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Bis(3-aminopyrazine-2-carboxylato-κ^2N^1,O)diaquamanganese(II) monohydrate

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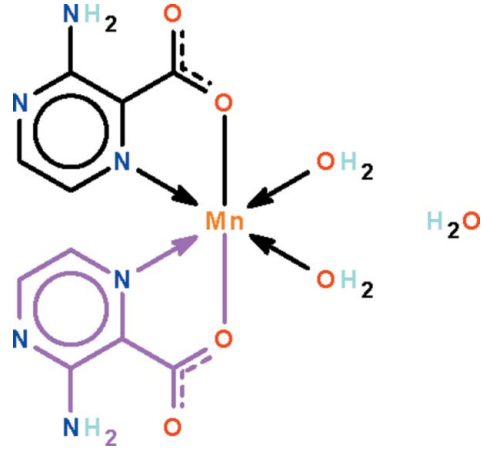
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.047; wR factor = 0.165; data-to-parameter ratio = 13.4.

In the title compound, $[Mn(C_5H_4N_3O_2)_2(H_2O)_2]\cdot H_2O$, the Mn^{II} cation, located on a twofold rotation axis, is N,O-chelated by two 3-aminopyrazine-2-carboxylate anions and coordinated by two water molecules in a distorted octahedral geometry. The uncoordinated water molecules lies on a twofold rotation axis. Adjacent molecules are linked by O—H···O and N—H···O hydrogen bonds into a three-dimensional network motif.

Related literature

For the isostructural magnesium analog, see: Ptasiewicz-Bak & Leciejewicz (1997); Marsh (2004).



Experimental

Crystal data

$[Mn(C_5H_4N_3O_2)_2(H_2O)_2]\cdot H_2O$ M_r = 385.21
Orthorhombic, *Fdd*2
a = 8.3107 (6) Å
b = 29.5862 (17) Å
c = 12.3791 (7) Å
V = 3043.8 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 293 K
0.15 × 0.10 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.875, T_{max} = 0.930
7239 measured reflections
1684 independent reflections
1086 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.165
S = 1.14
1684 reflections
126 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}
Absolute structure: Flack (1983), 775 Friedel pairs
Flack parameter: −0.02 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2^{i}	0.84 (7)	1.89 (3)	2.704 (7)	162 (9)
O1w—H12···N2^{ii}	0.84 (7)	2.02 (4)	2.792 (7)	152 (9)
O2w—H2···O1	0.84 (7)	2.10 (4)	2.902 (7)	159 (10)
N3—H31···O2	0.88 (7)	2.17 (9)	2.690 (8)	118 (8)
N3—H32···O2w^{iii}	0.88 (3)	2.15 (3)	3.001 (7)	161 (9)

Symmetry codes: (i) $-x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x-\frac{1}{4}, -y+\frac{3}{4}, z+\frac{1}{4}$; (iii) $-x-\frac{1}{4}, y+\frac{1}{4}, z-\frac{1}{4}$.

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: XU5022).

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Bis(3-aminopyrazine-2-carboxylato-κ^2N^1,O)diaquamanganese(II) monohydrate

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S1. Comment

The crystal structure of $Mg(H_2O)_2(C_5H_4N_3O_2)_2{\cdot}H_2O$ was described in the *Cc* space group (Ptasiewicz-Bak & Leciejewicz, 1997); the space group was revised to the *Fdd*2 space group (Marsh, 2004). The manganese analog (Scheme I) is isostructural; The water-coordinated manganese atom is *N*,*O*-chelated by the carboxylate ion (Fig. 2) in an octahedral environment. The mononuclear and lattice water both lie on a twofold rotation axis. Adjacent molecules are linked by O–H···O and N–H···O hydrogen bonds into a three-dimensional network motif.

S2. Experimental

Manganese acetate (1 mmol) and 2-aminopyrazine-3-carboxylic acid (2 mmol) and sodium hydroxide (2 mmol) were dissolved in a small volume of water to give a light yellow solution. Prismatic crystals separated from the solution after a few days.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C).

The amino H-atoms and water H-atoms were located in a difference Fourier map, and were refined with a distance restraints of N–H 0.88±0.01 and O–H 0.84±0.01 Å; their temperature factors were tied to those of the parent atoms by a factor of 1.5 times.

