

cis-Dichloridobis(5,5'-dimethyl-2,2'-bipyridine)manganese(II) 2.5-hydrate

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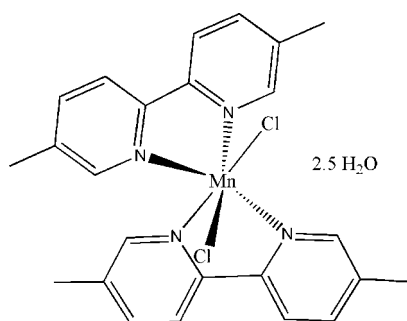
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in solvent or counterion; R factor = 0.043; wR factor = 0.150; data-to-parameter ratio = 21.4.

The metal site in the title compound $[\text{MnCl}_2(\text{C}_{12}\text{H}_{12}\text{N}_2)_2] \cdot 2.5\text{H}_2\text{O}$ has a distorted octahedral geometry, coordinated by four N atoms of two 5,5'-dimethyl-2,2'-dipyridine ligands and two Cl atoms. Two and a half water molecules of hydration per complex unit are observed in the crystal structure. The compounds extend along the c axis with $\text{O}-\text{H}\cdots\text{Cl}$, $\text{O}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and $\pi-\pi$ interactions [centroid-centroid distance = $3.70(2)$ Å] contributing substantially to the crystal packing. The Mn and one of the water O atoms, the latter being half-occupied, are located on special positions, in this case a rotation axis of order 2.

Related literature

For the structures and applications of bipyridine and analogous ligands, see: Hazell (2004); Bakir *et al.* (1992); Cordes *et al.* (1982); Hung-Low *et al.* (2009). For the structure and applications of 5,5'-dimethyl-2,2'-dipyridine, see: Marandi *et al.* (2009); van Albada *et al.* (2005). For weak intermolecular interactions, see: Calhorda (2000); Desiraju (1996); Janiak (2000).



Experimental

Crystal data

$[\text{MnCl}_2(\text{C}_{12}\text{H}_{12}\text{N}_2)_2] \cdot 2.5\text{H}_2\text{O}$
 $M_r = 539.35$
Monoclinic, $C2/c$
 $a = 18.6703(9)$ Å
 $b = 14.0598(4)$ Å
 $c = 12.0536(7)$ Å
 $\beta = 122.430(7)^\circ$

$V = 2670.6(2)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.72$ mm⁻¹
 $T = 293$ K
 $0.47 \times 0.35 \times 0.34$ mm

Data collection

Oxford Diffraction Xcalibur Atlas Gemini ultra diffractometer
Absorption correction: analytical [CrysAlis PRO (Oxford Diffraction, 2008) based on expressions derived by Clark & Reid (1995)]
 $T_{\min} = 0.470$, $T_{\max} = 0.697$

11860 measured reflections
3317 independent reflections
2499 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.150$
 $S = 1.09$
3317 reflections

155 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.72$ e Å⁻³
 $\Delta\rho_{\min} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1A}\cdots\text{Cl1}$	0.84	2.42	3.243 (3)	168
$\text{O1}-\text{H1B}\cdots\text{Cl1}^i$	0.81	2.73	3.358 (4)	136
$\text{O2}-\text{H2A}\cdots\text{O1}$	0.86	2.16	2.951 (6)	153
$\text{C3}-\text{H3}\cdots\text{O1}^{\text{ii}}$	0.93	2.49	3.257 (5)	140
$\text{C6}-\text{H6A}\cdots\text{Cl1}^i$	0.96	2.79	3.717 (4)	162

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

Data collection: CrysAlis PRO (Oxford Diffraction, 2008); cell refinement: CrysAlis PRO; data reduction: CrysAlis PRO; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2285).

