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Aquachlorido[4,4′-dimethyl-*N*,*N*′-(*o*-phenylene)bis(pyridine-2-carboxamidato)]manganese(III) dimethylformamide solvate

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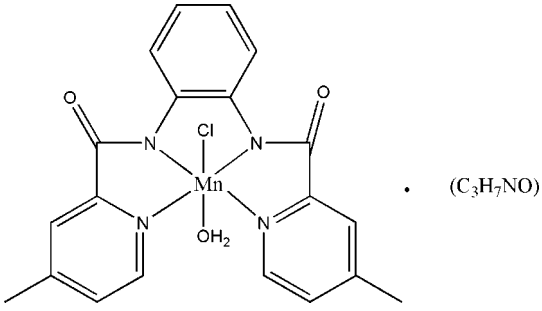
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.059; wR factor = 0.178; data-to-parameter ratio = 18.7.

In the title compound, $[Mn(C_{20}H_{16}N_4O_2)Cl(H_2O)]\cdot C_3H_7NO$, or [Mn(bmpb)Cl($H_2O$)]·DMF [$H_2$bmpb = 1,2-bis(4′-methylpyridine-2′-carboxamido)benzene and DMF is dimethylformamide], the Mn^{III} ion is six-coordinate in the form of a distorted octahedron with two pyridine and two deprotonated amide N atoms in the equatorial plane, while the two axial sites are occupied by a chloride ion and an O atom. The structure displays O—H···O hydrogen bonds.

Related literature

For the synthesis, see: Ray *et al.* (1993). For other related literature, see: Larson *et al.* (1992); Liang *et al.* (2007); Hureau *et al.* (2005).



· (C_3H_7NO)

Experimental

Crystal data

$[Mn(C_{20}H_{16}N_4O_2)Cl(H_2O)]\cdot C_3H_7NO$
M_r = 525.87
Monoclinic, $P2_1/c$
a = 11.7182 (15) Å
b = 15.503 (2) Å
c = 14.0158 (19) Å
β = 99.892 (3)°
V = 2508.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 294 (2) K
0.24 × 0.16 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.856, T_{max} = 0.924
16639 measured reflections
5805 independent reflections
2687 reflections with $I > 2\sigma(I)$
R_{int} = 0.087

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.178
S = 1.01
5805 reflections
310 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O1^{i}	0.86	1.90	2.728 (3)	162.3
O1W—H1WB···O3	0.86	1.78	2.627 (5)	170.2

Symmetry code: (i) $-x, -y, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve 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: BT2573).

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supplementary materials

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Aquachlorido[4,4'-dimethyl-*N*,*N*'-(*o*-phenylene)bis(pyridine-2-carboxamidato)]manganese(III) dimethylformamide solvate

L. Yang, Z. Jiang and X.-G. Zhou

Comment

Manganese complexes are involved in numerous biological redox reactions performed by metalloenzymes (Larson *et al.*, 1992). The carboxamide [–C(O)NH–] group, ubiquitous throughout nature in the primary structure of proteins, is an important ligand for coordination chemists. On the other hand, pyridine carboxamides, a burgeoning class of multidentate ligands containing this linkage, are available from condensation reactions. Here we describe the coordination chemistry of manganese(III) with a tetradentate pyridine carboxamide ligand prepared from 4-methylpyridine carboxylic acid and 1,2-diaminobenzene.

