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catena-Poly[[aqua(4,4′-bipyridine-κ^2N,N')manganese(II)]-μ-3-(4-carboxylatophenoxy)propionato-$\kappa^3O:O',O''$]

Li-Li Kong,[a] Shan Gao,[a] Li-Hua Huo[a] and Seik Weng Ng[b]*

[a]School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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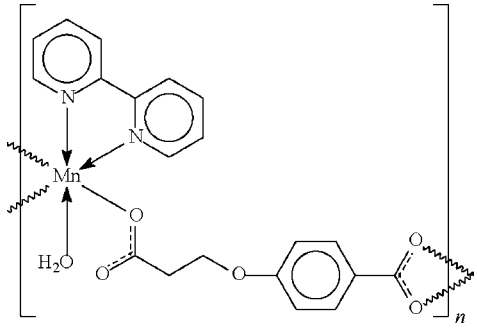
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.089; data-to-parameter ratio = 16.5.

In the crystal structure of the polymeric title compound, $[Mn(C_{10}H_8N_2)(C_{10}H_8O_5)(H_2O)]_n$, the Mn^{II} atom is O,O'-chelated by the aromatic carboxylate end of the 3-(4-carboxylatophenoxy)propionate dianion and is covalently bonded (through one O atom) by the aliphatic carboxylate end of another dianion; it is also coordinated by a water molecule. The compound adopts a helical chain structure that propagates along the c axis of the orthorhombic unit cell. The coordinated water molecule engages in both intrachain and interchain hydrogen bonding; the interchain hydrogen bonds result in a honeycomb motif. The compound crystallizes as a 0.36:0.64 inversion twin.

Related literature

For the structure of 3-(4-carboxyphenoxy)propionic acid, see: Gao & Ng (2006). For the crystal structure of a Co^{II} complex with the 3-(4-carboxylatophenoxy)propionate dianion, see: Xiao *et al.* (2006).



Experimental

Crystal data

$[Mn(C_{10}H_8N_2)(C_{10}H_8O_5)(H_2O)]$
M_r = 437.30
Orthorhombic, $P2_12_12_1$
a = 6.7770 (3) Å
b = 16.2626 (6) Å
c = 17.3730 (5) Å
V = 1914.71 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 295 (2) K
0.35 × 0.29 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.624, T_{max} = 0.880
18852 measured reflections
4362 independent reflections
3057 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.089
S = 0.95
4362 reflections
264 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Flack (1983), with 1860 Friedel pairs
Flack parameter: 0.36 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W2···O2	0.86 (1)	1.82 (2)	2.658 (3)	164 (6)
O1W—H1W1···O4^{i}	0.85 (1)	1.96 (1)	2.797 (3)	170 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2488).

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supplementary materials

Acta Cryst. (2007). E**63**, m2851 [**doi:10.1107/S160053680705218X**]

catena-Poly[[aqua(4,4'-bipyridine-κ^2N,N')manganese(II)]-μ-3-(4-carboxylatophenoxy)propionato-$\kappa^3O:O',O''$]

L.-L. Kong, S. Gao, L.-H. Huo and S. W. Ng

Experimental

Manganese dichloride hexahydrate (2 mmol), 3-(4-carboxylatophenoxy)propionic acid (2 mmol) and 2,2'-bipyridine (2 mmol) were dissolved in a 3:1 ethanol–water solution. Aqueous 0.1 *M* sodium hydroxide was added until the solution registered a pH of 7. The solution was set aside for the growth of crystal over several days. CH&N analysis. Calc. for $C_{20}H_{18}N_2O_6Mn$: C 54.93, H 4.15, N 6.41%. Found: C 54.94, H 4.13, N 6.42%.

Refinement

The C-bound H atoms were placed in calculated positions [C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C)], and were included in the refinement in the riding-model approximation. The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O—H = 0.85 (1) Å; their U_{iso}(H) values were freely refined.

