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Chlorido[*N*,*N*,*N*′,*N*′-tetrakis(benzimidazol-2-ylmethyl)ethane-1,2-diamine]manganese(II) chloride monohydrate

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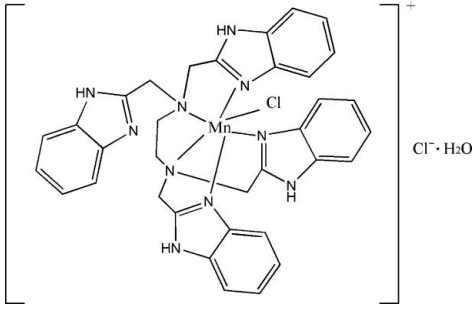
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.127; data-to-parameter ratio = 18.0.

In the title compound, $[MnCl(C_{34}H_{32}N_{10})]Cl\cdot H_2O$, the Mn^{II} ion is in a distorted octahedral coordination environment. The crystal structure is stabilized by extensive hydrogen bonding.

Related literature

Some work related to this study has been published (Chen *et al.*, 2004; Liao *et al.*, 2001) and the disordered solvent molecule was treated using the SQUEEZE routine in *PLATON* (Spek, 2003).

For related literature, see: Hendriks *et al.* (1982); Suresh *et al.* (2006).



Experimental

Crystal data

$[MnCl(C_{34}H_{32}N_{10})]Cl\cdot H_2O$
M_r = 724.55
Triclinic, $P\overline{1}$
a = 9.790 (2) Å
b = 12.657 (3) Å
c = 16.039 (4) Å
α = 76.380 (4)°
β = 84.743 (4)°
γ = 77.753 (4)°
V = 1885.8 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 299 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.901, T_{max} = 0.949
20876 measured reflections
8156 independent reflections
6487 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.127
S = 1.06
8156 reflections
453 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected bond angles (°).

N5—Mn1—N7	156.40 (6)	N3—Mn1—Cl1	105.02 (5)
N5—Mn1—N3	98.35 (6)	N1—Mn1—Cl1	174.68 (4)
N7—Mn1—N3	95.05 (6)	N5—Mn1—N2	85.00 (6)
N5—Mn1—N1	74.97 (6)	N7—Mn1—N2	73.08 (6)
N7—Mn1—N1	90.68 (6)	N3—Mn1—N2	145.62 (6)
N3—Mn1—N1	72.89 (6)	N1—Mn1—N2	75.08 (6)
N5—Mn1—Cl1	100.73 (4)	Cl1—Mn1—N2	107.93 (5)
N7—Mn1—Cl1	94.39 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···N10^{i}	0.835 (10)	2.065 (11)	2.884 (3)	167 (3)
N4—H4A···Cl2^{ii}	0.851 (10)	2.308 (11)	3.147 (2)	169 (2)
N8—H8···O3^{iii}	0.855 (10)	1.922 (12)	2.755 (3)	164 (2)
N9—H9···Cl1^{iv}	0.847 (10)	2.485 (15)	3.242 (2)	149 (2)
C19—H19B···Cl1^{iv}	0.97	2.69	3.607 (3)	157
N6—H6A···Cl2	0.843 (10)	2.454 (16)	3.1920 (19)	147 (2)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

The authors thank Xianggao Meng for help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2366).

References

Bruker (2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Z.-F., Liao, Z.-R., Li, D.-F., Li, W.-K. & Meng, X.-G. (2004). *J. Inorg. Biochem.* **98**, 1315–1318.
Hendriks, M. J., Birker, J. M. W. L., van Rijn, J., Verschoor, G. C. & Reedijk, J. (1982). *J. Am. Chem. Soc.* **104**, 3607–3617.
Liao, Z.-R., Zheng, X.-F., Luo, B.-S., Shen, L.-R., Li, D.-F., Liu, H.-L. & Zhao, W. (2001). *Polyhedron*, **20**, 2813–2821.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (2001). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Suresh, J., Raja, V. P. A., Perumal, S. & Natarajan, S. (2006). *Acta Cryst.* E**62**, o3307–o3309.

supplementary materials

Acta Cryst. (2007). E**63**, m1571-m1572 [**doi:10.1107/S1600536807021034**]

Chlorido[*N*,*N*,*N*',*N*'-tetrakis(benzimidazol-2-ylmethyl)ethane-1,2-diamine]manganese(II) chloride monohydrate

Y.-M. Pei, C.-S. Zhou, X.-G. Meng, L. Wang and C.-L. Liu

Comment

Recently, studies of ligands containing polybenzimidazole groups and their metal coordination compounds have been widely carried out (Chen *et al.*, 2004; Liao *et al.*,2001). In a continuation of our work, we report herein the crystal structure of the title compound (I).

In the molecular structure of (I) (Fig. 1) the Mn^{II} is coordinated by three benzimidazole N atoms, two amino N atoms of an edtb ligand and one chloride anion, forming a distorted octahedron coordination geometry. Unlike the related structure (Chen *et al.*, 2004), in (I) there is an uncoordinated benzimidazole group extending away from the central Mn atom.

There are a number of N(or C)–H···Cl, N–H···O and O–H···N hydrogen bonds which stabilize the crystal structure (Table 2 & Fig. 2).

Experimental

The ligand *N*,*N*,*N*',*N*'-tetrakis(benzimidazol-2-ylmethyl)ethane-1,2-diamine (edtb) was synthesized as reported by Hendriks, *et al.* (1982).

The edtb (0.58 g, 1.0 mmol) in 20 ml hot absolute methanol was added slowly to $MnCl_2 \cdot 4H_2O$ (0.20 g, 1.0 mmol) solution of 10 ml me thanol. The mixture was stirred for 1 h. After filtration, the brownish solution was allowed to stand at room temperature. Yellow block-shaped crystals suitable for X-ray analysis were obtained in several days in 55% yield.

