Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-5-cyanopyridinium nitrate

Jing Dai

Ordered Matter Science Research Center, College of Chemistry and Chemical Engineering, Southeast University, Nanjing 210096, People's Republic of China
Correspondence e-mail: fudavid88@yahoo.com.cn

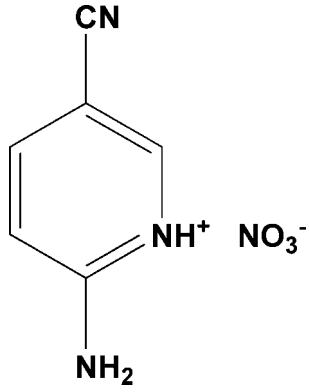
Received 26 August 2008; accepted 2 September 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.127; data-to-parameter ratio = 12.7.

In the title compound, $C_6H_6N_3^+\cdot NO_3^-$, the packing is consolidatedby N—H···N and N—H···O hydrogen bonds.

Related literature

For the chemisty of amine derivatives, see: Manzur *et al.* (2007); Ismayilov *et al.* (2007); Austria *et al.* (2007); Wen (2008).



Experimental

Crystal data

$C_6H_6N_3^+\cdot NO_3^-$
M_r = 182.15
Monoclinic, $P2_1/n$
a = 4.6475 (9) Å
b = 12.713 (3) Å
c = 13.417 (3) Å
β = 97.91 (3)°
V = 785.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 298 (2) K
0.25 × 0.15 × 0.15 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.975, T_{max} = 0.981
8053 measured reflections
1798 independent reflections
1163 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.127
S = 1.07
1798 reflections
142 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O2^{i}	0.90 (2)	2.05 (3)	2.941 (3)	169 (2)
N1—H1···O1^{i}	0.92 (3)	1.82 (3)	2.733 (2)	170 (2)
N2—H2C···O3	0.83 (3)	2.10 (3)	2.926 (3)	174 (3)

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

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* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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: WK2092).

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.
Wen, X.-C. (2008). *Acta Cryst.* E**64**, o1461.

supporting information

Acta Cryst. (2008). E**64**, o1899 [doi:10.1107/S1600536808028031]

2-Amino-5-cyanopyridinium nitrate

Jing Dai

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; Wen 2008). We report here the crystal structure of the title compound.

In the title compound (Fig. 1), the N1 atom of the pyridine ring is protonated. The nitrile group and the pyridinium ring are essentially coplanar. The nitrile group C6≡N3 bond length of 1.133 (3)Å is within the normal range. Crystal cohesion is enforced by N—H···N and N—H···O hydrogen bonds (Table 1, Fig. 2).

S2. Experimental

6-aminonicotinonitrile (3 mmol) was dissolved in the solution of ethanol (20 ml) and nitric acid (1 ml), and evaporated in the air affording colorless block crystals of this compound suitable for X-ray analysis.

S3. Refinement

All H atoms were located in difference Fourier maps and refined freely.

