

## (2-Pyridylmethyl)ammonium nitrate

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## Key indicators

Single-crystal X-ray study

T = 150 K

Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$ 

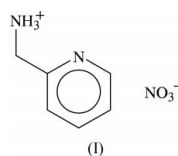
R factor = 0.043

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>.The single-crystal structure of (2-pyridylmethyl)ammonium nitrate,  $\text{C}_6\text{H}_9\text{N}_2^+\cdot\text{NO}_3^-$ , 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.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)  $\text{\AA}$ , are comparable with the bonds reported in the  $\text{AgNO}_3$  complex, and cause the formation of a two-dimensional network with the  $b$  and  $c$  axes as the base vectors (Fig. 2).

## Experimental

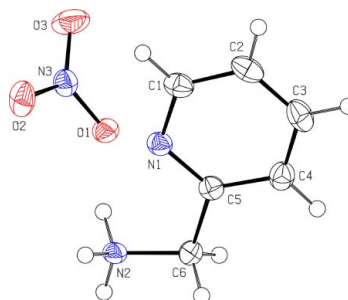
2-(Aminomethyl)pyridine (2.16 g, 0.02 mol) was dissolved in ethanol (5 ml) and added to a stirred ethanol solution of *o*-vanillin (3.04 g, 0.02 mol). The reaction mixture was stirred overnight. The solvent was removed using a rotary evaporator to give a red residue, which was recrystallized from the 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,  $P2_1/c$   
 $a = 8.2492(4) \text{ \AA}$   
 $b = 10.4014(5) \text{ \AA}$   
 $c = 9.3850(5) \text{ \AA}$   
 $\beta = 105.171(4)^\circ$   
 $V = 777.20(7) \text{ \AA}^3$   
 $Z = 4$   
 $D_x = 1.463 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 Cell parameters from 59  
 reflections, based on  $\psi$ - $\chi$  scan  
 (Duisenberg *et al.*, 2000)  
 $\theta = 5.5\text{--}20.8^\circ$   
 $\mu = 0.12 \text{ mm}^{-1}$   
 $T = 150(2) \text{ K}$   
 Block, colourless  
 $0.2 \times 0.1 \times 0.1 \text{ mm}$

## Data collection

Nonius KappaCCD diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: none  
 18 148 measured reflections  
 1774 independent reflections  
 1228 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.057$   
 $\theta_{\text{max}} = 27.4^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -13 \rightarrow 13$   
 $l = -12 \rightarrow 12$

## 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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$N2\text{--}H2A\cdots O2^i$	0.958 (19)	2.155 (18)	2.8817 (19)	131.7 (15)
$N2\text{--}H2A\cdots N1^i$	0.958 (19)	2.345 (18)	3.037 (2)	128.7 (13)
$N2\text{--}H2B\cdots O1^{ii}$	0.925 (18)	1.931 (18)	2.8237 (19)	161.4 (16)
$N2\text{--}H2B\cdots O3^{ii}$	0.925 (18)	2.440 (19)	3.110 (2)	129.3 (15)
$N2\text{--}H2C\cdots O1$	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 ( $C\text{--}H = 0.95 \text{ \AA}$ ) and constrained to ride on their parent atoms with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ . The H atoms on the N atom were found in a difference electron-density map and refined with  $U_{\text{iso}} = 1.5U_{\text{eq}}(N)$ .

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EvalCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS86* (Shel-

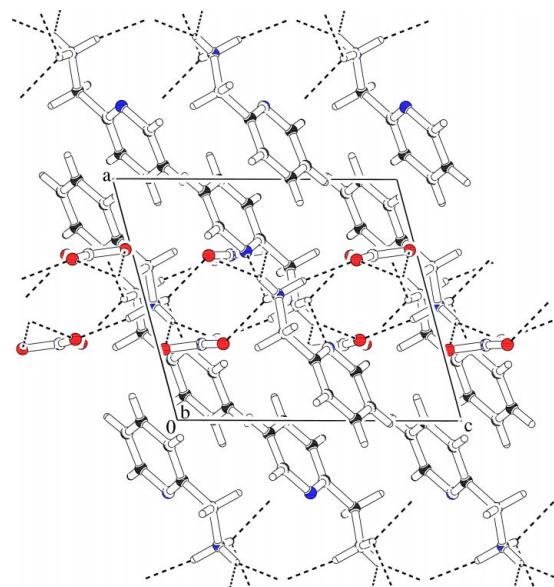


Figure 2

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

drick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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