Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chlorido{4,4′-dimethoxy-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]-diphenolato}methanolmanganese(III)

Naser Eltaher Eltayeb,[a]‡ Siang Guan Teoh,[a] Suchada Chantrapromma,[b]* Hoong-Kun Fun[c]* and Kamarulazizi Ibrahim[d]

[a]School of Chemical Science, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [d]School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: suchada.c@psu.ac.th, hkfun@usm.my

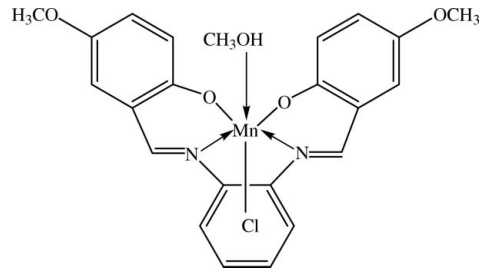
Received 12 November 2007; accepted 20 November 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.044; wR factor = 0.112; data-to-parameter ratio = 15.0.

In the title complex, $[Mn(C_{22}H_{18}N_2O_4)Cl(CH_3OH)]$, the Mn^{III} centre is in a distorted octahedral geometry, with the N_2O_2 tetradentate Schiff base ligand in the equatorial plane and the chloride ion and methanol molecule in the axial positions. The dihedral angles between the two outer phenolate rings and the central benzene ring of the tetradentate ligand are 4.08 (14) and 13.61 (14)°. One of the two methoxy substituents on the outer phenolate rings lies almost in the plane of the ring to which it is bound, whereas the other methoxy group is twisted significantly from the corresponding benzene ring plane. In the crystal structure, weak intermolecular C—H···Cl interactions link the molecules into infinite chains along the b axis, and these chains are further connected by O—H···O hydrogen bonds, weak C—H···O and C—H···Cl interactions into sheets parallel to the ab plane. The crystal structure is further stabilized by C—H···π interactions.

Related literature

For values of bond lengths, see Allen *et al.* (1987). For related structures, see, for example: Eltayeb *et al.* (2007); Habibi *et al.* (2007); Mitra *et al.* (2006); Naskar *et al.* (2004). For information on the applications of manganese complexes, see, for example: Dixit & Srinivasan (1988); Glatzel *et al.* (2004); Lu *et al.* (2006); Stallings *et al.* (1985).



Experimental

Crystal data

$[Mn(C_{22}H_{18}N2O4)Cl(CH_4O)]$
M_r = 496.82
Monoclinic, $P2_1/c$
a = 12.2105 (8) Å
b = 7.5497 (5) Å
c = 22.4197 (15) Å
β = 90.404 (1)°
V = 2066.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 100.0 (1) K
0.31 × 0.16 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.785, T_{max} = 0.931
10970 measured reflections
4429 independent reflections
3418 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.113
S = 1.05
4429 reflections
296 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 benzene rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1O5···O1^{i}	0.81 (4)	2.54 (4)	3.183 (3)	138 (3)
O5—H1O5···O2^{i}	0.81 (4)	2.37 (4)	2.998 (3)	135 (3)
C7—H7A···Cl1	0.93	2.69	3.519 (3)	148
C14—H14A···O4^{ii}	0.93	2.47	3.222 (4)	138
C23—H23B···Cl1^{iii}	0.96	2.83	3.488 (4)	127
C2—H2A···$Cg2^{iv}$	0.93	2.86	3.507 (3)	128
C9—H9A···$Cg1^{iv}$	0.93	2.98	3.577 (3)	124
C22—H22C···$Cg2^{ii}$	0.96	2.64	3.453 (3)	143

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government, the Ministry of Science, Technology and Innovation (MOSTI) and Universiti Sains Malaysia for an E-Science Fund research

‡ On study leave from the International University of Africa, Sudan.

