Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[*trans*-diaquamanganese(II)]-di-μ-3-pyridylacetato]

Su-Ni Qin, Fu-Pei Liang,* Zi-Lu Chen and Yan-Lin Cai

College of Chemistry and Chemical Engineering, Guangxi Normal University, Yucai Road 15, Guilin 541004, People's Republic of China
Correspondence e-mail: fliangoffice@yahoo.com

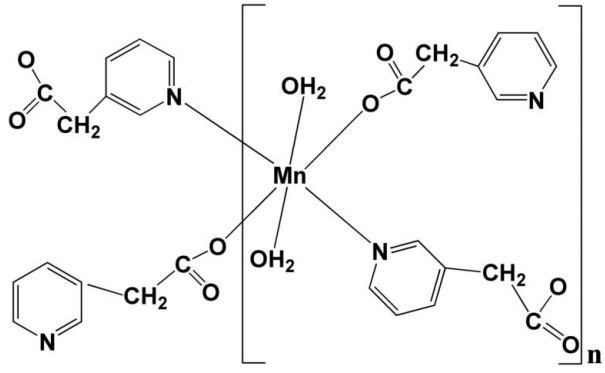
Received 19 April 2007; accepted 24 April 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.072; wR factor = 0.138; data-to-parameter ratio = 12.0.

The title manganese(II) coordination polymer, $[Mn(C_7H_6NO_2)_2(H_2O)_2]_n$, which was obtained from a solvothermal reaction of 3-pyridylacetic acid hydrochloride with $Mn(ClO_4)_2\cdot 6H_2O$, is centrosymmetric, so pairs of equivalent ligands lie *trans* to each other in a slightly distorted octahedral geometry such that the Mn^{II} center is coordinated by two pyridyl N atoms [Mn—N = 2.287 (4) Å], two carboxylate O atoms [Mn—O = 2.129 (3) Å] and two water molecules [Mn—O = 2.179 (3) Å]. Each unit is further extended into two-dimensional sheets with a rhombic grid through sharing Mn^{II} ions, 3-pyridylacetate anionic ligands and intramolecular O—H···O hydrogen bonds with angles at hydrogen of 147°. Adjacent two-dimensional layers are connected *via* intermolecular O—H···O and weak C—H···O hydrogen-bonding contacts, resulting in a three-dimensional framework with oxygen as a trifurcated acceptor atom.

Related literature

Related complexes of 4-pyridylacetate and 3-pyridylacetate have been reported (Li *et al.*, 2004; Du *et al.*, 2006; Martin *et al.*, 2007).



Experimental

Crystal data

$[Mn(C_7H_6NO_2)_2(H_2O)_2]$
M_r = 363.23
Monoclinic, $P2_1/n$
a = 9.260 (2) Å
b = 8.7283 (18) Å
c = 9.671 (2) Å
β = 106.788 (3)°
V = 748.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 298 (2) K
0.10 × 0.08 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.914, T_{max} = 0.947
3717 measured reflections
1274 independent reflections
770 reflections with $I > 2\sigma(I)$
R_{int} = 0.170

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.138
S = 0.99
1274 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H9···O2^{i}	0.85	2.01	2.763 (5)	147
O3—H8···O2^{ii}	0.85	1.90	2.707 (5)	158
C5—H5···O2^{iii}	0.93	2.56	3.409 (7)	152

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

We acknowledge financial support from the Program for Hundred Outstanding Young Teachers in Higher Education Institutions of Guangxi, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2014).

