

catena-Poly[[manganese(II)- μ -[*N,N,N',N'*-tetrakis(2-pyridylmethyl)hexane-1,6-diamine]] bis(perchlorate) acetone disolvate dihydrate]

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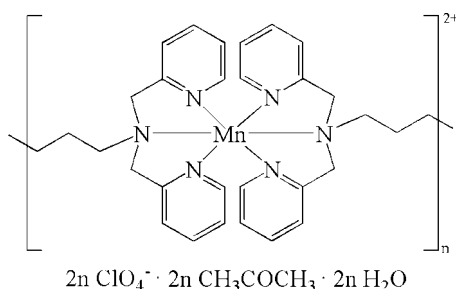
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Key indicators: single-crystal X-ray study; $T = 243$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; H-atom completeness 93%; R factor = 0.073; wR factor = 0.227; data-to-parameter ratio = 18.5.

The title compound, $[\text{Mn}(\text{C}_{30}\text{H}_{36}\text{N}_6)](\text{ClO}_4)_2 \cdot 2\text{C}_3\text{H}_6\text{O} \cdot 2\text{H}_2\text{O}$, consists of a cationic complex polymer with counter-anions and solvent molecules. In the cationic polymer, Mn^{2+} ions are bridged by the hexadentate ligand *N,N,N',N'*-tetrakis(2-pyridylmethyl)hexane-1,6-diamine (tphn) to form a one-dimensional chain structure along the c axis. The repeat unit of the polymer, $\text{Mn}^{\text{II}}(\text{tphn})$, is disposed about a twofold axis passing through the Mn atom. The coordination geometry around the Mn centre is distorted octahedral.

Related literature

For related literature, see: Jensen *et al.* (1997).



Experimental

Crystal data

$[\text{Mn}(\text{C}_{30}\text{H}_{36}\text{N}_6)](\text{ClO}_4)_2 \cdot 2\text{C}_3\text{H}_6\text{O} \cdot 2\text{H}_2\text{O}$
 $M_r = 886.68$
 Monoclinic, $C2/c$
 $a = 18.7266$ (16) Å
 $b = 14.5252$ (12) Å
 $c = 15.2375$ (13) Å

$\beta = 94.782$ (2) $^\circ$
 $V = 4130.3$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.52$ mm⁻¹
 $T = 243$ (2) K
 $0.20 \times 0.18 \times 0.15$ mm

Data collection

Bruker SMART 1000 CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\text{min}} = 0.707$, $T_{\text{max}} = 0.926$

16555 measured reflections
 4248 independent reflections
 2171 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.073$
 $wR(F^2) = 0.227$
 $S = 0.92$
 4248 reflections

230 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.86$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2266).

References

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 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
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supplementary materials

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catena-Poly[[manganese(II)- μ -[*N,N,N',N'*-tetrakis(2-pyridylmethyl)hexane-1,6-diamine]] bis(perchlorate) acetone disolvate dihydrate]

I.-C. Hwang and K. Ha

Comment

The title compound consists of cationic complex polymer with counter anions (ClO_4) and solvents (acetone and water). In the cation polymer, Mn^{2+} ions are bridged by the hexadentate ligand, *N,N,N',N'*-tetrakis(2-pyridylmethyl)-1,6-diaminohexane (tphn), and the constitutional repeating unit of the polymer, $\text{Mn}^{\text{II}}(\text{tphn})$, is disposed about a twofold axis passing through the Mn atom (Fig. 1). The Mn ion is six-coordinated in a distorted octahedral structure by three N atoms from one tphn ligand and three N atoms from another tphn ligand in the facial positions, respectively. The Mn—N(pyridyl) bond lengths (2.267 (4) and 2.217 (4) Å) are slightly longer than the Mn—N(amine) bond length (2.369 (4) Å). The polymer reveals a one-dimensional chain structure along the *c* axis (Fig. 2).

