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Anilinium nitrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.172
Data-to-parameter ratio = 22.2

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

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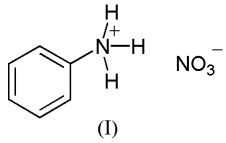
The crystal structure of anilinium nitrate, $C_6H_8N^+\cdot NO_3^-$, consists of alternating organic and inorganic layers. The organic layer contains the aromatic groups, and the inorganic layer is comprised of the ammonium groups and nitrate ions. A hydrogen-bonding network of N—H···O interactions is established in the inorganic layer.

Comment

The crystal structure of anilinium nitrate, (I), was determined as part of an ongoing study of the structural characteristics of organic–inorganic layered compounds. A related structure, that of benzylammonium nitrate ($C_7H_{10}N^+\cdot NO_3^-$), has been reported previously (Rademeyer, 2003).



(I)

One anilinium cation and one nitrate anion comprise the asymmetric unit of the title compound. The molecular structure of (I) and the atomic numbering used are shown in Fig. 1. As illustrated in Fig. 2, the crystal structure is comprised of alternating organic and inorganic layers, with the aromatic groups packing in the organic layer, and the ammonium groups and nitrate anions constituting the inorganic layer.

In the organic layer, aromatic groups are interdigitated and close to perpendicular to the layer plane, with the plane through the aromatic group (r.m.s. deviation 0.0035 Å) forming an angle of 88.31 (11)° with the layer plane. In the case of benzylammonium nitrate, the cations are tilted relative to the ionic layer. In (I), neighbouring pairs of anilinium cations pack in alternating opposite directions when viewed down the *b* axis (Fig. 2). No intermolecular π–π interactions are evident in the organic layer, and the shortest centroid-to-centroid distance between aromatic rings is 4.024 (2) Å. This

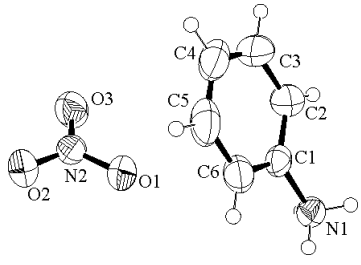


Figure 1
The molecular structure of (I), showing the atomic numbering scheme and displacement ellipsoids at the 50% probability level (*ORTEP*-3; Farrugia, 1997).

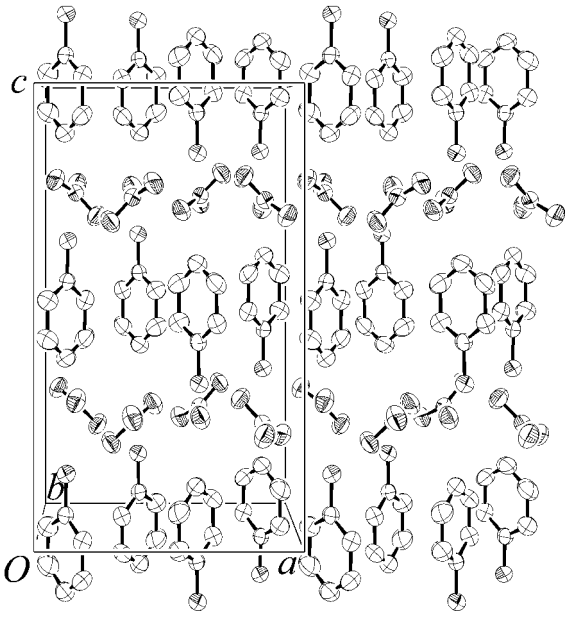


Figure 2
Packing diagram (*ORTEP*-3; Farrugia, 1997) for (I), viewed along the *b* axis. H atoms have been omitted for clarity.

distance is shorter than the value of 4.978 (5) Å found for benzylammonium nitrate.

