Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-3-carboxypyrazin-1-ium nitrate monohydrate

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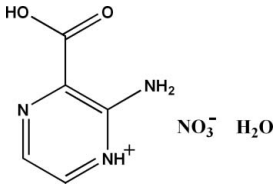
Received 18 January 2011; accepted 24 January 2011

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 13.8.

In crystal structure of the title compound, $C_5H_6N_3O_2^+\cdot NO_3^-\cdot H_2O$, intermolecular N—H···O, O—H···N and O—H···O hydrogen bonds link the cations, anions and water molecules into ribbons extending in [$\bar{1}$10]. Weak intermolecular C—H···O hydrogen bonds further link these ribbons into sheets parallel to ($\bar{1}\bar{1}$3).

Related literature

For similar compounds, see: Berrah *et al.* (2005*a*,*b*); Bouacida *et al.* (2005, 2009); Dobson & Gerkin (1996). For hydrogen-bond graph-set motifs, see: Etter *et al.* (1990); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_5H_6N_3O_2^+\cdot NO_3^-\cdot H_2O$
M_r = 220.15
Triclinic, $P\bar{1}$
a = 5.1277 (4) Å
b = 7.6368 (6) Å
c = 12.1571 (10) Å
α = 97.872 (3)°
β = 100.588 (3)°
γ = 106.194 (3)°
V = 440.37 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 150 K
0.58 × 0.49 × 0.42 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.773, T_{max} = 0.938
5333 measured reflections
1967 independent reflections
1693 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.03
1967 reflections
143 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1W^{i}	0.84	1.69	2.5233 (17)	168
O1W—H1W···O5^{ii}	0.80 (3)	1.93 (3)	2.7152 (18)	167 (3)
O1W—H2W···O1	0.88 (3)	2.39 (3)	2.8825 (19)	116 (2)
O1W—H2W···N4	0.88 (3)	1.99 (3)	2.8566 (18)	170 (2)
N2—H2A···O5	0.88	2.01	2.8549 (17)	161
N2—H2B···O2	0.88	2.08	2.7163 (17)	128
N2—H2B···O2^{iii}	0.88	2.20	2.9125 (18)	137
N3—H3···O4	0.88	1.91	2.7825 (16)	174
C4—H4A···O4^{iv}	0.95	2.24	3.1818 (17)	169

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

Data collection: *APEX2* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick,2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We are grateful to the LCATM Laboratory, Université Larbi Ben M'Hidi, Oum El Bouaghi, Algeria, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5043).

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supporting information

Acta Cryst. (2011). E**67**, o525–o526 [doi:10.1107/S1600536811003126]

2-Amino-3-carboxypyrazin-1-ium nitrate monohydrate

Fadila Berrah, Amira Ouakkaf, Sofiane Bouacida and Thierry Roisnel

S1. Comment

As a part of our search for new hybrid compounds based on protonated amines (Berrah *et al.* 2005*a,b*; Bouacida *et al.* 2005; 2009), we present the crystal structure of the title compound, (I).

The asymmetric unit of (I) contains one cation, one anion and one water molecule linked trough hydrogen bonds (Fig. 1). Bond distances and angles are similar to those encountered in analogous compounds (Berrah *el al.* 2005*a,b*; Dobson & Gerkin, 1996).

The crystal packing in the title structure can be described by considering sheets parallel to (-1-13) plane (Fig. 2). A sheet is an alternation of ribbons joined by a weak hyrogen bonds C4—H4···O4 and extended in direction [-110] (Fig. 2, Table 1). 3-Amino-pyrazinium 2-carboxylic acid cations, of the same ribbon, form centrosymetric dimers *via* N2—H2B···O2 hyrogen bonds. Each dimer is surrounded by two NO_3^- anions and four H_2O molecules, and all its atoms (except C5) are involved in N—H···O, O—H···N and O—H···O H-bonds. While nitrate anions are only acceptor of H-bonds, water molecules are at the same time donor and acceptor (Table 1). The resulting 2D hydrogen-bonded network exhibit rings with $R_4^4(8)$, $R_2^4(10)$, $R_2^2(8)$, $R_3^3(10)$, $R_2^2(4)$ and $R_2^1(5)$ graph set motifs (Etter *et al.*, 1990; Bernstein *et al.*, 1995) (Fig. 2).

S2. Experimental

The title compound was synthesized by reacting 3-amino-pyrazine 2- carboxylic acid with some excess of nitric acid in aqueous solution. Slow evaporation leads to well crystallized yellow needles.