Experimental

To a solution of *N,N,N',N'*-tetrakis(2-pyridylmethyl)-1,6-diaminohexane (0.50 g, 1.04 mmol) in EtOH (15 ml) was added $\text{Mn}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (0.38 g, 1.05 mmol) and stirred for 1 h at room temperature. The formed precipitate was separated by filtration and washed with EtOH and dried, to give a dark yellow powder (0.48 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from a acetone/ H_2O (1:1) solution.

Refinement

H atoms were positioned geometrically and allowed to ride on their respective carrier atoms [C—H = 0.94 (aromatic), 0.98 (CH_2) or 0.97 Å (CH_3) and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ or $1.5U_{\text{eq}}$ (methyl C)]. The solvent molecules were highly disordered, and then the atoms of acetone and water were refined with isotropic thermal parameters, as a result it reflects on large value of the *R* factor. The H atoms of the solvent H_2O molecules could neither be located from Fourier difference maps nor added geometrically.

Figures

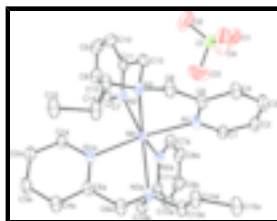


Fig. 1. The structure of the constitutional repeating unit of the title compound [Symmetry code: (*a*) $-x, y, 1/2 - z$]. Displacement ellipsoids are drawn at the 20% probability level. H atoms and the solvent molecules have been omitted for clarity.

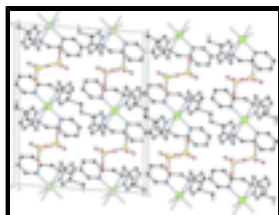


Fig. 2. View of the unit-cell contents and chain structure of the title compound. H atoms and the solvent molecules have been omitted for clarity.

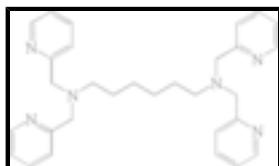


Fig. 3. The *N,N,N',N'*-tetrakis(2-pyridylmethyl)hexane-1,6-diamine ligand.

catena-Poly[[manganese(II)- μ -[*N,N,N',N'*-tetrakis(2-pyridylmethyl)hexane-1,6-diamine]] diperchlorate acetone disolvate dihydrate]

Crystal data

[Mn(C₃₀H₃₆N₆)](ClO₄)₂·2C₃H₆O·2H₂O

M_r = 886.68

Monoclinic, *C2/c*

Hall symbol: -C 2yc

a = 18.7266 (16) Å

b = 14.5252 (12) Å

c = 15.2375 (13) Å

β = 94.782 (2)°

V = 4130.3 (6) Å³

Z = 4

*F*₀₀₀ = 1860

D_x = 1.426 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 2085 reflections

θ = 2.2–21.0°

μ = 0.52 mm⁻¹

T = 243 (2) K

Block, yellow

0.20 × 0.18 × 0.15 mm

Data collection

Bruker SMART 1000 CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 243(2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2000)

