

Dichlorido[1-(2-pyridyl)ethanone oximate][1-(2-pyridyl)ethanone oxime]-manganese(III)

Jian Zuo,^a Jianmin Dou,^{a*} Dacheng Li,^a Daqi Wang^a and Yuying Sun^b

^aSchool of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China, and ^bAnalytical and Testing Center of Beihua University, People's Republic of China
Correspondence e-mail: dougroup@163.com

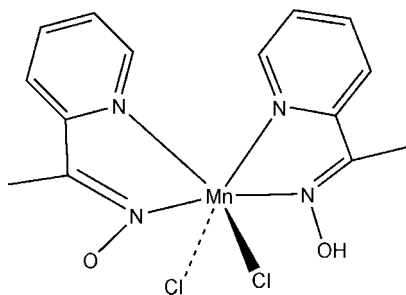
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.038; wR factor = 0.105; data-to-parameter ratio = 14.9.

The title complex, $[\text{MnCl}_2(\text{C}_7\text{H}_7\text{N}_2\text{O})(\text{C}_7\text{H}_8\text{N}_2\text{O})]$ or $[\text{MnCl}_2\{(\text{py})\text{C}(\text{Me})\text{NOH}\}\{(\text{py})\text{C}(\text{Me})\text{NO}\}]$ (py is pyridyl), has been prepared by the reaction of $(\text{py})\text{C}(\text{Me})\text{NOH}$ with MnCl_2 . The metal ion is coordinated by a chloride ligand, an N,N' -chelating $(\text{py})\text{C}(\text{Me})\text{NOH}$ molecule and a $(\text{py})\text{C}(\text{Me})\text{NO}$ molecule. The six-coordinate molecule is the *cis-cis-trans* isomer considering the positions of the coordinated Cl atoms, pyridyl and oxime N atoms, respectively. There is an intramolecular $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bond. The molecules are linked by intermolecular $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds.

Related literature

For the use of oximes, see: Chaudhuri (2003). For theoretical research, see: Pavlishchuk *et al.* (2003); Bokach *et al.* (2002). For the properties of related complexes, see: Kopylovich *et al.* (2002); Clerac *et al.* (2002).



Experimental

Crystal data

$[\text{MnCl}_2(\text{C}_7\text{H}_7\text{N}_2\text{O})(\text{C}_7\text{H}_8\text{N}_2\text{O})]$
 $M_r = 397.14$
 Monoclinic, $P2_1/n$
 $a = 8.908$ (4) Å
 $b = 10.590$ (5) Å
 $c = 18.555$ (8) Å
 $\beta = 92.604$ (5)°
 $V = 1748.5$ (14) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.07$ mm⁻¹
 $T = 298$ (2) K
 $0.56 \times 0.54 \times 0.21$ mm

Data collection

Siemens SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.585$, $T_{\max} = 0.806$
 8539 measured reflections
 3091 independent reflections
 2202 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.105$
 $S = 1.00$
 3091 reflections
 208 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.35$ e Å⁻³
 $\Delta\rho_{\min} = -0.27$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Mn1—N4	2.231 (3)	Mn1—N3	2.338 (3)
Mn1—N2	2.252 (3)	Mn1—Cl2	2.4254 (11)
Mn1—N1	2.288 (3)	Mn1—Cl1	2.4840 (13)
N4—Mn1—N2	152.45 (10)	N2—Mn1—Cl2	87.35 (8)
N4—Mn1—N1	91.34 (9)	N1—Mn1—Cl2	157.17 (7)
N2—Mn1—N1	69.88 (9)	N3—Mn1—Cl2	95.40 (7)
N4—Mn1—N3	69.06 (9)	N4—Mn1—Cl1	85.82 (7)
N2—Mn1—N3	89.15 (9)	N2—Mn1—Cl1	112.52 (7)
N1—Mn1—N3	86.28 (9)	N1—Mn1—Cl1	88.10 (7)
N4—Mn1—Cl2	110.57 (7)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{Cl13}-\text{H13}\cdots\text{Cl1}^{\text{i}}$	0.93	2.90	3.821 (4)	170
$\text{C5}-\text{H5}\cdots\text{Cl1}^{\text{ii}}$	0.93	2.83	3.592 (4)	140
$\text{O1}-\text{H1}\cdots\text{Cl2}^{\text{iii}}$	0.82	2.89	3.385 (3)	121
$\text{O1}-\text{H1}\cdots\text{Cl2}$	0.82	2.48	3.166 (3)	141

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXS97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); 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: KP2148).

