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Aqua(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')bis(4-hydroxybenzoato)-κO,-κ^2O,O'-manganese(II)–2,9-dimethyl-1,10-phenanthroline–ethanol–water (1/1/1/1)

Xiao-Peng Xuan* and Pei-Zheng Zhao

Department of Chemistry, Henan Normal University, Xinxiang 453007, People's Republic of China
Correspondence e-mail: xpxuan@henannu.edu.cn

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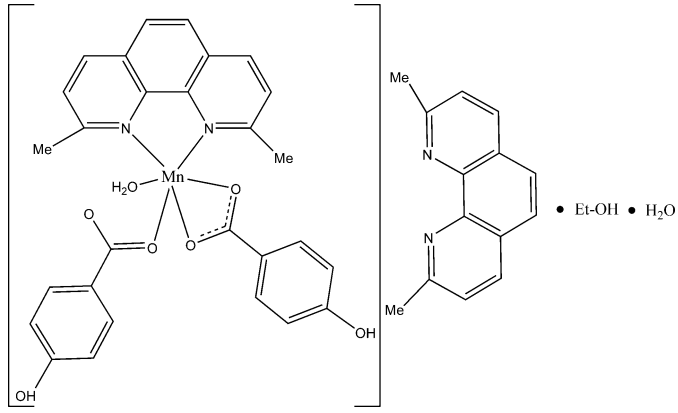
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.128; data-to-parameter ratio = 14.3.

In the title compound, $[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)(H_2O)]\cdot C_{14}H_{12}N_2\cdot C_2H_6O\cdot H_2O$, the Mn^{II} ion is six-coordinated by two N atoms of a 2,9-dimethyl-1,10-phenanthroline (dmphen) ligand, two carboxylate O atoms of one 4-hydroxybenzoate anion, one carboxylate O atom of another 4-hydroxybenzoate anion and one O atom of a water molecule. The resulting coordination geometry is a pseudo-square pyramid, considering the bidentate 4-hydroxybenzoate anion as an apical ligand. The separation between the Mn atom and the non-bonded carboxylate O atom of the monodentate benzoate anion is 3.520 (3) Å, much larger than the distance expected for an Mn—O bond. The crystal structure is stabilized through O—H···N and O—H···O hydrogen bonds involving the uncoordinated dmphen and the ethanol and water solvent molecules, and by π–π interaction between the uncoordinated and neighboring coordinated dmphen molecules, with a centroid–centroid separation of 3.812 (5) Å.

Related literature

For structures of related Mn^{II} complexes, see: Pan *et al.* (2006); Su *et al.* (2005); Wang *et al.* (2003, 2004); Xiao (2005); Xuan *et al.* (2007); Yang *et al.* (2006); Zhang (2006); Zhao *et al.* (2007).



Experimental

Crystal data

$[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)(H_2O)]\cdot C_{14}H_{12}N_2\cdot C_2H_6O\cdot H_2O$
M_r = 827.77
Monoclinic, $P2_1/c$
a = 15.9080 (12) Å
b = 18.4137 (14) Å
c = 15.4744 (11) Å
β = 115.585 (1)°
V = 4088.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 297 (2) K
0.48 × 0.35 × 0.29 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.838, T_{max} = 0.896
30925 measured reflections
7614 independent reflections
5682 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.128
S = 1.03
7614 reflections
532 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O4	2.1413 (17)	Mn1—N1	2.2755 (18)
Mn1—O7	2.1562 (17)	Mn1—N2	2.2974 (18)
Mn1—O1	2.2277 (17)	Mn1—O2	2.3258 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O9^{i}	0.82	1.83	2.651 (4)	176
O6—H6···O2^{ii}	0.82	1.83	2.640 (2)	169
O7—H1W···O5	0.82	1.83	2.613 (2)	158
O7—H2W···N4	0.84	2.24	2.998 (3)	151
O8—H8···O5^{iii}	0.82	1.88	2.685 (3)	167
O9—H4W···N4^{iv}	0.84	2.28	3.061 (3)	155

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve

  doi:10.1107/S1600536807061077

structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2148).

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supplementary materials

Acta Cryst. (2007). E**63**, m3180-m3181 [**doi:10.1107/S1600536807061077**]

Aqua(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')bis(4-hydroxybenzoato)-$\kappa O,\kappa^2 O,O'$-manganese(II)-2,9-dimethyl-1,10-phenanthroline-ethanol-water (1/1/1/1)

X.-P. Xuan and P.-Z. Zhao

Comment

Crystal structures of Mn^{II} complexes of 1,10-phenanthroline or its derivatives combined with benzoic anions have been reported (Pan *et al.*, 2006; Su *et al.*, 2005; Wang *et al.*, 2003; Wang *et al.*, 2004; Xiao, 2005; Yang *et al.*, 2006; Zhang, 2006). Recently, as part of our ongoing studies (Xuan *et al.*, 2007; Zhao *et al.*, 2007) of mixed-ligand complexes, we have reported the structure of Mn^{II} complexes (Zhao *et al.*, 2007). In this paper, we present the crystal structure of a Mn^{II} complex of 2,9-dimethyl-1,10-phenanthroline (dmphen) and 4-hydroxybenzoate anion, which is not very different to that our previously reported complex, which was obtained by reaction of dmphen, sodium 3-hydroxybenzoate and $Mn(NO_3)_2$ aqueous solutions (Xuan *et al.*, 2007).

As shown in Fig. 1, the structure unit of (I) is composed of a Mn^{II} complex, $[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)(H_2O)]$, one non-coordinated dmphen molecule, one ethanol and one water molecule. Two N atoms from one dmphen ligand, three O atoms from monodentate and bidentate carboxyl groups of two 4-hydroxybenzoate anions, and one O atom from water are coordinated to the Mn^{II} ion in a strongly distorted arrangement. The coordination geometry around the metal centre may be described as a distorted square pyramidal arrangement, considering the bidentate benzoate anion placed in the apical position. The corresponding bond lengths are listed in Table 1. Additionally, the non-bonding separation between Mn atom and the carboxyl O atoms of monodentate benzoate anion is 3.520 (3) Å, much larger than the distance expected for a Mn—O bond.

