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trans-Bis(acetato-κO)diaquabis(2-aminopyrazine-κN^4)manganese(II) dihydrate

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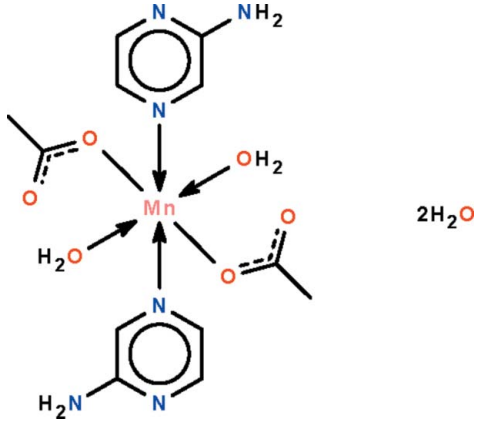
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.159; data-to-parameter ratio = 15.2.

The Mn^{II} atom in the title compound, $[Mn(CH_3COO)_2(C_4H_5N_3)_2(H_2O)_2]\cdot 2H_2O$, is situated on a center of inversion and shows an octahedral coordination polyhedron made up by four O atoms and two N atoms. The octahedron is somewhat tetragonally distorted owing to the longer Mn—N bond [2.323 (3) Å]. The mononuclear complex molecule and uncoordinated water molecules are linked by O—H···N, N—H···O and O—H···O hydrogen bonds, generating a three-dimensional network.

Related literature

For the crystal structure of manganese acetate dihydrate, see: Cheng & Wang (1991).



Experimental

Crystal data

$[Mn(C_2H_3O_2)_2(C_4H_5N_3)_2(H_2O)_2]\cdot 2H_2O$
M_r = 435.31
Triclinic, $P\overline{1}$
a = 7.0761 (7) Å
b = 8.5411 (8) Å
c = 9.5162 (10) Å
α = 100.866 (3)°
β = 105.036 (3)°
γ = 110.250 (3)°
V = 495.92 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 293 K
0.10 × 0.08 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.932, T_{max} = 0.965
4911 measured reflections
2249 independent reflections
1558 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.159
S = 1.07
2249 reflections
148 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −1.01 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2	0.84 (1)	1.89 (2)	2.690 (4)	160 (5)
O1w—H12···N2^{i}	0.84 (1)	2.02 (2)	2.837 (4)	165 (5)
O2w—H21···O1^{ii}	0.84 (1)	2.02 (1)	2.851 (4)	171 (4)
O2w—H22···O2^{iii}	0.84 (1)	1.90 (2)	2.726 (5)	167 (5)
N3—H31···O2w	0.88 (1)	1.98 (1)	2.859 (5)	178 (6)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (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: IM2304).

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trans-Bis(acetato-κO)diaquabis(2-aminopyrazine-κN^4)manganese(II) dihydrate

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S1. Comment

There are few crystal structure studies of *N*-heterocyclic adducts of manganese acetate, the latter crystallizing as a dihydrate (Cheng & Wang, 1991). Other first-row transition metal acetates furnish a large number of adducts. The Mn^{II} atom in $Mn(H_2O)_2(C_2H_3O_2)_2(C_4H_5N_3)_2 \times 2\ H_2O$ (Scheme I, Fig. 1) shows an octahedral coordination polyhedron made up by four O atoms and two N atoms. The octahedron is somewhat tetragonally distorted owing to the longer Mn–N bond. The mononuclear complex molecule and lattice water molecules are linked hydrogen bonds to generate a three-dimensional network (Table 1, Fig. 2).

S2. Experimental

To an aqueous solution of 2-aminopyrazine (1 mmol) was added manganese acetate tetrahydrate (1 mmol). The mixture was stirred for 30 min and then filtered. Colorless crystals of the title complex 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 using the riding model approximation, with U(H) set to 1.2U(C). The amino and water H-atoms were located in a difference Fourier map, and were refined with distance restraints N–H 0.88±0.01 Å, O–H 0.84±0.01 Å and H···H 1.37±0.01 Å; their temperature factors were refined.

The largest peaks/holes in the final difference Fourier map were found in close vicinity of Mn1.