Refinement

All H atoms bonded to C atoms were placed in calclulated positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, with U_{iso}(H) = 1.2U_{eq}(C). H atoms bonded to N atoms were located in a difference map and were refined with distance restraints of N—H =0.86 (1) Å and U_{iso}(H) =1.2U_{eq}(N). Similarly located water H atoms were refined with distance restraints of O–H = 0.82 (1) Å, H–H=1.39 (1) Å and U_{iso}(H)=1.5U_{eq}(O). During the refinement of the structure, electron density peaks were located that were believed to be highly disordered solvent molecule molecules (possibly methanol and water solvent). Attempts made to model the solvent molecules were not successful. The SQUEEZE option in *PLATON* (Spek, 2003) indicated there was a solvent cavity of volume 276.0 $Å^3$ containing approximately 26 electrons. In the final cycles of refinement, this contribution to the electron density was removed from the observed data. The density, the F(000) value, the molecular weight and the formula are given without taking into account the results obtained with the SQUEEZE option *PLATON* (Spek, 2003). Similar treatment of disordered solvent molecules were carried out by Suresh *et al.* (2006) and references cited therein.

Figures

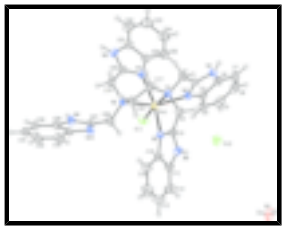


Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids and H atoms as small spheres.

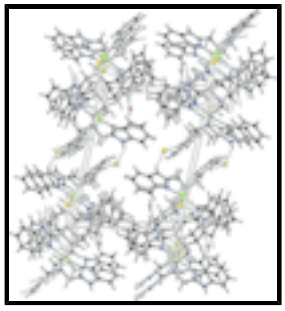


Fig. 2. Part of the crystal structure of (I), showing hydrogen bonds as dashed lines.

Chlorido[*N*,*N*,*N*',*N*'-tetrakis(benzimidazol-2-ylmethyl)ethane-1,2- diamine]manganese(II) chloride monohydrate

Crystal data

$[MnCl(C_{34}H_{32}N_{10})]Cl·H_2O$	$Z = 2$
$M_r = 724.55$	$F_{000} = 750$
Triclinic, $P\overline{1}$	$D_x = 1.276$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.790$ (2) Å	Cell parameters from 8006 reflections
$b = 12.657$ (3) Å	$\theta = 2.4$–27.2º
$c = 16.039$ (4) Å	$\mu = 0.53$ mm^{-1}
$\alpha = 76.380$ (4)º	$T = 299$ (2) K
$\beta = 84.743$ (4)º	Block, yellow
$\gamma = 77.753$ (4)º	0.20 × 0.10 × 0.10 mm
$V = 1885.8$ (8) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	8156 independent reflections
Radiation source: fine focus sealed Siemens Mo tube	6487 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 298$(2) K	$\theta_{max} = 27.0$º
0.3° wide ω exposures scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -12 \rightarrow 12$
$T_{min} = 0.901$, $T_{max} = 0.949$	$k = -16 \rightarrow 16$

20876 measured reflections

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.127$

$S = 1.06$

8156 reflections

453 parameters

7 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0763P)^2 + 0.1012P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.003$

$\Delta\rho_{max} = 0.41$ e Å^{-3}

$\Delta\rho_{min} = -0.18$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.87099 (3)	0.97239 (2)	0.217963 (17)	0.03531 (10)
Cl1	1.11136 (6)	0.95010 (5)	0.16532 (4)	0.06023 (17)
Cl2	0.55649 (7)	0.70808 (6)	0.54994 (4)	0.06850 (19)
C1	0.6092 (2)	1.08254 (18)	0.31676 (14)	0.0442 (5)
H1A	0.5343	1.0785	0.3607	0.053*
H1B	0.5801	1.1472	0.2713	0.053*
C2	0.7393 (2)	1.09219 (16)	0.35430 (12)	0.0399 (4)
C3	0.9568 (2)	1.07967 (16)	0.37531 (12)	0.0402 (4)
C4	1.1023 (2)	1.0563 (2)	0.37460 (14)	0.0512 (5)
H4	1.1551	1.0073	0.3434	0.061*
C5	1.1646 (3)	1.1088 (2)	0.42214 (16)	0.0602 (6)
H5	1.2617	1.0954	0.4224	0.072*
C6	1.0875 (3)	1.1808 (2)	0.46945 (16)	0.0636 (7)
H6	1.1344	1.2147	0.5003	0.076*

