

## Dichlorido(methanol- $\kappa$ O)[2-(2-pyridyl-methoxy)-1,10-phenanthroline- $\kappa^3$ N,N',N'']manganese(II)

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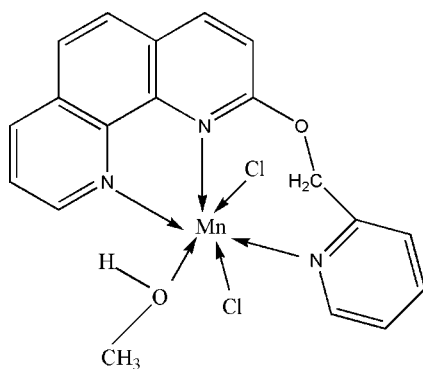
Received 7 June 2008; accepted 19 June 2008

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.090; data-to-parameter ratio = 16.5.

In the title mononuclear complex,  $[\text{MnCl}_2(\text{C}_{18}\text{H}_{13}\text{N}_3\text{O})(\text{CH}_4\text{O})]$ , the  $\text{Mn}^{\text{II}}$  ion assumes a distorted octahedral geometry. There is a  $\pi$ - $\pi$  stacking interaction between the phenanthroline ligand and the pyridine ring of a neighboring complex [centroid-to-centroid distance 3.5518 (13) Å]. The crystal structure also contains weak intermolecular  $\text{O}-\text{H}\cdots\text{Cl}$  hydrogen bonds that link neighboring complex molecules into a one-dimensional chain along the  $b$  axis.

### Related literature

For related structures, see: Liu *et al.* (2008); Li *et al.* (2008).



### Experimental

#### Crystal data

$[\text{MnCl}_2(\text{C}_{18}\text{H}_{13}\text{N}_3\text{O})(\text{CH}_4\text{O})]$   
 $M_r = 445.20$   
 Monoclinic,  $P2_1/n$   
 $a = 10.0390$  (16) Å  
 $b = 13.667$  (2) Å  
 $c = 13.583$  (2) Å  
 $\beta = 92.874$  (2)°

$V = 1861.2$  (5) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.02$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 $0.38 \times 0.18 \times 0.13$  mm

#### Data collection

Bruker SMART APEX CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2008)  
 $T_{\text{min}} = 0.699$ ,  $T_{\text{max}} = 0.879$

10717 measured reflections  
 4048 independent reflections  
 3278 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.033$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.090$   
 $S = 1.01$   
 4048 reflections  
 245 parameters

1 restraint  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.28$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H10}\cdots\text{Cl1}^i$	0.80	2.39	3.1581 (16)	161

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and local programs.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2150).

### References

- Bruker (1997). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Li, H. L. & Liu, Q. S. (2008). *Acta Cryst.* **E64**, m847.  
 Liu, Q. S., Liu, L. D. & Shi, J. M. (2008). *Acta Cryst.* **C64**, m58–m60.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

**supplementary materials**

*Acta Cryst.* (2008). E64, m962 [ doi:10.1107/S1600536808018631 ]

## Dichlorido(methanol- $\kappa O$ )[2-(2-pyridylmethoxy)-1,10-phenanthroline- $\kappa^3 N, N', N''$ ]manganese(II)

H. L. Li and H. Chao

### Comment

Derivatives of 1,10-phenanthroline play an important role in modern coordination chemistry and many complexes have been reported with different substituent groups (Li *et al.* 2008; Liu *et al.* 2008), but no complex with (pyridyl-2-yl)methoxy as substituent has been published. We report here the crystal structure of the title complex, Fig1.

Compound (I) is a monomer, in which the Mn atom adopts a distorted octahedral geometry completed by two N-atom donors from 1,10-phenanthroline, one N atom from pyridine ring, two Cl atom and one O atom from methanol molecule. In neighboring monomers, there is a strong  $\pi$ - $\pi$  interaction between 1,10-phenanthroline ligand and pyridine ring with a centroid-to-centroid distance of 3.5518 (13) Å. In addition, the crystal structure contains O—H $\cdots$ Cl hydrogen bonds that made the neighboring complexes connect into a one-dimensional chain along *b* axis as shown in Fig. 2.