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supplementary materials

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Dichlorido[1-(2-pyridyl)ethanone oximato][1-(2-pyridyl)ethanone oxime]manganese(III)

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Comment

There is currently a renewed interest in the coordination chemistry of oximes (Chaudhuri, 2003; Pavlishchuk *et al.*, 2003; Bokach *et al.*, 2002) and their application of metal ion/oxime systems as simple and efficient catalysts (Kopylovich *et al.*, 2002) and use of oxim ligands in synthesis of coordination polymers with interesting magnetic properties (Clerac *et al.*, 2002). Due to the above reasons, we used (py)C(Me)NOH as ligand, and obtained the title complex $[\text{MnCl}_2\{(\text{py})\text{C}(\text{Me})\text{NOH}\}\{(\text{py})\text{C}(\text{Me})\text{NO}\}]$.

The complex (Fig. 1) consists of two methyl(2-pyridyl)ketooxime, Mn^{2+} and two Cl^{1-} . The coordination geometry around the Mn centre is a distorted octahedron with a MnN_4Cl_2 ligand (Table 1). The N1 atom of methyl(2-pyridyl)ketooxime and Cl2 occupy the axial sites. The N2, N3, N4 and Cl1 are in the equatorial plane. The six-coordinate molecule is the *cis-cis-trans* isomer considering the positions of the coordinated chlorine atoms, pyridyl and oxime nitrogen atoms, respectively. The arrangement of the oxime groups seems unfavourable, most probably due to the steric hindrance of the methyl groups. There is an intramolecular O1—H1 \cdots Cl2 hydrogen bond. The molecules are linked into a three-dimensional-network by intermolecular O1—H1 \cdots Cl2, C5—H5 \cdots Cl1, C13—H13 \cdots Cl1 hydrogen bonds (Table 2, Fig. 2).

Experimental

A solution of MnCl_2 (0.126 g, 1.0 mmol) in MeOH (10 ml) was added to a solution of (py)C(Me)NOH (0.136 g, 1.0 mmol) in MeOH (10 ml). The resulting yellow solution was stirred for about 5 h and was then allowed to slowly concentrate by solvent evaporation at room temperature. Yellow block crystals suitable for X-ray diffraction were obtained within a week. The elemental analysis calculated for $\text{C}_{14}\text{H}_{15}\text{N}_4\text{O}_2\text{Cl}_2\text{Mn}$: C 42.34, H 3.81, N 14.11%; found: C 42.31, H 4.29, N 14.26%.

Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms with O—H 0.82, C—H 0.96 (methyl) Å [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O}, \text{C})$] and C—H 0.93 (pyridyl) Å [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$].

Figures

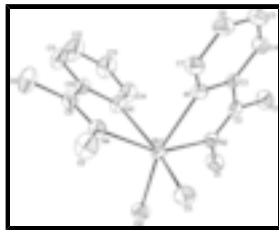


Fig. 1. The structure of the title complex showing the 30% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond O1—H1 \cdots Cl2 is shown.
Fig. 2. The crystal structure with hydrogen bonds shown as dashed lines.

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Crystal data

$[\text{MnCl}_2(\text{C}_7\text{H}_7\text{N}_2\text{O}_1)(\text{C}_7\text{H}_8\text{N}_2\text{O}_1)]$	$F_{000} = 808$
$M_r = 397.14$	$D_x = 1.509 \text{ Mg m}^{-3}$
Monoclinic, $P2(1)/n$	Mo $K\alpha$ radiation
Hall symbol: $-P2_1n$	$\lambda = 0.71073 \text{ \AA}$
$a = 8.908 (4) \text{ \AA}$	Cell parameters from 2984 reflections
$b = 10.590 (5) \text{ \AA}$	$\theta = 2.2\text{--}26.9^\circ$
$c = 18.555 (8) \text{ \AA}$	$\mu = 1.07 \text{ mm}^{-1}$
$\beta = 92.604 (5)^\circ$	$T = 298 (2) \text{ K}$
$V = 1748.5 (14) \text{ \AA}^3$	Block, yellow
$Z = 4$	$0.56 \times 0.54 \times 0.21 \text{ mm}$

