metal-organic compounds

[Bis(1*H*-benzimidazol-2-ylmethyl)amine-$\kappa^3 N,N',N''$]dichlorido(methanol)-manganese(II)

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In the title compound, $[MnCl_2(C_{16}H_{15}N_5)(CH_4O)]$, the manganese(II) cation is six-coordinate, forming a distorted octahedral configuration with bis(1*H*-benzimidazol-2-yl-methyl)amine (IDB) serving as a neutral tridentate chelating ligand. Two imine and one amine N atoms from IDB and one Cl anion form the equatorial plane. The two axial positions are occupied by the methanol O atom and the other Cl anion. By a combination of two N–H···Cl and one O–H···Cl hydrogen bonds, molecules are linked into a three-dimensional network which is strengthened by weak C—H···π and π–π interactions [interplanar spacing = 3.343 (1) Å, ring-centroid separation = 3.728 (3) Å, corresponding to a ring offset of 1.650 (1) Å].

Related literature

For related literature, see: Calderazzo *et al.* (2003); Gross *et al.* (2000); Liao *et al.* (2000); Meng *et al.* (2006*a,b*); Xu *et al.* (2003); Yu *et al.* (2006).
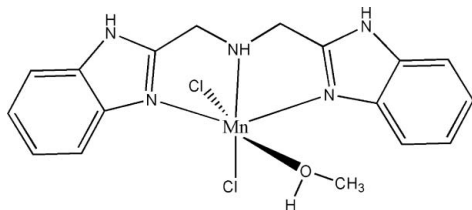
Experimental

Crystal data

$[MnCl_2(C_{16}H_{15}N_5)(CH_4O)]$
M_r = 435.21
Monoclinic, $P2_1/n$
a = 7.2064 (6) Å
b = 13.8208 (11) Å
c = 19.3825 (15) Å
β = 100.608 (2)°
V = 1897.5 (3) Å³
Z = 4
Mo $K\alpha$ radiation
μ = 0.99 mm⁻¹
T = 297 (2) K
$0.20 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.826, T_{max} = 0.907
14752 measured reflections
4112 independent reflections
2639 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.129
S = 0.95
4112 reflections
248 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.52 e Å⁻³
$\Delta\rho_{min}$ = −0.35 e Å⁻³

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

$Cg1$ is the centroid of the C11–C16 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···Cl1[i]	0.842 (18)	2.43 (2)	3.215 (3)	156 (3)
N2—H2A···Cl1[ii]	0.871 (18)	2.49 (3)	3.233 (3)	144 (3)
O1—H1C···Cl1[iii]	0.80 (5)	2.34 (5)	3.129 (3)	168 (5)
C6—H6···$Cg1$[iv]	0.93	2.75	3.354 (5)	124

Symmetry codes: (i) $-x + \frac{5}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 2, -y + 1, -z$; (iii) $x - 1, y, z$; (iv) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 2001); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2061).

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supplementary materials

[Bis(1*H*-benzimidazol-2-ylmethyl)amine-$\kappa^3 N,N',N''$]dichlorido(methanol)manganese(II)

H. Zhang, A. Wumaierjiang and X.-G. Meng

Comment

Di(2-benzimidazolylmethyl)imine (IDB) is a very often used organic N-containing ligand in preparing for metal model complexes aming to mimic the active sites found in natural metalloproteins (Calderazzo *et al.*, 2003; Xu *et al.*, 2003; Gross *et al.*, 2000). In a continuation of our studies on the molecular and supramolecular structure in IDB-containing analogas (Meng *et al.*, 2006*a*, 2006*b*; Yu *et al.*, 2006; Liao *et al.*, 2000), now we report the structure of the **I**.

Compound **I** have similar unit-cell parameters to the earlier reported ferrous complex (Calderazzo *et al.*, 2003). However, except for the discussion of the metal coordination bond lengths and bond angles in earlier paper, no any description involved with the crystall packing has been given. As expected, the Mn(II) cation in **I** displays a distorted octahedral coordination geometry which is very simiar to the recently reported analog in which the coordinated ethanol molecule is displaced by methanol here (Yu *et al.*, 2006). Atoms N1/N3/N5/Cl2 from the equatorial plane and the axial positions are occupied by methanol O atom and the Cl1 anion (Fig.1). The Mn—N$_{amine}$ distance is about 0.22Å longer than those between the Mn—N$_{imine}$ distance. The Mn—Cl bond length involving the axial atom Cl1 is about 0.21Å longer than that involving the equatorial atom Cl2.