The final difference Fourier map was featureless.

The second value in the WGHT is somewhat large. Using a smaller value led to a deeper hole in the final difference Fourier map and a larger *Goodness-of-fit*.

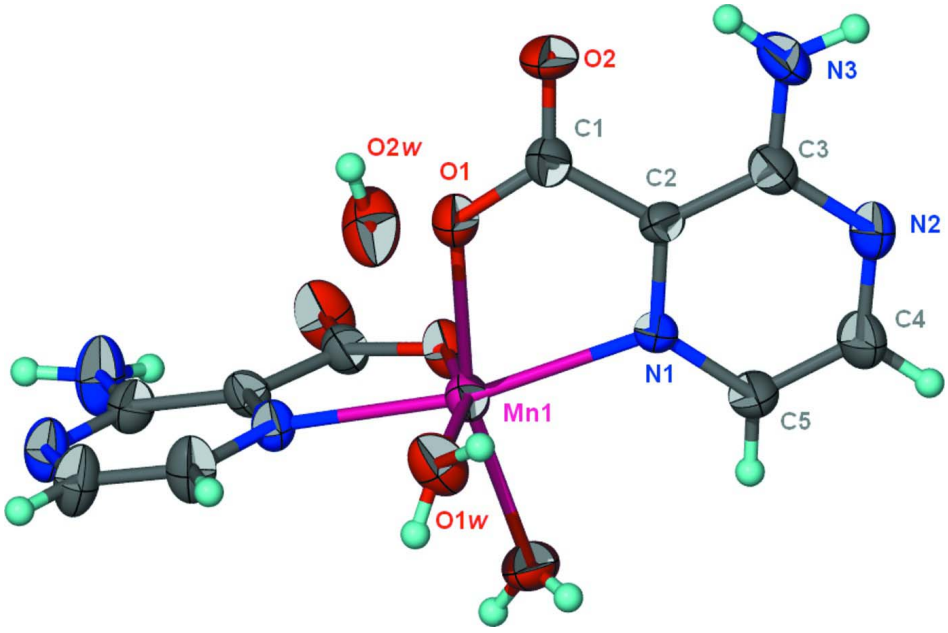

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Mn(H_2O)_2(C_5H_4N_3O_2)_2{\cdot}H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The Mn and lattice water molecule lie on a twofold rotation axis. Symmetry-related atoms are not labeled.