C7	0.9446 (3)	1.2040 (2)	0.47242 (15)	0.0577 (6)
H7	0.8932	1.2519	0.5050	0.069*
C8	0.8793 (2)	1.15160 (17)	0.42380 (13)	0.0444 (5)
C9	0.6374 (2)	0.88249 (17)	0.35197 (13)	0.0433 (5)
H9A	0.5498	0.8579	0.3533	0.052*
H9B	0.6440	0.9012	0.4065	0.052*
C10	0.7564 (2)	0.79014 (16)	0.34047 (12)	0.0371 (4)
C11	0.8914 (2)	0.62402 (17)	0.36215 (14)	0.0454 (5)
C12	0.9565 (3)	0.5139 (2)	0.38902 (18)	0.0659 (7)
H12	0.9187	0.4656	0.4337	0.079*
C13	1.0806 (3)	0.4800 (2)	0.3457 (2)	0.0751 (8)
H13	1.1271	0.4066	0.3614	0.090*
C14	1.1386 (3)	0.5522 (2)	0.2794 (2)	0.0683 (7)
H14	1.2226	0.5259	0.2521	0.082*
C15	1.0743 (2)	0.66171 (18)	0.25345 (16)	0.0537 (5)
H15	1.1128	0.7098	0.2089	0.064*
C16	0.9500 (2)	0.69731 (16)	0.29630 (13)	0.0398 (4)
C17	0.5418 (2)	0.98934 (19)	0.21419 (14)	0.0471 (5)
H17A	0.5241	1.0645	0.1796	0.056*
H17B	0.4533	0.9729	0.2405	0.056*
C18	0.6014 (2)	0.90988 (18)	0.15694 (13)	0.0443 (5)
H18A	0.6230	0.8350	0.1917	0.053*
H18B	0.5321	0.9120	0.1168	0.053*
C19	0.6979 (3)	1.03940 (18)	0.03887 (14)	0.0526 (5)
H19A	0.5974	1.0612	0.0336	0.063*
H19B	0.7389	1.0229	−0.0151	0.063*
C20	0.7528 (2)	1.13286 (16)	0.05581 (12)	0.0415 (4)
C21	0.8023 (2)	1.29872 (18)	0.03526 (14)	0.0465 (5)
C22	0.8184 (3)	1.4076 (2)	0.00745 (17)	0.0625 (6)
H22	0.7959	1.4478	−0.0477	0.075*
C23	0.8689 (3)	1.4538 (2)	0.0644 (2)	0.0710 (8)
H23	0.8777	1.5277	0.0482	0.085*
C24	0.9071 (3)	1.3929 (2)	0.14568 (19)	0.0633 (6)
H24	0.9438	1.4264	0.1819	0.076*
C25	0.8922 (2)	1.28452 (18)	0.17394 (16)	0.0527 (5)
H25	0.9180	1.2443	0.2285	0.063*
C26	0.8371 (2)	1.23728 (16)	0.11812 (13)	0.0425 (4)
C27	0.8169 (2)	0.84426 (19)	0.07694 (14)	0.0471 (5)
H27A	0.8430	0.7839	0.1261	0.057*
H27B	0.9024	0.8666	0.0503	0.057*
C28	0.7526 (2)	0.80061 (16)	0.01401 (13)	0.0410 (4)
C29	0.7187 (2)	0.76308 (17)	−0.10898 (13)	0.0431 (4)
C30	0.7182 (3)	0.7509 (2)	−0.19289 (14)	0.0555 (6)
H30	0.7730	0.7857	−0.2369	0.067*
C31	0.6319 (3)	0.6843 (2)	−0.20722 (17)	0.0619 (7)
H31	0.6282	0.6742	−0.2625	0.074*
C32	0.5511 (3)	0.6322 (2)	−0.14177 (19)	0.0658 (7)
H32	0.4940	0.5884	−0.1543	0.079*
C33	0.5523 (3)	0.64310 (19)	−0.05903 (17)	0.0554 (6)

H33	0.4982	0.6070	−0.0152	0.067*
C34	0.6384 (2)	0.71082 (16)	−0.04299 (13)	0.0417 (4)
N1	0.63796 (16)	0.98180 (13)	0.28227 (10)	0.0377 (3)
N2	0.72994 (18)	0.93848 (13)	0.10858 (10)	0.0412 (4)
N3	0.86515 (17)	1.04362 (13)	0.33155 (10)	0.0395 (4)
N4	0.7413 (2)	1.15652 (15)	0.40989 (12)	0.0468 (4)
H4A	0.6662 (16)	1.1952 (18)	0.4266 (15)	0.056*
N5	0.86186 (16)	0.80181 (13)	0.28470 (10)	0.0373 (3)
N6	0.76745 (19)	0.68611 (14)	0.38818 (11)	0.0446 (4)
H6A	0.709 (2)	0.6652 (19)	0.4270 (12)	0.053*
N7	0.80471 (18)	1.13265 (13)	0.12867 (10)	0.0427 (4)
N8	0.7508 (2)	1.22867 (15)	−0.00237 (11)	0.0490 (4)
H8	0.712 (2)	1.245 (2)	−0.0505 (10)	0.059*
N9	0.7908 (2)	0.82004 (15)	−0.07105 (11)	0.0469 (4)
H9	0.845 (2)	0.8612 (17)	−0.0990 (14)	0.056*
N10	0.66146 (19)	0.73513 (14)	0.03392 (11)	0.0456 (4)
O3	0.5832 (2)	0.3045 (2)	0.85843 (11)	0.0745 (5)
H3A	0.586 (3)	0.312 (3)	0.8063 (7)	0.112*
H3B	0.5049 (19)	0.299 (3)	0.8824 (18)	0.112*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.04063 (18)	0.03138 (16)	0.03312 (16)	−0.00702 (12)	−0.00128 (11)	−0.00574 (11)
Cl1	0.0523 (3)	0.0513 (3)	0.0703 (4)	−0.0121 (3)	0.0189 (3)	−0.0064 (3)
Cl2	0.0570 (4)	0.0882 (5)	0.0553 (3)	−0.0074 (3)	0.0099 (3)	−0.0170 (3)
C1	0.0394 (11)	0.0460 (11)	0.0481 (11)	−0.0003 (9)	−0.0046 (9)	−0.0185 (9)
C2	0.0452 (11)	0.0369 (10)	0.0366 (10)	−0.0053 (8)	−0.0031 (8)	−0.0084 (8)
C3	0.0464 (11)	0.0397 (10)	0.0345 (9)	−0.0139 (8)	−0.0067 (8)	−0.0017 (8)
C4	0.0468 (12)	0.0569 (13)	0.0478 (12)	−0.0118 (10)	−0.0042 (9)	−0.0051 (10)
C5	0.0531 (14)	0.0727 (17)	0.0561 (14)	−0.0267 (12)	−0.0152 (11)	0.0009 (12)
C6	0.0824 (19)	0.0700 (16)	0.0481 (13)	−0.0398 (14)	−0.0201 (12)	−0.0034 (12)
C7	0.0789 (18)	0.0573 (14)	0.0452 (12)	−0.0247 (12)	−0.0061 (11)	−0.0163 (10)
C8	0.0563 (13)	0.0393 (11)	0.0389 (10)	−0.0149 (9)	−0.0054 (9)	−0.0048 (8)
C9	0.0391 (10)	0.0445 (11)	0.0432 (11)	−0.0063 (8)	0.0037 (8)	−0.0075 (9)
C10	0.0390 (10)	0.0377 (10)	0.0356 (9)	−0.0104 (8)	−0.0039 (8)	−0.0068 (8)
C11	0.0505 (12)	0.0365 (10)	0.0476 (11)	−0.0100 (9)	−0.0074 (9)	−0.0028 (9)
C12	0.0762 (18)	0.0393 (12)	0.0729 (17)	−0.0086 (12)	−0.0054 (14)	0.0040 (11)
C13	0.0788 (19)	0.0382 (13)	0.096 (2)	0.0074 (12)	−0.0110 (16)	−0.0050 (13)
C14	0.0573 (15)	0.0476 (14)	0.093 (2)	0.0070 (11)	−0.0019 (14)	−0.0183 (13)
C15	0.0504 (13)	0.0423 (12)	0.0657 (14)	−0.0062 (10)	0.0041 (11)	−0.0116 (10)
C16	0.0417 (11)	0.0338 (10)	0.0437 (10)	−0.0061 (8)	−0.0065 (8)	−0.0077 (8)
C17	0.0404 (11)	0.0544 (13)	0.0483 (12)	−0.0034 (9)	−0.0109 (9)	−0.0173 (10)
C18	0.0443 (11)	0.0480 (12)	0.0447 (11)	−0.0096 (9)	−0.0098 (9)	−0.0147 (9)
C19	0.0736 (15)	0.0485 (12)	0.0380 (11)	−0.0147 (11)	−0.0132 (10)	−0.0077 (9)
C20	0.0458 (11)	0.0396 (10)	0.0364 (10)	−0.0058 (8)	−0.0017 (8)	−0.0055 (8)
C21	0.0452 (11)	0.0431 (11)	0.0471 (11)	−0.0076 (9)	−0.0034 (9)	−0.0021 (9)
C22	0.0679 (16)	0.0460 (13)	0.0659 (15)	−0.0157 (12)	−0.0068 (12)	0.0078 (11)

