Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aquachlorido{4,4′-dibromo-2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}manganese(III)

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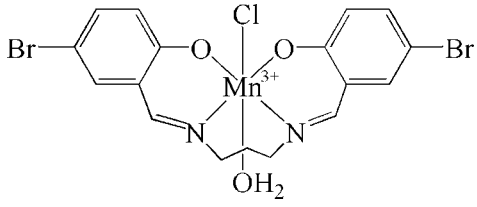
Received 2 August 2007; accepted 10 August 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.034; wR factor = 0.062; data-to-parameter ratio = 13.4.

In the title complex, $[Mn(C_{17}H_{14}Br_2N_2O_2)Cl(H_2O)]$, the Mn^{III} ion is six-coordinated by the tetradentate *N*,*N*′-bis(5-bromosalicylidene)-1,3-diiminopropane dianion (Brsalpn), Cl and water ligands in a distorted octahedral geometry. The complexes are assembled through intermolecular hydrogen bonds and π–π interactions (the centroid–centroid distance is 3.844 Å and the dihedral angle between the ring planes is 13.5°) along the *c* axis.

Related literature

For related literature, see: Mitra *et al.* (2006).



Experimental

Crystal data

$[Mn(C_{17}H_{14}Br_2N_2O_2)Cl(H_2O)]$
M_r = 546.53
Monoclinic, $P2_1/c$
a = 13.2369 (14) Å
b = 10.2666 (11) Å
c = 13.8635 (15) Å
β = 96.434 (2)°
V = 1872.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.14 mm^{-1}
T = 293 (2) K
0.12 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.448, T_{max} = 0.598
10208 measured reflections
3263 independent reflections
2153 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.062
S = 0.84
3263 reflections
243 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn—O2	1.882 (2)	Mn—N1	2.039 (3)
Mn—O1	1.894 (2)	Mn—O3*W*	2.342 (4)
Mn—N2	2.009 (3)	Mn—Cl	2.5852 (13)
O2—Mn—O1	85.46 (9)	N2—Mn—N1	92.70 (11)
O2—Mn—N2	91.32 (10)	O3*W*—Mn—Cl	170.43 (10)
O1—Mn—N1	90.68 (10)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*W*—H3*A*···O1^{i}	0.71 (4)	2.31 (5)	2.989 (4)	159 (5)
O3*W*—H3*B*···Cl^{ii}	0.76 (5)	2.48 (5)	3.236 (4)	174 (6)

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

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*.

This research was supported in part by the BK21 program from the Ministry of Education and Human Resources Development, Republic of Korea.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ER2038).

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supplementary materials

Acta Cryst. (2007). E**63**, m2365 [**doi:10.1107/S1600536807039815**]

Aquachlorido{4,4'-dibromo-2,2'-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}manganese(III)

I.-C. Hwang and K. Ha

Comment

In the title complex, Mn^{3+} ion is six-coordinated by two N and two O atoms from the tetradentate ligand, *N*,*N*'-bis(5-bromosalicylidene)-1,3- diiminopropane dianion (Brsalpn), occupying the four equatorial positions, one Cl atom and one O atom from water ligand 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 90.68 (10)°–92.70 (11)° and the O1—Mn—O2 bond angle is 85.46 (9)°. The apical O3w—Mn—Cl bond angle is 170.43 (10)° (Table 1). The Mn—N bond lengths (2.039 (3) and 2.009 (3) Å) are longer than the Mn—O bond (1.894 (2) and 1.882 (2) Å), but the bond distance between the Mn atom and the O atom of the water ligand is considerably long with 2.342 (4) Å. The compound displays the intermolecular hydrogen bonds between the O atom of the water and the O atom of the chelate ligand or Cl anion (Table 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: 1 − *x*, 1 − *y*, 1 − *z*), the centroid-centroid distance is 3.844 Å and the dihedral angle between the ring planes is 13.5°. The compounds are assembled through these hydrogen-bonding and π-π interactions along the *c* axis (Fig. 2).

