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Diaqua[*N*,*N*′-bis(salicylidene)propane-diamine(2−)]manganese(III) chloride

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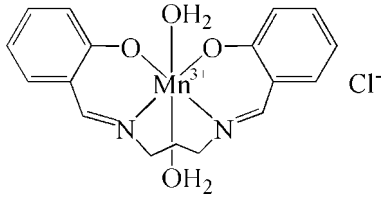
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.069; data-to-parameter ratio = 12.5.

The title compound (systematic name: diaqua{2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}manganese(III) chloride), $[Mn(C_{17}H_{16}N_2O_2)(H_2O)_2]Cl$, consists of an Mn^{III} cation complex and a counter-anion. In the complex, the Mn^{3+} ion is six-coordinated by the dianion of the tetradentate ligand *N*,*N*′-bis(salicylidene)-1,3-diaminopropane and two water molecules in a distorted octahedral geometry. The molecules are assembled through intermolecular O—H···Cl and O—H···O hydrogen bonds and π–π interactions [the centroid–centroid distance is 3.865 Å and the dihedral angle between the ring planes is 12.9°] along the *a* axis.

Related literature

For related literature, see: Gohdes & Armstrong (1992); Huang *et al.* (2002).



Experimental

Crystal data

$[Mn(C_{17}H_{16}N_2O_2)(H_2O)_2]Cl$
M_r = 406.74
Triclinic, $P\overline{1}$
a = 7.6540 (8) Å
b = 10.2633 (10) Å
c = 11.5050 (12) Å
α = 102.622 (2)°
β = 92.777 (2)°
γ = 92.852 (2)°
V = 879.21 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 293 (2) K
0.30 × 0.15 × 0.03 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.857, T_{max} = 0.973
12748 measured reflections
3030 independent reflections
2333 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.069
S = 0.95
3030 reflections
242 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn—O1	1.8843 (14)	Mn—N2	2.0369 (18)
Mn—O2	1.8861 (15)	Mn—O3*W*	2.195 (2)
Mn—N1	2.0191 (18)	Mn—O4*W*	2.240 (2)
O1—Mn—O2	84.41 (6)	N1—Mn—N2	94.19 (8)
O1—Mn—N1	90.39 (7)	O3*W*—Mn—O4*W*	173.95 (8)
O2—Mn—N2	91.01 (7)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*W*—H3*A*···Cl	0.78 (3)	2.27 (3)	3.033 (2)	166 (3)
O3*W*—H3*B*···O1^{i}	0.79 (3)	2.00 (3)	2.782 (3)	172 (3)
O4*W*—H4*A*···Cl^{ii}	0.84 (3)	2.36 (3)	3.192 (2)	173 (3)
O4*W*—H4*B*···O2^{iii}	0.72 (2)	2.15 (2)	2.864 (3)	169 (3)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2127).

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supplementary materials

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Diaqua[*N*,*N*'-bis(salicylidene)propanediamine(2-)]manganese(III) chloride

I.-C. Hwang and K. Ha

Comment

The crystal structure of the title compound consists of cation complex $[Mn(salpn)(H_2O)_2]^+$ (salpn = *N*,*N*'-bis(salicylidene)-1,3-diiminopropane dianion) and a chloride counter anion. Mn^{III} ion is six-coordinated by two N and two O atoms from the tetradentate ligand (salpn) occupying the four equatorial positions and two O atoms of water molecules in the axial positions (Fig.1). The coordination environment around the Mn centre is distorted octahedral. Within the equatorial plane, the chelating angles lie in the range of 90.39 (7)°–94.19 (8)° and the O1—Mn—O2 bond angle is 84.41 (6)°. The apical O3w—Mn—O4w bond angle is 173.95 (8)° (Table 1). The Mn—N bond lengths [2.0190 (18) and 2.0369 (18) Å] are longer than the Mn—O bond [1.8843 (14) and 1.8861 (15) Å] but the bond distances between the Mn atom and the O atoms of the water ligands are considerably longer [2.195 (2) and 2.240 (2) Å]. The compound displays the intermolecular hydrogen bonds between the O atoms of the water molecules and the O atoms of the chelate ligand, and water molecules and Cl anions (Table 2, Fig. 2). Moreover, there are intermolecular π-π interactions between the adjacent benzene rings. For *Cg*1 (the centroid of six-membered ring C1–C6) and $Cg2^i$ (ring C12–C17; symmetry code i: −*x*, 1 − *y*, −*z*), the centroid-centroid distance is 3.865 Å and the dihedral angle between the ring planes is 12.9°. The compounds are assembled through these hydrogen-bonding and π-π interactions along the *a* axis (Fig. 2).