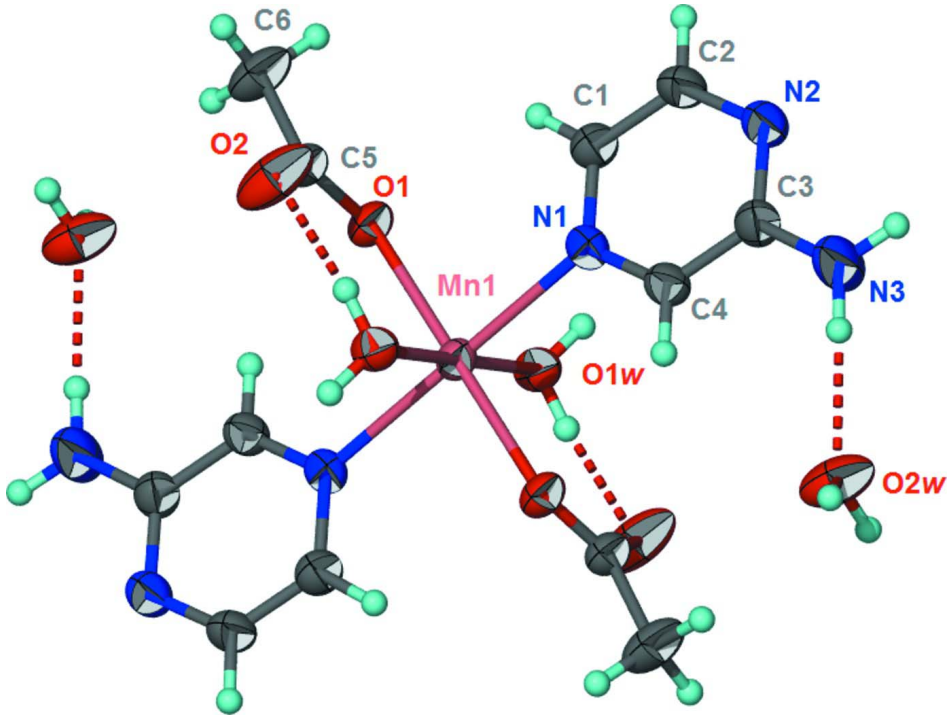

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Mn(H_2O)_2(C_2H_3O_2)_2(C_4H_5N_3)_2 \times 2\ H_2O$ at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

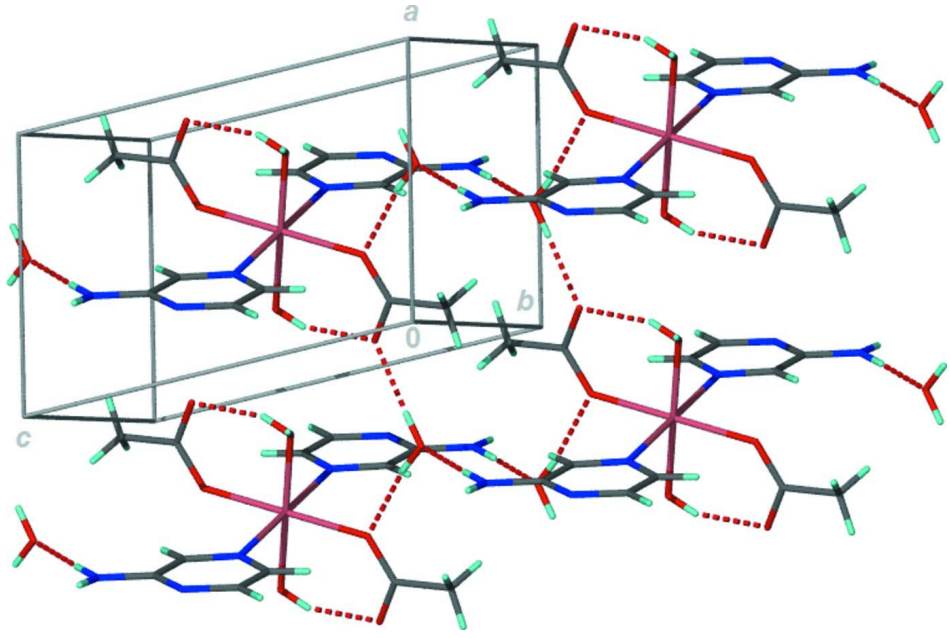

Figure 2

Three-dimensional hydrogen-bonded network of the title compound. Hydrogen bonds are depicted as dashed lines.

