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

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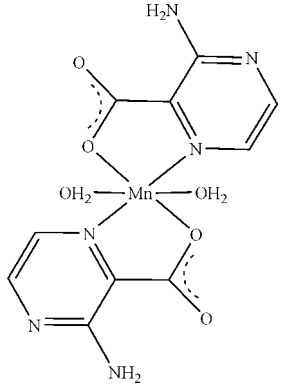
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.096; data-to-parameter ratio = 10.9.

The Mn^{II} atom in the title compound, $[Mn(C_5H_4N_3O_2)_2(H_2O)_2]$, exhibits an octahedral geometry comprising the two O atoms and two N atoms from two 3-aminopyrazine-2-carboxylate ligands, which act as chelating ligands, and two water molecules. An intramolecular N—H···O hydrogen bond occurs. In the crystal, N—H···O, O—H···N and O—H···O hydrogen bonds link adjacent molecules into a three-dimensional network. The molecule lies on a twofold rotation axis.

Related literature

For the nickel(II) analog, see: Ptasiewicz-Bak & Leciejewicz (1999).



Experimental

Crystal data

$[Mn(C_5H_4N_3O_2)_2(H_2O)_2]$ M_r = 367.20
Monoclinic, $C2/c$
a = 7.9257 (11) Å
b = 12.6994 (18) Å
c = 13.663 (2) Å
β = 91.903 (2)°
V = 1374.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 296 K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.889, T_{max} = 0.924
3373 measured reflections
1221 independent reflections
1114 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.096
S = 1.09
1221 reflections
112 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3C···O1^{i}	0.86	2.33	3.044 (3)	141
N3—H3D···O2	0.86	2.07	2.703 (4)	130
O3—H3B···N2^{ii}	0.89 (1)	1.95 (1)	2.833 (3)	170 (3)
O3—H3A···O2^{iii}	0.89 (1)	1.75 (1)	2.637 (3)	171 (3)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5015).

References

Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ptasiewicz-Bak, H. & Leciejewicz, J. (1999). *Pol. J. Chem.* **73**, 717–725.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, m1228 [doi:10.1107/S1600536810034835]

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

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S1. Experimental

The title complex was obtained as the main phase from the hydrothermal reaction of manganese sulfate tetrahydrate (0.0189 g) and 3-aminopyrazine-2-carboxylic acid (0.0913 g) in a 1:2 molar ratio. The reactants along with water were placed in a Teflon-lined stainless steel Parr bomb; the bomb was held at 413 K for three days. After cooling to room temperature, pink crystals were obtained.

S2. Refinement

All H atoms attached to C atoms and O atom from organic ligand were generated in idealized positions and constrained to ride on their parental C atoms, with C—H=0.93 Å, N—H=0.86 Å and and U_{iso}(H) = 1.5U(C). The water H-atoms were located in a difference Fouier map, and were refined with a distance restraint of O–H 0.88+0.01 Å; their temperature factors were also tied to those of the O-atom.

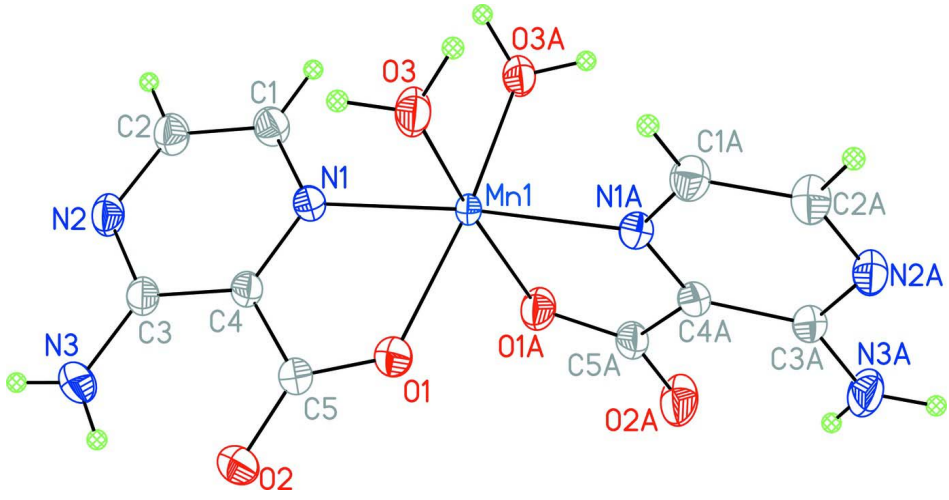

Figure 1

A view of the molecular structure with the atom-labling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

