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Bis(7-amino-2,4-dimethyl-1,8-naphthyridine)dichloridomanganese(II) methanol disolvate

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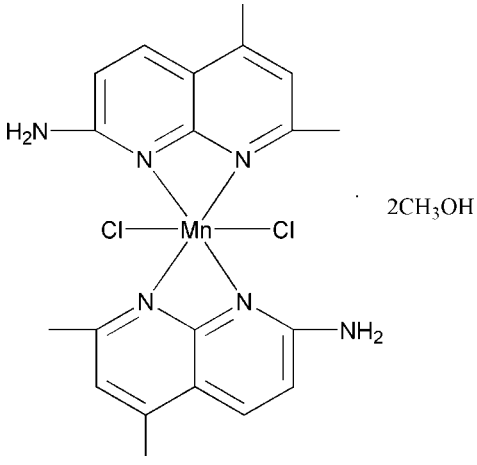
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.125; data-to-parameter ratio = 15.4.

In the title compound, $[MnCl_2(C_{10}H_{11}N_3)_2]\cdot 2CH_3OH$, both naphthyridine ligands coordinate to the Mn^{II} ion *via* two N atoms in a bidentate chelating mode. The Mn^{II} centre is furthermore coordinated by two Cl ligands to form an octahedral geometry. In addition, there are two methanol molecules in the asymmetric unit. The crystal packing is stabilized by O—H···Cl, N—H···O and N—H···Cl hydrogen bonds.

Related literature

For related literature, see: Bayer (1979); Gavrilova & Bosnich (2004); Jin *et al.* (2007); Mintert & Sheldrick (1995*a*,*b*); Oskui *et al.* (1999); Oskui & Sheldrick (1999).



Experimental

Crystal data

$[MnCl_2(C_{10}H_{11}N_3)_2]\cdot 2CH_3OH$
M_r = 536.36
Triclinic, $P\overline{1}$
a = 9.637 (3) Å
b = 10.649 (3) Å
c = 14.442 (4) Å
α = 79.178 (4)°
β = 78.343 (4)°
γ = 65.894 (4)°
V = 1315.7 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 298 (2) K
0.41 × 0.22 × 0.17 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.753, T_{max} = 0.885
6933 measured reflections
4597 independent reflections
2867 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.125
S = 1.02
4597 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···Cl1^{i}	0.82	2.35	3.162 (3)	169
O1—H1···Cl1^{ii}	0.82	2.41	3.183 (3)	158
N6—H6*B*···O1	0.86	2.10	2.960 (4)	173
N6—H6*A*···Cl1	0.86	2.55	3.359 (4)	158
N3—H3*B*···O2^{iii}	0.86	2.04	2.895 (4)	175
N3—H3*A*···Cl2	0.86	2.49	3.318 (4)	161

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996; data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); 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: BT2572).

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supplementary materials

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Bis(7-amino-2,4-dimethyl-1,8-naphthyridine)dichloridomanganese(II) methanol disolvate

S. Jin and D. Wang

Comment

Molecular structures and chemical properties of transition metal complexes of 1,8-naphthyridine (napy) and its derivatives have received much attention, because the ligands can link to metals with several coordination modes such as monodentate, chelating bidentate, and dinuclear bridging binding fashion (Gavrilova & Bosnich, 2004). 5,7-dimethyl-1,8-naphthyridin-2-amine are potentially tridentate ligands and are capable of linking two to four metal atoms together to form metal aggregates having metal–metal interactions (Oskui *et al.*, 1999; Mintert & Sheldrick, 1995*a*,b; Oskui & Sheldrick, 1999). The coordination chemistry of 5,7-dimethyl-1,8-naphthyridine-2-amine (*L*) has not been well studied before although a Mn(II) complex ($Mn_{(L)}2_{Cl}2$) (Bayer, 1979) was once described in a US patent. As an extension of our work (Jin *et al.*, 2007), the title complex ($Mn_{(L)}2(Cl)_{2)\cdot 2(C}H_3O_H$) is reported here.