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supplementary materials

Acta Cryst. (2011). E67, m906-m907 [doi:10.1107/S1600536811021805]

***cis*-Dichloridobis(5,5'-dimethyl-2,2'-bipyridine)manganese(II) 2.5-hydrate**

L. B. Lopes, C. C. Corrêa and R. Diniz

Comment

Bipyridine and analogous ligands are commonly used in the formation of different complexes with a general variety of transition metals (Hazell, 2004; Bakir *et al.*, 1992; Cordes *et al.*, 1982; Hung-Low *et al.*, 2009;). The ligand 5,5'-Dimethyl-2,2'-dipyridine (abbreviated as dmdpy) acts as a chelator and usually gives rise to monomeric compounds (Marandi *et al.*, 2009). Only a limited number of X-ray crystal structures with the ligand dmdpy has been published (van Albada *et al.*, 2005). In this study we used the ligand 5,5'-dimethyl-2,2'-dipyridine and manganese chloride tetrahydrate. This mixture resulted in the compound $[\text{Mn}(\text{C}_{12}\text{H}_{12}\text{N}_2)_2\text{Cl}_2] \times 2.5 \text{ H}_2\text{O}$ (Scheme 1).

The molecular structure of the complex unit of the title compound $[\text{Mn}(\text{C}_{12}\text{H}_{12}\text{N}_2)_2\text{Cl}_2] \times 2.5 \text{ H}_2\text{O}$ is shown in Figure 1. The metal site is coordinated by four nitrogen atoms N1, N2, N1ⁱ and N2ⁱ of the ligand dmdpy and two chlorides Cl1 and Cl1ⁱ adopting a distorted octahedral geometry as evidenced by the Mn—N1 distances (2.3111 (19) Å), Mn—N2 (2.245 (2) Å) and Mn—Cl1 (2.4702 (6) Å). The Mn atom is located in a special position, which in this case is a rotation axis of order 2.

The compound crystallizes in the monoclinic system and its unit cell is shown in Figure 2. The compound $[\text{Mn}(\text{C}_{12}\text{H}_{12}\text{N}_2)_2\text{Cl}_2] \times 2.5 \text{ H}_2\text{O}$ is a complex that stretches along the crystallographic *c* axis with the molecular entities being interconnected by weak hydrogen bonds (Desiraju, 1996; Calhorda, 2000) shown in Figure 2. These hydrogen bonds are formed by the interaction between oxygen atoms of water molecules O1 and O2 and the chlorine atom Cl1 which is coordinated to the metal. The distances O1—O2 and O1—Cl1 are 2.951 (6) Å and 3.243 (3) Å, respectively. π - π interactions between aromatic rings of the nitrogen ligand dmdpy are also shown in Figure 2. These interactions contribute substantially to the crystal packing (Janiak, 2000). In this compound the centroid-centroid distance is 3.70 (2) Å, and there was a substantial overlap between the aromatic rings of the ligand dmdpy, being centroid-plane distance of 3.45 (1) Å and the horizontal displacement of 1.37 (2) Å.

Experimental

All chemicals were obtained commercially and used without further purification. The complex was synthesized by mixing of 0.38 mmol of dmdpy dissolved in ethanol and 0.38 mmol of $\text{MnCl}_2 \times 4 \text{ H}_2\text{O}$ dissolved in water. The mixture was placed under agitation for 40 h. After a few weeks, yellow single crystals suitable for the analysis of X-ray diffraction were obtained (yield: 39%).

Refinement

H atoms were positioned geometrically and refined using the riding model approximation with C—H = 0.95 Å, and $U_{\text{iso}}(\text{H})$ was refined in group. H atoms of water molecule were located from electron density map, fixed in these positions and assigned the same isotropic displacement parameters for all H atoms.

Figures

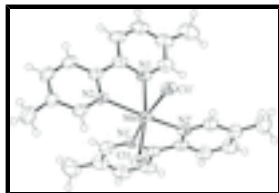


Fig. 1. Molecular structure of the complex unit of the title compound $[\text{Mn}(\text{C}_{12}\text{H}_{12}\text{N}_2)_2\text{Cl}_2] \times 2.5 \text{ H}_2\text{O}$. Water molecules were omitted for better visualization. Symmetry code: $i (1 - x, y, 1/2 - z)$.

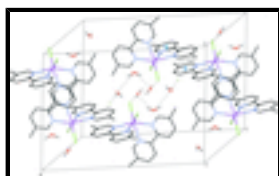


Fig. 2. Unit cell of the compound $[\text{Mn}(\text{C}_{12}\text{H}_{12}\text{N}_2)_2\text{Cl}_2] \times 2.5 \text{ H}_2\text{O}$ ($z = 4$), hydrogen bonds chain extending along the c axis and π - π interactions between the rings aromatic ligand dm-dpy are depicted as dashed lines.