grant (No. PKIMIA/613308) and facilities. The International University of Africa (Sudan) is acknowledged for providing study leave to NEE. The authors also thank Universiti Sains Malaysia for the Fundamental Research Grant Scheme (FRGS) (grant No. 203/PFIZIK/671064).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2438).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12A) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Dixit, P. S. & Srinivasan, K. (1988). *Inorg. Chem.* **27**, 4507–4509.
Eltayeb, N. E., Teoh, S. G., Chantrapromma, S., Fun, H.-K. & Ibrahim, K. (2007). *Acta Cryst.* E**63**, o3234–o3235.
Glatzel, P., Bergmann, U., Yano, J., Visser, H., Robblee, J. H., Gu, W., de Groot, F. M. F., Christou, G., Pecoraro, V. L., Cramer, S. P. & Yachandra, V. K. (2004). *J. Am. Chem. Soc.* **126**, 9946–9959.
Habibi, M. H., Askari, E., Chantrapromma, S. & Fun, H.-K. (2007). *Acta Cryst.* E**63**, m2905–m2906.
Lu, Z., Yuan, M., Pan, F., Gao, S., Zhang, D. & Zhu, D. (2006). *Inorg. Chem.* **45**, 3538–3548.
Mitra, K., Biswas, S., Lucas, C. R. & Adhikary, B. (2006). *Inorg. Chim. Acta*, **359**, 1997–2003.
Naskar, S., Biswas, S., Mishra, D., Adhikary, B., Falvello, L. R., Soler, T., Schwalbe, C. H. & Chattopadhyay, S. K. (2004). *Inorg. Chim. Acta*, **357**, 4257–4264.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stallings, W. C., Pattridge, K. A., Strong, R. K. & Ludwig, M. L. (1985). *J. Biol. Chem.* **260**, 16424–16432.

supplementary materials

Acta Cryst. (2007). E**63**, m3193-m3194 [**doi:10.1107/S1600536807061363**]

Chlorido{4,4'-dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato}methanolmanganese(III)

N. E. Eltayeb, S. G. Teoh, S. Chantrapromma, H.-K. Fun and K. Ibrahim

Comment

Manganese complexes with Schiff base have attracted considerable interest in the past decades and recently, due to their variety of applications in chemistry, biology, physics and advanced materials. They have been used as models for oxygen-evolving complex of photosystem II (Glatzel *et al.*, 2004), catalysis (Dixit & Srinivasan, 1988), single-molecule magnet (Lu *et al.*, 2006) and as active sites of manganese-containing metal enzymes (Stallings *et al.*, 1985). Recently, we reported the crystal structure of 4,4'-Dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenol (Eltayeb *et al.*, 2007). We have extended our synthesis to the title Mn(III) complex and herein its crystal structure is reported.

In the title complex molecule (Fig. 1), Mn^{III} coordinates with the tetradentate Schiff base ligand in the equatorial plane (N1, N2, O1 and O2) and the chloride ion and methanol molecule in the axial positions. The Mn1—N1 and Mn1—N2 distances of 1.987 (2) Å and 1.995 (2) Å, and the Mn1—O1 and Mn1—O2 distances of 1.8634 (19) and 1.8746 (19) Å, respectively are in the same range as those in other six coordinated Mn^{III} complexes of Schiff base ligands (Habibi *et al.*, 2007; Mitra *et al.*, 2006; Naskar *et al.*, 2004). The Mn1—O5 = 2.423 (2) Å and Mn1—Cl1 = 2.4846 (8) Å bonds were elongated as had also been found previously (Habibi *et al.*, 2007). The dihedral angles between the two outer benzene rings (C1–C6) and (C8–C13) and the central benzene ring (C15–C20) are 4.08 (14)° and 13.61 (14)° respectively. One of the two methoxy groups is almost coplanar with the attached benzene ring as indicated by the torsion angle C22—O3—C4—C3 of 4.9 (4)°, whereas another methoxy group is twisted from the mean plane of the attached benzene with the torsion angle C21—O3—C4—C3 = 33.3 (4)°. Bond lengths and angles in the Schiff base ligand are very similar to those reported for the other Mn^{III} complexes with similar ligands (Habibi *et al.*, 2007; Mitra *et al.*, 2006; Naskar *et al.*, 2004) and other bond lengths and angles observed in the structure are also normal (Allen *et al.*, 1987).

In the crystal packing (Fig. 2), weak C—H···Cl interactions (Table 1) link the molecules into infinite chains along the [0 1 0] direction. These chains are further connected into sheets parallel to the *ab* plane by O—H···O hydrogen bonds, weak C—H···O and C—H···Cl interactons (Table 1). The crystal is further stabilized by C—H···π interactions (Table 1); Cg_1 and Cg_2 are the centroids of C1–C6 and C8–C13 benzene rings, respectively.