Figures

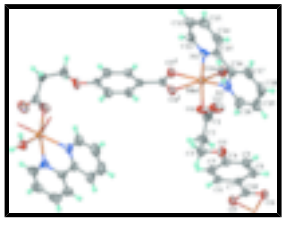


Fig. 1. Part of the polymeric structure of the title compound, showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. Symmetry code: (i) 5/2 − *x*, 1 − *y*, *z* − 1/2.

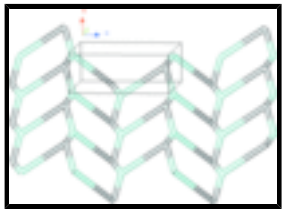


Fig. 2. Layer structure of the hydrogen-bonded network as illustrated by *OLEX* (Dolomanov *et al.*, 2003).

catena-Poly[[aqua(4,4'-bipyridine-κ$^2N,N'$)manganese(II)]- μ-3-(4-carboxylatophenoxy)propionato-κ$^3O:O',O''$]

Crystal data

$[Mn(C_{10}H_8N_2)(C_{10}H_8O_5)(H_2O)]$	F_{000} = 900
M_r = 437.30	D_x = 1.517 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 13538 reflections

a = 6.7770 (3) Å	θ = 3.0–27.5º
b = 16.2626 (6) Å	μ = 0.73 mm^{-1}
c = 17.3730 (5) Å	T = 295 (2) K
V = 1914.71 (12) $Å^3$	Prism, yellow
Z = 4	0.35 × 0.29 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	4362 independent reflections
Radiation source: fine-focus sealed tube	3057 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 3.2º
ω scans	$h = -8 \rightarrow 8$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -21 \rightarrow 21$
T_{min} = 0.624, T_{max} = 0.880	$l = -22 \rightarrow 22$
18852 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.089	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.95	$\Delta\rho_{max}$ = 0.34 e $Å^{-3}$
4362 reflections	$\Delta\rho_{min}$ = −0.30 e $Å^{-3}$
264 parameters	Extinction correction: none
2 restraints	Absolute structure: Flack (1983), with 1860 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.36 (2)
Secondary atom site location: difference Fourier map	

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

	x	y	z	U_{iso}*/U_{eq}
Mn1	0.75683 (7)	0.39945 (2)	0.849961 (18)	0.03710 (11)
O1	0.8310 (3)	0.52190 (13)	0.86239 (14)	0.0622 (6)
O2	0.5582 (4)	0.59275 (14)	0.84588 (16)	0.0803 (7)
O3	0.9809 (3)	0.64933 (14)	0.98274 (10)	0.0552 (6)
O4	1.4164 (3)	0.61980 (12)	1.30356 (9)	0.0430 (4)
O5	1.6748 (3)	0.61228 (13)	1.22776 (9)	0.0459 (5)
O1W	0.4470 (3)	0.43660 (15)	0.85866 (13)	0.0520 (5)