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Crystal data

$[\text{MnCl}_2(\text{C}_{12}\text{H}_{12}\text{N}_2)_2] \cdot 2.5 \text{ H}_2\text{O}$

$M_r = 539.35$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 18.6703 (9) \text{ \AA}$

$b = 14.0598 (4) \text{ \AA}$

$c = 12.0536 (7) \text{ \AA}$

$\beta = 122.430 (7)^\circ$

$V = 2670.6 (2) \text{ \AA}^3$

$Z = 4$

$F(000) = 1120$

$D_x = 1.341 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 6304 reflections

$\theta = 2.9\text{--}29.4^\circ$

$\mu = 0.72 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Prismatic, yellow

$0.47 \times 0.35 \times 0.34 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur Atlas Gemini ultra diffractometer

Radiation source: Enhance (Mo) X-ray Source graphite

Detector resolution: $10.4186 \text{ pixels mm}^{-1}$

ω scans

Absorption correction: analytical

[*CrysAlis PRO* (Oxford Diffraction, 2008) based on expressions derived by Clark & Reid (1995)]

$T_{\min} = 0.470$, $T_{\max} = 0.697$

11860 measured reflections

3317 independent reflections

2499 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 29.4^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -25 \rightarrow 23$

$k = -14 \rightarrow 18$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

$$R[F^2 > 2\sigma(F^2)] = 0.043$$

$$wR(F^2) = 0.150$$

$$S = 1.09$$

3317 reflections

155 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.094P)^2 + 0.4813P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.72 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL*

Absolute structure: no

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mn	0.5000	0.31073 (3)	0.2500	0.03326 (18)	
Cl1	0.56731 (3)	0.43196 (4)	0.42532 (6)	0.0429 (2)	
N1	0.42155 (12)	0.19415 (12)	0.0968 (2)	0.0391 (4)	
N2	0.38759 (11)	0.27687 (13)	0.26398 (18)	0.0359 (4)	
C1	0.37348 (15)	0.32044 (16)	0.3488 (2)	0.0407 (5)	
H1	0.4120	0.3667	0.4034	0.049*	
C5	0.33239 (14)	0.20969 (15)	0.1835 (2)	0.0368 (5)	
C4	0.26252 (15)	0.18577 (17)	0.1891 (3)	0.0466 (6)	
H4	0.2249	0.1393	0.1334	0.056*	
C2	0.30477 (16)	0.30103 (17)	0.3606 (3)	0.0447 (6)	
C3	0.24897 (16)	0.2312 (2)	0.2779 (3)	0.0523 (7)	
H3	0.2023	0.2150	0.2824	0.063*	
C7	0.35069 (14)	0.16493 (14)	0.0903 (2)	0.0386 (5)	
C8	0.29693 (17)	0.09802 (17)	-0.0022 (2)	0.0511 (6)	
H8	0.2475	0.0794	-0.0072	0.061*	
C11	0.43965 (16)	0.15765 (17)	0.0132 (2)	0.0477 (6)	
H11	0.4884	0.1792	0.0182	0.057*	
C10	0.39085 (19)	0.08913 (18)	-0.0818 (3)	0.0552 (7)	
C9	0.3180 (2)	0.05955 (18)	-0.0865 (3)	0.0580 (7)	
H9	0.2833	0.0135	-0.1470	0.070*	
C6	0.2939 (2)	0.3543 (2)	0.4579 (3)	0.0689 (9)	
H6A	0.3391	0.3995	0.5036	0.103*	
H6B	0.2950	0.3105	0.5199	0.103*	

