Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[diaqua(ethanol)bis(μ_3-pyridine-2,3-dicarboxylato)dimanganese(II)] monohydrate]

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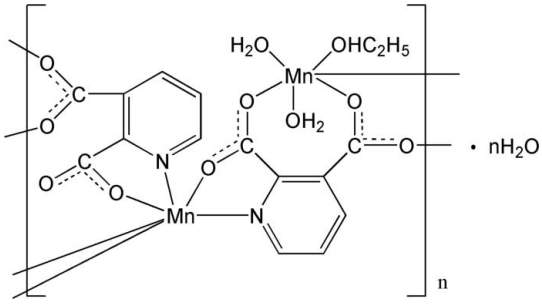
Received 18 July 2009; accepted 12 August 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.124; data-to-parameter ratio = 14.9.

The title compound, $\{[Mn_2(C_7H_3NO_4)_2(C_2H_5OH)(H_2O)_2]\cdot H_2O\}_n$, is a three-dimensional polymer. There are two symmetry-independent Mn^{II} centres with different coordination environments: one Mn^{II} atom is coordinated by four O atoms from four ligands and two N atoms from two ligands, the other Mn^{II} atom is coordinated by three O atoms from two ligands, two water O atoms and the O atom of an ethanol molecule. The crystal structure is stabilized by O—H···O hydrogen bonds.

Related literature

For a related structure, see: Li & Li (2004).



Experimental

Crystal data

$[Mn_2(C_7H_3NO_4)_2(C_2H_6O)(H_2O)_2]\cdot H_2O$
M_r = 540.20
Triclinic, $P\overline{1}$
a = 8.4972 (3) Å
b = 10.2676 (4) Å
c = 12.6508 (4) Å
α = 72.661 (3)°
β = 74.859 (3)°
γ = 70.588 (3)°
V = 977.43 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.36 mm^{-1}
T = 293 K
0.34 × 0.23 × 0.19 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.765, T_{max} = 0.876 (expected range = 0.674–0.772)
11238 measured reflections
4623 independent reflections
3432 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.124
S = 1.04
4623 reflections
310 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O3^{i}	0.827 (18)	2.29 (3)	3.083 (3)	161 (5)
O1W—H1B···O1	0.872 (18)	2.51 (4)	2.847 (4)	104 (3)
O1W—H1B···O3W^{i}	0.872 (18)	2.63 (5)	3.034 (4)	109 (4)
O2W—H2B···O5^{ii}	0.833 (18)	1.91 (2)	2.730 (3)	168 (5)
O3W—H3B···O1W	0.777 (16)	2.14 (2)	2.893 (4)	162 (3)
O3W—H3A···O6^{ii}	0.793 (16)	1.99 (2)	2.699 (3)	150 (4)
O9—H9A···O8^{iii}	0.821 (19)	2.10 (3)	2.776 (3)	140 (3)
O9—H9A···O4^{iv}	0.821 (19)	2.319 (18)	3.006 (3)	142 (3)

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $x-1, y+1, z$; (iii) $-x+2, -y+1, -z$; (iv) $x-1, y, z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors thank the Science Foundation of Liaoning Medical University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5015).

References

Li, L.-J. & Li, Y. (2004). *J. Mol. Struct.* pp. 199–203.
Oxford Diffraction (2006). *CrysAlis RED* and *CrysAlis CCD*. Oxford Diffraction Ltd, Abingdon, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2009). E**65**, m1092 [**doi:10.1107/S1600536809031948**]

Poly[[diaqua(ethanol)bis(μ_3-pyridine-2,3-dicarboxylato)dimanganese(II)] monohydrate]

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Comment

The title compound possesses two crystallographically unique manganese cations (Fig. 1, Table 1). The Mn(1) cation :is coordinated by four oxygen atoms from four *L* ligands and two N atoms from two *L* ligands. Mn(2) cation is coordinated by three oxygen atoms from two *L* ligands, two water molecules and one ethanol molecule . The Mn—O and Mn—N distances are within the normal range observed in the structure of Li & Li (2004). In the title compound, the manganese centres are bridged by *L* ligands to form an infinite two-dimensional layer structure. Further, the water molecules and ethanol are involved in formation of hydrogen-bonding interations, leading to a three-dimensional structure.