In the supramolecular structrue formed by a combination of N(O)···Cl1 hydrogen bonds, C–H···π and π···π interactions, molecules are linked into a three-dimensional network which can be easily analyzed in terms of several substructures listed below.

Firstly, methanol O1 atom in the initial molecule (*x*, *y*, *z*) acting as H-bonding donor, *via* H1C, to the equatorial Cl1^{iii} atom so forming by tranlation a one-dimensional chain running parallel to the [1 0 0] direction. Similarly, imine N4 atom in the initial molecule acts as H-bonding donor to another Cl1^i atom, producing the other one-dimensional chains along the [0 1 0] direction, but this time generated by the 2_1 axis. These two types of H-bondings suffices linked the molecules **I** into a two-dimensional network (Fig.2) running parallel to the [0 0 1] direction.

Secondly, the third H-bonding N2–H2A···Cl1^{ii} linked the reference and symmetry related molecules into a centrosymmetric $R_2^2(16)$ ring centered at (1, 1/2, 0). Propagation by inversion of this interaction then generates the simple three-dimensional network (Fig.3).

The crystal packing is stablized by C–H···π and π–π interactions. The initial N2/N3/C2/C3/C8 imidazole ring and N2^{iv}/N3^{iv}/C2^{iv}/C3^{iv}/C8^{iv} have an interplanar spacing of 3.343 (1) Å; the ring-centroid separation is 3.728 (3) Å, corresponding to a ring offset of 1.650 (1) Å. Symmetry codes: (i) 5/2 − *x*, 1/2 + *y*, 1/2 − *z*; (ii) 2 − *x*,1 − *y*,-*z*; (iii) *x* − 1, *y*, *z*; (iv) 1 − *x*, 1 − *y*,-*z*.

supplementary materials

Experimental

All reagents and solvents were used as obtained without further purification. Compound **I** was synthesized by refluxing stoichiometric quantities (1:1 molar ratio) of IDB (0.28 g, 1.0 mmol) and manganese(II) chloride tetrahydrate (0.20 g, 1 mmol) in methanol (20 ml) at 333 K for 2 h. The solution was cooled to room temperature, filtered and evaporated to obtain the product (yield 40%). Block colourless crystals of **I** suitable for X-ray single-crystal diffraction were grown by slow evaporation of the methanol solution.

Refinement

H atoms bonded to carbon atoms were located at the geometrical positions with C–H = 0.93Å (aromatic), 0.97Å (methylene) and 0.96Å (methyl); Uĩso~(H) = 1.2U~eq~(aromatic and methylene C) and $1.5U_{eq}$(methyl C). All the other H atoms were located from the difference maps with the constraints of $U_{iso}(H) = 1.2U_{eq}(N)$ or $1.5U_{eq}(O)$ and the N (or O)–H distances were refined freely. *Cg*1 is the centroid defined by phenyl atoms C11/C16.
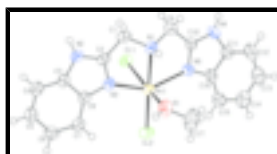
Figures

Fig. 1. Molecular structure of **I**, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The H atoms are presented as spheres at arbitrary radius.
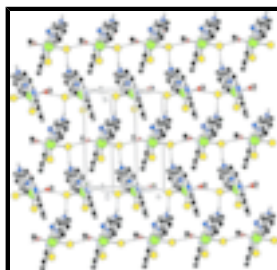
Fig. 2. Part of the crystal structure of **I**, showing the formation of the two-dimensional network running parallel to the [0 0 1] direction. Hydrogen bonding are shown as dashed lines. For the sake of clarity, H atoms not involved in the motif have been omitted.
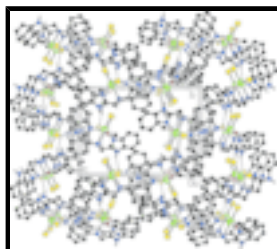
Fig. 3. Part of the crystal structure of **I**, showing the formation of the three-dimensional network. Hydrogen bonding are shown as dashed lines. For the sake of clarity, H atoms not involved in the motif have been omitted.