trans-Bis(acetato-κO)diaquabis(2-aminopyrazine-κN^4)manganese(II) dihydrate

Crystal data

$[Mn(C_2H_3O_2)_2(C_4H_5N_3)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 435.31$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.0761$ (7) Å
$b = 8.5411$ (8) Å
$c = 9.5162$ (10) Å
$\alpha = 100.866$ (3)°
$\beta = 105.036$ (3)°
$\gamma = 110.250$ (3)°
$V = 495.92$ (9) Å^3
$Z = 1$
$F(000) = 227$
$D_x = 1.458$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3626 reflections
$\theta = 3.3$–$27.5°$
$\mu = 0.72$ mm^{-1}
$T = 293$ K
Prism, colorless
0.10 × 0.08 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.932$, $T_{max} = 0.965$
4911 measured reflections
2249 independent reflections
1558 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -8\rightarrow 9$
$k = -11\rightarrow 11$
$l = -12\rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.159$
$S = 1.07$
2249 reflections
148 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.7384P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -1.01$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.021 (8)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.5000	0.5000	0.5000	0.0358 (3)
O1	0.6700 (4)	0.6113 (3)	0.7465 (3)	0.0413 (6)
O2	0.9808 (5)	0.5959 (6)	0.7684 (4)	0.0826 (12)
O1W	0.7647 (4)	0.4463 (3)	0.4659 (3)	0.0414 (6)
H11	0.858 (6)	0.503 (5)	0.553 (3)	0.082 (18)*
H12	0.763 (8)	0.346 (3)	0.440 (5)	0.09 (2)*
O2W	0.4054 (5)	0.6764 (5)	−0.0904 (4)	0.0719 (10)
H21	0.470 (6)	0.649 (7)	−0.147 (4)	0.085 (18)*
H22	0.273 (2)	0.636 (6)	−0.141 (4)	0.084 (18)*
N1	0.6498 (5)	0.7758 (4)	0.4722 (3)	0.0406 (7)
N2	0.7601 (5)	1.1077 (4)	0.4338 (4)	0.0464 (8)

N3	0.6301 (9)	0.9802 (5)	0.1732 (4)	0.0738 (13)
H31	0.562 (9)	0.888 (5)	0.091 (4)	0.111*
H32	0.654 (10)	1.085 (4)	0.163 (7)	0.111*
C1	0.7478 (6)	0.9231 (5)	0.5927 (4)	0.0465 (9)
H1	0.7803	0.9147	0.6914	0.056*
C2	0.7999 (7)	1.0845 (5)	0.5717 (4)	0.0476 (9)
H2	0.8665	1.1830	0.6576	0.057*
C3	0.6692 (7)	0.9628 (5)	0.3141 (4)	0.0448 (9)
C4	0.6154 (6)	0.7964 (5)	0.3351 (4)	0.0408 (8)
H4	0.5537	0.6977	0.2497	0.049*
C5	0.8583 (6)	0.6370 (5)	0.8229 (4)	0.0428 (8)
C6	0.9380 (8)	0.7229 (7)	0.9942 (5)	0.0659 (13)
H6A	1.0903	0.7569	1.0363	0.099*
H6B	0.8658	0.6414	1.0402	0.099*
H6C	0.9085	0.8248	1.0145	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0395 (5)	0.0376 (4)	0.0301 (4)	0.0194 (3)	0.0089 (3)	0.0084 (3)
O1	0.0417 (14)	0.0507 (15)	0.0297 (12)	0.0216 (12)	0.0082 (10)	0.0099 (11)
O2	0.0530 (19)	0.146 (3)	0.0437 (17)	0.054 (2)	0.0102 (14)	0.0016 (19)
O1W	0.0385 (14)	0.0421 (15)	0.0414 (15)	0.0189 (11)	0.0122 (12)	0.0067 (12)
O2W	0.0502 (19)	0.097 (3)	0.0474 (18)	0.0277 (19)	0.0103 (15)	−0.0094 (17)
N1	0.0447 (17)	0.0347 (15)	0.0428 (17)	0.0181 (13)	0.0142 (14)	0.0116 (13)
N2	0.057 (2)	0.0371 (16)	0.0435 (17)	0.0194 (14)	0.0172 (15)	0.0115 (14)
N3	0.124 (4)	0.048 (2)	0.042 (2)	0.030 (2)	0.022 (2)	0.0184 (17)
C1	0.054 (2)	0.045 (2)	0.0352 (19)	0.0192 (17)	0.0118 (16)	0.0099 (16)
C2	0.055 (2)	0.0359 (19)	0.041 (2)	0.0151 (17)	0.0117 (17)	0.0050 (16)
C3	0.055 (2)	0.042 (2)	0.0385 (19)	0.0226 (17)	0.0156 (17)	0.0115 (16)
C4	0.047 (2)	0.0354 (18)	0.0382 (19)	0.0155 (15)	0.0159 (16)	0.0093 (15)
C5	0.045 (2)	0.044 (2)	0.0321 (18)	0.0159 (16)	0.0069 (15)	0.0099 (15)
C6	0.059 (3)	0.094 (4)	0.033 (2)	0.034 (3)	0.0049 (19)	0.005 (2)

Geometric parameters (Å, º)