Experimental

$Mn(CH_3COO)_3{\cdot}2H_2O$ (1.00 g, 3.73 mmol), NaCl (0.22 g, 3.76 mmol) and *N*,*N*'-bis(salicylidene)-1,3-diiminopropane (H_2salpn; 1.06 g, 3.75 mmol) in EtOH (70 ml) and H_2O (10 ml) were stirred for 3 h at room temparature and then filtered. The solvent was reduced to 2 ml, the residue washed with acetone and dried under vacuum, to give a dark green powder (0.79 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from a MeOH solution. MS (FAB): m/*z* 335 $(Mn(salpn)^+)$; IR (KBr): 3446 cm^{-1} (broad).

Refinement

H atoms were positioned geometrically and allowed to ride on their respective carrier atoms [C—H = 0.93 (sp^2) or 0.97 Å (sp^3) and $U_{iso}(H) = 1.2U_{eq}(C)$]. The H atoms of the water ligands were localized from Fourier difference maps and refined with isotropic thermal parameters.

Figures

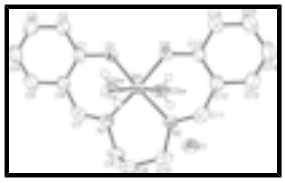

Fig. 1. The structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms at C atoms have been omitted for clarity.

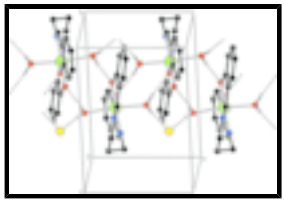

Fig. 2. View of the crystal packing of (I). Hydrogen-bond interactions are drawn with dashed lines.

diaqua{2,2'-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}manganese(III) chloride

Crystal data

$[Mn(C_{17}H_{16}N_2O_2)(H_2O)_2]Cl$	$Z = 2$
$M_r = 406.74$	$F_{000} = 420$
Triclinic, $P\overline{1}$	$D_x = 1.536$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.6540$ (8) Å	Cell parameters from 3154 reflections
$b = 10.2633$ (10) Å	$\theta = 2.4$–23.6º
$c = 11.5050$ (12) Å	$\mu = 0.93$ mm^{-1}
$\alpha = 102.622$ (2)º	$T = 293$ (2) K
$\beta = 92.777$ (2)º	Plate, green
$\gamma = 92.852$ (2)º	0.30 × 0.15 × 0.03 mm
$V = 879.21$ (16) Å^3	

Data collection

Bruker SMART 1000 CCD diffractometer	3030 independent reflections
Radiation source: fine-focus sealed tube	2333 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
$T = 293(2)$ K	$\theta_{max} = 25.1$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -9 \rightarrow 8$
$T_{min} = 0.857$, $T_{max} = 0.973$	$k = -12 \rightarrow 10$
12748 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.069$	$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{max} < 0.001$
3030 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
242 parameters	$\Delta\rho_{min} = -0.20$ 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 $F^2 > 2$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}
Mn	0.24240 (5)	0.35744 (3)	0.06024 (3)	0.03003 (12)
O1	0.2431 (2)	0.39908 (14)	−0.09134 (13)	0.0359 (4)
O2	0.2259 (2)	0.54309 (14)	0.11629 (13)	0.0369 (4)
O3W	0.5292 (3)	0.3795 (2)	0.0863 (2)	0.0482 (5)
H3A	0.572 (4)	0.349 (3)	0.137 (2)	0.062 (11)*
H3B	0.586 (4)	0.444 (3)	0.084 (2)	0.064 (11)*
O4W	−0.0482 (3)	0.3126 (2)	0.03569 (19)	0.0421 (5)
H4A	−0.106 (4)	0.300 (3)	0.093 (2)	0.065 (10)*
H4B	−0.087 (3)	0.357 (3)	0.003 (2)	0.040 (10)*
N1	0.2679 (2)	0.16265 (17)	−0.01432 (17)	0.0326 (5)
N2	0.2398 (3)	0.32827 (19)	0.22969 (16)	0.0337 (5)
C1	0.1984 (3)	0.3203 (2)	−0.1983 (2)	0.0322 (6)
C2	0.1508 (3)	0.3789 (3)	−0.2925 (2)	0.0419 (7)
H2	0.1505	0.4715	−0.2804	0.050*
C3	0.1044 (4)	0.2999 (3)	−0.4032 (2)	0.0527 (8)
H3	0.0691	0.3398	−0.4650	0.063*
C4	0.1090 (4)	0.1626 (3)	−0.4248 (2)	0.0601 (9)
H4	0.0798	0.1107	−0.5009	0.072*
C5	0.1565 (4)	0.1040 (3)	−0.3341 (2)	0.0519 (8)
H5	0.1607	0.0114	−0.3487	0.062*
C6	0.1995 (3)	0.1809 (2)	−0.2188 (2)	0.0357 (6)

