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2-Amino-5-cyanopyridinium chloride

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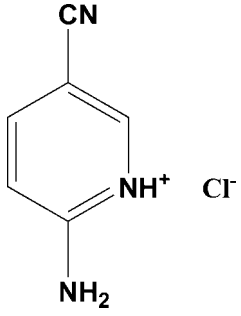
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.103; data-to-parameter ratio = 18.2.

In the crystal structure of the title compound, $C_6H_6N_3^+\cdot Cl^-$, cohesion is maintained by cation–anion N—H···Cl and cation–cation N—H···N hydrogen bonds, which link the ions into a three-dimensional network.

Related literature

For the use of tetrazole derivatives in coordination chemisty, see: Manzur *et al.* (2007); Ismayilov *et al.* (2007); Austria *et al.* (2007).



Experimental

Crystal data

$C_6H_6N_3^+\cdot Cl^-$
M_r = 155.59
Monoclinic, $P2_1/c$
a = 4.0937 (8) Å
b = 11.856 (2) Å
c = 14.842 (3) Å
β = 94.95 (3)°
V = 717.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 298 (2) K
0.18 × 0.15 × 0.15 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.922, T_{max} = 0.935
7307 measured reflections
1652 independent reflections
1252 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.102
S = 1.06
1652 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl1	0.86	2.29	3.0818 (18)	153
N3—H3A···Cl1	0.86	2.65	3.363 (2)	141
N3—H3A···N1^{i}	0.86	2.53	3.046 (3)	120
N3—H3B···Cl1^{ii}	0.86	2.37	3.216 (2)	167

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL/PC*.

This work was supported by a Start-up Grant from Southeast University to Professor Ren-Gen Xiong.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2232).

References

Austria, C., Zhang, J. & Valle, H. (2007). *Inorg. Chem.* **46**, 6283–6290.
Ismayilov, R. H., Wang, W. Z. & Lee, G. H. (2007). *Dalton Trans.* pp. 2898–2907.
Manzur, J., Vega, A. & Garcia, A. M. (2007). *Eur. J. Inorg. Chem.* **35**, 5500–5510.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2008). E**64**, o1461 [**doi:10.1107/S1600536808020783**]

2-Amino-5-cyanopyridinium chloride

X.-C. Wen

Comment

In the past five years, we have focused on the chemistry of amine derivatives because of their multiple coordination modes as ligands to metal ions and for the construction of novel metal-organic frameworks (Manzur *et al.* 2007; Ismayilov *et al.* 2007; Austria *et al.* 2007). Herein the crystal structure of the title compound, 6-aminonicotinonitrile-1-ium chloride, is reported.

In the title compound (Fig.1), the N2 atom of the pyridine ring is protonated. The nitrile group and the pyridine ring are nearly coplanar, as indicated by the dihedral angle of 86.71 (14)° formed by the C≡N vector with the normal to the pyridine plane. Crystal cohesion is enforced by cation-anion N—H···Cl and cation-cation N—H···N hydrogen bonds (Table 1, Fig. 2) linking molecules into a three-dimensional network.

Experimental

6-Aminonicotinonitrile-1-ium chloride (3 mmol) was dissolved in ethanol (20 ml) and evaporated in the air affording colourless block-shaped crystals suitable for X-ray analysis.

Refinement

All H atoms were fixed geometrically and treated as riding, with C–H = 0.93 Å, N–H =0.86 Å, and with U_{iso}(H) =1.2Ueq(C, N).

Figures

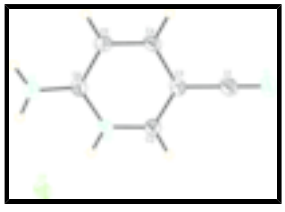


Fig. 1. A view of the title compound with the atom-numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

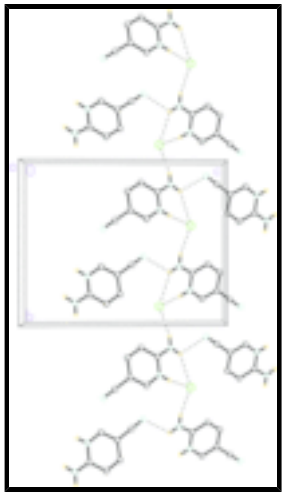


Fig. 2. Partial crystal packing of the title compound viewed along the *a* axis showing H bonding pattern as dashed lines. Hydrogen atoms not involved in hydrogen bonding are omitted for clarity.