Experimental

A mixture of pyridine-2,3-dicarboxylic acid (0.05 g, 0.3 mmol), $MnAc_2.4H_2O$ (0.07 g, 0.3 mmol), EtOH (3 ml) and H_2O (7 ml) was sealed in a 17 ml Teflon-lined stainless-steel cotainer. The container was heated to 140 °C and held at this temperature for 72 h. It was then cooled to room temperature at a rate of 10 °C.h^{-1}. The colorless blocks were collected in 35% yield.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H)= 1.2U_{eq}(C). H-atoms bonded to water molecules were located in a different Fourier map and refined isotropically.

Figures

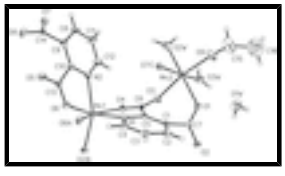


Fig. 1. Anisotropic displacement ellipsoid (30%) plot of the title compound showing the co-ordination environment around the Mn atoms. [symmetry code: (A) -*x* + 3, -*y* + 1, -*z*; (B) -*x* + 2, -*y* + 1,-*z* + 1; (*c*) -*x* + 2, -*y* + 1, -*z*].

Poly[[diaqua(ethanol)bis(μ$_3$-pyridine-2,3-dicarboxylato)dimanganese(II)] monohydrate]

Crystal data

$[Mn_2(C_7H_3NO_4)_2(C_2H_6O)(H_2O)_2]\cdot H_2O$	Z = 2
M_r = 540.20	F_{000} = 548
Triclinic, $P\overline{1}$	D_x = 1.835 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 8.4972 (3) Å	Cell parameters from 4623 reflections

b = 10.2676 (4) Å	θ = 1.7–29.3º
c = 12.6508 (4) Å	μ = 1.36 mm^{-1}
α = 72.661 (3)º	T = 293 K
β = 74.859 (3)º	Block, colorless
γ = 70.588 (3)º	0.34 × 0.23 × 0.19 mm
V = 977.43 (6) Å^3	

