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2,4-Diamino-6-methyl-1,3,5-triazin-1-ium nitrate

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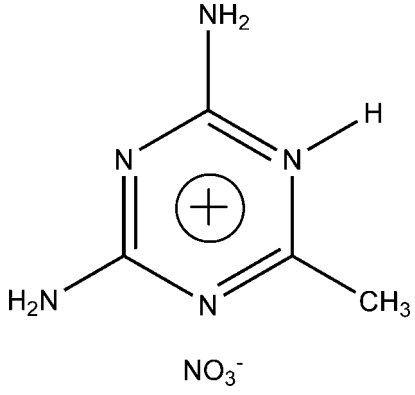
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.178; data-to-parameter ratio = 13.5.

In the title salt, $C_4H_8N_5^+\cdot NO_3^-$, a ring N atom of 2,6-diamino-4-methyltriazine is protonated. Each anion is connected to three neighbouring cations by multiple N—H···O hydrogen bonds which, together with N—H···N contacts, generate a layer structure.

Related literature

For 2,6-diamino-4-methyltriazine compounds, see: Kaczmarek *et al.* (2008); Perpétuo & Janczak (2007); Portalone & Colapietro (2007); Wijaya *et al.* (2004); Xiao (2008).



Experimental

Crystal data

$C_4H_8N_5^+\cdot NO_3^-$
M_r = 188.16
Monoclinic, $P2_1/n$
a = 7.667 (1) Å
b = 10.338 (2) Å
c = 9.977 (1) Å
β = 93.384 (2)°
V = 789.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 291 (2) K
0.13 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
4763 measured reflections
1867 independent reflections
1202 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.178
S = 1.00
1867 reflections
138 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3	0.88 (2)	2.62 (2)	3.414 (3)	150 (3)
N2—H2···O2	0.88 (2)	2.00 (3)	2.831 (3)	156 (3)
N4—H4D···O1^{i}	0.87 (2)	2.17 (2)	3.031 (3)	175 (2)
N4—H4E···N3^{ii}	0.87 (3)	2.24 (3)	3.105 (3)	177 (2)
N5—H5B···O3	0.90 (1)	2.20 (1)	3.083 (3)	167 (3)
N5—H5A···O3^{iii}	0.89 (1)	2.13 (1)	3.014 (3)	174 (3)
N5—H5A···O1^{iii}	0.89 (1)	2.49 (2)	3.046 (3)	121 (2)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2537).

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supporting information

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2,4-Diamino-6-methyl-1,3,5-triazin-1-ium nitrate

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S1. Comment

The crystal structures of 2,6-diamino-4-methayltriazine with methanol and ethanol solvates (Kaczmarek *et al.*, 2008; Xiao, 2008) and its trifluoroacetate, dimesylamide and hydrogenchlorate (Perpétuo & Janczak 2007; Wijaya *et al.*, 2004; Portalone *et al.*, 2007) have been reported in literature. In this paper, we report the X-ray single-crystal structure of 2,4-diamino-6-methyl-1,3,5-triazin-1-ium nitrate (I).

The molecular structure of (I) is illustrated in Fig. 1. The bond distances and bond angles are similar to those reported structures. All the non-hydrogen atoms of cations and nitrate anions are coplanar with the mean deviation from least-squares plane is 0.0745 (3) Å. The proton is suggested to be delocalized within the aromatic ring although it is added to one of the nitrogen atoms. The molecules of (I) form a layer structure where intermolecular N—H···O, N—H···N hydrogen bonds are found between adjacent molecules (Table 1). Every nitrate is connected with three neighboring cations by multiple N—H···O hydrogen contacts (Fig. 2).

S2. Experimental

Experimental The title compound was obtained as a by-product from the reaction between $CuNO_3.3H_2O$ (180 mg, 1.0 mmol) and 2,6-diamino-4-methayltriazine (935 mg, 5.0 mmol) in methanol (30 ml). Colourless crystals of (I) were obtained by slow evaporation of the mother liquid at room temperature in air after one week. Anal.Calcd. for $C_4H_8N_6O_3$: C: 25.55; H: 4.29; N: 44.67%. Found: C: 25.45; H: 4.34; N: 44.56%. Main FT—IR absorptions (KBr, cm^{-1}): 3384 (b, s), 2396 (*m*), 1763 (*m*), 1624 (*s*), 1384 (*s*), 825 (*m*), and 456 (*m*).