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H6C	0.2405	0.3872	0.4128	0.103*	
C12	0.4172 (2)	0.0531 (2)	-0.1719 (3)	0.0782 (10)	
H12A	0.4692	0.0834	-0.1506	0.117*	
H12B	0.3737	0.0673	-0.2613	0.117*	
H12C	0.4257	-0.0145	-0.1614	0.117*	
O1	0.5956 (2)	0.4141 (2)	0.7145 (3)	0.1311 (14)	
H1A	0.5803	0.4187	0.6356	0.197*	
H1B	0.5699	0.4548	0.7272	0.197*	
O2	0.5000	0.2629 (5)	0.7500	0.112 (3)	0.50
H2A	0.5382	0.2904	0.7422	0.168*	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn	0.0241 (3)	0.0282 (3)	0.0388 (3)	0.000	0.0111 (2)	0.000
C11	0.0341 (3)	0.0394 (3)	0.0431 (3)	-0.0026 (2)	0.0127 (3)	-0.0082 (2)
N1	0.0330 (10)	0.0304 (9)	0.0398 (10)	0.0005 (7)	0.0101 (8)	-0.0025 (7)
N2	0.0286 (9)	0.0321 (9)	0.0364 (9)	-0.0054 (7)	0.0105 (8)	0.0017 (7)
C1	0.0339 (11)	0.0390 (12)	0.0416 (12)	-0.0089 (9)	0.0153 (10)	-0.0011 (9)
C5	0.0307 (11)	0.0281 (10)	0.0350 (11)	-0.0042 (8)	0.0067 (9)	0.0071 (8)
C4	0.0370 (12)	0.0404 (13)	0.0477 (14)	-0.0143 (10)	0.0130 (11)	0.0020 (10)
C2	0.0415 (13)	0.0437 (13)	0.0475 (14)	-0.0073 (10)	0.0230 (11)	0.0053 (10)
C3	0.0403 (13)	0.0560 (16)	0.0563 (15)	-0.0153 (12)	0.0231 (12)	0.0050 (12)
C7	0.0364 (11)	0.0249 (9)	0.0354 (11)	-0.0015 (9)	0.0065 (9)	0.0046 (8)
C8	0.0501 (14)	0.0383 (12)	0.0428 (13)	-0.0147 (11)	0.0102 (12)	-0.0001 (10)
C11	0.0422 (13)	0.0402 (12)	0.0487 (14)	0.0020 (10)	0.0163 (11)	-0.0068 (11)
C10	0.0615 (17)	0.0373 (13)	0.0454 (14)	0.0039 (12)	0.0146 (13)	-0.0061 (10)
C9	0.0666 (18)	0.0354 (13)	0.0454 (15)	-0.0120 (12)	0.0125 (13)	-0.0077 (10)
C6	0.0645 (18)	0.080 (2)	0.079 (2)	-0.0247 (17)	0.0493 (17)	-0.0175 (17)
C12	0.092 (3)	0.068 (2)	0.060 (2)	0.0055 (18)	0.0315 (19)	-0.0192 (15)
O1	0.166 (3)	0.157 (3)	0.110 (2)	0.121 (3)	0.101 (2)	0.068 (2)
O2	0.092 (5)	0.047 (4)	0.135 (7)	0.000	0.020 (5)	0.000

Geometric parameters (\AA , $^\circ$)

Mn—C11	2.4702 (6)	C7—C8	1.391 (3)
Mn—N1	2.3111 (19)	C8—C9	1.382 (5)
Mn—N2	2.245 (2)	C9—C10	1.394 (6)
O1—H1B	0.8100	C10—C12	1.502 (6)
O1—H1A	0.8400	C10—C11	1.397 (4)
O2—H2A	0.8600	C1—H1	0.9300
O2—H2A ⁱ	0.8600	C3—H3	0.9300
N1—C11	1.326 (4)	C4—H4	0.9300
N1—C7	1.347 (3)	C6—H6A	0.9600
N2—C5	1.350 (2)	C6—H6B	0.9600
N2—C1	1.334 (3)	C6—H6C	0.9600
C1—C2	1.391 (5)	C8—H8	0.9300
C2—C3	1.389 (4)	C9—H9	0.9300

