

## Andrei S. Batsanov

Department of Chemistry, University of  
Durham, South Road, Durham DH1 3LE,  
EnglandCorrespondence e-mail:  
a.s.batsanov@durham.ac.uk

## Key indicators

Single-crystal X-ray study  
 $T = 290\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.050  
 $wR$  factor = 0.157  
Data-to-parameter ratio = 12.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## Pyridinium nitrate at 290 K

A previous structural study [Serewicz *et al.* (1965). *J. Phys. Chem.* **69**, 1915–1921] of pyridinium nitrate,  $\text{C}_5\text{H}_6\text{N}^+\cdot\text{NO}_3^-$ , has been repeated at 290 K.

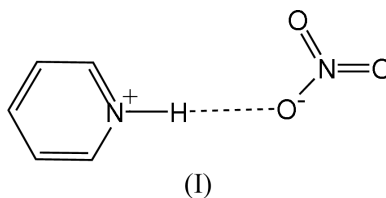
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## Comment

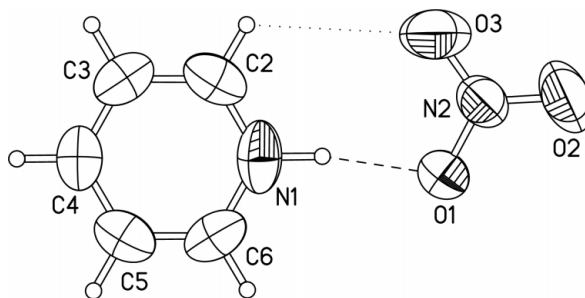
The crystal structure of pyridinium nitrate, (I), as determined by Serewicz *et al.* (1965), implied the existence of a strong hydrogen bond between the pyridinium and nitrate ions, but the precision of the data (measured at room temperature by the Weissenberg method) was insufficient to locate H atoms directly. We have redetermined this structure at two temperatures in the course of screening for materials suitable for neutron-diffraction and charge-density studies of hydrogen bonds. The 290 K structure (Fig. 1 and Table 1) is reported here. The results reported by Serewicz *et al.* (1965) are essentially confirmed, though the unit cell is slightly larger than reported previously (without s.u. values):  $a = 3.905$ ,  $b = 12.286$ ,  $c = 13.470\text{ \AA}$ ,  $\beta = 90.5^\circ$  and  $V = 646\text{ \AA}^3$ .



For the low-temperature results and the general discussion, see Batsanov (2004).

## Experimental

The crystals of (I) were grown by slow evaporation, at room temperature, of an aqueous solution of equimolar amounts of pyridine and nitric acid.



**Figure 1**

The molecular structure of (I) at 290 K. Displacement ellipsoids are drawn at the 50% probability level. The dashed and dotted lines indicate strong and weak hydrogen bonds, respectively.

## Crystal data

$C_5H_6N^+ \cdot NO_3^-$   
 $M_r = 142.12$   
 Monoclinic,  $P2_1/c$   
 $a = 3.9015$  (6) Å  
 $b = 12.324$  (2) Å  
 $c = 13.503$  (2) Å  
 $\beta = 90.57$  (1)°  
 $V = 649.2$  (2) Å<sup>3</sup>  
 $Z = 4$

## Data collection

Bruker APEX CCD area-detector  
 diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 5258 measured reflections  
 1154 independent reflections

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.050$   
 $wR(F^2) = 0.157$   
 $S = 1.04$   
 1154 reflections  
 95 parameters  
 H atoms treated by a mixture of  
 independent and constrained  
 refinement

$D_x = 1.454$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1107  
 reflections  
 $\theta = 2.2$ – $22.4$ °  
 $\mu = 0.12$  mm<sup>-1</sup>  
 $T = 290$  (2) K  
 Plate, colourless  
 $0.42 \times 0.37 \times 0.03$  mm

735 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.073$   
 $\theta_{max} = 25.0$ °  
 $h = -4 \rightarrow 4$   
 $k = -14 \rightarrow 14$   
 $l = -16 \rightarrow 16$

$w = 1/[\sigma^2(F_o^2) + (0.086P)^2 + 0.0078P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.003$   
 $\Delta\rho_{max} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.13$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

N1—C2	1.328 (4)	C5—C6	1.337 (4)
N1—C6	1.338 (4)	O1—N2	1.251 (2)
C2—C3	1.352 (4)	O2—N2	1.217 (3)
C3—C4	1.343 (4)	O3—N2	1.225 (3)
C4—C5	1.337 (4)		
C2—N1—C6	121.0 (2)	C5—C6—N1	119.5 (2)
N1—C2—C3	119.8 (2)	O2—N2—O3	122.1 (2)
C4—C3—C2	119.1 (2)	O2—N2—O1	119.5 (2)
C5—C4—C3	120.6 (2)	O3—N2—O1	118.4 (2)
C6—C5—C4	120.0 (2)		

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1 <sup>i</sup> ···O1	0.94 (4)	1.86 (4)	2.787 (3)	171 (3)
N1—H1 <sup>i</sup> ···O3	0.94 (4)	2.45 (4)	3.149 (3)	131 (3)
C2—H2 <sup>i</sup> ···O3	0.93	2.78	3.307 (4)	117
C2—H2 <sup>i</sup> ···O2 <sup>i</sup>	0.93	2.56	3.177 (3)	124
C3—H3 <sup>i</sup> ···O2 <sup>ii</sup>	0.93	2.67	3.324 (3)	128
C4—H4 <sup>i</sup> ···O3 <sup>iii</sup>	0.93	2.70	3.330 (3)	126
C5—H5 <sup>i</sup> ···O3 <sup>iii</sup>	0.93	2.77	3.365 (4)	123
C6—H6 <sup>i</sup> ···O1 <sup>iv</sup>	0.93	2.38	3.196 (3)	146
C6—H6 <sup>i</sup> ···O2 <sup>iv</sup>	0.93	2.68	3.456 (3)	141

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

All H atoms were located in a difference Fourier map. Atom H1 was refined in isotropic approximation [ $N-H = 0.94$  (4) Å], other H atoms were treated as riding in idealized positions, with  $C-H = 0.93$  Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ .

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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## References

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