Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chlorido{4,4′-dichloro-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}(methanol-κO)-manganese(III)

Naser Eltaher Eltayeb,[a]‡ Siang Guan Teoh,[a] Suchada Chantrapromma,[b]§ Hoong-Kun Fun[c]* and Rohana Adnan[a]

[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, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hkfun@usm.my

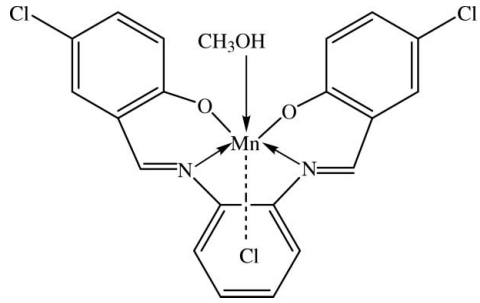
Received 23 November 2007; accepted 28 November 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.108; data-to-parameter ratio = 19.8.

In the title complex, $[Mn(C_{20}H_{12}Cl_2N_2O_2)Cl(CH_3OH)]$, the Mn^{III} atom is in an octahedral coordination geometry with the N_2O_2 atoms of the doubly-deprotonated Schiff base forming a square around it. The chloride ion and the O atom of the methanol molecule occupy the other two positions of the octahedron. The dihedral angle between the two outer phenolate rings of the tetradentate ligand is 20.27 (12)°. The central phenylene ring makes dihedral angles of 18.62 (12) and 6.02 (12)° with the two outer phenolate rings. Hydrogen bonds of the O—H···Cl type link the molecules into an infinite chain along [010]. These chains are arranged into sheets parallel to the *ab* plane and these sheets are connected by weak C—H···Cl interactions into a three-dimensional network. The crystal structure is further stabilized by C—H···π interactions.

Related literature

For related structures see, for examples: Eltayeb *et al.* (2007); Habibi *et al.* (2007); Mitra *et al.* (2006); Naskar *et al.* (2004). For related literature on 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

$[Mn(C_{20}H_{12}Cl_2N_2O_2)Cl(CH_4O)]$
M_r = 505.65
Monoclinic, $P2_1/c$
a = 15.9183 (4) Å
b = 6.6305 (2) Å
c = 23.3399 (6) Å
β = 124.672 (2)°
V = 2025.99 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 100.0 (1) K
0.56 × 0.09 × 0.04 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.584, T_{max} = 0.963
22773 measured reflections
5384 independent reflections
4153 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
S = 1.09
5384 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1*O*3···Cl1^{i}	0.76	2.36	3.1093 (19)	165
C12—H12*A*···Cl1^{ii}	0.93	2.81	3.725 (3)	170
C14—H14*A*···Cl1^{ii}	0.93	2.72	3.606 (3)	159
C2—H2*A*···*Cg*3^{iii}	0.93	3.02	3.890 (3)	158
C16—H16*A*···*Cg*2^{iv}	0.93	3.35	3.880 (3)	119
C18—H18*A*···*Cg*1^{iii}	0.93	2.96	3.640 (3)	131

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, -y+2, -z+1$. *Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, C8–C13 and C15–C20 benzene rings, respectively.

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, Ministry of Science, Technology and Innovation (MOSTI) and Universiti Sains Malaysia for the E-Science Fund research grant (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

‡ On study leave from International University of Africa, Sudan.
§ Additional correspondence author, email: suchada.c@psu.ac.th.

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: NG2401).

References

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**, m3193–m3194.
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.

supporting information

Acta Cryst. (2008). E**64**, m124–m125 [https://doi.org/10.1107/S1600536807064240]

Chlorido{4,4′-dichloro-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}(methanol-κO)manganese(III)

Naser Eltaher Eltayeb, Siang Guan Teoh, Suchada Chantrapromma, Hoong-Kun Fun and Rohana Adnan

S1. Comment

The coordination chemistry of manganese complexes in various oxidation states and in various combinations of nitrogen and oxygen donor environment has been extensively investigated, especially manganese complexes with Schiff base ligands which have attracted considerable interest in the past decades and recently, due to their importance and 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 Mn^{III} with Schiff base ligand (Eltayeb *et al.*, 2007) and herein the crystal structure of the Mn^{III} complex with 2,2′-{1,2-phenylenebis(nitrilomethylidyne)}bis(4-chlorophenol) is reported.