In the crystal structure, the complex is stabilizing by π–π interactions between the free and coordinated dmphen. The centroid (ring C4···C7/C11/C12) to centroid (ring C38···C41/N3/C42) separation is 3.812 (5) Å.

A structural feature of (I) is the extensive network of hydrogen bonds (Table 2 and Fig. 2). The coordinated water participates in hydrogen bonds with the O atom of benzoate and to the N atoms of uncoordinated dmphen molecule. The 4-hydroxybenzoate ligand and the uncoordinated ethanol also form hydrogen bonds with carbonyl O atom of neighboring benzoate and with lattice water molecule.

Experimental

The reaction of 4-hydroxybenzoate (0.069 g, 0.5 mmol) and NaOH (0.018 g, 0.5 mmol) in ethanol/water *(v*:*v*=1:1, 10 ml) at room temperature for 1 h. produced a colorless solutions, to which 2,9-dimethyl-1,10-phenanthroline ($C_{14}H_{12}N_2{\cdot}0.5H_2O$, 0.109 g, 0.5 mmol) and a 50% $Mn(NO_3)_2$ aqueous solution (0.146 g, 0.5 mmol) in ethanol/water *(v*:*v*=2:1, 10 ml) mixture was added. The resulting solution was stirred for 5 h. at 323 K and then a yellow precipitate was filtered. Yellow single crystals of (I) were obtained by slow evaporation of the filtrate over 2 days.

Refinement

C-bonded H atoms were placed in calculated positions, with C—H = 0.93 (aromatic CH), 0.97 (methylene CH_2) or C—H = 0.96 Å (methyl CH_3), and refined in the riding-model approximation with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl groups and $U_{iso}(H) = 1.2U_{eq}(C)$ otherwise. Hydroxyl and water H atoms were found in a difference map and their coordinates fixed. Isotropic displacement parameters were fixed to $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

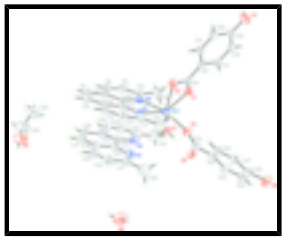

Fig. 1. The structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

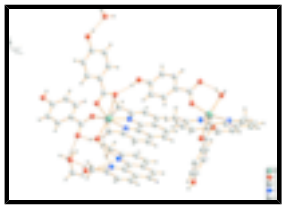

Fig. 2. Crystal packing of (I) showing the formation of hydrogen-bonds drawn as dashed lines.

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Crystal data

$[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)(H_2O)]\cdot C_{14}H_{12}N_2\cdot C_2H_6O\cdot H_2O$	$F_{000} = 1732$
$M_r = 827.77$	$D_x = 1.345$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 8290 reflections
$a = 15.9080$ (12) Å	$\theta = 2.6$–$24.1°$
$b = 18.4137$ (14) Å	$\mu = 0.38$ mm^{-1}
$c = 15.4744$ (11) Å	$T = 297$ (2) K
$\beta = 115.5850$ (10)°	Block, yellow
$V = 4088.4$ (5) Å^3	0.48 × 0.35 × 0.29 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	7614 independent reflections
Radiation source: fine-focus sealed tube	5682 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$

T = 293(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 1997)

T_{min} = 0.838, T_{max} = 0.896

30925 measured reflections

θ_{max} = 25.5º

θ_{min} = 2.6º

h = −19→19

k = −22→22

l = −18→18

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.042

$wR(F^2)$ = 0.128

S = 1.03

7614 reflections

532 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 1.2395P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.29 e Å^{-3}

$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.39251 (2)	0.324065 (17)	0.10749 (2)	0.04676 (12)
O1	0.49765 (11)	0.29788 (10)	0.05292 (11)	0.0607 (4)
O2	0.55171 (11)	0.31851 (9)	0.20570 (12)	0.0612 (4)
O3	0.91738 (15)	0.20101 (14)	0.17976 (18)	0.0953 (7)
H3	0.9556	0.2035	0.2360	0.143*
O4	0.36118 (12)	0.21099 (9)	0.10766 (12)	0.0621 (4)
O5	0.22988 (13)	0.18962 (9)	−0.02313 (13)	0.0723 (5)
O6	0.34146 (14)	−0.13266 (9)	0.12067 (12)	0.0716 (5)
H6	0.3770	−0.1421	0.1764	0.107*
O7	0.26701 (12)	0.32769 (9)	−0.02475 (13)	0.0676 (5)
H1W	0.2456	0.2866	−0.0390	0.101*
H2W	0.2261	0.3565	−0.0255	0.101*
O8	−0.0490 (2)	0.84383 (19)	0.0833 (2)	0.1286 (10)
H8	−0.1056	0.8406	0.0646	0.193*
O9	0.03962 (15)	0.20203 (14)	0.3624 (2)	0.1172 (9)
H3W	0.0509	0.2343	0.4049	0.176*
H4W	0.0622	0.1629	0.3911	0.176*
N1	0.39368 (12)	0.36568 (10)	0.24646 (13)	0.0482 (4)
N2	0.38111 (12)	0.44827 (10)	0.09324 (13)	0.0494 (4)
N3	0.13868 (14)	0.38424 (12)	0.07226 (16)	0.0631 (5)
N4	0.12798 (16)	0.44918 (12)	−0.09163 (16)	0.0694 (6)
C1	0.41119 (17)	0.32609 (14)	0.32510 (17)	0.0567 (6)
C2	0.42060 (19)	0.35868 (17)	0.41084 (19)	0.0684 (7)
H2	0.4336	0.3301	0.4647	0.082*