C23	0.0720 (17)	0.0419 (13)	0.097 (2)	−0.0219 (12)	−0.0014 (15)	−0.0019 (13)
C24	0.0687 (16)	0.0483 (13)	0.0801 (18)	−0.0223 (12)	−0.0067 (13)	−0.0173 (12)
C25	0.0590 (14)	0.0447 (12)	0.0568 (13)	−0.0165 (10)	−0.0105 (11)	−0.0072 (10)
C26	0.0424 (11)	0.0338 (10)	0.0484 (11)	−0.0069 (8)	−0.0023 (9)	−0.0039 (8)
C27	0.0489 (12)	0.0522 (12)	0.0458 (11)	−0.0121 (10)	−0.0053 (9)	−0.0187 (9)
C28	0.0456 (11)	0.0391 (10)	0.0404 (10)	−0.0081 (9)	−0.0016 (8)	−0.0132 (8)
C29	0.0447 (11)	0.0412 (11)	0.0437 (11)	−0.0019 (9)	−0.0034 (9)	−0.0155 (9)
C30	0.0649 (15)	0.0576 (14)	0.0414 (11)	0.0023 (11)	−0.0043 (10)	−0.0176 (10)
C31	0.0724 (16)	0.0589 (15)	0.0555 (14)	0.0136 (12)	−0.0259 (13)	−0.0302 (12)
C32	0.0642 (16)	0.0579 (15)	0.0855 (19)	−0.0012 (12)	−0.0214 (14)	−0.0383 (14)
C33	0.0572 (14)	0.0483 (13)	0.0681 (15)	−0.0134 (10)	−0.0035 (11)	−0.0245 (11)
C34	0.0443 (11)	0.0369 (10)	0.0460 (11)	−0.0045 (8)	−0.0033 (8)	−0.0158 (8)
N1	0.0355 (8)	0.0378 (8)	0.0400 (8)	−0.0033 (6)	−0.0066 (6)	−0.0105 (7)
N2	0.0529 (10)	0.0391 (9)	0.0338 (8)	−0.0118 (7)	−0.0049 (7)	−0.0090 (7)
N3	0.0397 (9)	0.0416 (9)	0.0375 (8)	−0.0056 (7)	−0.0044 (7)	−0.0102 (7)
N4	0.0511 (11)	0.0439 (10)	0.0479 (10)	−0.0054 (8)	−0.0010 (8)	−0.0188 (8)
N5	0.0372 (8)	0.0330 (8)	0.0390 (8)	−0.0044 (6)	−0.0004 (7)	−0.0056 (6)
N6	0.0498 (10)	0.0395 (9)	0.0425 (9)	−0.0140 (8)	0.0025 (8)	−0.0022 (7)
N7	0.0531 (10)	0.0352 (9)	0.0397 (9)	−0.0092 (7)	−0.0082 (7)	−0.0052 (7)
N8	0.0589 (11)	0.0450 (10)	0.0383 (9)	−0.0088 (8)	−0.0103 (8)	0.0022 (8)
N9	0.0548 (11)	0.0498 (10)	0.0406 (9)	−0.0203 (8)	0.0070 (8)	−0.0133 (8)
N10	0.0553 (10)	0.0448 (10)	0.0411 (9)	−0.0174 (8)	0.0031 (8)	−0.0134 (7)
O3	0.0684 (12)	0.1107 (16)	0.0462 (9)	−0.0287 (11)	−0.0056 (8)	−0.0102 (10)

Geometric parameters (Å, °)