S3. Refinement

H atoms of water molecule were located in difference Fourier map and included in the subsequent refinement with $U_{iso}(H) = 1.5U_{eq}(O)$. The remaining H atoms were localized on Fourier maps but introduced in calculated positions and treated as riding on their parent atoms, with C—H = 0.95 Å, O—H = 0.84 Å and N—H = 0.88 Å, and with $U_{iso}(H) = 1.2$ U_{eq}(C or N) and U_{iso}(H = 1.5 U_{eq}(O).

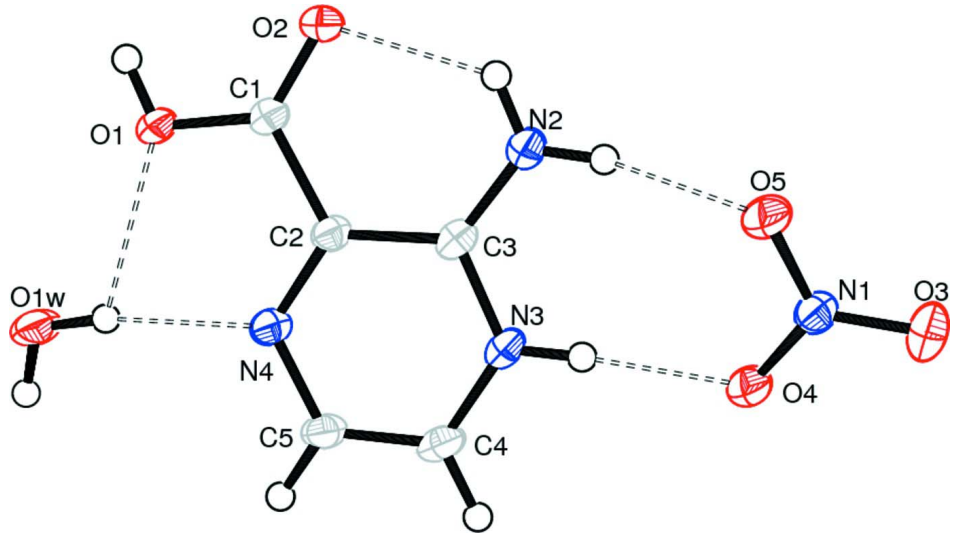

Figure 1

Ortep-3 (Farrugia, 1997) view of (I) showing the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