C3	0.41081 (19)	0.43131 (17)	0.4155 (2)	0.0704 (7)
H3A	0.4164	0.4526	0.4723	0.084*
C4	0.39219 (17)	0.47455 (14)	0.33455 (19)	0.0613 (6)
C5	0.3805 (2)	0.55136 (17)	0.3346 (2)	0.0786 (8)
H5	0.3828	0.5741	0.3892	0.094*
C6	0.3665 (2)	0.59097 (16)	0.2571 (3)	0.0810 (9)
H6A	0.3577	0.6408	0.2583	0.097*
C7	0.36476 (17)	0.55819 (13)	0.1724 (2)	0.0650 (7)
C8	0.3549 (2)	0.59773 (15)	0.0915 (3)	0.0785 (9)
H8A	0.3456	0.6477	0.0897	0.094*
C9	0.3588 (2)	0.56367 (16)	0.0159 (2)	0.0773 (8)
H9	0.3517	0.5903	−0.0379	0.093*
C10	0.37371 (16)	0.48792 (14)	0.01812 (18)	0.0597 (6)
C11	0.37580 (15)	0.48233 (12)	0.16950 (17)	0.0508 (5)
C12	0.38662 (15)	0.43933 (12)	0.25134 (16)	0.0494 (5)
C13	0.4220 (2)	0.24625 (15)	0.3212 (2)	0.0781 (8)
H13A	0.3638	0.2253	0.2776	0.117*
H13B	0.4402	0.2260	0.3839	0.117*
H13C	0.4689	0.2358	0.2996	0.117*
C14	0.3833 (2)	0.45073 (17)	−0.0631 (2)	0.0761 (8)
H14A	0.4359	0.4185	−0.0382	0.114*
H14B	0.3924	0.4864	−0.1035	0.114*
H14C	0.3278	0.4234	−0.0996	0.114*
C15	0.56467 (15)	0.29844 (11)	0.13417 (16)	0.0468 (5)
C16	0.65894 (15)	0.27431 (11)	0.14719 (16)	0.0449 (5)
C17	0.67156 (17)	0.24486 (12)	0.07141 (17)	0.0533 (6)
H17	0.6208	0.2408	0.0118	0.064*
C18	0.75787 (19)	0.22137 (13)	0.0825 (2)	0.0624 (6)
H18	0.7654	0.2026	0.0305	0.075*
C19	0.83286 (18)	0.22581 (13)	0.1710 (2)	0.0637 (7)
C20	0.82175 (17)	0.25559 (14)	0.2474 (2)	0.0649 (7)
H20	0.8726	0.2595	0.3069	0.078*
C21	0.73571 (16)	0.27942 (13)	0.23550 (18)	0.0570 (6)
H21	0.7287	0.2993	0.2873	0.068*
C22	0.29848 (18)	0.16912 (12)	0.05170 (18)	0.0542 (6)
C23	0.30779 (16)	0.08987 (12)	0.07469 (16)	0.0501 (5)
C24	0.25473 (19)	0.03984 (14)	0.00593 (17)	0.0658 (7)
H24	0.2099	0.0565	−0.0526	0.079*
C25	0.2665 (2)	−0.03391 (14)	0.02191 (17)	0.0678 (7)
H25	0.2308	−0.0663	−0.0260	0.081*
C26	0.33145 (17)	−0.05972 (13)	0.10953 (16)	0.0535 (6)
C28	0.37170 (16)	0.06317 (13)	0.16186 (17)	0.0556 (6)
H28	0.4082	0.0955	0.2094	0.067*
C29	−0.0294 (4)	0.8918 (3)	0.0229 (4)	0.1507 (19)
H29A	−0.0326	0.9415	0.0422	0.181*
H29B	−0.0763	0.8859	−0.0425	0.181*
C30	0.0611 (4)	0.8789 (4)	0.0266 (4)	0.191 (3)
H30A	0.1080	0.8875	0.0905	0.286*
H30B	0.0708	0.9110	−0.0171	0.286*

H30C	0.0650	0.8295	0.0089	0.286*
C31	0.38257 (17)	−0.01054 (13)	0.17998 (17)	0.0562 (6)
H31	0.4245	−0.0271	0.2400	0.067*
C32	0.1190 (2)	0.47937 (19)	−0.1722 (2)	0.0876 (10)
C33	0.1057 (3)	0.5574 (2)	−0.1856 (3)	0.1069 (13)
H33	0.0996	0.5790	−0.2423	0.128*
C34	0.1024 (2)	0.5978 (2)	−0.1147 (3)	0.1032 (12)
H34	0.0940	0.6477	−0.1233	0.124*
C35	0.1111 (2)	0.56769 (17)	−0.0302 (3)	0.0835 (9)
C36	0.1091 (2)	0.60876 (17)	0.0469 (3)	0.0931 (11)
H36	0.1003	0.6588	0.0405	0.112*
C37	0.1196 (2)	0.5759 (2)	0.1291 (3)	0.0972 (11)
H37	0.1198	0.6042	0.1790	0.117*
C38	0.13028 (18)	0.50068 (17)	0.1414 (2)	0.0748 (8)
C39	0.1398 (2)	0.4645 (2)	0.2233 (2)	0.0897 (10)
H39	0.1403	0.4911	0.2747	0.108*
C40	0.1484 (2)	0.3919 (2)	0.2308 (2)	0.0904 (10)
H40	0.1557	0.3686	0.2869	0.108*
C41	0.14627 (19)	0.35185 (19)	0.1528 (2)	0.0733 (8)
C42	0.13143 (16)	0.45694 (15)	0.06545 (19)	0.0619 (6)
C43	0.12330 (16)	0.49098 (14)	−0.0211 (2)	0.0649 (7)
C44	0.1229 (3)	0.4319 (2)	−0.2477 (2)	0.1203 (15)
H44A	0.1516	0.3865	−0.2199	0.180*
H44B	0.1587	0.4552	−0.2762	0.180*
H44C	0.0608	0.4232	−0.2959	0.180*
C45	0.1509 (3)	0.27153 (19)	0.1570 (3)	0.0997 (11)
H45A	0.0889	0.2520	0.1302	0.150*
H45B	0.1836	0.2562	0.2225	0.150*
H45C	0.1832	0.2543	0.1211	0.150*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0449 (2)	0.0421 (2)	0.0498 (2)	−0.00200 (14)	0.01706 (16)	−0.00229 (14)
O1	0.0475 (9)	0.0748 (11)	0.0512 (10)	0.0047 (8)	0.0131 (8)	−0.0028 (8)
O2	0.0491 (9)	0.0756 (12)	0.0551 (10)	0.0016 (8)	0.0189 (8)	−0.0130 (8)
O3	0.0675 (13)	0.1065 (16)	0.1183 (18)	0.0300 (13)	0.0461 (13)	0.0013 (16)
O4	0.0667 (11)	0.0482 (9)	0.0594 (10)	−0.0117 (8)	0.0157 (8)	−0.0055 (8)
O5	0.0697 (12)	0.0508 (10)	0.0739 (12)	−0.0078 (8)	0.0099 (10)	0.0021 (9)
O6	0.0917 (14)	0.0484 (10)	0.0559 (10)	−0.0067 (9)	0.0141 (10)	0.0064 (8)
O7	0.0510 (10)	0.0485 (9)	0.0821 (12)	−0.0015 (7)	0.0087 (9)	−0.0013 (9)
O8	0.1011 (19)	0.152 (3)	0.121 (2)	−0.007 (2)	0.0372 (18)	0.0329 (19)
O9	0.0689 (14)	0.0969 (17)	0.152 (2)	0.0177 (12)	0.0154 (14)	0.0402 (16)
N1	0.0447 (10)	0.0469 (11)	0.0511 (11)	−0.0005 (8)	0.0189 (8)	−0.0008 (8)
N2	0.0423 (10)	0.0448 (10)	0.0553 (11)	−0.0017 (8)	0.0157 (9)	0.0064 (9)
N3	0.0536 (12)	0.0656 (14)	0.0652 (14)	0.0015 (10)	0.0210 (10)	−0.0015 (11)
N4	0.0671 (14)	0.0637 (14)	0.0631 (14)	−0.0099 (11)	0.0147 (11)	0.0072 (11)
C1	0.0541 (14)	0.0645 (15)	0.0503 (13)	−0.0013 (11)	0.0216 (11)	0.0020 (12)