S3. Refinement

The methyl H atoms were placed in geometrically idealized positions and refined as riding, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). The H atoms bonded to the N atoms were located in the difference synthesis. Four restraints are used to restrain the bond lengths of N2—H2, N4—H4D, N5—H5A and N5—H5B in order to give similar N—H distances. In addition, one restraint is used to restrain the distance of atoms N1 and H5A so that it is simiar to that between atoms N1 and H4D.

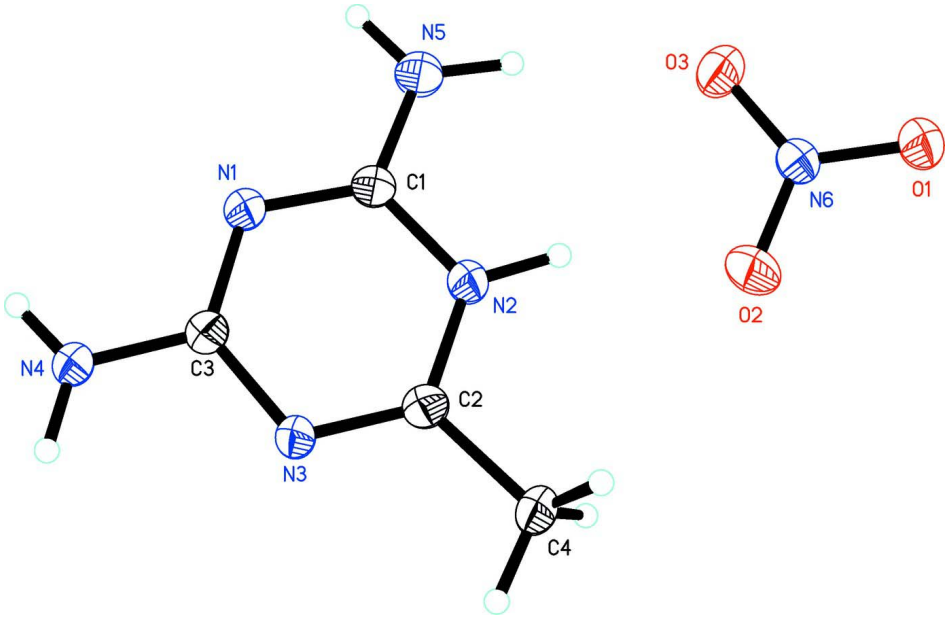

Figure 1

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

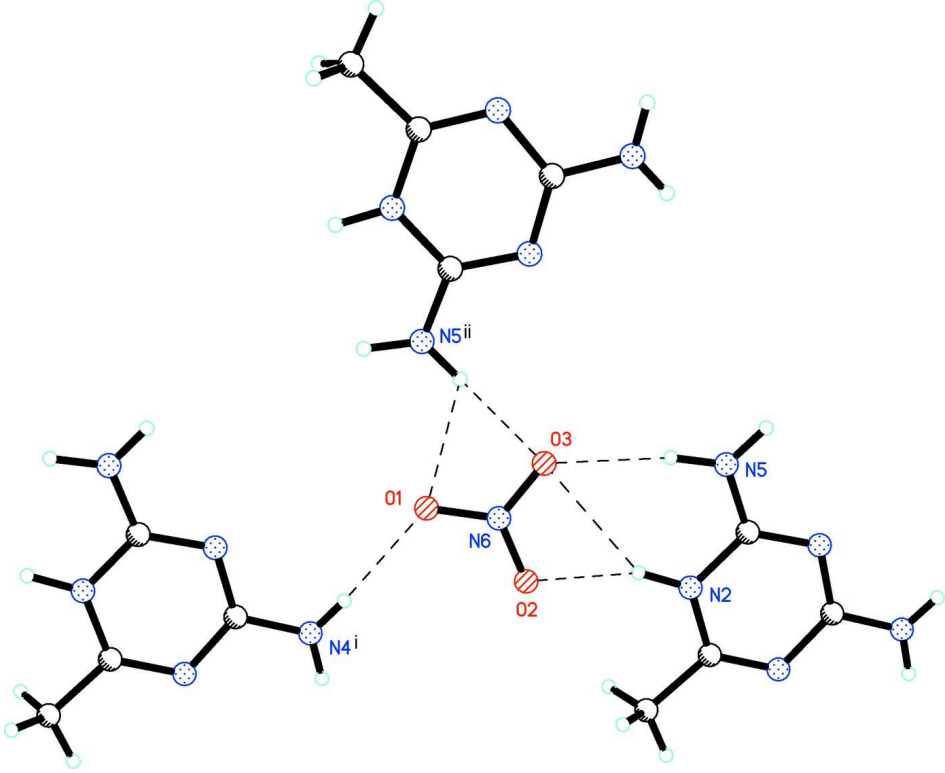

Figure 2

Perspective view of the hydrogen bonding interactions related to every nitrate anion where the hydrogen bonds are shown as dashed lines. [Symmetry codes: (i) *x*, *y*-1, *z*; (ii) -*x*-1/2, *y*-1/2, -*z*+3/2.]

2,4-Diamino-6-methyl-1,3,5-triazin-1-ium nitrate

Crystal data

$C_4H_8N_5^+ \cdot NO_3^-$
$M_r = 188.16$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.667$ (1) Å
$b = 10.338$ (2) Å
$c = 9.977$ (1) Å
$\beta = 93.384$ (2)°
$V = 789.4$ (2) Å^3
$Z = 4$
$F(000) = 392$
$D_x = 1.583$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1324 reflections
$\theta = 2.8$–26.0°
$\mu = 0.14$ mm^{-1}
$T = 291$ K
Block, colourless
0.13 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
4763 measured reflections
1867 independent reflections
1202 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.8°$
$h = -8 \rightarrow 10$
$k = -12 \rightarrow 13$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.178$
$S = 1.00$
1867 reflections
138 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.106P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Special details

Experimental. The structure was solved by direct methods (Bruker, 2000) and successive difference Fourier syntheses.
Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.0367 (3)	0.2000 (2)	0.8411 (2)	0.0350 (5)