Mn1—N5	2.1889 (16)	C18—N2	1.482 (3)
Mn1—N7	2.1978 (17)	C18—H18A	0.9700
Mn1—N3	2.2063 (17)	C18—H18B	0.9700
Mn1—N1	2.4071 (17)	C19—N2	1.484 (3)
Mn1—Cl1	2.4078 (8)	C19—C20	1.487 (3)
Mn1—N2	2.4938 (17)	C19—H19A	0.9700
C1—N1	1.470 (3)	C19—H19B	0.9700
C1—C2	1.497 (3)	C20—N7	1.315 (3)
C1—H1A	0.9700	C20—N8	1.342 (3)
C1—H1B	0.9700	C21—N8	1.379 (3)
C2—N3	1.316 (3)	C21—C22	1.383 (3)
C2—N4	1.345 (3)	C21—C26	1.404 (3)
C3—C4	1.392 (3)	C22—C23	1.370 (4)
C3—C8	1.393 (3)	C22—H22	0.9300
C3—N3	1.395 (2)	C23—C24	1.388 (4)
C4—C5	1.375 (3)	C23—H23	0.9300
C4—H4	0.9300	C24—C25	1.375 (3)
C5—C6	1.380 (4)	C24—H24	0.9300
C5—H5	0.9300	C25—C26	1.388 (3)
C6—C7	1.366 (4)	C25—H25	0.9300
C6—H6	0.9300	C26—N7	1.395 (3)
C7—C8	1.404 (3)	C27—N2	1.476 (3)
C7—H7	0.9300	C27—C28	1.499 (3)

C8—N4	1.376 (3)	C27—H27A	0.9700
C9—N1	1.473 (3)	C27—H27B	0.9700
C9—C10	1.497 (3)	C28—N10	1.312 (3)
C9—H9A	0.9700	C28—N9	1.360 (3)
C9—H9B	0.9700	C29—N9	1.374 (3)
C10—N5	1.312 (2)	C29—C34	1.384 (3)
C10—N6	1.346 (2)	C29—C30	1.391 (3)
C11—N6	1.386 (3)	C30—C31	1.380 (4)
C11—C12	1.388 (3)	C30—H30	0.9300
C11—C16	1.399 (3)	C31—C32	1.381 (4)
C12—C13	1.381 (4)	C31—H31	0.9300
C12—H12	0.9300	C32—C33	1.367 (4)
C13—C14	1.393 (4)	C32—H32	0.9300
C13—H13	0.9300	C33—C34	1.401 (3)
C14—C15	1.377 (3)	C33—H33	0.9300
C14—H14	0.9300	C34—N10	1.388 (3)
C15—C16	1.384 (3)	N4—H4A	0.851 (10)
C15—H15	0.9300	N6—H6A	0.843 (10)
C16—N5	1.399 (2)	N8—H8	0.855 (10)
C17—N1	1.479 (3)	N9—H9	0.847 (10)
C17—C18	1.511 (3)	O3—H3A	0.819 (10)
C17—H17A	0.9700	O3—H3B	0.835 (10)
C17—H17B	0.9700		
N5—Mn1—N7	156.40 (6)	C20—C19—H19B	109.3
N5—Mn1—N3	98.35 (6)	H19A—C19—H19B	108.0
N7—Mn1—N3	95.05 (6)	N7—C20—N8	112.80 (18)
N5—Mn1—N1	74.97 (6)	N7—C20—C19	124.59 (18)
N7—Mn1—N1	90.68 (6)	N8—C20—C19	122.59 (18)
N3—Mn1—N1	72.89 (6)	N8—C21—C22	133.0 (2)
N5—Mn1—Cl1	100.73 (4)	N8—C21—C26	105.36 (18)
N7—Mn1—Cl1	94.39 (5)	C22—C21—C26	121.6 (2)
N3—Mn1—Cl1	105.02 (5)	C23—C22—C21	117.3 (2)
N1—Mn1—Cl1	174.68 (4)	C23—C22—H22	121.4
N5—Mn1—N2	85.00 (6)	C21—C22—H22	121.4
N7—Mn1—N2	73.08 (6)	C22—C23—C24	121.6 (2)
N3—Mn1—N2	145.62 (6)	C22—C23—H23	119.2
N1—Mn1—N2	75.08 (6)	C24—C23—H23	119.2
Cl1—Mn1—N2	107.93 (5)	C25—C24—C23	121.7 (2)
N1—C1—C2	108.90 (16)	C25—C24—H24	119.2
N1—C1—H1A	109.9	C23—C24—H24	119.2
C2—C1—H1A	109.9	C24—C25—C26	117.6 (2)
N1—C1—H1B	109.9	C24—C25—H25	121.2
C2—C1—H1B	109.9	C26—C25—H25	121.2
H1A—C1—H1B	108.3	C25—C26—N7	131.23 (19)
N3—C2—N4	112.98 (18)	C25—C26—C21	120.19 (19)
N3—C2—C1	122.85 (17)	N7—C26—C21	108.58 (18)
N4—C2—C1	124.03 (18)	N2—C27—C28	116.69 (18)
C4—C3—C8	120.7 (2)	N2—C27—H27A	108.1
C4—C3—N3	130.4 (2)	C28—C27—H27A	108.1