The crystal structure of the title compound is represented in Figure 1. A s shown in Fig. 1, the mononuclear Mn^{III} ion is six-coordinated, forming a distorted octahedron with two pyridine and two deprotonated amide N atoms in the equatorial plane, while the two axial sites are occupied by Cl ion and O atom provided by a water molecule. The Mn—*N*(amide) distances of *ca* 1.92 Å are significantly shorter than the Mn—*N*(pyridine) distances of *ca* 2.07 Å, both of which are appreciably shorter than the Mn—N distances found in related Mn—N4 complexes such as *cis*-[Mn^{II}(mep)Cl_2] and [Mn^{III}(mpp)Cl(OH_2)](ClO_4) [mep = *N*,*N*'-dimethyl-*N*,*N*'- bis(2-pyridylmethyl)ethane-1,2-diamino, mpp = *N*,*N*'-dimethyl-*N*,*N*'-bis(2-pyridylmethyl)propane-1,2-diamino] (Hureau *et al.*, 2005). The Mn—*N*(amide) and Mn—*N*(pyridine) distances are also comparable to those of [Mn(bpc)Cl(DMF)] [H_2bpc =1,2- bis(2- pyridinecarboxamido)-4,5-dichlorobenzene] (Liang *et al.*, 2007). The Mn—Cl distance at 2.463 Å is very similar to what is observed for [(mpp)MnCl(OH_2)](ClO_4)(Hureau *et al.*, 2005). However, The Mn—O distance (*ca* 2.27 Å) in the title compound is longer than the corresponding Mn—O distances (*ca* 2.19 Å) in [(mpp)MnCl(OH_2)](ClO_4) (Hureau *et al.*, 2005), due to the distinctive hydrogen-bond effect.

Experimental

The title complex was prepared in a manner similar to the literature by the reaction of manganese(III) acetate and H_2bmpb in DMF in the presence of triethylamine (Ray *et al.*, 1993). Single crystals suitable for X-ray analysis were obtained by slow diffusion of diethyl ether into a DMF solution of the complex. Selected IR data (KBr, cm^{-1}): 2950 (*m*), 1630 (amide I band, s), 1600(amide II band, s), 1480 (*s*), 1350 (*s*), 1165(*s*), 1020 (*m*), 850 (*m*). Analysis calculated for $C_{23}H_{25}ClMnN_5O_4$: C 52.53, H 4.79, Cl 6.74, N 13.32, %; found:*C* 52.87, H 4.32, Cl 6.78 N 12.58%. MS (FAB): 399 ($[Mn(bmpb)]^+$).

Refinement

All H atoms were fixed geometrically and treated as riding on their parent atoms with O—H =0.86 Å, $C_{aromatic}$—H = 0.93 Å and C_{methyl}—H = 0.96 Å with U_{iso}(H)= 1.2U_{eq}(C,*O*) or U_{iso}(H) = 1.5U_{eq}(C_{methyl}).

Figures

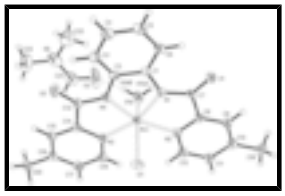


Fig. 1. A view of anion of the title complex with displacement ellipsoids drawn at the 30% propability level. The dashed line depicts an intermolecular hydrogen bond.

Aquachlorido[4,4'-dimethyl-*N*,*N*'-(*o*-phenylene)bis(pyridine-2- carboxamidato)]manganese(III) dimethylformamide solvate

Crystal data

$[Mn(C_{20}H_{16}N_4O_2)Cl(H_2O)]\cdot C_3H_7NO$	F_{000} = 1088
M_r = 525.87	D_x = 1.392 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.7182 (15) Å	Cell parameters from 4879 reflections
b = 15.503 (2) Å	θ = 1–27.5º
c = 14.0158 (19) Å	μ = 0.67 mm^{-1}
β = 99.892 (3)º	T = 294 (2) K
V = 2508.4 (6) Å^3	Prism, black
Z = 4	0.24 × 0.16 × 0.12 mm

Data collection

Bruker CCD area-detector diffractometer	5805 independent reflections
Radiation source: fine-focus sealed tube	2687 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.087
T = 294(2) K	θ_{max} = 27.6º
phi and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→15
T_{min} = 0.856, T_{max} = 0.924	k = −20→17
16639 measured reflections	l = −18→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H-atom parameters constrained
$wR(F^2)$ = 0.178	$w = 1/[\sigma^2(F_o^2) + (0.075P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$