Data collection

Oxford Diffraction Gemini R Ultra diffractometer	4623 independent reflections
Radiation source: fine-focus sealed tube	3432 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 29.3º
T = 293 K	θ_{min} = 1.7º
ω scans	h = −10→11
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	k = −11→14
T_{min} = 0.765, T_{max} = 0.876	l = −17→16
11238 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.124	$w = 1/[\sigma^2(F_o^2) + (0.0787P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4623 reflections	$\Delta\rho_{max}$ = 0.72 e Å^{-3}
310 parameters	$\Delta\rho_{min}$ = −0.89 e Å^{-3}
10 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	1.27969 (5)	0.49235 (4)	0.24918 (3)	0.02484 (13)
Mn2	0.59087 (5)	0.85545 (4)	0.26515 (3)	0.02779 (14)
C1	0.7656 (3)	0.5490 (3)	0.4552 (2)	0.0231 (5)
C2	0.7464 (4)	0.4128 (3)	0.4991 (2)	0.0308 (6)
H2	0.6522	0.3986	0.5534	0.037*
C3	0.8660 (4)	0.2984 (3)	0.4627 (3)	0.0336 (7)
H3	0.8522	0.2074	0.4900	0.040*
C4	1.0063 (4)	0.3234 (3)	0.3846 (3)	0.0336 (7)
H4	1.0883	0.2469	0.3604	0.040*
C5	0.9105 (3)	0.5653 (3)	0.3738 (2)	0.0228 (5)
C6	0.9532 (3)	0.7047 (3)	0.3163 (2)	0.0230 (5)
C7	0.6300 (3)	0.6661 (3)	0.5036 (2)	0.0247 (6)
C8	1.2344 (5)	0.6470 (3)	−0.1599 (3)	0.0461 (9)
H8	1.2322	0.6728	−0.2366	0.055*
C9	1.3034 (4)	0.5069 (3)	−0.1091 (2)	0.0262 (6)
C10	1.3014 (3)	0.4728 (3)	0.0062 (2)	0.0248 (6)
C11	1.1694 (6)	0.7478 (4)	−0.0978 (3)	0.0575 (11)
H11	1.1259	0.8428	−0.1317	0.069*
C12	1.1699 (5)	0.7052 (3)	0.0170 (3)	0.0510 (10)
H12	1.1226	0.7727	0.0600	0.061*
C13	1.3785 (4)	0.3243 (3)	0.0709 (2)	0.0280 (6)
C14	1.3882 (4)	0.4007 (3)	−0.1817 (2)	0.0247 (6)
C15	0.1882 (8)	0.9931 (7)	0.2423 (7)	0.112 (2)
H17A	0.1739	1.0126	0.1650	0.135*
H17B	0.2214	1.0725	0.2473	0.135*
C16	0.0088 (13)	1.0105 (12)	0.3108 (9)	0.186 (4)
H18A	−0.0615	1.1033	0.2827	0.279*
H18B	0.0118	0.9994	0.3884	0.279*
H18C	−0.0368	0.9399	0.3044	0.279*
N1	1.0296 (3)	0.4528 (2)	0.34232 (19)	0.0269 (5)
N2	1.2358 (3)	0.5708 (2)	0.06771 (19)	0.0311 (5)
O1	0.5328 (3)	0.7618 (2)	0.44223 (16)	0.0346 (5)
O2	0.6140 (3)	0.6560 (2)	0.60686 (16)	0.0359 (5)
O3	0.8368 (3)	0.8183 (2)	0.31103 (17)	0.0329 (5)
O9	0.3290 (3)	0.8821 (3)	0.2514 (3)	0.0522 (7)
O4	1.1066 (2)	0.6962 (2)	0.27672 (16)	0.0301 (4)
O3W	0.5052 (4)	1.0585 (2)	0.3092 (2)	0.0479 (6)
O5	1.4375 (3)	0.2271 (2)	0.02105 (17)	0.0443 (6)
O6	1.3777 (3)	0.3112 (2)	0.17400 (15)	0.0346 (5)
O1W	0.2771 (5)	0.9922 (4)	0.5189 (3)	0.0725 (9)
O7	1.3037 (3)	0.3305 (2)	−0.19511 (16)	0.0308 (4)
O8	1.5393 (3)	0.3966 (2)	−0.22933 (17)	0.0375 (5)
O2W	0.6507 (4)	0.9652 (3)	0.0894 (2)	0.0520 (6)
H9A	0.316 (3)	0.806 (3)	0.253 (4)	0.078*
H3A	0.502 (6)	1.1229 (18)	0.2557 (19)	0.078*

