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2-Aminopyrimidinium nitrate

Xiao-Li Cheng,[a] Shan Gao[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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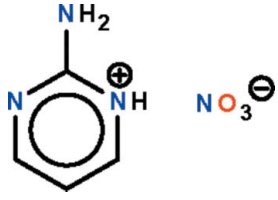
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.120; data-to-parameter ratio = 9.8.

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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supporting information

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S1. 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.

S2. 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.

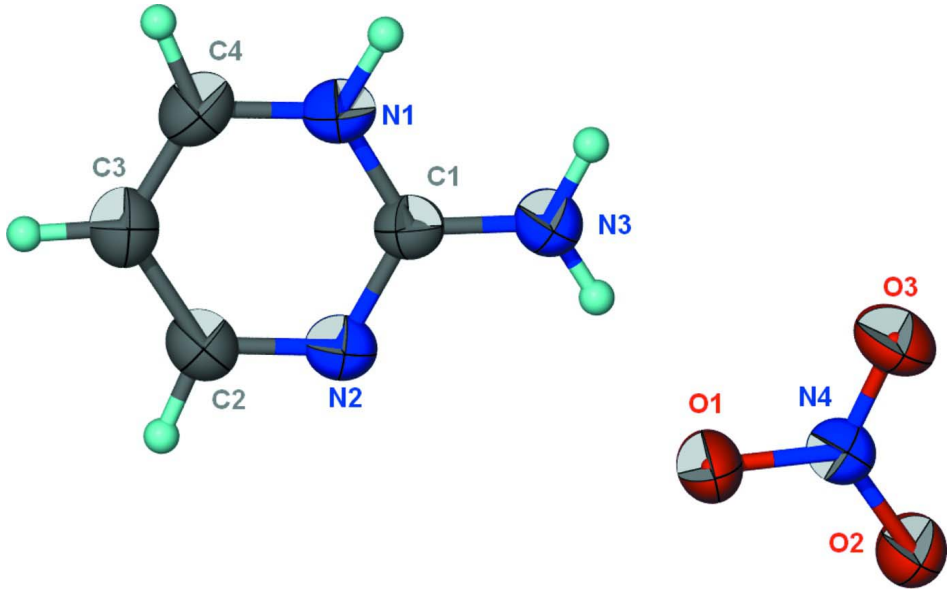

Figure 1

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

$C_4H_6N_3^+\cdot NO_3^-$
M_r = 158.13
Monoclinic, $C2/c$
Hall symbol: -C 2yc
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
F(000) = 656
D_x = 1.528 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3773 reflections

θ = 3.3–27.5°
μ = 0.13 mm^{-1}
T = 293 K

Prism, colorless
0.25 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
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
θ_{max} = 25.0°, θ_{min} = 3.3°
h = −14→14
k = −7→7
l = −21→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.120
S = 0.99
1210 reflections
124 parameters
6 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0773P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 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, º)

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, º)

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*.