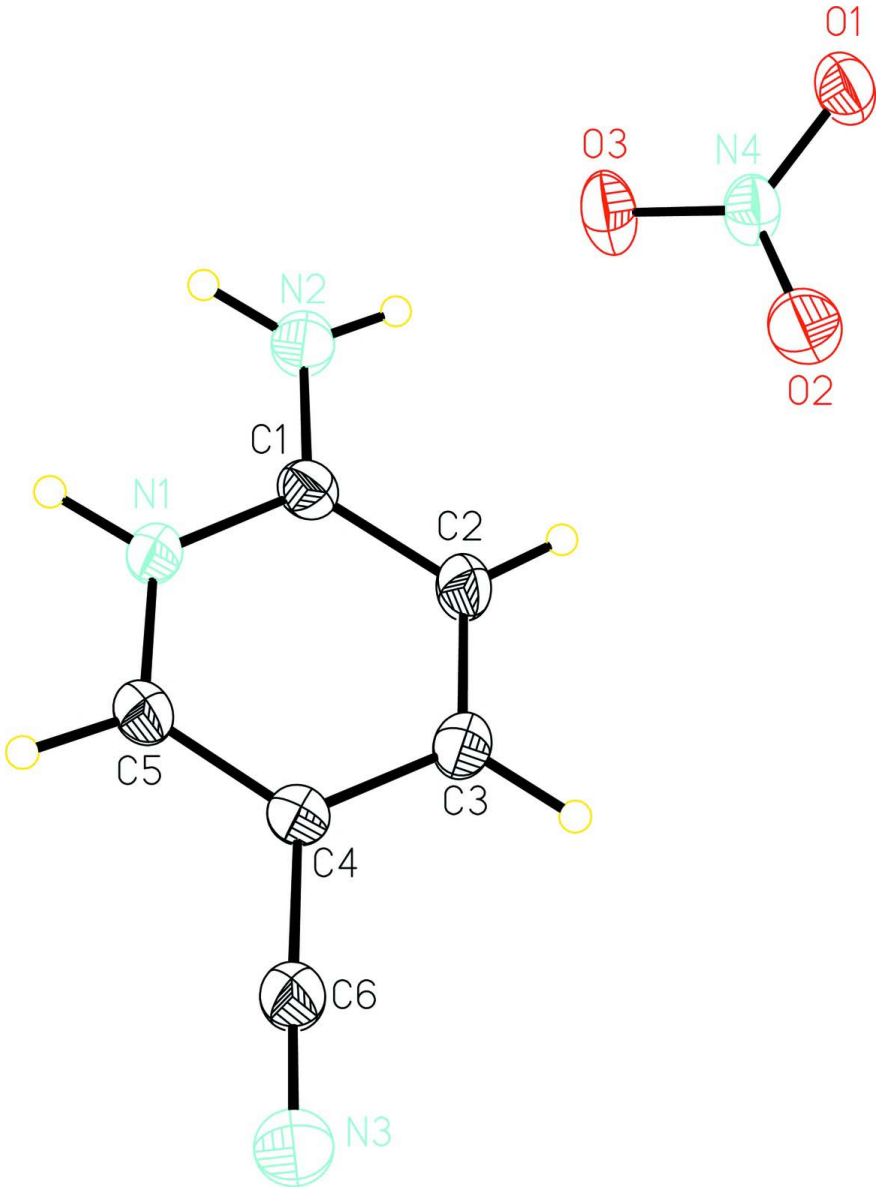


Figure 1

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

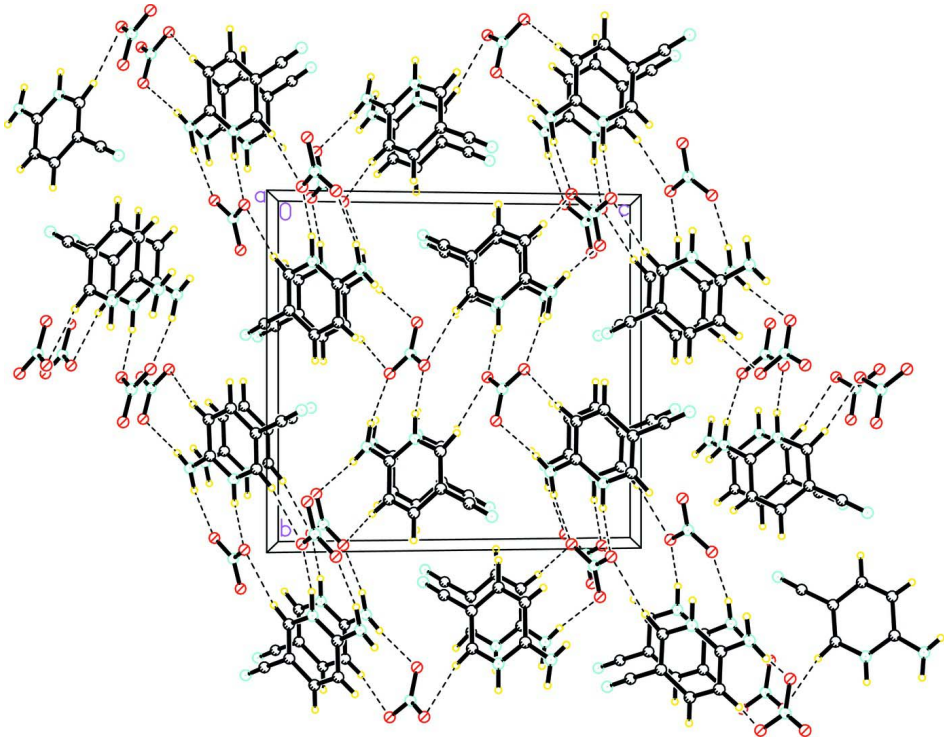


Figure 2

The crystal packing of the title compound viewed along the *a* axis and all hydrogen atoms not involved in hydrogen bonding (dashed lines) were omitted for clarity.

2-Amino-5-cyanopyridinium nitrate

Crystal data

$C_6H_6N_3^+\cdot NO_3^-$
$M_r = 182.15$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 4.6475\ (9)$ Å
$b = 12.713\ (3)$ Å
$c = 13.417\ (3)$ Å
$\beta = 97.91\ (3)°$
$V = 785.1\ (3)$ Å^3
$Z = 4$
$F(000) = 376$
$D_x = 1.541$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1796 reflections
$\theta = 3.1–27.5°$
$\mu = 0.13$ mm^{-1}
$T = 298$ K
Block, colourless
0.25 × 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)
$T_{min} = 0.975$, $T_{max} = 0.981$
8053 measured reflections
1798 independent reflections
1163 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -6\rightarrow6$
$k = -16\rightarrow16$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.127$
$S = 1.07$
1798 reflections
142 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.1542P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C2	0.7591 (5)	0.86151 (17)	0.31844 (17)	0.0428 (5)