It is interesting to note that although the unit cell is almost metrically orthorhombic, the space group is actually monoclinic.

Experimental

The title compound was synthesized by adding 5-methoxy-2-hydroxybenzaldehyde (0.4 ml, 4 mmol) to a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol 95% (20 ml). The mixture was refluxed with stirring for half an hour. Manganese chloride tetrahydrate (0.394 g, 2 mmol) in ethanol (10 ml) was then added, followed by triethylamine (0.5 ml, 3.6 mmol). The mixture was refluxed at room temperature for three hours. A brown precipitate was obtained, washed with

ethanol (about 5 ml), dried, and then washed with copious quantities of diethyl ether. Brown single crystals of the title compound suitable for X-ray structure determination were recrystalized from methanol by slow evaporation of the solvent at room temperature over several days.

Refinement

H atom (H1O5) of the methanol molecule was located from the difference map and refined isotropically. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the ranges 0.93–0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 0.68 Å from H23C and the deepest hole is located at 0.52 Å from C23.

Figures

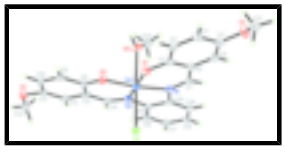


Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering.

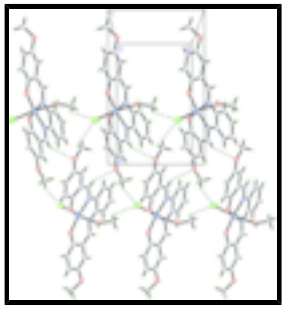


Fig. 2. The crystal packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

Chlorido{4,4'-dimethoxy-2,2'-[1,2- phenylenebis(nitrilomethylidyne)]diphenolato}methanolmanganese(III)

Crystal data

[Mn($C_{22}H_{18}N2O4$)Cl(CH_4O)]	F_{000} = 1024
M_r = 496.82	D_x = 1.597 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4429 reflections
a = 12.2105 (8) Å	θ = 4.9–27.0º
b = 7.5497 (5) Å	μ = 0.81 mm^{-1}
c = 22.4197 (15) Å	*T* = 100.0 (1) K
β = 90.404 (1)º	Plate, black
V = 2066.7 (2) Å^3	0.31 × 0.16 × 0.09 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	4429 independent reflections
Radiation source: fine-focus sealed tube	3418 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.047$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 27.0^{o}$
$T = 100.0(1)$ K	$\theta_{min} = 4.9^{o}$
ω scans	$h = -12 \rightarrow 15$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -9 \rightarrow 9$
$T_{min} = 0.785$, $T_{max} = 0.931$	$l = -28 \rightarrow 28$
10970 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
$R[F^2 > 2\sigma(F^2)] = 0.044$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.113$	$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 1.7319P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = <0.001$
4429 reflections	$\Delta\rho_{max} = 1.44$ e $Å^{-3}$
296 parameters	$\Delta\rho_{min} = -0.40$ e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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}
Mn1	0.40972 (3)	0.52000 (6)	0.147831 (18)	0.01839 (13)
Cl1	0.33383 (6)	0.27719 (9)	0.08519 (3)	0.02167 (17)