5805 reflections	$\Delta\rho_{max} = 0.57$ e Å^{-3}
310 parameters	$\Delta\rho_{min} = -0.41$ 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}
Mn1	0.29430 (4)	0.02350 (4)	0.62328 (4)	0.04348 (16)
Cl1	0.42626 (8)	0.13481 (7)	0.57974 (8)	0.0620 (3)
O1	−0.0071 (2)	0.13130 (16)	0.49219 (18)	0.0549 (7)
O1W	0.2130 (2)	−0.10901 (18)	0.6296 (2)	0.0699 (9)
H1WA	0.1476	−0.1260	0.5981	0.084*
H1WB	0.2234	−0.1360	0.6841	0.084*
O2	0.3918 (3)	0.0425 (2)	0.9130 (2)	0.0834 (10)
N1	0.1508 (2)	0.08875 (18)	0.6048 (2)	0.0427 (7)
N2	0.2379 (2)	0.00161 (18)	0.4774 (2)	0.0452 (8)
N3	0.4375 (2)	−0.04517 (18)	0.6902 (2)	0.0453 (8)
N4	0.2958 (2)	0.05783 (19)	0.7554 (2)	0.0463 (8)
C1	0.1261 (3)	0.1318 (2)	0.6878 (3)	0.0433 (9)
C2	0.2085 (3)	0.1156 (2)	0.7712 (3)	0.0463 (9)
C3	0.1998 (3)	0.1578 (3)	0.8564 (3)	0.0620 (12)
H3A	0.2556	0.1493	0.9113	0.074*
C4	0.1080 (4)	0.2124 (3)	0.8596 (3)	0.0701 (13)
H4A	0.1017	0.2399	0.9174	0.084*
C5	0.0266 (4)	0.2269 (3)	0.7800 (3)	0.0668 (13)
H5A	−0.0346	0.2641	0.7841	0.080*
C6	0.0334 (3)	0.1872 (2)	0.6927 (3)	0.0533 (11)
H6A	−0.0228	0.1973	0.6383	0.064*
C7	0.0855 (3)	0.0923 (2)	0.5156 (3)	0.0440 (9)
C8	0.1376 (3)	0.0425 (2)	0.4426 (3)	0.0435 (9)
C9	0.0869 (3)	0.0375 (2)	0.3471 (3)	0.0537 (11)
H9A	0.0173	0.0660	0.3259	0.064*
C10	0.1382 (4)	−0.0096 (3)	0.2818 (3)	0.0567 (11)
C11	0.2401 (4)	−0.0520 (3)	0.3179 (3)	0.0646 (12)
H11A	0.2769	−0.0853	0.2769	0.078*

