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(3-Aminopyrazin-4-ium-2-carboxylate-κ^2N^1,O)diaquazinc(II) dinitrate

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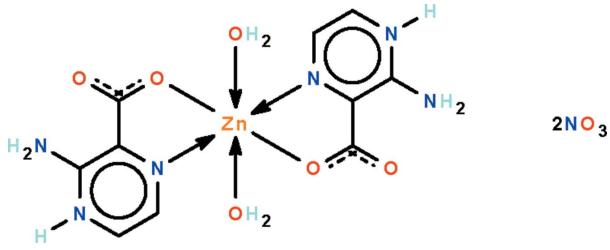
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.060; wR factor = 0.175; data-to-parameter ratio = 13.7.

The water-coordinated Zn^{II} atom in the title salt, $[Zn(C_5H_5N_3O_2)_2(H_2O)_2](NO_3)_2$, is N,O-chelated by a zwitterionic aminopyraziniocarboxylate unit; the metal atom, which lies on a center of inversion, shows an octahedral coordination. The nitrate ion interacts indirectly, through N—H···O hydrogen bonds. In the crystal, adjacent cations and anions are connected by O—H···O hydrogen bonds into a three-dimensional network motif. The crystal studied was a non-merohedral twin with two minor components of 15.1 (1) and 8.0 (1)%.

Related literature

For a related structure, see: Tayebee *et al.* (2008). For the treatment of non-merohedral twins, see: Spek (2003).



Experimental

Crystal data

$[Zn(C_5H_5N_3O_2)_2(H_2O)_2](NO_3)_2$
M_r = 503.66
Monoclinic, $P2_1/c$
a = 13.4676 (14) Å
b = 9.7059 (9) Å
c = 6.6682 (6) Å
β = 96.610 (3)°
V = 865.84 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.51 mm^{-1}
T = 293 K
0.24 × 0.21 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.580, T_{max} = 1.000
8164 measured reflections
1983 independent reflections
1739 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.175
S = 1.15
1983 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.37 e Å^{-3}
$\Delta\rho_{min}$ = −1.66 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O1^{i}	0.82	2.17	2.895 (5)	148
O1w—H1w2···O2^{ii}	0.82	1.99	2.752 (6)	154
N2—H2···O3	0.88	1.86	2.703 (6)	161
N3—H31···O4	0.88	2.14	2.981 (6)	161
N3—H32···O5^{iii}	0.88	2.33	2.994 (7)	133

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (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, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2064).

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supplementary materials

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(3-Aminopyrazin-4-ium-2-carboxylate-κ^2N^1,O)diaquazinc(II) dinitrate

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Comment

3-Aminopyrazine-2-carboxylic acid forms a number of aqua complexes with divalent transition metals in which the metal atom is *N*,*O*-chelated by the monoanion. In an attempt at the solution synthesis of the zinc derivative, the sodium ion used as a reactant is incorporated into the crystal structure (Tayebee *et al.*, 2008). In the present study, the attempt by a hydrothermal route yielded $Zn(H_2O)_2(C_5H_5N_3O_2)_2\ 2NO_3$ (Scheme I, Fig. 1). The water-coordinated zinc atom in the salt is *N*,*O*-chelated by a zwitterionic aminopyraziniocarboxylate unit; the metal atom, which lies on a center of inversion, shows octahedral coordination. The nitrate ion interacts indirectly, through N–H···O hydrogen bonds. Adjacent cations and anions are connected by O–H···O hydrogen bonds into a three-dimensional network motif.

Experimental

Zinc nitrate hexahydrate (0.30 g, 1 mmol), 3-aminopyrazine-2-carboxylic acid (0.28 g, 2 mmol), and sodium hydroxide (0.08 g 2 mmol) were dissolved in a H_2O/DMF (12 ml, *v*/*v* = 2:1) solution. The mixture was sealed in a 25- ml Teflon-lined stainless steel bomb and held at 443 K for 3 d. The bomb was gradually cooled to room temperature, and yellow crystals were obtained after several days.

Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93, N–H 0.88, O–H 0.82 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C,*N*,*O*). The crystal is a non-merohedral twin, with two minor components of 15.1 (1)% and 8.0 (1)%; *PLATON* (Spek, 2003) was used to separate the diffraction intensities into three domains. The final difference Fourier map had a peak at 0.92 Å from Zn1 and a hole at 0.98 Å from H1w2.

Figures

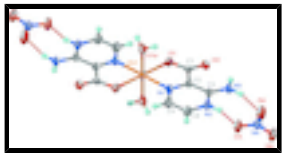

Fig. 1. Displacement ellipsoid plot of $Zn(H_2O)_2(C_5H_5N_3O_2)_2\ 2NO_3$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. Unlabeled atoms are related to labeled atoms by 1 - *x*, 1 - *y*, 1 - *z*.

