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2-Aminopyrimidinium nitrate

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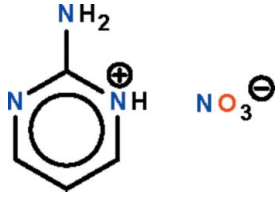
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.120; data-to-parameter ratio = 9.8.

In the title compound, $C_4H_6N_3^+\cdot NO_3^-$, the cation is coplanar with the anion (r.m.s. deviation = 0.048 Å), and links to the anion *via* an N—H···O hydrogen bond, forming an ion pair. In the crystal, adjacent ion pairs are further linked by N—H···O hydrogen bonds into linear chains running along the *b* axis.

Related literature

For the crystal structures of the 2-aminopyrimidinium salts of other mineral acids, see: Czupiński *et al.* (2005); Lee *et al.* (2003); Ye *et al.* (2002).



Experimental

Crystal data

$C_4H_6N_3^+\cdot NO_3^-$
M_r = 158.13
Monoclinic, $C2/c$
a = 12.632 (2) Å
b = 6.2160 (8) Å
c = 17.727 (2) Å
β = 99.009 (3)°
V = 1374.8 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.968, T_{max} = 0.981
5139 measured reflections
1210 independent reflections
823 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.120
S = 0.99
1210 reflections
124 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.87 (1)	1.87 (1)	2.742 (2)	177 (2)
N3—H11···O1	0.86 (1)	1.99 (1)	2.850 (3)	178 (2)
N3—H12···O2^{i}	0.85 (1)	2.05 (1)	2.901 (2)	178 (2)

Symmetry code: (i) $x, y-1, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2705).

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supplementary materials

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2-Aminopyrimidinium nitrate

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Experimental

To an aqueous solution of 2-aminopyrimidine (0.19 g, 2 mmol) was added chromium nitrate nonahydrate (0.80 g, 2 mmol). The pale green solution was set aside for several days. Colorless crystals of the organic salt were isolated.

Refinement

Carbon-bound H-atoms generated geometrically [C–H 0.93 Å, U(H) 1.2U_{eq}(C)]. The nitrogen-bound H-atoms were refined with a distance restraint of N–H 0.86±0.01 Å; their temperature factors were refined.

Figures

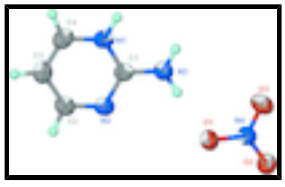

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $[C_4H_6N_4][NO_3]$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Aminopyrimidinium nitrate

Crystal data

$C_4H_6N_3^+\cdot NO_3^-$	F(000) = 656
M_r = 158.13	D_x = 1.528 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3773 reflections
a = 12.632 (2) Å	θ = 3.3–27.5°
b = 6.2160 (8) Å	μ = 0.13 mm^{-1}
c = 17.727 (2) Å	T = 293 K
β = 99.009 (3)°	Prism, colorless
V = 1374.8 (3) Å^3	0.25 × 0.20 × 0.15 mm
Z = 8	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	1210 independent reflections
Radiation source: fine-focus sealed tube	823 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.028

ω scan	θ_{max} = 25.0°, θ_{min} = 3.3°
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	h = −14→14
T_{min} = 0.968, T_{max} = 0.981	k = −7→7
5139 measured reflections	l = −21→20

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.039	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.120	H atoms treated by a mixture of independent and constrained refinement
S = 0.99	$w = 1/[\sigma^2(F_o^2) + (0.0773P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
1210 reflections	$(\Delta/\sigma)_{max}$ = 0.001
124 parameters	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
6 restraints	$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.61627 (16)	1.0844 (3)	0.47003 (8)	0.0892 (6)
O2	0.63012 (12)	1.3264 (2)	0.38605 (8)	0.0711 (5)
O3	0.61420 (14)	0.9926 (3)	0.35358 (9)	0.0797 (5)
N1	0.62478 (13)	0.3594 (3)	0.59174 (10)	0.0568 (5)
N2	0.62700 (13)	0.7155 (3)	0.63460 (9)	0.0575 (5)
N3	0.62544 (15)	0.6380 (3)	0.50731 (10)	0.0633 (5)
N4	0.62009 (13)	1.1341 (3)	0.40181 (9)	0.0560 (5)
C1	0.62639 (15)	0.5716 (3)	0.57800 (10)	0.0501 (5)
C2	0.62721 (17)	0.6376 (4)	0.70374 (12)	0.0616 (6)
C3	0.62702 (18)	0.4200 (4)	0.72104 (13)	0.0669 (6)
C4	0.62560 (17)	0.2810 (4)	0.66282 (13)	0.0638 (6)
H1	0.6222 (17)	0.268 (3)	0.5539 (10)	0.074 (7)*
H11	0.6213 (19)	0.7733 (19)	0.4964 (16)	0.083 (8)*
H12	0.6282 (16)	0.547 (3)	0.4718 (9)	0.068 (7)*
H2	0.6222 (18)	0.749 (3)	0.7401 (13)	0.079 (7)*
H3	0.628 (2)	0.378 (4)	0.7724 (10)	0.087 (7)*
H4	0.6234 (17)	0.130 (3)	0.6655 (12)	0.068 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1669 (17)	0.0547 (10)	0.0505 (9)	0.0094 (10)	0.0311 (9)	0.0031 (7)
O2	0.1061 (12)	0.0523 (10)	0.0576 (9)	−0.0043 (8)	0.0217 (8)	0.0025 (7)
O3	0.1178 (13)	0.0620 (11)	0.0620 (9)	−0.0010 (9)	0.0227 (8)	−0.0182 (8)