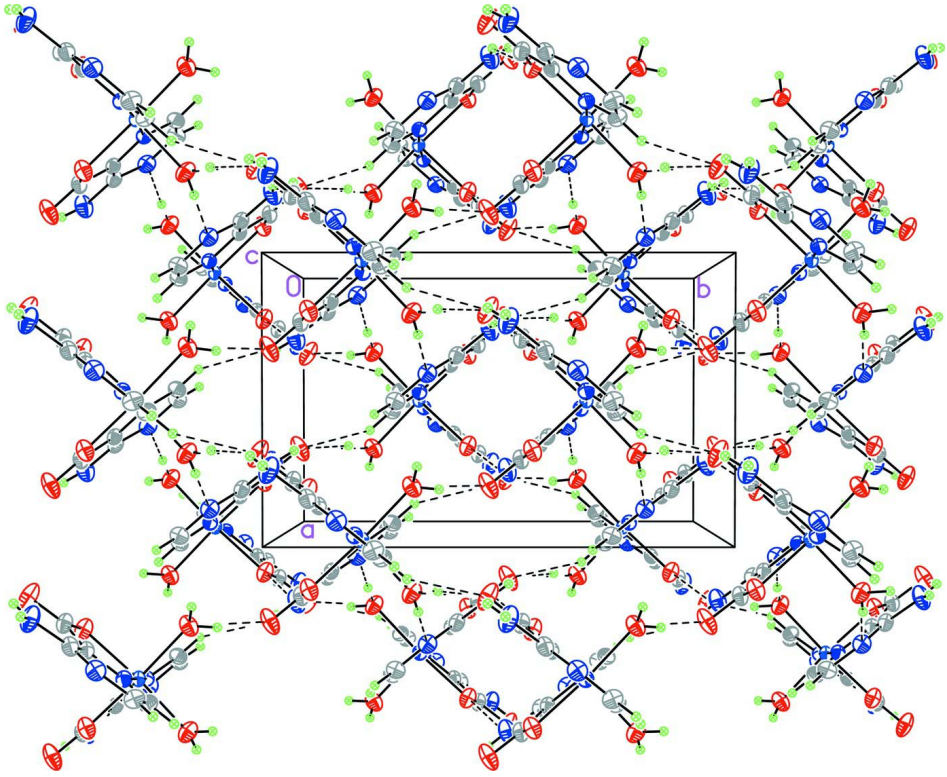

Figure 2

Three dimensional network of the title complex connected through hydrogen bonding.

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

Crystal data

$[Mn(C_5H_4N_3O_2)_2(H_2O)_2]$
$M_r = 367.20$
Monoclinic, $C2/c$
$a = 7.9257$ (11) Å
$b = 12.6994$ (18) Å
$c = 13.663$ (2) Å
$\beta = 91.903$ (2)°
$V = 1374.4$ (3) Å^3
$Z = 4$
$F(000) = 748$
$D_x = 1.775$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 117 reflections
$\theta = 2.5$–18.9°
$\mu = 1.01$ mm^{-1}
$T = 296$ K
Block, pink
0.12 × 0.10 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.889$, $T_{max} = 0.924$
3373 measured reflections
1221 independent reflections
1114 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.1°$, $\theta_{min} = 3.0°$
$h = -7 \rightarrow 9$
$k = -15 \rightarrow 15$
$l = -16 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.096$
$S = 1.09$
1221 reflections
112 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 1.9431P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0048 (10)

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}
Mn1	0.5000	0.30461 (4)	0.2500	0.0254 (2)
O1	0.6806 (3)	0.42418 (16)	0.23675 (14)	0.0466 (5)
O2	0.8132 (3)	0.52317 (18)	0.12895 (17)	0.0645 (7)
O3	0.6893 (3)	0.19335 (16)	0.26050 (16)	0.0475 (5)
N1	0.5308 (3)	0.31144 (16)	0.09621 (16)	0.0332 (5)
N2	0.5990 (3)	0.3363 (2)	−0.09977 (17)	0.0425 (6)
N3	0.7654 (4)	0.4795 (2)	−0.0636 (2)	0.0573 (8)
H3C	0.7829	0.4858	−0.1251	0.069*
H3D	0.8113	0.5231	−0.0225	0.069*
C1	0.4598 (3)	0.2483 (2)	0.0281 (2)	0.0396 (7)
H1	0.3855	0.1957	0.0463	0.048*
C2	0.4971 (4)	0.2615 (2)	−0.0691 (2)	0.0430 (7)
H2	0.4485	0.2158	−0.1151	0.052*
C3	0.6674 (4)	0.4023 (2)	−0.0320 (2)	0.0386 (6)
C4	0.6355 (3)	0.3870 (2)	0.0689 (2)	0.0342 (6)
C5	0.7160 (4)	0.4498 (2)	0.1509 (2)	0.0406 (7)
H3B	0.764 (3)	0.181 (2)	0.2150 (18)	0.049*
H3A	0.678 (4)	0.1343 (15)	0.295 (2)	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0323 (3)	0.0239 (3)	0.0203 (3)	0.000	0.0081 (2)	0.000