### Experimental

10 ml methanol solution of (2-((pyridin-2-yl)methoxy)-1,10-phenanthroline (0.1200 g, 0.418 mmol) was added into 15 ml methanol solution of MnCl<sub>2</sub>·4H<sub>2</sub>O (0.0827 g, 0.418 mmol) and the mixture was stirred for a few minutes. The colorless single crystals were obtained after the filtrate had been allowed to stand at room temperature for a week.

### Refinement

H atoms from the hydroxyl group of methanol was located in a difference Fourier map with O—H = 0.80 Å and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ ; Other H atoms were placed in calculated positions with C—H = 0.96 Å for methyl group, C—H = 0.97 Å for methylene group and C—H = 0.93 Å for other H atoms, and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl group and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for other H atoms.

### Figures

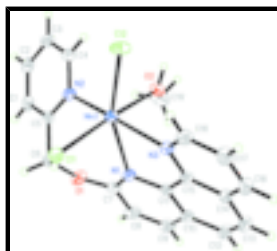


Fig. 1. Structure of the title complex with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

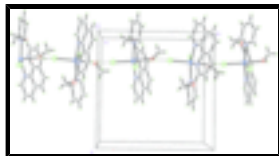


Fig. 2. A view of the packing in the crystal structure. Intermolecular Hydrogen bonds as dashed lines.

## Dichlorido(methanol- $\kappa$ O)[2-(2-pyridylmethoxy)-1,10-phenanthroline- $\kappa^3$ N,N',N'']manganese(II)

### Crystal data

[MnCl<sub>2</sub>(C<sub>18</sub>H<sub>13</sub>N<sub>3</sub>O)(CH<sub>4</sub>O)]

$M_r = 445.20$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 10.0390$  (16) Å

$b = 13.667$  (2) Å

$c = 13.583$  (2) Å

$\beta = 92.874$  (2)°

$V = 1861.2$  (5) Å<sup>3</sup>

$Z = 4$

$F_{000} = 908$

$D_x = 1.589$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 3203 reflections

$\theta = 2.5$ – $25.7$ °

$\mu = 1.02$  mm<sup>-1</sup>

$T = 298$  (2) K

Block, colorless

$0.38 \times 0.18 \times 0.13$  mm

### Data collection

Bruker SMART APEX CCD  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 2008)

$T_{\min} = 0.699$ ,  $T_{\max} = 0.879$

10717 measured reflections

4048 independent reflections

3278 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\text{max}} = 27.0$ °

$\theta_{\text{min}} = 2.1$ °

$h = -12 \rightarrow 12$

$k = -13 \rightarrow 17$

$l = -15 \rightarrow 17$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.090$

$S = 1.01$

4048 reflections

245 parameters

1 restraint

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.29$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.25$  e Å<sup>-3</sup>

