Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-5-cyanopyridinium chloride

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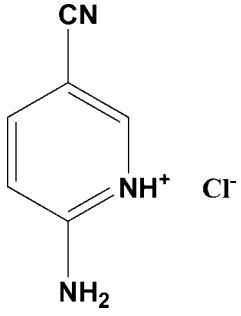
Received 30 June 2008; accepted 4 July 2008

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.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

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

2-Amino-5-cyanopyridinium chloride

Xiao-Chun Wen

S1. 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.

S2. 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.

S3. 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).

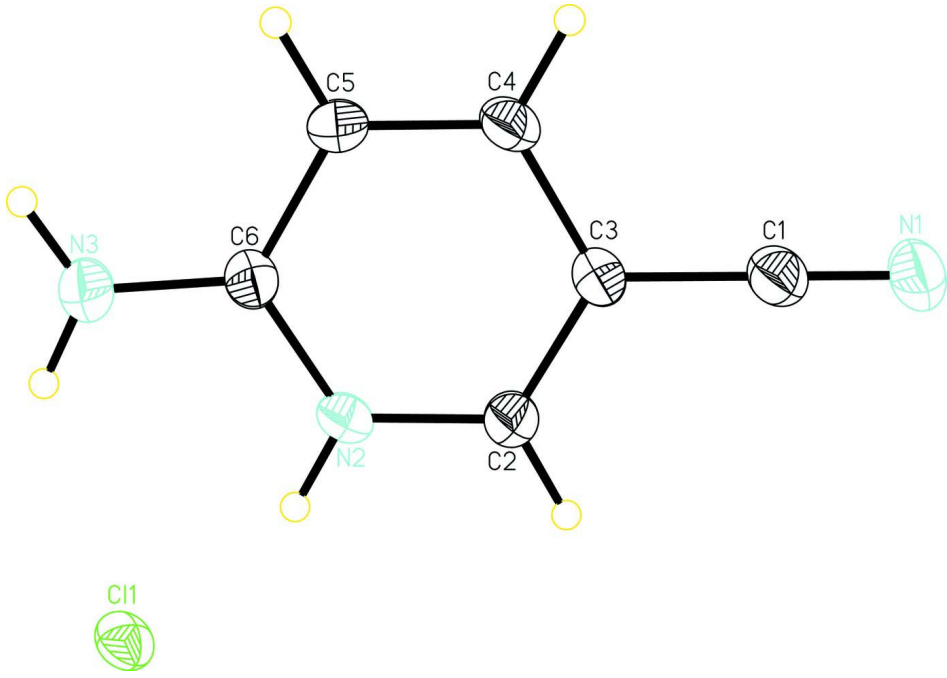

Figure 1

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

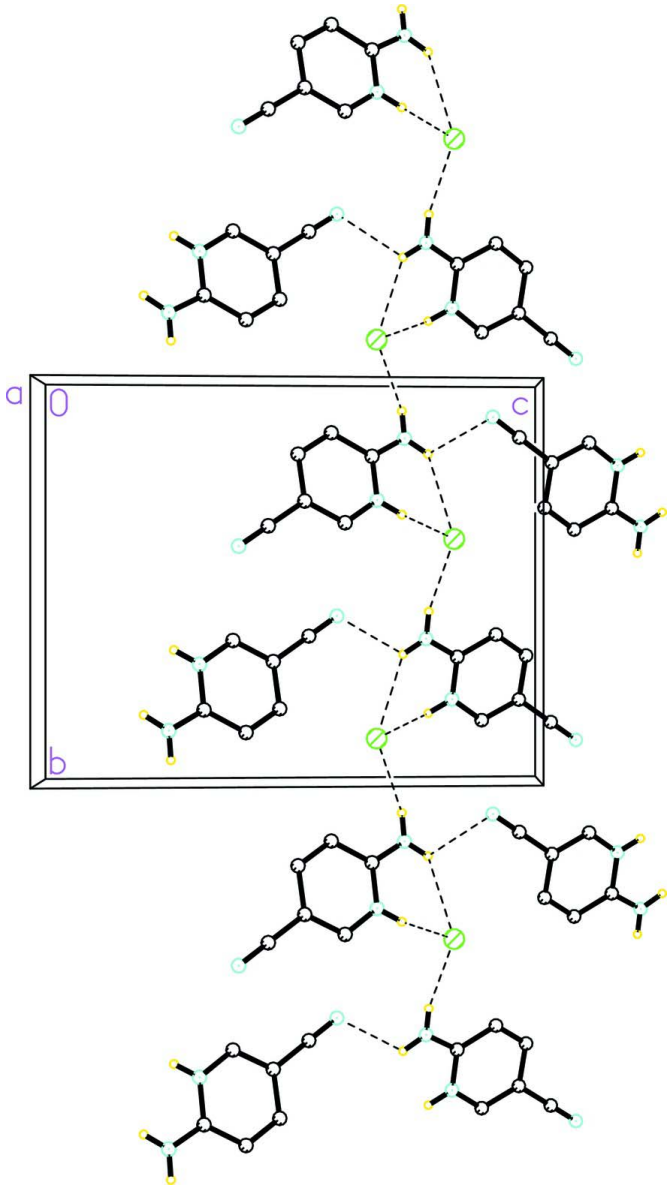

Figure 2

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

$C_6H_6N_3^+\cdot Cl^-$
M_r = 155.59
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
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
F(000) = 320
D_x = 1.440 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1250 reflections
θ = 2.3–24.4°
μ = 0.45 mm^{-1}

T = 298 K
Block, colourless

0.18 × 0.15 × 0.15 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
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
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −5→5
k = −15→15
l = −19→19

Refinement

Refinement on F^2
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
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
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.2213P]$ 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}

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 (Å²)

	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, º)

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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Cl1	0.86	2.29	3.0818 (18)	153
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