

Poly[di- μ -*cis*-cyclohexane-1,4-dicarboxylato- μ -*trans*-cyclohexane-1,4-dicarboxylato-bis[dipyrido[3,2-*a*:2',3'-*c*]-phenazine]trimanganese(II)]

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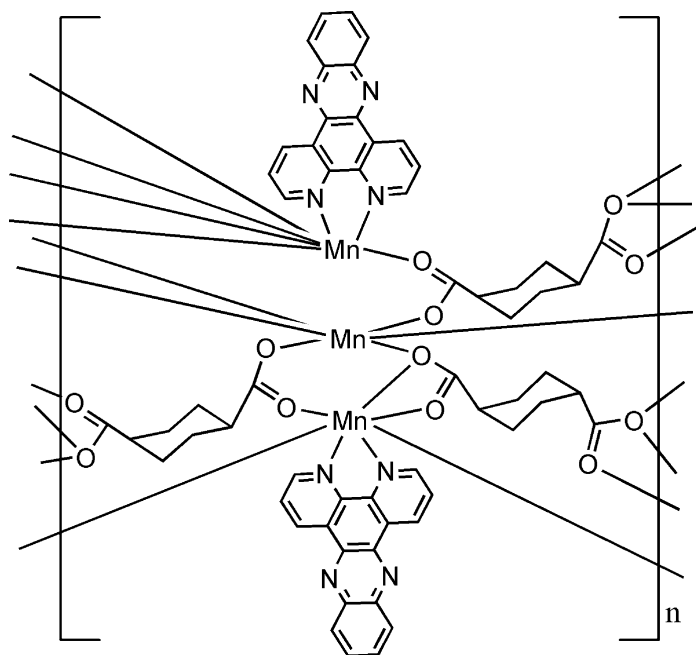
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.060; wR factor = 0.176; data-to-parameter ratio = 15.5.

In the title compound, $[\text{Mn}_3(\text{C}_8\text{H}_{10}\text{O}_4)_3(\text{C}_{18}\text{H}_{10}\text{N}_4)_2]$, one Mn atom and one cyclohexane-1,4-dicarboxylate (chdc) ligand are located on centres of inversion. One of the two independent Mn atoms is seven-coordinate, binding to five carboxylate O atoms from different chdc ligands and two phenanthrene N atoms from a dipyrido[3,2-*a*:2',3'-*c*]phenazine (*L*) ligand, while the second Mn atom is six-coordinate, binding to six carboxylate O atoms from different chdc ligands. The *cis*-chdc ligands bridge the trinuclear Mn^{II} clusters, forming chains, which are further linked into a three-dimensional network.

Related literature

For related structures, see: De (2007); Li (2007).



Experimental

Crystal data

$[\text{Mn}_3(\text{C}_8\text{H}_{10}\text{O}_4)_3(\text{C}_{18}\text{H}_{10}\text{N}_4)_2]$
 $M_r = 1239.90$
Triclinic, $P\bar{1}$
 $a = 8.5730$ (17) Å
 $b = 10.614$ (2) Å
 $c = 14.846$ (3) Å
 $\alpha = 77.34$ (3)°
 $\beta = 81.99$ (3)°

$\gamma = 82.67$ (3)°
 $V = 1298.6$ (4) Å³
 $Z = 1$
Mo $K\alpha$ radiation
 $\mu = 0.80$ mm⁻¹
 $T = 293$ (2) K
0.33 × 0.22 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID
diffractometer
Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.762$, $T_{\max} = 0.863$

12776 measured reflections
5830 independent reflections
3707 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.176$
 $S = 1.05$
5830 reflections

376 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.64$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.74$ e Å⁻³

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); 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: BT2704).

References

- De, G. (2007). *Acta Cryst.* **E63**, m1748–m1749.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Li, Y.-J. (2007). *Acta Cryst.* **E63**, m1654–m1655.
- Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2008). E64, m781-m782 [doi:10.1107/S1600536808012737]

Poly[di- μ -cis-cyclohexane-1,4-dicarboxylato- μ -trans-cyclohexane-1,4-dicarboxylato-bis[dipyrido[3,2-*a*:2',3'-*c*]phenazine]trimanganese(II)]

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Comment

1,4-Cyclohexanedicarboxylic acid (H₂chdc), as a flexible multidentate ligand, has been extensively studied in the chemistry of coordination polymers (De, 2007; Li, 2007). Here, we report a new Mn^{II} coordination polymer with chdc ligand, namely [Mn₃(cis-chdc)₃(trans-chdc)(*L*)₂] (I), where *L* = dipyrido[3,2-*a*:2',3'-*c*]-phenazine.