O1	0.54569 (15)	0.4197 (3)	0.16522 (8)	0.0216 (4)
O2	0.35701 (15)	0.4359 (3)	0.22087 (8)	0.0213 (4)
O3	0.95200 (16)	0.5459 (3)	0.06780 (10)	0.0297 (5)
O4	−0.03870 (16)	0.5087 (3)	0.33444 (9)	0.0232 (4)
O5	0.4667 (2)	0.7850 (3)	0.20047 (10)	0.0315 (5)
H1O5	0.494 (3)	0.786 (5)	0.2333 (17)	0.031 (10)*
N1	0.46456 (18)	0.6480 (3)	0.07661 (9)	0.0174 (5)
N2	0.27412 (18)	0.6576 (3)	0.12943 (9)	0.0176 (5)
C1	0.6420 (2)	0.4531 (4)	0.14052 (12)	0.0186 (6)
C2	0.7347 (2)	0.3746 (4)	0.16562 (12)	0.0217 (6)
H2A	0.7271	0.3030	0.1991	0.026*
C3	0.8376 (2)	0.4009 (4)	0.14186 (13)	0.0230 (6)
H3A	0.8984	0.3478	0.1596	0.028*
C4	0.8506 (2)	0.5071 (4)	0.09128 (13)	0.0235 (6)
C5	0.7607 (2)	0.5857 (4)	0.06544 (12)	0.0210 (6)
H5A	0.7695	0.6555	0.0316	0.025*
C6	0.6549 (2)	0.5620 (4)	0.08945 (12)	0.0190 (6)
C7	0.5661 (2)	0.6517 (4)	0.05965 (11)	0.0192 (6)
H7A	0.5826	0.7172	0.0257	0.023*
C8	0.2602 (2)	0.4633 (4)	0.24474 (12)	0.0183 (5)
C9	0.2400 (2)	0.3840 (4)	0.30091 (12)	0.0208 (6)
H9A	0.2948	0.3176	0.3194	0.025*
C10	0.1404 (2)	0.4039 (4)	0.32845 (12)	0.0217 (6)
H10A	0.1292	0.3518	0.3655	0.026*
C11	0.0562 (2)	0.5007 (4)	0.30186 (12)	0.0198 (6)
C12	0.0729 (2)	0.5807 (4)	0.24731 (12)	0.0199 (6)
H12A	0.0165	0.6446	0.2293	0.024*
C13	0.1760 (2)	0.5657 (4)	0.21846 (12)	0.0190 (6)
C14	0.1870 (2)	0.6559 (4)	0.16251 (12)	0.0192 (6)
H14A	0.1265	0.7188	0.1487	0.023*
C15	0.2781 (2)	0.7462 (4)	0.07338 (12)	0.0184 (5)
C16	0.1906 (2)	0.8325 (4)	0.04637 (12)	0.0223 (6)
H16A	0.1230	0.8370	0.0652	0.027*
C17	0.2044 (2)	0.9122 (4)	−0.00878 (12)	0.0234 (6)
H17A	0.1460	0.9709	−0.0268	0.028*
C18	0.3051 (2)	0.9049 (4)	−0.03733 (12)	0.0217 (6)
H18A	0.3133	0.9579	−0.0745	0.026*
C19	0.3924 (2)	0.8201 (4)	−0.01116 (12)	0.0198 (6)
H19A	0.4596	0.8157	−0.0304	0.024*
C20	0.3798 (2)	0.7401 (4)	0.04479 (12)	0.0182 (5)
C21	1.0340 (2)	0.4101 (4)	0.07311 (14)	0.0278 (7)
H21A	1.0979	0.4444	0.0512	0.042*
H21B	1.0058	0.3010	0.0573	0.042*
H21C	1.0532	0.3942	0.1144	0.042*
C22	−0.1303 (2)	0.5962 (4)	0.30732 (13)	0.0254 (6)
H22A	−0.1912	0.5943	0.3342	0.038*
H22B	−0.1501	0.5363	0.2710	0.038*
H22C	−0.1112	0.7167	0.2986	0.038*
C23	0.4505 (3)	0.9679 (5)	0.18215 (16)	0.0392 (8)