Experimental

$Mn(CH_3COO)_3{\cdot}2H_2O$ (0.50 g, 1.86 mmol), NaCl (0.11 g, 1.88 mmol) and *N*,*N*'-bis(5-bromosalicylidene)-1,3-diiminopropane (H_2Brsalpn; 0.83 g, 1.89 mmol) in EtOH (70 ml) and H_2O (3 ml) were stirred for 3 h at room temparature and then filtered. The solvent was removed, the residue washed with water and acetone, and dried under vacuum, to give a dark green powder (0.76 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from a MeOH solution. MS (FAB): m/*z* 491, 493, 495 $(Mn(Brsalpn)^{+})$; IR (KBr): 3358 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 ligand were localized from Fourier difference maps and refined with isotropic thermal parameters.

Figures

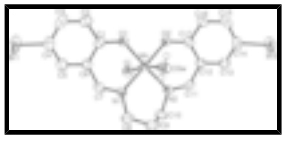

Fig. 1. The structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level. H atoms at C atoms have been omitted for clarity.

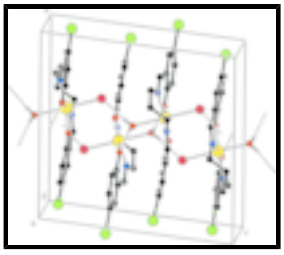

Fig. 2. View of the unit-cell contents of the title complex. Hydrogen-bond interactions are drawn with dashed lines.

Aquachlorido{4,4'-dibromo-2,2'-[propane-1,3- diylbis(nitrilomethylidyne)]diphenolato}manganese(III)

Crystal data

$[Mn(C_{17}H_{14}Br_2N_2O_2)Cl(H_2O)]$	F_{000} = 1072
M_r = 546.53	D_x = 1.939 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2295 reflections
a = 13.2369 (14) Å	θ = 2.5–23.9º
b = 10.2666 (11) Å	μ = 5.14 mm^{-1}
c = 13.8635 (15) Å	T = 293 (2) K
β = 96.434 (2)º	Plate, green
V = 1872.2 (3) Å^3	0.12 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD diffractometer	3263 independent reflections
Radiation source: fine-focus sealed tube	2153 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 293(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −15→7
T_{min} = 0.448, T_{max} = 0.598	k = −11→12
10208 measured reflections	l = −16→14

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
$wR(F^2)$ = 0.062	$w = 1/[\sigma^2(F_o^2) + (0.0243P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.84	$(\Delta/\sigma)_{max}$ = 0.001

3263 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
243 parameters	$\Delta\rho_{min} = -0.63$ 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.40515 (4)	0.33233 (5)	0.37376 (4)	0.02959 (16)
Br1	−0.06136 (4)	0.73006 (5)	0.33024 (4)	0.07213 (19)
Br2	0.94384 (3)	0.14805 (5)	0.41859 (4)	0.06350 (17)
Cl	0.33221 (7)	0.31177 (9)	0.19346 (7)	0.0414 (3)
O1	0.36286 (17)	0.5071 (2)	0.38667 (19)	0.0353 (7)
O2	0.53279 (17)	0.4039 (2)	0.35665 (18)	0.0351 (7)
O3W	0.4692 (3)	0.3130 (4)	0.5376 (3)	0.0461 (9)
H3A	0.497 (4)	0.368 (4)	0.556 (4)	0.07 (2)*
H3B	0.441 (4)	0.282 (5)	0.577 (4)	0.12 (3)*
N1	0.2690 (2)	0.2666 (3)	0.4099 (2)	0.0294 (8)
N2	0.4567 (2)	0.1510 (2)	0.3550 (2)	0.0299 (8)
C1	0.2688 (3)	0.5545 (3)	0.3745 (3)	0.0327 (10)
C2	0.2529 (3)	0.6879 (4)	0.3601 (3)	0.0410 (11)
H2	0.3087	0.7426	0.3585	0.049*
C3	0.1571 (3)	0.7398 (4)	0.3481 (3)	0.0506 (12)
H3	0.1486	0.8291	0.3393	0.061*
C4	0.0723 (3)	0.6597 (4)	0.3491 (3)	0.0497 (12)
C5	0.0858 (3)	0.5299 (4)	0.3645 (3)	0.0475 (11)
H5	0.0294	0.4762	0.3661	0.057*
C6	0.1836 (3)	0.4754 (4)	0.3779 (3)	0.0358 (10)
C7	0.1904 (3)	0.3399 (3)	0.4022 (3)	0.0368 (10)
H7	0.1299	0.3001	0.4139	0.044*
C8	0.2479 (3)	0.1309 (3)	0.4385 (3)	0.0455 (12)
H8A	0.2293	0.1323	0.5042	0.055*
H8B	0.1895	0.0995	0.3965	0.055*
C9	0.3307 (3)	0.0379 (4)	0.4349 (4)	0.0604 (15)
H9A	0.3033	−0.0491	0.4407	0.072*
H9B	0.3799	0.0524	0.4911	0.072*