H1A	0.224 (6)	1.047 (3)	0.561 (3)	0.078*
H1B	0.312 (6)	0.911 (3)	0.565 (3)	0.078*
H3B	0.444 (5)	1.058 (3)	0.367 (2)	0.078*
H2B	0.575 (4)	1.039 (3)	0.070 (3)	0.078*
H2A	0.735 (4)	0.957 (5)	0.034 (3)	0.078*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0302 (2)	0.0226 (2)	0.0194 (2)	−0.00310 (17)	−0.00298 (15)	−0.00753 (16)
Mn2	0.0325 (2)	0.0222 (2)	0.0268 (2)	−0.00084 (18)	−0.01131 (17)	−0.00549 (17)
C1	0.0275 (13)	0.0246 (14)	0.0169 (11)	−0.0044 (11)	−0.0081 (10)	−0.0041 (10)
C2	0.0356 (16)	0.0301 (16)	0.0276 (14)	−0.0129 (13)	−0.0044 (12)	−0.0045 (12)
C3	0.0442 (18)	0.0216 (14)	0.0356 (15)	−0.0107 (13)	−0.0084 (13)	−0.0044 (12)
C4	0.0388 (17)	0.0234 (15)	0.0388 (16)	−0.0042 (12)	−0.0078 (13)	−0.0117 (12)
C5	0.0274 (13)	0.0202 (13)	0.0212 (12)	−0.0025 (10)	−0.0097 (10)	−0.0051 (10)
C6	0.0282 (14)	0.0227 (13)	0.0202 (12)	−0.0050 (11)	−0.0074 (10)	−0.0078 (10)
C7	0.0280 (14)	0.0244 (14)	0.0221 (13)	−0.0078 (11)	−0.0059 (10)	−0.0040 (11)
C8	0.071 (2)	0.0328 (18)	0.0285 (15)	0.0059 (16)	−0.0250 (15)	−0.0073 (13)
C9	0.0315 (14)	0.0242 (14)	0.0237 (13)	−0.0045 (11)	−0.0094 (11)	−0.0065 (11)
C10	0.0270 (13)	0.0227 (14)	0.0240 (13)	−0.0031 (11)	−0.0061 (10)	−0.0071 (10)
C11	0.094 (3)	0.0254 (18)	0.0385 (18)	0.0162 (18)	−0.0316 (19)	−0.0071 (15)
C12	0.080 (3)	0.0265 (17)	0.0387 (18)	0.0139 (16)	−0.0243 (17)	−0.0165 (14)
C13	0.0343 (15)	0.0239 (14)	0.0243 (13)	−0.0040 (12)	−0.0064 (11)	−0.0070 (11)
C14	0.0335 (15)	0.0207 (13)	0.0177 (12)	−0.0019 (11)	−0.0094 (10)	−0.0034 (10)
C15	0.076 (4)	0.094 (5)	0.180 (7)	−0.020 (3)	−0.040 (4)	−0.038 (5)
C16	0.156 (9)	0.191 (10)	0.215 (11)	−0.085 (8)	−0.053 (8)	0.007 (8)
N1	0.0295 (12)	0.0221 (12)	0.0276 (11)	−0.0033 (9)	−0.0053 (9)	−0.0078 (9)
N2	0.0400 (14)	0.0230 (12)	0.0258 (12)	0.0030 (10)	−0.0099 (10)	−0.0088 (10)
O1	0.0335 (11)	0.0334 (12)	0.0268 (10)	0.0020 (9)	−0.0081 (8)	−0.0024 (8)
O2	0.0414 (12)	0.0378 (12)	0.0232 (10)	0.0020 (10)	−0.0093 (8)	−0.0110 (9)
O3	0.0318 (11)	0.0210 (10)	0.0471 (12)	−0.0023 (8)	−0.0143 (9)	−0.0089 (9)
O9	0.0416 (13)	0.0287 (13)	0.0922 (19)	0.0047 (10)	−0.0303 (13)	−0.0227 (13)
O4	0.0300 (10)	0.0247 (10)	0.0336 (10)	−0.0071 (8)	0.0011 (8)	−0.0102 (8)
O3W	0.0725 (18)	0.0252 (12)	0.0428 (13)	0.0015 (12)	−0.0236 (13)	−0.0089 (10)
O5	0.0772 (17)	0.0218 (11)	0.0275 (11)	0.0061 (10)	−0.0203 (11)	−0.0094 (9)
O6	0.0564 (14)	0.0230 (10)	0.0195 (9)	0.0006 (9)	−0.0126 (9)	−0.0058 (8)
O1W	0.078 (2)	0.083 (2)	0.074 (2)	−0.0251 (19)	−0.0054 (17)	−0.0475 (18)
O7	0.0334 (11)	0.0302 (11)	0.0317 (10)	−0.0053 (9)	−0.0095 (8)	−0.0120 (9)
O8	0.0367 (12)	0.0396 (12)	0.0402 (12)	−0.0140 (10)	0.0035 (9)	−0.0199 (10)
O2W	0.0574 (16)	0.0420 (15)	0.0408 (13)	−0.0039 (12)	−0.0133 (11)	0.0058 (11)