H23A	0.4206	1.0344	0.2147	0.059*
H23B	0.4007	0.9718	0.1489	0.059*
H23C	0.5194	1.0183	0.1708	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0203 (2)	0.0188 (2)	0.0160 (2)	0.00112 (17)	−0.00294 (15)	0.00307 (16)
Cl1	0.0268 (3)	0.0194 (3)	0.0187 (3)	−0.0018 (3)	−0.0012 (3)	0.0005 (3)
O1	0.0216 (10)	0.0217 (10)	0.0214 (10)	0.0033 (8)	−0.0030 (8)	0.0062 (8)
O2	0.0231 (10)	0.0242 (11)	0.0164 (9)	0.0030 (8)	−0.0023 (8)	0.0035 (8)
O3	0.0224 (10)	0.0312 (12)	0.0354 (12)	0.0036 (9)	0.0040 (9)	0.0100 (10)
O4	0.0238 (10)	0.0244 (11)	0.0215 (10)	0.0037 (8)	0.0013 (8)	0.0036 (8)
O5	0.0466 (14)	0.0247 (12)	0.0230 (11)	0.0033 (10)	−0.0162 (10)	−0.0033 (9)
N1	0.0221 (11)	0.0146 (11)	0.0155 (10)	−0.0006 (9)	−0.0039 (9)	−0.0004 (9)
N2	0.0228 (11)	0.0167 (11)	0.0133 (10)	0.0017 (9)	−0.0028 (9)	0.0005 (9)
C1	0.0211 (13)	0.0173 (14)	0.0175 (13)	−0.0011 (11)	−0.0027 (10)	−0.0050 (11)
C2	0.0283 (15)	0.0168 (14)	0.0198 (13)	−0.0015 (11)	−0.0050 (11)	0.0036 (11)
C3	0.0224 (14)	0.0207 (15)	0.0257 (14)	0.0007 (11)	−0.0051 (11)	0.0004 (12)
C4	0.0227 (14)	0.0225 (15)	0.0254 (14)	−0.0009 (12)	0.0016 (11)	−0.0009 (12)
C5	0.0273 (15)	0.0170 (14)	0.0187 (13)	−0.0016 (11)	−0.0021 (11)	0.0000 (11)
C6	0.0231 (14)	0.0168 (14)	0.0172 (12)	0.0014 (11)	−0.0021 (10)	−0.0020 (10)
C7	0.0265 (14)	0.0172 (14)	0.0140 (12)	−0.0017 (11)	−0.0030 (11)	−0.0019 (10)
C8	0.0227 (13)	0.0148 (13)	0.0173 (12)	0.0005 (11)	−0.0033 (10)	−0.0013 (10)
C9	0.0256 (14)	0.0180 (14)	0.0188 (13)	0.0016 (11)	−0.0058 (11)	0.0002 (11)
C10	0.0311 (15)	0.0163 (14)	0.0176 (13)	−0.0010 (12)	−0.0001 (11)	0.0008 (11)
C11	0.0238 (14)	0.0176 (14)	0.0180 (13)	−0.0030 (11)	−0.0009 (11)	−0.0025 (11)
C12	0.0236 (14)	0.0177 (14)	0.0184 (13)	0.0024 (11)	−0.0042 (11)	0.0000 (11)
C13	0.0241 (14)	0.0164 (14)	0.0166 (12)	−0.0010 (11)	−0.0007 (11)	−0.0014 (10)
C14	0.0229 (14)	0.0157 (13)	0.0189 (13)	0.0015 (11)	−0.0048 (11)	−0.0016 (11)
C15	0.0243 (14)	0.0141 (13)	0.0166 (12)	−0.0008 (11)	−0.0046 (10)	0.0022 (10)
C16	0.0245 (14)	0.0226 (15)	0.0196 (13)	0.0002 (12)	−0.0017 (11)	0.0013 (11)
C17	0.0274 (15)	0.0216 (15)	0.0211 (14)	0.0020 (12)	−0.0081 (11)	0.0022 (12)
C18	0.0300 (15)	0.0175 (14)	0.0176 (13)	−0.0018 (12)	−0.0043 (11)	0.0028 (11)
C19	0.0251 (14)	0.0160 (14)	0.0182 (13)	−0.0013 (11)	−0.0038 (11)	0.0011 (11)
C20	0.0244 (14)	0.0128 (13)	0.0174 (12)	−0.0011 (11)	−0.0071 (11)	0.0002 (10)
C21	0.0225 (14)	0.0304 (17)	0.0303 (16)	0.0055 (13)	−0.0044 (12)	0.0000 (13)
C22	0.0258 (15)	0.0257 (16)	0.0247 (14)	0.0036 (12)	0.0001 (12)	0.0024 (12)
C23	0.050 (2)	0.0298 (19)	0.0379 (19)	0.0003 (16)	−0.0156 (16)	0.0002 (15)

Geometric parameters (Å, °)

Mn1—O1	1.8634 (19)	C8—C9	1.418 (4)
Mn1—O2	1.8746 (19)	C9—C10	1.376 (4)
Mn1—N1	1.987 (2)	C9—H9A	0.9300
Mn1—N2	1.995 (2)	C10—C11	1.392 (4)
Mn1—O5	2.423 (2)	C10—H10A	0.9300
Mn1—Cl1	2.4846 (8)	C11—C12	1.380 (4)
O1—C1	1.328 (3)	C12—C13	1.424 (4)