Data collection

Siemens SMART CCD area-detector diffractometer	3091 independent reflections
Radiation source: fine-focus sealed tube	2202 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.051$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.2^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 10$
$T_{\text{min}} = 0.585$, $T_{\text{max}} = 0.806$	$k = -12 \rightarrow 10$
8539 measured reflections	$l = -21 \rightarrow 22$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.6261P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.105$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
3091 reflections	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$
208 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\sigma(F^2)$ 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.15081 (5)	0.24776 (4)	0.13664 (2)	0.03510 (16)
C11	0.05850 (10)	0.22964 (9)	0.26055 (5)	0.0536 (3)
C12	-0.04571 (9)	0.13122 (9)	0.07088 (5)	0.0522 (3)
N1	0.3852 (3)	0.2859 (2)	0.18742 (13)	0.0365 (6)
N2	0.3083 (3)	0.0899 (2)	0.10980 (14)	0.0400 (6)
N3	0.2301 (3)	0.3592 (2)	0.03647 (13)	0.0417 (6)
N4	0.0901 (3)	0.4516 (3)	0.14395 (14)	0.0430 (7)
O1	0.2664 (2)	-0.0104 (2)	0.06551 (13)	0.0569 (6)
H1	0.1760	-0.0066	0.0554	0.085*
O2	0.0174 (3)	0.4952 (3)	0.20388 (13)	0.0680 (7)
C1	0.5587 (4)	-0.0045 (4)	0.10622 (19)	0.0577 (10)
H1A	0.5060	-0.0714	0.0810	0.087*
H1B	0.6111	-0.0379	0.1483	0.087*
H1C	0.6294	0.0332	0.0752	0.087*
C2	0.4482 (3)	0.0938 (3)	0.12842 (16)	0.0365 (7)
C3	0.4945 (3)	0.2005 (3)	0.17488 (16)	0.0355 (7)
C4	0.6376 (3)	0.2146 (4)	0.20532 (19)	0.0483 (9)
H4	0.7128	0.1572	0.1951	0.058*
C5	0.6676 (4)	0.3144 (4)	0.2510 (2)	0.0557 (10)
H5	0.7632	0.3239	0.2727	0.067*
C6	0.5578 (4)	0.3997 (4)	0.26474 (19)	0.0523 (9)
H6	0.5764	0.4677	0.2956	0.063*
C7	0.4185 (3)	0.3815 (3)	0.23132 (18)	0.0466 (8)
H7	0.3434	0.4398	0.2400	0.056*
C8	0.0950 (5)	0.6723 (4)	0.1065 (2)	0.0685 (11)
H8A	0.0158	0.6842	0.1392	0.103*
H8B	0.0653	0.7073	0.0603	0.103*
H8C	0.1843	0.7139	0.1251	0.103*
C9	0.1253 (3)	0.5351 (3)	0.09853 (17)	0.0419 (8)
C10	0.2051 (3)	0.4845 (3)	0.03611 (16)	0.0401 (7)
C11	0.2517 (4)	0.5605 (4)	-0.0193 (2)	0.0654 (11)
H11	0.2319	0.6467	-0.0193	0.078*
C12	0.3272 (5)	0.5069 (5)	-0.0742 (2)	0.0829 (14)