C2	0.0698 (17)	0.084 (2)	0.0543 (15)	−0.0007 (15)	0.0293 (13)	0.0008 (14)
C3	0.0652 (17)	0.092 (2)	0.0570 (16)	−0.0001 (15)	0.0290 (13)	−0.0151 (15)
C4	0.0488 (14)	0.0654 (16)	0.0677 (16)	−0.0015 (12)	0.0230 (12)	−0.0172 (13)
C5	0.0767 (19)	0.0677 (18)	0.088 (2)	0.0037 (15)	0.0320 (17)	−0.0252 (17)
C6	0.0743 (19)	0.0497 (16)	0.110 (3)	0.0041 (14)	0.0310 (18)	−0.0211 (17)
C7	0.0511 (14)	0.0441 (13)	0.091 (2)	0.0001 (11)	0.0224 (13)	0.0000 (13)
C8	0.0745 (19)	0.0415 (14)	0.112 (3)	0.0009 (13)	0.0336 (18)	0.0106 (16)
C9	0.0734 (19)	0.0582 (16)	0.096 (2)	0.0009 (14)	0.0325 (17)	0.0298 (16)
C10	0.0486 (14)	0.0578 (15)	0.0681 (16)	−0.0047 (11)	0.0209 (12)	0.0144 (12)
C11	0.0376 (11)	0.0433 (12)	0.0651 (15)	−0.0009 (9)	0.0163 (10)	−0.0034 (11)
C12	0.0384 (11)	0.0501 (13)	0.0582 (14)	−0.0007 (9)	0.0193 (10)	−0.0039 (11)
C13	0.106 (2)	0.0619 (17)	0.0565 (16)	−0.0002 (16)	0.0252 (16)	0.0108 (13)
C14	0.0815 (19)	0.082 (2)	0.0679 (17)	−0.0070 (15)	0.0350 (15)	0.0170 (15)
C15	0.0478 (12)	0.0379 (11)	0.0511 (13)	−0.0042 (9)	0.0181 (11)	−0.0004 (10)
C16	0.0450 (12)	0.0342 (10)	0.0534 (13)	0.0009 (9)	0.0192 (10)	0.0027 (9)
C17	0.0583 (14)	0.0440 (12)	0.0543 (13)	0.0004 (11)	0.0211 (11)	0.0001 (10)
C18	0.0687 (17)	0.0527 (14)	0.0728 (17)	0.0059 (12)	0.0371 (14)	−0.0039 (12)
C19	0.0580 (15)	0.0484 (14)	0.091 (2)	0.0105 (11)	0.0376 (15)	0.0046 (13)
C20	0.0498 (14)	0.0663 (16)	0.0677 (16)	0.0074 (12)	0.0151 (12)	0.0011 (13)
C21	0.0523 (14)	0.0594 (15)	0.0564 (14)	0.0057 (11)	0.0209 (12)	−0.0020 (11)
C22	0.0587 (15)	0.0498 (13)	0.0542 (14)	−0.0062 (11)	0.0244 (12)	−0.0037 (11)
C23	0.0533 (13)	0.0465 (12)	0.0498 (13)	−0.0086 (10)	0.0217 (11)	−0.0028 (10)
C24	0.0778 (18)	0.0542 (15)	0.0459 (13)	−0.0120 (13)	0.0083 (12)	0.0080 (11)
C25	0.0867 (19)	0.0488 (14)	0.0475 (14)	−0.0189 (13)	0.0097 (13)	0.0001 (11)
C26	0.0605 (14)	0.0480 (13)	0.0501 (13)	−0.0067 (11)	0.0221 (11)	0.0034 (10)
C28	0.0501 (13)	0.0544 (14)	0.0551 (14)	−0.0054 (11)	0.0159 (11)	−0.0126 (11)
C29	0.127 (4)	0.174 (5)	0.146 (4)	−0.019 (3)	0.055 (3)	0.049 (4)
C30	0.124 (4)	0.311 (9)	0.161 (5)	0.017 (5)	0.085 (4)	0.056 (5)
C31	0.0514 (13)	0.0585 (15)	0.0485 (13)	0.0010 (11)	0.0118 (11)	0.0001 (11)
C32	0.084 (2)	0.089 (2)	0.071 (2)	−0.0223 (17)	0.0150 (16)	0.0118 (17)
C33	0.103 (3)	0.098 (3)	0.094 (3)	−0.013 (2)	0.019 (2)	0.039 (2)
C34	0.085 (2)	0.075 (2)	0.121 (3)	−0.0080 (18)	0.019 (2)	0.024 (2)
C35	0.0578 (17)	0.0647 (18)	0.106 (2)	−0.0042 (14)	0.0153 (16)	0.0041 (18)
C36	0.0678 (19)	0.0547 (17)	0.140 (3)	0.0021 (14)	0.029 (2)	−0.024 (2)
C37	0.076 (2)	0.089 (3)	0.118 (3)	0.0023 (18)	0.033 (2)	−0.028 (2)
C38	0.0488 (15)	0.078 (2)	0.087 (2)	−0.0008 (13)	0.0194 (14)	−0.0221 (17)
C39	0.077 (2)	0.118 (3)	0.078 (2)	0.000 (2)	0.0366 (17)	−0.020 (2)
C40	0.082 (2)	0.121 (3)	0.072 (2)	−0.005 (2)	0.0371 (17)	−0.003 (2)
C41	0.0592 (16)	0.098 (2)	0.0610 (17)	0.0005 (15)	0.0243 (13)	0.0014 (16)
C42	0.0422 (13)	0.0677 (17)	0.0675 (16)	−0.0010 (11)	0.0158 (12)	−0.0076 (13)
C43	0.0439 (13)	0.0505 (14)	0.0835 (19)	−0.0032 (11)	0.0115 (13)	−0.0078 (13)
C44	0.149 (4)	0.138 (4)	0.068 (2)	−0.033 (3)	0.041 (2)	0.009 (2)
C45	0.119 (3)	0.093 (2)	0.093 (2)	0.009 (2)	0.051 (2)	0.0252 (19)