O2—C8	1.318 (3)	C12—H12A	0.9300
O3—C4	1.380 (3)	C13—C14	1.435 (4)
O3—C21	1.438 (4)	C14—H14A	0.9300
O4—C11	1.375 (3)	C15—C16	1.387 (4)
O4—C22	1.431 (3)	C15—C20	1.402 (4)
O5—C23	1.454 (4)	C16—C17	1.386 (4)
O5—H1O5	0.81 (4)	C16—H16A	0.9300
N1—C7	1.299 (3)	C17—C18	1.391 (4)
N1—C20	1.433 (3)	C17—H17A	0.9300
N2—C14	1.301 (3)	C18—C19	1.371 (4)
N2—C15	1.425 (3)	C18—H18A	0.9300
C1—C2	1.392 (4)	C19—C20	1.402 (4)
C1—C6	1.419 (4)	C19—H19A	0.9300
C2—C3	1.383 (4)	C21—H21A	0.9600
C2—H2A	0.9300	C21—H21B	0.9600
C3—C4	1.399 (4)	C21—H21C	0.9600
C3—H3A	0.9300	C22—H22A	0.9600
C4—C5	1.372 (4)	C22—H22B	0.9600
C5—C6	1.415 (4)	C22—H22C	0.9600
C5—H5A	0.9300	C23—H23A	0.9600
C6—C7	1.439 (4)	C23—H23B	0.9600
C7—H7A	0.9300	C23—H23C	0.9600
C8—C13	1.411 (4)		
O1—Mn1—O2	89.45 (8)	C10—C9—H9A	119.6
O1—Mn1—N1	93.50 (9)	C8—C9—H9A	119.6
O2—Mn1—N1	170.62 (9)	C9—C10—C11	121.2 (3)
O1—Mn1—N2	172.56 (9)	C9—C10—H10A	119.4
O2—Mn1—N2	93.87 (9)	C11—C10—H10A	119.4
N1—Mn1—N2	82.20 (9)	O4—C11—C12	125.6 (3)
O1—Mn1—O5	88.91 (8)	O4—C11—C10	114.7 (2)
O2—Mn1—O5	87.34 (8)	C12—C11—C10	119.7 (3)
N1—Mn1—O5	83.82 (9)	C11—C12—C13	120.3 (3)
N2—Mn1—O5	84.60 (9)	C11—C12—H12A	119.9
O1—Mn1—Cl1	98.44 (7)	C13—C12—H12A	119.9
O2—Mn1—Cl1	96.59 (7)	C8—C13—C12	119.8 (2)
N1—Mn1—Cl1	91.79 (7)	C8—C13—C14	123.5 (2)
N2—Mn1—Cl1	87.80 (7)	C12—C13—C14	116.6 (2)
O5—Mn1—Cl1	171.67 (6)	N2—C14—C13	125.8 (3)
C1—O1—Mn1	128.77 (17)	N2—C14—H14A	117.1
C8—O2—Mn1	128.03 (17)	C13—C14—H14A	117.1
C4—O3—C21	116.3 (2)	C16—C15—C20	119.9 (2)
C11—O4—C22	117.0 (2)	C16—C15—N2	125.1 (2)
C23—O5—Mn1	127.49 (19)	C20—C15—N2	115.1 (2)
C23—O5—H1O5	108 (3)	C17—C16—C15	119.7 (3)
Mn1—O5—H1O5	125 (3)	C17—C16—H16A	120.2
C7—N1—C20	122.1 (2)	C15—C16—H16A	120.2
C7—N1—Mn1	124.98 (19)	C16—C17—C18	120.4 (3)
C20—N1—Mn1	112.94 (17)	C16—C17—H17A	119.8
C14—N2—C15	122.7 (2)	C18—C17—H17A	119.8