C7	0.2451 (3)	0.1126 (2)	−0.1270 (2)	0.0377 (6)
H7	0.2599	0.0215	−0.1515	0.045*
C8	0.3028 (3)	0.0704 (2)	0.0646 (2)	0.0430 (7)
H8A	0.4188	0.0921	0.1041	0.052*
H8B	0.2992	−0.0207	0.0178	0.052*
C9	0.1670 (3)	0.0818 (2)	0.1566 (2)	0.0449 (7)
H9A	0.0539	0.0919	0.1189	0.054*
H9B	0.1589	−0.0006	0.1848	0.054*
C10	0.2061 (4)	0.1967 (2)	0.2614 (2)	0.0495 (7)
H10A	0.1079	0.2027	0.3122	0.059*
H10B	0.3079	0.1783	0.3073	0.059*
C11	0.2778 (3)	0.4259 (3)	0.3199 (2)	0.0413 (6)
H11	0.2845	0.4030	0.3938	0.050*
C12	0.3113 (3)	0.5647 (2)	0.3226 (2)	0.0392 (6)
C13	0.3625 (4)	0.6512 (3)	0.4327 (2)	0.0556 (8)
H13	0.3753	0.6166	0.5007	0.067*
C14	0.3938 (4)	0.7852 (3)	0.4417 (3)	0.0665 (9)
H14	0.4276	0.8416	0.5150	0.080*
C15	0.3746 (4)	0.8359 (3)	0.3408 (3)	0.0618 (9)
H15	0.3981	0.9269	0.3463	0.074*
C16	0.3215 (4)	0.7547 (2)	0.2322 (2)	0.0494 (7)
H16	0.3090	0.7912	0.1653	0.059*
C17	0.2863 (3)	0.6180 (2)	0.2213 (2)	0.0350 (6)
Cl	0.74037 (10)	0.24095 (6)	0.24821 (6)	0.0510 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn	0.0350 (2)	0.0248 (2)	0.0309 (2)	−0.00026 (16)	0.00138 (15)	0.00799 (15)
O1	0.0526 (12)	0.0253 (9)	0.0292 (9)	−0.0035 (8)	−0.0001 (8)	0.0063 (7)
O2	0.0535 (12)	0.0242 (9)	0.0313 (9)	0.0030 (8)	−0.0043 (8)	0.0039 (7)
O3W	0.0357 (13)	0.0492 (13)	0.0670 (14)	−0.0081 (10)	−0.0038 (10)	0.0330 (11)
O4W	0.0391 (13)	0.0447 (12)	0.0472 (12)	0.0052 (9)	0.0019 (10)	0.0201 (10)
N1	0.0321 (13)	0.0261 (11)	0.0404 (12)	0.0009 (9)	0.0018 (9)	0.0094 (9)
N2	0.0358 (13)	0.0331 (12)	0.0351 (11)	0.0005 (9)	0.0007 (9)	0.0144 (10)
C1	0.0319 (15)	0.0328 (14)	0.0300 (13)	−0.0027 (11)	0.0046 (11)	0.0033 (11)
C2	0.0523 (19)	0.0384 (15)	0.0349 (14)	−0.0030 (13)	0.0023 (12)	0.0094 (12)
C3	0.062 (2)	0.060 (2)	0.0358 (15)	−0.0107 (16)	−0.0035 (13)	0.0154 (14)
C4	0.083 (2)	0.0532 (19)	0.0348 (16)	−0.0251 (17)	−0.0012 (15)	−0.0026 (14)
C5	0.067 (2)	0.0385 (16)	0.0438 (17)	−0.0130 (14)	0.0032 (14)	−0.0004 (13)
C6	0.0381 (17)	0.0315 (14)	0.0349 (14)	−0.0050 (12)	0.0033 (11)	0.0034 (11)
C7	0.0369 (17)	0.0241 (13)	0.0498 (17)	−0.0014 (11)	0.0071 (12)	0.0034 (12)
C8	0.0489 (19)	0.0294 (14)	0.0543 (17)	0.0075 (12)	0.0014 (13)	0.0164 (12)
C9	0.0469 (19)	0.0348 (15)	0.0596 (18)	−0.0001 (13)	0.0035 (14)	0.0254 (14)
C10	0.064 (2)	0.0445 (16)	0.0465 (16)	−0.0010 (14)	0.0029 (14)	0.0264 (14)
C11	0.0411 (17)	0.0531 (17)	0.0323 (14)	0.0011 (13)	−0.0003 (12)	0.0157 (13)
C12	0.0420 (18)	0.0407 (16)	0.0323 (14)	0.0012 (13)	−0.0024 (12)	0.0036 (12)
C13	0.064 (2)	0.059 (2)	0.0394 (16)	0.0050 (16)	−0.0098 (14)	0.0044 (14)

