Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

4-Aminopyridinium nitrate

Melanie Rademeyer

School of Chemistry, University of KwaZulu-Natal, Howard College Campus, Durban 4041, South Africa

Correspondence e-mail:
rademeyerm@ukzn.ac.za

Received 21 June 2005
Accepted 29 June 2005
Online 13 July 2005

Key indicators

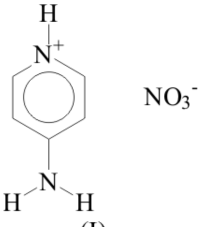
Single-crystal X-ray study
T = 200 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.116
Data-to-parameter ratio = 20.6

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

The structure of the organic–inorganic hybrid material 4-aminopyridinium nitrate, $C_5H_7N_2^+\cdot NO_3^-$, exhibits classical and bifurcated strong N—H···O hydrogen-bonding interactions, as well as weaker C—H···O interactions. Organic 4-aminopyridinium cations and inorganic nitrate anions interact to form a one-dimensional hydrogen-bonded ribbon in the *a* direction. Neighbouring ribbons interact to form two-dimensional corrugated hydrogen-bonded sheets parallel to the *ac* plane.

Comment

The crystal structure of 4-aminopyridinium nitrate, (I), has been determined as part of an ongoing investigation into the effect of various anions on the structures and hydrogen-bonding connectivities of organic–inorganic hybrid compounds. The crystal structures of two polymorphs of 4-aminopyridinium perchlorate have been reported previously (Czupinski *et al.*, 2002), these being the only examples of structures that could be located in the literature containing a 4-aminopyridinium cation and a non-metallic polyatomic anion.



(I)

The molecular structure of (I), as well as the atomic numbering scheme employed, are illustrated in Fig. 1. One 4-aminopyridinium cation and one discrete nitrate anion comprise the asymmetric unit.

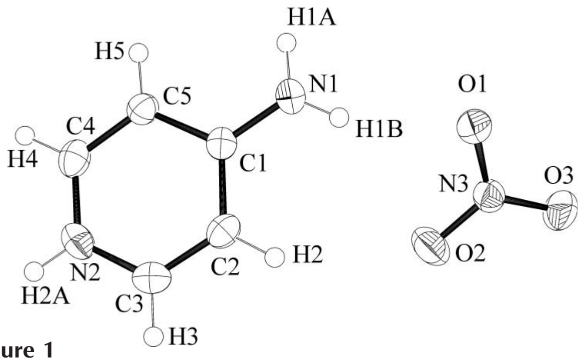


Figure 1
The molecular structure of (I), showing the atomic numbering scheme and with displacement ellipsoids at the 50% probability level.

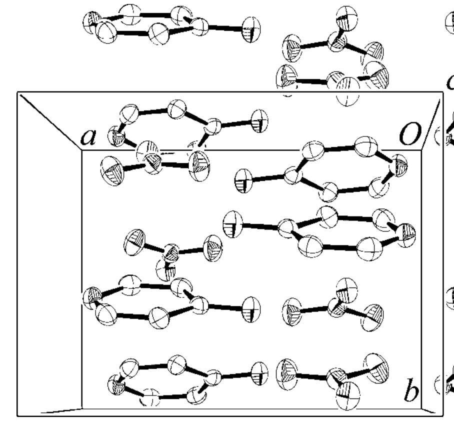


Figure 2
A packing diagram for (I), viewed down the *c* axis. H atoms have been omitted for clarity.

The molecular packing is illustrated in Fig. 2. Alternating pairs of cations and anions pack parallel to the *ab* plane. N—O bond lengths for the nitrate anion range from 1.2383 (15) to 1.2632 (15) Å, and O—N—O bond angles range from 118.48 (12) to 121.80 (13)°.

4-Aminopyridinium cations and nitrate anions interact *via* N—H···O hydrogen bonds (Table 1). The structure can be considered as consisting of one-dimensional hydrogen-bonded ribbons extending in the *a* direction, as illustrated in Fig. 3. Each ribbon consists of alternating cations and anions, with the aromatic groups of the organic cations being parallel. In the ribbon, each cation interacts with two different nitrate anions *via* hydrogen-bonding interactions. Within a cation, atom N1 forms a bifurcated interaction through atom H1*B* to atom O1 of an anion. On the opposite side of the molecule, atom N2 interacts with atom O1($x - 1, y, z$) through a classical hydrogen bond involving atom H2*A*.