Extinction correction: none

Primary atom site location: structure-invariant direct methods

*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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1526 (2)	0.79472 (15)	0.58696 (17)	0.0372 (5)
H1	0.0945	0.7746	0.6342	0.045*
C2	0.2736 (2)	0.83666 (16)	0.61481 (17)	0.0409 (6)
H2	0.2988	0.8449	0.6811	0.049*
C3	0.3567 (2)	0.86618 (16)	0.54275 (17)	0.0399 (5)
H3	0.4390	0.8944	0.5596	0.048*
C4	0.3163 (2)	0.85338 (16)	0.44621 (17)	0.0373 (5)
H4	0.3726	0.8743	0.3981	0.045*
C5	0.1191 (2)	0.78311 (14)	0.48767 (16)	0.0308 (5)
C6	-0.01179 (19)	0.73705 (16)	0.45422 (16)	0.0355 (5)
H6A	-0.0034	0.7067	0.3903	0.043*
H6B	-0.0349	0.6865	0.5005	0.043*
C7	-0.1580 (2)	0.84967 (15)	0.36073 (17)	0.0331 (5)
C8	-0.2826 (2)	0.89726 (17)	0.36516 (18)	0.0409 (6)
H8	-0.3257	0.9010	0.4241	0.049*
C9	-0.3375 (2)	0.93711 (16)	0.28180 (19)	0.0420 (6)
H9	-0.4195	0.9687	0.2829	0.050*
C10	-0.2712 (2)	0.93111 (14)	0.19319 (18)	0.0361 (5)
C11	-0.14608 (19)	0.88455 (14)	0.19628 (16)	0.0293 (5)
C12	-0.3287 (2)	0.96695 (16)	0.1018 (2)	0.0461 (6)
H12	-0.4100	0.9996	0.1010	0.055*
C13	-0.2673 (2)	0.95437 (17)	0.0167 (2)	0.0476 (6)
H13	-0.3079	0.9764	-0.0422	0.057*
C14	-0.1406 (2)	0.90753 (15)	0.01644 (17)	0.0375 (5)
C15	-0.0780 (2)	0.87583 (14)	0.10597 (16)	0.0309 (5)
C16	-0.0753 (3)	0.88884 (18)	-0.07041 (18)	0.0499 (7)
H16	-0.1147	0.9070	-0.1311	0.060*
C17	0.0457 (3)	0.84415 (18)	-0.06574 (18)	0.0474 (6)
H17	0.0891	0.8303	-0.1230	0.057*
C18	0.1037 (2)	0.81939 (16)	0.02599 (17)	0.0395 (5)
H18	0.1878	0.7907	0.0286	0.047*