C14	0.080 (3)	0.056 (2)	0.0490 (19)	0.0029 (18)	−0.0205 (17)	−0.0141 (16)
C15	0.075 (2)	0.0373 (17)	0.064 (2)	−0.0030 (15)	−0.0143 (17)	−0.0030 (15)
C16	0.066 (2)	0.0327 (15)	0.0455 (16)	0.0004 (14)	−0.0073 (14)	0.0037 (13)
C17	0.0353 (16)	0.0304 (14)	0.0370 (14)	0.0043 (11)	0.0007 (11)	0.0021 (11)
Cl	0.0629 (5)	0.0414 (4)	0.0525 (4)	0.0080 (3)	0.0046 (3)	0.0176 (3)

Geometric parameters (Å, °)

Mn—O1	1.8843 (14)	C5—C6	1.403 (3)
Mn—O2	1.8861 (15)	C5—H5	0.9300
Mn—N1	2.0191 (18)	C6—C7	1.429 (3)
Mn—N2	2.0369 (18)	C7—H7	0.9300
Mn—O3W	2.195 (2)	C8—C9	1.510 (3)
Mn—O4W	2.240 (2)	C8—H8A	0.9700
O1—C1	1.335 (2)	C8—H8B	0.9700
O2—C17	1.330 (3)	C9—C10	1.498 (3)
O3W—H3A	0.78 (3)	C9—H9A	0.9700
O3W—H3B	0.79 (3)	C9—H9B	0.9700
O4W—H4A	0.84 (3)	C10—H10A	0.9700
O4W—H4B	0.72 (2)	C10—H10B	0.9700
N1—C7	1.285 (3)	C11—C12	1.428 (3)
N1—C8	1.473 (3)	C11—H11	0.9300
N2—C11	1.286 (3)	C12—C17	1.400 (3)
N2—C10	1.488 (3)	C12—C13	1.404 (3)
C1—C2	1.392 (3)	C13—C14	1.365 (4)
C1—C6	1.399 (3)	C13—H13	0.9300
C2—C3	1.372 (3)	C14—C15	1.376 (4)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.379 (4)	C15—C16	1.372 (3)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.358 (3)	C16—C17	1.392 (3)
C4—H4	0.9300	C16—H16	0.9300
O1—Mn—O2	84.41 (6)	C1—C6—C7	122.7 (2)
O1—Mn—N1	90.39 (7)	C5—C6—C7	118.0 (2)
O2—Mn—N1	174.54 (7)	N1—C7—C6	127.4 (2)
O1—Mn—N2	175.42 (7)	N1—C7—H7	116.3
O2—Mn—N2	91.01 (7)	C6—C7—H7	116.3
N1—Mn—N2	94.19 (8)	N1—C8—C9	109.7 (2)
O1—Mn—O3W	93.00 (8)	N1—C8—H8A	109.7
O2—Mn—O3W	91.15 (8)	C9—C8—H8A	109.7
N1—Mn—O3W	87.45 (8)	N1—C8—H8B	109.7
N2—Mn—O3W	87.16 (8)	C9—C8—H8B	109.7
O1—Mn—O4W	90.08 (8)	H8A—C8—H8B	108.2
O2—Mn—O4W	94.33 (7)	C10—C9—C8	113.6 (2)
N1—Mn—O4W	87.33 (7)	C10—C9—H9A	108.8
N2—Mn—O4W	90.18 (8)	C8—C9—H9A	108.8
O3W—Mn—O4W	173.95 (8)	C10—C9—H9B	108.8
C1—O1—Mn	129.05 (14)	C8—C9—H9B	108.8
C17—O2—Mn	127.51 (14)	H9A—C9—H9B	107.7