In the title complex molecule (Fig. 1), Mn^{III} coordinates with the dianionic tetradentate Schiff base ligand through two imine N atoms and two phenolato O atoms in the basal plane (N1, N2, O1 and O2) and the chloride ion and methanol molecule in the axial positions. The in-plane Mn—O distances [Mn1—O1 = 1.8834 (15) Å and Mn1—O2 = 1.8668 (16) Å] and Mn—N distances [Mn1—N1 = 1.9860 (19) Å and Mn1—N2 = 2.0005 (18) Å are quite similar to that observed in other six coordination Mn^{III} complexes of Schiff base ligands (Eltayeb *et al.*, 2007; Habibi *et al.*, 2007; Mitra *et al.*, 2006; Naskar *et al.*, 2004). The two axially ligated chloride ion and methanol molecule experience the usual Jahn Teller distortion of the Mn^{III} oxidation state, which was indicated by the Mn1—O5 = 2.3247 (19) Å and Mn1—Cl1 = 2.5493 (7) Å bond elongation as have been found previously (Eltayeb *et al.*, 2007; Habibi *et al.*, 2007). The dihedral angle between the two outer phenolate rings [(C1–C6) and C15–C20) of the tetradentate ligand is 20.27 (12) °. The central benzene ring (C8–C13) makes the dihedral angles of 18.62(12 ° and 6.02 (12) ° with the two outer phenolate rings respectively. Bond lengths and angles in the Schiff base ligand are very similar to those reported for the other Mn^{III} complexes with similar ligands (Eltayeb *et al.*, 2007; Habibi *et al.*, 2007; Mitra *et al.*, 2006; Naskar *et al.*, 2004).

In the crystal packing (Fig. 2), O—H···Cl hydrogen bonds [O3—H1O3···Cl1; symmetry code x, 1 + y, z (Table 1)] link the molecules into infinite chains along the [0 1 0] direction. These chains are arranged into sheets parallel to the *ab* plane and these sheets are connect by weak C—H···Cl interactons (Table 1). The crystal is further stabilized by C—H···π interactions (Table 1); Cg_1, Cg_2 and Cg_3 are the centroids of C1–C6, C8–C13 and C15–C20 benzene rings, respectively.

S2. Experimental

The title compound was synthesized by adding 5-chloro-2-hydroxybenzaldehyde (0.626 g, 4 mmol) into a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol 95% (30 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 by about 5 ml e thanol, dried, and then washed with copious quantities of diethyl ether. Brown single crystals of the title compound suitable for *x*-ray structure determination were recrystallized from methanol by slow evaporation of the solvent at room temperature over several days.

S3. Refinement

All 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 H21A and the deepest hole is located at 0.35 Å from C21.