Geometric parameters (Å, °)

Mn1—O4	2.1413 (17)	C15—C16	1.492 (3)
Mn1—O7	2.1562 (17)	C16—C17	1.383 (3)
Mn1—O1	2.2277 (17)	C16—C21	1.388 (3)

Mn1—N1	2.2755 (18)	C17—C18	1.378 (3)
Mn1—N2	2.2974 (18)	C17—H17	0.9300
Mn1—O2	2.3258 (16)	C18—C19	1.376 (4)
Mn1—C15	2.630 (2)	C18—H18	0.9300
O1—C15	1.249 (3)	C19—C20	1.382 (4)
O2—C15	1.265 (3)	C20—C21	1.372 (3)
O3—C19	1.370 (3)	C20—H20	0.9300
O3—H3	0.8200	C21—H21	0.9300
O4—C22	1.262 (3)	C22—C23	1.494 (3)
O5—C22	1.258 (3)	C23—C28	1.382 (3)
O6—C26	1.355 (3)	C23—C24	1.385 (3)
O6—H6	0.8200	C24—C25	1.378 (3)
O7—H1W	0.8200	C24—H24	0.9300
O7—H2W	0.8363	C25—C26	1.387 (3)
O8—C29	1.415 (5)	C25—H25	0.9300
O8—H8	0.8200	C26—C31	1.380 (3)
O9—H3W	0.8460	C28—C31	1.381 (3)
O9—H4W	0.8418	C28—H28	0.9300
N1—C1	1.341 (3)	C29—C30	1.436 (7)
N1—C12	1.366 (3)	C29—H29A	0.9700
N2—C10	1.334 (3)	C29—H29B	0.9700
N2—C11	1.371 (3)	C30—H30A	0.9600
N3—C41	1.340 (3)	C30—H30B	0.9600
N3—C42	1.344 (3)	C30—H30C	0.9600
N4—C32	1.316 (4)	C31—H31	0.9300
N4—C43	1.363 (3)	C32—C33	1.453 (5)
C1—C2	1.404 (4)	C32—C44	1.481 (5)
C1—C13	1.484 (4)	C33—C34	1.346 (5)
C2—C3	1.352 (4)	C33—H33	0.9300
C2—H2	0.9300	C34—C35	1.371 (5)
C3—C4	1.404 (4)	C34—H34	0.9300
C3—H3A	0.9300	C35—C36	1.424 (5)
C4—C12	1.410 (3)	C35—C43	1.424 (4)
C4—C5	1.426 (4)	C36—C37	1.353 (5)
C5—C6	1.337 (4)	C36—H36	0.9300
C5—H5	0.9300	C37—C38	1.398 (5)
C6—C7	1.433 (4)	C37—H37	0.9300
C6—H6A	0.9300	C38—C39	1.381 (5)
C7—C8	1.397 (4)	C38—C42	1.432 (4)
C7—C11	1.411 (3)	C39—C40	1.344 (5)
C8—C9	1.353 (4)	C39—H39	0.9300
C8—H8A	0.9300	C40—C41	1.402 (4)
C9—C10	1.413 (4)	C40—H40	0.9300
C9—H9	0.9300	C41—C45	1.481 (5)
C10—C14	1.495 (4)	C42—C43	1.433 (4)
C11—C12	1.439 (3)	C44—H44A	0.9600
C13—H13A	0.9600	C44—H44B	0.9600
C13—H13B	0.9600	C44—H44C	0.9600
C13—H13C	0.9600	C45—H45A	0.9600