(3-Aminopyrazin-4-ium-2-carboxylate-κ^2N^1,O)diaquazinc(II) dinitrate

Crystal data

$[Zn(C_5H_5N_3O_2)_2(H_2O)_2](NO_3)_2$	$F(000) = 512$
$M_r = 503.66$	$D_x = 1.932$ Mg m^{-3}

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 13.4676 (14) Å
b = 9.7059 (9) Å
c = 6.6682 (6) Å
β = 96.610 (3)°
V = 865.84 (14) Å^3
Z = 2

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7197 reflections
θ = 3.1–27.5°
μ = 1.51 mm^{-1}
T = 293 K
Prism, yellow
0.24 × 0.21 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
graphite
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.580, T_{max} = 1.000
8164 measured reflections

1983 independent reflections
1739 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −17→17
k = −11→12
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.175
S = 1.15
1983 reflections
145 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 4.4842P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.37 e Å^{-3}
$\Delta\rho_{min}$ = −1.66 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.5000	0.5000	0.5000	0.0239 (3)
O1	0.5443 (3)	0.7058 (4)	0.5390 (6)	0.0286 (8)
O2	0.6686 (3)	0.8494 (4)	0.4874 (6)	0.0302 (8)
O3	1.0229 (3)	0.4552 (5)	0.2346 (9)	0.0472 (12)
O4	1.0421 (4)	0.6731 (5)	0.2591 (11)	0.0630 (17)
O5	1.1600 (3)	0.5475 (5)	0.1631 (8)	0.0452 (11)
O1W	0.5552 (3)	0.4400 (5)	0.8042 (6)	0.0388 (10)
H1W1	0.5111	0.3991	0.8552	0.058*
H1W2	0.5717	0.5089	0.8710	0.058*

N1	0.6477 (3)	0.4895 (4)	0.4259 (7)	0.0280 (10)
N2	0.8377 (3)	0.5065 (5)	0.3357 (8)	0.0288 (9)
H2	0.9001	0.5100	0.3091	0.035*
N3	0.8428 (3)	0.7410 (5)	0.3867 (8)	0.0331 (11)
H31	0.9044	0.7417	0.3544	0.040*
H32	0.8146	0.8183	0.4193	0.040*
N4	1.0755 (3)	0.5598 (5)	0.2176 (8)	0.0320 (10)
C1	0.6305 (4)	0.7331 (5)	0.4932 (8)	0.0235 (10)
C2	0.6923 (4)	0.6113 (5)	0.4370 (7)	0.0221 (9)
C3	0.7931 (4)	0.6243 (5)	0.3862 (8)	0.0245 (10)
C4	0.7906 (4)	0.3840 (6)	0.3245 (10)	0.0357 (12)
H4	0.8231	0.3057	0.2849	0.043*
C5	0.6951 (4)	0.3757 (6)	0.3717 (10)	0.0358 (13)
H5	0.6625	0.2910	0.3664	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0173 (4)	0.0251 (4)	0.0306 (5)	−0.0034 (3)	0.0077 (3)	0.0000 (3)
O1	0.0223 (17)	0.0259 (17)	0.039 (2)	0.0009 (14)	0.0117 (15)	−0.0037 (16)
O2	0.0281 (18)	0.0218 (17)	0.041 (2)	0.0008 (14)	0.0031 (16)	−0.0001 (15)
O3	0.031 (2)	0.026 (2)	0.089 (4)	−0.0043 (18)	0.024 (2)	−0.003 (2)
O4	0.048 (3)	0.025 (2)	0.124 (5)	0.001 (2)	0.045 (3)	−0.010 (3)
O5	0.023 (2)	0.040 (2)	0.075 (3)	−0.0003 (17)	0.020 (2)	−0.003 (2)
O1W	0.042 (2)	0.041 (2)	0.033 (2)	−0.0187 (19)	0.0033 (18)	0.0027 (18)
N1	0.023 (2)	0.024 (2)	0.039 (3)	−0.0002 (16)	0.0121 (18)	0.0015 (18)
N2	0.0153 (18)	0.037 (2)	0.035 (2)	0.0016 (17)	0.0058 (17)	0.0005 (19)
N3	0.023 (2)	0.031 (2)	0.046 (3)	−0.0061 (18)	0.011 (2)	0.000 (2)
N4	0.027 (2)	0.027 (2)	0.043 (3)	0.0000 (18)	0.0092 (19)	0.000 (2)
C1	0.022 (2)	0.025 (2)	0.023 (2)	0.0004 (18)	0.0022 (18)	−0.0004 (19)
C2	0.021 (2)	0.022 (2)	0.023 (2)	0.0012 (18)	0.0043 (18)	0.0022 (18)
C3	0.020 (2)	0.030 (3)	0.024 (2)	−0.0011 (18)	0.0035 (18)	0.000 (2)
C4	0.032 (3)	0.027 (3)	0.049 (3)	0.006 (2)	0.011 (3)	−0.003 (3)
C5	0.036 (3)	0.021 (2)	0.052 (4)	−0.001 (2)	0.013 (3)	−0.001 (2)

Geometric parameters (Å, °)