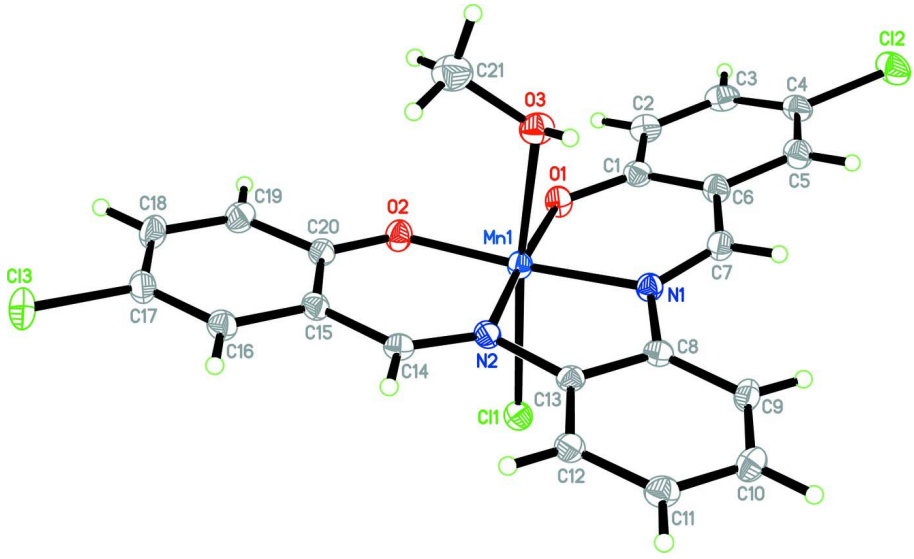


Figure 1

The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

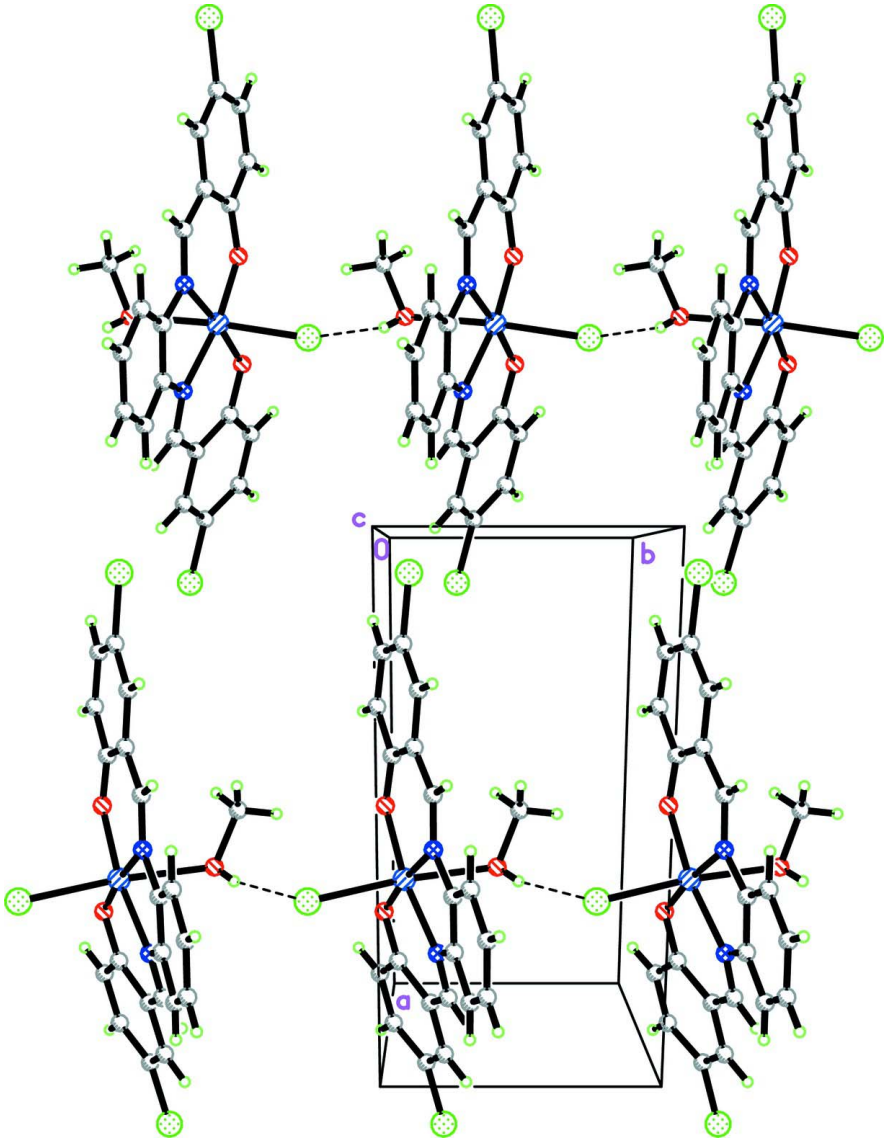


Figure 2

The crystal packing of (I), viewed along the *c* axis showing the chains running along [0 1 0] direction. Hydrogen bonds are drawn as dash lines.