Bis(3-aminopyrazine-2-carboxylato-κ^2N^1,O)diaquamanganese(II) monohydrate

Crystal data

$[Mn(C_5H_4N_3O_2)_2(H_2O)_2]{\cdot}H_2O$
$M_r = 385.21$
Orthorhombic, *Fdd*2
Hall symbol: F 2 -2d
$a = 8.3107\ (6)$ Å
$b = 29.5862\ (17)$ Å
$c = 12.3791\ (7)$ Å
$V = 3043.8\ (3)$ Å^3
$Z = 8$
$F(000) = 1576$
$D_x = 1.681$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4731 reflections
$\theta = 3.0$–$27.4°$
$\mu = 0.92$ mm^{-1}
$T = 293$ K
Prism, yellow
0.15 × 0.10 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.875$, $T_{max} = 0.930$
7239 measured reflections
1684 independent reflections
1086 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.0°$
$h = -10 \rightarrow 10$
$k = -38 \rightarrow 38$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.165$
$S = 1.14$
1684 reflections
126 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
$w = 1/[\sigma^2(F_o^2) + (0.0722P)^2 + 15.3101P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.90$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0014 (3)
Absolute structure: Flack (1983), 775 Friedel pairs
Absolute structure parameter: −0.02 (5)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.2500	0.2500	0.53687 (11)	0.0378 (4)
O1	0.0649 (6)	0.26569 (16)	0.4190 (4)	0.0457 (11)
O2	−0.0500 (7)	0.31796 (16)	0.3169 (4)	0.0606 (16)
O1W	0.0675 (8)	0.24512 (17)	0.6593 (4)	0.0561 (16)
H11	0.084 (11)	0.225 (2)	0.706 (5)	0.084*
H12	0.006 (9)	0.267 (2)	0.675 (8)	0.084*
O2W	−0.2500	0.2500	0.5133 (9)	0.069 (3)
H2	−0.164 (7)	0.248 (4)	0.478 (7)	0.104*
N1	0.2472 (6)	0.32757 (14)	0.5175 (4)	0.0348 (13)
N2	0.2176 (7)	0.41941 (18)	0.4774 (5)	0.0515 (16)
N3	0.0251 (9)	0.4054 (2)	0.3489 (6)	0.0634 (19)
H31	−0.048 (9)	0.391 (3)	0.311 (7)	0.095*
H32	0.035 (11)	0.4344 (8)	0.335 (8)	0.095*
C1	0.0468 (8)	0.30645 (19)	0.3886 (5)	0.0409 (14)
C2	0.1439 (7)	0.34192 (19)	0.4439 (5)	0.0349 (12)
C3	0.1271 (8)	0.3890 (2)	0.4229 (5)	0.0427 (14)
C4	0.3184 (10)	0.4035 (2)	0.5501 (7)	0.0587 (19)
H4	0.3808	0.4241	0.5886	0.070*
C5	0.3368 (9)	0.3572 (2)	0.5727 (6)	0.0503 (17)
H5	0.4095	0.3474	0.6248	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0457 (7)	0.0301 (6)	0.0376 (7)	0.0012 (7)	0.000	0.000
O1	0.051 (3)	0.035 (2)	0.051 (3)	−0.001 (2)	−0.009 (2)	0.000 (2)
O2	0.076 (4)	0.050 (2)	0.055 (4)	0.010 (2)	−0.035 (3)	0.000 (2)
O1W	0.070 (4)	0.048 (3)	0.050 (3)	0.010 (3)	0.019 (3)	0.008 (2)
O2W	0.044 (4)	0.055 (4)	0.109 (10)	−0.009 (4)	0.000	0.000
N1	0.041 (2)	0.030 (2)	0.033 (4)	−0.001 (2)	−0.009 (3)	0.003 (2)
N2	0.056 (4)	0.039 (3)	0.059 (4)	−0.015 (3)	−0.008 (3)	0.004 (3)

N3	0.075 (5)	0.042 (3)	0.073 (5)	−0.001 (3)	−0.029 (4)	0.019 (3)
C1	0.050 (4)	0.033 (3)	0.040 (3)	0.001 (3)	−0.001 (3)	−0.003 (3)
C2	0.041 (3)	0.034 (3)	0.030 (3)	0.002 (2)	−0.008 (3)	−0.003 (2)
C3	0.046 (4)	0.037 (3)	0.044 (4)	−0.001 (3)	−0.001 (3)	0.006 (3)
C4	0.063 (4)	0.045 (4)	0.068 (5)	−0.019 (3)	−0.014 (4)	0.013 (4)
C5	0.055 (4)	0.043 (3)	0.053 (4)	−0.007 (3)	−0.021 (3)	0.006 (3)

Geometric parameters (Å, º)