References

Bruker (1998). *SMART* (Version 5.051), *SAINT* (Versions 5.01), *SHELXTL* (Version 6.02) and *SADABS* (Version 2.0). Bruker AXS Inc., Madison, Wisconsin, USA.
Du, M., Li, C.-P. & Zhao, X.-J. (2006). *Cryst. Growth Des.* **6**, 335–341.
Li, X., Cao, R., Sun, Y.-Q., Shi, Q., Yuan, D.-Q., Sun, D.-F., Bi, W.-H. & Hong, M.-C. (2004). *Cryst. Growth Des.* **4**, 255–261.
Martin, D.-P., Springsteen, C.-H. & LaDuca, R.-L. (2007). *Inorg. Chim. Acta*, **360**, 599–606.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

 doi:10.1107/S1600536807020466

supplementary materials

Acta Cryst. (2007). E**63**, m1551 [**doi:10.1107/S1600536807020466**]

catena-Poly[[*trans*-diaquamanganese(II)]-di-μ-3-pyridylacetato]

S.-N. Qin, F.-P. Liang, Z.-L. Chen and Y.-L. Cai

Comment

The molecule of the title complex (I), which is similar to the described for $[M(\mathrm{Hpya})_2(\mathrm{H_2O})_2]_n$ (M = Cu, Co, Mn, Ni, Zn, Cd; Hpya = 4-pyridylacetic acid) (Li *et al.*, 2004; Du *et al.*,

2006) and $[M(\text{3-pyridylacetato})_2(\mathrm{H_2O})_2]_n$ (M = Ni, Co) (Martin *et al.*, 2007), is centrosymmetric, so pairs of equivalent ligands lie *trans* to each other in a slightly distorted octahedral geometry. The Mn^{II} center is six-coordinated by two pyridyl nitrogen atoms from two 3-pyridylacetate ligands in the axial positions, two carboxylate oxygen atoms from another two 3-pyridylacetate ligands and two oxygen atoms from two water molecules in the equatorial plane. Each 3-pyridylacetate anion uses its pyridine nitrogen atom and one carboxylate oxygen atom to connect two Mn^{II} ions. Four 3-pyridylacetate anionic ligands and four Mn^{II} ions form a tetragon with a side length of 8.763 Å and a diagonal measurement of 15.199 * 8.728 Å based on the Mn—Mn distances. The tetragon is further extended into a two-dimensional framework with a rhombic grid through sharing Mn^{II} ions, 3-pyridylacetate anionic ligands and intramolecular O—H···O hydrogen bonds with angles at hydrogen of 147 ° (Fig. 1).

Adjacent two-dimensional layers are connected *via* intermolecular O—H···O and weak C—H···O hydrogen-bonding contacts, resulting in a three-dimensional framework structure with oxygen as a trifurcated acceptor atom (Fig. 2).

Experimental

A mixture of 3-pyridylacetic acid hydrochloride (0.0174 g, 0.1 mmol), $Mn(ClO_4)_2\cdot 6H_2O$(0.0181 g, 0.05 mmol), $NaClO_4\cdot 6H_2O$ (0.0150 g, 0.07 mmol), NaOH (0.0080 g, 0.2 mmol), THF (5 ml) and water (2.5 ml) was sealed in a 25 ml Teflon-lined stainless-steel reactor and heated to 333 K for 96 h, yielding colourless crystals of (I) suitable for X-ray analysis. Elemental analysis for $C_{14}H_{16}MnN_2O_6$, calculated: C 46.29, H 4.44, N 7.71%; found: C 45.09, H 4.97, N 7.15%.

Refinement

H atoms of the water molecules were located in a difference map. H atoms bonded to C atoms were placed at calulated positions and treated using a riding-model approximation [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

Figures

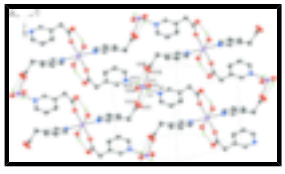


Fig. 1. Principal connectivity of the coordination polymer two-dimensional structure (I), showing 50% probability displacement ellipsoids. All H atoms except H9 have been omitted for clarity. Symmetry codes: (i) $1-x,-y,-z$; (ii) $1/2-x,y-1/2,1/2-z$; (iii) $1/2+x,1/2-y,z-1/2$.