[Bis(1*H*-benzimidazol-2-ylmethyl)amine- κ³*N*,*N*',*N*'']dichlorido(methanol)manganese(II)

Crystal data

[MnCl₂(C₁₆H₁₅N₅)(CH₄O)]	$F_{000} = 892$
$M_r = 435.21$	$D_x = 1.523$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo *K*α radiation

Hall symbol: -P 2yn

$a = 7.2064\ (6)$ Å

$b = 13.8208\ (11)$ Å

$c = 19.3825\ (15)$ Å

$\beta = 100.608\ (2)°$

$V = 1897.5\ (3)$ Å^3

$Z = 4$

$\lambda = 0.71073$ Å

Cell parameters from 752 reflections

$\theta = 2.6–21.0°$

$\mu = 0.99$ mm^{-1}

$T = 297\ (2)$ K

Block, colorless

$0.20 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine focus sealed Siemens Mo tube

Monochromator: graphite

$T = 297(2)$ K

0.3° wide ω–scans

Absorption correction: multi-scan (SADABS; (Sheldrick, 2001)

$T_{min} = 0.826$, $T_{max} = 0.907$

14752 measured reflections

4112 independent reflections

2639 reflections with $I > 2\sigma(I)$

$R_{int} = 0.068$

$\theta_{max} = 27.0°$

$\theta_{min} = 1.8°$

$h = -9 \rightarrow 9$

$k = -17 \rightarrow 17$

$l = -23 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.129$

$S = 0.95$

4112 reflections

248 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.52$ e Å^{-3}

$\Delta\rho_{min} = -0.35$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Mn1	0.91501 (7)	0.48326 (3)	0.21677 (3)	0.03220 (17)
C1	0.8660 (5)	0.6318 (2)	0.08502 (18)	0.0388 (8)
H1A	0.9896	0.6395	0.0726	0.047*
H1B	0.7838	0.6819	0.0612	0.047*
C2	0.7881 (5)	0.5346 (2)	0.06223 (17)	0.0342 (8)
C3	0.6897 (5)	0.4104 (2)	−0.00642 (17)	0.0350 (8)
C4	0.6300 (5)	0.3455 (3)	−0.06046 (19)	0.0431 (9)
H4	0.6173	0.3638	−0.1073	0.052*
C5	0.5906 (5)	0.2535 (3)	−0.0419 (2)	0.0479 (10)
H5	0.5513	0.2080	−0.0769	0.058*
C6	0.6082 (5)	0.2261 (3)	0.0288 (2)	0.0476 (10)
H6	0.5803	0.1628	0.0396	0.057*
C7	0.6658 (5)	0.2910 (3)	0.08260 (19)	0.0433 (9)
H7	0.6758	0.2729	0.1294	0.052*
C8	0.7082 (5)	0.3840 (2)	0.06417 (17)	0.0338 (8)
C9	1.0263 (6)	0.7083 (3)	0.19505 (18)	0.0469 (10)
H9A	0.9746	0.7732	0.1950	0.056*
H9B	1.1301	0.7096	0.1696	0.056*
C10	1.0954 (5)	0.6761 (2)	0.26850 (17)	0.0372 (8)
C11	1.2508 (5)	0.6760 (2)	0.37731 (19)	0.0392 (9)
C12	1.3639 (6)	0.6942 (3)	0.4423 (2)	0.0540 (11)
H12	1.4338	0.7509	0.4511	0.065*
C13	1.3668 (6)	0.6248 (3)	0.4922 (2)	0.0564 (11)
H13	1.4383	0.6353	0.5366	0.068*
C14	1.2677 (6)	0.5393 (3)	0.4793 (2)	0.0557 (11)
H14	1.2742	0.4939	0.5151	0.067*
C15	1.1584 (6)	0.5197 (3)	0.4140 (2)	0.0461 (9)
H15	1.0923	0.4619	0.4052	0.055*
C16	1.1519 (5)	0.5898 (2)	0.36275 (18)	0.0368 (8)
C17	0.6031 (7)	0.5393 (5)	0.3127 (3)	0.0925 (18)
H17A	0.7198	0.5321	0.3454	0.139*