Zn1—O1	2.092 (4)	N1—C2	1.324 (6)
Zn1—O1^{i}	2.092 (4)	N1—C5	1.346 (7)
Zn1—N1^{i}	2.107 (4)	N2—C4	1.345 (7)
Zn1—N1	2.107 (4)	N2—C3	1.353 (7)
Zn1—O1w^{i}	2.158 (4)	N2—H2	0.8800
Zn1—O1w	2.158 (4)	N3—C3	1.315 (7)
O1—C1	1.262 (6)	N3—H31	0.8800
O2—C1	1.242 (6)	N3—H32	0.8800
O3—N4	1.250 (6)	C1—C2	1.517 (7)
O4—N4	1.232 (7)	C2—C3	1.442 (7)
O5—N4	1.240 (6)	C4—C5	1.362 (8)

O1W—H1W1	0.8200	C4—H4	0.9300
O1W—H1W2	0.8200	C5—H5	0.9300
O1—Zn1—O1^{i}	180.0	C4—N2—H2	118.6
O1—Zn1—N1^{i}	100.84 (15)	C3—N2—H2	118.6
O1^{i}—Zn1—N1^{i}	79.16 (15)	C3—N3—H31	120.0
O1—Zn1—N1	79.16 (15)	C3—N3—H32	120.0
O1^{i}—Zn1—N1	100.84 (15)	H31—N3—H32	120.0
N1^{i}—Zn1—N1	180.0	O4—N4—O5	121.5 (5)
O1—Zn1—O1W^{i}	85.51 (16)	O4—N4—O3	118.6 (5)
O1^{i}—Zn1—O1W^{i}	94.49 (16)	O5—N4—O3	119.9 (5)
N1^{i}—Zn1—O1W^{i}	88.56 (18)	O2—C1—O1	126.4 (5)
N1—Zn1—O1W^{i}	91.44 (18)	O2—C1—C2	117.4 (4)
O1—Zn1—O1W	94.49 (16)	O1—C1—C2	116.2 (4)
O1^{i}—Zn1—O1W	85.51 (16)	N1—C2—C3	119.9 (4)
N1^{i}—Zn1—O1W	91.44 (18)	N1—C2—C1	116.8 (4)
N1—Zn1—O1W	88.56 (18)	C3—C2—C1	123.2 (4)
O1W^{i}—Zn1—O1W	180.0	N3—C3—N2	119.2 (4)
C1—O1—Zn1	115.3 (3)	N3—C3—C2	124.6 (5)
Zn1—O1W—H1W1	109.5	N2—C3—C2	116.2 (5)
Zn1—O1W—H1W2	109.5	N2—C4—C5	119.4 (5)
H1W1—O1W—H1W2	109.5	N2—C4—H4	120.3
C2—N1—C5	121.5 (5)	C5—C4—H4	120.3
C2—N1—Zn1	112.2 (3)	N1—C5—C4	120.2 (5)
C5—N1—Zn1	126.3 (4)	N1—C5—H5	119.9
C4—N2—C3	122.8 (4)	C4—C5—H5	119.9
N1^{i}—Zn1—O1—C1	−176.2 (4)	C5—N1—C2—C1	178.1 (5)
N1—Zn1—O1—C1	3.8 (4)	Zn1—N1—C2—C1	−1.6 (6)
O1W^{i}—Zn1—O1—C1	−88.5 (4)	O2—C1—C2—N1	−174.0 (5)
O1W—Zn1—O1—C1	91.5 (4)	O1—C1—C2—N1	5.0 (7)
O1—Zn1—N1—C2	−0.9 (4)	O2—C1—C2—C3	2.6 (7)
O1^{i}—Zn1—N1—C2	179.1 (4)	O1—C1—C2—C3	−178.3 (5)
O1W^{i}—Zn1—N1—C2	84.2 (4)	C4—N2—C3—N3	−177.5 (6)
O1W—Zn1—N1—C2	−95.8 (4)	C4—N2—C3—C2	2.7 (8)
O1—Zn1—N1—C5	179.4 (5)	N1—C2—C3—N3	178.0 (5)
O1^{i}—Zn1—N1—C5	−0.6 (5)	C1—C2—C3—N3	1.4 (8)
O1W^{i}—Zn1—N1—C5	−95.5 (5)	N1—C2—C3—N2	−2.2 (7)
O1W—Zn1—N1—C5	84.5 (5)	C1—C2—C3—N2	−178.8 (5)
Zn1—O1—C1—O2	173.2 (4)	C3—N2—C4—C5	−2.2 (10)
Zn1—O1—C1—C2	−5.7 (6)	C2—N1—C5—C4	−0.7 (10)
C5—N1—C2—C3	1.3 (8)	Zn1—N1—C5—C4	179.0 (5)
Zn1—N1—C2—C3	−178.4 (4)	N2—C4—C5—N1	1.1 (10)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O1^{ii}	0.82	2.17	2.895 (5)	148
O1w—H1w2···O2^{iii}	0.82	1.99	2.752 (6)	154
N2—H2···O3	0.88	1.86	2.703 (6)	161
N3—H31···O4	0.88	2.14	2.981 (6)	161
N3—H32···O5^{iv}	0.88	2.33	2.994 (7)	133

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

Fig. 1