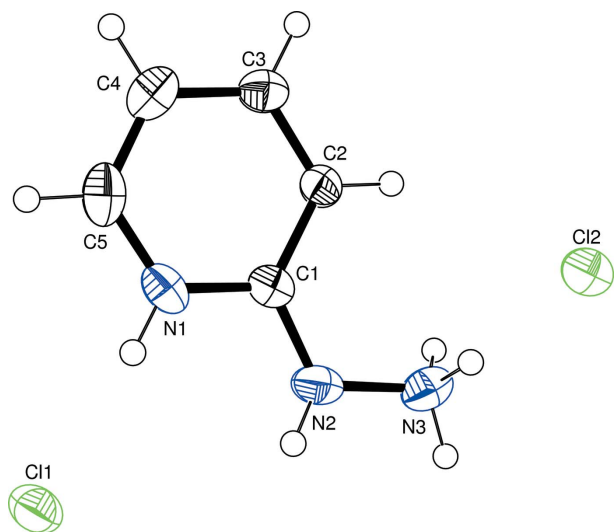


The asymmetric unit of (I) (Fig. 1 and Table 1) contains a hydrazinopyridine ring, protonated at the pyridine N1 and hydrazine N3 atoms, and two  $\text{Cl}^-$  anions multiply hydrogen-bonded to the  $\text{N}-\text{H}$  groups.

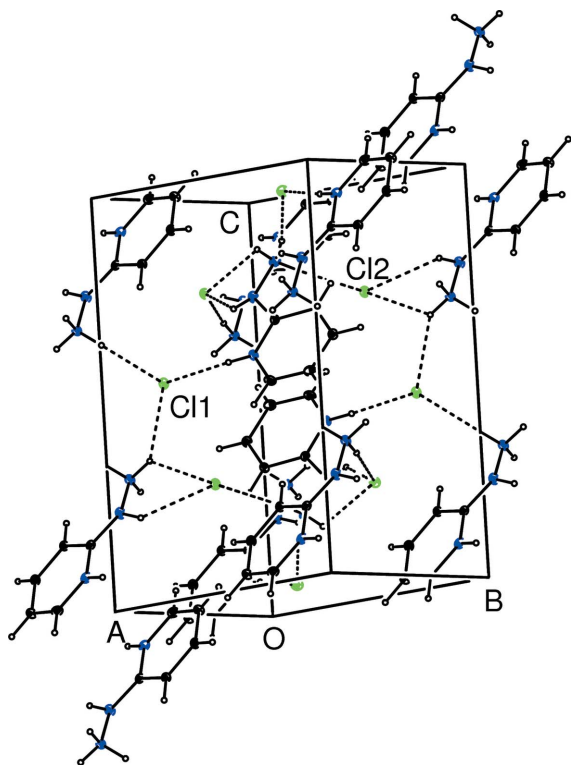
In the crystal structure of (I), there are six types of hydrogen bonds between the N and  $\text{Cl}^-$  anions, forming a three-dimensional network (Fig. 2 and Table 2). Each  $\text{Cl}^-$  anion forms three hydrogen bonds with N atoms, and the hydrazine unit forms  $R_2^1(5)$  motifs (Etter, 1990) with the  $\text{Cl}^-$  anions (Fig. 2). The aromatic ring plane is inclined at  $5.66$  ( $9^\circ$ ) to the  $\text{C}1-\text{N}2-\text{N}3-\text{H}3\text{A}$  plane, and the  $\text{Cl}1$  anion is coplanar with the pyridinium cation [deviation  $0.0060$  ( $6$ ) Å; Fig. 1].

## Experimental

2-Hydrazinopyridine (100 mg) was dissolved in diethyl ether (5 ml) and concentrated HCl was added until a precipitate was obtained. The precipitate was filtered off, dissolved in water and filtered again. Slow evaporation of the solvent afforded single crystals of (I) [m.p. 485–486 K (decomposition)].


**Figure 1**

A view of the asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.


**Figure 2**

A packing diagram for (I), with hydrogen bonds drawn as dashed lines.

#### Crystal data

$C_5H_9N_3^{2+} \cdot 2Cl^-$   
 $M_r = 182.05$   
 Monoclinic,  $P2_1/n$   
 $a = 7.3787$  (11) Å  
 $b = 8.5682$  (9) Å  
 $c = 12.637$  (2) Å  
 $\beta = 93.179$  (12)°  
 $V = 797.70$  (19) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.516$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.74$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
 Block, brown  
 $0.58 \times 0.47 \times 0.31$  mm

#### Data collection

Stoe IPDS II diffractometer  
 $\omega$  scans  
 Absorption correction: integration  
 (*X-RED32*; Stoe & Cie, 2002)  
 $T_{min} = 0.684$ ,  $T_{max} = 0.826$

4066 measured reflections  
 1564 independent reflections  
 1388 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.024$   
 $\theta_{max} = 26.0^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.026$   
 $wR(F^2) = 0.068$   
 $S = 1.05$   
 1564 reflections  
 95 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.2627P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.20$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

C1—N1	1.338 (2)	C5—N1	1.345 (2)
C1—N2	1.356 (2)	N2—N3	1.410 (2)
N1—C1—N2	115.51 (14)	N2—C1—C2	125.76 (14)
N1—C1—C2	118.71 (14)	C1—N2—N3	118.95 (14)
N1—C1—N2—N3	−174.86 (13)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1 $\cdots$ Cl1	0.86	2.17	3.0259 (14)	175
N3—H3A $\cdots$ Cl2 <sup>i</sup>	0.89	2.55	3.1441 (15)	125
N3—H3A $\cdots$ Cl1 <sup>ii</sup>	0.89	2.61	3.1674 (15)	121
N3—H3B $\cdots$ Cl2	0.89	2.19	3.0730 (16)	173
N3—H3C $\cdots$ Cl1 <sup>iii</sup>	0.89	2.21	3.0800 (15)	167
N2—H2A $\cdots$ Cl2 <sup>i</sup>	0.83 (3)	2.49 (3)	3.1092 (15)	132.6 (19)

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

Atom H2A was located in a difference map and refined isotropically [ $N-H = 0.83$  (3) Å]. All other H atoms were refined using the riding-model approximation, with  $C-H = 0.93$  Å and  $N-H = 0.86$  Å, and with  $U_{iso}(H) = 1.2U_{eq}(C,N)$ .

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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