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H12	0.3610	0.5571	-0.1112	0.099*
C13	0.3526 (5)	0.3809 (5)	-0.0744 (2)	0.0735 (12)
H13	0.4027	0.3431	-0.1117	0.088*
C14	0.3025 (4)	0.3100 (4)	-0.01807 (19)	0.0596 (10)
H14	0.3202	0.2235	-0.0181	0.072*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0341 (3)	0.0337 (3)	0.0380 (3)	0.0027 (2)	0.0069 (2)	-0.0009 (2)
C11	0.0518 (5)	0.0658 (7)	0.0444 (5)	0.0005 (4)	0.0167 (4)	0.0051 (4)
C12	0.0456 (5)	0.0547 (6)	0.0558 (5)	-0.0049 (4)	-0.0042 (4)	-0.0049 (4)
N1	0.0355 (14)	0.0350 (15)	0.0394 (14)	0.0000 (11)	0.0056 (11)	-0.0044 (12)
N2	0.0417 (15)	0.0315 (15)	0.0469 (16)	0.0014 (11)	0.0039 (12)	-0.0030 (13)
N3	0.0533 (16)	0.0377 (17)	0.0350 (14)	0.0049 (13)	0.0112 (12)	0.0002 (12)
N4	0.0471 (15)	0.0430 (17)	0.0396 (14)	0.0097 (13)	0.0105 (12)	-0.0047 (13)
O1	0.0545 (14)	0.0466 (15)	0.0691 (16)	0.0009 (11)	-0.0037 (12)	-0.0186 (14)
O2	0.0813 (18)	0.0650 (18)	0.0600 (15)	0.0189 (14)	0.0304 (14)	-0.0164 (14)
C1	0.054 (2)	0.053 (2)	0.067 (2)	0.0174 (18)	0.0070 (18)	-0.011 (2)
C2	0.0404 (18)	0.0336 (18)	0.0360 (17)	0.0069 (14)	0.0077 (14)	0.0069 (15)
C3	0.0335 (17)	0.0365 (18)	0.0370 (17)	0.0009 (14)	0.0088 (13)	0.0098 (15)
C4	0.0340 (18)	0.052 (2)	0.060 (2)	0.0043 (15)	0.0057 (16)	0.0054 (18)
C5	0.041 (2)	0.063 (3)	0.063 (2)	-0.0115 (18)	-0.0058 (17)	0.002 (2)
C6	0.051 (2)	0.051 (2)	0.054 (2)	-0.0119 (17)	-0.0011 (17)	-0.0055 (18)
C7	0.0432 (19)	0.045 (2)	0.053 (2)	0.0011 (15)	0.0079 (15)	-0.0063 (17)
C8	0.098 (3)	0.039 (2)	0.069 (3)	0.015 (2)	0.005 (2)	-0.003 (2)
C9	0.0428 (18)	0.039 (2)	0.0429 (19)	0.0059 (15)	-0.0059 (14)	-0.0022 (16)
C10	0.0445 (18)	0.0369 (19)	0.0386 (17)	0.0011 (15)	0.0007 (14)	0.0056 (16)
C11	0.083 (3)	0.049 (2)	0.065 (3)	0.003 (2)	0.010 (2)	0.017 (2)
C12	0.111 (4)	0.085 (4)	0.056 (3)	0.004 (3)	0.037 (3)	0.027 (3)
C13	0.096 (3)	0.083 (4)	0.044 (2)	0.012 (3)	0.029 (2)	0.007 (2)
C14	0.078 (3)	0.057 (3)	0.045 (2)	0.013 (2)	0.0207 (19)	0.0011 (19)

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

Mn1—N4	2.231 (3)	C4—C5	1.375 (5)
Mn1—N2	2.252 (3)	C4—H4	0.9300
Mn1—N1	2.288 (3)	C5—C6	1.364 (5)
Mn1—N3	2.338 (3)	C5—H5	0.9300
Mn1—C12	2.4254 (11)	C6—C7	1.375 (4)
Mn1—C11	2.4840 (13)	C6—H6	0.9300
N1—C7	1.325 (4)	C7—H7	0.9300
N1—C3	1.357 (4)	C8—C9	1.486 (5)
N2—C2	1.278 (4)	C8—H8A	0.9600
N2—O1	1.385 (3)	C8—H8B	0.9600
N3—C14	1.331 (4)	C8—H8C	0.9600
N3—C10	1.345 (4)	C9—C10	1.486 (4)
N4—C9	1.271 (4)	C10—C11	1.383 (5)
N4—O2	1.391 (3)	C11—C12	1.368 (6)