C12	0.2873 (3)	−0.0450 (3)	0.4147 (3)	0.0582 (11)
H12A	0.3563	−0.0737	0.4376	0.070*
C13	0.3800 (3)	0.0274 (3)	0.8262 (3)	0.0517 (10)
C14	0.4618 (3)	−0.0318 (2)	0.7858 (3)	0.0455 (9)
C15	0.5545 (3)	−0.0706 (2)	0.8444 (3)	0.0500 (10)
H15A	0.5691	−0.0596	0.9106	0.060*
C16	0.6255 (3)	−0.1261 (2)	0.8037 (3)	0.0507 (10)
C17	0.5988 (3)	−0.1395 (3)	0.7056 (3)	0.0585 (11)
H17A	0.6440	−0.1767	0.6757	0.070*
C18	0.5048 (3)	−0.0981 (3)	0.6506 (3)	0.0573 (11)
H18A	0.4887	−0.1077	0.5841	0.069*
C19	0.0836 (4)	−0.0150 (3)	0.1775 (3)	0.0816 (15)
H19A	0.0764	0.0419	0.1500	0.122*
H19B	0.0082	−0.0407	0.1721	0.122*
H19C	0.1311	−0.0497	0.1432	0.122*
C20	0.7271 (3)	−0.1707 (3)	0.8662 (3)	0.0672 (13)
H20A	0.7838	−0.1859	0.8271	0.101*
H20B	0.7005	−0.2220	0.8939	0.101*
H20C	0.7614	−0.1325	0.9170	0.101*
O3	0.2566 (4)	−0.2053 (4)	0.7859 (4)	0.215 (3)
N5	0.2985 (4)	−0.1807 (3)	0.9457 (5)	0.1136 (19)
C21	0.3201 (5)	−0.2117 (4)	0.8616 (5)	0.113 (2)
H21A	0.3899	−0.2403	0.8622	0.135*
C22	0.1947 (7)	−0.1350 (6)	0.9424 (6)	0.187 (4)
H22A	0.1688	−0.1142	0.8778	0.281*
H22B	0.2072	−0.0871	0.9864	0.281*
H22C	0.1370	−0.1725	0.9608	0.281*
C23	0.3818 (6)	−0.1888 (5)	1.0310 (5)	0.157 (3)
H23A	0.4456	−0.2229	1.0177	0.236*
H23B	0.3472	−0.2165	1.0803	0.236*
H23C	0.4090	−0.1327	1.0529	0.236*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0350 (3)	0.0512 (3)	0.0443 (3)	0.0053 (3)	0.0072 (2)	−0.0028 (3)
Cl1	0.0529 (5)	0.0601 (6)	0.0785 (7)	−0.0063 (5)	0.0268 (5)	−0.0082 (5)
O1	0.0447 (14)	0.0578 (17)	0.0600 (17)	0.0097 (13)	0.0026 (13)	0.0087 (13)
O1W	0.0550 (16)	0.0710 (19)	0.075 (2)	−0.0168 (14)	−0.0118 (14)	0.0187 (16)
O2	0.0782 (19)	0.115 (3)	0.0513 (19)	0.0413 (18)	−0.0050 (15)	−0.0195 (17)
N1	0.0363 (15)	0.0497 (18)	0.0422 (17)	−0.0003 (14)	0.0071 (13)	−0.0009 (14)
N2	0.0398 (16)	0.0475 (18)	0.0481 (18)	−0.0007 (14)	0.0066 (14)	−0.0016 (14)
N3	0.0397 (16)	0.0483 (19)	0.0474 (19)	0.0026 (14)	0.0060 (14)	−0.0056 (14)
N4	0.0363 (15)	0.0553 (19)	0.0471 (18)	0.0079 (14)	0.0064 (14)	−0.0022 (15)
C1	0.0381 (18)	0.040 (2)	0.053 (2)	−0.0005 (16)	0.0104 (17)	−0.0022 (17)
C2	0.0423 (19)	0.041 (2)	0.058 (2)	0.0059 (17)	0.0147 (18)	−0.0037 (18)
C3	0.063 (2)	0.063 (3)	0.060 (3)	0.011 (2)	0.010 (2)	−0.009 (2)
C4	0.070 (3)	0.067 (3)	0.074 (3)	0.018 (2)	0.015 (2)	−0.021 (2)

C5	0.055 (2)	0.053 (3)	0.095 (3)	0.014 (2)	0.020 (2)	−0.009 (2)
C6	0.042 (2)	0.049 (2)	0.070 (3)	0.0067 (18)	0.0124 (19)	0.003 (2)
C7	0.0376 (19)	0.037 (2)	0.058 (2)	−0.0066 (16)	0.0102 (18)	0.0058 (18)
C8	0.0390 (19)	0.041 (2)	0.050 (2)	−0.0031 (16)	0.0071 (17)	0.0077 (17)
C9	0.053 (2)	0.055 (3)	0.052 (2)	−0.0071 (19)	0.0039 (19)	0.010 (2)
C10	0.065 (3)	0.057 (2)	0.047 (2)	−0.019 (2)	0.007 (2)	0.000 (2)
C11	0.071 (3)	0.070 (3)	0.056 (3)	−0.009 (2)	0.019 (2)	−0.009 (2)
C12	0.054 (2)	0.065 (3)	0.058 (3)	0.007 (2)	0.013 (2)	−0.007 (2)
C13	0.046 (2)	0.063 (3)	0.045 (2)	0.007 (2)	0.0024 (18)	−0.008 (2)
C14	0.0376 (18)	0.046 (2)	0.052 (2)	0.0015 (17)	0.0057 (17)	−0.0040 (18)
C15	0.045 (2)	0.055 (2)	0.048 (2)	−0.0004 (19)	0.0014 (18)	−0.0031 (19)
C16	0.0375 (19)	0.047 (2)	0.068 (3)	0.0014 (18)	0.0089 (18)	0.006 (2)
C17	0.048 (2)	0.060 (3)	0.070 (3)	0.011 (2)	0.015 (2)	−0.007 (2)
C18	0.051 (2)	0.066 (3)	0.055 (2)	0.008 (2)	0.0115 (19)	−0.009 (2)
C19	0.105 (4)	0.090 (3)	0.049 (3)	−0.020 (3)	0.010 (3)	−0.001 (2)
C20	0.056 (2)	0.069 (3)	0.076 (3)	0.013 (2)	0.008 (2)	0.008 (2)
O3	0.173 (4)	0.262 (6)	0.166 (4)	−0.105 (4)	−0.094 (3)	0.137 (4)
N5	0.078 (3)	0.081 (3)	0.176 (6)	0.003 (3)	0.006 (3)	−0.001 (3)
C21	0.080 (4)	0.098 (4)	0.154 (6)	−0.018 (3)	0.004 (4)	0.052 (4)
C22	0.166 (7)	0.259 (11)	0.134	−0.005 (8)	0.017 (6)	−0.035 (7)
C23	0.176 (7)	0.166 (7)	0.111 (6)	−0.031 (6)	−0.026 (5)	0.007 (5)