C14—H14A	0.9600	C45—H45B	0.9600
C14—H14B	0.9600	C45—H45C	0.9600
C14—H14C	0.9600		
O4—Mn1—O7	84.88 (6)	C18—C17—C16	121.3 (2)
O4—Mn1—O1	90.19 (7)	C18—C17—H17	119.4
O7—Mn1—O1	100.72 (7)	C16—C17—H17	119.4
O4—Mn1—N1	103.49 (7)	C19—C18—C17	119.6 (2)
O7—Mn1—N1	120.85 (7)	C19—C18—H18	120.2
O1—Mn1—N1	136.89 (6)	C17—C18—H18	120.2
O4—Mn1—N2	163.62 (7)	O3—C19—C18	118.1 (3)
O7—Mn1—N2	82.86 (6)	O3—C19—C20	122.0 (3)
O1—Mn1—N2	102.72 (7)	C18—C19—C20	119.9 (2)
N1—Mn1—N2	73.95 (7)	C21—C20—C19	120.0 (2)
O4—Mn1—O2	98.32 (6)	C21—C20—H20	120.0
O7—Mn1—O2	157.25 (7)	C19—C20—H20	120.0
O1—Mn1—O2	56.93 (6)	C20—C21—C16	120.9 (2)
N1—Mn1—O2	80.51 (6)	C20—C21—H21	119.6
N2—Mn1—O2	97.18 (6)	C16—C21—H21	119.6
O4—Mn1—C15	93.01 (7)	O5—C22—O4	124.2 (2)
O7—Mn1—C15	128.99 (7)	O5—C22—C23	118.0 (2)
O1—Mn1—C15	28.28 (6)	O4—C22—C23	117.7 (2)
N1—Mn1—C15	109.21 (7)	C28—C23—C24	117.4 (2)
N2—Mn1—C15	103.14 (7)	C28—C23—C22	122.4 (2)
O2—Mn1—C15	28.76 (6)	C24—C23—C22	120.1 (2)
C15—O1—Mn1	94.06 (14)	C25—C24—C23	121.8 (2)
C15—O2—Mn1	89.08 (13)	C25—C24—H24	119.1
C19—O3—H3	109.5	C23—C24—H24	119.1
C22—O4—Mn1	135.11 (16)	C24—C25—C26	119.9 (2)
C26—O6—H6	109.5	C24—C25—H25	120.0
Mn1—O7—H1W	109.5	C26—C25—H25	120.0
Mn1—O7—H2W	115.4	O6—C26—C31	123.6 (2)
H1W—O7—H2W	110.7	O6—C26—C25	117.5 (2)
C29—O8—H8	109.5	C31—C26—C25	118.9 (2)
H3W—O9—H4W	107.1	C31—C28—C23	121.5 (2)
C1—N1—C12	118.7 (2)	C31—C28—H28	119.3
C1—N1—Mn1	126.04 (15)	C23—C28—H28	119.3
C12—N1—Mn1	114.80 (14)	O8—C29—C30	111.9 (5)
C10—N2—C11	119.0 (2)	O8—C29—H29A	109.2
C10—N2—Mn1	127.01 (17)	C30—C29—H29A	109.2
C11—N2—Mn1	113.86 (14)	O8—C29—H29B	109.2
C41—N3—C42	119.1 (2)	C30—C29—H29B	109.2
C32—N4—C43	119.9 (3)	H29A—C29—H29B	107.9
N1—C1—C2	121.4 (2)	C29—C30—H30A	109.5
N1—C1—C13	119.0 (2)	C29—C30—H30B	109.5
C2—C1—C13	119.7 (2)	H30A—C30—H30B	109.5
C3—C2—C1	120.4 (3)	C29—C30—H30C	109.5
C3—C2—H2	119.8	H30A—C30—H30C	109.5
C1—C2—H2	119.8	H30B—C30—H30C	109.5
C2—C3—C4	119.9 (2)	C26—C31—C28	120.3 (2)

C2—C3—H3A	120.1	C26—C31—H31	119.8
C4—C3—H3A	120.1	C28—C31—H31	119.8
C3—C4—C12	117.4 (2)	N4—C32—C33	120.1 (3)
C3—C4—C5	122.6 (3)	N4—C32—C44	118.3 (3)
C12—C4—C5	120.0 (3)	C33—C32—C44	121.6 (3)
C6—C5—C4	120.8 (3)	C34—C33—C32	119.0 (3)
C6—C5—H5	119.6	C34—C33—H33	120.5
C4—C5—H5	119.6	C32—C33—H33	120.5
C5—C6—C7	121.4 (3)	C33—C34—C35	122.1 (4)
C5—C6—H6A	119.3	C33—C34—H34	118.9
C7—C6—H6A	119.3	C35—C34—H34	118.9
C8—C7—C11	117.1 (3)	C34—C35—C36	123.7 (4)
C8—C7—C6	123.4 (3)	C34—C35—C43	116.6 (3)
C11—C7—C6	119.5 (3)	C36—C35—C43	119.7 (3)
C9—C8—C7	120.3 (3)	C37—C36—C35	120.8 (3)
C9—C8—H8A	119.9	C37—C36—H36	119.6
C7—C8—H8A	119.9	C35—C36—H36	119.6
C8—C9—C10	120.4 (3)	C36—C37—C38	122.0 (3)
C8—C9—H9	119.8	C36—C37—H37	119.0
C10—C9—H9	119.8	C38—C37—H37	119.0
N2—C10—C9	120.8 (3)	C39—C38—C37	124.2 (3)
N2—C10—C14	118.6 (2)	C39—C38—C42	116.6 (3)
C9—C10—C14	120.6 (2)	C37—C38—C42	119.3 (3)
N2—C11—C7	122.3 (2)	C40—C39—C38	121.7 (3)
N2—C11—C12	118.51 (19)	C40—C39—H39	119.2
C7—C11—C12	119.1 (2)	C38—C39—H39	119.2
N1—C12—C4	122.2 (2)	C39—C40—C41	119.1 (3)
N1—C12—C11	118.6 (2)	C39—C40—H40	120.5
C4—C12—C11	119.1 (2)	C41—C40—H40	120.5
C1—C13—H13A	109.5	N3—C41—C40	121.7 (3)
C1—C13—H13B	109.5	N3—C41—C45	117.9 (3)
H13A—C13—H13B	109.5	C40—C41—C45	120.4 (3)
C1—C13—H13C	109.5	N3—C42—C38	121.8 (3)
H13A—C13—H13C	109.5	N3—C42—C43	118.6 (2)
H13B—C13—H13C	109.5	C38—C42—C43	119.6 (3)
C10—C14—H14A	109.5	N4—C43—C35	122.2 (3)
C10—C14—H14B	109.5	N4—C43—C42	119.1 (2)
H14A—C14—H14B	109.5	C35—C43—C42	118.6 (3)
C10—C14—H14C	109.5	C32—C44—H44A	109.5
H14A—C14—H14C	109.5	C32—C44—H44B	109.5
H14B—C14—H14C	109.5	H44A—C44—H44B	109.5
O1—C15—O2	119.5 (2)	C32—C44—H44C	109.5
O1—C15—C16	120.3 (2)	H44A—C44—H44C	109.5
O2—C15—C16	120.2 (2)	H44B—C44—H44C	109.5
O1—C15—Mn1	57.67 (12)	C41—C45—H45A	109.5
O2—C15—Mn1	62.16 (12)	C41—C45—H45B	109.5
C16—C15—Mn1	172.95 (15)	H45A—C45—H45B	109.5
C17—C16—C21	118.2 (2)	C41—C45—H45C	109.5
C17—C16—C15	120.5 (2)	H45A—C45—H45C	109.5