Neigbouring one-dimensional ribbons are connected through the strong bifurcated hydrogen-bonding interactions N1—H1*A*···O2($x, \frac{1}{2} - y, \frac{1}{2} + z$) and N1—H1*B*···O2, to form corrugated two-dimensional sheets, as illustrated in Fig. 4. It is noteworthy that atom O3 is not involved in strong hydrogen-bonding interactions and exhibits a short N—O bond of 1.2383 (15) Å, whereas the N—O bonds participating in strong hydrogen bonds (N3—O1 and N3—O2) are elongated. In the two-dimensional sheet, however, two additional, weaker C—H···O interactions involving atom O3 are present, namely C3—H3···O1($1 - x, 1 - y, -z$) and C4—H4···O3($x, \frac{1}{2} - y, \frac{1}{2} + z$), at distances of 3.364 (3) and 3.387 (3) Å, respectively.

Thus, in terms of the connectivity observed in this structure, the nitrate anion can be described as a four-connecting node with bifurcated and normal hydrogen bonds, resulting in a two-dimensional sheet structure. Stacking of the two-dimensional sheets in the *b* cell direction gives the complete crystal structure.

Experimental

4-Aminopyridinium nitrate was prepared by the dropwise addition of nitric acid (70%, Aldrich) to a chloroform (99%, Saarchem) solution of 4-aminopyridine (98+%, Aldrich), in stoichiometric amounts. The solution was left to evaporate to dryness at room temperature. A colourless needle crystal of (I) was cut to dimensions 0.2 × 0.2 × 0.2 mm and employed in the diffraction study.

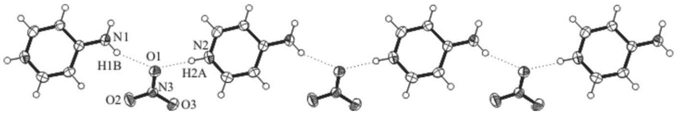


Figure 3
A view of the one-dimensional hydrogen-bonded (dashed lines) chain, parallel to the *a* axis.

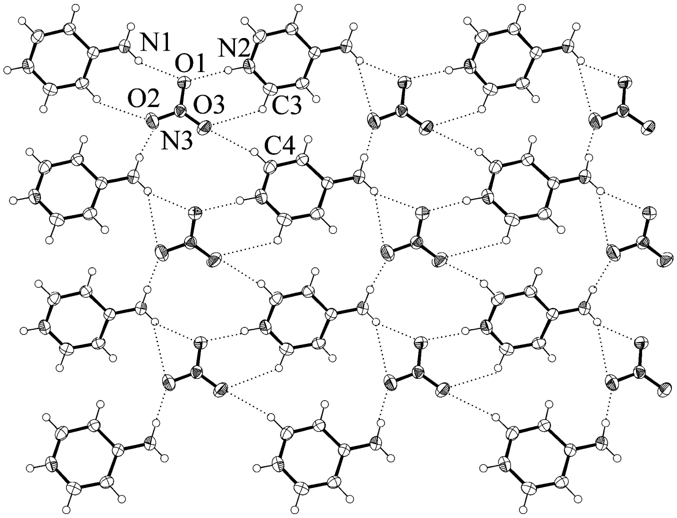


Figure 4
A view of two-dimensional hydrogen-bonded (dashed lines) sheet, parallel to the *ac* plane.

Crystal data

$C_5H_7N_2^+ \cdot NO_3^-$
$M_r = 157.14$
Monoclinic, $P2_1/c$
$a = 9.192$ (4) Å
$b = 6.996$ (4) Å
$c = 10.869$ (5) Å
$\beta = 93.60$ (4)°
$V = 697.5$ (6) Å^3
$Z = 4$
$D_x = 1.496$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 209 reflections
$\theta = 2$–30°
$\mu = 0.13$ mm^{-1}
$T = 200$ (2) K
Fragment cut from needle, colourless
0.20 × 0.20 × 0.20 mm

Data collection

Oxford Excalibur2 diffractometer
ω–2θ scans
6090 measured reflections
2220 independent reflections
1369 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 31.8°$
$h = -13 \rightarrow 13$
$k = -10 \rightarrow 8$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.116$
$S = 0.94$
2220 reflections
108 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$B\cdots$O2	0.86 (2)	2.58 (2)	3.302 (2)	143 (2)
N1—H1$B\cdots$O1	0.86 (2)	2.14 (2)	2.952 (2)	159 (2)
N2—H2$A\cdots$O1^{i}	0.88 (2)	1.90 (2)	2.784 (2)	175 (2)
N2—H2$A\cdots$O3^{i}	0.88 (2)	2.66 (2)	3.218 (2)	122 (2)
N2—H2$A\cdots$N3^{i}	0.88 (2)	2.63 (2)	3.421 (2)	149 (2)

Symmetry codes: (i) $x-1, y, z$.

All H atoms involved in hydrogen bonding (H1*A*, H1*B* and H2*A*) were located in a difference map and refined independently. All other H atoms were placed in calculated positions, with an aromatic C—H distance of 0.93 Å, and were refined using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *CrysAlisCCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlisCCD*; data reduction: *CrysAlisRED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXL97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

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

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