Geometric parameters (Å, °)

Mn1—N4	1.923 (3)	C10—C11	1.382 (6)
Mn1—N1	1.941 (3)	C10—C19	1.495 (5)
Mn1—N2	2.066 (3)	C11—C12	1.380 (5)
Mn1—N3	2.071 (3)	C11—H11A	0.9300
Mn1—O1W	2.273 (3)	C12—H12A	0.9300
Mn1—Cl1	2.4628 (12)	C13—C14	1.506 (5)
O1—C7	1.237 (4)	C14—C15	1.382 (5)
O1W—H1WA	0.8582	C15—C16	1.386 (5)
O1W—H1WB	0.8600	C15—H15A	0.9300
O2—C13	1.223 (5)	C16—C17	1.373 (6)
N1—C7	1.351 (4)	C16—C20	1.519 (5)
N1—C1	1.413 (4)	C17—C18	1.389 (5)
N2—C12	1.343 (5)	C17—H17A	0.9300
N2—C8	1.350 (4)	C18—H18A	0.9300
N3—C18	1.324 (5)	C19—H19A	0.9600
N3—C14	1.337 (5)	C19—H19B	0.9600
N4—C13	1.358 (4)	C19—H19C	0.9600
N4—C2	1.405 (4)	C20—H20A	0.9600
C1—C6	1.396 (5)	C20—H20B	0.9600
C1—C2	1.405 (5)	C20—H20C	0.9600
C2—C3	1.380 (5)	O3—C21	1.190 (7)
C3—C4	1.376 (5)	N5—C21	1.336 (8)
C3—H3A	0.9300	N5—C22	1.401 (9)
C4—C5	1.356 (6)	N5—C23	1.413 (7)
C4—H4A	0.9300	C21—H21A	0.9300