C2	0.3207 (3)	0.2520 (2)	0.9243 (2)	0.0368 (5)
C3	0.2268 (3)	0.0451 (2)	0.9114 (2)	0.0340 (5)

C4	0.4496 (3)	0.3560 (2)	0.9556 (3)	0.0488 (6)
H4A	0.5589	0.3183	0.9872	0.073*
H4B	0.4074	0.4113	1.0239	0.073*
H4C	0.4661	0.4057	0.8761	0.073*
H2	0.129 (4)	0.372 (2)	0.858 (3)	0.067 (9)*
H4D	0.189 (3)	−0.137 (2)	0.909 (2)	0.034 (6)*
H4E	0.371 (4)	−0.096 (2)	0.965 (3)	0.044 (7)*
N1	0.0678 (2)	0.07622 (17)	0.85890 (19)	0.0366 (5)
N2	0.1626 (2)	0.29135 (19)	0.87137 (19)	0.0373 (5)
N3	0.3580 (2)	0.13121 (17)	0.94713 (19)	0.0358 (5)
N4	0.2668 (3)	−0.07814 (18)	0.9311 (2)	0.0415 (5)
N5	−0.1161 (3)	0.2428 (2)	0.7917 (2)	0.0484 (6)
H5A	−0.193 (3)	0.1810 (18)	0.771 (3)	0.082 (9)*
H5B	−0.131 (4)	0.3288 (11)	0.783 (3)	0.066 (9)*
N6	0.0038 (2)	0.61218 (18)	0.84158 (19)	0.0391 (5)
O1	−0.0186 (2)	0.73101 (16)	0.84536 (19)	0.0515 (5)
O2	0.1471 (2)	0.56484 (18)	0.8772 (2)	0.0582 (6)
O3	−0.1190 (3)	0.54094 (17)	0.7991 (2)	0.0596 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0308 (11)	0.0347 (12)	0.0391 (11)	0.0002 (8)	−0.0019 (8)	0.0011 (9)
C2	0.0326 (12)	0.0345 (12)	0.0426 (12)	−0.0011 (9)	−0.0030 (9)	−0.0022 (9)
C3	0.0316 (11)	0.0309 (11)	0.0394 (11)	−0.0013 (8)	0.0010 (9)	−0.0007 (8)
C4	0.0425 (14)	0.0299 (12)	0.0722 (16)	−0.0060 (9)	−0.0120 (12)	−0.0034 (11)
N1	0.0307 (10)	0.0306 (10)	0.0478 (11)	−0.0016 (7)	−0.0035 (8)	0.0007 (8)
N2	0.0337 (10)	0.0280 (10)	0.0493 (11)	0.0009 (7)	−0.0056 (8)	0.0022 (8)
N3	0.0315 (10)	0.0263 (9)	0.0488 (11)	−0.0008 (7)	−0.0054 (8)	−0.0018 (7)
N4	0.0322 (11)	0.0284 (11)	0.0629 (13)	−0.0031 (8)	−0.0070 (9)	0.0015 (8)
N5	0.0351 (11)	0.0422 (13)	0.0661 (13)	0.0015 (9)	−0.0122 (9)	0.0049 (10)
N6	0.0357 (11)	0.0339 (10)	0.0474 (11)	0.0038 (8)	−0.0007 (8)	0.0017 (8)
O1	0.0459 (10)	0.0359 (10)	0.0719 (12)	0.0047 (7)	−0.0045 (8)	−0.0026 (8)
O2	0.0414 (11)	0.0514 (12)	0.0796 (14)	0.0133 (8)	−0.0134 (9)	0.0030 (9)
O3	0.0468 (11)	0.0408 (10)	0.0896 (14)	−0.0073 (8)	−0.0107 (10)	−0.0001 (9)