C10	0.3850 (3)	0.0414 (3)	0.3472 (3)	0.0418 (11)
H10A	0.4215	−0.0396	0.3413	0.050*
H10B	0.3366	0.0516	0.2897	0.050*
C11	0.5502 (3)	0.1228 (3)	0.3483 (3)	0.0333 (10)
H11	0.5645	0.0371	0.3326	0.040*
C12	0.6348 (3)	0.2111 (3)	0.3627 (3)	0.0304 (9)
C13	0.7313 (3)	0.1549 (4)	0.3738 (3)	0.0384 (10)
H13	0.7385	0.0653	0.3672	0.046*
C14	0.8149 (3)	0.2313 (4)	0.3943 (3)	0.0391 (10)
C15	0.8056 (3)	0.3657 (4)	0.3990 (3)	0.0418 (11)
H15	0.8633	0.4173	0.4112	0.050*
C16	0.7113 (3)	0.4223 (3)	0.3856 (3)	0.0358 (10)
H16	0.7059	0.5126	0.3880	0.043*
C17	0.6227 (3)	0.3467 (3)	0.3683 (3)	0.0311 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn	0.0280 (3)	0.0247 (3)	0.0364 (4)	−0.0021 (2)	0.0049 (3)	−0.0010 (3)
Br1	0.0565 (3)	0.0848 (4)	0.0714 (4)	0.0366 (3)	−0.0093 (3)	−0.0064 (3)
Br2	0.0318 (3)	0.0806 (4)	0.0771 (4)	0.0098 (2)	0.0022 (2)	−0.0028 (3)
Cl	0.0484 (6)	0.0408 (6)	0.0344 (7)	−0.0017 (4)	0.0020 (5)	0.0012 (5)
O1	0.0310 (15)	0.0251 (14)	0.051 (2)	−0.0002 (11)	0.0073 (13)	−0.0034 (12)
O2	0.0283 (14)	0.0278 (14)	0.050 (2)	−0.0007 (11)	0.0073 (13)	0.0013 (12)
O3W	0.050 (2)	0.044 (2)	0.042 (2)	−0.0127 (16)	−0.0021 (17)	−0.0044 (17)
N1	0.0314 (18)	0.0261 (18)	0.031 (2)	−0.0011 (14)	0.0062 (15)	0.0004 (14)
N2	0.0300 (18)	0.0226 (17)	0.037 (2)	−0.0051 (13)	0.0015 (15)	−0.0036 (14)
C1	0.045 (3)	0.028 (2)	0.025 (3)	0.0051 (18)	0.0042 (19)	−0.0048 (18)
C2	0.051 (3)	0.035 (3)	0.037 (3)	−0.0011 (19)	0.007 (2)	−0.004 (2)
C3	0.072 (3)	0.039 (3)	0.041 (3)	0.021 (2)	0.009 (2)	0.001 (2)
C4	0.039 (3)	0.060 (3)	0.049 (3)	0.014 (2)	−0.001 (2)	−0.006 (2)
C5	0.036 (2)	0.051 (3)	0.055 (4)	0.001 (2)	0.001 (2)	−0.006 (2)
C6	0.032 (2)	0.035 (2)	0.040 (3)	0.0033 (18)	0.0002 (19)	−0.0054 (19)
C7	0.029 (2)	0.040 (2)	0.042 (3)	−0.0068 (18)	0.0073 (19)	−0.003 (2)
C8	0.049 (3)	0.031 (2)	0.058 (4)	−0.0046 (19)	0.013 (2)	0.006 (2)
C9	0.064 (3)	0.033 (3)	0.088 (5)	−0.008 (2)	0.028 (3)	0.007 (2)
C10	0.042 (2)	0.031 (2)	0.054 (3)	−0.0095 (18)	0.010 (2)	−0.011 (2)
C11	0.039 (2)	0.024 (2)	0.037 (3)	0.0029 (17)	0.0061 (19)	0.0012 (18)
C12	0.031 (2)	0.029 (2)	0.032 (3)	−0.0002 (16)	0.0055 (18)	0.0019 (17)
C13	0.037 (2)	0.036 (2)	0.042 (3)	0.0010 (19)	0.007 (2)	0.000 (2)
C14	0.026 (2)	0.056 (3)	0.035 (3)	0.0068 (19)	0.0042 (18)	0.003 (2)
C15	0.031 (2)	0.060 (3)	0.035 (3)	−0.013 (2)	0.0048 (19)	−0.006 (2)
C16	0.035 (2)	0.037 (2)	0.036 (3)	−0.0066 (18)	0.0069 (19)	−0.0008 (19)
C17	0.031 (2)	0.037 (2)	0.027 (3)	−0.0028 (18)	0.0086 (18)	0.0012 (18)