C8—C3—N3	108.90 (18)	N2—C27—H27B	108.1
C5—C4—C3	117.0 (2)	C28—C27—H27B	108.1
C5—C4—H4	121.5	H27A—C27—H27B	107.3
C3—C4—H4	121.5	N10—C28—N9	112.32 (18)
C4—C5—C6	122.1 (2)	N10—C28—C27	125.14 (18)
C4—C5—H5	119.0	N9—C28—C27	122.42 (18)
C6—C5—H5	119.0	N9—C29—C34	105.17 (17)
C7—C6—C5	122.2 (2)	N9—C29—C30	132.7 (2)
C7—C6—H6	118.9	C34—C29—C30	122.1 (2)
C5—C6—H6	118.9	C31—C30—C29	116.4 (2)
C6—C7—C8	116.5 (2)	C31—C30—H30	121.8
C6—C7—H7	121.7	C29—C30—H30	121.8
C8—C7—H7	121.7	C30—C31—C32	121.8 (2)
N4—C8—C3	105.75 (18)	C30—C31—H31	119.1
N4—C8—C7	132.8 (2)	C32—C31—H31	119.1
C3—C8—C7	121.5 (2)	C33—C32—C31	122.0 (2)
N1—C9—C10	111.66 (16)	C33—C32—H32	119.0
N1—C9—H9A	109.3	C31—C32—H32	119.0
C10—C9—H9A	109.3	C32—C33—C34	117.2 (2)
N1—C9—H9B	109.3	C32—C33—H33	121.4
C10—C9—H9B	109.3	C34—C33—H33	121.4
H9A—C9—H9B	107.9	C29—C34—N10	110.07 (17)
N5—C10—N6	112.84 (17)	C29—C34—C33	120.5 (2)
N5—C10—C9	124.15 (17)	N10—C34—C33	129.5 (2)
N6—C10—C9	123.00 (17)	C1—N1—C9	110.72 (16)
N6—C11—C12	132.7 (2)	C1—N1—C17	111.94 (16)
N6—C11—C16	105.43 (17)	C9—N1—C17	112.47 (16)
C12—C11—C16	121.9 (2)	C1—N1—Mn1	105.12 (12)
C13—C12—C11	116.3 (2)	C9—N1—Mn1	108.33 (11)
C13—C12—H12	121.9	C17—N1—Mn1	107.90 (12)
C11—C12—H12	121.9	C27—N2—C18	112.46 (16)
C12—C13—C14	122.2 (2)	C27—N2—C19	112.10 (16)
C12—C13—H13	118.9	C18—N2—C19	111.78 (17)
C14—C13—H13	118.9	C27—N2—Mn1	105.26 (12)
C15—C14—C13	121.4 (2)	C18—N2—Mn1	104.54 (11)
C15—C14—H14	119.3	C19—N2—Mn1	110.21 (12)
C13—C14—H14	119.3	C2—N3—C3	105.15 (16)
C14—C15—C16	117.3 (2)	C2—N3—Mn1	113.98 (13)
C14—C15—H15	121.4	C3—N3—Mn1	138.25 (13)
C16—C15—H15	121.4	C2—N4—C8	107.21 (17)
C15—C16—N5	130.39 (19)	C2—N4—H4A	121.2 (17)
C15—C16—C11	121.03 (19)	C8—N4—H4A	131.3 (17)
N5—C16—C11	108.57 (18)	C10—N5—C16	105.76 (16)
N1—C17—C18	111.77 (17)	C10—N5—Mn1	115.66 (12)
N1—C17—H17A	109.3	C16—N5—Mn1	137.62 (13)
C18—C17—H17A	109.3	C10—N6—C11	107.40 (16)
N1—C17—H17B	109.3	C10—N6—H6A	124.5 (17)
C18—C17—H17B	109.3	C11—N6—H6A	128.1 (17)
H17A—C17—H17B	107.9	C20—N7—C26	105.59 (16)

N2—C18—C17	111.39 (17)	C20—N7—Mn1	118.21 (13)
N2—C18—H18A	109.4	C26—N7—Mn1	133.69 (13)
C17—C18—H18A	109.4	C20—N8—C21	107.65 (17)
N2—C18—H18B	109.4	C20—N8—H8	124.6 (17)
C17—C18—H18B	109.4	C21—N8—H8	127.0 (17)
H18A—C18—H18B	108.0	C28—N9—C29	107.41 (17)
N2—C19—C20	111.61 (17)	C28—N9—H9	129.4 (17)
N2—C19—H19A	109.3	C29—N9—H9	123.1 (17)
C20—C19—H19A	109.3	C28—N10—C34	105.03 (17)
N2—C19—H19B	109.3	H3A—O3—H3B	114.4 (18)
N1—C1—C2—N3	22.5 (3)	N3—Mn1—N2—C27	−157.38 (12)
N1—C1—C2—N4	−162.06 (19)	N1—Mn1—N2—C27	−135.62 (13)
C8—C3—C4—C5	−1.2 (3)	Cl1—Mn1—N2—C27	39.81 (13)
N3—C3—C4—C5	177.1 (2)	N5—Mn1—N2—C18	58.80 (12)
C3—C4—C5—C6	0.6 (3)	N7—Mn1—N2—C18	−112.34 (13)
C4—C5—C6—C7	0.4 (4)	N3—Mn1—N2—C18	−38.70 (17)
C5—C6—C7—C8	−0.8 (4)	N1—Mn1—N2—C18	−16.95 (12)
C4—C3—C8—N4	179.73 (19)	Cl1—Mn1—N2—C18	158.48 (11)
N3—C3—C8—N4	1.1 (2)	N5—Mn1—N2—C19	179.06 (14)
C4—C3—C8—C7	0.9 (3)	N7—Mn1—N2—C19	7.92 (14)
N3—C3—C8—C7	−177.77 (18)	N3—Mn1—N2—C19	81.56 (17)
C6—C7—C8—N4	−178.3 (2)	N1—Mn1—N2—C19	103.31 (14)
C6—C7—C8—C3	0.1 (3)	Cl1—Mn1—N2—C19	−81.26 (14)
N1—C9—C10—N5	11.4 (3)	N4—C2—N3—C3	−0.4 (2)
N1—C9—C10—N6	−170.01 (18)	C1—C2—N3—C3	175.43 (18)
N6—C11—C12—C13	178.6 (3)	N4—C2—N3—Mn1	−165.50 (13)
C16—C11—C12—C13	−1.5 (4)	C1—C2—N3—Mn1	10.3 (2)
C11—C12—C13—C14	0.7 (4)	C4—C3—N3—C2	−178.9 (2)
C12—C13—C14—C15	−0.2 (5)	C8—C3—N3—C2	−0.4 (2)
C13—C14—C15—C16	0.4 (4)	C4—C3—N3—Mn1	−19.6 (3)
C14—C15—C16—N5	−179.9 (2)	C8—C3—N3—Mn1	158.89 (15)
C14—C15—C16—C11	−1.2 (3)	N5—Mn1—N3—C2	−95.69 (14)
N6—C11—C16—C15	−178.22 (19)	N7—Mn1—N3—C2	64.83 (14)
C12—C11—C16—C15	1.8 (3)	N1—Mn1—N3—C2	−24.33 (13)
N6—C11—C16—N5	0.8 (2)	Cl1—Mn1—N3—C2	160.76 (13)
C12—C11—C16—N5	−179.2 (2)	N2—Mn1—N3—C2	−2.3 (2)
N1—C17—C18—N2	−64.5 (2)	N5—Mn1—N3—C3	106.22 (19)
N2—C19—C20—N7	−9.5 (3)	N7—Mn1—N3—C3	−93.26 (19)
N2—C19—C20—N8	172.27 (19)	N1—Mn1—N3—C3	177.6 (2)
N8—C21—C22—C23	177.2 (2)	Cl1—Mn1—N3—C3	2.7 (2)
C26—C21—C22—C23	−0.5 (4)	N2—Mn1—N3—C3	−160.41 (16)
C21—C22—C23—C24	2.3 (4)	N3—C2—N4—C8	1.1 (2)
C22—C23—C24—C25	−2.1 (4)	C1—C2—N4—C8	−174.68 (19)
C23—C24—C25—C26	0.0 (4)	C3—C8—N4—C2	−1.3 (2)
C24—C25—C26—N7	−177.3 (2)	C7—C8—N4—C2	177.4 (2)
C24—C25—C26—C21	1.7 (3)	N6—C10—N5—C16	−0.1 (2)
N8—C21—C26—C25	−179.8 (2)	C9—C10—N5—C16	178.61 (18)
C22—C21—C26—C25	−1.4 (3)	N6—C10—N5—Mn1	−170.87 (13)
N8—C21—C26—N7	−0.6 (2)	C9—C10—N5—Mn1	7.8 (2)