C5—C6	1.384 (6)	C22—H22A	0.9600
C5—H5A	0.9300	C22—H22B	0.9600
C6—H6A	0.9300	C22—H22C	0.9600
C7—C8	1.492 (5)	C23—H23A	0.9600
C8—C9	1.371 (5)	C23—H23B	0.9600
C9—C10	1.386 (6)	C23—H23C	0.9600
C9—H9A	0.9300		
N4—Mn1—N1	81.29 (12)	C11—C10—C9	117.1 (4)
N4—Mn1—N2	161.16 (12)	C11—C10—C19	121.9 (4)
N1—Mn1—N2	80.28 (12)	C9—C10—C19	121.0 (4)
N4—Mn1—N3	80.40 (12)	C12—C11—C10	119.8 (4)
N1—Mn1—N3	160.75 (12)	C12—C11—H11A	120.1
N2—Mn1—N3	117.43 (12)	C10—C11—H11A	120.1
N4—Mn1—O1W	98.45 (12)	N2—C12—C11	122.8 (4)
N1—Mn1—O1W	96.71 (11)	N2—C12—H12A	118.6
N2—Mn1—O1W	79.93 (11)	C11—C12—H12A	118.6
N3—Mn1—O1W	80.21 (10)	O2—C13—N4	127.2 (4)
N4—Mn1—Cl1	98.18 (9)	O2—C13—C14	121.3 (3)
N1—Mn1—Cl1	99.69 (9)	N4—C13—C14	111.5 (3)
N2—Mn1—Cl1	88.73 (9)	N3—C14—C15	122.5 (3)
N3—Mn1—Cl1	88.75 (9)	N3—C14—C13	115.6 (3)
O1W—Mn1—Cl1	158.17 (9)	C15—C14—C13	121.9 (3)
Mn1—O1W—H1WA	126.9	C14—C15—C16	119.5 (4)
Mn1—O1W—H1WB	118.6	C14—C15—H15A	120.3
H1WA—O1W—H1WB	106.6	C16—C15—H15A	120.3
C7—N1—C1	125.5 (3)	C17—C16—C15	117.2 (3)
C7—N1—Mn1	118.9 (2)	C17—C16—C20	122.0 (4)
C1—N1—Mn1	115.6 (2)	C15—C16—C20	120.8 (4)
C12—N2—C8	117.6 (3)	C16—C17—C18	120.5 (4)
C12—N2—Mn1	129.4 (3)	C16—C17—H17A	119.7
C8—N2—Mn1	113.0 (2)	C18—C17—H17A	119.7
C18—N3—C14	118.5 (3)	N3—C18—C17	121.8 (4)
C18—N3—Mn1	128.5 (3)	N3—C18—H18A	119.1
C14—N3—Mn1	113.0 (2)	C17—C18—H18A	119.1
C13—N4—C2	124.3 (3)	C10—C19—H19A	109.5
C13—N4—Mn1	119.5 (2)	C10—C19—H19B	109.5
C2—N4—Mn1	116.2 (2)	H19A—C19—H19B	109.5
C6—C1—C2	119.9 (3)	C10—C19—H19C	109.5
C6—C1—N1	127.0 (3)	H19A—C19—H19C	109.5
C2—C1—N1	113.0 (3)	H19B—C19—H19C	109.5
C3—C2—C1	119.5 (3)	C16—C20—H20A	109.5
C3—C2—N4	127.0 (3)	C16—C20—H20B	109.5
C1—C2—N4	113.5 (3)	H20A—C20—H20B	109.5
C4—C3—C2	119.6 (4)	C16—C20—H20C	109.5
C4—C3—H3A	120.2	H20A—C20—H20C	109.5
C2—C3—H3A	120.2	H20B—C20—H20C	109.5
C5—C4—C3	121.2 (4)	C21—N5—C22	116.6 (6)
C5—C4—H4A	119.4	C21—N5—C23	120.4 (6)
C3—C4—H4A	119.4	C22—N5—C23	122.8 (7)