Geometric parameters (Å, °)

Mn—O2	1.882 (2)	C5—C6	1.403 (5)
Mn—O1	1.894 (2)	C5—H5	0.9300

Mn—N2	2.009 (3)	C6—C7	1.431 (5)
Mn—N1	2.039 (3)	C7—H7	0.9300
Mn—O3W	2.342 (4)	C8—C9	1.458 (5)
Mn—Cl	2.5852 (13)	C8—H8A	0.9700
Br1—C4	1.901 (4)	C8—H8B	0.9700
Br2—C14	1.905 (4)	C9—C10	1.481 (5)
O1—C1	1.330 (4)	C9—H9A	0.9700
O2—C17	1.321 (4)	C9—H9B	0.9700
O3W—H3A	0.71 (4)	C10—H10A	0.9700
O3W—H3B	0.76 (5)	C10—H10B	0.9700
N1—C7	1.279 (4)	C11—C12	1.438 (5)
N1—C8	1.483 (4)	C11—H11	0.9300
N2—C11	1.285 (4)	C12—C13	1.394 (5)
N2—C10	1.468 (4)	C12—C17	1.405 (4)
C1—C6	1.394 (5)	C13—C14	1.360 (5)
C1—C2	1.397 (5)	C13—H13	0.9300
C2—C3	1.368 (5)	C14—C15	1.387 (5)
C2—H2	0.9300	C15—C16	1.370 (5)
C3—C4	1.394 (5)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.405 (5)
C4—C5	1.358 (5)	C16—H16	0.9300
O2—Mn—O1	85.46 (9)	C5—C6—C7	116.8 (3)
O2—Mn—N2	91.32 (10)	N1—C7—C6	128.4 (3)
O1—Mn—N2	176.42 (10)	N1—C7—H7	115.8
O2—Mn—N1	172.37 (11)	C6—C7—H7	115.8
O1—Mn—N1	90.68 (10)	C9—C8—N1	116.2 (3)
N2—Mn—N1	92.70 (11)	C9—C8—H8A	108.2
O2—Mn—O3W	85.58 (13)	N1—C8—H8A	108.2
O1—Mn—O3W	93.86 (12)	C9—C8—H8B	108.2
N2—Mn—O3W	87.45 (12)	N1—C8—H8B	108.2
N1—Mn—O3W	88.12 (13)	H8A—C8—H8B	107.4
O2—Mn—Cl	98.82 (8)	C8—C9—C10	116.6 (4)
O1—Mn—Cl	94.96 (9)	C8—C9—H9A	108.1
N2—Mn—Cl	83.97 (9)	C10—C9—H9A	108.1
N1—Mn—Cl	88.05 (9)	C8—C9—H9B	108.1
O3W—Mn—Cl	170.43 (10)	C10—C9—H9B	108.1
C1—O1—Mn	128.1 (2)	H9A—C9—H9B	107.3
C17—O2—Mn	128.3 (2)	N2—C10—C9	109.1 (3)
Mn—O3W—H3A	114 (4)	N2—C10—H10A	109.9
Mn—O3W—H3B	125 (5)	C9—C10—H10A	109.9
H3A—O3W—H3B	111 (6)	N2—C10—H10B	109.9
C7—N1—C8	113.6 (3)	C9—C10—H10B	109.9
C7—N1—Mn	121.2 (2)	H10A—C10—H10B	108.3
C8—N1—Mn	125.1 (2)	N2—C11—C12	126.1 (3)
C11—N2—C10	116.2 (3)	N2—C11—H11	116.9
C11—N2—Mn	124.2 (2)	C12—C11—H11	116.9
C10—N2—Mn	119.6 (2)	C13—C12—C17	120.9 (3)
O1—C1—C6	122.1 (3)	C13—C12—C11	116.4 (3)
O1—C1—C2	120.0 (3)	C17—C12—C11	122.7 (3)