## supplementary materials

C19	0.0884 (3)	1.03698 (18)	0.3451 (2)	0.0593 (7)
H19A	-0.0056	1.0389	0.3283	0.089*
H19B	0.1245	1.1019	0.3419	0.089*
H19C	0.1031	1.0117	0.4106	0.089*
Cl1	0.10996 (5)	0.62442 (4)	0.24263 (4)	0.03925 (15)
Cl2	0.36834 (5)	0.82286 (5)	0.19848 (5)	0.04570 (17)
Mn1	0.14453 (3)	0.80494 (2)	0.25537 (2)	0.02795 (11)
N1	-0.08860 (16)	0.84415 (12)	0.28120 (13)	0.0288 (4)
N2	0.19883 (16)	0.81198 (12)	0.41697 (13)	0.0314 (4)
N3	0.04509 (16)	0.83459 (12)	0.10973 (13)	0.0304 (4)
O1	-0.11631 (14)	0.81011 (12)	0.44771 (12)	0.0424 (4)
O2	0.15254 (14)	0.97535 (10)	0.27729 (11)	0.0372 (4)
H10	0.2227	1.0012	0.2676	0.056*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0430 (13)	0.0372 (13)	0.0317 (12)	0.0068 (10)	0.0055 (10)	0.0042 (9)
C2	0.0529 (15)	0.0374 (13)	0.0315 (13)	0.0060 (11)	-0.0074 (11)	-0.0010 (10)
C3	0.0361 (12)	0.0417 (14)	0.0408 (14)	-0.0015 (10)	-0.0076 (10)	-0.0019 (10)
C4	0.0295 (11)	0.0426 (13)	0.0397 (14)	-0.0022 (9)	-0.0004 (10)	0.0040 (10)
C5	0.0294 (11)	0.0290 (11)	0.0340 (12)	0.0056 (8)	0.0021 (9)	0.0025 (9)
C6	0.0322 (11)	0.0375 (12)	0.0372 (13)	0.0016 (9)	0.0063 (9)	0.0059 (10)
C7	0.0260 (10)	0.0348 (12)	0.0386 (13)	-0.0033 (9)	0.0006 (9)	-0.0047 (9)
C8	0.0259 (11)	0.0466 (14)	0.0508 (15)	0.0023 (10)	0.0083 (10)	-0.0090 (11)
C9	0.0253 (11)	0.0357 (13)	0.0647 (17)	0.0054 (9)	-0.0015 (11)	-0.0082 (11)
C10	0.0283 (11)	0.0253 (11)	0.0539 (15)	0.0003 (9)	-0.0058 (10)	-0.0022 (10)
C11	0.0261 (10)	0.0225 (10)	0.0389 (13)	-0.0022 (8)	-0.0037 (9)	-0.0016 (8)
C12	0.0345 (12)	0.0364 (13)	0.0657 (18)	0.0071 (10)	-0.0153 (12)	0.0040 (12)
C13	0.0455 (14)	0.0414 (14)	0.0538 (17)	0.0008 (11)	-0.0184 (12)	0.0109 (11)
C14	0.0389 (12)	0.0306 (11)	0.0420 (14)	-0.0058 (10)	-0.0092 (10)	0.0066 (10)
C15	0.0290 (11)	0.0253 (11)	0.0376 (13)	-0.0056 (8)	-0.0043 (9)	0.0005 (9)
C16	0.0564 (16)	0.0565 (16)	0.0355 (15)	-0.0093 (13)	-0.0107 (12)	0.0141 (11)
C17	0.0545 (16)	0.0569 (16)	0.0309 (13)	-0.0074 (13)	0.0024 (11)	0.0023 (11)
C18	0.0364 (12)	0.0465 (14)	0.0356 (13)	-0.0016 (10)	0.0030 (10)	-0.0020 (10)
C19	0.0622 (17)	0.0401 (15)	0.078 (2)	-0.0018 (12)	0.0270 (15)	-0.0142 (13)
Cl1	0.0355 (3)	0.0310 (3)	0.0508 (4)	0.0014 (2)	-0.0029 (2)	-0.0018 (2)
Cl2	0.0283 (3)	0.0637 (4)	0.0460 (4)	-0.0058 (3)	0.0106 (2)	-0.0148 (3)
Mn1	0.02338 (17)	0.03248 (19)	0.02796 (19)	0.00096 (12)	0.00103 (13)	-0.00058 (13)
N1	0.0243 (9)	0.0298 (9)	0.0322 (10)	0.0001 (7)	-0.0003 (7)	-0.0021 (7)
N2	0.0266 (9)	0.0361 (10)	0.0313 (10)	-0.0010 (7)	0.0000 (8)	0.0022 (7)
N3	0.0273 (9)	0.0324 (10)	0.0312 (10)	-0.0013 (7)	-0.0004 (7)	0.0011 (7)
O1	0.0303 (8)	0.0628 (11)	0.0345 (9)	0.0104 (7)	0.0074 (7)	0.0018 (7)
O2	0.0357 (8)	0.0323 (8)	0.0443 (9)	-0.0042 (6)	0.0076 (7)	-0.0018 (7)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C1—C2	1.379 (3)	C12—C13	1.347 (3)
C1—C5	1.382 (3)	C12—H12	0.9300