H1W1	0.334 (2)	0.4252 (19)	0.8405 (17)	0.063 (10)*
H1W2	0.459 (9)	0.4888 (8)	0.853 (3)	0.16 (2)*
N1	0.7321 (4)	0.26198 (12)	0.86540 (11)	0.0413 (5)
N2	0.7755 (4)	0.37423 (14)	0.97641 (10)	0.0416 (5)
C1	0.7385 (5)	0.58737 (15)	0.85466 (13)	0.0463 (6)
C2	0.8625 (5)	0.66545 (18)	0.85678 (16)	0.0540 (8)
H2A	0.8992	0.6800	0.8046	0.065*
H2B	0.7827	0.7099	0.8773	0.065*
C3	1.0480 (5)	0.65767 (19)	0.90479 (14)	0.0494 (7)
H3A	1.1236	0.6098	0.8893	0.059*
H3B	1.1300	0.7062	0.8992	0.059*
C4	1.1170 (4)	0.64004 (19)	1.04023 (15)	0.0434 (8)
C5	1.3162 (4)	0.6315 (2)	1.02968 (15)	0.0447 (8)
H5	1.3696	0.6316	0.9804	0.054*
C6	1.4373 (4)	0.62257 (17)	1.09374 (14)	0.0391 (6)
H6	1.5725	0.6161	1.0868	0.047*
C7	1.3603 (4)	0.62311 (19)	1.16835 (14)	0.0360 (6)
C8	1.1573 (4)	0.6318 (2)	1.17619 (15)	0.0469 (9)
H8	1.1020	0.6323	1.2252	0.056*
C9	1.0369 (4)	0.6398 (2)	1.11337 (16)	0.0506 (8)
H9	0.9013	0.6450	1.1199	0.061*
C10	1.4908 (4)	0.61775 (16)	1.23693 (13)	0.0363 (6)
C11	0.7252 (5)	0.20784 (18)	0.80691 (16)	0.0535 (7)
H11	0.7117	0.2280	0.7571	0.064*
C12	0.7371 (6)	0.12452 (18)	0.8171 (2)	0.0664 (8)
H12	0.7305	0.0889	0.7753	0.080*
C13	0.7589 (5)	0.09507 (19)	0.8902 (2)	0.0682 (9)
H13	0.7694	0.0388	0.8986	0.082*
C14	0.7654 (5)	0.14913 (17)	0.95166 (18)	0.0583 (7)
H14	0.7786	0.1296	1.0017	0.070*
C15	0.7520 (5)	0.23271 (14)	0.93762 (14)	0.0423 (5)
C16	0.7595 (4)	0.29574 (16)	0.99965 (13)	0.0422 (6)
C17	0.7479 (5)	0.2761 (2)	1.07716 (14)	0.0574 (7)
H17	0.7367	0.2216	1.0928	0.069*
C18	0.7533 (6)	0.3384 (3)	1.13051 (15)	0.0713 (10)
H18	0.7459	0.3262	1.1827	0.086*
C19	0.7696 (5)	0.4191 (2)	1.10699 (16)	0.0672 (9)
H19	0.7728	0.4618	1.1426	0.081*
C20	0.7808 (5)	0.4344 (2)	1.02932 (15)	0.0547 (8)
H20	0.7924	0.4886	1.0128	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.03402 (19)	0.04224 (19)	0.03503 (17)	−0.0002 (2)	0.0009 (2)	0.00125 (15)
O1	0.0507 (13)	0.0422 (11)	0.0939 (16)	−0.0024 (10)	−0.0079 (12)	−0.0035 (11)
O2	0.0593 (15)	0.0597 (14)	0.122 (2)	0.0052 (12)	−0.0319 (15)	−0.0050 (15)
O3	0.0416 (12)	0.0877 (16)	0.0365 (9)	−0.0032 (11)	−0.0105 (8)	0.0006 (9)

