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Poly[[aqua(2,2-bipyridyl)(μ_3-pyridine-3,4-dicarboxylato)manganese(II)] monohydrate]

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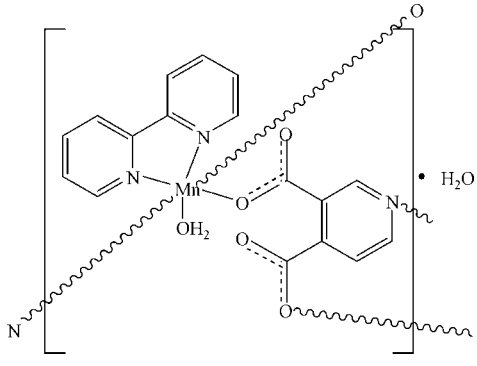
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.092; data-to-parameter ratio = 12.7.

In the title compound, $\{[Mn(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]\cdot H_2O\}_n$, the Mn(II) atom has a distorted *fac*-MnN_3O_3 octahedral coordination geometry, defined by one *N*,*N*′-chelating bipyridine molecule, one N-bonded pyridine-3,4-dicarboxylate (pdb) anion, two monodentate O-bonded pdb anions and one water molecule. Adjacent Mn^{II} ions are bridged by pairs of pdb ligands to form distinctive squares, which are further linked by other pdb ligands to result in a layered coordination polymer exhibiting a wave-like structure. Hydrogen bonds involving both the coordinated and uncoordinated water molecules help to consolidate the structure.

Related literature

For related literature, see: Biradha *et al.* (2000); Cao *et al.* (2003); Eddaoudi *et al.* (2001); Kortz *et al.* (2003); Moulton & Zaworotko (2001); Noro *et al.* (2000); Pan *et al.* (2003).



Experimental

Crystal data

$[Mn(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)].H_2O$
M_r = 412.26
Orthorhombic, *Pbca*
a = 15.614 (2) Å
b = 12.4561 (18) Å
c = 16.870 (3) Å
V = 3281.1 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 292 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
26510 measured reflections
3249 independent reflections
2562 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.01
3249 reflections
256 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O3^{i}	2.1091 (16)	Mn1—N2	2.2401 (19)
Mn1—O1	2.1303 (15)	Mn1—N1	2.2888 (18)
Mn1—O6	2.2221 (17)	Mn1—N4^{ii}	2.3552 (18)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O2^{iii}	0.84 (3)	2.01 (3)	2.838 (3)	174 (3)
O5—H2W···O4	0.85 (3)	1.93 (3)	2.779 (3)	170 (3)
O6—H3W···O5^{iv}	0.96 (3)	1.90 (4)	2.834 (2)	165 (3)
O6—H4W···O2	0.82	1.96	2.659 (2)	143

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

We thank Professors Ning-Hai Hu and Heng-Qing Jia from Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, for their help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2406).

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supplementary materials

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Poly[[aqua(2,2-bipyridyl)(μ_3-pyridine-3,4-dicarboxylato)manganese(II)] monohydrate]

X.-M. Li, Y.-L. Niu, Q.-W. Wang and B. Liu

Comment

Due to both their structural and topological novelty as well as for their potential applications as functional materials, the rational design of inorganic coordination networks has attracted much recent attention (Biradha *et al.*, 2000, Moulton *et al.*, 2001, Eddaoudi *et al.*, 2001, Cao *et al.*, 2003, Kortz *et al.*, 2003). To date, a variety of extended frameworks have been obtained through the use of polydentate ligands, such as polycarboxylic acids (Pan *et al.*, 2003, Noro *et al.*, 2000). Herein, we report the crystal structure of the title compound, (I), which shows a layered polymeric structure.

The Mn^{II} ion in (I) has a distorted octahedral coordination geometry, defined by three N atoms and three carboxyl O atoms from chelating bipy, pyridine-3,4-dicarboxylate (pdb) ligands and one water molecule (Fig. 1, Table 1) The polymeric layers in (I) feature squares constructed from two Mn^{II} ions bridged by two pdb ligands. Such squares are further connected by pdb ligands, forming a sheet (Fig. 2). A network of O—H···O hydrogen bonds arising from the water molecules (Table 2) helps to consolidate the structure.