Mn—O3W—H3A	117 (2)	N2—C10—C9	114.5 (2)
Mn—O3W—H3B	125 (2)	N2—C10—H10A	108.6
H3A—O3W—H3B	108 (3)	C9—C10—H10A	108.6
Mn—O4W—H4A	120.5 (19)	N2—C10—H10B	108.6
Mn—O4W—H4B	110 (2)	C9—C10—H10B	108.6
H4A—O4W—H4B	114 (3)	H10A—C10—H10B	107.6
C7—N1—C8	117.68 (19)	N2—C11—C12	129.1 (2)
C7—N1—Mn	123.57 (16)	N2—C11—H11	115.5
C8—N1—Mn	118.61 (15)	C12—C11—H11	115.5
C11—N2—C10	114.2 (2)	C17—C12—C13	119.2 (2)
C11—N2—Mn	120.71 (16)	C17—C12—C11	122.5 (2)
C10—N2—Mn	125.04 (16)	C13—C12—C11	118.2 (2)
O1—C1—C2	118.9 (2)	C14—C13—C12	121.1 (3)
O1—C1—C6	122.0 (2)	C14—C13—H13	119.4
C2—C1—C6	119.1 (2)	C12—C13—H13	119.4
C3—C2—C1	119.9 (2)	C13—C14—C15	119.2 (3)
C3—C2—H2	120.0	C13—C14—H14	120.4
C1—C2—H2	120.0	C15—C14—H14	120.4
C2—C3—C4	121.4 (3)	C16—C15—C14	121.2 (3)
C2—C3—H3	119.3	C16—C15—H15	119.4
C4—C3—H3	119.3	C14—C15—H15	119.4
C5—C4—C3	119.4 (2)	C15—C16—C17	120.6 (3)
C5—C4—H4	120.3	C15—C16—H16	119.7
C3—C4—H4	120.3	C17—C16—H16	119.7
C4—C5—C6	120.9 (3)	O2—C17—C16	119.2 (2)
C4—C5—H5	119.5	O2—C17—C12	122.2 (2)
C6—C5—H5	119.5	C16—C17—C12	118.6 (2)
C1—C6—C5	119.2 (2)		

O2—Mn—O1—C1	−156.77 (19)	C2—C1—C6—C5	1.4 (4)
N1—Mn—O1—C1	24.90 (19)	O1—C1—C6—C7	1.2 (4)
O3W—Mn—O1—C1	112.37 (19)	C2—C1—C6—C7	−179.4 (2)
O4W—Mn—O1—C1	−62.42 (19)	C4—C5—C6—C1	−2.0 (4)
O1—Mn—O2—C17	−150.14 (19)	C4—C5—C6—C7	178.8 (3)
N2—Mn—O2—C17	29.9 (2)	C8—N1—C7—C6	175.9 (2)
O3W—Mn—O2—C17	−57.24 (19)	Mn—N1—C7—C6	0.2 (3)
O4W—Mn—O2—C17	120.20 (19)	C1—C6—C7—N1	9.7 (4)
O1—Mn—N1—C7	−13.38 (19)	C5—C6—C7—N1	−171.1 (2)
N2—Mn—N1—C7	166.67 (18)	C7—N1—C8—C9	−122.8 (2)
O3W—Mn—N1—C7	−106.37 (19)	Mn—N1—C8—C9	53.1 (2)
O4W—Mn—N1—C7	76.68 (19)	N1—C8—C9—C10	−82.3 (3)
O1—Mn—N1—C8	170.94 (17)	C11—N2—C10—C9	−178.2 (2)
N2—Mn—N1—C8	−9.02 (17)	Mn—N2—C10—C9	−1.8 (3)
O3W—Mn—N1—C8	77.95 (17)	C8—C9—C10—N2	52.7 (3)
O4W—Mn—N1—C8	−99.00 (17)	C10—N2—C11—C12	−177.6 (3)
O2—Mn—N2—C11	−19.4 (2)	Mn—N2—C11—C12	5.8 (4)
N1—Mn—N2—C11	158.91 (19)	N2—C11—C12—C17	7.8 (4)
O3W—Mn—N2—C11	71.67 (19)	N2—C11—C12—C13	−175.6 (3)
O4W—Mn—N2—C11	−113.76 (19)	C17—C12—C13—C14	−2.2 (4)
O2—Mn—N2—C10	164.4 (2)	C11—C12—C13—C14	−178.9 (3)

