(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.

The single-crystal structure of (2-pyridylmethyl)ammonium nitrate, C₈H₈N₂⁺NO₃⁻, 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 (Dossing 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...A distances of between 2.8237 (19) and 3.110 (2) Å, are comparable with the bonds reported in the AgNO₃ 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

C₆H₉N₂⁺NO₃⁻

Mr = 171.16
Monoclinic, P2₁/c

a = 8.2492 (4) Å
b = 10.4014 (5) Å
c = 9.3850 (5) Å
β = 105.171 (4)
V = 777.20 (7) Å³
Z = 4

Dₐ = 1.463 Mg m⁻³

Mo Kα radiation

Cell parameters from 59 reflections, based on ψ-φ scan

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

ψ and φ scans

Absorption correction: none

18 148 measured reflections

1774 independent reflections

1228 reflections with I > 2σ(I)

Refinement

Refinement on F²

R[F² > 2σ(F²)] = 0.043
wR² = 0.097
S = 1.05

1774 reflections

118 parameters

H atoms treated by a mixture of independent and constrained refinement

w = 1/[σ²(Fo²) + (0.0364P)² + 0.3509P]

where P = (Fo² + 2Fc²)/3

Δρmax = 0.19 e Å⁻³

Δρmin = −0.23 e Å⁻³

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(eq)(H) = 1.2Ueq(C). The H atoms on the N atom were found in a difference electron-density map and refined with Ueq(C) = 1.5Ueq(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 (Sheldrick, 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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References