C21—C16—C15	121.2 (2)	H45B—C45—H45C	109.5
O4—Mn1—O1—C15	−96.01 (14)	N2—C11—C12—C4	172.7 (2)
O7—Mn1—O1—C15	179.17 (13)	C7—C11—C12—C4	−4.2 (3)
N1—Mn1—O1—C15	14.16 (18)	Mn1—O1—C15—O2	−6.8 (2)
N2—Mn1—O1—C15	94.16 (14)	Mn1—O1—C15—C16	172.09 (17)
O2—Mn1—O1—C15	3.81 (12)	Mn1—O2—C15—O1	6.5 (2)
O4—Mn1—O2—C15	81.01 (14)	Mn1—O2—C15—C16	−172.40 (17)
O7—Mn1—O2—C15	−15.6 (2)	O4—Mn1—C15—O1	84.79 (14)
O1—Mn1—O2—C15	−3.75 (12)	O7—Mn1—C15—O1	−1.05 (17)
N1—Mn1—O2—C15	−176.60 (14)	N1—Mn1—C15—O1	−169.81 (13)
N2—Mn1—O2—C15	−104.28 (13)	N2—Mn1—C15—O1	−92.48 (14)
O7—Mn1—O4—C22	2.1 (2)	O2—Mn1—C15—O1	−173.4 (2)
O1—Mn1—O4—C22	−98.6 (2)	O4—Mn1—C15—O2	−101.86 (13)
N1—Mn1—O4—C22	122.7 (2)	O7—Mn1—C15—O2	172.30 (12)
N2—Mn1—O4—C22	43.8 (4)	O1—Mn1—C15—O2	173.4 (2)
O2—Mn1—O4—C22	−155.2 (2)	N1—Mn1—C15—O2	3.55 (14)
C15—Mn1—O4—C22	−126.8 (2)	N2—Mn1—C15—O2	80.88 (14)
O4—Mn1—N1—C1	25.45 (19)	O1—C15—C16—C17	−5.9 (3)
O7—Mn1—N1—C1	117.53 (18)	O2—C15—C16—C17	172.9 (2)
O1—Mn1—N1—C1	−79.7 (2)	O1—C15—C16—C21	175.3 (2)
N2—Mn1—N1—C1	−171.29 (19)	O2—C15—C16—C21	−5.9 (3)
O2—Mn1—N1—C1	−70.91 (18)	C21—C16—C17—C18	−0.3 (3)
C15—Mn1—N1—C1	−72.64 (19)	C15—C16—C17—C18	−179.1 (2)
O4—Mn1—N1—C12	−162.76 (14)	C16—C17—C18—C19	1.3 (4)
O7—Mn1—N1—C12	−70.68 (16)	C17—C18—C19—O3	179.1 (2)
O1—Mn1—N1—C12	92.10 (16)	C17—C18—C19—C20	−1.8 (4)
N2—Mn1—N1—C12	0.51 (14)	O3—C19—C20—C21	−179.7 (3)
O2—Mn1—N1—C12	100.88 (15)	C18—C19—C20—C21	1.2 (4)
C15—Mn1—N1—C12	99.15 (15)	C19—C20—C21—C16	−0.2 (4)
O4—Mn1—N2—C10	−95.8 (3)	C17—C16—C21—C20	−0.3 (3)
O7—Mn1—N2—C10	−53.96 (18)	C15—C16—C21—C20	178.5 (2)
O1—Mn1—N2—C10	45.47 (19)	Mn1—O4—C22—O5	−4.5 (4)
N1—Mn1—N2—C10	−178.98 (19)	Mn1—O4—C22—C23	173.87 (16)
O2—Mn1—N2—C10	103.10 (18)	O5—C22—C23—C28	−169.7 (2)
C15—Mn1—N2—C10	74.50 (19)	O4—C22—C23—C28	11.8 (4)
O4—Mn1—N2—C11	79.9 (3)	O5—C22—C23—C24	13.7 (4)
O7—Mn1—N2—C11	121.72 (15)	O4—C22—C23—C24	−164.8 (2)
O1—Mn1—N2—C11	−138.85 (14)	C28—C23—C24—C25	−1.9 (4)
N1—Mn1—N2—C11	−3.30 (14)	C22—C23—C24—C25	174.9 (3)
O2—Mn1—N2—C11	−81.22 (14)	C23—C24—C25—C26	1.4 (4)
C15—Mn1—N2—C11	−109.82 (15)	C24—C25—C26—O6	−178.7 (3)
C12—N1—C1—C2	1.1 (3)	C24—C25—C26—C31	0.9 (4)
Mn1—N1—C1—C2	172.65 (18)	C24—C23—C28—C31	0.1 (4)
C12—N1—C1—C13	−178.0 (2)	C22—C23—C28—C31	−176.6 (2)
Mn1—N1—C1—C13	−6.5 (3)	O6—C26—C31—C28	176.9 (2)
N1—C1—C2—C3	0.9 (4)	C25—C26—C31—C28	−2.6 (4)
C13—C1—C2—C3	−179.9 (3)	C23—C28—C31—C26	2.2 (4)
C1—C2—C3—C4	−0.7 (4)	C43—N4—C32—C33	1.0 (4)
C2—C3—C4—C12	−1.4 (4)	C43—N4—C32—C44	−178.9 (3)