N4	0.0550 (4)	0.94943 (14)	0.12683 (14)	0.0456 (5)
N2	0.4566 (4)	0.71680 (19)	0.25422 (16)	0.0509 (5)
O1	−0.1866 (3)	0.98288 (12)	0.08728 (13)	0.0604 (5)
O2	0.2162 (4)	1.00628 (14)	0.18518 (14)	0.0651 (5)
O3	0.1266 (4)	0.85819 (13)	0.10891 (13)	0.0610 (5)
N1	0.8152 (4)	0.69031 (15)	0.38842 (14)	0.0406 (4)
C3	0.9809 (5)	0.89511 (17)	0.38692 (17)	0.0435 (5)
C5	1.0356 (4)	0.72284 (18)	0.45750 (17)	0.0402 (5)
C6	1.3541 (5)	0.86115 (17)	0.53382 (18)	0.0476 (6)
C1	0.6718 (4)	0.75525 (16)	0.31857 (15)	0.0379 (5)
C4	1.1235 (4)	0.82498 (16)	0.45893 (16)	0.0388 (5)
N3	1.5342 (5)	0.89264 (16)	0.59161 (18)	0.0684 (7)
H5	1.126 (4)	0.6708 (16)	0.5011 (15)	0.036 (5)*
H2A	0.655 (4)	0.9049 (16)	0.2716 (15)	0.033 (5)*
H3	1.041 (4)	0.9695 (19)	0.3867 (16)	0.051 (6)*
H2B	0.401 (5)	0.650 (2)	0.2641 (17)	0.048 (7)*
H1	0.764 (5)	0.620 (2)	0.389 (2)	0.067 (8)*
H2C	0.370 (6)	0.761 (3)	0.216 (2)	0.082 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0473 (13)	0.0351 (11)	0.0432 (12)	0.0020 (9)	−0.0043 (11)	0.0098 (10)
N4	0.0556 (12)	0.0365 (10)	0.0425 (10)	0.0046 (9)	−0.0013 (9)	0.0013 (9)