O4	0.0323 (10)	0.0623 (12)	0.0345 (9)	−0.0020 (9)	−0.0001 (7)	−0.0047 (9)
O5	0.0272 (9)	0.0720 (13)	0.0384 (8)	−0.0008 (9)	−0.0003 (7)	−0.0006 (9)
O1W	0.0320 (11)	0.0665 (14)	0.0575 (12)	−0.0004 (10)	−0.0075 (10)	−0.0060 (11)
N1	0.0358 (12)	0.0418 (11)	0.0463 (11)	−0.0026 (12)	0.0065 (11)	0.0015 (8)
N2	0.0355 (13)	0.0551 (13)	0.0343 (10)	0.0031 (12)	−0.0014 (10)	0.0001 (9)
C1	0.0552 (16)	0.0467 (15)	0.0372 (11)	0.0002 (18)	−0.0109 (17)	0.0007 (10)
C2	0.067 (2)	0.0483 (17)	0.0465 (15)	−0.0065 (15)	−0.0132 (16)	0.0111 (14)
C3	0.0527 (18)	0.0541 (18)	0.0415 (14)	−0.0061 (15)	−0.0048 (13)	0.0042 (13)
C4	0.0365 (16)	0.053 (2)	0.0410 (15)	−0.0059 (14)	−0.0084 (12)	−0.0012 (13)
C5	0.0441 (18)	0.0559 (19)	0.0340 (13)	−0.0014 (13)	0.0012 (11)	−0.0039 (12)
C6	0.0301 (14)	0.0441 (17)	0.0430 (14)	0.0004 (12)	−0.0002 (11)	−0.0040 (13)
C7	0.0324 (14)	0.0366 (15)	0.0390 (14)	−0.0029 (12)	−0.0028 (10)	−0.0005 (12)
C8	0.0320 (15)	0.072 (2)	0.0369 (14)	−0.0050 (15)	0.0030 (12)	0.0040 (14)
C9	0.0287 (15)	0.078 (2)	0.0450 (15)	−0.0031 (14)	0.0005 (12)	0.0018 (15)
C10	0.0331 (14)	0.0375 (14)	0.0382 (13)	−0.0027 (11)	−0.0006 (11)	−0.0020 (11)
C11	0.052 (2)	0.0538 (16)	0.0549 (15)	−0.0053 (17)	0.0077 (16)	−0.0043 (13)
C12	0.058 (2)	0.0512 (17)	0.090 (2)	−0.008 (2)	0.009 (2)	−0.0167 (16)
C13	0.0519 (18)	0.0401 (15)	0.113 (3)	−0.001 (2)	0.007 (2)	0.0007 (16)
C14	0.0363 (16)	0.0584 (18)	0.0803 (19)	0.0010 (19)	−0.0009 (18)	0.0230 (15)
C15	0.0232 (11)	0.0463 (14)	0.0574 (14)	0.0021 (16)	0.0056 (16)	0.0111 (11)
C16	0.0206 (11)	0.0627 (15)	0.0433 (12)	0.0054 (17)	0.0015 (14)	0.0114 (11)
C17	0.0384 (15)	0.086 (2)	0.0478 (14)	0.004 (2)	0.0042 (16)	0.0209 (14)
C18	0.0448 (17)	0.133 (3)	0.0355 (13)	0.007 (3)	0.0048 (16)	0.0119 (17)
C19	0.049 (2)	0.109 (3)	0.0435 (15)	0.004 (2)	0.0008 (17)	−0.0165 (16)
C20	0.049 (2)	0.0719 (18)	0.0436 (14)	0.0053 (17)	−0.0027 (14)	−0.0088 (13)

Geometric parameters (Å, °)

Mn1—O1	2.065 (2)	C5—C6	1.391 (4)
Mn1—O5^{i}	2.181 (2)	C5—H5	0.93
Mn1—O1W	2.190 (2)	C6—C7	1.398 (3)
Mn1—N2	2.2384 (18)	C6—H6	0.93
Mn1—N1	2.258 (2)	C7—C8	1.390 (4)
Mn1—O4^{i}	2.377 (2)	C7—C10	1.487 (3)
Mn1—C10^{i}	2.619 (2)	C8—C9	1.368 (4)
O1—C1	1.243 (3)	C8—H8	0.93
O2—C1	1.234 (4)	C9—H9	0.93
O3—C4	1.368 (3)	C10—Mn1^{ii}	2.619 (2)
O3—C3	1.435 (3)	C11—C12	1.369 (4)
O4—C10	1.263 (3)	C11—H11	0.93
O5—C10	1.260 (3)	C12—C13	1.365 (5)
O1W—H1W1	0.85 (1)	C12—H12	0.93
O1W—H1W2	0.86 (1)	C13—C14	1.384 (5)
N1—C11	1.345 (3)	C13—H13	0.93
N1—C15	1.349 (3)	C14—C15	1.384 (4)
N2—C16	1.343 (3)	C14—H14	0.93
N2—C20	1.343 (3)	C15—C16	1.488 (4)
C1—C2	1.523 (4)	C16—C17	1.386 (3)