C1—H1	0.9300	C13—C14	1.424 (3)
C2—C3	1.377 (3)	C13—H13	0.9300
C2—H2	0.9300	C14—C16	1.402 (3)
C3—C4	1.364 (3)	C14—C15	1.409 (3)
C3—H3	0.9300	C15—N3	1.357 (3)
C4—N2	1.350 (3)	C16—C17	1.358 (3)
C4—H4	0.9300	C16—H16	0.9300
C5—N2	1.340 (3)	C17—C18	1.390 (3)
C5—C6	1.507 (3)	C17—H17	0.9300
C6—O1	1.448 (2)	C18—N3	1.323 (3)
C6—H6A	0.9700	C18—H18	0.9300
C6—H6B	0.9700	C19—O2	1.425 (3)
C7—N1	1.316 (3)	C19—H19A	0.9600
C7—O1	1.347 (3)	C19—H19B	0.9600
C7—C8	1.414 (3)	C19—H19C	0.9600
C8—C9	1.349 (3)	Cl1—Mn1	2.4961 (7)
C8—H8	0.9300	Cl2—Mn1	2.4248 (7)
C9—C10	1.407 (3)	Mn1—N3	2.2082 (18)
C9—H9	0.9300	Mn1—N2	2.2370 (18)
C10—C11	1.407 (3)	Mn1—O2	2.3487 (14)
C10—C12	1.430 (3)	Mn1—N1	2.4434 (17)
C11—N1	1.379 (3)	O2—H10	0.8048
C11—C15	1.439 (3)		
C2—C1—C5	118.9 (2)	N3—C15—C11	118.23 (18)
C2—C1—H1	120.6	C14—C15—C11	119.99 (19)
C5—C1—H1	120.6	C17—C16—C14	119.8 (2)
C3—C2—C1	118.9 (2)	C17—C16—H16	120.1
C3—C2—H2	120.6	C14—C16—H16	120.1
C1—C2—H2	120.6	C16—C17—C18	119.0 (2)
C4—C3—C2	119.0 (2)	C16—C17—H17	120.5
C4—C3—H3	120.5	C18—C17—H17	120.5
C2—C3—H3	120.5	N3—C18—C17	123.2 (2)
N2—C4—C3	123.3 (2)	N3—C18—H18	118.4
N2—C4—H4	118.3	C17—C18—H18	118.4
C3—C4—H4	118.3	O2—C19—H19A	109.5
N2—C5—C1	122.74 (19)	O2—C19—H19B	109.5
N2—C5—C6	116.75 (19)	H19A—C19—H19B	109.5
C1—C5—C6	120.5 (2)	O2—C19—H19C	109.5
O1—C6—C5	110.41 (17)	H19A—C19—H19C	109.5
O1—C6—H6A	109.6	H19B—C19—H19C	109.5
C5—C6—H6A	109.6	N3—Mn1—N2	161.46 (6)
O1—C6—H6B	109.6	N3—Mn1—O2	86.71 (6)
C5—C6—H6B	109.6	N2—Mn1—O2	80.09 (6)
H6A—C6—H6B	108.1	N3—Mn1—Cl2	94.62 (5)
N1—C7—O1	122.89 (18)	N2—Mn1—Cl2	97.14 (5)
N1—C7—C8	124.5 (2)	O2—Mn1—Cl2	85.06 (4)
O1—C7—C8	112.6 (2)	N3—Mn1—N1	72.25 (6)
C9—C8—C7	118.4 (2)	N2—Mn1—N1	92.16 (6)
C9—C8—H8	120.8	O2—Mn1—N1	77.95 (5)