Chlorido{4,4′-dichloro-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato- κ^4O,N,N',O'}(methanol-κO)manganese(III)

Crystal data

$[Mn(C_{20}H_{12}N_2O_2Cl_2)Cl(CH_4O)]$
$M_r = 505.65$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.9183\ (4)$ Å
$b = 6.6305\ (2)$ Å
$c = 23.3399\ (6)$ Å
$\beta = 124.672\ (2)°$
$V = 2025.99\ (10)$ Å^3
$Z = 4$
$F(000) = 1024$
$D_x = 1.658$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5384 reflections
$\theta = 1.5–29.0°$
$\mu = 1.07$ mm^{-1}

T = 100 K
Needle, brown

0.56 × 0.09 × 0.04 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Radiation source: medium-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.584, T_{max} = 0.963

22773 measured reflections
5384 independent reflections
4153 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 29.0°, θ_{min} = 1.6°
h = −21→21
k = −9→9
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
S = 1.09
5384 reflections
272 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.9163P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.38124 (2)	0.58871 (6)	0.592785 (16)	0.01538 (10)
Cl1	0.34939 (4)	0.25637 (10)	0.52850 (3)	0.01860 (13)
Cl2	−0.09275 (5)	0.72592 (12)	0.56471 (3)	0.02870 (16)
Cl3	0.92504 (4)	0.60705 (12)	0.74512 (3)	0.02954 (17)
O1	0.31347 (12)	0.5137 (3)	0.63441 (8)	0.0189 (4)
O2	0.50867 (12)	0.5203 (3)	0.67240 (8)	0.0189 (4)
O3	0.39833 (13)	0.9150 (3)	0.63460 (8)	0.0220 (4)
H1O3	0.3759	0.9889	0.6041	0.026*
N1	0.25509 (14)	0.7054 (3)	0.51017 (9)	0.0158 (4)
N2	0.44238 (14)	0.6915 (3)	0.54358 (9)	0.0150 (4)
C1	0.22094 (17)	0.5628 (4)	0.61572 (12)	0.0184 (5)
C2	0.18875 (18)	0.4945 (4)	0.65745 (12)	0.0220 (5)
H2A	0.2325	0.4155	0.6963	0.026*