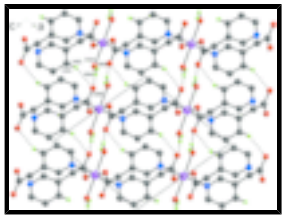


Fig. 2. Intermolecular hydrogen bonding contacts between the two-dimensional polymer layers in *ac* plane. For clarity, only H5, H8 and H9 were used. Symmetry codes: (i) $x-1,2+y,z$; (ii) $-x,2-y,1-z$; (iii) $-1/2-x,1/2+y,1/2-z$.

catena-Poly[[*trans*-diaquamanganese(II)]-di-μ-(3-pyridyl)acetato]

Crystal data

$[Mn(C_7H_6NO_2)_2(H_2O)_2]$	$F_{000} = 374$
$M_r = 363.23$	$D_x = 1.612$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1227 reflections
$a = 9.260$ (2) Å	$\theta = 2.6–28.0°$
$b = 8.7283$ (18) Å	$\mu = 0.92$ mm^{-1}
$c = 9.671$ (2) Å	$T = 298$ (2) K
$\beta = 106.788$ (3)°	Block, colourless
$V = 748.3$ (3) Å^3	0.10 × 0.08 × 0.06 mm
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	1274 independent reflections
Radiation source: fine-focus sealed tube	770 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.170$
$T = 298$(2) K	$\theta_{max} = 25.0°$
φ and ω scans	$\theta_{min} = 2.7°$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -10\rightarrow7$
$T_{min} = 0.914$, $T_{max} = 0.947$	$k = -10\rightarrow10$
3717 measured reflections	$l = -11\rightarrow11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.072$	H-atom parameters constrained
$wR(F^2) = 0.138$	$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
1274 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
106 parameters	$\Delta\rho_{min} = -0.56$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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	0.0000	0.0000	0.0273 (4)
N1	0.2917 (5)	0.0792 (5)	0.0622 (4)	0.0297 (11)
O1	0.0346 (5)	0.2775 (4)	0.4250 (4)	0.0376 (10)
O2	0.1985 (5)	0.1665 (4)	0.6121 (4)	0.0433 (11)
O3	0.6360 (4)	0.0553 (4)	0.2185 (4)	0.0375 (10)
H8	0.7067	0.0017	0.2725	0.056*
H9	0.6703	0.1460	0.2219	0.056*
C1	0.1243 (7)	0.1730 (6)	0.4810 (6)	0.0284 (13)
C2	0.1421 (8)	0.0417 (6)	0.3840 (6)	0.0387 (16)
H2A	0.2328	−0.0146	0.4328	0.046*
H2B	0.0574	−0.0275	0.3721	0.046*
C3	0.2762 (7)	0.0467 (6)	0.1934 (5)	0.0283 (14)
H3A	0.3539	−0.0058	0.2588	0.034*
C4	0.1512 (6)	0.0869 (6)	0.2364 (5)	0.0269 (13)
C5	0.0392 (7)	0.1676 (6)	0.1404 (6)	0.0341 (14)
H5	−0.0462	0.1982	0.1653	0.041*
C6	0.0546 (7)	0.2029 (6)	0.0071 (6)	0.0376 (15)
H6	−0.0205	0.2573	−0.0594	0.045*
C7	0.1825 (7)	0.1567 (6)	−0.0273 (6)	0.0347 (15)
H7	0.1918	0.1816	−0.1178	0.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0316 (8)	0.0291 (6)	0.0210 (6)	−0.0029 (7)	0.0074 (5)	−0.0003 (6)
N1	0.030 (3)	0.035 (2)	0.022 (2)	0.003 (3)	0.004 (2)	0.002 (2)
O1	0.053 (3)	0.028 (2)	0.027 (2)	0.009 (2)	0.005 (2)	−0.0021 (17)
O2	0.052 (3)	0.039 (2)	0.032 (2)	0.008 (2)	0.001 (2)	−0.0002 (19)
O3	0.041 (3)	0.038 (2)	0.027 (2)	−0.001 (2)	−0.0010 (18)	−0.0040 (16)
C1	0.029 (4)	0.027 (3)	0.031 (3)	−0.005 (3)	0.012 (3)	0.001 (3)
C2	0.054 (4)	0.032 (3)	0.035 (3)	0.007 (3)	0.021 (3)	0.005 (2)