*T*_{min} = 0.707, *T*_{max} = 0.926

16555 measured reflections

4248 independent reflections

2171 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.056

θ_{max} = 26.4°

θ_{min} = 1.8°

h = -23→22

k = -18→18

l = -19→12

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.073

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.227$	$w = 1/[\sigma^2(F_o^2) + (0.132P)^2]$
$S = 0.92$	where $P = (F_o^2 + 2F_c^2)/3$
4248 reflections	$(\Delta/\sigma)_{\max} < 0.001$
230 parameters	$\Delta\rho_{\max} = 0.86 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.49 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > \sigma(F^2)$ 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn	0.0000	0.26386 (6)	0.2500	0.0436 (3)
N1	0.0765 (2)	0.2265 (2)	0.1478 (2)	0.0488 (10)
N2	0.0500 (2)	0.3736 (2)	0.3356 (3)	0.0509 (10)
N3	0.1019 (2)	0.1940 (3)	0.3248 (2)	0.0523 (10)
C1	0.0736 (3)	0.2587 (3)	0.0651 (3)	0.0508 (12)
H1	0.0380	0.3022	0.0478	0.061*
C2	0.1189 (3)	0.2322 (4)	0.0046 (3)	0.0588 (13)
H2	0.1138	0.2562	-0.0529	0.071*
C3	0.1713 (3)	0.1710 (4)	0.0281 (3)	0.0688 (15)
H3	0.2030	0.1514	-0.0128	0.083*
C4	0.1773 (3)	0.1378 (4)	0.1134 (4)	0.0661 (15)
H4	0.2139	0.0961	0.1318	0.079*
C5	0.1285 (3)	0.1670 (3)	0.1715 (3)	0.0547 (13)
C6	0.1313 (3)	0.1281 (3)	0.2638 (3)	0.0637 (15)
H6A	0.1037	0.0707	0.2633	0.076*
H6B	0.1811	0.1138	0.2843	0.076*
C7	0.0191 (3)	0.4531 (3)	0.3588 (3)	0.0620 (14)
H7	-0.0277	0.4657	0.3345	0.074*
C8	0.0512 (4)	0.5154 (4)	0.4146 (4)	0.0718 (16)
H8	0.0276	0.5700	0.4285	0.086*
C9	0.1186 (4)	0.4969 (4)	0.4502 (4)	0.087 (2)
H9	0.1423	0.5393	0.4891	0.104*
C10	0.1522 (3)	0.4176 (5)	0.4301 (4)	0.0754 (17)
H10	0.1986	0.4045	0.4556	0.090*
C11	0.1176 (3)	0.3571 (3)	0.3721 (3)	0.0551 (13)

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C12	0.1520 (3)	0.2711 (4)	0.3387 (4)	0.0605 (13)
H12A	0.1722	0.2853	0.2829	0.073*
H12B	0.1915	0.2525	0.3811	0.073*
C13	0.0935 (3)	0.1483 (4)	0.4109 (3)	0.0632 (14)
H13A	0.1411	0.1307	0.4369	0.076*
H13B	0.0741	0.1936	0.4503	0.076*
C14	0.0467 (3)	0.0653 (3)	0.4084 (3)	0.0650 (15)
H14A	0.0723	0.0132	0.3846	0.078*
H14B	0.0036	0.0768	0.3690	0.078*
C15	0.0251 (3)	0.0406 (3)	0.4997 (4)	0.0738 (17)
H15A	0.0685	0.0267	0.5380	0.089*
H15B	0.0020	0.0941	0.5244	0.089*
Cl	0.23323 (9)	0.43776 (12)	0.17809 (10)	0.0844 (6)
O1	0.2592 (2)	0.4928 (3)	0.1128 (3)	0.1020 (15)
O2	0.2566 (4)	0.4597 (4)	0.2616 (3)	0.150 (3)
O3	0.1583 (3)	0.4373 (6)	0.1717 (5)	0.193 (4)
O4	0.2472 (4)	0.3424 (4)	0.1612 (4)	0.154 (2)
O1S	0.4558 (3)	0.2153 (4)	0.3938 (5)	0.139 (2)*
C1S	0.4137 (6)	0.2292 (8)	0.3337 (8)	0.150 (4)*
C2S	0.3836 (7)	0.1745 (10)	0.2604 (9)	0.231 (6)*
H2S1	0.3393	0.2025	0.2358	0.346*
H2S2	0.3738	0.1128	0.2807	0.346*
H2S3	0.4174	0.1714	0.2156	0.346*
C3S	0.3406 (7)	0.2371 (9)	0.3732 (9)	0.302 (10)*
H3S1	0.3151	0.2906	0.3488	0.453*
H3S2	0.3482	0.2436	0.4367	0.453*
H3S3	0.3125	0.1822	0.3591	0.453*
O1W	0.4390 (7)	0.3332 (9)	0.2678 (9)	0.416 (9)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn	0.0622 (7)	0.0285 (5)	0.0426 (6)	0.000	0.0197 (5)	0.000
N1	0.066 (3)	0.034 (2)	0.048 (2)	0.0046 (19)	0.0172 (19)	0.0045 (17)
N2	0.072 (3)	0.034 (2)	0.050 (2)	-0.0020 (18)	0.023 (2)	-0.0016 (17)
N3	0.077 (3)	0.040 (2)	0.043 (2)	0.013 (2)	0.021 (2)	0.0066 (17)
C1	0.069 (3)	0.041 (3)	0.044 (3)	-0.002 (2)	0.015 (2)	0.003 (2)
C2	0.077 (4)	0.061 (3)	0.040 (3)	-0.007 (3)	0.016 (3)	-0.002 (2)
C3	0.083 (4)	0.076 (4)	0.052 (3)	0.003 (3)	0.029 (3)	-0.010 (3)
C4	0.078 (4)	0.060 (3)	0.063 (4)	0.018 (3)	0.027 (3)	-0.006 (3)
C5	0.074 (3)	0.041 (3)	0.052 (3)	0.005 (2)	0.023 (3)	-0.003 (2)
C6	0.091 (4)	0.050 (3)	0.054 (3)	0.024 (3)	0.026 (3)	0.003 (2)
C7	0.090 (4)	0.040 (3)	0.060 (3)	0.001 (3)	0.025 (3)	-0.004 (2)
C8	0.120 (5)	0.044 (3)	0.055 (3)	-0.010 (3)	0.025 (4)	-0.010 (3)
C9	0.142 (7)	0.060 (4)	0.061 (4)	-0.029 (4)	0.018 (4)	-0.017 (3)
C10	0.084 (4)	0.084 (4)	0.058 (4)	-0.024 (3)	0.004 (3)	-0.007 (3)
C11	0.073 (4)	0.054 (3)	0.042 (3)	-0.008 (3)	0.020 (3)	0.004 (2)
C12	0.065 (3)	0.066 (3)	0.052 (3)	0.004 (3)	0.014 (3)	0.007 (3)