C4—C5—C6	120.9 (4)	O3—C21—N5	124.9 (7)
C4—C5—H5A	119.5	O3—C21—H21A	117.5
C6—C5—H5A	119.5	N5—C21—H21A	117.5
C5—C6—C1	118.7 (4)	N5—C22—H22A	109.5
C5—C6—H6A	120.6	N5—C22—H22B	109.5
C1—C6—H6A	120.6	H22A—C22—H22B	109.5
O1—C7—N1	126.6 (3)	N5—C22—H22C	109.5
O1—C7—C8	121.0 (3)	H22A—C22—H22C	109.5
N1—C7—C8	112.4 (3)	H22B—C22—H22C	109.5
N2—C8—C9	122.0 (3)	N5—C23—H23A	109.5
N2—C8—C7	115.3 (3)	N5—C23—H23B	109.5
C9—C8—C7	122.6 (3)	H23A—C23—H23B	109.5
C8—C9—C10	120.7 (4)	N5—C23—H23C	109.5
C8—C9—H9A	119.7	H23A—C23—H23C	109.5
C10—C9—H9A	119.7	H23B—C23—H23C	109.5
N4—Mn1—N1—C7	−177.1 (3)	C1—C2—C3—C4	2.6 (6)
N2—Mn1—N1—C7	−1.0 (2)	N4—C2—C3—C4	−179.9 (4)
N3—Mn1—N1—C7	−159.0 (3)	C2—C3—C4—C5	−1.2 (7)
O1W—Mn1—N1—C7	−79.5 (3)	C3—C4—C5—C6	−0.1 (7)
Cl1—Mn1—N1—C7	86.0 (2)	C4—C5—C6—C1	−0.2 (6)
N4—Mn1—N1—C1	5.2 (2)	C2—C1—C6—C5	1.6 (5)
N2—Mn1—N1—C1	−178.7 (3)	N1—C1—C6—C5	−176.8 (4)
N3—Mn1—N1—C1	23.3 (5)	C1—N1—C7—O1	−2.1 (6)
O1W—Mn1—N1—C1	102.7 (2)	Mn1—N1—C7—O1	−179.6 (3)
Cl1—Mn1—N1—C1	−91.7 (2)	C1—N1—C7—C8	177.7 (3)
N4—Mn1—N2—C12	−167.7 (4)	Mn1—N1—C7—C8	0.2 (4)
N1—Mn1—N2—C12	−179.7 (3)	C12—N2—C8—C9	0.0 (5)
N3—Mn1—N2—C12	−7.7 (4)	Mn1—N2—C8—C9	178.8 (3)
O1W—Mn1—N2—C12	−81.0 (3)	C12—N2—C8—C7	179.2 (3)
Cl1—Mn1—N2—C12	80.2 (3)	Mn1—N2—C8—C7	−2.0 (4)
N4—Mn1—N2—C8	13.6 (5)	O1—C7—C8—N2	−179.0 (3)
N1—Mn1—N2—C8	1.6 (2)	N1—C7—C8—N2	1.2 (4)
N3—Mn1—N2—C8	173.7 (2)	O1—C7—C8—C9	0.2 (5)
O1W—Mn1—N2—C8	100.3 (2)	N1—C7—C8—C9	−179.5 (3)
Cl1—Mn1—N2—C8	−98.4 (2)	N2—C8—C9—C10	−0.8 (5)
N4—Mn1—N3—C18	178.9 (3)	C7—C8—C9—C10	−179.9 (3)
N1—Mn1—N3—C18	160.8 (3)	C8—C9—C10—C11	1.4 (6)
N2—Mn1—N3—C18	5.3 (4)	C8—C9—C10—C19	−179.7 (4)
O1W—Mn1—N3—C18	78.5 (3)	C9—C10—C11—C12	−1.2 (6)
Cl1—Mn1—N3—C18	−82.6 (3)	C19—C10—C11—C12	179.9 (4)
N4—Mn1—N3—C14	−1.4 (2)	C8—N2—C12—C11	0.2 (6)
N1—Mn1—N3—C14	−19.6 (5)	Mn1—N2—C12—C11	−178.4 (3)
N2—Mn1—N3—C14	−175.0 (2)	C10—C11—C12—N2	0.4 (6)
O1W—Mn1—N3—C14	−101.8 (3)	C2—N4—C13—O2	2.3 (7)
Cl1—Mn1—N3—C14	97.1 (2)	Mn1—N4—C13—O2	−179.1 (4)
N1—Mn1—N4—C13	175.0 (3)	C2—N4—C13—C14	−178.9 (3)
N2—Mn1—N4—C13	163.0 (3)	Mn1—N4—C13—C14	−0.3 (4)
N3—Mn1—N4—C13	0.9 (3)	C18—N3—C14—C15	0.4 (5)
O1W—Mn1—N4—C13	79.4 (3)	Mn1—N3—C14—C15	−179.3 (3)