Experimental

Compound (I) was prepared from a mixture of $Mn(CH_3CO_2)_2{\cdot}4H_2O$ (0.120 g, 0.5 mmol), pyridine-3,4-dicarboxylic acid (0.083 g, 0.5 mmol), 2,2-bipyridine (0.078 g, 0.5 mmol) and H_2O (18 ml) in a 30 ml Teflon-lined autoclave under autogenous pressure at 423 K for 5 d. After cooling to room temperature, yellow crystals suitable for X-ray structure analysis were obtained. Analysis, calculated for $C_{17}H_{15}MnN_3O_6$: C 49.5, H 3.7, N 10.2%; found: C 49.4, H 3.6, N 10.0%.

Refinement

The C-bonded H atoms and H4W were generated geometrically (C—H = 0.93 Å, O—H =0.82 Å) and refined as riding with U_{iso}(H)= 1.2U_{eq}(C) or U_{iso}(H4W) = 0.05 Å^2. The other H atoms of the water molecules were located in difference maps and their positions and U_{iso} values were freely refined.

Figures

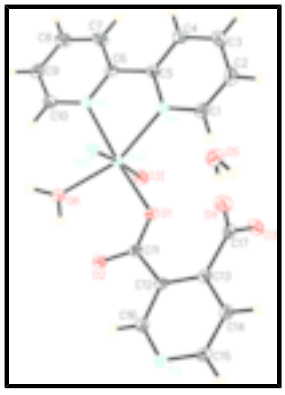

Fig. 1. The asymmetric unit of (I) expanded to show the coordination of the Mn atom drawn with 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). Atoms O3I and N4I are at the symmetry positions (1 − *x*, −*y*, −*z*) and (1/2 − *x*, 3/2 − *y*, *z*) respectively.

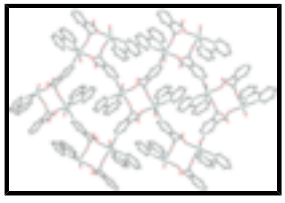

Fig. 2. Part of a polymeric layer in (I). Mn atoms are represented by green hatched spheres, N atoms by blue dotted spheres, O atoms by red grid spheres, and C atoms by grey spheres. H atoms have been omitted for clarity.

Poly[[aqua(2,2-bipyridyl)(μ$_3$pyridine-3,4-dicarboxylato)manganese(II)] monohydrate]

Crystal data

$[Mn(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]\cdot H_2O$	F_{000} = 1688
M_r = 412.26	D_x = 1.669 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	θ = 2.4–26.1°
a = 15.614 (2) Å	μ = 0.85 mm^{-1}
b = 12.4561 (18) Å	*T* = 292 (2) K
c = 16.870 (3) Å	Block, yellow
V = 3281.1 (8) Å^3	0.10 × 0.10 × 0.10 mm
Z = 8	

Data collection

Bruker SMART CCD diffractometer	2562 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.073
Monochromator: graphite	θ_{max} = 26.1°
T = 292(2) K	θ_{min} = 2.4°
ω scans	*h* = −19→19
Absorption correction: none	*k* = −15→15
26510 measured reflections	*l* = −20→20
3249 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
3249 reflections	$\Delta\rho_{max} = 0.55$ e Å^{-3}
256 parameters	$\Delta\rho_{min} = -0.55$ 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	0.43851 (2)	0.18948 (3)	−0.06880 (2)	0.02453 (12)
C13	0.31857 (13)	−0.12791 (17)	0.07018 (13)	0.0244 (5)
O2	0.30663 (11)	0.00140 (13)	−0.12384 (10)	0.0383 (4)
O1	0.38982 (9)	0.04326 (11)	−0.02127 (9)	0.0296 (4)
N2	0.51764 (11)	0.25010 (14)	0.03251 (11)	0.0264 (4)
O5	0.26473 (12)	0.13867 (14)	0.26106 (12)	0.0387 (4)
C16	0.22594 (13)	−0.15776 (17)	−0.04054 (13)	0.0257 (5)
H16A	0.2094	−0.1383	−0.0915	0.031*
N4	0.18302 (11)	−0.23754 (15)	−0.00607 (11)	0.0295 (4)
N1	0.49150 (11)	0.35320 (15)	−0.10606 (11)	0.0269 (4)
C14	0.27565 (14)	−0.21355 (18)	0.10597 (15)	0.0321 (5)
H14A	0.2913	−0.2358	0.1566	0.038*
C15	0.20980 (15)	−0.26556 (19)	0.06634 (14)	0.0331 (6)
H4A	0.1829	−0.3229	0.0914	0.040*
C1	0.52431 (15)	0.20098 (19)	0.10279 (15)	0.0339 (6)
H1A	0.4924	0.1391	0.1117	0.041*
C2	0.57649 (16)	0.2385 (2)	0.16233 (15)	0.0422 (6)