N1—Mn—N2—C10	−17.3 (2)	C12—C13—C14—C15	0.0 (5)
O3W—Mn—N2—C10	−104.5 (2)	C13—C14—C15—C16	1.3 (5)
O4W—Mn—N2—C10	70.0 (2)	C14—C15—C16—C17	−0.3 (5)
Mn—O1—C1—C2	158.04 (17)	Mn—O2—C17—C16	156.36 (19)
Mn—O1—C1—C6	−22.6 (3)	Mn—O2—C17—C12	−25.4 (3)
O1—C1—C2—C3	180.0 (2)	C15—C16—C17—O2	176.3 (2)
C6—C1—C2—C3	0.6 (4)	C15—C16—C17—C12	−1.9 (4)
C1—C2—C3—C4	−2.1 (4)	C13—C12—C17—O2	−175.1 (2)
C2—C3—C4—C5	1.5 (4)	C11—C12—C17—O2	1.5 (4)
C3—C4—C5—C6	0.5 (4)	C13—C12—C17—C16	3.1 (4)
O1—C1—C6—C5	−178.0 (2)	C11—C12—C17—C16	179.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3W—H3A···Cl	0.78 (3)	2.27 (3)	3.033 (2)	166 (3)
O3W—H3B···O1^{i}	0.79 (3)	2.00 (3)	2.782 (3)	172 (3)
O4W—H4A···Cl^{ii}	0.84 (3)	2.36 (3)	3.192 (2)	173 (3)
O4W—H4B···O2^{iii}	0.72 (2)	2.15 (2)	2.864 (3)	169 (3)

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

Fig. 1

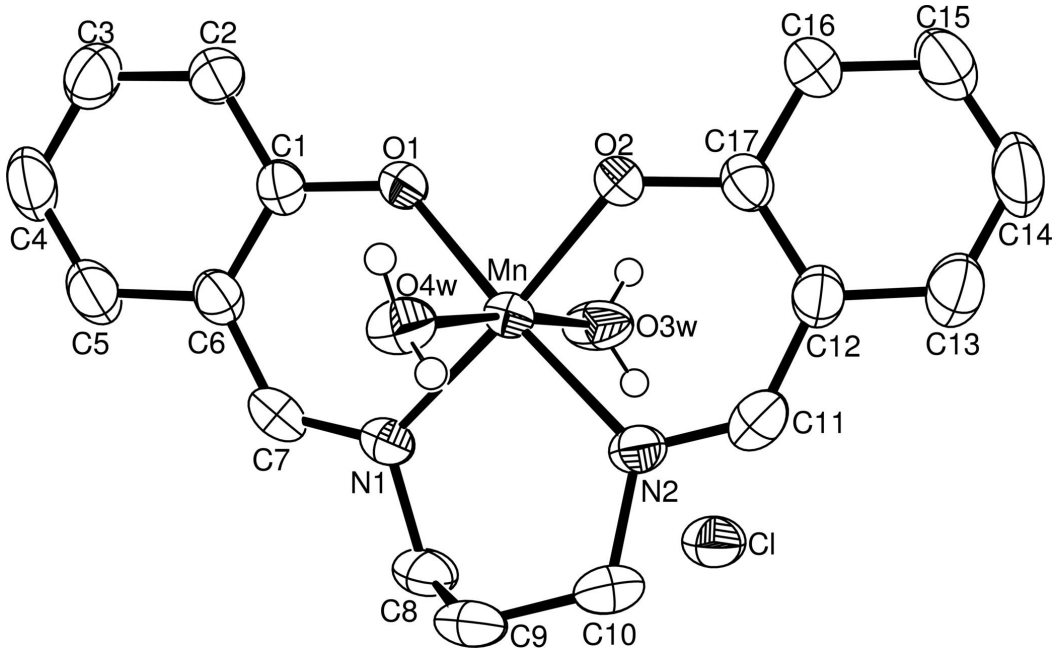
C3
C2
C16
C15
C1
O1
O2
C17
C4
C14
O4w
Mn
O3w
C5
C6
C12
C13
C7
C11
N1
N2
Cl
C8
C9
C10

Fig. 2