Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

2-Aminopyridinium nitrate

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Received 27 July 2006
Accepted 21 December 2006

Strong N—H···O interactions are present in the crystal structure of the title organic–inorganic hybrid material, $C_5H_7N_2^+\cdot NO_3^-$. Organic 2-aminopyridinium cations and discrete nitrate anions interact to form hydrogen-bonded ribbons. There are two cations and two anions in the asymmetric unit.

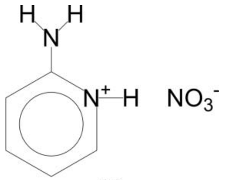
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.122
Data-to-parameter ratio = 23.9

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

Comment

The structure of 2-aminopyridinium nitrate, (I), was determined as part of an ongoing study of the structural characteristics of organic–inorganic hybrid materials. The crystal structure of the sulfate salt of 2-aminopyridinium has been reported previously (Jebas *et al.*, 2006), and appears to be the only report in the literature of a structure consisting of 2-aminopyridinium cations and non-metallic inorganic anions.



(I)

The molecular structure of (I) and the atomic labelling scheme employed are illustrated in Fig. 1. The asymmetric unit contains two crystallographically independent 2-aminopyridinium cations and two crystallographically independent isolated nitrate anions. Only the pyridinium N atoms of the cations are protonated, while the amine groups remain unprotonated, resulting in a charge of +1 for each cation.

Fig. 2 illustrates the layered molecular packing in the structure. The inorganic layer contains the discrete nitrate anions, and alternates with the organic layer which consists of the 2-aminopyridinium cations. Neighbouring cations in the

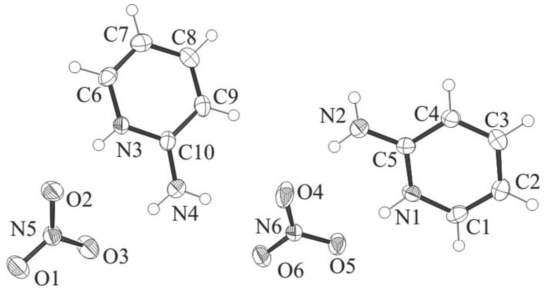


Figure 1
The asymmetric unit of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

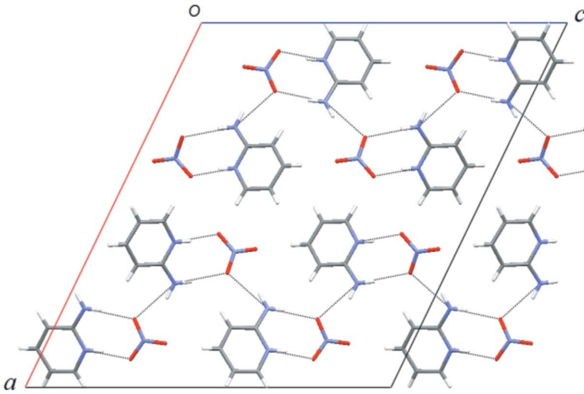


Figure 2
Molecular packing and hydrogen-bonding interactions (dashed lines), viewed down the *b* axis.

organic layer differ in the orientation of the amino groups, as illustrated in Fig. 2. In the inorganic layer, N—O bond lengths range from 1.234 (1) to 1.260 (1) Å, and O—N—O bond angles fall between 118.8 (1) and 121.3 (1)°.

2-Aminopyridinium cations and nitrate anions interact *via* strong charge-assisted N—H···O hydrogen bonds, which are listed in Table 1. One-dimensional corrugated hydrogen-bonded ribbons are formed. Neighbouring hydrogen-bonded ribbons form sheets, and stacking of the sheets results in the three-dimensional structure. However, the ribbons or sheets do not interact *via* non-covalent interactions.

Experimental

2-Aminopyridinium nitrate was prepared by the dropwise addition of HNO_3 (0.64 ml, 70%, Aldrich) to a solution of 2-aminopyridine (0.506 g, 98%, Aldrich) in 20 ml chloroform The salt was re-crystallized from distilled water, and colourless crystals formed on evaporation at room temperature.

Crystal data

$C_5H_7N_2^+ \cdot NO_3^-$
$M_r = 157.14$
Monoclinic, $P2/c$
$a = 21.5559$ (11) Å
$b = 3.6473$ (1) Å
$c = 19.4851$ (8) Å
$\beta = 115.752$ (4)°
$V = 1379.79$ (10) Å^3
$Z = 8$
$D_x = 1.513$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.13$ mm^{-1}
$T = 120$ (2) K
Needle, colourless
0.40 × 0.20 × 0.15 mm

Data collection

Oxford Diffraction Excalibur2 diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.949$, $T_{max} = 0.983$
20896 measured reflections
4939 independent reflections
3460 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 34.2°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.122$
$S = 1.05$
4939 reflections
207 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.2988P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2	0.866 (16)	1.956 (16)	2.7983 (13)	164 (2)
N4—H4B···O4	0.86	2.18	2.9564 (14)	150
N4—H4A···O3	0.86	2.06	2.8959 (13)	164
N1—H1A···O5	0.920 (16)	1.878 (16)	2.7790 (13)	166 (2)
N2—H2A···O4	0.86	2.04	2.8915 (14)	170
N2—H2B···O3^{i}	0.86	2.10	2.8856 (13)	152
N4—H4B···O6	0.86	2.45	3.2450 (14)	154

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

The pyridinium H atoms (H1*A* and H3*A*) were located in a Fourier map and their positions refined. This resulted in the best placement of these atoms in the hydrogen-bonding network. All other H atoms were placed in calculated positions, with aromatic C—H distances of 0.93 Å and amine N—H distances of 0.86 Å, and were refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$ of the parent atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2003); 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) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

The author acknowledges funding received for this work from the University of KwaZulu-Natal Research Office, and from the National Research Foundation (GUN: 2054350).

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