C2—C3—C4—C5	179.6 (3)	N4—C32—C33—C34	−0.2 (5)
C3—C4—C5—C6	177.4 (3)	C44—C32—C33—C34	179.7 (4)
C12—C4—C5—C6	−1.6 (4)	C32—C33—C34—C35	−0.1 (6)
C4—C5—C6—C7	−1.4 (5)	C33—C34—C35—C36	179.3 (3)
C5—C6—C7—C8	−176.8 (3)	C33—C34—C35—C43	−0.4 (5)
C5—C6—C7—C11	1.6 (4)	C34—C35—C36—C37	−178.9 (3)
C11—C7—C8—C9	−1.9 (4)	C43—C35—C36—C37	0.8 (5)
C6—C7—C8—C9	176.5 (3)	C35—C36—C37—C38	−1.9 (5)
C7—C8—C9—C10	−0.5 (4)	C36—C37—C38—C39	−179.0 (3)
C11—N2—C10—C9	−1.2 (3)	C36—C37—C38—C42	0.9 (5)
Mn1—N2—C10—C9	174.27 (18)	C37—C38—C39—C40	178.9 (3)
C11—N2—C10—C14	177.6 (2)	C42—C38—C39—C40	−0.9 (5)
Mn1—N2—C10—C14	−6.9 (3)	C38—C39—C40—C41	−0.9 (5)
C8—C9—C10—N2	2.2 (4)	C42—N3—C41—C40	−1.1 (4)
C8—C9—C10—C14	−176.6 (3)	C42—N3—C41—C45	177.9 (3)
C10—N2—C11—C7	−1.4 (3)	C39—C40—C41—N3	2.0 (5)
Mn1—N2—C11—C7	−177.44 (17)	C39—C40—C41—C45	−177.0 (3)
C10—N2—C11—C12	−178.2 (2)	C41—N3—C42—C38	−0.9 (4)
Mn1—N2—C11—C12	5.7 (2)	C41—N3—C42—C43	−180.0 (2)
C8—C7—C11—N2	2.9 (3)	C39—C38—C42—N3	1.9 (4)
C6—C7—C11—N2	−175.5 (2)	C37—C38—C42—N3	−178.0 (3)
C8—C7—C11—C12	179.7 (2)	C39—C38—C42—C43	−179.0 (2)
C6—C7—C11—C12	1.3 (3)	C37—C38—C42—C43	1.1 (4)
C1—N1—C12—C4	−3.5 (3)	C32—N4—C43—C35	−1.6 (4)
Mn1—N1—C12—C4	−175.89 (17)	C32—N4—C43—C42	178.8 (2)
C1—N1—C12—C11	174.7 (2)	C34—C35—C43—N4	1.2 (4)
Mn1—N1—C12—C11	2.3 (2)	C36—C35—C43—N4	−178.5 (3)
C3—C4—C12—N1	3.6 (3)	C34—C35—C43—C42	−179.2 (3)
C5—C4—C12—N1	−177.4 (2)	C36—C35—C43—C42	1.2 (4)
C3—C4—C12—C11	−174.6 (2)	N3—C42—C43—N4	−3.3 (3)
C5—C4—C12—C11	4.4 (3)	C38—C42—C43—N4	177.6 (2)
N2—C11—C12—N1	−5.6 (3)	N3—C42—C43—C35	177.0 (2)
C7—C11—C12—N1	177.5 (2)	C38—C42—C43—C35	−2.1 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O9^{i}	0.82	1.83	2.651 (4)	176
O6—H6···O2^{ii}	0.82	1.83	2.640 (2)	169
O7—H1W···O5	0.82	1.83	2.613 (2)	158
O7—H2W···N3	0.84	2.51	3.186 (3)	139
O7—H2W···N4	0.84	2.24	2.998 (3)	151
O8—H8···O5^{iii}	0.82	1.88	2.685 (3)	167
O9—H3W···O8^{iv}	0.85	2.03	2.727 (4)	140
O9—H4W···N3^{v}	0.84	2.67	3.336 (3)	137
O9—H4W···N4^{v}	0.84	2.28	3.061 (3)	155

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

Fig. 1

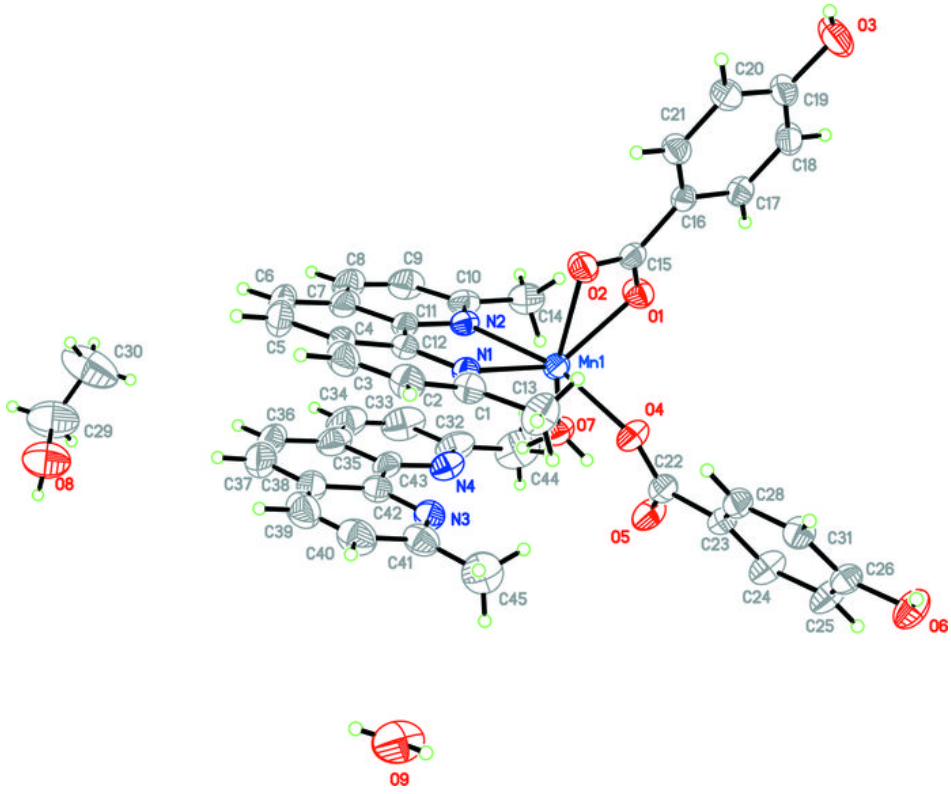
O3
C20
C19
C21
C18
C16
C17
C15
O2
O1
C6
C8
C9
C10
C7
C14
C11
N2
C5
C4
C12
N1
Mn1
C3
C34
C33
C2
C13
C1
C36
C32
O7
O4
C35
C43
N4
C22
C37
C38
C44
C28
C42
N3
O5
C23
C31
C39
C40
C41
C26
C24
C45
C25
O6
C30
C29
O8
O9

Fig. 2