## supplementary materials

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C7—C8—H8	120.8	C12—Mn1—N1	158.93 (5)
C8—C9—C10	120.2 (2)	N3—Mn1—C11	93.68 (5)
C8—C9—H9	119.9	N2—Mn1—C11	97.86 (5)
C10—C9—H9	119.9	O2—Mn1—C11	173.00 (4)
C11—C10—C9	117.5 (2)	C12—Mn1—C11	101.86 (2)
C11—C10—C12	120.1 (2)	N1—Mn1—C11	95.50 (4)
C9—C10—C12	122.4 (2)	C7—N1—C11	116.55 (17)
N1—C11—C10	122.8 (2)	C7—N1—Mn1	132.87 (14)
N1—C11—C15	118.89 (17)	C11—N1—Mn1	109.35 (13)
C10—C11—C15	118.28 (19)	C5—N2—C4	117.19 (19)
C13—C12—C10	121.3 (2)	C5—N2—Mn1	124.45 (13)
C13—C12—H12	119.4	C4—N2—Mn1	118.23 (14)
C10—C12—H12	119.4	C18—N3—C15	118.45 (19)
C12—C13—C14	120.5 (2)	C18—N3—Mn1	122.74 (14)
C12—C13—H13	119.8	C15—N3—Mn1	118.68 (14)
C14—C13—H13	119.8	C7—O1—C6	121.52 (17)
C16—C14—C15	117.6 (2)	C19—O2—Mn1	130.86 (14)
C16—C14—C13	122.7 (2)	C19—O2—H10	105.9
C15—C14—C13	119.7 (2)	Mn1—O2—H10	116.0
N3—C15—C14	121.8 (2)		
C5—C1—C2—C3	0.5 (3)	C11—Mn1—N1—C7	87.71 (18)
C1—C2—C3—C4	0.3 (3)	N3—Mn1—N1—C11	-13.64 (12)
C2—C3—C4—N2	-0.8 (3)	N2—Mn1—N1—C11	156.13 (12)
C2—C1—C5—N2	-0.8 (3)	O2—Mn1—N1—C11	76.75 (12)
C2—C1—C5—C6	179.61 (19)	C12—Mn1—N1—C11	39.8 (2)
N2—C5—C6—O1	-93.6 (2)	C11—Mn1—N1—C11	-105.76 (12)
C1—C5—C6—O1	86.0 (2)	C1—C5—N2—C4	0.4 (3)
N1—C7—C8—C9	2.4 (3)	C6—C5—N2—C4	179.96 (18)
O1—C7—C8—C9	-177.8 (2)	C1—C5—N2—Mn1	-175.49 (14)
C7—C8—C9—C10	-0.1 (3)	C6—C5—N2—Mn1	4.1 (2)
C8—C9—C10—C11	-1.4 (3)	C3—C4—N2—C5	0.4 (3)
C8—C9—C10—C12	176.2 (2)	C3—C4—N2—Mn1	176.55 (17)
C9—C10—C11—N1	1.0 (3)	N3—Mn1—N2—C5	67.7 (3)
C12—C10—C11—N1	-176.65 (18)	O2—Mn1—N2—C5	112.92 (16)
C9—C10—C11—C15	178.68 (18)	C12—Mn1—N2—C5	-163.39 (15)
C12—C10—C11—C15	1.0 (3)	N1—Mn1—N2—C5	35.55 (16)
C11—C10—C12—C13	2.2 (3)	C11—Mn1—N2—C5	-60.30 (16)
C9—C10—C12—C13	-175.4 (2)	N3—Mn1—N2—C4	-108.1 (2)
C10—C12—C13—C14	-2.1 (3)	O2—Mn1—N2—C4	-62.89 (15)
C12—C13—C14—C16	177.1 (2)	C12—Mn1—N2—C4	20.79 (15)
C12—C13—C14—C15	-1.2 (3)	N1—Mn1—N2—C4	-140.26 (15)
C16—C14—C15—N3	4.4 (3)	C11—Mn1—N2—C4	123.88 (15)
C13—C14—C15—N3	-177.20 (19)	C17—C18—N3—C15	0.4 (3)
C16—C14—C15—C11	-174.03 (19)	C17—C18—N3—Mn1	-175.35 (17)
C13—C14—C15—C11	4.4 (3)	C14—C15—N3—C18	-3.7 (3)
N1—C11—C15—N3	-4.9 (3)	C11—C15—N3—C18	174.77 (18)
C10—C11—C15—N3	177.29 (17)	C14—C15—N3—Mn1	172.26 (14)
N1—C11—C15—C14	173.53 (17)	C11—C15—N3—Mn1	-9.3 (2)
C10—C11—C15—C14	-4.2 (3)	N2—Mn1—N3—C18	154.10 (19)