H2A	0.5797	0.2024	0.2105	0.051*
C12	0.29349 (13)	−0.10105 (16)	−0.00670 (12)	0.0227 (5)
C11	0.33328 (13)	−0.01213 (16)	−0.05444 (13)	0.0242 (5)
C10	0.47938 (15)	0.40019 (19)	−0.17620 (14)	0.0332 (5)
H10A	0.4357	0.3740	−0.2083	0.040*
C9	0.52727 (16)	0.48483 (19)	−0.20416 (15)	0.0368 (6)
H9A	0.5160	0.5157	−0.2532	0.044*
C5	0.56416 (13)	0.33975 (18)	0.01934 (13)	0.0255 (5)
C4	0.61805 (15)	0.38030 (19)	0.07749 (14)	0.0347 (6)
H4B	0.6503	0.4416	0.0677	0.042*
C3	0.62353 (16)	0.3293 (2)	0.14975 (16)	0.0428 (6)
H3A	0.6588	0.3564	0.1894	0.051*
C6	0.55396 (13)	0.39158 (18)	−0.05899 (13)	0.0261 (5)
C7	0.60589 (17)	0.4750 (2)	−0.08444 (15)	0.0442 (7)
H7A	0.6502	0.4993	−0.0522	0.053*
C8	0.59225 (18)	0.5219 (2)	−0.15697 (16)	0.0456 (7)
H8A	0.6268	0.5782	−0.1739	0.055*
C17	0.38450 (14)	−0.06848 (17)	0.11963 (12)	0.0263 (5)
O3	0.45903 (10)	−0.10620 (13)	0.12223 (10)	0.0372 (4)
O4	0.35811 (11)	0.00841 (14)	0.15903 (10)	0.0412 (4)
O6	0.36338 (11)	0.18742 (13)	−0.18066 (10)	0.0335 (4)
H4W	0.3344	0.1326	−0.1825	0.050*
H1W	0.2400 (18)	0.100 (2)	0.2944 (18)	0.053 (9)*
H2W	0.2883 (19)	0.093 (3)	0.2303 (18)	0.064 (10)*
H3W	0.322 (2)	0.241 (3)	−0.195 (2)	0.080 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.02398 (19)	0.01951 (19)	0.0301 (2)	−0.00234 (13)	−0.00148 (14)	0.00011 (13)
C13	0.0207 (10)	0.0215 (11)	0.0309 (12)	0.0045 (8)	0.0042 (9)	−0.0009 (9)
O2	0.0512 (10)	0.0328 (9)	0.0309 (10)	−0.0135 (8)	−0.0092 (8)	0.0064 (7)
O1	0.0304 (8)	0.0228 (8)	0.0356 (9)	−0.0064 (7)	−0.0020 (7)	0.0023 (7)
N2	0.0245 (9)	0.0243 (10)	0.0304 (11)	−0.0005 (8)	0.0017 (8)	0.0009 (8)
O5	0.0482 (11)	0.0335 (10)	0.0342 (10)	0.0002 (9)	0.0064 (9)	0.0004 (9)
C16	0.0287 (11)	0.0239 (11)	0.0245 (11)	0.0004 (9)	0.0007 (9)	0.0005 (9)
N4	0.0278 (10)	0.0269 (10)	0.0337 (11)	−0.0040 (8)	−0.0004 (9)	0.0010 (8)
N1	0.0250 (10)	0.0260 (10)	0.0297 (11)	−0.0031 (8)	−0.0018 (8)	0.0023 (8)
C14	0.0333 (13)	0.0332 (13)	0.0297 (13)	−0.0003 (10)	−0.0022 (10)	0.0074 (10)
C15	0.0325 (13)	0.0280 (13)	0.0388 (14)	−0.0083 (10)	0.0009 (11)	0.0063 (10)
C1	0.0320 (12)	0.0322 (14)	0.0376 (14)	−0.0019 (10)	0.0020 (11)	0.0073 (11)
C2	0.0431 (15)	0.0502 (17)	0.0334 (15)	0.0013 (12)	−0.0033 (12)	0.0115 (12)
C12	0.0224 (10)	0.0181 (11)	0.0275 (12)	0.0005 (8)	0.0047 (9)	−0.0023 (9)
C11	0.0233 (11)	0.0176 (11)	0.0317 (13)	0.0013 (9)	0.0015 (9)	−0.0017 (9)
C10	0.0330 (13)	0.0352 (14)	0.0314 (13)	−0.0052 (10)	−0.0044 (10)	0.0013 (10)
C9	0.0444 (14)	0.0333 (14)	0.0328 (14)	−0.0035 (11)	0.0013 (11)	0.0069 (11)
C5	0.0223 (11)	0.0241 (11)	0.0301 (12)	0.0007 (9)	0.0012 (9)	−0.0026 (9)
C4	0.0347 (13)	0.0306 (13)	0.0387 (15)	−0.0080 (10)	−0.0065 (11)	−0.0003 (10)