C2—C3	1.514 (4)	C17—C18	1.375 (5)
C2—H2A	0.97	C17—H17	0.93
C2—H2B	0.97	C18—C19	1.378 (5)
C3—H3A	0.97	C18—H18	0.93
C3—H3B	0.97	C19—C20	1.374 (4)
C4—C5	1.369 (4)	C19—H19	0.93
C4—C9	1.382 (4)	C20—H20	0.93
O1—Mn1—O5^{i}	97.72 (9)	C4—C5—C6	119.0 (3)
O1—Mn1—O1W	87.71 (9)	C4—C5—H5	120.5
O5^{i}—Mn1—O1W	107.15 (8)	C6—C5—H5	120.5
O1—Mn1—N2	93.46 (9)	C5—C6—C7	121.4 (3)
O5^{i}—Mn1—N2	158.00 (8)	C5—C6—H6	119.3
O1W—Mn1—N2	92.12 (9)	C7—C6—H6	119.3
O1—Mn1—N1	163.82 (9)	C8—C7—C6	117.5 (3)
O5^{i}—Mn1—N1	92.57 (8)	C8—C7—C10	121.1 (3)
O1W—Mn1—N1	101.18 (9)	C6—C7—C10	121.4 (3)
N2—Mn1—N1	72.91 (8)	C9—C8—C7	121.4 (3)
O1—Mn1—O4^{i}	86.31 (8)	C9—C8—H8	119.3
O5^{i}—Mn1—O4^{i}	57.36 (6)	C7—C8—H8	119.3
O1W—Mn1—O4^{i}	162.32 (7)	C8—C9—C4	120.0 (3)
N2—Mn1—O4^{i}	104.83 (7)	C8—C9—H9	120.0
N1—Mn1—O4^{i}	88.80 (8)	C4—C9—H9	120.0
O1—Mn1—C10^{i}	91.29 (9)	O5—C10—O4	120.8 (2)
O5^{i}—Mn1—C10^{i}	28.63 (7)	O5—C10—C7	119.4 (2)
O1W—Mn1—C10^{i}	135.01 (8)	O4—C10—C7	119.7 (2)
N2—Mn1—C10^{i}	132.79 (8)	O5—C10—Mn1^{ii}	56.02 (12)
N1—Mn1—C10^{i}	91.82 (8)	O4—C10—Mn1^{ii}	64.93 (12)
O4^{i}—Mn1—C10^{i}	28.76 (6)	C7—C10—Mn1^{ii}	174.76 (19)
C1—O1—Mn1	133.8 (2)	N1—C11—C12	123.3 (3)
C4—O3—C3	119.1 (2)	N1—C11—H11	118.4
C10—O4—Mn1^{ii}	86.31 (14)	C12—C11—H11	118.4
C10—O5—Mn1^{ii}	95.35 (15)	C11—C12—C13	118.3 (3)
Mn1—O1W—H1W1	141 (2)	C11—C12—H12	120.9
Mn1—O1W—H1W2	100 (4)	C13—C12—H12	120.9
H1W1—O1W—H1W2	105 (5)	C12—C13—C14	119.9 (3)
C11—N1—C15	118.4 (2)	C12—C13—H13	120.1
C11—N1—Mn1	124.11 (18)	C14—C13—H13	120.1
C15—N1—Mn1	116.90 (16)	C13—C14—C15	119.1 (3)
C16—N2—C20	119.3 (2)	C13—C14—H14	120.5
C16—N2—Mn1	117.68 (15)	C15—C14—H14	120.5
C20—N2—Mn1	122.65 (19)	N1—C15—C14	121.1 (2)
O2—C1—O1	125.0 (3)	N1—C15—C16	115.7 (2)
O2—C1—C2	119.3 (3)	C14—C15—C16	123.1 (2)
O1—C1—C2	115.7 (3)	N2—C16—C17	121.1 (2)
C3—C2—C1	113.7 (2)	N2—C16—C15	116.09 (19)