C14—N2—Mn1	123.88 (18)	C19—C18—C17	120.5 (3)
C15—N2—Mn1	113.16 (17)	C19—C18—H18A	119.7
O1—C1—C2	118.0 (2)	C17—C18—H18A	119.7
O1—C1—C6	123.4 (2)	C18—C19—C20	119.6 (3)
C2—C1—C6	118.6 (2)	C18—C19—H19A	120.2
C3—C2—C1	121.4 (3)	C20—C19—H19A	120.2
C3—C2—H2A	119.3	C19—C20—C15	119.9 (2)
C1—C2—H2A	119.3	C19—C20—N1	124.8 (2)
C2—C3—C4	120.2 (3)	C15—C20—N1	115.3 (2)
C2—C3—H3A	119.9	O3—C21—H21A	109.5
C4—C3—H3A	119.9	O3—C21—H21B	109.5
C5—C4—O3	117.6 (3)	H21A—C21—H21B	109.5
C5—C4—C3	119.7 (3)	O3—C21—H21C	109.5
O3—C4—C3	122.6 (3)	H21A—C21—H21C	109.5
C4—C5—C6	121.0 (3)	H21B—C21—H21C	109.5
C4—C5—H5A	119.5	O4—C22—H22A	109.5
C6—C5—H5A	119.5	O4—C22—H22B	109.5
C5—C6—C1	119.1 (2)	H22A—C22—H22B	109.5
C5—C6—C7	116.8 (2)	O4—C22—H22C	109.5
C1—C6—C7	124.1 (2)	H22A—C22—H22C	109.5
N1—C7—C6	124.8 (2)	H22B—C22—H22C	109.5
N1—C7—H7A	117.6	O5—C23—H23A	109.5
C6—C7—H7A	117.6	O5—C23—H23B	109.5
O2—C8—C13	124.7 (2)	H23A—C23—H23B	109.5
O2—C8—C9	117.1 (2)	O5—C23—H23C	109.5
C13—C8—C9	118.1 (2)	H23A—C23—H23C	109.5
C10—C9—C8	120.8 (3)	H23B—C23—H23C	109.5
O2—Mn1—O1—C1	−162.9 (2)	C20—N1—C7—C6	−179.8 (2)
N1—Mn1—O1—C1	8.2 (2)	Mn1—N1—C7—C6	0.7 (4)
O5—Mn1—O1—C1	−75.6 (2)	C5—C6—C7—N1	−178.2 (3)
Cl1—Mn1—O1—C1	100.5 (2)	C1—C6—C7—N1	1.9 (4)
O1—Mn1—O2—C8	175.8 (2)	Mn1—O2—C8—C13	−0.3 (4)
N2—Mn1—O2—C8	2.4 (2)	Mn1—O2—C8—C9	179.84 (18)
O5—Mn1—O2—C8	86.8 (2)	O2—C8—C9—C10	−179.0 (3)
Cl1—Mn1—O2—C8	−85.8 (2)	C13—C8—C9—C10	1.1 (4)
O1—Mn1—O5—C23	136.6 (3)	C8—C9—C10—C11	0.7 (4)
O2—Mn1—O5—C23	−133.9 (3)	C22—O4—C11—C12	4.9 (4)
N1—Mn1—O5—C23	42.9 (3)	C22—O4—C11—C10	−175.8 (2)
N2—Mn1—O5—C23	−39.8 (3)	C9—C10—C11—O4	179.7 (2)
O1—Mn1—N1—C7	−4.5 (2)	C9—C10—C11—C12	−1.0 (4)
N2—Mn1—N1—C7	169.4 (2)	O4—C11—C12—C13	178.7 (3)
O5—Mn1—N1—C7	84.0 (2)	C10—C11—C12—C13	−0.5 (4)
Cl1—Mn1—N1—C7	−103.1 (2)	O2—C8—C13—C12	177.5 (3)
O1—Mn1—N1—C20	175.94 (18)	C9—C8—C13—C12	−2.5 (4)
N2—Mn1—N1—C20	−10.16 (17)	O2—C8—C13—C14	−1.4 (4)
O5—Mn1—N1—C20	−95.53 (18)	C9—C8—C13—C14	178.6 (3)
Cl1—Mn1—N1—C20	77.38 (17)	C11—C12—C13—C8	2.3 (4)
O2—Mn1—N2—C14	−4.2 (2)	C11—C12—C13—C14	−178.7 (3)
N1—Mn1—N2—C14	−175.6 (2)	C15—N2—C14—C13	178.1 (3)