C3	0.0401 (15)	0.0492 (17)	0.0391 (15)	−0.0034 (12)	−0.0112 (12)	−0.0023 (12)
C6	0.0250 (11)	0.0220 (11)	0.0311 (13)	−0.0016 (9)	0.0015 (9)	−0.0033 (9)
C7	0.0466 (16)	0.0447 (16)	0.0412 (16)	−0.0250 (13)	−0.0087 (12)	0.0040 (12)
C8	0.0552 (16)	0.0407 (16)	0.0408 (16)	−0.0225 (13)	−0.0001 (13)	0.0075 (12)
C17	0.0298 (12)	0.0271 (12)	0.0219 (12)	0.0013 (10)	0.0031 (9)	0.0041 (9)
O3	0.0258 (9)	0.0431 (10)	0.0428 (11)	0.0092 (7)	−0.0034 (7)	−0.0098 (8)
O4	0.0454 (10)	0.0365 (10)	0.0416 (11)	0.0110 (8)	−0.0012 (8)	−0.0153 (8)
O6	0.0355 (9)	0.0281 (9)	0.0370 (10)	−0.0046 (7)	−0.0038 (8)	−0.0006 (7)

Geometric parameters (Å, °)

Mn1—O3^{i}	2.1091 (16)	C15—H4A	0.9300
Mn1—O1	2.1303 (15)	C1—C2	1.375 (4)
Mn1—O6	2.2221 (17)	C1—H1A	0.9300
Mn1—N2	2.2401 (19)	C2—C3	1.365 (4)
Mn1—N1	2.2888 (18)	C2—H2A	0.9300
Mn1—N4^{ii}	2.3552 (18)	C12—C11	1.504 (3)
C13—C12	1.395 (3)	C10—C9	1.376 (3)
C13—C14	1.397 (3)	C10—H10A	0.9300
C13—C17	1.518 (3)	C9—C8	1.370 (4)
O2—C11	1.254 (3)	C9—H9A	0.9300
O1—C11	1.252 (2)	C5—C4	1.388 (3)
N2—C1	1.338 (3)	C5—C6	1.479 (3)
N2—C5	1.351 (3)	C4—C3	1.377 (4)
O5—H1W	0.83 (3)	C4—H4B	0.9300
O5—H2W	0.86 (3)	C3—H3A	0.9300
C16—N4	1.332 (3)	C6—C7	1.386 (3)
C16—C12	1.392 (3)	C7—C8	1.372 (4)
C16—H16A	0.9300	C7—H7A	0.9300
N4—C15	1.337 (3)	C8—H8A	0.9300
N4—Mn1^{iii}	2.3552 (18)	C17—O4	1.236 (3)
N1—C10	1.334 (3)	C17—O3	1.256 (2)
N1—C6	1.345 (3)	O3—Mn1^{i}	2.1091 (16)
C14—C15	1.387 (3)	O6—H4W	0.8200
C14—H14A	0.9300	O6—H3W	0.96 (3)
O3^{i}—Mn1—O1	90.63 (6)	C3—C2—C1	119.1 (2)
O3^{i}—Mn1—O6	91.82 (6)	C3—C2—H2A	120.4
O1—Mn1—O6	96.97 (6)	C1—C2—H2A	120.4
O3^{i}—Mn1—N2	94.21 (6)	C16—C12—C13	118.18 (19)
O1—Mn1—N2	101.41 (6)	C16—C12—C11	117.85 (19)
O6—Mn1—N2	160.57 (6)	C13—C12—C11	123.94 (19)
O3^{i}—Mn1—N1	92.67 (7)	O1—C11—O2	125.2 (2)
O1—Mn1—N1	173.81 (6)	O1—C11—C12	117.24 (19)
O6—Mn1—N1	88.16 (6)	O2—C11—C12	117.50 (18)
N2—Mn1—N1	73.13 (7)	N1—C10—C9	124.3 (2)
O3^{i}—Mn1—N4^{ii}	173.24 (7)	N1—C10—H10A	117.9
O1—Mn1—N4^{ii}	82.73 (6)	C9—C10—H10A	117.9