Mn1—O1W^{i}	2.149 (6)	N1—C5	1.338 (8)
Mn1—O1W	2.149 (6)	N2—C4	1.316 (10)
Mn1—O1	2.170 (5)	N2—C3	1.352 (8)
Mn1—O1^{i}	2.170 (5)	N3—C3	1.339 (8)
Mn1—N1^{i}	2.308 (4)	N3—H31	0.88 (7)
Mn1—N1	2.308 (4)	N3—H32	0.88 (3)
O1—C1	1.273 (7)	C1—C2	1.490 (8)
O2—C1	1.245 (8)	C2—C3	1.424 (8)
O1W—H11	0.84 (7)	C4—C5	1.409 (9)
O1W—H12	0.84 (7)	C4—H4	0.9300
O2W—H2	0.84 (7)	C5—H5	0.9300
N1—C2	1.322 (7)		
O1W^{i}—Mn1—O1W	90.3 (4)	C5—N1—Mn1	126.3 (4)
O1W^{i}—Mn1—O1	163.73 (16)	C4—N2—C3	117.2 (6)
O1W—Mn1—O1	89.33 (18)	C3—N3—H31	129 (7)
O1W^{i}—Mn1—O1^{i}	89.33 (18)	C3—N3—H32	115 (6)
O1W—Mn1—O1^{i}	163.73 (16)	H31—N3—H32	115 (9)
O1—Mn1—O1^{i}	95.5 (3)	O2—C1—O1	123.1 (6)
O1W^{i}—Mn1—N1^{i}	97.65 (18)	O2—C1—C2	119.0 (5)
O1W—Mn1—N1^{i}	90.79 (18)	O1—C1—C2	117.9 (6)
O1—Mn1—N1^{i}	98.61 (18)	N1—C2—C3	120.2 (5)
O1^{i}—Mn1—N1^{i}	73.16 (17)	N1—C2—C1	116.2 (5)
O1W^{i}—Mn1—N1	90.79 (18)	C3—C2—C1	123.5 (5)
O1W—Mn1—N1	97.65 (18)	N3—C3—N2	116.9 (6)
O1—Mn1—N1	73.16 (17)	N3—C3—C2	122.7 (6)
O1^{i}—Mn1—N1	98.61 (18)	N2—C3—C2	120.3 (6)
N1^{i}—Mn1—N1	168.0 (3)	N2—C4—C5	123.5 (7)
C1—O1—Mn1	119.0 (4)	N2—C4—H4	118.2
Mn1—O1W—H11	115 (6)	C5—C4—H4	118.2
Mn1—O1W—H12	122 (7)	N1—C5—C4	118.4 (6)
H11—O1W—H12	119 (10)	N1—C5—H5	120.8
C2—N1—C5	120.2 (5)	C4—C5—H5	120.8
C2—N1—Mn1	113.4 (4)		
O1W^{i}—Mn1—O1—C1	14.2 (12)	Mn1—N1—C2—C3	179.6 (5)
O1W—Mn1—O1—C1	102.9 (5)	C5—N1—C2—C1	−178.6 (6)
O1^{i}—Mn1—O1—C1	−92.7 (5)	Mn1—N1—C2—C1	1.0 (7)
N1^{i}—Mn1—O1—C1	−166.4 (5)	O2—C1—C2—N1	−178.5 (6)

N1—Mn1—O1—C1	4.7 (5)	O1—C1—C2—N1	3.0 (9)
O1W^{i}—Mn1—N1—C2	179.9 (4)	O2—C1—C2—C3	3.0 (9)
O1W—Mn1—N1—C2	−89.8 (4)	O1—C1—C2—C3	−175.5 (6)
O1—Mn1—N1—C2	−2.8 (4)	C4—N2—C3—N3	−179.9 (8)
O1^{i}—Mn1—N1—C2	90.4 (4)	C4—N2—C3—C2	−0.7 (10)
N1^{i}—Mn1—N1—C2	44.8 (4)	N1—C2—C3—N3	179.6 (7)
O1W^{i}—Mn1—N1—C5	−0.6 (6)	C1—C2—C3—N3	−1.9 (10)
O1W—Mn1—N1—C5	89.8 (6)	N1—C2—C3—N2	0.5 (10)
O1—Mn1—N1—C5	176.8 (6)	C1—C2—C3—N2	178.9 (6)
O1^{i}—Mn1—N1—C5	−90.0 (6)	C3—N2—C4—C5	0.5 (13)
N1^{i}—Mn1—N1—C5	−135.6 (5)	C2—N1—C5—C4	−0.2 (10)
Mn1—O1—C1—O2	175.7 (5)	Mn1—N1—C5—C4	−179.8 (5)
Mn1—O1—C1—C2	−5.8 (8)	N2—C4—C5—N1	0.0 (13)
C5—N1—C2—C3	0.0 (9)		

Symmetry code: (i) −*x*+1/2, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O2^{ii}	0.84 (7)	1.89 (3)	2.704 (7)	162 (9)
O1w—H12···N2^{iii}	0.84 (7)	2.02 (4)	2.792 (7)	152 (9)
O2w—H2···O1	0.84 (7)	2.10 (4)	2.902 (7)	159 (10)
N3—H31···O2	0.88 (7)	2.17 (9)	2.690 (8)	118 (8)
N3—H32···O2w^{iv}	0.88 (3)	2.15 (3)	3.001 (7)	161 (9)

Symmetry codes: (ii) −*x*, −*y*+1/2, *z*+1/2; (iii) *x*−1/4, −*y*+3/4, *z*+1/4; (iv) −*x*−1/4, *y*+1/4, *z*−1/4.