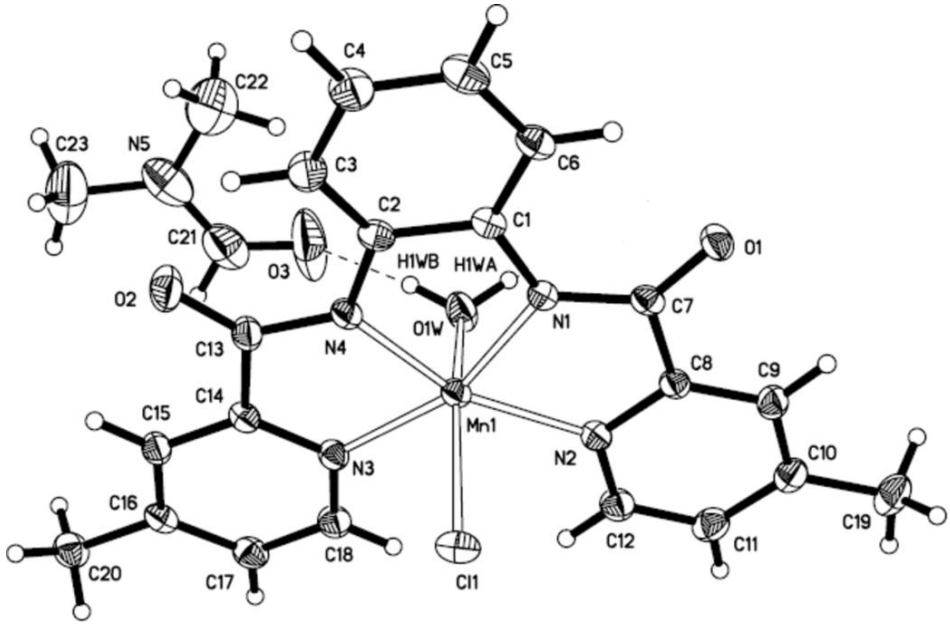
Cl1—Mn1—N4—C13	−86.4 (3)	C18—N3—C14—C13	−178.6 (3)
N1—Mn1—N4—C2	−6.4 (2)	Mn1—N3—C14—C13	1.7 (4)
N2—Mn1—N4—C2	−18.3 (5)	O2—C13—C14—N3	177.9 (4)
N3—Mn1—N4—C2	179.6 (3)	N4—C13—C14—N3	−1.0 (5)
O1W—Mn1—N4—C2	−101.9 (3)	O2—C13—C14—C15	−1.0 (6)
Cl1—Mn1—N4—C2	92.3 (2)	N4—C13—C14—C15	−180.0 (3)
C7—N1—C1—C6	−2.1 (6)	N3—C14—C15—C16	−0.4 (6)
Mn1—N1—C1—C6	175.4 (3)	C13—C14—C15—C16	178.6 (3)
C7—N1—C1—C2	179.3 (3)	C14—C15—C16—C17	−0.1 (5)
Mn1—N1—C1—C2	−3.1 (4)	C14—C15—C16—C20	−179.2 (3)
C6—C1—C2—C3	−2.9 (5)	C15—C16—C17—C18	0.6 (6)
N1—C1—C2—C3	175.8 (3)	C20—C16—C17—C18	179.6 (4)
C6—C1—C2—N4	179.3 (3)	C14—N3—C18—C17	0.1 (6)
N1—C1—C2—N4	−2.0 (4)	Mn1—N3—C18—C17	179.8 (3)
C13—N4—C2—C3	7.4 (6)	C16—C17—C18—N3	−0.6 (6)
Mn1—N4—C2—C3	−171.2 (3)	C22—N5—C21—O3	−2.2 (10)
C13—N4—C2—C1	−175.0 (3)	C23—N5—C21—O3	−177.5 (6)
Mn1—N4—C2—C1	6.4 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O1^{i}	0.86	1.90	2.728 (3)	162.3
O1W—H1WB···O3i	0.86	1.78	2.627 (5)	170.2

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

Fig. 1


C4
C5
C22
C23
N5
C3
C6
C2
C1
C21
O3
H1WB
H1WA
O1
O2
O1W
N1
C7
C13
N4
C8
C9
C14
C15
Mn1
N3
N2
C10
C16
C19
C12
C11
C20
C17
C18
Cl1