C3	0.09306 (19)	0.5431 (4)	0.64153 (12)	0.0231 (6)
H3A	0.0728	0.4952	0.6694	0.028*
C4	0.02714 (17)	0.6633 (4)	0.58403 (12)	0.0214 (5)
C5	0.05423 (18)	0.7289 (4)	0.54092 (12)	0.0210 (5)
H5A	0.0088	0.8059	0.5019	0.025*
C6	0.15150 (17)	0.6792 (4)	0.55588 (12)	0.0183 (5)
C7	0.17185 (17)	0.7418 (4)	0.50609 (11)	0.0183 (5)
H7A	0.1211	0.8146	0.4677	0.022*
C8	0.26702 (17)	0.7624 (4)	0.45641 (11)	0.0152 (5)
C9	0.18680 (17)	0.8169 (4)	0.38927 (11)	0.0189 (5)
H9A	0.1200	0.8163	0.3769	0.023*
C10	0.20691 (18)	0.8716 (4)	0.34132 (11)	0.0198 (5)
H10A	0.1535	0.9084	0.2965	0.024*
C11	0.30626 (18)	0.8721 (4)	0.35933 (12)	0.0198 (5)
H11A	0.3189	0.9102	0.3265	0.024*
C12	0.38699 (17)	0.8165 (4)	0.42562 (11)	0.0173 (5)
H12A	0.4535	0.8174	0.4375	0.021*
C13	0.36721 (16)	0.7592 (4)	0.47441 (11)	0.0148 (4)
C14	0.53947 (17)	0.6908 (4)	0.56893 (11)	0.0163 (5)
H14A	0.5587	0.7369	0.5403	0.020*
C15	0.61905 (16)	0.6240 (4)	0.63775 (11)	0.0159 (5)
C16	0.72077 (17)	0.6399 (4)	0.65662 (12)	0.0189 (5)
H16A	0.7333	0.6881	0.6247	0.023*
C17	0.80005 (17)	0.5842 (4)	0.72182 (12)	0.0211 (5)
C18	0.78387 (18)	0.5105 (4)	0.77090 (12)	0.0227 (5)
H18A	0.8391	0.4758	0.8154	0.027*
C19	0.68541 (18)	0.4893 (4)	0.75304 (11)	0.0210 (5)
H19A	0.6748	0.4376	0.7855	0.025*
C20	0.60042 (17)	0.5451 (4)	0.68617 (11)	0.0165 (5)
C21	0.4985 (2)	0.9955 (5)	0.69176 (13)	0.0304 (6)
H21A	0.4901	1.1303	0.7027	0.046*
H21B	0.5444	0.9968	0.6775	0.046*
H21C	0.5261	0.9116	0.7322	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.01368 (16)	0.0184 (2)	0.01457 (16)	0.00078 (15)	0.00836 (13)	0.00217 (15)
Cl1	0.0184 (3)	0.0183 (3)	0.0200 (2)	−0.0003 (2)	0.0115 (2)	0.0002 (2)
Cl2	0.0230 (3)	0.0326 (4)	0.0394 (3)	−0.0020 (3)	0.0231 (3)	−0.0054 (3)
Cl3	0.0130 (3)	0.0404 (4)	0.0285 (3)	0.0003 (3)	0.0078 (2)	−0.0028 (3)
O1	0.0176 (7)	0.0222 (10)	0.0184 (7)	0.0017 (8)	0.0112 (6)	0.0044 (7)
O2	0.0162 (7)	0.0230 (10)	0.0164 (7)	0.0010 (8)	0.0087 (6)	0.0033 (7)
O3	0.0265 (9)	0.0200 (10)	0.0194 (7)	0.0006 (8)	0.0130 (7)	0.0015 (7)
N1	0.0153 (8)	0.0171 (11)	0.0151 (8)	0.0004 (8)	0.0086 (7)	0.0011 (8)
N2	0.0145 (8)	0.0158 (11)	0.0153 (8)	0.0012 (8)	0.0088 (7)	0.0006 (8)
C1	0.0179 (10)	0.0187 (14)	0.0201 (10)	−0.0025 (10)	0.0116 (9)	−0.0034 (10)
C2	0.0247 (12)	0.0209 (14)	0.0224 (11)	−0.0028 (11)	0.0146 (10)	−0.0015 (11)

C3	0.0263 (12)	0.0258 (15)	0.0248 (11)	−0.0079 (12)	0.0191 (10)	−0.0060 (11)
C4	0.0175 (11)	0.0230 (14)	0.0273 (11)	−0.0049 (11)	0.0149 (10)	−0.0085 (11)
C5	0.0172 (10)	0.0220 (14)	0.0246 (11)	−0.0017 (11)	0.0124 (9)	−0.0024 (11)
C6	0.0168 (10)	0.0193 (13)	0.0202 (10)	−0.0011 (10)	0.0114 (9)	−0.0005 (10)
C7	0.0158 (10)	0.0214 (14)	0.0165 (9)	0.0013 (10)	0.0085 (8)	0.0019 (10)
C8	0.0173 (10)	0.0143 (12)	0.0162 (9)	−0.0007 (10)	0.0110 (8)	−0.0002 (9)
C9	0.0133 (10)	0.0237 (14)	0.0158 (10)	0.0010 (10)	0.0061 (8)	0.0005 (10)
C10	0.0195 (11)	0.0204 (14)	0.0153 (10)	0.0007 (11)	0.0073 (9)	0.0031 (10)
C11	0.0251 (12)	0.0180 (13)	0.0185 (10)	0.0021 (11)	0.0136 (9)	0.0018 (10)
C12	0.0161 (10)	0.0180 (13)	0.0182 (10)	−0.0008 (10)	0.0100 (9)	−0.0023 (10)
C13	0.0170 (10)	0.0118 (12)	0.0148 (9)	0.0001 (10)	0.0085 (8)	−0.0014 (9)
C14	0.0189 (10)	0.0145 (13)	0.0166 (9)	−0.0002 (10)	0.0108 (9)	−0.0014 (9)
C15	0.0158 (10)	0.0128 (12)	0.0182 (10)	0.0019 (10)	0.0092 (9)	0.0002 (9)
C16	0.0181 (11)	0.0165 (13)	0.0214 (10)	0.0002 (10)	0.0109 (9)	−0.0022 (10)
C17	0.0141 (10)	0.0203 (14)	0.0244 (11)	0.0008 (10)	0.0082 (9)	−0.0028 (11)
C18	0.0173 (11)	0.0222 (15)	0.0189 (10)	0.0042 (11)	0.0044 (9)	0.0007 (11)
C19	0.0214 (11)	0.0218 (14)	0.0174 (10)	0.0008 (11)	0.0096 (9)	0.0017 (10)
C20	0.0166 (10)	0.0127 (12)	0.0174 (10)	0.0015 (10)	0.0079 (8)	−0.0009 (9)
C21	0.0342 (14)	0.0317 (17)	0.0294 (13)	−0.0008 (14)	0.0206 (12)	−0.0032 (13)