C6—C1—C2	117.9 (3)	C14—C13—C12	119.9 (4)
C3—C2—C1	121.4 (4)	C14—C13—H13	120.1
C3—C2—H2	119.3	C12—C13—H13	120.1
C1—C2—H2	119.3	C13—C14—C15	120.6 (3)
C2—C3—C4	120.4 (4)	C13—C14—Br2	118.0 (3)
C2—C3—H3	119.8	C15—C14—Br2	121.4 (3)
C4—C3—H3	119.8	C16—C15—C14	120.0 (3)
C5—C4—C3	119.2 (4)	C16—C15—H15	120.0
C5—C4—Br1	119.9 (3)	C14—C15—H15	120.0
C3—C4—Br1	120.8 (3)	C15—C16—C17	121.2 (4)
C4—C5—C6	121.0 (4)	C15—C16—H16	119.4
C4—C5—H5	119.5	C17—C16—H16	119.4
C6—C5—H5	119.5	O2—C17—C12	122.8 (3)
C1—C6—C5	120.0 (4)	O2—C17—C16	119.9 (3)
C1—C6—C7	123.0 (3)	C12—C17—C16	117.3 (3)
O2—Mn—O1—C1	158.8 (3)	C2—C1—C6—C5	1.6 (6)
N1—Mn—O1—C1	−27.8 (3)	O1—C1—C6—C7	5.1 (6)
O3W—Mn—O1—C1	−116.0 (3)	C2—C1—C6—C7	−173.3 (4)
Cl—Mn—O1—C1	60.3 (3)	C4—C5—C6—C1	−0.7 (6)
O1—Mn—O2—C17	159.2 (3)	C4—C5—C6—C7	174.5 (4)
N2—Mn—O2—C17	−22.4 (3)	C8—N1—C7—C6	178.8 (4)
O3W—Mn—O2—C17	64.9 (3)	Mn—N1—C7—C6	−6.2 (6)
Cl—Mn—O2—C17	−106.5 (3)	C1—C6—C7—N1	−11.3 (7)
O1—Mn—N1—C7	20.3 (3)	C5—C6—C7—N1	173.6 (4)
N2—Mn—N1—C7	−158.5 (3)	C7—N1—C8—C9	171.4 (4)
O3W—Mn—N1—C7	114.2 (3)	Mn—N1—C8—C9	−3.4 (5)
Cl—Mn—N1—C7	−74.6 (3)	N1—C8—C9—C10	−45.4 (5)
O1—Mn—N1—C8	−165.2 (3)	C11—N2—C10—C9	123.7 (4)
N2—Mn—N1—C8	16.0 (3)	Mn—N2—C10—C9	−57.0 (4)
O3W—Mn—N1—C8	−71.4 (3)	C8—C9—C10—N2	78.4 (5)
Cl—Mn—N1—C8	99.9 (3)	C10—N2—C11—C12	−173.9 (4)
O2—Mn—N2—C11	7.4 (3)	Mn—N2—C11—C12	6.8 (5)
N1—Mn—N2—C11	−166.1 (3)	N2—C11—C12—C13	165.8 (4)
O3W—Mn—N2—C11	−78.1 (3)	N2—C11—C12—C17	−12.4 (6)
Cl—Mn—N2—C11	106.1 (3)	C17—C12—C13—C14	2.7 (6)
O2—Mn—N2—C10	−171.9 (3)	C11—C12—C13—C14	−175.5 (4)
N1—Mn—N2—C10	14.6 (3)	C12—C13—C14—C15	−3.6 (6)
O3W—Mn—N2—C10	102.6 (3)	C12—C13—C14—Br2	175.2 (3)
Cl—Mn—N2—C10	−73.1 (3)	C13—C14—C15—C16	1.8 (6)
Mn—O1—C1—C6	19.6 (5)	Br2—C14—C15—C16	−176.9 (3)
Mn—O1—C1—C2	−162.0 (3)	C14—C15—C16—C17	0.8 (6)
O1—C1—C2—C3	−179.5 (4)	Mn—O2—C17—C12	23.2 (5)
C6—C1—C2—C3	−0.9 (6)	Mn—O2—C17—C16	−157.8 (3)
C1—C2—C3—C4	−0.7 (6)	C13—C12—C17—O2	178.9 (3)
C2—C3—C4—C5	1.6 (7)	C11—C12—C17—O2	−3.0 (6)
C2—C3—C4—Br1	−178.8 (3)	C13—C12—C17—C16	−0.1 (5)
C3—C4—C5—C6	−0.9 (7)	C11—C12—C17—C16	178.0 (3)
Br1—C4—C5—C6	179.5 (3)	C15—C16—C17—O2	179.3 (3)
O1—C1—C6—C5	−179.9 (4)	C15—C16—C17—C12	−1.7 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3W—H3A···O1^{i}	0.71 (4)	2.31 (5)	2.989 (4)	159 (5)
O3W—H3B···Cl^{ii}	0.76 (5)	2.48 (5)	3.236 (4)	174 (6)

