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Nicotinium nitrate monohydrate

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.137
Data-to-parameter ratio = 11.9

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

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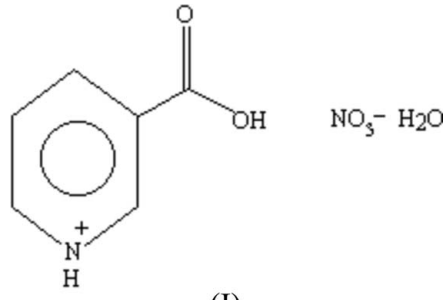
In the title compound, $C_6H_6NO_2^+\cdot NO_3^-\cdot H_2O$, the nicotinium cation is essentially planar. N—H···O, O—H···O and C—H···O hydrogen bonds link the molecules into layers parallel to the $(10\bar{1})$ plane.

Comment

Nicotinic acid (vitamin B3), known as niacin, is a lipid lowering agent widely used to treat hypertriglyceridemia by the inhibition of lipolysis in adipose tissue (Athimoolam & Rajaram, 2005). The nicotinic acid complex 5-methylpyrazine-2-carboxylic acid-4-oxide is a commonly used drug for the treatment of hypercholesterolemia (Lorenzen *et al.*, 2001). Coordination complexes of nicotinic acid with metals such as Sn possess antitumour activity greater than the well known *cis*-platin or doxorubicin (Gielen *et al.*, 1992). The enzyme nicotinic acid mononucleotide adenyltransferase is essential for the synthesis of nicotinamide adenine dinucleotide in all living cells and is a potential target for antibiotics (Kim *et al.*, 2004). As a part of our investigation of inorganic salts of nicotinic acid, we report here the crystal structure of nicotinium nitrate monohydrate, (I).



(I)

The asymetric unit of (I) contains a nicotinium cation, a nitrate anion and a water molecule (Fig. 1). Protonation of atom N1 of nicotine results in a widening of the C2—N1—C6 angle to 122.9 (3)°, compared with 118.9 (3)° in unprotonated nicotinic acid (Kutoglu & Scheringer, 1983). The nicotinium cation is essentially planar, with a maximum deviation from the mean plane of 0.048 (2) Å for atom O1.

The crystal packing is stabilized by N—H···O, O—H···O and C—H···O hydrogen bonds (Table 1), which link the molecules into layers parallel to the $(10\bar{1})$ plane (Fig. 2).

Experimental

Nitric acid was added dropwise to an aqueous solution of nicotinic acid, in stoichiometric amounts. The solution was heated at 323 K for

2 h. Colourless block-shaped crystals of (I) were obtained by slow evaporation over a period of one week.

Crystal data

$C_6H_6NO_2^+\cdot NO_3^-\cdot H_2O$
$M_r = 204.14$
Monoclinic, $P2_1/n$
$a = 6.6539\ (7)$ Å
$b = 12.3682\ (15)$ Å
$c = 10.1814\ (15)$ Å
$\beta = 100.967\ (7)^\circ$
$V = 822.59\ (18)$ Å^3
$Z = 4$
$D_x = 1.641$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.15$ mm^{-1}
$T = 120\ (2)$ K
Block, colourless
0.2 × 0.2 × 0.07 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.970$, $T_{max} = 0.990$
6153 measured reflections
1604 independent reflections
894 reflections with $I > 2\sigma(I)$
$R_{int} = 0.109$
$\theta_{max} = 26.1^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.137$
$S = 0.98$
1604 reflections
135 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ 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
N1—H1···O3^{i}	0.86	1.93	2.782 (3)	170
O1—H1A···O6	0.82	1.77	2.587 (3)	180
O6—H6A···O5	0.93 (5)	1.92 (5)	2.843 (3)	171 (4)
O6—H6B···O3^{ii}	0.88 (5)	1.96 (5)	2.825 (3)	173 (5)
C2—H2···O2^{iii}	0.93	2.43	3.173 (4)	137
C4—H4···O1^{iv}	0.93	2.46	3.262 (4)	144
C6—H6···O5^{i}	0.93	2.35	3.051 (4)	132
C6—H6···O4^{iv}	0.93	2.32	3.013 (4)	131

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

Water H atoms were located in a difference map and refined freely [O—H = 0.88 (5) and 0.93 (5) Å]. All other H atoms were placed in calculated positions, with C—H = 0.93 Å, O—H = 0.82 Å and N—H = 0.86 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C,N)$ and $1.5U_{eq}(O)$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

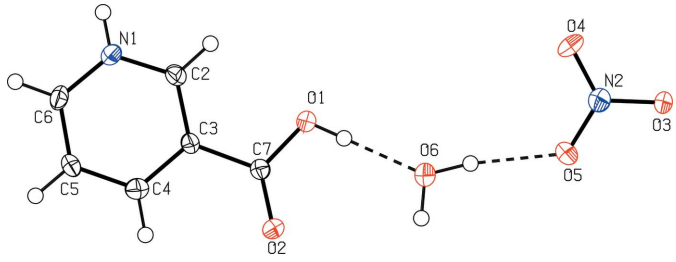


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme, with 50% probability displacement ellipsoids. Hydrogen bonds are drawn as dashed lines.

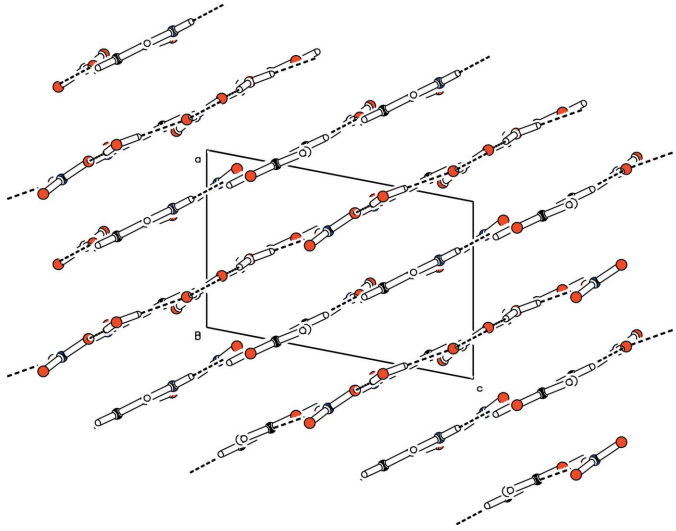


Figure 2
A packing diagram for (I), viewed down the *b* axis. Hydrogen bonds are drawn as dashed lines.

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