In (I) the Mn1 atom is seven-coordinate binding to five carboxylate O atoms from different chdc ligands, and two phenanthrene N atoms from *L* ligand (Fig. 1 and Table 1). The Mn2 atom is six-coordinate binding to six carboxylate O atoms from different chdc ligands (Fig. 1 and Table 1). Interestingly, the chdc ligands bridge neighboring Mn^{II} atoms to give a trinuclear Mn^{II} cluster. The cis-chdc ligands bridge the trinuclear Mn^{II} clusters to form a chain structure, which are further linked into a 3D network structure (Fig. 2). One Mn atom and one 1,4-cyclohexanedicarboxylate molecule are located on a centre of inversion.

Experimental

A mixture of Mn(NO₃)₂·2H₂O (1 mmol), H₂chdc (1 mmol) and *L* (1 mmol) was dissolved in 12 ml distilled water, followed by addition of triethylamine until the pH value of the system was approximately 5.5. The resulting solution was sealed in a 23-ml Teflon-lined stainless steel autoclave and heated at 175°C for 8 days under autogenous pressure. The reaction vessel was then slowly cooled to room temperature. Pale yellow block-like crystals of (I) suitable for single-crystal X-ray diffraction analysis were obtained from the resulting solution.

Refinement

C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures



Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (i) $x-1, y, z$; (ii) $2-x, 1-y, -z$; (iii) $3-x, 1-y, -z$; (iv) $2-x, 2-y, -z$.

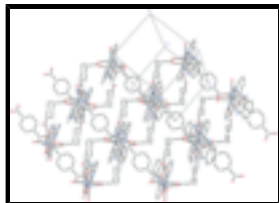


Fig. 2. Packing diagram of (I).

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Crystal data

[Mn₃(C₈H₁₀O₄)₃(C₁₈H₁₀N₄)₂]

$M_r = 1239.90$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.5730$ (17) Å

$b = 10.614$ (2) Å

$c = 14.846$ (3) Å

$\alpha = 77.34$ (3)°

$\beta = 81.99$ (3)°

$\gamma = 82.67$ (3)°

$V = 1298.6$ (4) Å³

$Z = 1$

$F_{000} = 637$

$D_x = 1.585$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 8527 reflections

$\theta = 3.0$ – 27.5 °

$\mu = 0.80$ mm⁻¹

$T = 293$ (2) K

Block, pale yellow

$0.33 \times 0.22 \times 0.19$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Radiation source: rotating anode

Monochromator: graphite

Detector resolution: 10.0 pixels mm⁻¹

$T = 293$ (2) K

ω scans

Absorption correction: multi-scan
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.762$, $T_{\max} = 0.863$

12776 measured reflections

5830 independent reflections

3707 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

$\theta_{\max} = 27.5$ °

$\theta_{\min} = 3.1$ °

$h = -11 \rightarrow 11$

$k = -13 \rightarrow 13$

$l = -16 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.176$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0908P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.05$ $(\Delta/\sigma)_{\max} < 0.001$
 5830 reflections $\Delta\rho_{\max} = 0.64 \text{ e } \text{\AA}^{-3}$
 376 parameters $\Delta\rho_{\min} = -0.74 \text{ e } \text{\AA}^{-3}$
 Primary atom site location: structure-invariant direct methods Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.3154 (5)	0.6357 (5)	0.2263 (4)	0.0481 (12)
H1	1.3426	0.6017	0.1729	0.058*
C2	1.4234 (5)	0.7038 (5)	0.2518 (4)	0.0542 (13)
H2	1.5216	0.7137	0.2169	0.065*
C3	1.3834 (5)	0.7570 (5)	0.3297 (4)	0.0513 (13)
H3	1.4535	0.8044	0.3476	0.062*
C4	1.2354 (5)	0.7384 (4)	0.3817 (3)	0.0361 (9)
C5	1.1352 (4)	0.6662 (4)	0.3517 (3)	0.0322 (9)
C6	0.9812 (5)	0.6398 (4)	0.4043 (3)	0.0312 (8)
C7	0.7506 (5)	0.5439 (4)	0.4195 (3)	0.0428 (10)
H7	0.6873	0.4949	0.3977	0.051*
C8	0.6944 (5)	0.5891 (5)	0.5002 (3)	0.0448 (11)
H8	0.5957	0.5702	0.5314	0.054*
C9	0.7855 (5)	0.6617 (4)	0.5334 (3)	0.0405 (10)
H9	0.7504	0.6915	0.5879	0.049*
C10	0.9314 (5)	0.6901 (4)	0.4842 (3)	0.0334 (9)
C11	1.0314 (5)	0.7716 (4)	0.5137 (3)	0.0320 (9)
C12	1.1837 (5)	0.7951 (4)	0.4643 (3)	0.0361 (9)
C13	1.2187 (5)	0.9248 (4)	0.5624 (3)	0.0368 (9)
C14	1.3088 (5)	1.0088 (5)	0.5907 (4)	0.0467 (11)
H14	1.4085	1.0250	0.5597	0.056*
C15	1.2492 (5)	1.0660 (4)	0.6635 (3)	0.0455 (11)
H15	1.3096	1.1204	0.6821	0.055*
C16	1.0994 (6)	1.0448 (4)	0.7108 (3)	0.0451 (11)
H16	1.0602	1.0862	0.7596	0.054*
C17	1.0108 (6)	0.9640 (5)	0.6856 (3)	0.0459 (11)
H17	0.9116	0.9492	0.7178	0.055*

