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2,6-Dimethylpyridinium nitrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.077
Data-to-parameter ratio = 18.0

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

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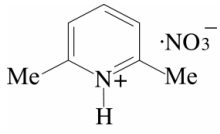
In the crystal structure of the title compound, $C_7H_{10}N^+\cdot NO_3^-$, the cations and anions are linked by N—H···O and C—H···O hydrogen bonds to form a supramolecular structure.

Comment

Crystal structures of a few 2,6-dimethylpyridinium complexes have been reported previously (Jin *et al.*, 2000; Pan *et al.*, 2001). We report here the structure of the title salt, (I), obtained from 2,6-dimethylpyridine and nitric acid.



(I)

The asymmetric unit of (I) consists of one 2,6-dimethylpyridinium cation and one nitrate anion linked by a N1—H1···O3 hydrogen bond and a C7—H7···O2 interaction (Fig. 1 and Table 2). In the crystal structure, the cations and anions are linked by a number of C—H···O interactions to form a network. Part of the network around a nitrate anion is shown in Fig. 2. In the network, the nitrate anion is arranged nearly parallel to two symmetry-related cations [dihedral angle 12.33 (6)°], but it is inclined to the other cation (N1/C1–C7) with a dihedral angle of 60.42 (3)°. The network is further stabilized by π–π-stacking interactions involving pyridinium rings at (*x*, *y*, *z*) and ($\frac{1}{2}-x$, $\frac{3}{2}-y$, $-z$), respectively, with a centroid–centroid separation of 3.558 (1) Å.

The bond lengths in (I) have normal values. In comparison with pyridine, the C—N—C angle in the pyridinium ring is usually widened. For example, the C—N—C angle in 2,6-dimethylpyridine (Bond *et al.*, 2001) is 119.0 (3)°, and 120° in its 1:1 complex with urea (Lee & Wallwork, 1965). In the 1:1 complex of 4-methylpyridine and pentachlorophenol, which has been crystallized as a salt at 80 K and a neutral adduct at 295 K, the C—N—C angles are 119.9 (2) and 118.0 (4)°, respectively (Malarski *et al.*, 1987, 1996). In the salts of 2,6-dimethylpyridinium hydrogen phthalate and 2,6-dimethylpyridinium fumarate (Jin *et al.*, 2000; Pan *et al.*, 2001), this angle is widened to 123.83 (2) and 123.92 (17)°, respectively. A similar feature is also observed in the title salt, with a C1—N1—C5 angle of 124.90 (13)°.

Experimental

2,6–Dimethylpyridine and aqueous nitric acid, in an equimolar ratio, were mixed together. Crystals of (I) formed in the resulting solution by slow evaporation for a month at 293 K.

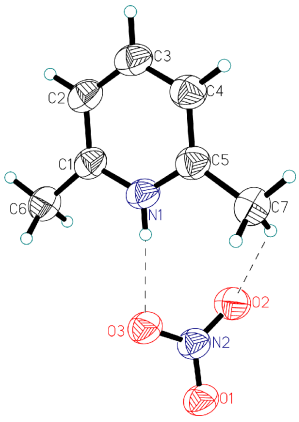


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

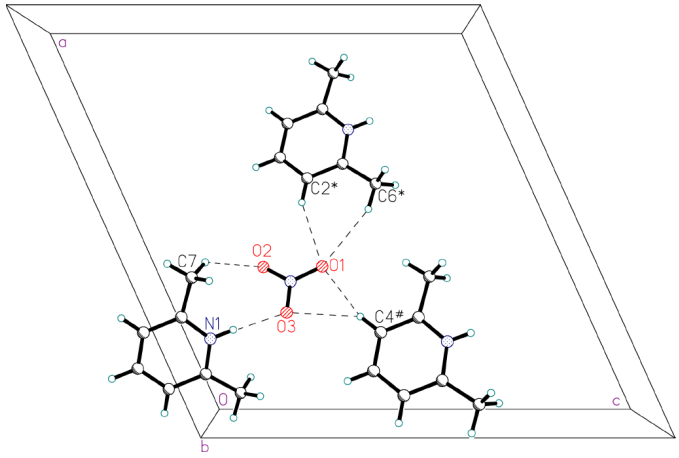


Figure 2
A view of the hydrogen bonding network around a nitrate anion. The symmetry code for atoms C2* and C6* is $(\frac{1}{2}+x, \frac{3}{2}-y, \frac{1}{2}+z)$ and that for C4# is $(x, 2-y, \frac{1}{2}+z)$.

Crystal data

$C_7H_{10}N^+\cdot NO_3^-$
$M_r = 170.17$
Monoclinic, $C2/c$
$a = 15.918$ (3) Å
$b = 7.560$ (1) Å
$c = 15.924$ (3) Å
$\beta = 114.26$ (1)°
$V = 1747.1$ (5) Å^3
$Z = 8$
$D_x = 1.294$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 782 reflections
$\theta = 2.8$–19.8°
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.3 × 0.2 × 0.2 mm

Data collection

Bruker SMART Apex CCD area-detector diffractometer
φ and ω scans
5170 measured reflections
2069 independent reflections
1091 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 28.1°$
$h = -13 \rightarrow 20$
$k = -9 \rightarrow 9$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.077$
$S = 0.86$
2069 reflections
115 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.07$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.3313 (16)	C5—N1	1.3271 (16)
C1—C2	1.3581 (17)	C5—C7	1.4747 (17)
C1—C6	1.4817 (18)	N2—O2	1.2107 (13)
C2—C3	1.3534 (19)	N2—O1	1.2176 (12)
C3—C4	1.3506 (18)	N2—O3	1.2342 (13)
C4—C5	1.3661 (17)		
N1—C1—C2	117.63 (14)	N1—C5—C7	118.23 (12)
N1—C1—C6	117.52 (12)	C4—C5—C7	124.53 (14)
C2—C1—C6	124.84 (13)	C5—N1—C1	124.90 (13)
N1—C5—C4	117.24 (14)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.827 (12)	1.912 (13)	2.7364 (17)	175.5 (11)
C2—H2···O1^{i}	0.93	2.51	3.3567 (19)	152
C4—H4···O1^{ii}	0.93	2.44	3.3438 (18)	165
C4—H4···O3^{ii}	0.93	2.54	3.3463 (18)	145
C6—H6B···O1^{i}	0.96	2.57	3.4700 (17)	156
C7—H7C···O2	0.96	2.58	3.3723 (16)	140

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

Atom H1 was located in a difference Fourier map and refined isotropically; all other H atoms were placed in calculated positions and allowed to ride on their parent atoms. A rotating group model was used for the methyl groups.

Data collection: *SMART* (Bruker, 2000); cell refinement: SMART; data reduction: *SAINT-Plus* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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