Geometric parameters (Å, °)

Mn1—O8^{i}	2.127 (2)	C9—C10	1.392 (4)
Mn1—O6	2.1612 (19)	C9—C14	1.510 (4)
Mn1—O2^{ii}	2.178 (2)	C10—N2	1.339 (3)
Mn1—O4	2.1874 (19)	C10—C13	1.515 (4)

Mn1—N1	2.247 (2)	C11—C12	1.386 (5)
Mn1—N2	2.281 (2)	C11—H11	0.9300
Mn2—O1	2.1542 (19)	C12—N2	1.333 (4)
Mn2—O3W	2.158 (2)	C12—H12	0.9300
Mn2—O7^{iii}	2.1653 (19)	C13—O5	1.235 (3)
Mn2—O2W	2.184 (2)	C13—O6	1.269 (3)
Mn2—O3	2.195 (2)	C14—O7	1.244 (3)
Mn2—O9	2.196 (3)	C14—O8	1.260 (3)
C1—C2	1.390 (4)	C15—O9	1.353 (6)
C1—C5	1.406 (4)	C15—C16	1.526 (11)
C1—C7	1.516 (4)	C15—H17A	0.9700
C2—C3	1.382 (4)	C15—H17B	0.9700
C2—H2	0.9300	C16—H18A	0.9600
C3—C4	1.378 (4)	C16—H18B	0.9600
C3—H3	0.9300	C16—H18C	0.9600
C4—N1	1.337 (4)	O2—Mn1^{ii}	2.178 (2)
C4—H4	0.9300	O9—H9A	0.821 (19)
C5—N1	1.344 (3)	O3W—H3A	0.793 (16)
C5—C6	1.515 (4)	O3W—H3B	0.777 (16)
C6—O3	1.251 (3)	O1W—H1A	0.827 (18)
C6—O4	1.252 (3)	O1W—H1B	0.872 (18)
C7—O2	1.254 (3)	O7—Mn2^{iii}	2.1653 (19)
C7—O1	1.262 (3)	O8—Mn1^{i}	2.127 (2)
C8—C11	1.368 (5)	O2W—H2B	0.833 (18)
C8—C9	1.383 (4)	O2W—H2A	0.863 (18)
C8—H8	0.9300		
O8^{i}—Mn1—O6	113.83 (8)	C8—C9—C10	117.8 (2)
O8^{i}—Mn1—O2^{ii}	87.96 (9)	C8—C9—C14	118.9 (2)
O6—Mn1—O2^{ii}	84.30 (7)	C10—C9—C14	123.1 (2)
O8^{i}—Mn1—O4	80.75 (8)	N2—C10—C9	122.1 (3)
O6—Mn1—O4	155.64 (8)	N2—C10—C13	114.9 (2)
O2^{ii}—Mn1—O4	116.80 (7)	C9—C10—C13	122.9 (2)
O8^{i}—Mn1—N1	146.77 (8)	C8—C11—C12	118.4 (3)
O6—Mn1—N1	98.13 (9)	C8—C11—H11	120.8
O2^{ii}—Mn1—N1	86.36 (8)	C12—C11—H11	120.8
O4—Mn1—N1	72.82 (8)	N2—C12—C11	122.3 (3)
O8^{i}—Mn1—N2	96.47 (9)	N2—C12—H12	118.8
O6—Mn1—N2	72.70 (8)	C11—C12—H12	118.8
O2^{ii}—Mn1—N2	156.42 (8)	O5—C13—O6	125.1 (3)
O4—Mn1—N2	86.78 (8)	O5—C13—C10	119.0 (2)
N1—Mn1—N2	101.68 (9)	O6—C13—C10	115.9 (2)
O1—Mn2—O3W	87.17 (9)	O7—C14—O8	125.0 (2)
O1—Mn2—O7^{iii}	101.72 (8)	O7—C14—C9	118.8 (2)
O3W—Mn2—O7^{iii}	170.69 (9)	O8—C14—C9	116.0 (2)
O1—Mn2—O2W	175.41 (10)	O9—C15—C16	130.6 (7)
O3W—Mn2—O2W	88.54 (10)	O9—C15—H17A	104.6