O1	0.0624 (13)	0.0430 (11)	0.0349 (11)	−0.0126 (10)	0.0109 (9)	−0.0046 (9)
O2	0.0916 (18)	0.0529 (14)	0.0506 (14)	−0.0358 (13)	0.0258 (13)	−0.0123 (11)
O3	0.0556 (13)	0.0492 (13)	0.0389 (12)	0.0155 (10)	0.0185 (10)	0.0073 (9)
N1	0.0350 (12)	0.0326 (12)	0.0324 (12)	−0.0001 (9)	0.0070 (9)	0.0017 (9)
N2	0.0480 (14)	0.0488 (14)	0.0314 (12)	0.0033 (11)	0.0100 (10)	0.0017 (11)
N3	0.083 (2)	0.0478 (15)	0.0422 (15)	−0.0173 (14)	0.0232 (14)	0.0036 (12)
C1	0.0380 (15)	0.0445 (16)	0.0364 (15)	−0.0049 (12)	0.0022 (11)	−0.0001 (13)
C2	0.0429 (16)	0.0516 (17)	0.0347 (15)	−0.0040 (14)	0.0034 (12)	−0.0018 (13)
C3	0.0444 (16)	0.0358 (14)	0.0363 (15)	0.0057 (12)	0.0127 (12)	0.0038 (12)
C4	0.0380 (14)	0.0307 (13)	0.0346 (14)	0.0032 (11)	0.0113 (11)	0.0014 (11)
C5	0.0501 (17)	0.0339 (14)	0.0386 (16)	−0.0052 (13)	0.0162 (13)	−0.0027 (12)

Geometric parameters (Å, º)

Mn1—O3^{i}	2.062 (2)	N1—C1	1.337 (3)
Mn1—O3	2.062 (2)	N2—C2	1.324 (4)
Mn1—O1	2.099 (2)	N2—C3	1.350 (4)
Mn1—O1^{i}	2.099 (2)	N3—C3	1.332 (4)
Mn1—N1	2.125 (2)	N3—H3C	0.8600
Mn1—N1^{i}	2.125 (2)	N3—H3D	0.8600
O1—C5	1.257 (3)	C1—C2	1.381 (4)
O2—C5	1.252 (3)	C1—H1	0.9300
O3—H3B	0.887 (10)	C2—H2	0.9300
O3—H3A	0.891 (10)	C3—C4	1.422 (4)
N1—C4	1.330 (3)	C4—C5	1.501 (4)
O3^{i}—Mn1—O3	93.50 (13)	C1—N1—Mn1	127.13 (18)
O3^{i}—Mn1—O1	170.52 (8)	C2—N2—C3	117.6 (2)
O3—Mn1—O1	90.29 (9)	C3—N3—H3C	120.0
O3^{i}—Mn1—O1^{i}	90.29 (9)	C3—N3—H3D	120.0
O3—Mn1—O1^{i}	170.52 (8)	H3C—N3—H3D	120.0
O1—Mn1—O1^{i}	87.32 (12)	N1—C1—C2	119.9 (3)
O3^{i}—Mn1—N1	93.80 (8)	N1—C1—H1	120.1
O3—Mn1—N1	89.40 (8)	C2—C1—H1	120.1
O1—Mn1—N1	77.54 (8)	N2—C2—C1	123.0 (3)
O1^{i}—Mn1—N1	99.02 (8)	N2—C2—H2	118.5
O3^{i}—Mn1—N1^{i}	89.40 (8)	C1—C2—H2	118.5
O3—Mn1—N1^{i}	93.80 (8)	N3—C3—N2	117.4 (3)
O1—Mn1—N1^{i}	99.02 (8)	N3—C3—C4	122.6 (3)
O1^{i}—Mn1—N1^{i}	77.54 (8)	N2—C3—C4	120.0 (3)
N1—Mn1—N1^{i}	175.33 (11)	N1—C4—C3	120.2 (2)
C5—O1—Mn1	116.20 (18)	N1—C4—C5	115.3 (2)
Mn1—O3—H3B	125 (2)	C3—C4—C5	124.5 (2)
Mn1—O3—H3A	122 (2)	O2—C5—O1	125.1 (3)
H3B—O3—H3A	107 (3)	O2—C5—C4	117.8 (2)

C4—N1—C1	119.3 (2)	O1—C5—C4	117.2 (2)
C4—N1—Mn1	113.60 (17)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*C*···O1^{ii}	0.86	2.33	3.044 (3)	141
N3—H3*D*···O2	0.86	2.07	2.703 (4)	130
O3—H3*B*···N2^{iii}	0.89 (1)	1.95 (1)	2.833 (3)	170 (3)
O3—H3*A*···O2^{iv}	0.89 (1)	1.75 (1)	2.637 (3)	171 (3)

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