C22—C21—C26—N7	177.7 (2)	C15—C16—N5—C10	178.4 (2)
N2—C27—C28—N10	−78.5 (3)	C11—C16—N5—C10	−0.4 (2)
N2—C27—C28—N9	105.8 (2)	C15—C16—N5—Mn1	−13.9 (4)
N9—C29—C30—C31	179.0 (2)	C11—C16—N5—Mn1	167.21 (15)
C34—C29—C30—C31	0.6 (3)	N7—Mn1—N5—C10	−69.2 (2)
C29—C30—C31—C32	−0.3 (3)	N3—Mn1—N5—C10	54.70 (14)
C30—C31—C32—C33	−0.3 (4)	N1—Mn1—N5—C10	−14.98 (13)
C31—C32—C33—C34	0.7 (4)	Cl1—Mn1—N5—C10	161.82 (13)
N9—C29—C34—N10	−0.2 (2)	N2—Mn1—N5—C10	−90.85 (14)
C30—C29—C34—N10	178.56 (19)	N7—Mn1—N5—C16	123.9 (2)
N9—C29—C34—C33	−178.98 (19)	N3—Mn1—N5—C16	−112.11 (19)
C30—C29—C34—C33	−0.2 (3)	N1—Mn1—N5—C16	178.2 (2)
C32—C33—C34—C29	−0.4 (3)	Cl1—Mn1—N5—C16	−5.0 (2)
C32—C33—C34—N10	−178.9 (2)	N2—Mn1—N5—C16	102.34 (19)
C2—C1—N1—C9	77.9 (2)	N5—C10—N6—C11	0.6 (2)
C2—C1—N1—C17	−155.78 (17)	C9—C10—N6—C11	−178.14 (18)
C2—C1—N1—Mn1	−38.91 (18)	C12—C11—N6—C10	179.1 (3)
C10—C9—N1—C1	−136.64 (17)	C16—C11—N6—C10	−0.8 (2)
C10—C9—N1—C17	97.29 (19)	N8—C20—N7—C26	1.1 (2)
C10—C9—N1—Mn1	−21.87 (19)	C19—C20—N7—C26	−177.2 (2)
C18—C17—N1—C1	158.62 (18)	N8—C20—N7—Mn1	−163.37 (14)
C18—C17—N1—C9	−76.0 (2)	C19—C20—N7—Mn1	18.3 (3)
C18—C17—N1—Mn1	43.4 (2)	C25—C26—N7—C20	178.8 (2)
N5—Mn1—N1—C1	138.30 (13)	C21—C26—N7—C20	−0.3 (2)
N7—Mn1—N1—C1	−60.67 (12)	C25—C26—N7—Mn1	−20.3 (4)
N3—Mn1—N1—C1	34.40 (12)	C21—C26—N7—Mn1	160.69 (15)
Cl1—Mn1—N1—C1	101.9 (5)	N5—Mn1—N7—C20	−35.9 (3)
N2—Mn1—N1—C1	−132.95 (13)	N3—Mn1—N7—C20	−160.38 (15)
N5—Mn1—N1—C9	19.90 (12)	N1—Mn1—N7—C20	−87.50 (15)
N7—Mn1—N1—C9	−179.07 (12)	Cl1—Mn1—N7—C20	94.09 (15)
N3—Mn1—N1—C9	−83.99 (13)	N2—Mn1—N7—C20	−13.33 (15)
Cl1—Mn1—N1—C9	−16.4 (5)	N5—Mn1—N7—C26	165.01 (17)
N2—Mn1—N1—C9	108.66 (13)	N3—Mn1—N7—C26	40.50 (19)
N5—Mn1—N1—C17	−102.10 (13)	N1—Mn1—N7—C26	113.38 (19)
N7—Mn1—N1—C17	58.93 (13)	Cl1—Mn1—N7—C26	−65.03 (19)
N3—Mn1—N1—C17	154.01 (14)	N2—Mn1—N7—C26	−172.4 (2)
Cl1—Mn1—N1—C17	−138.5 (4)	N7—C20—N8—C21	−1.5 (3)
N2—Mn1—N1—C17	−13.35 (12)	C19—C20—N8—C21	176.9 (2)
C28—C27—N2—C18	62.6 (2)	C22—C21—N8—C20	−176.8 (3)
C28—C27—N2—C19	−64.3 (2)	C26—C21—N8—C20	1.2 (2)
C28—C27—N2—Mn1	175.86 (15)	N10—C28—N9—C29	0.1 (2)
C17—C18—N2—C27	159.79 (17)	C27—C28—N9—C29	176.31 (19)
C17—C18—N2—C19	−73.1 (2)	C34—C29—N9—C28	0.1 (2)
C17—C18—N2—Mn1	46.13 (18)	C30—C29—N9—C28	−178.5 (2)
C20—C19—N2—C27	−119.4 (2)	N9—C28—N10—C34	−0.3 (2)
C20—C19—N2—C18	113.2 (2)	C27—C28—N10—C34	−176.32 (19)
C20—C19—N2—Mn1	−2.6 (2)	C29—C34—N10—C28	0.3 (2)
N5—Mn1—N2—C27	−59.88 (13)	C33—C34—N10—C28	178.9 (2)
N7—Mn1—N2—C27	128.99 (13)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3B···N10^{i}	0.835 (10)	2.065 (11)	2.884 (3)	167 (3)
N4—H4A···Cl2^{ii}	0.851 (10)	2.308 (11)	3.147 (2)	169 (2)
N8—H8···O3^{iii}	0.855 (10)	1.922 (12)	2.755 (3)	164 (2)
N9—H9···Cl1^{iv}	0.847 (10)	2.485 (15)	3.242 (2)	149 (2)
C19—H19B···Cl1^{iv}	0.97	2.69	3.607 (3)	157
N6—H6A···Cl2	0.843 (10)	2.454 (16)	3.1920 (19)	147 (2)