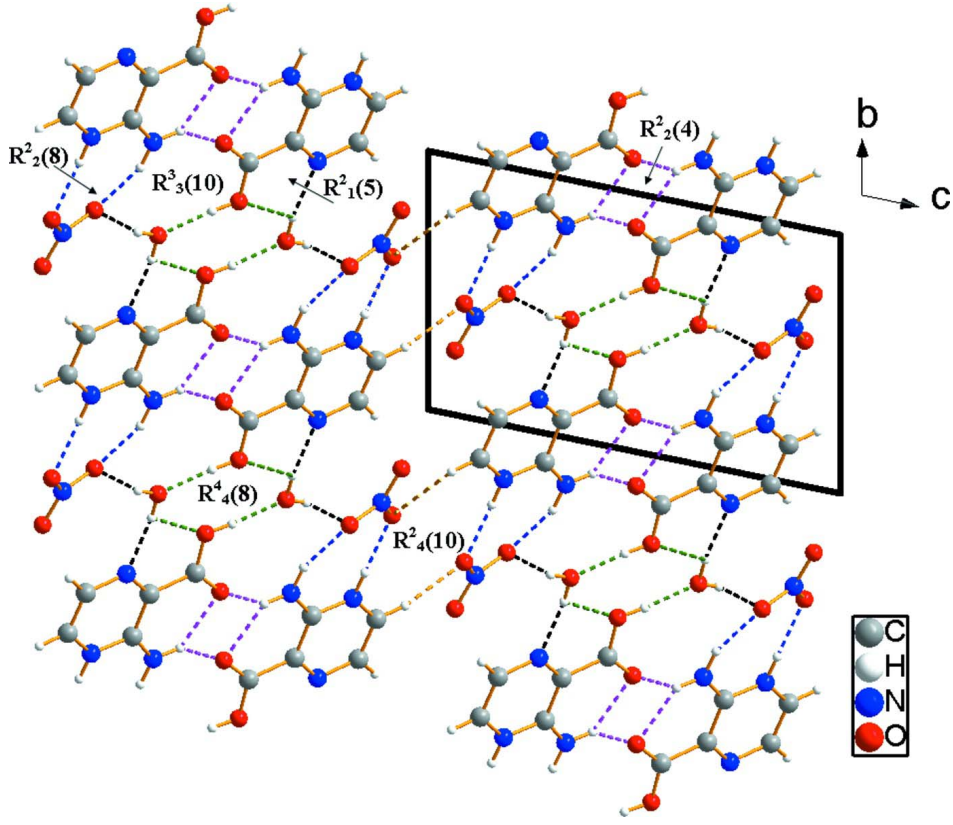

Figure 2

DIAMOND (Brandenburg & Berndt, 2001) view of a portion of hydrogen-bonded sheet in (I) showing the graph set motif notations. Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_5H_6N_3O_2^+ \cdot NO_3^- \cdot H_2O$
$M_r = 220.15$
Triclinic, $P\overline{1}$
$a = 5.1277$ (4) Å
$b = 7.6368$ (6) Å
$c = 12.1571$ (10) Å
$\alpha = 97.872$ (3)°
$\beta = 100.588$ (3)°
$\gamma = 106.194$ (3)°
$V = 440.37$ (6) Å^3
$Z = 2$
$F(000) = 228$
$D_x = 1.66$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2815 reflections
$\theta = 2.8$–$27.5°$
$\mu = 0.15$ mm^{-1}
$T = 150$ K
Prism, yellow
0.58 × 0.49 × 0.42 mm

Data collection

Bruker APEXII diffractometer
Graphite monochromator
CCD rotation images, thin slices scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min} = 0.773$, $T_{max} = 0.938$
5333 measured reflections
1967 independent reflections
1693 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.097$
$S = 1.03$
1967 reflections
143 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.1681P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

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	0.3536 (3)	0.81463 (18)	0.56444 (11)	0.0213 (3)
C2	0.5373 (3)	0.93343 (17)	0.67594 (11)	0.0196 (3)
C3	0.5053 (3)	1.11068 (18)	0.71720 (11)	0.0206 (3)

C4	0.8826 (3)	1.14836 (19)	0.87398 (11)	0.0243 (3)
H4A	1.0058	1.2218	0.9434	0.029*
C5	0.9034 (3)	0.97938 (19)	0.83049 (11)	0.0239 (3)
H5	1.0420	0.9354	0.8702	0.029*
N1	0.4633 (3)	1.60420 (16)	0.88650 (10)	0.0226 (3)
N2	0.3198 (3)	1.18108 (16)	0.66687 (11)	0.0270 (3)
H2A	0.3137	1.2905	0.6980	0.032*
H2B	0.2019	1.1188	0.6021	0.032*
N3	0.6850 (2)	1.20958 (15)	0.81712 (10)	0.0228 (3)
H3	0.6719	1.3181	0.8460	0.027*
N4	0.7294 (2)	0.87393 (15)	0.73168 (9)	0.0219 (3)
O1	0.3992 (2)	0.65591 (14)	0.54062 (9)	0.0303 (3)
H1	0.3004	0.5977	0.4759	0.045*
O2	0.1873 (2)	0.86840 (14)	0.50431 (9)	0.0288 (3)
O3	0.4414 (2)	1.75010 (14)	0.93506 (9)	0.0326 (3)
O4	0.6850 (2)	1.56230 (14)	0.91237 (9)	0.0279 (3)
O5	0.2640 (2)	1.49165 (15)	0.80957 (9)	0.0337 (3)
O1W	0.8473 (3)	0.53972 (18)	0.65527 (11)	0.0490 (4)
H1W	0.979 (6)	0.543 (4)	0.704 (3)	0.074*
H2W	0.793 (6)	0.637 (4)	0.671 (2)	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0231 (6)	0.0211 (6)	0.0170 (6)	0.0071 (5)	0.0009 (5)	0.0001 (5)
C2	0.0215 (6)	0.0196 (6)	0.0156 (6)	0.0051 (5)	0.0021 (5)	0.0017 (5)
C3	0.0209 (6)	0.0205 (6)	0.0174 (6)	0.0035 (5)	0.0043 (5)	−0.0001 (5)
C4	0.0246 (7)	0.0254 (7)	0.0157 (6)	0.0011 (5)	0.0002 (5)	0.0009 (5)
C5	0.0236 (7)	0.0255 (7)	0.0178 (6)	0.0050 (5)	−0.0014 (5)	0.0029 (5)
N1	0.0265 (6)	0.0208 (5)	0.0185 (6)	0.0066 (5)	0.0036 (5)	0.0014 (4)
N2	0.0284 (6)	0.0234 (6)	0.0255 (6)	0.0119 (5)	−0.0023 (5)	−0.0038 (5)
N3	0.0253 (6)	0.0195 (5)	0.0189 (6)	0.0049 (5)	0.0017 (5)	−0.0029 (4)
N4	0.0242 (6)	0.0212 (5)	0.0173 (6)	0.0055 (5)	0.0011 (4)	0.0023 (4)
O1	0.0380 (6)	0.0252 (5)	0.0214 (5)	0.0159 (4)	−0.0088 (4)	−0.0075 (4)
O2	0.0300 (5)	0.0276 (5)	0.0243 (5)	0.0135 (4)	−0.0071 (4)	−0.0016 (4)
O3	0.0406 (6)	0.0231 (5)	0.0337 (6)	0.0116 (5)	0.0108 (5)	−0.0023 (4)
O4	0.0256 (5)	0.0275 (5)	0.0250 (5)	0.0093 (4)	−0.0031 (4)	−0.0030 (4)
O1W	0.0619 (9)	0.0472 (7)	0.0308 (6)	0.0396 (7)	−0.0220 (6)	−0.0188 (5)
O5	0.0284 (6)	0.0316 (6)	0.0316 (6)	0.0109 (4)	−0.0085 (4)	−0.0070 (4)