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C18	1.0681 (5)	0.9021 (4)	0.6110 (3)	0.0372 (9)
C19	1.2088 (4)	0.3188 (4)	0.1441 (3)	0.0330 (9)
C20	1.3374 (4)	0.2042 (4)	0.1547 (3)	0.0329 (9)
H20	1.2888	0.1277	0.1496	0.039*
C21	1.4043 (5)	0.1721 (4)	0.2488 (3)	0.0371 (9)
H21A	1.3173	0.1678	0.2983	0.044*
H21B	1.4648	0.0875	0.2559	0.044*
C22	1.5100 (4)	0.2725 (4)	0.2577 (3)	0.0329 (9)
H22A	1.5559	0.2449	0.3158	0.039*
H22B	1.4464	0.3547	0.2590	0.039*
C23	1.6420 (4)	0.2913 (4)	0.1774 (3)	0.0344 (9)
H23	1.7047	0.2070	0.1790	0.041*
C24	1.7540 (5)	0.3865 (4)	0.1871 (3)	0.0371 (10)
C25	1.5739 (5)	0.3280 (4)	0.0842 (3)	0.0389 (10)
H25A	1.5112	0.4115	0.0797	0.047*
H25B	1.6598	0.3359	0.0340	0.047*
C26	1.4706 (5)	0.2260 (5)	0.0744 (3)	0.0416 (10)
H26A	1.5359	0.1447	0.0726	0.050*
H26B	1.4248	0.2535	0.0161	0.050*
C27	0.9657 (5)	0.7352 (4)	0.0992 (3)	0.0360 (9)
C28	0.9835 (5)	0.8607 (4)	0.0286 (3)	0.0426 (10)
H28	1.0018	0.8391	-0.0332	0.051*
C29	1.1322 (5)	0.9177 (4)	0.0430 (3)	0.0400 (10)
H29A	1.1198	0.9368	0.1047	0.048*
H29B	1.2236	0.8544	0.0383	0.048*
C30	0.8404 (5)	0.9579 (4)	0.0298 (3)	0.0423 (10)
H30A	0.8166	0.9787	0.0910	0.051*
H30B	0.7501	0.9206	0.0172	0.051*
N1	1.1746 (4)	0.6163 (3)	0.2743 (2)	0.0364 (8)
N2	0.8915 (4)	0.5678 (3)	0.3718 (2)	0.0340 (8)
N3	1.2766 (4)	0.8696 (4)	0.4881 (3)	0.0407 (9)
N4	0.9733 (4)	0.8249 (3)	0.5858 (2)	0.0380 (8)
O1	1.1606 (4)	0.3541 (3)	0.0659 (2)	0.0532 (9)
O2	1.1563 (3)	0.3674 (3)	0.2134 (2)	0.0397 (7)
O3	1.8227 (4)	0.4527 (4)	0.1177 (3)	0.0595 (10)
O4	1.7807 (4)	0.3935 (3)	0.2666 (2)	0.0532 (9)
O5	0.8733 (4)	0.7288 (3)	0.1720 (2)	0.0461 (8)
O6	1.0573 (3)	0.6357 (3)	0.0822 (2)	0.0365 (7)
Mn1	0.97563 (7)	0.51832 (6)	0.22819 (4)	0.02964 (19)
Mn2	1.0000	0.5000	0.0000	0.0292 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.043 (2)	0.049 (3)	0.057 (3)	-0.008 (2)	0.005 (2)	-0.025 (2)
C2	0.038 (2)	0.069 (3)	0.063 (3)	-0.019 (2)	0.008 (2)	-0.031 (3)
C3	0.039 (2)	0.059 (3)	0.066 (3)	-0.016 (2)	0.001 (2)	-0.031 (3)
C4	0.036 (2)	0.034 (2)	0.040 (2)	-0.0096 (17)	0.0023 (18)	-0.0130 (19)