The complex was obtained as colorless crystals by reacting of manganese chloride tetrahydrate and *L* in methanol. The compound is air stable and light insensitive. The complex does not dissolve in water and common organic solvent. The molecular structure of the compound is shown in Fig. 1. Both of the two *L* coordinate to the metal with two N atoms in a bidentate chelating fashion. Two chloride anions coordinate to the Mn ion to complete its octahedral geometry. The amine group of 5,7-dimethyl-1,8-naphthyridin-2-amine does not show any bonding interaction with the Mn atoms. The Mn—N bond distances range from 2.231 (3) to 2.453 (3) Å. The Mn—Cl bond distances are 2.4166 (14) and 2.4699 (12) Å. The two naphthyridine rings are almost perpendicular to each other.

Experimental

All reagents and solvents were used as obtained without further purification. The CHN elemental analyses were performed on a Perkin–Elmer elemental analyzer.

To an methanol solution of manganese chloride tetrahydrate (40 mg, 0.2 mmol) was added *L* (34.8 mg, 0.2 mmol) in 10 ml of methanol. The solution was stirred for a few minutes, then the solution was filtered. After standing the solution at room temperature for several days, colorless block crystals were isolated. Yield: 32.2 mg, 60%. Anal. Calcd. for $C_{22}H_{30}Cl_2Mn_N6_O2$: C, 49.22; H, 5.59; N, 15.66. Found: C, 49.17; H, 5.50; N, 15.62.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with O—H = 0.82 Å, N—H = 0.90 Å and C—H = 0.96 Å and U(H) set to $1.2U_{eq}$(C,*N*,*O*).

Figures

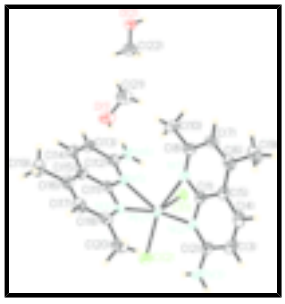

Fig. 1. The structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

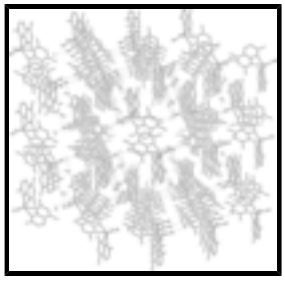

Fig. 2. Three dimensional network structure connected *via* pi-pi interaction and hydrogen bonds.

Bis(7-amino-2,4-dimethyl-1,8-naphthyridine)dichloridomanganese(II) methanol disolvate

Crystal data

$[MnCl_2(C_{10}H_{11}N_3)_2]\cdot 2CH_3OH$	$Z = 2$
$M_r = 536.36$	$F_{000} = 558$
Triclinic, $P\overline{1}$	$D_x = 1.354$ Mg m^{-3}
$a = 9.637$ (3) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.649$ (3) Å	Cell parameters from 1874 reflections
$c = 14.442$ (4) Å	$\theta = 2.4$–23.2°
$\alpha = 79.178$ (4)°	$\mu = 0.73$ mm^{-1}
$\beta = 78.343$ (4)°	$T = 298$ (2) K
$\gamma = 65.894$ (4)°	Block, colourless
$V = 1315.7$ (7) Å^3	0.41 × 0.22 × 0.17 mm

Data collection

Siemens SMART CCD area-detector diffractometer	4597 independent reflections
Radiation source: fine-focus sealed tube	2867 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 298$(2) K	$\theta_{max} = 25.0^\circ$
φ and ω scans	$\theta_{min} = 1.5^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9\rightarrow11$
$T_{min} = 0.753$, $T_{max} = 0.885$	$k = -12\rightarrow11$
6933 measured reflections	$l = -17\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.125$	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.4067P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
4597 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
298 parameters	$\Delta\rho_{min} = -0.24$ 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 $F^2 > 2$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	0.03600 (6)	0.77674 (5)	0.25965 (4)	0.04575 (19)
Cl1	0.05456 (13)	0.98490 (10)	0.29881 (7)	0.0636 (3)
Cl2	−0.24018 (12)	0.85917 (13)	0.27296 (7)	0.0760 (4)
N1	0.2973 (3)	0.7055 (3)	0.1725 (2)	0.0449 (7)
N2	0.0861 (3)	0.7875 (3)	0.10128 (19)	0.0449 (7)
N3	−0.1387 (4)	0.8679 (4)	0.0390 (2)	0.0736 (10)
H3A	−0.1879	0.8741	0.0958	0.088*
H3B	−0.1880	0.8911	−0.0090	0.088*
N4	0.0720 (3)	0.5423 (3)	0.29246 (19)	0.0434 (7)
N5	0.1309 (3)	0.6444 (3)	0.39243 (19)	0.0440 (7)
N6	0.1863 (4)	0.7605 (3)	0.4883 (2)	0.0711 (10)
H6A	0.1532	0.8348	0.4497	0.085*
H6B	0.2206	0.7620	0.5385	0.085*
O1	0.2760 (4)	0.7735 (3)	0.6695 (2)	0.0863 (10)
H1	0.2054	0.8466	0.6822	0.130*
O2	0.7131 (4)	0.9445 (4)	0.8698 (2)	0.0924 (10)
H2	0.7655	0.9740	0.8266	0.139*
C1	0.2407 (4)	0.7379 (3)	0.0889 (2)	0.0436 (8)