O1—H1	0.8200	C11—H11	0.9300
C1—C2	1.503 (4)	C12—C13	1.354 (6)
C1—H1A	0.9600	C12—H12	0.9300
C1—H1B	0.9600	C13—C14	1.377 (5)
C1—H1C	0.9600	C13—H13	0.9300
C2—C3	1.469 (4)	C14—H14	0.9300
C3—C4	1.378 (4)		
N4—Mn1—N2	152.45 (10)	N1—C3—C2	115.4 (3)
N4—Mn1—N1	91.34 (9)	C4—C3—C2	123.6 (3)
N2—Mn1—N1	69.88 (9)	C5—C4—C3	119.1 (3)
N4—Mn1—N3	69.06 (9)	C5—C4—H4	120.5
N2—Mn1—N3	89.15 (9)	C3—C4—H4	120.5
N1—Mn1—N3	86.28 (9)	C6—C5—C4	120.2 (3)
N4—Mn1—C12	110.57 (7)	C6—C5—H5	119.9
N2—Mn1—C12	87.35 (8)	C4—C5—H5	119.9
N1—Mn1—C12	157.17 (7)	C5—C6—C7	117.6 (3)
N3—Mn1—C12	95.40 (7)	C5—C6—H6	121.2
N4—Mn1—C11	85.82 (7)	C7—C6—H6	121.2
N2—Mn1—C11	112.52 (7)	N1—C7—C6	123.8 (3)
N1—Mn1—C11	88.10 (7)	N1—C7—H7	118.1
N3—Mn1—C11	154.09 (7)	C6—C7—H7	118.1
C12—Mn1—C11	99.47 (4)	C9—C8—H8A	109.5
C7—N1—C3	118.2 (3)	C9—C8—H8B	109.5
C7—N1—Mn1	124.3 (2)	H8A—C8—H8B	109.5
C3—N1—Mn1	117.4 (2)	C9—C8—H8C	109.5
C2—N2—O1	114.7 (2)	H8A—C8—H8C	109.5
C2—N2—Mn1	121.7 (2)	H8B—C8—H8C	109.5
O1—N2—Mn1	123.18 (17)	N4—C9—C8	124.3 (3)
C14—N3—C10	117.9 (3)	N4—C9—C10	114.0 (3)
C14—N3—Mn1	125.5 (2)	C8—C9—C10	121.7 (3)
C10—N3—Mn1	116.5 (2)	N3—C10—C11	121.5 (3)
C9—N4—O2	115.9 (3)	N3—C10—C9	115.9 (3)
C9—N4—Mn1	124.4 (2)	C11—C10—C9	122.6 (3)
O2—N4—Mn1	119.5 (2)	C12—C11—C10	119.1 (4)
N2—O1—H1	109.5	C12—C11—H11	120.5
C2—C1—H1A	109.5	C10—C11—H11	120.5
C2—C1—H1B	109.5	C13—C12—C11	119.9 (4)
H1A—C1—H1B	109.5	C13—C12—H12	120.0
C2—C1—H1C	109.5	C11—C12—H12	120.0
H1A—C1—H1C	109.5	C12—C13—C14	118.3 (4)
H1B—C1—H1C	109.5	C12—C13—H13	120.8
N2—C2—C3	115.3 (3)	C14—C13—H13	120.8
N2—C2—C1	123.1 (3)	N3—C14—C13	123.3 (4)
C3—C2—C1	121.5 (3)	N3—C14—H14	118.4
N1—C3—C4	121.0 (3)	C13—C14—H14	118.4
N4—Mn1—N1—C7	26.1 (3)	C11—Mn1—N4—O2	-5.3 (2)
N2—Mn1—N1—C7	-174.5 (3)	O1—N2—C2—C3	179.4 (2)
N3—Mn1—N1—C7	95.0 (3)	Mn1—N2—C2—C3	6.4 (4)

