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(2-Pyridylmethyl)ammonium nitrate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.097
Data-to-parameter ratio = 15.0

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

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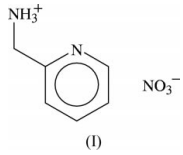
The single-crystal structure of (2-pyridylmethyl)ammonium nitrate, $C_6H_9N_2^+\cdot NO_3^-$, is presented, in what is only the third reported structure containing this cation. The structure contains extensively hydrogen-bonded layers.

Comment

During research into novel chelating ligands, the crystal structure of the title compound, (I), was determined (Fig. 1). The structure of the (2-pyridylmethyl)ammonium cation has only been determined twice previously, once in a silver nitrate complex (Sailaja *et al.*, 2001) and once as the pyridine-2-carboxylate salt (Døssing *et al.*, 2001). In both of these structures, four hydrogen bonds were formed from the ammonium group.



(I)

In (I), five hydrogen bonds are formed between the ammonium group and nitrate O atoms. These bonds, with D—H$\cdots A$ distances of between 2.8237 (19) and 3.110 (2) Å, are comparable with the bonds reported in the $AgNO_3$ complex, and cause the formation of a two-dimensional network with the b and c axes as the base vectors (Fig. 2).

Experimental

2-(Aminomethyl)pyridine (2.16 g, 0.02 mol) was dissolved in ethanol (5 ml) and added to a stirred ethanol solution of *o*-vanillin (3.04 g, 0.02 mol). The reaction mixture was stirred overnight. The solvent was removed using a rotary evaporator to give a red residue, which was recrystallized from the minimum amount of hot methanol, yielding good quality single crystals.

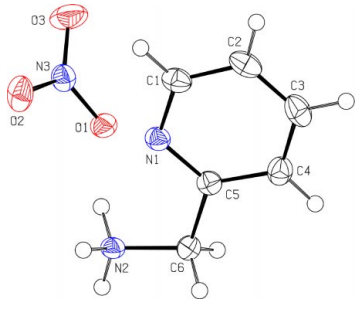


Figure 1
View of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

Crystal data

$C_6H_9N_2^+\cdot NO_3^-$
M_r = 171.16
Monoclinic, $P2_1/c$
a = 8.2492 (4) Å
b = 10.4014 (5) Å
c = 9.3850 (5) Å
β = 105.171 (4)°
V = 777.20 (7) Å^3
Z = 4
D_x = 1.463 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 59 reflections, based on ψ–χ scan (Duisenberg *et al.*, 2000)
θ = 5.5–20.8°
μ = 0.12 mm^{-1}
T = 150 (2) K
Block, colourless
0.2 × 0.1 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
18 148 measured reflections
1774 independent reflections
1228 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 27.4°
$h = -10 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.097
S = 1.05
1774 reflections
118 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.3509P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.958 (19)	2.155 (18)	2.8817 (19)	131.7 (15)
N2—H2A···N1^{i}	0.958 (19)	2.345 (18)	3.037 (2)	128.7 (13)
N2—H2B···O1^{ii}	0.925 (18)	1.931 (18)	2.8237 (19)	161.4 (16)
N2—H2B···O3^{ii}	0.925 (18)	2.440 (19)	3.110 (2)	129.3 (15)
N2—H2C···O1	0.942 (18)	1.923 (18)	2.8412 (18)	164.3 (16)

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

The aromatic H atoms were placed in geometrically idealized positions (C—H = 0.95 Å) and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C). The H atoms on the N atom were found in a difference electron-density map and refined with U_{iso} = 1.5U_{eq}(N).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EvalCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

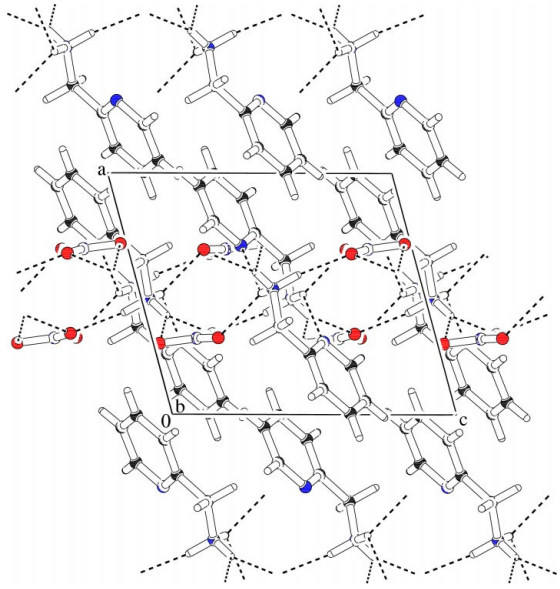


Figure 2
The two-dimensional network structure of (I). Hydrogen bonds are shown as dashed lines.

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