Geometric parameters (Å, º)

C1—O2	1.2162 (17)	C5—H5	0.9500
C1—O1	1.3017 (16)	N1—O3	1.2314 (14)
C1—C2	1.5050 (18)	N1—O4	1.2621 (15)
C2—N4	1.3132 (17)	N1—O5	1.2635 (15)
C2—C3	1.4420 (17)	N2—H2A	0.8800
C3—N2	1.3150 (18)	N2—H2B	0.8800

C3—N3	1.3580 (17)	N3—H3	0.8800
C4—N3	1.3488 (18)	O1—H1	0.8400
C4—C5	1.3663 (19)	O1W—H1W	0.81 (3)
C4—H4A	0.9500	O1W—H2W	0.88 (3)
C5—N4	1.3520 (17)		

O2—C1—O1	125.51 (12)	C4—C5—H5	119.6
O2—C1—C2	121.65 (11)	O3—N1—O4	121.00 (12)
O1—C1—C2	112.82 (12)	O3—N1—O5	120.97 (12)
N4—C2—C3	121.68 (12)	O4—N1—O5	118.02 (11)
N4—C2—C1	118.46 (11)	C3—N2—H2A	120.0
C3—C2—C1	119.83 (12)	C3—N2—H2B	120.0
N2—C3—N3	118.84 (12)	H2A—N2—H2B	120.0
N2—C3—C2	125.70 (12)	C4—N3—C3	122.72 (11)
N3—C3—C2	115.46 (12)	C4—N3—H3	118.6
N3—C4—C5	119.16 (12)	C3—N3—H3	118.6
N3—C4—H4A	120.4	C2—N4—C5	120.09 (11)
C5—C4—H4A	120.4	C1—O1—H1	109.5
N4—C5—C4	120.89 (13)	H1W—O1W—H2W	110 (3)
N4—C5—H5	119.6		

O2—C1—C2—N4	−174.02 (13)	N3—C4—C5—N4	0.1 (2)
O1—C1—C2—N4	4.43 (18)	C5—C4—N3—C3	−0.5 (2)
O2—C1—C2—C3	4.1 (2)	N2—C3—N3—C4	−179.55 (13)
O1—C1—C2—C3	−177.47 (12)	C2—C3—N3—C4	0.68 (19)
N4—C2—C3—N2	179.80 (13)	C3—C2—N4—C5	0.1 (2)
C1—C2—C3—N2	1.8 (2)	C1—C2—N4—C5	178.13 (12)
N4—C2—C3—N3	−0.45 (19)	C4—C5—N4—C2	0.1 (2)
C1—C2—C3—N3	−178.48 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1*W*^{i}	0.84	1.69	2.5233 (17)	168
O1*W*—H1*W*···O5^{ii}	0.80 (3)	1.93 (3)	2.7152 (18)	167 (3)
O1*W*—H2*W*···O1	0.88 (3)	2.39 (3)	2.8825 (19)	116 (2)
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