Geometric parameters (Å, º)

Mn1—O2	1.8668 (16)	C7—H7A	0.9300
Mn1—O1	1.8834 (15)	C8—C9	1.393 (3)
Mn1—N1	1.9860 (19)	C8—C13	1.399 (3)
Mn1—N2	2.0005 (18)	C9—C10	1.376 (3)
Mn1—O3	2.3247 (19)	C9—H9A	0.9300
Mn1—Cl1	2.5493 (7)	C10—C11	1.386 (3)
Cl2—C4	1.743 (2)	C10—H10A	0.9301
Cl3—C17	1.745 (2)	C11—C12	1.385 (3)
O1—C1	1.317 (3)	C11—H11A	0.9299
O2—C20	1.315 (3)	C12—C13	1.396 (3)
O3—C21	1.479 (3)	C12—H12A	0.9300
O3—H1O3	0.7642	C14—C15	1.437 (3)
N1—C7	1.296 (3)	C14—H14A	0.9302
N1—C8	1.423 (3)	C15—C16	1.420 (3)
N2—C14	1.303 (3)	C15—C20	1.421 (3)
N2—C13	1.429 (3)	C16—C17	1.364 (3)
C1—C2	1.408 (3)	C16—H16A	0.9300
C1—C6	1.419 (3)	C17—C18	1.398 (3)
C2—C3	1.385 (3)	C18—C19	1.381 (3)
C2—H2A	0.9298	C18—H18A	0.9300
C3—C4	1.391 (4)	C19—C20	1.414 (3)
C3—H3A	0.9300	C19—H19A	0.9298
C4—C5	1.372 (3)	C21—H21A	0.9600
C5—C6	1.419 (3)	C21—H21B	0.9600
C5—H5A	0.9300	C21—H21C	0.9600
C6—C7	1.434 (3)		