H17B	0.5121	0.4941	0.3241	0.139*
H17C	0.5565	0.6040	0.3153	0.139*
Cl1	1.22979 (12)	0.45919 (6)	0.16820 (5)	0.0397 (2)
Cl2	0.92642 (16)	0.32687 (7)	0.27362 (5)	0.0570 (3)
N1	0.8810 (4)	0.6417 (2)	0.16111 (15)	0.0381 (7)
H1D	0.779 (3)	0.660 (3)	0.1722 (18)	0.046*
N2	0.7420 (4)	0.5069 (2)	−0.00540 (15)	0.0390 (7)
H2A	0.753 (5)	0.543 (2)	−0.0413 (14)	0.047*
N3	0.7698 (4)	0.46425 (19)	0.10614 (14)	0.0341 (7)
N4	1.2130 (4)	0.7290 (2)	0.31645 (17)	0.0445 (8)
H4A	1.238 (5)	0.7869 (15)	0.3082 (18)	0.053*
N5	1.0545 (4)	0.59134 (19)	0.29307 (14)	0.0344 (7)
O1	0.6339 (4)	0.5209 (2)	0.24405 (15)	0.0537 (8)
H1C	0.538 (7)	0.498 (3)	0.222 (3)	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0362 (3)	0.0311 (3)	0.0296 (3)	−0.0019 (2)	0.0069 (2)	0.0009 (2)
C1	0.037 (2)	0.039 (2)	0.041 (2)	0.0014 (16)	0.0091 (16)	0.0113 (16)
C2	0.032 (2)	0.039 (2)	0.0318 (19)	0.0018 (15)	0.0055 (15)	0.0052 (15)
C3	0.0258 (19)	0.047 (2)	0.0329 (19)	0.0029 (15)	0.0074 (15)	−0.0024 (16)
C4	0.040 (2)	0.055 (2)	0.036 (2)	0.0002 (18)	0.0122 (17)	−0.0039 (17)
C5	0.046 (2)	0.054 (2)	0.045 (2)	−0.0026 (19)	0.0109 (18)	−0.0135 (19)
C6	0.044 (2)	0.043 (2)	0.057 (3)	−0.0089 (18)	0.0147 (19)	−0.0004 (19)
C7	0.045 (2)	0.048 (2)	0.038 (2)	−0.0049 (18)	0.0123 (17)	0.0033 (17)
C8	0.0249 (18)	0.044 (2)	0.0323 (18)	−0.0026 (15)	0.0045 (14)	0.0004 (15)
C9	0.062 (3)	0.035 (2)	0.046 (2)	−0.0116 (18)	0.015 (2)	0.0004 (17)
C10	0.044 (2)	0.034 (2)	0.036 (2)	−0.0037 (15)	0.0146 (17)	−0.0064 (15)
C11	0.035 (2)	0.039 (2)	0.044 (2)	−0.0013 (16)	0.0108 (17)	−0.0080 (17)
C12	0.045 (3)	0.058 (3)	0.058 (3)	−0.007 (2)	0.005 (2)	−0.021 (2)
C13	0.053 (3)	0.058 (3)	0.052 (3)	0.007 (2)	−0.007 (2)	−0.011 (2)
C14	0.061 (3)	0.058 (3)	0.047 (2)	0.012 (2)	0.004 (2)	0.004 (2)
C15	0.050 (2)	0.039 (2)	0.049 (2)	0.0008 (18)	0.0064 (19)	−0.0021 (18)
C16	0.036 (2)	0.038 (2)	0.038 (2)	0.0001 (15)	0.0099 (16)	−0.0084 (16)
C17	0.066 (3)	0.147 (5)	0.072 (3)	−0.011 (3)	0.033 (3)	−0.042 (3)
Cl1	0.0371 (5)	0.0421 (5)	0.0412 (5)	0.0014 (4)	0.0109 (4)	0.0014 (4)
Cl2	0.0804 (8)	0.0424 (6)	0.0490 (6)	−0.0045 (5)	0.0138 (5)	0.0134 (4)
N1	0.0419 (19)	0.0393 (17)	0.0360 (17)	−0.0008 (14)	0.0150 (14)	−0.0014 (13)
N2	0.0452 (19)	0.0418 (18)	0.0307 (17)	0.0015 (14)	0.0088 (14)	0.0059 (13)
N3	0.0335 (17)	0.0389 (16)	0.0287 (15)	0.0015 (12)	0.0026 (12)	0.0006 (12)
N4	0.052 (2)	0.0340 (17)	0.050 (2)	−0.0144 (15)	0.0159 (16)	−0.0113 (15)
N5	0.0339 (17)	0.0329 (16)	0.0373 (16)	−0.0025 (12)	0.0087 (13)	−0.0051 (12)
O1	0.0311 (15)	0.077 (2)	0.0546 (18)	−0.0044 (14)	0.0127 (13)	−0.0170 (15)