C2	0.0140 (5)	0.8224 (4)	0.0253 (3)	0.0544 (10)
C3	0.0983 (5)	0.8106 (4)	−0.0680 (3)	0.0621 (11)
H3	0.0470	0.8367	−0.1209	0.075*
C4	0.2517 (5)	0.7617 (4)	−0.0791 (3)	0.0625 (11)
H4	0.3063	0.7539	−0.1401	0.075*
C5	0.3329 (5)	0.7213 (4)	0.0003 (2)	0.0497 (9)
C6	0.4929 (5)	0.6667 (4)	−0.0013 (3)	0.0596 (11)
C7	0.5471 (5)	0.6343 (4)	0.0835 (3)	0.0644 (11)
H7	0.6526	0.5981	0.0843	0.077*
C8	0.4486 (5)	0.6537 (4)	0.1696 (3)	0.0554 (10)
C9	0.6011 (5)	0.6424 (5)	−0.0936 (3)	0.0815 (14)
H9A	0.6051	0.7289	−0.1251	0.122*
H9B	0.5650	0.6034	−0.1339	0.122*
H9C	0.7018	0.5796	−0.0806	0.122*
C10	0.5090 (5)	0.6191 (5)	0.2626 (3)	0.0782 (13)
H10A	0.4275	0.6625	0.3111	0.117*
H10B	0.5896	0.6522	0.2572	0.117*
H10C	0.5485	0.5205	0.2794	0.117*
C11	0.1292 (4)	0.5249 (3)	0.3733 (2)	0.0414 (8)
C12	0.1846 (4)	0.6429 (4)	0.4704 (3)	0.0502 (9)
C13	0.2383 (4)	0.5185 (4)	0.5337 (3)	0.0564 (10)
H13	0.2750	0.5189	0.5884	0.068*
C14	0.2361 (4)	0.4015 (4)	0.5147 (3)	0.0568 (10)
H14	0.2713	0.3211	0.5565	0.068*
C15	0.1809 (4)	0.3981 (4)	0.4314 (2)	0.0485 (9)
C16	0.1720 (5)	0.2840 (4)	0.4025 (3)	0.0572 (10)
C17	0.1094 (5)	0.3053 (4)	0.3206 (3)	0.0591 (11)
H17	0.1008	0.2313	0.3002	0.071*
C18	0.0586 (4)	0.4350 (4)	0.2675 (3)	0.0517 (9)
C19	0.2261 (6)	0.1429 (4)	0.4589 (3)	0.0798 (14)
H19A	0.3153	0.1289	0.4859	0.120*
H19B	0.2515	0.0732	0.4178	0.120*
H19C	0.1461	0.1367	0.5091	0.120*
C20	−0.0165 (5)	0.4602 (5)	0.1806 (3)	0.0722 (12)
H20A	−0.1079	0.4408	0.1979	0.108*
H20B	0.0532	0.4008	0.1346	0.108*
H20C	−0.0428	0.5552	0.1536	0.108*
C21	0.4129 (6)	0.7950 (6)	0.6425 (4)	0.1003 (17)
H21A	0.4127	0.8616	0.6791	0.150*
H21B	0.4220	0.8290	0.5760	0.150*
H21C	0.4980	0.7091	0.6537	0.150*
C22	0.5636 (6)	1.0004 (5)	0.8526 (5)	0.118 (2)
H22A	0.5028	0.9640	0.9024	0.177*
H22B	0.5588	0.9771	0.7926	0.177*
H22C	0.5247	1.0993	0.8507	0.177*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0506 (4)	0.0454 (3)	0.0389 (3)	−0.0156 (3)	−0.0108 (2)	−0.0012 (2)
Cl1	0.0821 (8)	0.0473 (6)	0.0639 (6)	−0.0256 (5)	−0.0129 (6)	−0.0079 (5)
Cl2	0.0492 (6)	0.1008 (9)	0.0613 (7)	−0.0161 (6)	−0.0116 (5)	0.0040 (6)