C13	0.090 (4)	0.058 (3)	0.044 (3)	0.023 (3)	0.020 (3)	0.011 (2)
C14	0.109 (4)	0.039 (3)	0.051 (3)	0.019 (3)	0.030 (3)	0.010 (2)
C15	0.128 (5)	0.043 (3)	0.054 (3)	0.024 (3)	0.031 (3)	0.018 (3)
Cl	0.0958 (12)	0.0966 (13)	0.0642 (10)	-0.0439 (9)	0.0265 (8)	-0.0183 (8)
O1	0.112 (3)	0.128 (4)	0.069 (3)	-0.052 (3)	0.022 (2)	-0.005 (3)
O2	0.236 (7)	0.152 (5)	0.067 (3)	-0.110 (5)	0.034 (4)	-0.023 (3)
O3	0.101 (4)	0.273 (10)	0.208 (8)	-0.031 (5)	0.041 (4)	0.073 (7)
O4	0.240 (7)	0.108 (5)	0.124 (5)	-0.010 (5)	0.079 (5)	-0.030 (4)

Geometric parameters (Å, °)

Mn—N2	2.217 (4)	C9—H9	0.9400
Mn—N2 ⁱ	2.217 (4)	C10—C11	1.370 (7)
Mn—N1 ⁱ	2.267 (4)	C10—H10	0.9400
Mn—N1	2.267 (4)	C11—C12	1.514 (7)
Mn—N3	2.369 (4)	C12—H12A	0.9800
Mn—N3 ⁱ	2.369 (4)	C12—H12B	0.9800
N1—C5	1.331 (6)	C13—C14	1.489 (7)
N1—C1	1.341 (6)	C13—H13A	0.9800
N2—C7	1.352 (6)	C13—H13B	0.9800
N2—C11	1.360 (6)	C14—C15	1.524 (7)
N3—C12	1.465 (6)	C14—H14A	0.9800
N3—C6	1.472 (6)	C14—H14B	0.9800
N3—C13	1.490 (6)	C15—C15 ⁱⁱ	1.509 (11)
C1—C2	1.360 (7)	C15—H15A	0.9800
C1—H1	0.9400	C15—H15B	0.9800
C2—C3	1.350 (7)	Cl—O2	1.349 (5)
C2—H2	0.9400	Cl—O1	1.395 (4)
C3—C4	1.382 (7)	Cl—O3	1.399 (6)
C3—H3	0.9400	Cl—O4	1.437 (6)
C4—C5	1.390 (6)	O1S—C1S	1.175 (11)
C4—H4	0.9400	C1S—C2S	1.446 (15)
C5—C6	1.513 (7)	C1S—C3S	1.546 (15)
C6—H6A	0.9800	C2S—H2S1	0.9700
C6—H6B	0.9800	C2S—H2S2	0.9700
C7—C8	1.349 (7)	C2S—H2S3	0.9700
C7—H7	0.9400	C3S—H3S1	0.9700
C8—C9	1.359 (8)	C3S—H3S2	0.9700
C8—H8	0.9400	C3S—H3S3	0.9700
C9—C10	1.359 (9)		
N2—Mn—N2 ⁱ	88.1 (2)	C8—C9—C10	120.7 (6)
N2—Mn—N1 ⁱ	91.59 (13)	C8—C9—H9	119.7
N2 ⁱ —Mn—N1 ⁱ	108.42 (14)	C10—C9—H9	119.7
N2—Mn—N1	108.42 (14)	C9—C10—C11	119.0 (6)
N2 ⁱ —Mn—N1	91.59 (13)	C9—C10—H10	120.5
N1 ⁱ —Mn—N1	152.33 (19)	C11—C10—H10	120.5
N2—Mn—N3	74.99 (14)	N2—C11—C10	121.7 (5)