In the inorganic layer, trigonal planar nitrate anions are tilted by 44.48 (6)° relative to the layer plane. A hydrogen-bonding network of N—H···O hydrogen bonds is established between ammonium groups and nitrate anions. This network extends in two dimensions in the inorganic layer, parallel to the *ab* plane. Atom N1 is hydrogen bonded to five O atoms in three different nitrate ions through one normal and four bifurcated hydrogen bonds. In the nitrate ion, N—O bond lengths differ significantly, with values of 1.232 (2) (N2—O2), 1.238 (2) (N2—O1) and 1.348 (2) Å (N2—O3). The N2—O3 bond, which is engaged in strong hydrogen bonding [H1*C*···O3 interaction of 1.81 (2) Å], is elongated. Hydrogen-bonding parameters are listed in Table 1, and the interactions are illustrated in Fig. 3. The same number and type of hydrogen-bonding interactions were observed in the benzylammonium structure.

Experimental

Anilinium nitrate was prepared by the dropwise addition of concentrated nitric acid (70%, Aldrich) to a solution of aniline (99%, Aldrich) in chloroform. The resulting precipitate was filtered. Good-quality single crystals were obtained by recrystallization from water at room temperature.

Crystal data

$C_6H_8N^+\cdot NO_3^-$
M_r = 156.14
Orthorhombic, *Pbca*
a = 9.255 (4) Å
b = 10.161 (4) Å
c = 16.188 (5) Å
V = 1522.4 (10) Å^3
Z = 8
D_x = 1.369 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 833 reflections
θ = 2–31°
μ = 0.11 mm^{-1}
T = 293 (2) K
Block, light brown
0.40 × 0.20 × 0.20 mm

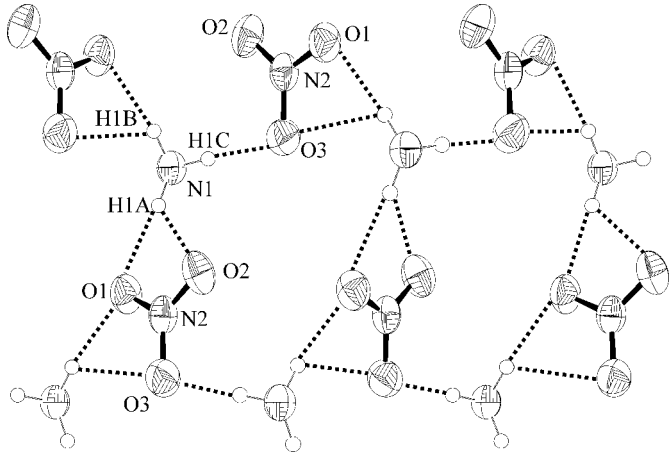


Figure 3
Hydrogen-bonding interactions (dashed lines) in the inorganic layer, viewed down the *c* axis (*ORTEP*3; Farrugia, 1997).

Data collection

Oxford Diffraction Excalibur2 diffractometer
ω–2θ scans
13 740 measured reflections
2485 independent reflections
1306 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 34.4°
$h = -13 \rightarrow 14$
$k = -13 \rightarrow 12$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.172
S = 1.06
2485 reflections
112 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0769P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.92 (2)	2.13 (2)	3.046 (2)	179 (2)
N1—H1A···O2^{i}	0.92 (2)	2.59 (2)	3.272 (2)	131 (2)
N1—H1C···O3^{ii}	0.88 (2)	1.81 (2)	2.689 (2)	177 (2)
N1—H1B···O1^{iii}	0.91 (2)	1.99 (2)	2.880 (2)	167 (2)
N1—H1B···O3^{iii}	0.91 (2)	2.50 (2)	3.036 (2)	118 (2)

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

H atoms bonded to C atoms were placed in calculated positions (C—H = 0.93 Å) and were refined using a riding model with U_{iso}(H) = 1.2U_{eq}(parent atom). For the ammonium group, H atoms were placed as observed in a Fourier map and refined. The N—H bond lengths lie in the range 0.88 (2)–0.92 (2) Å.

Data collection: *CrysAlisCCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlisCCD*; data reduction: *CrysAlisRED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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