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

Fig. 1

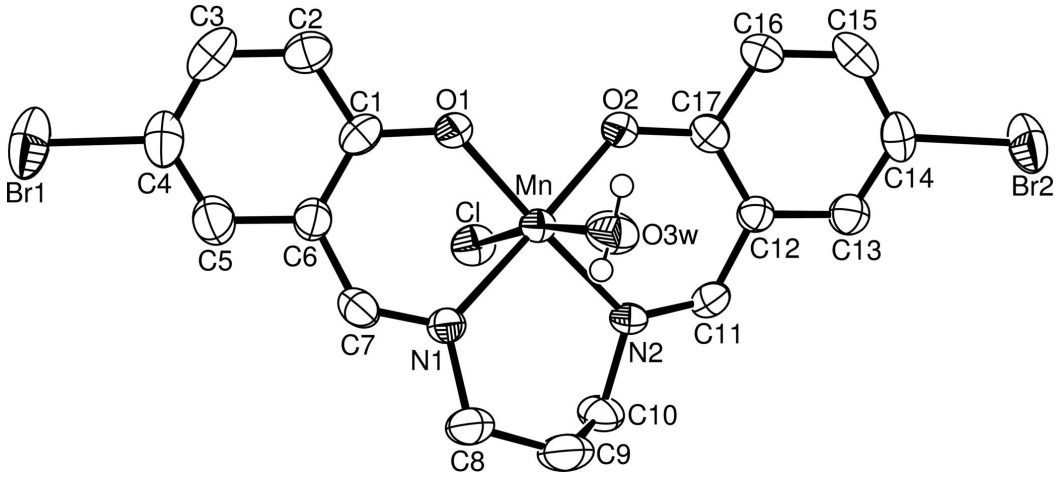
C3
C2
C16
C15
C1
O1
O2
C17
Br1
C4
Mn
C14
Br2
Cl
O3w
C5
C6
C12
C13
C7
N1
N2
C11
C10
C8
C9

Fig. 2