N2	0.0512 (12)	0.0424 (12)	0.0529 (12)	−0.0048 (10)	−0.0146 (10)	0.0011 (10)
O1	0.0532 (10)	0.0445 (9)	0.0766 (12)	0.0102 (8)	−0.0156 (9)	−0.0064 (8)
O2	0.0615 (11)	0.0566 (11)	0.0698 (11)	0.0031 (8)	−0.0179 (9)	−0.0180 (9)
O3	0.0770 (12)	0.0405 (9)	0.0599 (11)	0.0171 (8)	−0.0098 (9)	−0.0044 (8)
N1	0.0405 (10)	0.0306 (10)	0.0478 (11)	−0.0032 (8)	−0.0041 (8)	0.0032 (8)
C3	0.0471 (13)	0.0323 (12)	0.0492 (13)	−0.0021 (10)	−0.0003 (11)	0.0029 (10)
C5	0.0394 (11)	0.0383 (12)	0.0408 (12)	0.0034 (9)	−0.0025 (10)	0.0052 (10)
C6	0.0495 (14)	0.0373 (12)	0.0515 (14)	−0.0002 (10)	−0.0089 (12)	0.0008 (10)
C1	0.0356 (11)	0.0399 (12)	0.0370 (11)	0.0027 (9)	0.0007 (9)	0.0003 (9)
C4	0.0355 (11)	0.0377 (12)	0.0414 (11)	−0.0002 (9)	−0.0014 (9)	0.0020 (10)
N3	0.0697 (14)	0.0501 (13)	0.0755 (16)	−0.0045 (11)	−0.0249 (13)	−0.0036 (11)

Geometric parameters (Å, º)

C2—C3	1.352 (3)	N1—C5	1.348 (3)
C2—C1	1.411 (3)	N1—C1	1.354 (3)
C2—H2A	0.92 (2)	N1—H1	0.92 (3)
N4—O3	1.239 (2)	C3—C4	1.411 (3)
N4—O2	1.239 (2)	C3—H3	0.99 (2)
N4—O1	1.249 (2)	C5—C4	1.361 (3)
N2—C1	1.322 (3)	C5—H5	0.94 (2)
N2—H2B	0.90 (2)	C6—N3	1.133 (3)
N2—H2C	0.83 (3)	C6—C4	1.440 (3)
C3—C2—C1	119.6 (2)	C2—C3—H3	119.4 (13)
C3—C2—H2A	123.7 (12)	C4—C3—H3	120.0 (13)
C1—C2—H2A	116.7 (12)	N1—C5—C4	120.1 (2)
O3—N4—O2	120.89 (19)	N1—C5—H5	116.3 (12)
O3—N4—O1	119.08 (18)	C4—C5—H5	123.6 (12)
O2—N4—O1	120.00 (18)	N3—C6—C4	177.9 (2)
C1—N2—H2B	117.2 (15)	N2—C1—N1	118.9 (2)
C1—N2—H2C	115 (2)	N2—C1—C2	123.1 (2)
H2B—N2—H2C	127 (3)	N1—C1—C2	118.07 (19)
C5—N1—C1	123.0 (2)	C5—C4—C3	118.77 (19)
C5—N1—H1	117.7 (16)	C5—C4—C6	120.53 (19)
C1—N1—H1	119.4 (17)	C3—C4—C6	120.69 (19)
C2—C3—C4	120.5 (2)		
C1—C2—C3—C4	−0.6 (3)	C3—C2—C1—N1	0.2 (3)
C1—N1—C5—C4	−0.2 (3)	N1—C5—C4—C3	−0.3 (3)
C5—N1—C1—N2	−179.4 (2)	N1—C5—C4—C6	178.5 (2)
C5—N1—C1—C2	0.2 (3)	C2—C3—C4—C5	0.6 (3)
C3—C2—C1—N2	179.8 (2)	C2—C3—C4—C6	−178.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O2^{i}	0.90 (2)	2.05 (3)	2.941 (3)	169 (2)

N1—H1···O1^{i}	0.92 (3)	1.82 (3)	2.733 (2)	170 (2)
N1—H1···N4^{i}	0.92 (3)	2.62 (3)	3.505 (3)	161 (2)
N2—H2*C*···O3	0.83 (3)	2.10 (3)	2.926 (3)	174 (3)

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