N1	0.0466 (19)	0.0405 (17)	0.0457 (17)	−0.0131 (15)	−0.0121 (14)	−0.0028 (13)
N2	0.0467 (19)	0.0462 (18)	0.0384 (16)	−0.0137 (15)	−0.0107 (14)	−0.0013 (13)
N3	0.057 (2)	0.104 (3)	0.051 (2)	−0.018 (2)	−0.0218 (18)	−0.0040 (19)
N4	0.0463 (18)	0.0482 (18)	0.0388 (16)	−0.0209 (15)	−0.0084 (14)	−0.0033 (13)
N5	0.0527 (19)	0.0428 (17)	0.0413 (16)	−0.0222 (15)	−0.0124 (14)	−0.0005 (13)
N6	0.109 (3)	0.069 (2)	0.055 (2)	−0.045 (2)	−0.034 (2)	−0.0028 (17)
O1	0.065 (2)	0.101 (2)	0.080 (2)	−0.0100 (19)	−0.0094 (17)	−0.0327 (18)
O2	0.073 (2)	0.132 (3)	0.074 (2)	−0.046 (2)	−0.0337 (18)	0.0206 (19)
C1	0.049 (2)	0.0359 (19)	0.045 (2)	−0.0161 (17)	−0.0083 (18)	−0.0013 (16)
C2	0.057 (3)	0.050 (2)	0.054 (3)	−0.018 (2)	−0.015 (2)	−0.0012 (18)
C3	0.078 (3)	0.068 (3)	0.039 (2)	−0.026 (2)	−0.016 (2)	−0.0006 (19)
C4	0.081 (3)	0.063 (3)	0.041 (2)	−0.031 (2)	0.007 (2)	−0.0085 (19)
C5	0.060 (3)	0.044 (2)	0.044 (2)	−0.0191 (19)	−0.007 (2)	−0.0045 (17)
C6	0.061 (3)	0.047 (2)	0.067 (3)	−0.023 (2)	0.004 (2)	−0.008 (2)
C7	0.043 (2)	0.066 (3)	0.077 (3)	−0.017 (2)	−0.002 (2)	−0.010 (2)
C8	0.050 (3)	0.050 (2)	0.067 (3)	−0.019 (2)	−0.017 (2)	−0.0002 (19)
C9	0.070 (3)	0.084 (3)	0.081 (3)	−0.032 (3)	0.024 (3)	−0.021 (3)
C10	0.059 (3)	0.092 (3)	0.083 (3)	−0.026 (3)	−0.032 (2)	0.007 (3)
C11	0.040 (2)	0.044 (2)	0.040 (2)	−0.0179 (17)	−0.0021 (16)	−0.0032 (16)
C12	0.056 (2)	0.056 (2)	0.044 (2)	−0.026 (2)	−0.0086 (18)	−0.0068 (18)
C13	0.061 (3)	0.068 (3)	0.040 (2)	−0.024 (2)	−0.0177 (19)	0.0034 (19)
C14	0.056 (3)	0.053 (2)	0.048 (2)	−0.014 (2)	−0.0062 (19)	0.0090 (18)
C15	0.050 (2)	0.043 (2)	0.045 (2)	−0.0143 (18)	−0.0051 (18)	0.0002 (17)
C16	0.057 (3)	0.047 (2)	0.061 (3)	−0.019 (2)	0.002 (2)	−0.0045 (19)
C17	0.061 (3)	0.048 (2)	0.071 (3)	−0.025 (2)	0.003 (2)	−0.018 (2)
C18	0.048 (2)	0.058 (3)	0.054 (2)	−0.024 (2)	−0.0019 (18)	−0.0147 (19)
C19	0.098 (4)	0.047 (3)	0.088 (3)	−0.026 (3)	−0.012 (3)	0.002 (2)
C20	0.069 (3)	0.091 (3)	0.072 (3)	−0.037 (3)	−0.015 (2)	−0.025 (2)
C21	0.083 (4)	0.107 (4)	0.108 (4)	−0.027 (3)	−0.017 (3)	−0.023 (3)
C22	0.090 (4)	0.080 (4)	0.190 (7)	−0.035 (3)	−0.058 (4)	0.014 (4)