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N2 ⁱ —Mn—N3	151.06 (14)	N2—C11—C12	114.5 (4)
N1 ⁱ —Mn—N3	95.57 (14)	C10—C11—C12	123.7 (5)
N1—Mn—N3	72.42 (13)	N3—C12—C11	113.2 (4)
N2—Mn—N3 ⁱ	151.06 (14)	N3—C12—H12A	108.9
N2 ⁱ —Mn—N3 ⁱ	74.98 (14)	C11—C12—H12A	108.9
N1 ⁱ —Mn—N3 ⁱ	72.42 (13)	N3—C12—H12B	108.9
N1—Mn—N3 ⁱ	95.57 (14)	C11—C12—H12B	108.9
N3—Mn—N3 ⁱ	129.2 (2)	H12A—C12—H12B	107.7
C5—N1—C1	116.9 (4)	C14—C13—N3	116.3 (4)
C5—N1—Mn	117.4 (3)	C14—C13—H13A	108.2
C1—N1—Mn	125.7 (3)	N3—C13—H13A	108.2
C7—N2—C11	116.6 (4)	C14—C13—H13B	108.2
C7—N2—Mn	126.8 (4)	N3—C13—H13B	108.2
C11—N2—Mn	116.6 (3)	H13A—C13—H13B	107.4
C12—N3—C6	108.7 (4)	C13—C14—C15	111.6 (5)
C12—N3—C13	109.1 (4)	C13—C14—H14A	109.3
C6—N3—C13	109.8 (4)	C15—C14—H14A	109.3
C12—N3—Mn	102.8 (3)	C13—C14—H14B	109.3
C6—N3—Mn	107.7 (3)	C15—C14—H14B	109.3
C13—N3—Mn	118.3 (3)	H14A—C14—H14B	108.0
N1—C1—C2	124.1 (5)	C15 ⁱⁱ —C15—C14	113.7 (6)
N1—C1—H1	118.0	C15 ⁱⁱ —C15—H15A	108.8
C2—C1—H1	118.0	C14—C15—H15A	108.8
C3—C2—C1	119.2 (5)	C15 ⁱⁱ —C15—H15B	108.8
C3—C2—H2	120.4	C14—C15—H15B	108.8
C1—C2—H2	120.4	H15A—C15—H15B	107.7
C2—C3—C4	118.7 (5)	O2—Cl—O1	115.6 (3)
C2—C3—H3	120.7	O2—Cl—O3	108.1 (5)
C4—C3—H3	120.7	O1—Cl—O3	111.1 (4)
C3—C4—C5	119.1 (5)	O2—Cl—O4	110.3 (4)
C3—C4—H4	120.5	O1—Cl—O4	110.2 (3)
C5—C4—H4	120.5	O3—Cl—O4	100.4 (5)
N1—C5—C4	122.1 (5)	O1S—C1S—C2S	134.4 (12)
N1—C5—C6	117.6 (4)	O1S—C1S—C3S	105.5 (11)
C4—C5—C6	120.3 (5)	C2S—C1S—C3S	92.3 (9)
N3—C6—C5	111.0 (4)	C1S—C2S—H2S1	109.5
N3—C6—H6A	109.4	C1S—C2S—H2S2	109.5
C5—C6—H6A	109.4	H2S1—C2S—H2S2	109.5
N3—C6—H6B	109.4	C1S—C2S—H2S3	109.5
C5—C6—H6B	109.4	H2S1—C2S—H2S3	109.5
H6A—C6—H6B	108.0	H2S2—C2S—H2S3	109.5
C8—C7—N2	124.1 (6)	C1S—C3S—H3S1	109.5
C8—C7—H7	118.0	C1S—C3S—H3S2	109.5
N2—C7—H7	118.0	H3S1—C3S—H3S2	109.5
C7—C8—C9	117.9 (6)	C1S—C3S—H3S3	109.5
C7—C8—H8	121.0	H3S1—C3S—H3S3	109.5
C9—C8—H8	121.0	H3S2—C3S—H3S3	109.5