2-Amino-5-cyanopyridinium chloride

Crystal data

$C_6H_6N_3^+ \cdot Cl^-$	F_{000} = 320
M_r = 155.59	D_x = 1.440 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1250 reflections
a = 4.0937 (8) Å	θ = 2.3–24.4º
b = 11.856 (2) Å	μ = 0.45 mm^{-1}
c = 14.842 (3) Å	T = 298 (2) K
β = 94.95 (3)º	Block, colourless
V = 717.7 (2) Å^3	0.18 × 0.15 × 0.15 mm
Z = 4	

Data collection

Rigaku Mercury2 diffractometer	1652 independent reflections
Radiation source: fine-focus sealed tube	1252 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 27.5º
T = 298(2) K	θ_{min} = 3.3º
ω scans	h = −5→5
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −15→15
T_{min} = 0.922, T_{max} = 0.935	l = −19→19
7307 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.102$

$S = 1.06$

1652 reflections

91 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.2213P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.21$ e Å^{-3}

$\Delta\rho_{min} = -0.23$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.44244 (14)	0.60704 (5)	0.17252 (4)	0.0459 (2)
N2	0.0652 (4)	0.69979 (14)	0.32749 (11)	0.0377 (4)
H2A	0.1041	0.6650	0.2787	0.045*
C2	−0.0884 (5)	0.64335 (18)	0.39019 (14)	0.0385 (5)
H2B	−0.1506	0.5687	0.3801	0.046*
N3	0.3183 (5)	0.85595 (16)	0.27271 (13)	0.0507 (5)
H3A	0.3567	0.8175	0.2256	0.061*
H3B	0.3816	0.9250	0.2777	0.061*
C3	−0.1527 (5)	0.69550 (17)	0.46837 (13)	0.0352 (5)
C1	−0.3034 (6)	0.63422 (18)	0.53757 (15)	0.0442 (5)
C6	0.1619 (5)	0.80885 (17)	0.33739 (13)	0.0355 (5)
C4	−0.0595 (5)	0.81008 (17)	0.48174 (14)	0.0398 (5)
H4A	−0.1029	0.8471	0.5346	0.048*
N1	−0.4184 (6)	0.58515 (18)	0.59282 (14)	0.0626 (6)
C5	0.0921 (5)	0.86506 (17)	0.41756 (15)	0.0414 (5)
H5A	0.1510	0.9403	0.4261	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0522 (3)	0.0472 (3)	0.0398 (3)	0.0063 (3)	0.0124 (2)	−0.0055 (2)
N2	0.0471 (10)	0.0364 (9)	0.0305 (9)	−0.0004 (8)	0.0091 (7)	−0.0073 (7)

C2	0.0442 (12)	0.0344 (11)	0.0376 (11)	−0.0020 (9)	0.0082 (9)	−0.0007 (9)
N3	0.0672 (13)	0.0442 (11)	0.0435 (11)	−0.0080 (10)	0.0207 (10)	−0.0001 (9)
C3	0.0370 (11)	0.0378 (11)	0.0313 (10)	0.0033 (9)	0.0063 (8)	0.0016 (8)
C1	0.0523 (13)	0.0414 (12)	0.0400 (12)	0.0027 (10)	0.0101 (10)	−0.0022 (10)
C6	0.0370 (11)	0.0366 (11)	0.0332 (10)	0.0022 (9)	0.0054 (9)	0.0028 (8)
C4	0.0486 (12)	0.0384 (11)	0.0334 (11)	0.0036 (10)	0.0104 (9)	−0.0066 (9)
N1	0.0862 (16)	0.0547 (13)	0.0514 (12)	−0.0085 (11)	0.0316 (12)	0.0009 (10)
C5	0.0530 (13)	0.0306 (11)	0.0419 (12)	−0.0015 (9)	0.0106 (10)	−0.0060 (9)

Geometric parameters (Å, °)