Geometric parameters (Å, °)

Mn1—N2	2.231 (3)	C7—C8	1.395 (5)
Mn1—N5	2.267 (3)	C7—H7	0.9300
Mn1—N4	2.344 (3)	C8—C10	1.495 (5)
Mn1—Cl2	2.4166 (14)	C9—H9A	0.9600
Mn1—N1	2.453 (3)	C9—H9B	0.9600
Mn1—Cl1	2.4699 (12)	C9—H9C	0.9600
N1—C8	1.327 (5)	C10—H10A	0.9600
N1—C1	1.353 (4)	C10—H10B	0.9600
N2—C2	1.331 (4)	C10—H10C	0.9600

N2—C1	1.347 (4)	C11—C15	1.403 (5)
N3—C2	1.332 (5)	C12—C13	1.426 (5)
N3—H3A	0.8600	C13—C14	1.333 (5)
N3—H3B	0.8600	C13—H13	0.9300
N4—C18	1.322 (4)	C14—C15	1.422 (5)
N4—C11	1.341 (4)	C14—H14	0.9300
N5—C12	1.326 (4)	C15—C16	1.396 (5)
N5—C11	1.359 (4)	C16—C17	1.374 (5)
N6—C12	1.332 (4)	C16—C19	1.505 (5)
N6—H6A	0.8600	C17—C18	1.392 (5)
N6—H6B	0.8600	C17—H17	0.9300
O1—C21	1.396 (5)	C18—C20	1.501 (5)
O1—H1	0.8200	C19—H19A	0.9600
O2—C22	1.371 (5)	C19—H19B	0.9600
O2—H2	0.8200	C19—H19C	0.9600
C1—C5	1.398 (5)	C20—H20A	0.9600
C2—C3	1.424 (5)	C20—H20B	0.9600
C3—C4	1.338 (5)	C20—H20C	0.9600
C3—H3	0.9300	C21—H21A	0.9600
C4—C5	1.420 (5)	C21—H21B	0.9600
C4—H4	0.9300	C21—H21C	0.9600
C5—C6	1.405 (5)	C22—H22A	0.9600
C6—C7	1.359 (6)	C22—H22B	0.9600
C6—C9	1.509 (5)	C22—H22C	0.9600
N2—Mn1—N5	140.98 (10)	C6—C9—H9B	109.5
N2—Mn1—N4	97.82 (10)	H9A—C9—H9B	109.5
N5—Mn1—N4	58.08 (9)	C6—C9—H9C	109.5
N2—Mn1—Cl2	97.46 (8)	H9A—C9—H9C	109.5
N5—Mn1—Cl2	113.38 (8)	H9B—C9—H9C	109.5
N4—Mn1—Cl2	94.45 (8)	C8—C10—H10A	109.5
N2—Mn1—N1	56.89 (10)	C8—C10—H10B	109.5
N5—Mn1—N1	89.71 (10)	H10A—C10—H10B	109.5
N4—Mn1—N1	88.28 (9)	C8—C10—H10C	109.5
Cl2—Mn1—N1	154.31 (8)	H10A—C10—H10C	109.5
N2—Mn1—Cl1	105.51 (8)	H10B—C10—H10C	109.5
N5—Mn1—Cl1	93.36 (7)	N4—C11—N5	112.1 (3)
N4—Mn1—Cl1	151.42 (8)	N4—C11—C15	123.8 (3)
Cl2—Mn1—Cl1	98.59 (5)	N5—C11—C15	124.1 (3)
N1—Mn1—Cl1	90.77 (7)	N5—C12—N6	118.4 (3)
C8—N1—C1	117.8 (3)	N5—C12—C13	120.6 (3)
C8—N1—Mn1	151.8 (3)	N6—C12—C13	121.0 (3)
C1—N1—Mn1	90.4 (2)	C14—C13—C12	120.3 (3)
C2—N2—C1	119.0 (3)	C14—C13—H13	119.9
C2—N2—Mn1	140.4 (3)	C12—C13—H13	119.9
C1—N2—Mn1	100.6 (2)	C13—C14—C15	120.9 (3)
C2—N3—H3A	120.0	C13—C14—H14	119.5
C2—N3—H3B	120.0	C15—C14—H14	119.5
H3A—N3—H3B	120.0	C16—C15—C11	117.6 (3)
C18—N4—C11	118.2 (3)	C16—C15—C14	127.2 (3)