C3	0.034 (4)	0.029 (3)	0.021 (3)	0.004 (3)	0.007 (3)	0.002 (2)
C4	0.033 (4)	0.025 (3)	0.021 (3)	−0.001 (3)	0.005 (3)	−0.002 (2)
C5	0.027 (4)	0.038 (3)	0.034 (3)	0.003 (3)	0.004 (3)	−0.006 (3)
C6	0.039 (4)	0.033 (3)	0.033 (3)	0.014 (3)	−0.002 (3)	0.001 (3)
C7	0.042 (4)	0.037 (3)	0.024 (3)	0.002 (3)	0.008 (3)	0.006 (3)

Geometric parameters (Å, °)

Mn1—O1^{i}	2.129 (3)	C1—C2	1.520 (7)
Mn1—O1^{ii}	2.129 (3)	C2—C4	1.507 (6)
Mn1—O3	2.179 (3)	C2—H2A	0.9700
Mn1—O3^{iii}	2.179 (3)	C2—H2B	0.9700
Mn1—N1^{iii}	2.287 (4)	C3—C4	1.383 (7)
Mn1—N1	2.287 (4)	C3—H3A	0.9300
N1—C7	1.313 (7)	C4—C5	1.370 (7)
N1—C3	1.348 (6)	C5—C6	1.372 (7)
O1—C1	1.247 (6)	C5—H5	0.9300
O1—Mn1^{iv}	2.129 (3)	C6—C7	1.380 (8)
O2—C1	1.257 (7)	C6—H6	0.9300
O3—H8	0.8500	C7—H7	0.9300
O3—H9	0.8500		
O1^{i}—Mn1—O1^{ii}	180	O1—C1—C2	117.4 (5)
O1^{i}—Mn1—O3	88.47 (14)	O2—C1—C2	117.6 (5)
O1^{ii}—Mn1—O3	91.53 (14)	C4—C2—C1	115.7 (4)
O1^{i}—Mn1—O3^{iii}	91.53 (14)	C4—C2—H2A	108.4
O1^{ii}—Mn1—O3^{iii}	88.47 (14)	C1—C2—H2A	108.4
O3—Mn1—O3^{iii}	180	C4—C2—H2B	108.4
O1^{i}—Mn1—N1^{iii}	92.02 (15)	C1—C2—H2B	108.4
O1^{ii}—Mn1—N1^{iii}	87.98 (15)	H2A—C2—H2B	107.4
O3—Mn1—N1^{iii}	91.54 (15)	N1—C3—C4	123.8 (5)
O3^{iii}—Mn1—N1^{iii}	88.46 (15)	N1—C3—H3A	118.1
O1^{i}—Mn1—N1	87.98 (15)	C4—C3—H3A	118.1
O1^{ii}—Mn1—N1	92.02 (15)	C5—C4—C3	117.5 (5)
O3—Mn1—N1	88.46 (15)	C5—C4—C2	122.5 (5)
O3^{iii}—Mn1—N1	91.54 (15)	C3—C4—C2	120.0 (5)
N1^{iii}—Mn1—N1	180	C4—C5—C6	119.2 (5)
C7—N1—C3	117.2 (5)	C4—C5—H5	120.4
C7—N1—Mn1	122.0 (3)	C6—C5—H5	120.4
C3—N1—Mn1	120.8 (4)	C5—C6—C7	119.4 (6)
C1—O1—Mn1^{iv}	131.8 (3)	C5—C6—H6	120.3
Mn1—O3—H8	126.9	C7—C6—H6	120.3
Mn1—O3—H9	110.4	N1—C7—C6	122.9 (5)
H8—O3—H9	106.1	N1—C7—H7	118.6
O1—C1—O2	124.9 (5)	C6—C7—H7	118.6