N2—C2	1.345 (2)	C3—C4	1.420 (3)
N2—C6	1.356 (3)	C3—C1	1.440 (3)
N2—H2A	0.8600	C1—N1	1.140 (3)
C2—C3	1.360 (3)	C6—C5	1.414 (3)
C2—H2B	0.9300	C4—C5	1.349 (3)
N3—C6	1.323 (3)	C4—H4A	0.9300
N3—H3A	0.8600	C5—H5A	0.9300
N3—H3B	0.8600		
C2—N2—C6	123.26 (17)	C4—C3—C1	120.62 (18)
C2—N2—H2A	118.4	N1—C1—C3	179.0 (3)
C6—N2—H2A	118.4	N3—C6—N2	118.60 (18)
N2—C2—C3	120.02 (19)	N3—C6—C5	123.9 (2)
N2—C2—H2B	120.0	N2—C6—C5	117.53 (18)
C3—C2—H2B	120.0	C5—C4—C3	119.85 (18)
C6—N3—H3A	120.0	C5—C4—H4A	120.1
C6—N3—H3B	120.0	C3—C4—H4A	120.1
H3A—N3—H3B	120.0	C4—C5—C6	120.34 (19)
C2—C3—C4	118.98 (18)	C4—C5—H5A	119.8
C2—C3—C1	120.37 (19)	C6—C5—H5A	119.8
C6—N2—C2—C3	−0.3 (3)	C2—C3—C4—C5	−0.4 (3)
N2—C2—C3—C4	0.9 (3)	C1—C3—C4—C5	177.6 (2)
N2—C2—C3—C1	−177.1 (2)	C3—C4—C5—C6	−0.7 (3)
C2—N2—C6—N3	178.4 (2)	N3—C6—C5—C4	−177.9 (2)
C2—N2—C6—C5	−0.8 (3)	N2—C6—C5—C4	1.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···Cl1	0.86	2.29	3.0818 (18)	153
N3—H3A···Cl1	0.86	2.65	3.363 (2)	141
N3—H3A···N1^{i}	0.86	2.53	3.046 (3)	120
N3—H3B···Cl1^{ii}	0.86	2.37	3.216 (2)	167

Symmetry codes: (i) *x*+1, −*y*+3/2, *z*−1/2; (ii) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

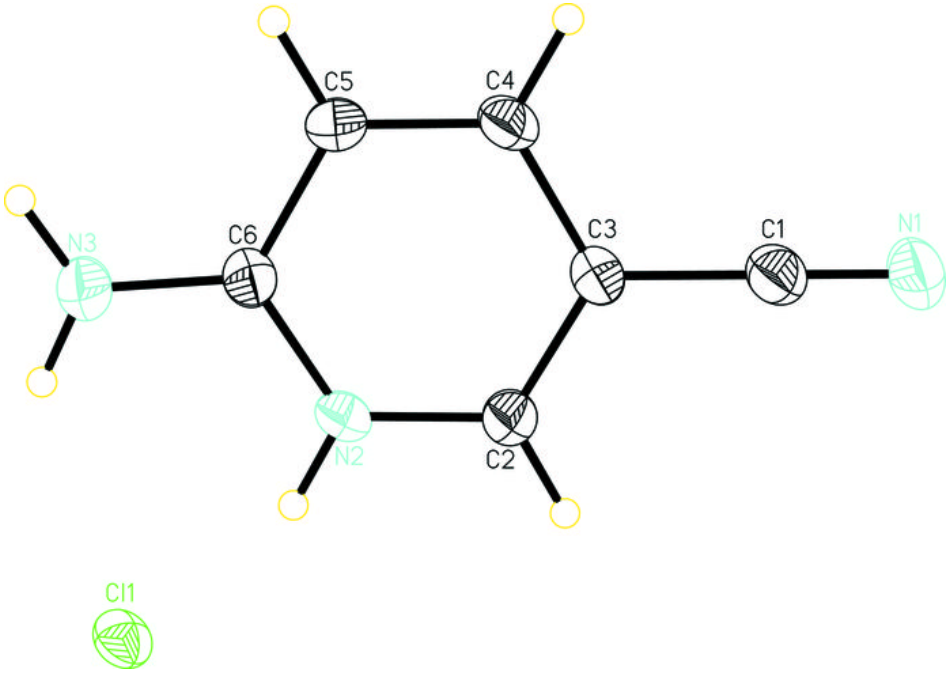


Fig. 2