C18—N4—Mn1	148.4 (2)	C11—C15—C14	115.2 (3)
C11—N4—Mn1	93.44 (19)	C17—C16—C15	117.4 (3)
C12—N5—C11	118.8 (3)	C17—C16—C19	120.7 (4)
C12—N5—Mn1	144.8 (2)	C15—C16—C19	121.8 (4)
C11—N5—Mn1	96.3 (2)	C16—C17—C18	121.6 (3)
C12—N6—H6A	120.0	C16—C17—H17	119.2
C12—N6—H6B	120.0	C18—C17—H17	119.2
H6A—N6—H6B	120.0	N4—C18—C17	121.3 (4)
C21—O1—H1	109.5	N4—C18—C20	116.9 (3)
C22—O2—H2	109.5	C17—C18—C20	121.7 (4)
N2—C1—N1	112.1 (3)	C16—C19—H19A	109.5
N2—C1—C5	124.4 (3)	C16—C19—H19B	109.5
N1—C1—C5	123.5 (3)	H19A—C19—H19B	109.5
N2—C2—N3	118.2 (4)	C16—C19—H19C	109.5
N2—C2—C3	120.7 (4)	H19A—C19—H19C	109.5
N3—C2—C3	121.1 (4)	H19B—C19—H19C	109.5
C4—C3—C2	119.5 (4)	C18—C20—H20A	109.5
C4—C3—H3	120.2	C18—C20—H20B	109.5
C2—C3—H3	120.2	H20A—C20—H20B	109.5
C3—C4—C5	121.5 (4)	C18—C20—H20C	109.5
C3—C4—H4	119.3	H20A—C20—H20C	109.5
C5—C4—H4	119.3	H20B—C20—H20C	109.5
C1—C5—C6	117.9 (3)	O1—C21—H21A	109.5
C1—C5—C4	115.0 (4)	O1—C21—H21B	109.5
C6—C5—C4	127.1 (4)	H21A—C21—H21B	109.5
C7—C6—C5	117.5 (4)	O1—C21—H21C	109.5
C7—C6—C9	121.1 (4)	H21A—C21—H21C	109.5
C5—C6—C9	121.4 (4)	H21B—C21—H21C	109.5
C6—C7—C8	121.7 (4)	O2—C22—H22A	109.5
C6—C7—H7	119.1	O2—C22—H22B	109.5
C8—C7—H7	119.1	H22A—C22—H22B	109.5
N1—C8—C7	121.6 (4)	O2—C22—H22C	109.5
N1—C8—C10	117.0 (4)	H22A—C22—H22C	109.5
C7—C8—C10	121.5 (4)	H22B—C22—H22C	109.5
C6—C9—H9A	109.5		
N2—Mn1—N1—C8	−177.8 (5)	N3—C2—C3—C4	−178.5 (4)
N5—Mn1—N1—C8	−19.2 (5)	C2—C3—C4—C5	−0.1 (6)
N4—Mn1—N1—C8	−77.3 (5)	N2—C1—C5—C6	−179.3 (3)
Cl2—Mn1—N1—C8	−174.0 (4)	N1—C1—C5—C6	0.7 (5)
Cl1—Mn1—N1—C8	74.1 (5)	N2—C1—C5—C4	0.2 (5)
N2—Mn1—N1—C1	−0.35 (18)	N1—C1—C5—C4	−179.8 (3)
N5—Mn1—N1—C1	158.21 (19)	C3—C4—C5—C1	−0.5 (5)
N4—Mn1—N1—C1	100.13 (19)	C3—C4—C5—C6	178.9 (4)
Cl2—Mn1—N1—C1	3.4 (3)	C1—C5—C6—C7	−0.3 (5)
Cl1—Mn1—N1—C1	−108.44 (18)	C4—C5—C6—C7	−179.7 (4)
N5—Mn1—N2—C2	143.0 (3)	C1—C5—C6—C9	178.6 (3)
N4—Mn1—N2—C2	95.7 (4)	C4—C5—C6—C9	−0.8 (6)
Cl2—Mn1—N2—C2	0.2 (4)	C5—C6—C7—C8	0.2 (6)
N1—Mn1—N2—C2	178.5 (4)	C9—C6—C7—C8	−178.8 (4)