C2—C6	1.494 (5)	C11—H11	0.9300
C3—C4	1.381 (4)	C12—H12B	0.9600
C4—C5	1.383 (4)	C12—H12C	0.9600
C5—C7	1.480 (3)	C12—H12A	0.9600
C11…C1	3.581 (3)	O1 ^{iv} …C3 ⁱⁱ	3.257 (5)
C11…O1	3.243 (3)	N1…N1 ⁱⁱ	3.259 (3)
C11…C11 ⁱⁱ	3.5759 (9)	N1…N2 ⁱⁱ	3.233 (3)
C11…N1 ⁱⁱ	3.3695 (18)	N1…N2	2.681 (3)
C11…O1 ⁱⁱⁱ	3.358 (4)	N2…C11 ⁱⁱ	3.337 (4)
O1…O2	2.951 (6)	C3…O1 ^v	3.257 (5)
O1…C11 ⁱⁱⁱ	3.358 (4)		
C11—Mn—N1	170.62 (6)	N1—C7—C5	116.49 (19)
C11—Mn—N2	98.59 (5)	C5—C7—C8	122.4 (3)
C11—Mn—C11 ⁱⁱ	92.74 (2)	C7—C8—C9	119.1 (3)
C11—Mn—N1 ⁱⁱ	89.55 (5)	C8—C9—C10	120.7 (3)
C11—Mn—N2 ⁱⁱ	98.24 (5)	C9—C10—C12	124.2 (3)
N1—Mn—N2	72.07 (8)	C11—C10—C12	120.2 (4)
C11 ⁱⁱ —Mn—N1	89.55 (5)	C9—C10—C11	115.6 (3)
N1—Mn—N1 ⁱⁱ	89.65 (7)	N1—C11—C10	124.8 (3)
N1—Mn—N2 ⁱⁱ	90.40 (8)	C2—C1—H1	118.00
C11 ⁱⁱ —Mn—N2	98.24 (5)	N2—C1—H1	118.00
N1 ⁱⁱ —Mn—N2	90.40 (8)	C4—C3—H3	120.00
N2—Mn—N2 ⁱⁱ	155.51 (7)	C2—C3—H3	120.00
C11 ⁱⁱ —Mn—N1 ⁱⁱ	170.62 (6)	C5—C4—H4	120.00
C11 ⁱⁱ —Mn—N2 ⁱⁱ	98.59 (5)	C3—C4—H4	120.00
N1 ⁱⁱ —Mn—N2 ⁱⁱ	72.07 (8)	C2—C6—H6C	109.00
H1A—O1—H1B	107.00	C2—C6—H6A	110.00
H2A—O2—H2A ⁱ	127.00	C2—C6—H6B	110.00
Mn—N1—C11	124.8 (2)	H6B—C6—H6C	109.00
Mn—N1—C7	116.40 (15)	H6A—C6—H6C	109.00
C7—N1—C11	118.7 (2)	H6A—C6—H6B	110.00
C1—N2—C5	118.9 (2)	C9—C8—H8	120.00
Mn—N2—C5	118.63 (17)	C7—C8—H8	120.00
Mn—N2—C1	122.49 (17)	C8—C9—H9	120.00
N2—C1—C2	124.1 (2)	C10—C9—H9	120.00
C3—C2—C6	123.5 (3)	N1—C11—H11	118.00
C1—C2—C3	116.3 (3)	C10—C11—H11	118.00
C1—C2—C6	120.2 (3)	C10—C12—H12B	109.00
C2—C3—C4	120.3 (3)	C10—C12—H12C	109.00
C3—C4—C5	119.6 (3)	H12A—C12—H12C	110.00
N2—C5—C7	116.4 (2)	H12B—C12—H12C	109.00
N2—C5—C4	120.8 (2)	H12A—C12—H12B	110.00
C4—C5—C7	122.8 (2)	C10—C12—H12A	109.00
N1—C7—C8	121.1 (2)		