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

Fig. 1

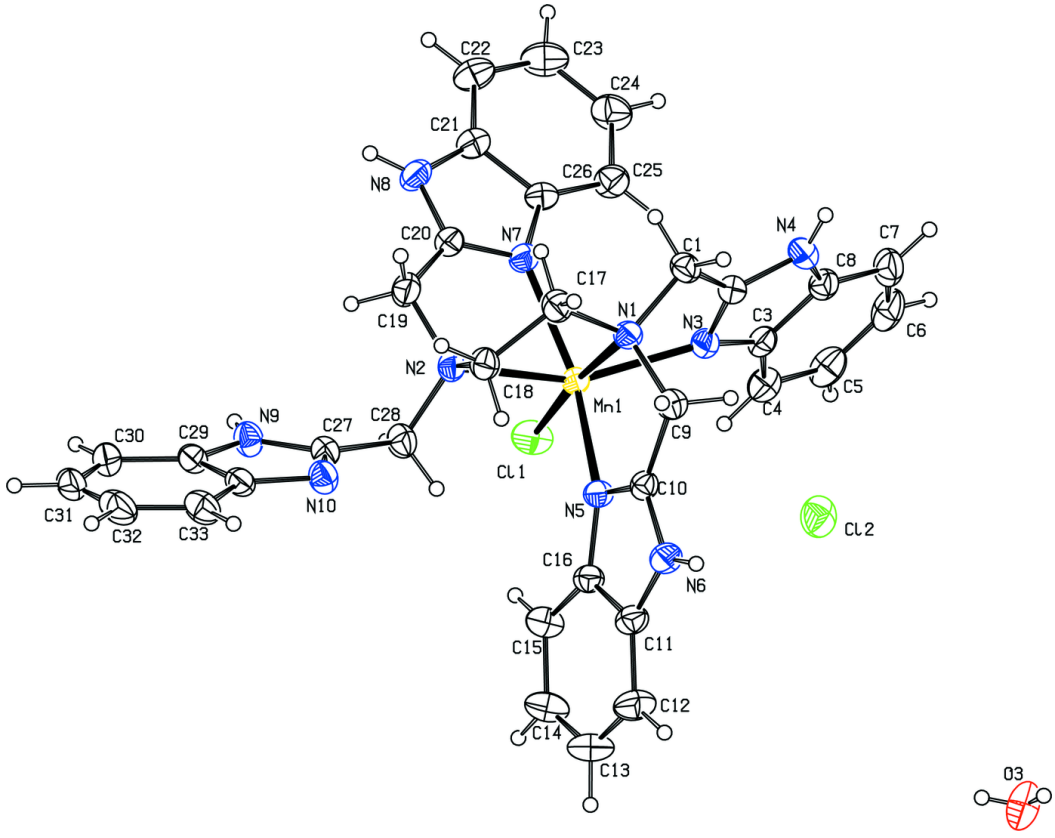

C22
C23
C24
C21
N8
C26
C25
C20
N7
C1
N4
C7
C8
C17
C19
N1
N3
C3
C6
N2
C18
Mn1
C4
C5
C9
C28
N9
C27
C30
C29
Cl1
C10
N5
Cl2
N10
C31
C32
C33
C16
N6
C15
C11
C12
C14
C13
O3

Fig. 2