Cl1—Mn1—N2—C2	−100.9 (4)	C1—N1—C8—C7	0.7 (5)
N5—Mn1—N2—C1	−35.1 (3)	Mn1—N1—C8—C7	177.8 (3)
N4—Mn1—N2—C1	−82.4 (2)	C1—N1—C8—C10	179.8 (3)
Cl2—Mn1—N2—C1	−177.99 (19)	Mn1—N1—C8—C10	−3.1 (7)
N1—Mn1—N2—C1	0.36 (18)	C6—C7—C8—N1	−0.3 (6)
Cl1—Mn1—N2—C1	80.9 (2)	C6—C7—C8—C10	−179.4 (4)
N2—Mn1—N4—C18	−35.6 (5)	C18—N4—C11—N5	−177.5 (3)
N5—Mn1—N4—C18	177.5 (5)	Mn1—N4—C11—N5	1.7 (3)
Cl2—Mn1—N4—C18	62.6 (5)	C18—N4—C11—C15	2.4 (5)
N1—Mn1—N4—C18	−91.8 (5)	Mn1—N4—C11—C15	−178.4 (3)
Cl1—Mn1—N4—C18	179.8 (4)	C12—N5—C11—N4	180.0 (3)
N2—Mn1—N4—C11	145.8 (2)	Mn1—N5—C11—N4	−1.8 (3)
N5—Mn1—N4—C11	−1.12 (19)	C12—N5—C11—C15	0.1 (5)
Cl2—Mn1—N4—C11	−115.98 (19)	Mn1—N5—C11—C15	178.4 (3)
N1—Mn1—N4—C11	89.6 (2)	C11—N5—C12—N6	179.7 (3)
Cl1—Mn1—N4—C11	1.2 (3)	Mn1—N5—C12—N6	2.7 (7)
N2—Mn1—N5—C12	119.4 (4)	C11—N5—C12—C13	−0.6 (5)
N4—Mn1—N5—C12	178.5 (5)	Mn1—N5—C12—C13	−177.6 (3)
Cl2—Mn1—N5—C12	−101.3 (4)	N5—C12—C13—C14	0.5 (6)
N1—Mn1—N5—C12	90.3 (4)	N6—C12—C13—C14	−179.8 (4)
Cl1—Mn1—N5—C12	−0.5 (4)	C12—C13—C14—C15	0.1 (6)
N2—Mn1—N5—C11	−58.0 (3)	N4—C11—C15—C16	0.2 (5)
N4—Mn1—N5—C11	1.11 (18)	N5—C11—C15—C16	180.0 (3)
Cl2—Mn1—N5—C11	81.3 (2)	N4—C11—C15—C14	−179.4 (3)
N1—Mn1—N5—C11	−87.1 (2)	N5—C11—C15—C14	0.4 (5)
Cl1—Mn1—N5—C11	−177.80 (19)	C13—C14—C15—C16	180.0 (4)
C2—N2—C1—N1	−179.2 (3)	C13—C14—C15—C11	−0.5 (5)
Mn1—N2—C1—N1	−0.6 (3)	C11—C15—C16—C17	−1.7 (5)
C2—N2—C1—C5	0.8 (5)	C14—C15—C16—C17	177.8 (4)
Mn1—N2—C1—C5	179.5 (3)	C11—C15—C16—C19	179.2 (3)
C8—N1—C1—N2	179.1 (3)	C14—C15—C16—C19	−1.3 (6)
Mn1—N1—C1—N2	0.5 (3)	C15—C16—C17—C18	0.9 (6)
C8—N1—C1—C5	−0.9 (5)	C19—C16—C17—C18	179.9 (4)
Mn1—N1—C1—C5	−179.5 (3)	C11—N4—C18—C17	−3.3 (5)
C1—N2—C2—N3	178.2 (3)	Mn1—N4—C18—C17	178.3 (3)
Mn1—N2—C2—N3	0.3 (6)	C11—N4—C18—C20	175.6 (3)
C1—N2—C2—C3	−1.4 (5)	Mn1—N4—C18—C20	−2.8 (7)
Mn1—N2—C2—C3	−179.4 (3)	C16—C17—C18—N4	1.7 (6)
N2—C2—C3—C4	1.1 (6)	C16—C17—C18—C20	−177.1 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···Cl1^{i}	0.82	2.35	3.162 (3)	169
O1—H1···Cl1^{ii}	0.82	2.41	3.183 (3)	158
N6—H6B···O1	0.86	2.10	2.960 (4)	173
N6—H6A···Cl1	0.86	2.55	3.359 (4)	158
N3—H3B···O2^{iii}	0.86	2.04	2.895 (4)	175