O6—Mn1—N4^{ii}	87.75 (6)	C8—C9—C10	117.5 (2)
N2—Mn1—N4^{ii}	88.36 (6)	C8—C9—H9A	121.3
N1—Mn1—N4^{ii}	94.06 (6)	C10—C9—H9A	121.3
C12—C13—C14	116.8 (2)	N2—C5—C4	120.7 (2)
C12—C13—C17	125.75 (19)	N2—C5—C6	116.74 (19)
C14—C13—C17	117.39 (19)	C4—C5—C6	122.5 (2)
C11—O1—Mn1	123.67 (14)	C3—C4—C5	119.7 (2)
C1—N2—C5	118.81 (19)	C3—C4—H4B	120.1
C1—N2—Mn1	124.39 (15)	C5—C4—H4B	120.1
C5—N2—Mn1	116.73 (15)	C2—C3—C4	119.1 (2)
H1W—O5—H2W	103 (3)	C2—C3—H3A	120.5
N4—C16—C12	125.5 (2)	C4—C3—H3A	120.5
N4—C16—H16A	117.2	N1—C6—C7	120.5 (2)
C12—C16—H16A	117.2	N1—C6—C5	116.75 (19)
C16—N4—C15	115.85 (19)	C7—C6—C5	122.7 (2)
C16—N4—Mn1^{iii}	119.81 (15)	C8—C7—C6	120.3 (2)
C15—N4—Mn1^{iii}	124.16 (15)	C8—C7—H7A	119.9
C10—N1—C6	118.1 (2)	C6—C7—H7A	119.9
C10—N1—Mn1	125.69 (15)	C9—C8—C7	119.3 (2)
C6—N1—Mn1	114.62 (14)	C9—C8—H8A	120.3
C15—C14—C13	120.3 (2)	C7—C8—H8A	120.3
C15—C14—H14A	119.9	O4—C17—O3	125.4 (2)
C13—C14—H14A	119.9	O4—C17—C13	116.58 (19)
N4—C15—C14	123.4 (2)	O3—C17—C13	117.72 (19)
N4—C15—H4A	118.3	C17—O3—Mn1^{i}	150.70 (16)
C14—C15—H4A	118.3	Mn1—O6—H4W	109.5
N2—C1—C2	122.5 (2)	Mn1—O6—H3W	124 (2)
N2—C1—H1A	118.7	H4W—O6—H3W	101.7
C2—C1—H1A	118.7		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1W···O2^{iv}	0.84 (3)	2.01 (3)	2.838 (3)	174 (3)
O5—H2W···O4	0.85 (3)	1.93 (3)	2.779 (3)	170 (3)
O6—H3W···O5^{v}	0.96 (3)	1.90 (4)	2.834 (2)	165 (3)
O6—H4W···O2	0.82	1.96	2.659 (2)	143