supplementary materials

Cl2—Mn1—N1—C7	-169.89 (19)	O1—N2—C2—C1	-1.8 (4)
Cl1—Mn1—N1—C7	-59.7 (2)	Mn1—N2—C2—C1	-174.8 (2)
N4—Mn1—N1—C3	-157.9 (2)	C7—N1—C3—C4	-1.8 (4)
N2—Mn1—N1—C3	1.4 (2)	Mn1—N1—C3—C4	-178.0 (2)
N3—Mn1—N1—C3	-89.0 (2)	C7—N1—C3—C2	177.3 (3)
Cl2—Mn1—N1—C3	6.1 (3)	Mn1—N1—C3—C2	1.0 (3)
Cl1—Mn1—N1—C3	116.3 (2)	N2—C2—C3—N1	-4.7 (4)
N4—Mn1—N2—C2	45.2 (3)	C1—C2—C3—N1	176.5 (3)
N1—Mn1—N2—C2	-4.4 (2)	N2—C2—C3—C4	174.3 (3)
N3—Mn1—N2—C2	81.9 (2)	C1—C2—C3—C4	-4.5 (5)
Cl2—Mn1—N2—C2	177.4 (2)	N1—C3—C4—C5	2.3 (5)
Cl1—Mn1—N2—C2	-83.5 (2)	C2—C3—C4—C5	-176.7 (3)
N4—Mn1—N2—O1	-127.2 (2)	C3—C4—C5—C6	-1.3 (5)
N1—Mn1—N2—O1	-176.8 (2)	C4—C5—C6—C7	-0.1 (5)
N3—Mn1—N2—O1	-90.5 (2)	C3—N1—C7—C6	0.3 (5)
Cl2—Mn1—N2—O1	5.0 (2)	Mn1—N1—C7—C6	176.2 (3)
Cl1—Mn1—N2—O1	104.1 (2)	C5—C6—C7—N1	0.6 (5)
N4—Mn1—N3—C14	179.7 (3)	O2—N4—C9—C8	0.6 (5)
N2—Mn1—N3—C14	16.9 (3)	Mn1—N4—C9—C8	-175.0 (2)
N1—Mn1—N3—C14	86.8 (3)	O2—N4—C9—C10	178.9 (2)
Cl2—Mn1—N3—C14	-70.3 (3)	Mn1—N4—C9—C10	3.2 (4)
Cl1—Mn1—N3—C14	164.7 (2)	C14—N3—C10—C11	0.6 (5)
N4—Mn1—N3—C10	2.6 (2)	Mn1—N3—C10—C11	177.9 (3)
N2—Mn1—N3—C10	-160.2 (2)	C14—N3—C10—C9	-179.4 (3)
N1—Mn1—N3—C10	-90.3 (2)	Mn1—N3—C10—C9	-2.1 (3)
Cl2—Mn1—N3—C10	112.6 (2)	N4—C9—C10—N3	-0.5 (4)
Cl1—Mn1—N3—C10	-12.4 (3)	C8—C9—C10—N3	177.8 (3)
N2—Mn1—N4—C9	36.6 (4)	N4—C9—C10—C11	179.5 (3)
N1—Mn1—N4—C9	82.2 (3)	C8—C9—C10—C11	-2.2 (5)
N3—Mn1—N4—C9	-3.3 (2)	N3—C10—C11—C12	-1.2 (6)
Cl2—Mn1—N4—C9	-91.2 (3)	C9—C10—C11—C12	178.7 (3)
Cl1—Mn1—N4—C9	170.2 (3)	C10—C11—C12—C13	1.3 (7)
N2—Mn1—N4—O2	-138.9 (2)	C11—C12—C13—C14	-0.8 (7)
N1—Mn1—N4—O2	-93.3 (2)	C10—N3—C14—C13	0.0 (6)
N3—Mn1—N4—O2	-178.8 (2)	Mn1—N3—C14—C13	-177.1 (3)
Cl2—Mn1—N4—O2	93.3 (2)	C12—C13—C14—N3	0.1 (7)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C13—H13 \cdots C11 ⁱ	0.93	2.90	3.821 (4)	170
C5—H5 \cdots C11 ⁱⁱ	0.93	2.83	3.592 (4)	140
O1—H1 \cdots Cl2 ⁱⁱⁱ	0.82	2.89	3.385 (3)	121
O1—H1 \cdots Cl2	0.82	2.48	3.166 (3)	141

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

Fig. 1