N2—Mn—N1—C5	83.1 (4)	Mn—N1—C1—C2	-177.6 (4)
N2 ⁱ —Mn—N1—C5	171.6 (3)	N1—C1—C2—C3	-1.2 (8)
N1 ⁱ —Mn—N1—C5	-51.2 (3)	C1—C2—C3—C4	-0.5 (8)
N3—Mn—N1—C5	16.1 (3)	C2—C3—C4—C5	1.3 (8)
N3 ⁱ —Mn—N1—C5	-113.4 (3)	C1—N1—C5—C4	-1.0 (7)
N2—Mn—N1—C1	-97.5 (4)	Mn—N1—C5—C4	178.5 (4)
N2 ⁱ —Mn—N1—C1	-9.0 (4)	C1—N1—C5—C6	-178.4 (4)
N1 ⁱ —Mn—N1—C1	128.2 (4)	Mn—N1—C5—C6	1.1 (6)
N3—Mn—N1—C1	-164.4 (4)	C3—C4—C5—N1	-0.6 (8)
N3 ⁱ —Mn—N1—C1	66.1 (4)	C3—C4—C5—C6	176.8 (5)
N2 ⁱ —Mn—N2—C7	40.4 (3)	C12—N3—C6—C5	-70.6 (5)
N1 ⁱ —Mn—N2—C7	-67.9 (4)	C13—N3—C6—C5	170.2 (4)
N1—Mn—N2—C7	131.5 (4)	Mn—N3—C6—C5	40.1 (5)
N3—Mn—N2—C7	-163.3 (4)	N1—C5—C6—N3	-29.4 (7)
N3 ⁱ —Mn—N2—C7	-13.0 (5)	C4—C5—C6—N3	153.2 (5)
N2 ⁱ —Mn—N2—C11	-143.1 (4)	C11—N2—C7—C8	0.3 (7)
N1 ⁱ —Mn—N2—C11	108.5 (3)	Mn—N2—C7—C8	176.7 (4)
N1—Mn—N2—C11	-52.1 (3)	N2—C7—C8—C9	-0.4 (8)
N3—Mn—N2—C11	13.1 (3)	C7—C8—C9—C10	-0.3 (9)
N3 ⁱ —Mn—N2—C11	163.5 (3)	C8—C9—C10—C11	1.1 (9)
N2—Mn—N3—C12	-30.5 (3)	C7—N2—C11—C10	0.6 (7)
N2 ⁱ —Mn—N3—C12	25.7 (4)	Mn—N2—C11—C10	-176.2 (4)
N1 ⁱ —Mn—N3—C12	-120.7 (3)	C7—N2—C11—C12	-175.4 (4)
N1—Mn—N3—C12	84.8 (3)	Mn—N2—C11—C12	7.8 (5)
N3 ⁱ —Mn—N3—C12	167.5 (3)	C9—C10—C11—N2	-1.2 (8)
N2—Mn—N3—C6	-145.2 (3)	C9—C10—C11—C12	174.4 (5)
N2 ⁱ —Mn—N3—C6	-89.0 (4)	C6—N3—C12—C11	159.4 (4)
N1 ⁱ —Mn—N3—C6	124.7 (3)	C13—N3—C12—C11	-80.9 (5)
N1—Mn—N3—C6	-29.8 (3)	Mn—N3—C12—C11	45.5 (4)
N3 ⁱ —Mn—N3—C6	52.8 (3)	N2—C11—C12—N3	-38.9 (6)
N2—Mn—N3—C13	89.7 (3)	C10—C11—C12—N3	145.2 (5)
N2 ⁱ —Mn—N3—C13	145.9 (3)	C12—N3—C13—C14	-177.3 (4)
N1 ⁱ —Mn—N3—C13	-0.5 (4)	C6—N3—C13—C14	-58.3 (6)
N1—Mn—N3—C13	-155.0 (4)	Mn—N3—C13—C14	65.8 (5)
N3 ⁱ —Mn—N3—C13	-72.3 (3)	N3—C13—C14—C15	-164.0 (4)
C5—N1—C1—C2	1.9 (7)	C13—C14—C15—C15 ⁱⁱ	177.3 (6)