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

Fig. 1

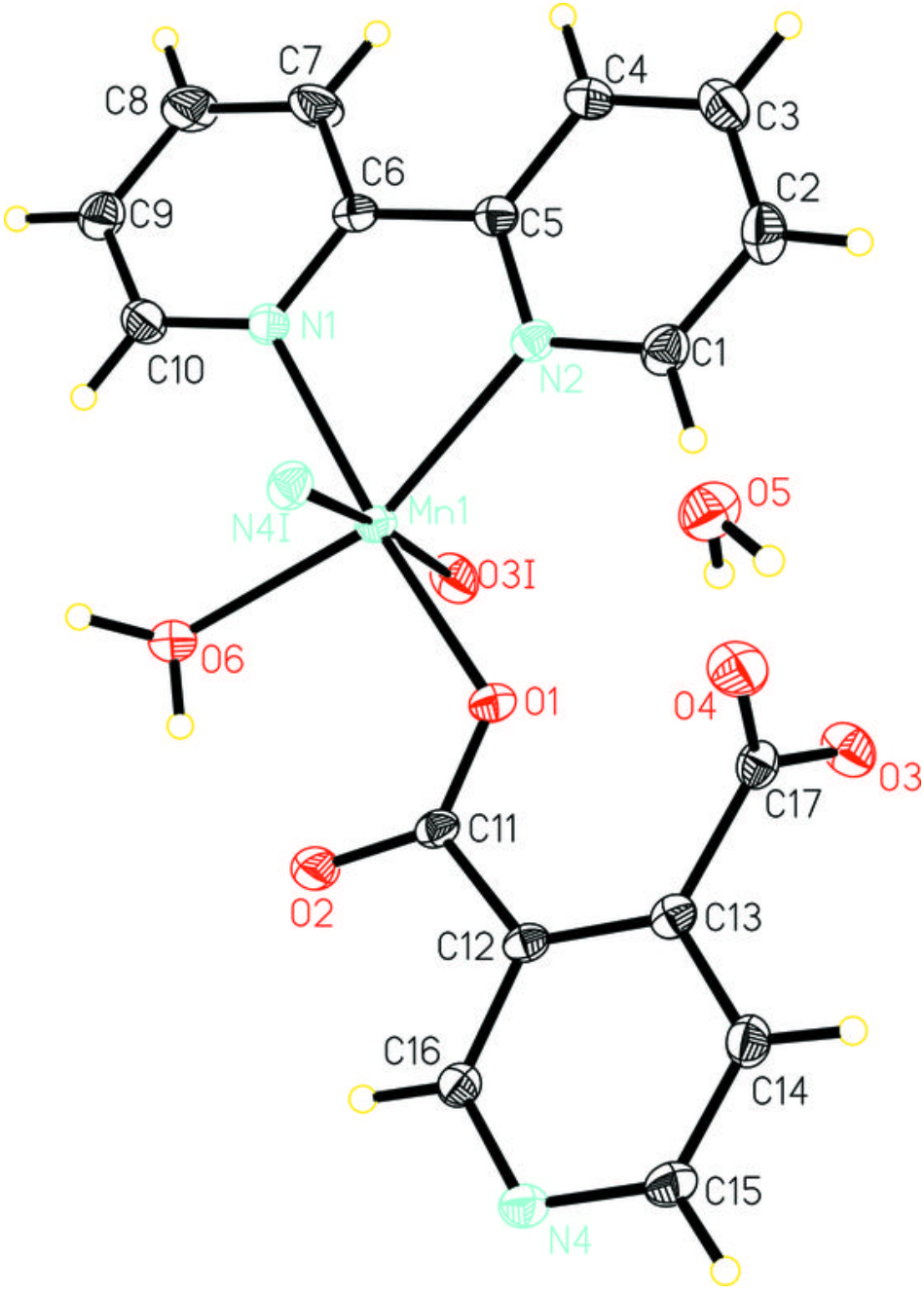
C7
C8
C4
C3
C6
C2
C9
C5
N1
C1
C10
N2
N4I
Mn1
O5
O3I
O6
O1
O4
O3
C17
C11
O2
C13
C12
C16
C14
C15
N4

Fig. 2