O5—Mn1—N2—C14	−91.1 (2)	Mn1—N2—C14—C13	4.0 (4)
Cl1—Mn1—N2—C14	92.3 (2)	C8—C13—C14—N2	−0.8 (4)
O2—Mn1—N2—C15	−178.80 (18)	C12—C13—C14—N2	−179.7 (3)
N1—Mn1—N2—C15	9.76 (18)	C14—N2—C15—C16	−3.1 (4)
O5—Mn1—N2—C15	94.24 (18)	Mn1—N2—C15—C16	171.7 (2)
Cl1—Mn1—N2—C15	−82.34 (18)	C14—N2—C15—C20	177.7 (2)
Mn1—O1—C1—C2	173.15 (19)	Mn1—N2—C15—C20	−7.6 (3)
Mn1—O1—C1—C6	−8.0 (4)	C20—C15—C16—C17	0.0 (4)
O1—C1—C2—C3	179.0 (3)	N2—C15—C16—C17	−179.2 (3)
C6—C1—C2—C3	0.1 (4)	C15—C16—C17—C18	0.5 (4)
C1—C2—C3—C4	−0.5 (4)	C16—C17—C18—C19	−0.5 (4)
C21—O3—C4—C5	−150.7 (3)	C17—C18—C19—C20	0.1 (4)
C21—O3—C4—C3	33.3 (4)	C18—C19—C20—C15	0.4 (4)
C2—C3—C4—C5	0.2 (4)	C18—C19—C20—N1	−179.9 (3)
C2—C3—C4—O3	176.2 (3)	C16—C15—C20—C19	−0.5 (4)
O3—C4—C5—C6	−175.7 (3)	N2—C15—C20—C19	178.8 (2)
C3—C4—C5—C6	0.5 (4)	C16—C15—C20—N1	179.8 (2)
C4—C5—C6—C1	−0.9 (4)	N2—C15—C20—N1	−0.9 (3)
C4—C5—C6—C7	179.2 (3)	C7—N1—C20—C19	9.7 (4)
O1—C1—C6—C5	−178.3 (2)	Mn1—N1—C20—C19	−170.7 (2)
C2—C1—C6—C5	0.6 (4)	C7—N1—C20—C15	−170.6 (2)
O1—C1—C6—C7	1.7 (4)	Mn1—N1—C20—C15	8.9 (3)
C2—C1—C6—C7	−179.5 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1O5···O1^{i}	0.81 (4)	2.54 (4)	3.183 (3)	138 (3)
O5—H1O5···O2^{i}	0.81 (4)	2.37 (4)	2.998 (3)	135 (3)
C7—H7A···Cl1i	0.93	2.69	3.519 (3)	148
C14—H14A···O4^{ii}	0.93	2.47	3.222 (4)	138
C23—H23B···Cl1^{iii}	0.96	2.83	3.488 (4)	127
C2—H2A···Cg2^{iv}	0.93	2.86	3.507 (3)	128
C9—H9A···Cg1^{iv}	0.93	2.98	3.577 (3)	124
C22—H22C···Cg2^{ii}	0.96	2.64	3.453 (3)	143

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

Fig. 1

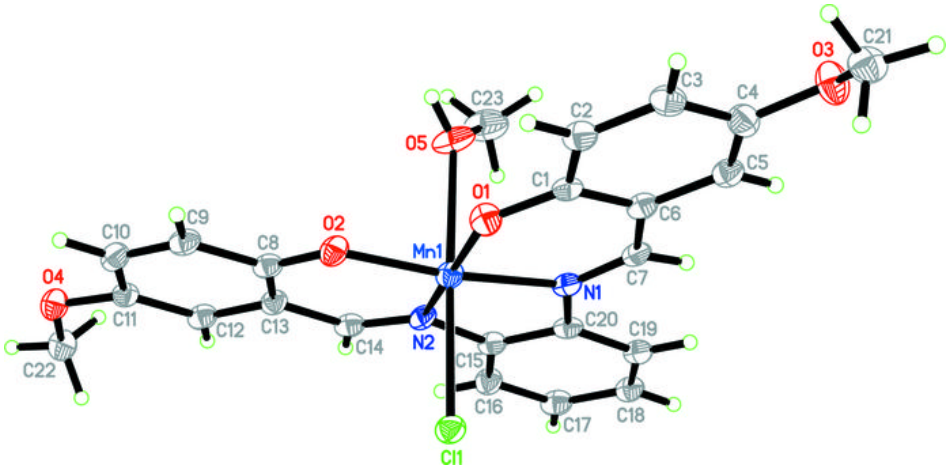

O3
C21
C3
C4
C23
C2
O5
C5
C1
O1
C6
C10
C9
O2
C8
Mn1
C7
O4
N1
C11
C12
C13
C14
N2
C20
C19
C22
C15
C16
C17
C18
Cl1

Fig. 2