C3—C2—H2A	108.8	C17—C16—C15	122.8 (2)
C1—C2—H2A	108.8	C18—C17—C16	118.9 (3)
C3—C2—H2B	108.8	C18—C17—H17	120.6
C1—C2—H2B	108.8	C16—C17—H17	120.6
H2A—C2—H2B	107.7	C17—C18—C19	120.3 (3)
O3—C3—C2	105.4 (2)	C17—C18—H18	119.8
O3—C3—H3A	110.7	C19—C18—H18	119.8
C2—C3—H3A	110.7	C20—C19—C18	117.9 (3)
O3—C3—H3B	110.7	C20—C19—H19	121.0
C2—C3—H3B	110.7	C18—C19—H19	121.0
H3A—C3—H3B	108.8	N2—C20—C19	122.5 (3)
C5—C4—O3	125.3 (3)	N2—C20—H20	118.7
C5—C4—C9	120.7 (3)	C19—C20—H20	118.7
O3—C4—C9	114.0 (3)		
$O5^{i}$—Mn1—O1—C1	88.7 (3)	C5—C6—C7—C8	0.8 (5)
O1W—Mn1—O1—C1	−18.3 (3)	C5—C6—C7—C10	−176.9 (3)
N2—Mn1—O1—C1	−110.3 (3)	C6—C7—C8—C9	−0.1 (6)
N1—Mn1—O1—C1	−142.3 (3)	C10—C7—C8—C9	177.6 (3)
$O4^{i}$—Mn1—O1—C1	145.1 (3)	C7—C8—C9—C4	−0.7 (6)
$C10^{i}$—Mn1—O1—C1	116.7 (3)	C5—C4—C9—C8	0.7 (5)
O1—Mn1—N1—C11	−141.2 (3)	O3—C4—C9—C8	−179.3 (3)
$O5^{i}$—Mn1—N1—C11	−11.6 (3)	$Mn1^{ii}$—O5—C10—O4	4.0 (3)
O1W—Mn1—N1—C11	96.4 (3)	$Mn1^{ii}$—O5—C10—C7	−176.9 (2)
N2—Mn1—N1—C11	−174.8 (3)	$Mn1^{ii}$—O4—C10—O5	−3.7 (3)
$O4^{i}$—Mn1—N1—C11	−68.9 (3)	$Mn1^{ii}$—O4—C10—C7	177.2 (2)
$C10^{i}$—Mn1—N1—C11	−40.3 (3)	C8—C7—C10—O5	−177.9 (3)
O1—Mn1—N1—C15	29.6 (5)	C6—C7—C10—O5	−0.3 (4)
$O5^{i}$—Mn1—N1—C15	159.2 (2)	C8—C7—C10—O4	1.2 (5)
O1W—Mn1—N1—C15	−92.7 (2)	C6—C7—C10—O4	178.8 (3)
N2—Mn1—N1—C15	−3.9 (2)	C15—N1—C11—C12	0.1 (5)
$O4^{i}$—Mn1—N1—C15	102.0 (2)	Mn1—N1—C11—C12	170.9 (3)
$C10^{i}$—Mn1—N1—C15	130.6 (2)	N1—C11—C12—C13	−0.6 (6)
O1—Mn1—N2—C16	−172.6 (2)	C11—C12—C13—C14	1.0 (6)
$O5^{i}$—Mn1—N2—C16	−52.0 (4)	C12—C13—C14—C15	−0.8 (6)
O1W—Mn1—N2—C16	99.5 (2)	C11—N1—C15—C14	0.1 (5)
N1—Mn1—N2—C16	−1.5 (2)	Mn1—N1—C15—C14	−171.3 (3)
$O4^{i}$—Mn1—N2—C16	−85.5 (2)	C11—N1—C15—C16	179.8 (3)
$C10^{i}$—Mn1—N2—C16	−77.7 (2)	Mn1—N1—C15—C16	8.3 (4)
O1—Mn1—N2—C20	14.6 (2)	C13—C14—C15—N1	0.3 (5)
$O5^{i}$—Mn1—N2—C20	135.2 (2)	C13—C14—C15—C16	−179.4 (3)
O1W—Mn1—N2—C20	−73.2 (2)	C20—N2—C16—C17	0.1 (5)
N1—Mn1—N2—C20	−174.3 (3)	Mn1—N2—C16—C17	−172.9 (2)
$O4^{i}$—Mn1—N2—C20	101.7 (2)	C20—N2—C16—C15	179.2 (3)
$C10^{i}$—Mn1—N2—C20	109.6 (2)	Mn1—N2—C16—C15	6.2 (4)
Mn1—O1—C1—O2	10.1 (5)	N1—C15—C16—N2	−9.7 (4)