Geometric parameters (Å, °)

Mn1—N5	2.209 (3)	C9—C10	1.487 (5)
Mn1—N3	2.222 (3)	C9—H9A	0.9700
Mn1—O1	2.247 (3)	C9—H9B	0.9700
Mn1—Cl2	2.4207 (10)	C10—N5	1.318 (4)
Mn1—N1	2.434 (3)	C10—N4	1.351 (4)
Mn1—Cl1	2.6322 (10)	C11—N4	1.373 (5)
C1—N1	1.465 (4)	C11—C16	1.390 (5)
C1—C2	1.492 (5)	C11—C12	1.391 (5)
C1—H1A	0.9700	C12—C13	1.361 (6)
C1—H1B	0.9700	C12—H12	0.9300
C2—N3	1.314 (4)	C13—C14	1.379 (6)
C2—N2	1.347 (4)	C13—H13	0.9300
C3—N2	1.385 (4)	C14—C15	1.389 (5)
C3—C4	1.386 (5)	C14—H14	0.9300
C3—C8	1.399 (4)	C15—C16	1.383 (5)
C4—C5	1.365 (5)	C15—H15	0.9300

C4—H4	0.9300	C16—N5	1.403 (4)
C5—C6	1.405 (5)	C17—O1	1.412 (5)
C5—H5	0.9300	C17—H17A	0.9600
C6—C7	1.380 (5)	C17—H17B	0.9600
C6—H6	0.9300	C17—H17C	0.9600
C7—C8	1.383 (5)	N1—H1D	0.839 (18)
C7—H7	0.9300	N2—H2A	0.871 (18)
C8—N3	1.399 (4)	N4—H4A	0.842 (18)
C9—N1	1.457 (4)	O1—H1C	0.80 (5)
N5—Mn1—N3	143.27 (10)	N5—C10—N4	112.7 (3)
N5—Mn1—O1	90.26 (10)	N5—C10—C9	123.7 (3)
N3—Mn1—O1	88.26 (10)	N4—C10—C9	123.6 (3)
N5—Mn1—Cl2	109.02 (8)	N4—C11—C16	105.6 (3)
N3—Mn1—Cl2	107.71 (8)	N4—C11—C12	132.2 (3)
O1—Mn1—Cl2	93.23 (8)	C16—C11—C12	122.2 (4)
N5—Mn1—N1	71.61 (10)	C13—C12—C11	116.5 (4)
N3—Mn1—N1	71.79 (10)	C13—C12—H12	121.8
O1—Mn1—N1	82.78 (10)	C11—C12—H12	121.8
Cl2—Mn1—N1	175.97 (8)	C12—C13—C14	122.4 (4)
N5—Mn1—Cl1	90.52 (7)	C12—C13—H13	118.8
N3—Mn1—Cl1	85.63 (8)	C14—C13—H13	118.8
O1—Mn1—Cl1	170.78 (8)	C13—C14—C15	121.3 (4)
Cl2—Mn1—Cl1	95.20 (4)	C13—C14—H14	119.3
N1—Mn1—Cl1	88.75 (7)	C15—C14—H14	119.3
N1—C1—C2	109.6 (3)	C16—C15—C14	117.2 (4)
N1—C1—H1A	109.7	C16—C15—H15	121.4
C2—C1—H1A	109.7	C14—C15—H15	121.4
N1—C1—H1B	109.7	C15—C16—C11	120.4 (3)
C2—C1—H1B	109.7	C15—C16—N5	130.3 (3)
H1A—C1—H1B	108.2	C11—C16—N5	109.3 (3)
N3—C2—N2	112.5 (3)	O1—C17—H17A	109.5
N3—C2—C1	123.5 (3)	O1—C17—H17B	109.5
N2—C2—C1	123.8 (3)	H17A—C17—H17B	109.5
N2—C3—C4	132.8 (3)	O1—C17—H17C	109.5
N2—C3—C8	105.1 (3)	H17A—C17—H17C	109.5
C4—C3—C8	122.1 (3)	H17B—C17—H17C	109.5
C5—C4—C3	117.0 (3)	C9—N1—C1	115.3 (3)
C5—C4—H4	121.5	C9—N1—Mn1	111.3 (2)
C3—C4—H4	121.5	C1—N1—Mn1	110.2 (2)
C4—C5—C6	121.5 (4)	C9—N1—H1D	107 (3)
C4—C5—H5	119.3	C1—N1—H1D	112 (3)
C6—C5—H5	119.3	Mn1—N1—H1D	100 (3)
C7—C6—C5	121.5 (4)	C2—N2—C3	107.8 (3)
C7—C6—H6	119.2	C2—N2—H2A	125 (2)
C5—C6—H6	119.2	C3—N2—H2A	127 (2)
C6—C7—C8	117.3 (3)	C2—N3—C8	105.6 (3)
C6—C7—H7	121.4	C2—N3—Mn1	116.9 (2)
C8—C7—H7	121.4	C8—N3—Mn1	134.2 (2)
C7—C8—C3	120.6 (3)	C10—N4—C11	107.6 (3)