N1	0.0695 (11)	0.0435 (11)	0.0575 (10)	0.0026 (7)	0.0104 (8)	−0.0033 (8)
N2	0.0713 (11)	0.0478 (10)	0.0543 (9)	0.0030 (8)	0.0126 (8)	−0.0039 (8)
N3	0.0928 (13)	0.0486 (13)	0.0504 (10)	0.0032 (9)	0.0174 (9)	−0.0014 (8)
N4	0.0677 (10)	0.0512 (11)	0.0506 (10)	0.0046 (8)	0.0144 (8)	−0.0020 (8)
C1	0.0535 (11)	0.0447 (12)	0.0520 (10)	0.0022 (8)	0.0077 (8)	−0.0022 (8)
C2	0.0742 (14)	0.0584 (15)	0.0533 (12)	0.0030 (10)	0.0131 (10)	−0.0047 (10)
C3	0.0787 (15)	0.0674 (15)	0.0559 (12)	0.0022 (11)	0.0146 (11)	0.0062 (12)
C4	0.0736 (14)	0.0500 (14)	0.0676 (13)	0.0011 (10)	0.0104 (11)	0.0089 (11)

Geometric parameters (Å, °)

O1—N4	1.257 (2)	N3—C1	1.318 (3)
O2—N4	1.239 (2)	N3—H11	0.86 (1)
O3—N4	1.221 (2)	N3—H12	0.85 (1)
N1—C1	1.342 (2)	C2—C3	1.387 (3)
N1—C4	1.350 (3)	C2—H2	0.953 (16)
N1—H1	0.87 (1)	C3—C4	1.344 (3)
N2—C2	1.318 (3)	C3—H3	0.944 (17)
N2—C1	1.344 (2)	C4—H4	0.942 (16)
C1—N1—C4	121.76 (19)	N3—C1—N2	119.96 (19)
C1—N1—H1	119.8 (16)	N1—C1—N2	121.17 (18)
C4—N1—H1	118.4 (17)	N2—C2—C3	124.4 (2)
C2—N2—C1	116.65 (18)	N2—C2—H2	111.8 (15)
C1—N3—H11	120.6 (19)	C3—C2—H2	123.6 (15)
C1—N3—H12	120.0 (16)	C4—C3—C2	117.2 (2)
H11—N3—H12	119 (3)	C4—C3—H3	123.9 (16)
O3—N4—O2	122.31 (17)	C2—C3—H3	118.9 (15)
O3—N4—O1	119.30 (18)	C3—C4—N1	118.8 (2)
O2—N4—O1	118.39 (16)	C3—C4—H4	126.9 (13)
N3—C1—N1	118.86 (18)	N1—C4—H4	114.3 (13)
C4—N1—C1—N3	−179.98 (18)	C1—N2—C2—C3	0.1 (3)
C4—N1—C1—N2	−1.2 (3)	N2—C2—C3—C4	−0.6 (3)
C2—N2—C1—N3	179.55 (19)	C2—C3—C4—N1	0.2 (3)
C2—N2—C1—N1	0.8 (3)	C1—N1—C4—C3	0.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.87 (1)	1.87 (1)	2.742 (2)	177 (2)
N3—H11···O1	0.86 (1)	1.99 (1)	2.850 (3)	178 (2)
N3—H12···O2^{i}	0.85 (1)	2.05 (1)	2.901 (2)	178 (2)

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1