Mn1—O1—C1—C2	−170.1 (2)	C14—C15—C16—N2	170.0 (3)
O2—C1—C2—C3	151.1 (3)	N1—C15—C16—C17	169.4 (3)
O1—C1—C2—C3	−28.7 (3)	C14—C15—C16—C17	−10.9 (5)
C4—O3—C3—C2	179.2 (2)	N2—C16—C17—C18	−0.1 (5)
C1—C2—C3—O3	−67.6 (3)	C15—C16—C17—C18	−179.1 (3)
C3—O3—C4—C5	−5.4 (5)	C16—C17—C18—C19	0.1 (6)
C3—O3—C4—C9	174.7 (3)	C17—C18—C19—C20	−0.2 (6)
O3—C4—C5—C6	180.0 (3)	C16—N2—C20—C19	−0.3 (5)
C9—C4—C5—C6	−0.1 (5)	Mn1—N2—C20—C19	172.4 (2)
C4—C5—C6—C7	−0.7 (5)	C18—C19—C20—N2	0.3 (5)

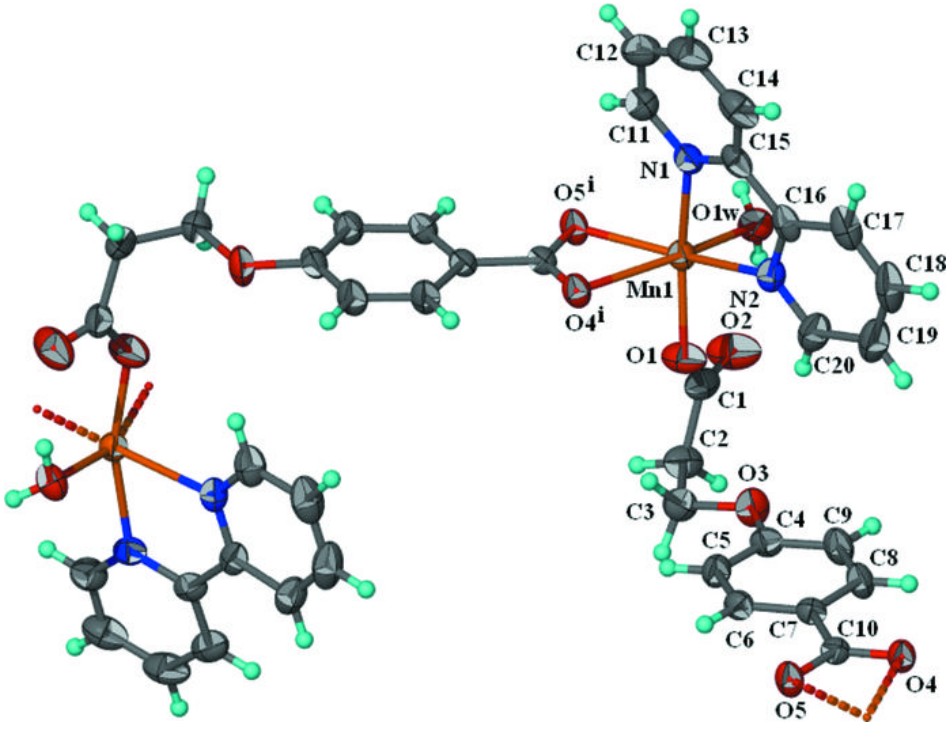
Symmetry codes: (i) −*x*+5/2, −*y*+1, *z*−1/2; (ii) −*x*+5/2, −*y*+1, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W2···O2	0.86 (1)	1.82 (2)	2.658 (3)	164 (6)
O1W—H1W1···O4^{iii}	0.85 (1)	1.96 (1)	2.797 (3)	170 (3)

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

Fig. 1


C13
C12
C14
C11
C15
N1
O5i
O1w
C16
C17
C18
Mn1
N2
O4i
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C19
O1
C20
C1
C2
O3
C3
C4
C9
C5
C8
C6
C7
C10
O4
O5

Fig. 2