O7^{iii}—Mn2—O2W	82.49 (9)	C16—C15—H17A	104.6
O1—Mn2—O3	80.79 (8)	O9—C15—H17B	104.6
O3W—Mn2—O3	89.55 (9)	C16—C15—H17B	104.6
O7^{iii}—Mn2—O3	89.15 (8)	H17A—C15—H17B	105.7
O2W—Mn2—O3	97.54 (10)	C15—C16—H18A	109.5
O1—Mn2—O9	89.22 (10)	C15—C16—H18B	109.5
O3W—Mn2—O9	88.39 (10)	H18A—C16—H18B	109.5
O7^{iii}—Mn2—O9	94.44 (8)	C15—C16—H18C	109.5
O2W—Mn2—O9	92.30 (11)	H18A—C16—H18C	109.5
O3—Mn2—O9	169.89 (10)	H18B—C16—H18C	109.5
C2—C1—C5	117.7 (2)	C4—N1—C5	119.6 (2)
C2—C1—C7	116.3 (2)	C4—N1—Mn1	123.72 (19)
C5—C1—C7	125.9 (2)	C5—N1—Mn1	115.42 (18)
C3—C2—C1	120.6 (3)	C12—N2—C10	119.0 (2)
C3—C2—H2	119.7	C12—N2—Mn1	125.7 (2)
C1—C2—H2	119.7	C10—N2—Mn1	114.86 (18)
C4—C3—C2	117.9 (3)	C7—O1—Mn2	128.11 (17)
C4—C3—H3	121.1	C7—O2—Mn1^{ii}	138.53 (18)
C2—C3—H3	121.1	C6—O3—Mn2	125.46 (18)
N1—C4—C3	122.9 (3)	C15—O9—Mn2	134.9 (3)
N1—C4—H4	118.6	C15—O9—H9A	114.7 (19)
C3—C4—H4	118.6	Mn2—O9—H9A	110.5 (19)
N1—C5—C1	121.3 (2)	C6—O4—Mn1	119.19 (17)
N1—C5—C6	113.3 (2)	Mn2—O3W—H3A	112.5 (18)
C1—C5—C6	125.5 (2)	Mn2—O3W—H3B	112.7 (18)
O3—C6—O4	124.6 (3)	H3A—O3W—H3B	127 (3)
O3—C6—C5	119.3 (2)	C13—O6—Mn1	121.35 (17)
O4—C6—C5	116.0 (2)	H1A—O1W—H1B	103 (3)
O2—C7—O1	123.2 (2)	C14—O7—Mn2^{iii}	124.82 (17)
O2—C7—C1	116.6 (2)	C14—O8—Mn1^{i}	138.76 (18)
O1—C7—C1	120.0 (2)	Mn2—O2W—H2B	113 (3)
C11—C8—C9	120.3 (3)	Mn2—O2W—H2A	137 (3)
C11—C8—H8	119.9	H2B—O2W—H2A	109 (3)
C9—C8—H8	119.9		
C5—C1—C2—C3	−0.4 (4)	C9—C10—N2—Mn1	−172.4 (2)
C7—C1—C2—C3	−178.2 (3)	C13—C10—N2—Mn1	5.5 (3)
C1—C2—C3—C4	2.0 (5)	O8^{i}—Mn1—N2—C12	−63.8 (3)
C2—C3—C4—N1	−0.9 (5)	O6—Mn1—N2—C12	−176.8 (3)
C2—C1—C5—N1	−2.4 (4)	O2^{ii}—Mn1—N2—C12	−163.6 (3)
C7—C1—C5—N1	175.2 (3)	O4—Mn1—N2—C12	16.5 (3)
C2—C1—C5—C6	179.8 (2)	N1—Mn1—N2—C12	88.2 (3)
C7—C1—C5—C6	−2.6 (4)	O8^{i}—Mn1—N2—C10	108.1 (2)
N1—C5—C6—O3	158.8 (2)	O6—Mn1—N2—C10	−4.9 (2)
C1—C5—C6—O3	−23.2 (4)	O2^{ii}—Mn1—N2—C10	8.3 (4)
N1—C5—C6—O4	−21.0 (3)	O4—Mn1—N2—C10	−171.6 (2)
C1—C5—C6—O4	156.9 (3)	N1—Mn1—N2—C10	−99.8 (2)
C2—C1—C7—O2	61.3 (4)	O2—C7—O1—Mn2	150.7 (2)