supplementary materials

N2—Mn—N1—C7	0.40 (15)	Mn—N2—C1—C2	-179.72 (19)
N2—Mn—N1—C11	177.7 (2)	C5—N2—C1—C2	0.1 (3)
Cl1 ⁱⁱ —Mn—N1—C7	-98.41 (15)	Mn—N2—C5—C4	179.52 (18)
Cl1 ⁱⁱ —Mn—N1—C11	78.9 (2)	Mn—N2—C5—C7	-1.1 (2)
N1 ⁱⁱ —Mn—N1—C7	90.94 (16)	C1—N2—C5—C4	-0.3 (3)
N1 ⁱⁱ —Mn—N1—C11	-91.8 (2)	C1—N2—C5—C7	179.10 (19)
N2 ⁱⁱ —Mn—N1—C7	163.01 (16)	N2—C1—C2—C3	0.4 (4)
N2 ⁱⁱ —Mn—N1—C11	-19.7 (2)	N2—C1—C2—C6	-179.4 (3)
Cl1—Mn—N2—C1	1.11 (17)	C1—C2—C3—C4	-0.7 (4)
Cl1—Mn—N2—C5	-178.73 (15)	C6—C2—C3—C4	179.1 (3)
N1—Mn—N2—C1	-179.78 (19)	C2—C3—C4—C5	0.5 (4)
N1—Mn—N2—C5	0.38 (15)	C3—C4—C5—N2	0.0 (4)
Cl1 ⁱⁱ —Mn—N2—C1	-92.95 (17)	C3—C4—C5—C7	-179.4 (2)
Cl1 ⁱⁱ —Mn—N2—C5	87.21 (16)	N2—C5—C7—N1	1.4 (3)
N1 ⁱⁱ —Mn—N2—C1	90.71 (17)	N2—C5—C7—C8	-176.9 (2)
N1 ⁱⁱ —Mn—N2—C5	-89.13 (16)	C4—C5—C7—N1	-179.2 (2)
N2 ⁱⁱ —Mn—N2—C1	134.05 (18)	C4—C5—C7—C8	2.5 (3)
N2 ⁱⁱ —Mn—N2—C5	-45.8 (3)	N1—C7—C8—C9	1.5 (3)
Mn—N1—C7—C5	-1.1 (2)	C5—C7—C8—C9	179.7 (2)
Mn—N1—C7—C8	177.24 (16)	C7—C8—C9—C10	-1.8 (4)
C11—N1—C7—C5	-178.5 (2)	C8—C9—C10—C11	0.8 (4)
C11—N1—C7—C8	-0.2 (3)	C8—C9—C10—C12	-178.3 (3)
Mn—N1—C11—C10	-178.1 (2)	C9—C10—C11—N1	0.6 (4)
C7—N1—C11—C10	-0.9 (4)	C12—C10—C11—N1	179.7 (3)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots Cl1	0.84	2.42	3.243 (3)	168
O1—H1B \cdots Cl1 ⁱⁱⁱ	0.81	2.73	3.358 (4)	136
O2—H2A \cdots O1	0.86	2.16	2.951 (6)	153
C3—H3 \cdots O1 ^v	0.93	2.49	3.257 (5)	140
C6—H6A \cdots Cl1 ⁱⁱⁱ	0.96	2.79	3.717 (4)	162

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

Fig. 1

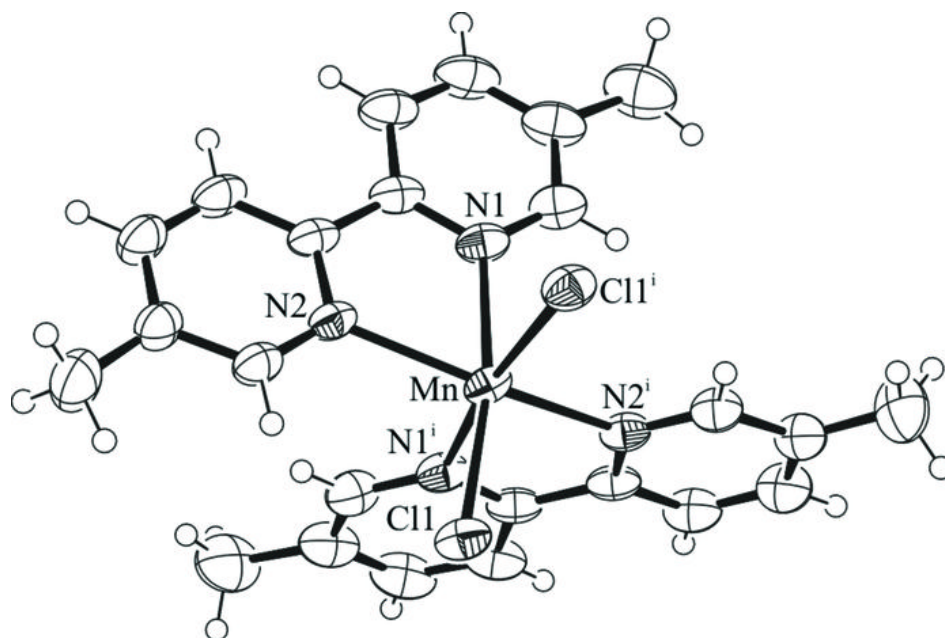


Fig. 2