O1^{i}—Mn1—N1—C7	−130.5 (4)	C7—N1—C3—C4	1.7 (8)
O1^{ii}—Mn1—N1—C7	49.5 (4)	Mn1—N1—C3—C4	−177.9 (4)
O3—Mn1—N1—C7	141.0 (4)	N1—C3—C4—C5	−1.6 (8)
O3^{iii}—Mn1—N1—C7	−39.0 (4)	N1—C3—C4—C2	178.3 (5)
O1^{i}—Mn1—N1—C3	49.1 (4)	C1—C2—C4—C5	−58.4 (7)
O1^{ii}—Mn1—N1—C3	−130.9 (4)	C1—C2—C4—C3	121.7 (6)
O3—Mn1—N1—C3	−39.4 (4)	C3—C4—C5—C6	0.8 (8)
O3^{iii}—Mn1—N1—C3	140.6 (4)	C2—C4—C5—C6	−179.1 (5)
Mn1^{iv}—O1—C1—O2	14.6 (8)	C4—C5—C6—C7	−0.2 (8)
Mn1^{iv}—O1—C1—C2	−166.9 (4)	C3—N1—C7—C6	−1.0 (8)
O1—C1—C2—C4	42.5 (7)	Mn1—N1—C7—C6	178.7 (4)
O2—C1—C2—C4	−139.0 (5)	C5—C6—C7—N1	0.3 (9)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H9···O2^{ii}	0.85	2.01	2.763 (5)	147
O3—H8···O2^{v}	0.85	1.90	2.707 (5)	158
C5—H5···O2^{vi}	0.93	2.56	3.409 (7)	152

Symmetry codes: (ii) *x*+1/2, −*y*+1/2, *z*−1/2; (v) −*x*+1, −*y*, −*z*+1; (vi) *x*−1/2, −*y*+1/2, *z*−1/2.

Fig. 1

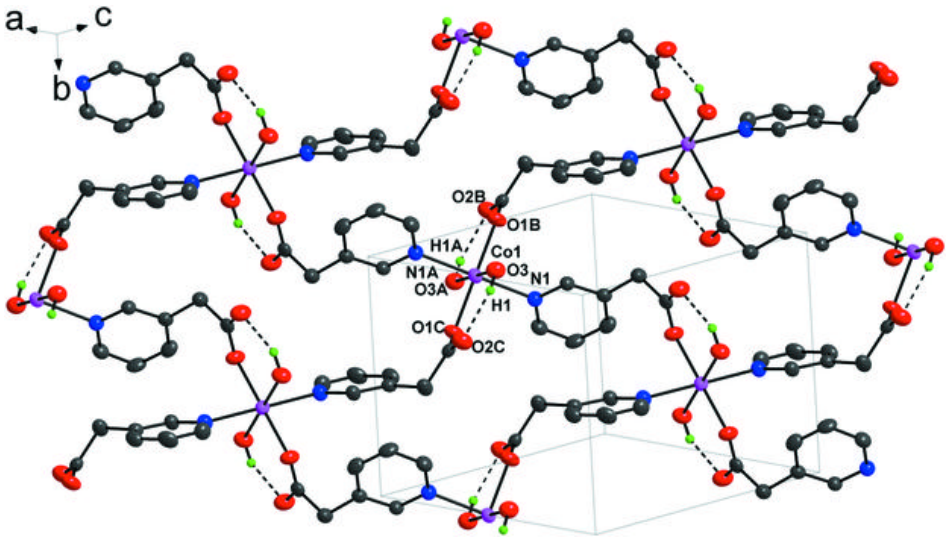


Fig. 2