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

Fig. 1

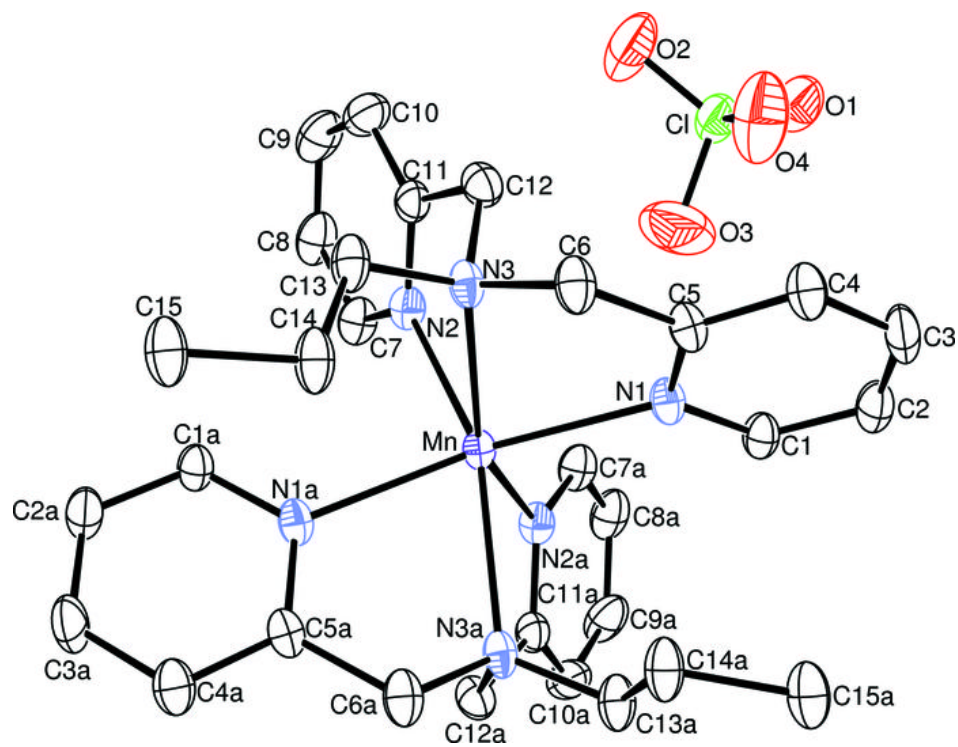


Fig. 2

