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Hydrazinium nitrate

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(O–N) = 0.001 Å
R factor = 0.028
wR factor = 0.072
Data-to-parameter ratio = 11.0

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

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The monoprotonated hydrazinium cation in the title compound, $N_2H_5^+\cdot NO_3^-$, forms several types of hydrogen bonds. Stronger ones, in which the H atoms attached to the protonated N atom take part, link cations and anions into layers. Less strong hydrogen bonds, with participation of H atoms attached to the non-protonated N atom, link the layers into a three-dimensional structure. In addition to hydrogen bonds, short contacts of 2.8607 (10) Å have been found between O and N atoms of neighbouring nitrate anions. Such contacts can correspond to a weak intermolecular interaction similar to that in organic compounds containing nitro groups.

Comment

Hydrazine and its derivatives are widely used in various chemical technologies. X-ray structural data available for several inorganic salts of mono- and diprotonated hydrazine (Conant & Roof, 1970; Jönsson & Hamilton, 1970; Jönsson & Liminga, 1971; Klapötke *et al.*, 1996; Kvick *et al.*, 1972; Liminga, 1966; Liminga & Lundgren, 1965; Nitta *et al.*, 1951) show the importance of hydrogen bonding in the formation of their crystal structures. We present here the structure of hydrazinium nitrate, (I), having a three-dimensional system of hydrogen bonds.

$^+H_3N—NH_2$ NO_3^-
(I)

The principal bond lengths and bond angles in the title compound, (I), are given in Table 1. Fig. 1 shows a molecular view of the structure. Each H atom of the monoprotonated hydrazinium cation takes part in hydrogen bonding (Table 2). H atoms attached to the protonated N atom give strong

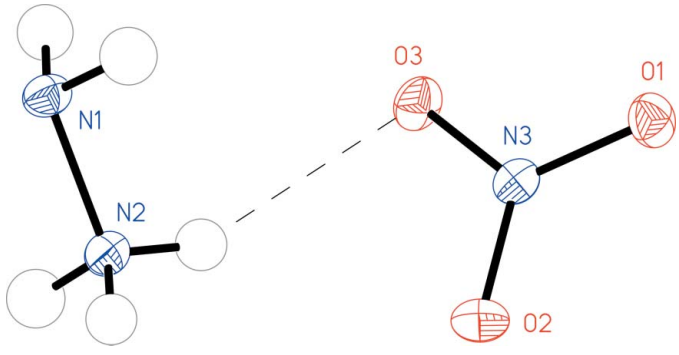

Figure 1
A view of $N_2H_5NO_3$, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. A dashed line indicates one hydrogen-bonding interaction.

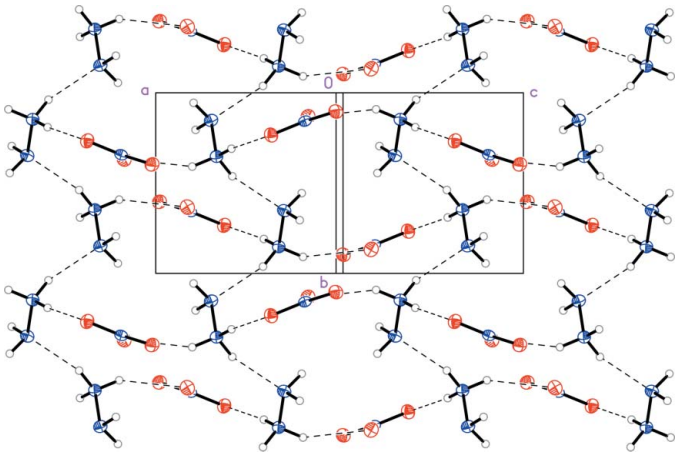

Figure 2
A net of stronger hydrogen bonds (dashed lines) in $N_2H_5NO_3$.

hydrogen bonds in which the acceptors are two O atoms of nitrate anions and the non-protonated N atom of a neighbouring cation. These hydrogen bonds link cations and anions into layers parallel to (101) (Fig. 2). Each of the smallest rings in these layers contains two nitrate anions and four hydrazinium cations. Less strong hydrogen bonds with participation of H atoms attached to the non-protonated N atom and O atoms of nitrate anions link the layers into a three-dimensional structure. In addition to hydrogen bonds, short contacts of 2.8607 (10) Å have been found between O and N atoms of neighbouring nitrate anions. Such contacts can correspond to a weak intermolecular interaction similar to that in organic compounds containing nitro groups (Platts *et al.*, 1995).

Experimental

For the preparation of (I), a stoichiometric amount of 14.7 *M* HNO_3 was added dropwise to pure hydrazine (5 ml) at 278 K. The pH of the resulting solution was about 4.5–5.0. The solution was kept at room temperature under a hood for slow evaporation of water. After two months, bulky colourless crystals were formed.

Crystal data

$N_2H_5^+\cdot NO_3^-$
M_r = 95.07
Monoclinic, $P2_1/n$
a = 7.9649 (4) Å
b = 5.6569 (3) Å
c = 8.1221 (3) Å
β = 91.340 (3)°
V = 365.85 (3) Å^3
Z = 4
D_x = 1.726 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2616 reflections
θ = 3.5–27.4°
μ = 0.17 mm^{-1}
T = 120 (2) K
Fragment, colourless
0.30 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: none
2616 measured reflections
824 independent reflections
772 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.4°
$h = -10 \rightarrow 9$
$k = -7 \rightarrow 6$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.072
S = 1.10
824 reflections
75 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 0.0639P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—N3	1.2558 (10)	O3—N3	1.2556 (10)
O2—N3	1.2516 (10)	N1—N2	1.4468 (11)
O2—N3—O3	120.10 (7)	O3—N3—O1	120.11 (7)
O2—N3—O1	119.79 (7)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.91 (2)	2.27 (1)	3.0657 (10)	145 (1)
N1—H2···O2^{ii}	0.90 (1)	2.21 (1)	3.0603 (11)	158 (1)
N2—H3···O1^{iii}	0.88 (1)	1.97 (1)	2.8386 (11)	173 (1)
N2—H4···O3	0.86 (1)	2.15 (1)	2.9245 (10)	150 (1)
N2—H5···N1^{iv}	0.89 (2)	2.04 (2)	2.8908 (11)	160 (1)

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

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

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