O2—Mn1—O1	92.25 (7)	C6—C7—H7A	117.3
O2—Mn1—N1	170.80 (9)	C9—C8—C13	120.02 (19)
O1—Mn1—N1	92.54 (7)	C9—C8—N1	124.35 (19)
O2—Mn1—N2	92.65 (7)	C13—C8—N1	115.63 (19)
O1—Mn1—N2	173.99 (8)	C10—C9—C8	119.7 (2)
N1—Mn1—N2	82.14 (8)	C10—C9—H9A	120.2
O2—Mn1—O3	90.40 (7)	C8—C9—H9A	120.2
O1—Mn1—O3	89.64 (7)	C9—C10—C11	120.5 (2)
N1—Mn1—O3	81.79 (8)	C9—C10—H10A	119.8
N2—Mn1—O3	86.84 (7)	C11—C10—H10A	119.8
O2—Mn1—Cl1	96.63 (6)	C12—C11—C10	120.8 (2)
O1—Mn1—Cl1	95.44 (6)	C12—C11—H11A	119.6
N1—Mn1—Cl1	90.72 (6)	C10—C11—H11A	119.6
N2—Mn1—Cl1	87.45 (6)	C11—C12—C13	119.2 (2)
O3—Mn1—Cl1	171.14 (4)	C11—C12—H12A	120.4
C1—O1—Mn1	128.67 (15)	C13—C12—H12A	120.4
C20—O2—Mn1	129.77 (14)	C12—C13—C8	119.9 (2)
C21—O3—Mn1	121.53 (16)	C12—C13—N2	125.09 (19)
C21—O3—H1O3	107.5	C8—C13—N2	115.00 (18)
Mn1—O3—H1O3	109.0	N2—C14—C15	124.9 (2)
C7—N1—C8	121.98 (19)	N2—C14—H14A	117.5
C7—N1—Mn1	124.80 (15)	C15—C14—H14A	117.6
C8—N1—Mn1	113.03 (14)	C16—C15—C20	119.9 (2)
C14—N2—C13	121.91 (18)	C16—C15—C14	116.6 (2)
C14—N2—Mn1	125.22 (15)	C20—C15—C14	123.5 (2)
C13—N2—Mn1	112.80 (13)	C17—C16—C15	119.6 (2)
O1—C1—C2	118.0 (2)	C17—C16—H16A	120.2
O1—C1—C6	124.0 (2)	C15—C16—H16A	120.2
C2—C1—C6	118.0 (2)	C16—C17—C18	121.6 (2)
C3—C2—C1	121.1 (2)	C16—C17—Cl3	119.44 (19)
C3—C2—H2A	119.4	C18—C17—Cl3	118.94 (18)
C1—C2—H2A	119.4	C19—C18—C17	119.7 (2)
C2—C3—C4	120.2 (2)	C19—C18—H18A	120.2
C2—C3—H3A	119.9	C17—C18—H18A	120.2
C4—C3—H3A	119.9	C18—C19—C20	121.0 (2)
C5—C4—C3	120.7 (2)	C18—C19—H19A	119.5
C5—C4—Cl2	119.3 (2)	C20—C19—H19A	119.5
C3—C4—Cl2	120.00 (18)	O2—C20—C19	118.0 (2)
C4—C5—C6	120.0 (2)	O2—C20—C15	123.8 (2)
C4—C5—H5A	120.0	C19—C20—C15	118.2 (2)
C6—C5—H5A	120.0	O3—C21—H21A	109.5
C5—C6—C1	119.9 (2)	O3—C21—H21B	109.5
C5—C6—C7	116.8 (2)	H21A—C21—H21B	109.5
C1—C6—C7	123.1 (2)	O3—C21—H21C	109.5
N1—C7—C6	125.4 (2)	H21A—C21—H21C	109.5
N1—C7—H7A	117.3	H21B—C21—H21C	109.5