Geometric parameters (Å, º)

C1—N1	1.311 (3)	C4—H4B	0.9600
C1—N5	1.321 (3)	C4—H4C	0.9600
C1—N2	1.371 (3)	N2—H2	0.88 (2)
C2—N3	1.298 (3)	N4—H4D	0.87 (2)
C2—N2	1.356 (3)	N4—H4E	0.87 (3)
C2—C4	1.481 (3)	N5—H5A	0.888 (10)
C3—N4	1.322 (3)	N5—H5B	0.900 (10)
C3—N1	1.337 (3)	N6—O2	1.236 (2)
C3—N3	1.375 (3)	N6—O1	1.241 (2)
C4—H4A	0.9600	N6—O3	1.249 (3)

N1—C1—N5	121.8 (2)	C1—N1—C3	116.22 (18)
N1—C1—N2	121.5 (2)	C2—N2—C1	118.7 (2)
N5—C1—N2	116.6 (2)	C2—N2—H2	126 (2)
N3—C2—N2	122.7 (2)	C1—N2—H2	115 (2)
N3—C2—C4	121.6 (2)	C2—N3—C3	115.26 (18)
N2—C2—C4	115.7 (2)	C3—N4—H4D	119.0 (17)
N4—C3—N1	119.2 (2)	C3—N4—H4E	117.7 (17)
N4—C3—N3	115.2 (2)	H4D—N4—H4E	123 (2)
N1—C3—N3	125.6 (2)	C1—N5—H5A	114.3 (16)
C2—C4—H4A	109.5	C1—N5—H5B	118 (2)
C2—C4—H4B	109.5	H5A—N5—H5B	128 (3)
H4A—C4—H4B	109.5	O2—N6—O1	120.34 (19)
C2—C4—H4C	109.5	O2—N6—O3	120.2 (2)
H4A—C4—H4C	109.5	O1—N6—O3	119.42 (18)
H4B—C4—H4C	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3	0.88 (2)	2.62 (2)	3.414 (3)	150 (3)
N2—H2···O2	0.88 (2)	2.00 (3)	2.831 (3)	156 (3)
N4—H4*D*···O1^{i}	0.87 (2)	2.17 (2)	3.031 (3)	175 (2)
N4—H4*E*···N3^{ii}	0.87 (3)	2.24 (3)	3.105 (3)	177 (2)
N5—H5*B*···O3	0.90 (1)	2.20 (1)	3.083 (3)	167 (3)
N5—H5*A*···O3^{iii}	0.89 (1)	2.13 (1)	3.014 (3)	174 (3)
N5—H5*A*···O1^{iii}	0.89 (1)	2.49 (2)	3.046 (3)	121 (2)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1, −*y*, −*z*+2; (iii) −*x*−1/2, *y*−1/2, −*z*+3/2.