C5—C1—C7—O2	−116.2 (3)	C1—C7—O1—Mn2	−34.5 (4)
C2—C1—C7—O1	−113.9 (3)	O3W—Mn2—O1—C7	−124.0 (3)
C5—C1—C7—O1	68.6 (4)	O7^{iii}—Mn2—O1—C7	53.2 (3)
C11—C8—C9—C10	1.0 (6)	O2W—Mn2—O1—C7	−103.1 (11)
C11—C8—C9—C14	−174.5 (4)	O3—Mn2—O1—C7	−34.0 (2)
C8—C9—C10—N2	−0.1 (5)	O9—Mn2—O1—C7	147.5 (2)
C14—C9—C10—N2	175.3 (3)	O1—C7—O2—Mn1^{ii}	171.5 (2)
C8—C9—C10—C13	−177.8 (3)	C1—C7—O2—Mn1^{ii}	−3.5 (4)
C14—C9—C10—C13	−2.4 (4)	O4—C6—O3—Mn2	134.9 (2)
C9—C8—C11—C12	−1.9 (7)	C5—C6—O3—Mn2	−44.9 (3)
C8—C11—C12—N2	2.0 (7)	O1—Mn2—O3—C6	85.2 (2)
N2—C10—C13—O5	178.0 (3)	O3W—Mn2—O3—C6	172.4 (2)
C9—C10—C13—O5	−4.2 (5)	O7^{iii}—Mn2—O3—C6	−16.8 (2)
N2—C10—C13—O6	−2.6 (4)	O2W—Mn2—O3—C6	−99.1 (2)
C9—C10—C13—O6	175.3 (3)	O9—Mn2—O3—C6	94.2 (5)
C8—C9—C14—O7	−94.3 (4)	C16—C15—O9—Mn2	−127.9 (8)
C10—C9—C14—O7	90.4 (3)	O1—Mn2—O9—C15	103.6 (6)
C8—C9—C14—O8	82.0 (4)	O3W—Mn2—O9—C15	16.4 (6)
C10—C9—C14—O8	−93.4 (3)	O7^{iii}—Mn2—O9—C15	−154.7 (6)
C3—C4—N1—C5	−1.8 (4)	O2W—Mn2—O9—C15	−72.1 (6)
C3—C4—N1—Mn1	164.6 (2)	O3—Mn2—O9—C15	94.7 (7)
C1—C5—N1—C4	3.5 (4)	O3—C6—O4—Mn1	−162.1 (2)
C6—C5—N1—C4	−178.5 (2)	C5—C6—O4—Mn1	17.7 (3)
C1—C5—N1—Mn1	−164.02 (19)	O8^{i}—Mn1—O4—C6	−167.4 (2)
C6—C5—N1—Mn1	14.0 (3)	O6—Mn1—O4—C6	63.3 (3)
O8^{i}—Mn1—N1—C4	−132.7 (2)	O2^{ii}—Mn1—O4—C6	−84.4 (2)
O6—Mn1—N1—C4	31.7 (2)	N1—Mn1—O4—C6	−7.78 (19)
O2^{ii}—Mn1—N1—C4	−52.0 (2)	N2—Mn1—O4—C6	95.5 (2)
O4—Mn1—N1—C4	−171.6 (2)	O5—C13—O6—Mn1	177.4 (3)
N2—Mn1—N1—C4	105.6 (2)	C10—C13—O6—Mn1	−2.1 (3)
O8^{i}—Mn1—N1—C5	34.2 (3)	O8^{i}—Mn1—O6—C13	−85.8 (2)
O6—Mn1—N1—C5	−161.41 (19)	O2^{ii}—Mn1—O6—C13	−171.0 (2)
O2^{ii}—Mn1—N1—C5	114.9 (2)	O4—Mn1—O6—C13	37.5 (3)
O4—Mn1—N1—C5	−4.62 (18)	N1—Mn1—O6—C13	103.5 (2)
N2—Mn1—N1—C5	−87.50 (19)	N2—Mn1—O6—C13	3.7 (2)
C11—C12—N2—C10	−1.1 (6)	O8—C14—O7—Mn2^{iii}	17.6 (4)
C11—C12—N2—Mn1	170.5 (3)	C9—C14—O7—Mn2^{iii}	−166.56 (17)
C9—C10—N2—C12	0.2 (5)	O7—C14—O8—Mn1^{i}	170.8 (2)
C13—C10—N2—C12	178.0 (3)	C9—C14—O8—Mn1^{i}	−5.2 (4)