Mn1—O1W^{i}	2.163 (3)	N2—C3	1.335 (5)
Mn1—O1W	2.163 (3)	N2—C2	1.336 (5)
Mn1—O1^{i}	2.181 (2)	N3—C3	1.344 (5)
Mn1—O1	2.181 (2)	N3—H31	0.879 (10)
Mn1—N1^{i}	2.323 (3)	N3—H32	0.878 (10)
Mn1—N1	2.323 (3)	C1—C2	1.366 (5)
O1—C5	1.260 (4)	C1—H1	0.9300
O2—C5	1.232 (5)	C2—H2	0.9300
O1W—H11	0.840 (10)	C3—C4	1.406 (5)
O1W—H12	0.841 (10)	C4—H4	0.9300
O2W—H21	0.838 (10)	C5—C6	1.516 (5)
O2W—H22	0.838 (10)	C6—H6A	0.9600

N1—C4	1.321 (5)	C6—H6B	0.9600
N1—C1	1.348 (5)	C6—H6C	0.9600
O1W^{i}—Mn1—O1W	180.000 (1)	C3—N3—H31	121 (4)
O1W^{i}—Mn1—O1^{i}	91.79 (10)	C3—N3—H32	119 (4)
O1W—Mn1—O1^{i}	88.21 (9)	H31—N3—H32	119 (6)
O1W^{i}—Mn1—O1	88.21 (10)	N1—C1—C2	120.9 (4)
O1W—Mn1—O1	91.79 (10)	N1—C1—H1	119.6
O1^{i}—Mn1—O1	180.000 (1)	C2—C1—H1	119.6
O1W^{i}—Mn1—N1^{i}	90.34 (10)	N2—C2—C1	123.2 (3)
O1W—Mn1—N1^{i}	89.66 (10)	N2—C2—H2	118.4
O1^{i}—Mn1—N1^{i}	89.93 (10)	C1—C2—H2	118.4
O1—Mn1—N1^{i}	90.07 (10)	N2—C3—N3	118.3 (4)
O1W^{i}—Mn1—N1	89.66 (10)	N2—C3—C4	120.7 (3)
O1W—Mn1—N1	90.34 (10)	N3—C3—C4	121.0 (3)
O1^{i}—Mn1—N1	90.07 (10)	N1—C4—C3	122.1 (3)
O1—Mn1—N1	89.93 (10)	N1—C4—H4	118.9
N1^{i}—Mn1—N1	180.000 (1)	C3—C4—H4	118.9
C5—O1—Mn1	128.8 (2)	O2—C5—O1	124.7 (3)
Mn1—O1W—H11	99 (3)	O2—C5—C6	118.0 (4)
Mn1—O1W—H12	125 (4)	O1—C5—C6	117.4 (4)
H11—O1W—H12	109 (2)	C5—C6—H6A	109.5
H21—O2W—H22	110 (2)	C5—C6—H6B	109.5
C4—N1—C1	116.8 (3)	H6A—C6—H6B	109.5
C4—N1—Mn1	120.7 (2)	C5—C6—H6C	109.5
C1—N1—Mn1	121.9 (2)	H6A—C6—H6C	109.5
C3—N2—C2	116.2 (3)	H6B—C6—H6C	109.5
O1W^{i}—Mn1—O1—C5	−175.9 (3)	C4—N1—C1—C2	2.6 (6)
O1W—Mn1—O1—C5	4.1 (3)	Mn1—N1—C1—C2	−168.1 (3)
N1^{i}—Mn1—O1—C5	93.7 (3)	C3—N2—C2—C1	−1.6 (6)
N1—Mn1—O1—C5	−86.3 (3)	N1—C1—C2—N2	−0.5 (6)
O1W^{i}—Mn1—N1—C4	−95.9 (3)	C2—N2—C3—N3	−178.7 (4)
O1W—Mn1—N1—C4	84.1 (3)	C2—N2—C3—C4	1.5 (6)
O1^{i}—Mn1—N1—C4	−4.2 (3)	C1—N1—C4—C3	−2.7 (5)
O1—Mn1—N1—C4	175.8 (3)	Mn1—N1—C4—C3	168.1 (3)
O1W^{i}—Mn1—N1—C1	74.3 (3)	N2—C3—C4—N1	0.7 (6)
O1W—Mn1—N1—C1	−105.7 (3)	N3—C3—C4—N1	−179.1 (4)
O1^{i}—Mn1—N1—C1	166.1 (3)	Mn1—O1—C5—O2	−2.8 (6)
O1—Mn1—N1—C1	−13.9 (3)	Mn1—O1—C5—C6	178.0 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O2	0.84 (1)	1.89 (2)	2.690 (4)	160 (5)
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N3—H31···O2w	0.88 (1)	1.98 (1)	2.859 (5)	178 (6)

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