N3—H3A···Cl2	0.86	2.49	3.318 (4)	161

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

Fig. 1

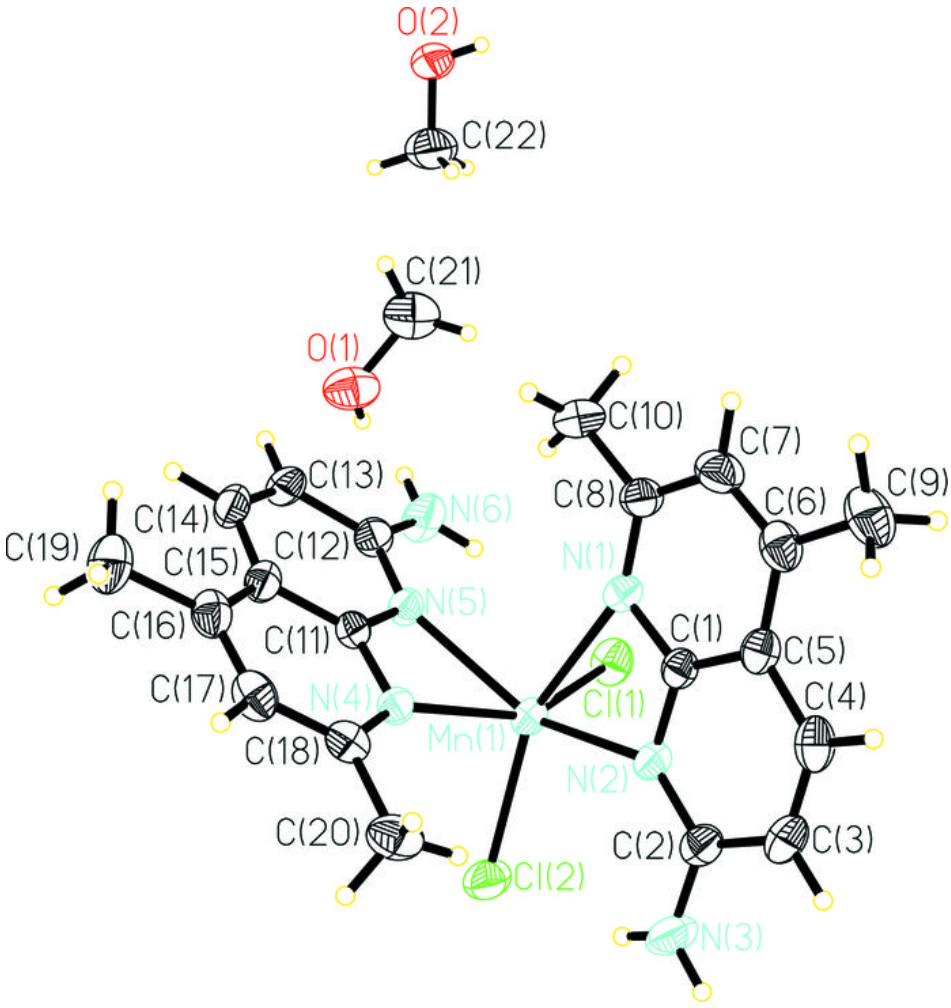

Fig. 2