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

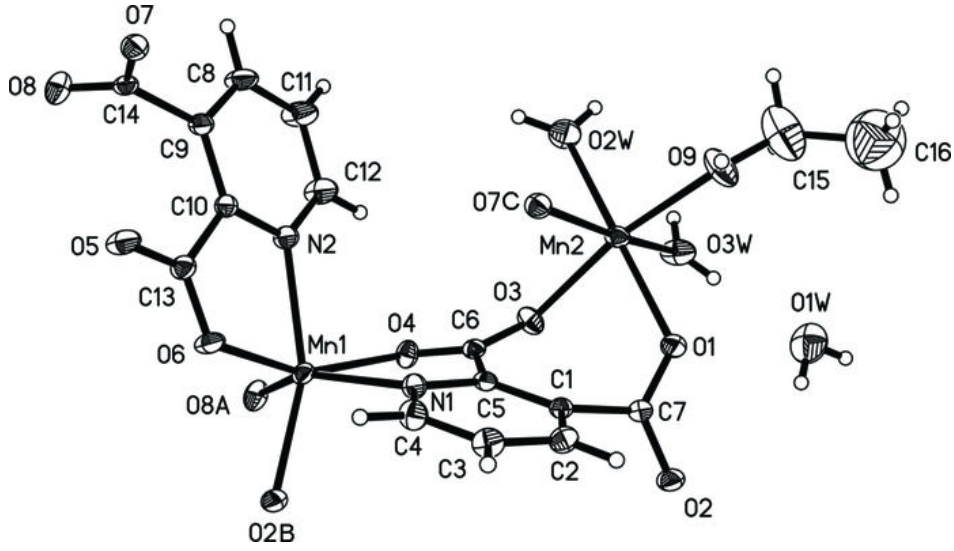
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1A···O3^{iv}	0.827 (18)	2.29 (3)	3.083 (3)	161 (5)
O1W—H1B···O1	0.872 (18)	2.51 (4)	2.847 (4)	104 (3)

O1W—H1B···O3W^{iv}	0.872 (18)	2.63 (5)	3.034 (4)	109 (4)
O2W—H2B···O5^{v}	0.833 (18)	1.91 (2)	2.730 (3)	168 (5)
O3W—H3B···O1W	0.777 (16)	2.14 (2)	2.893 (4)	162 (3)
O3W—H3A···O6^{v}	0.793 (16)	1.99 (2)	2.699 (3)	150 (4)
O9—H9A···O8^{iii}	0.821 (19)	2.10 (3)	2.776 (3)	140 (3)
O9—H9A···O4^{vi}	0.821 (19)	2.319 (18)	3.006 (3)	142 (3)

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

Fig. 1


O7
O8
C14
C8
C11
C9
C12
C10
N2
O5
C13
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Mn1
O8A
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C6
O3
N1
C5
C1
C7
C4
C3
C2
O2
O2W
O9
C15
C16
O7C
Mn2
O3W
O1W
O1