C7—C8—N3	130.4 (3)	C10—N4—H4A	121 (2)
C3—C8—N3	108.9 (3)	C11—N4—H4A	131 (2)
N1—C9—C10	109.2 (3)	C10—N5—C16	104.8 (3)
N1—C9—H9A	109.8	C10—N5—Mn1	117.6 (2)
C10—C9—H9A	109.8	C16—N5—Mn1	136.0 (2)
N1—C9—H9B	109.8	C17—O1—Mn1	124.6 (3)
C10—C9—H9B	109.8	C17—O1—H1C	107 (4)
H9A—C9—H9B	108.3	Mn1—O1—H1C	121 (4)
N1—C1—C2—N3	−11.2 (5)	C1—C2—N3—C8	−175.0 (3)
N1—C1—C2—N2	173.9 (3)	N2—C2—N3—Mn1	162.9 (2)
N2—C3—C4—C5	179.5 (4)	C1—C2—N3—Mn1	−12.5 (4)
C8—C3—C4—C5	−0.4 (5)	C7—C8—N3—C2	−179.7 (4)
C3—C4—C5—C6	0.6 (5)	C3—C8—N3—C2	−0.4 (4)
C4—C5—C6—C7	0.0 (6)	C7—C8—N3—Mn1	22.3 (5)
C5—C6—C7—C8	−0.8 (5)	C3—C8—N3—Mn1	−158.4 (2)
C6—C7—C8—C3	1.0 (5)	N5—Mn1—N3—C2	14.7 (3)
C6—C7—C8—N3	−179.8 (3)	O1—Mn1—N3—C2	102.8 (3)
N2—C3—C8—C7	179.7 (3)	Cl2—Mn1—N3—C2	−164.4 (2)
C4—C3—C8—C7	−0.4 (5)	N1—Mn1—N3—C2	19.8 (2)
N2—C3—C8—N3	0.3 (4)	Cl1—Mn1—N3—C2	−70.3 (2)
C4—C3—C8—N3	−179.8 (3)	N5—Mn1—N3—C8	170.7 (3)
N1—C9—C10—N5	11.3 (5)	O1—Mn1—N3—C8	−101.2 (3)
N1—C9—C10—N4	−171.4 (3)	Cl2—Mn1—N3—C8	−8.3 (3)
N4—C11—C12—C13	179.2 (4)	N1—Mn1—N3—C8	175.9 (3)
C16—C11—C12—C13	−2.7 (6)	Cl1—Mn1—N3—C8	85.7 (3)
C11—C12—C13—C14	1.7 (6)	N5—C10—N4—C11	−0.7 (4)
C12—C13—C14—C15	−0.1 (7)	C9—C10—N4—C11	−178.3 (3)
C13—C14—C15—C16	−0.6 (6)	C16—C11—N4—C10	0.5 (4)
C14—C15—C16—C11	−0.4 (5)	C12—C11—N4—C10	178.9 (4)
C14—C15—C16—N5	−179.5 (4)	N4—C10—N5—C16	0.7 (4)
N4—C11—C16—C15	−179.3 (3)	C9—C10—N5—C16	178.2 (3)
C12—C11—C16—C15	2.1 (5)	N4—C10—N5—Mn1	−167.3 (2)
N4—C11—C16—N5	−0.1 (4)	C9—C10—N5—Mn1	10.2 (4)
C12—C11—C16—N5	−178.7 (3)	C15—C16—N5—C10	178.8 (4)
C10—C9—N1—C1	−150.7 (3)	C11—C16—N5—C10	−0.4 (4)
C10—C9—N1—Mn1	−24.3 (4)	C15—C16—N5—Mn1	−16.6 (6)
C2—C1—N1—C9	153.1 (3)	C11—C16—N5—Mn1	164.3 (2)
C2—C1—N1—Mn1	26.1 (3)	N3—Mn1—N5—C10	−12.2 (3)
N5—Mn1—N1—C9	22.7 (2)	O1—Mn1—N5—C10	−99.7 (3)
N3—Mn1—N1—C9	−154.0 (3)	Cl2—Mn1—N5—C10	166.8 (2)
O1—Mn1—N1—C9	115.4 (2)	N1—Mn1—N5—C10	−17.4 (2)
Cl1—Mn1—N1—C9	−68.2 (2)	Cl1—Mn1—N5—C10	71.2 (2)
N5—Mn1—N1—C1	151.9 (2)	N3—Mn1—N5—C16	−175.4 (3)
N3—Mn1—N1—C1	−24.8 (2)	O1—Mn1—N5—C16	97.2 (3)
O1—Mn1—N1—C1	−115.4 (2)	Cl2—Mn1—N5—C16	3.7 (3)
Cl1—Mn1—N1—C1	61.0 (2)	N1—Mn1—N5—C16	179.5 (3)
N3—C2—N2—C3	−0.3 (4)	Cl1—Mn1—N5—C16	−92.0 (3)
C1—C2—N2—C3	175.1 (3)	N5—Mn1—O1—C17	−40.7 (4)
C4—C3—N2—C2	−180.0 (4)	N3—Mn1—O1—C17	176.0 (4)