C15—C14—C16—C17	-1.8 (3)	O2—Mn1—N3—C18	109.61 (17)
C13—C14—C16—C17	179.8 (2)	Cl2—Mn1—N3—C18	24.84 (16)
C14—C16—C17—C18	-1.2 (4)	N1—Mn1—N3—C18	-172.00 (18)
C16—C17—C18—N3	2.0 (4)	Cl1—Mn1—N3—C18	-77.39 (16)
O1—C7—N1—C11	177.43 (18)	N2—Mn1—N3—C15	-21.6 (3)
C8—C7—N1—C11	-2.8 (3)	O2—Mn1—N3—C15	-66.13 (14)
O1—C7—N1—Mn1	-16.8 (3)	Cl2—Mn1—N3—C15	-150.90 (14)
C8—C7—N1—Mn1	162.96 (16)	N1—Mn1—N3—C15	12.26 (13)
C10—C11—N1—C7	1.1 (3)	Cl1—Mn1—N3—C15	106.87 (14)
C15—C11—N1—C7	-176.61 (17)	N1—C7—O1—C6	-16.9 (3)
C10—C11—N1—Mn1	-167.94 (15)	C8—C7—O1—C6	163.28 (18)
C15—C11—N1—Mn1	14.4 (2)	C5—C6—O1—C7	100.3 (2)
N3—Mn1—N1—C7	179.82 (19)	N3—Mn1—O2—C19	114.2 (2)
N2—Mn1—N1—C7	-10.41 (18)	N2—Mn1—O2—C19	-52.8 (2)
O2—Mn1—N1—C7	-89.79 (18)	Cl2—Mn1—O2—C19	-150.9 (2)
Cl2—Mn1—N1—C7	-126.75 (17)	N1—Mn1—O2—C19	41.6 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H10...Cl1 <sup>i</sup>	0.80	2.39	3.1581 (16)	161

Symmetry codes: (i)  $-x+1/2, y+1/2, -z+1/2$ .

Fig. 1

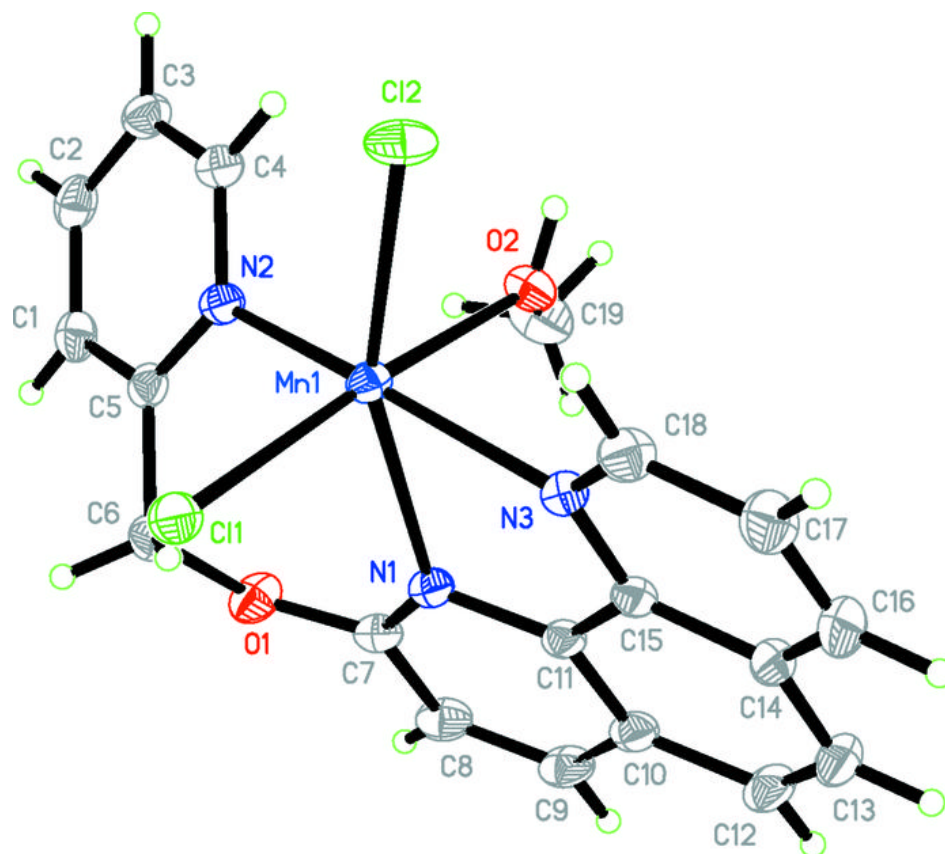


Fig. 2