O2—Mn1—O1—C1	162.1 (2)	C8—N1—C7—C6	176.2 (2)
N1—Mn1—O1—C1	−10.1 (2)	Mn1—N1—C7—C6	−9.2 (4)
O3—Mn1—O1—C1	71.7 (2)	C5—C6—C7—N1	−178.1 (2)
Cl1—Mn1—O1—C1	−101.0 (2)	C1—C6—C7—N1	−1.8 (4)
O1—Mn1—O2—C20	−174.3 (2)	C7—N1—C8—C9	−15.6 (4)
N2—Mn1—O2—C20	2.2 (2)	Mn1—N1—C8—C9	169.1 (2)
O3—Mn1—O2—C20	−84.6 (2)	C7—N1—C8—C13	165.0 (2)
Cl1—Mn1—O2—C20	89.9 (2)	Mn1—N1—C8—C13	−10.2 (3)
O2—Mn1—O3—C21	16.48 (16)	C13—C8—C9—C10	−1.4 (4)
O1—Mn1—O3—C21	108.72 (16)	N1—C8—C9—C10	179.3 (2)
N1—Mn1—O3—C21	−158.66 (16)	C8—C9—C10—C11	0.2 (4)
N2—Mn1—O3—C21	−76.15 (16)	C9—C10—C11—C12	0.4 (4)
O1—Mn1—N1—C7	12.8 (2)	C10—C11—C12—C13	0.1 (4)
N2—Mn1—N1—C7	−164.4 (2)	C11—C12—C13—C8	−1.3 (4)
O3—Mn1—N1—C7	−76.5 (2)	C11—C12—C13—N2	177.6 (2)
Cl1—Mn1—N1—C7	108.3 (2)	C9—C8—C13—C12	1.9 (4)
O1—Mn1—N1—C8	−172.10 (17)	N1—C8—C13—C12	−178.7 (2)
N2—Mn1—N1—C8	10.70 (17)	C9—C8—C13—N2	−177.1 (2)
O3—Mn1—N1—C8	98.63 (17)	N1—C8—C13—N2	2.3 (3)
Cl1—Mn1—N1—C8	−76.62 (16)	C14—N2—C13—C12	4.8 (4)
O2—Mn1—N2—C14	1.1 (2)	Mn1—N2—C13—C12	−172.3 (2)
N1—Mn1—N2—C14	173.5 (2)	C14—N2—C13—C8	−176.3 (2)
O3—Mn1—N2—C14	91.4 (2)	Mn1—N2—C13—C8	6.6 (3)
Cl1—Mn1—N2—C14	−95.4 (2)	C13—N2—C14—C15	−179.7 (2)
O2—Mn1—N2—C13	178.13 (16)	Mn1—N2—C14—C15	−2.9 (4)
N1—Mn1—N2—C13	−9.49 (16)	N2—C14—C15—C16	−178.3 (2)
O3—Mn1—N2—C13	−91.62 (16)	N2—C14—C15—C20	1.7 (4)
Cl1—Mn1—N2—C13	81.60 (16)	C20—C15—C16—C17	−1.8 (4)
Mn1—O1—C1—C2	−177.18 (18)	C14—C15—C16—C17	178.3 (2)
Mn1—O1—C1—C6	3.2 (4)	C15—C16—C17—C18	0.3 (4)
O1—C1—C2—C3	179.0 (2)	C15—C16—C17—Cl3	−179.2 (2)
C6—C1—C2—C3	−1.4 (4)	C16—C17—C18—C19	1.2 (4)
C1—C2—C3—C4	−0.8 (4)	Cl3—C17—C18—C19	−179.3 (2)
C2—C3—C4—C5	2.5 (4)	C17—C18—C19—C20	−1.3 (4)
C2—C3—C4—Cl2	−179.4 (2)	Mn1—O2—C20—C19	176.37 (18)
C3—C4—C5—C6	−1.9 (4)	Mn1—O2—C20—C15	−3.8 (4)
Cl2—C4—C5—C6	180.0 (2)	C18—C19—C20—O2	179.7 (2)
C4—C5—C6—C1	−0.4 (4)	C18—C19—C20—C15	−0.1 (4)
C4—C5—C6—C7	176.1 (2)	C16—C15—C20—O2	−178.2 (2)
O1—C1—C6—C5	−178.4 (2)	C14—C15—C20—O2	1.8 (4)
C2—C1—C6—C5	2.0 (4)	C16—C15—C20—C19	1.7 (4)
O1—C1—C6—C7	5.4 (4)	C14—C15—C20—C19	−178.4 (2)
C2—C1—C6—C7	−174.2 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1*O*3···Cl1^{i}	0.76	2.36	3.1093 (19)	165

C12—H12*A*···Cl1^{ii}	0.93	2.81	3.725 (3)	170
C14—H14*A*···Cl1^{ii}	0.93	2.72	3.606 (3)	159
C2—H2*A*···*Cg*3^{iii}	0.93	3.02	3.890 (3)	158
C16—H16*A*···*Cg*2^{iv}	0.93	3.35	3.880 (3)	119
C18—H18*A*···*Cg*1^{iii}	0.93	2.96	3.640 (3)	131

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y-1/2, -z+3/2$; (iv) $-x+1, -y+2, -z+1$.