C8—C3—N2—C2	0.0 (4)	Cl2—Mn1—O1—C17	68.4 (4)
N2—C2—N3—C8	0.4 (4)	N1—Mn1—O1—C17	−112.1 (4)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···Cl1[i]	0.842 (18)	2.43 (2)	3.215 (3)	156 (3)
N2—H2A···Cl1[ii]	0.871 (18)	2.49 (3)	3.233 (3)	144 (3)
O1—H1C···Cl1[iii]	0.80 (5)	2.34 (5)	3.129 (3)	168 (5)
C6—H6···Cg1[iv]	0.93	2.75	3.354 (5)	124

Symmetry codes: (i) $-x+5/2, y+1/2, -z+1/2$; (ii) $-x+2, -y+1, -z$; (iii) $x-1, y, z$; (iv) $-x+3/2, y-1/2, -z+1/2$.
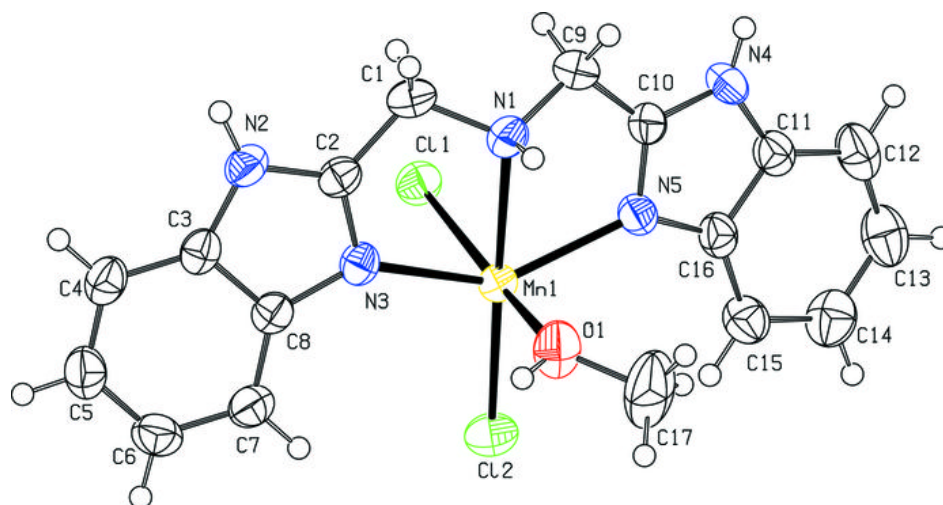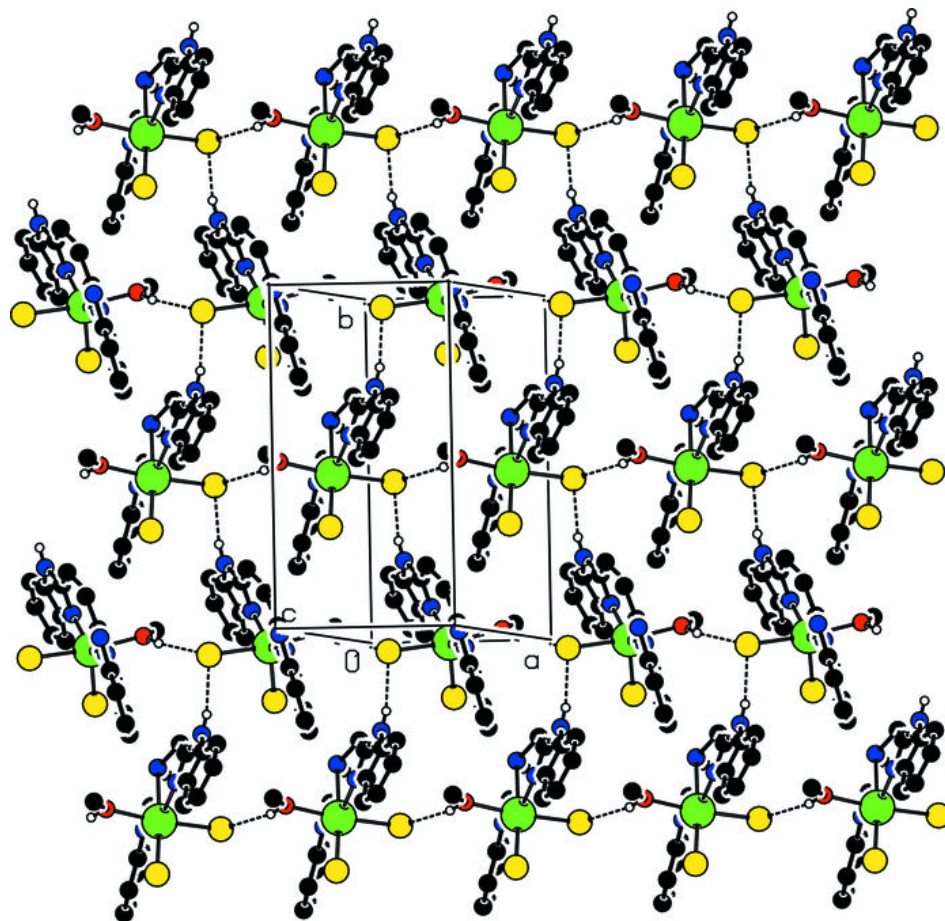
Fig. 1

Fig. 2

Fig. 3