C5	0.033 (2)	0.031 (2)	0.036 (2)	-0.0062 (16)	-0.0048 (17)	-0.0108 (18)
C6	0.038 (2)	0.0253 (19)	0.033 (2)	-0.0071 (16)	-0.0100 (17)	-0.0067 (17)
C7	0.042 (2)	0.041 (2)	0.050 (3)	-0.0163 (19)	-0.006 (2)	-0.013 (2)
C8	0.035 (2)	0.057 (3)	0.047 (3)	-0.017 (2)	0.007 (2)	-0.020 (2)
C9	0.042 (2)	0.044 (3)	0.039 (2)	-0.0143 (19)	0.0044 (19)	-0.015 (2)
C10	0.036 (2)	0.029 (2)	0.038 (2)	-0.0105 (16)	-0.0045 (18)	-0.0087 (18)
C11	0.038 (2)	0.029 (2)	0.033 (2)	-0.0069 (16)	-0.0070 (17)	-0.0105 (17)
C12	0.036 (2)	0.035 (2)	0.042 (2)	-0.0061 (17)	-0.0077 (18)	-0.015 (2)
C13	0.038 (2)	0.032 (2)	0.044 (3)	-0.0054 (17)	-0.0104 (19)	-0.0127 (19)
C14	0.037 (2)	0.054 (3)	0.058 (3)	-0.010 (2)	-0.005 (2)	-0.028 (2)
C15	0.047 (3)	0.042 (3)	0.057 (3)	-0.008 (2)	-0.013 (2)	-0.023 (2)
C16	0.057 (3)	0.043 (3)	0.042 (3)	-0.007 (2)	-0.007 (2)	-0.020 (2)
C17	0.052 (3)	0.051 (3)	0.040 (3)	-0.019 (2)	0.004 (2)	-0.020 (2)
C18	0.041 (2)	0.034 (2)	0.040 (2)	-0.0120 (18)	-0.0062 (19)	-0.0084 (19)
C19	0.033 (2)	0.0235 (19)	0.044 (2)	-0.0064 (16)	-0.0099 (18)	-0.0058 (18)
C20	0.031 (2)	0.0238 (19)	0.047 (2)	-0.0073 (15)	-0.0061 (18)	-0.0107 (18)
C21	0.036 (2)	0.030 (2)	0.044 (3)	-0.0092 (17)	-0.0082 (18)	0.0013 (19)
C22	0.0299 (19)	0.037 (2)	0.034 (2)	-0.0113 (16)	-0.0075 (16)	-0.0051 (18)
C23	0.0288 (19)	0.030 (2)	0.047 (3)	-0.0068 (16)	-0.0013 (18)	-0.0136 (19)
C24	0.031 (2)	0.037 (2)	0.047 (3)	-0.0098 (17)	0.0017 (19)	-0.017 (2)
C25	0.038 (2)	0.044 (2)	0.037 (2)	-0.0093 (18)	-0.0001 (18)	-0.013 (2)
C26	0.035 (2)	0.052 (3)	0.044 (3)	-0.0067 (19)	-0.0022 (19)	-0.022 (2)
C27	0.047 (2)	0.028 (2)	0.037 (2)	-0.0106 (18)	-0.009 (2)	-0.0073 (18)
C28	0.053 (3)	0.026 (2)	0.048 (3)	-0.0078 (18)	-0.001 (2)	-0.0045 (19)
C29	0.039 (2)	0.031 (2)	0.047 (3)	-0.0050 (18)	-0.003 (2)	-0.003 (2)
C30	0.045 (2)	0.032 (2)	0.050 (3)	-0.0124 (18)	-0.005 (2)	-0.004 (2)
N1	0.0386 (18)	0.0342 (19)	0.039 (2)	-0.0080 (15)	-0.0005 (15)	-0.0128 (16)
N2	0.0337 (17)	0.0320 (18)	0.040 (2)	-0.0101 (14)	-0.0060 (15)	-0.0099 (16)
N3	0.0353 (18)	0.045 (2)	0.049 (2)	-0.0119 (15)	-0.0009 (16)	-0.0233 (19)
N4	0.0442 (19)	0.041 (2)	0.0338 (19)	-0.0150 (16)	-0.0048 (16)	-0.0112 (16)
O1	0.069 (2)	0.0470 (19)	0.048 (2)	0.0177 (16)	-0.0304 (17)	-0.0172 (16)
O2	0.0408 (16)	0.0360 (16)	0.0435 (18)	0.0027 (12)	-0.0073 (14)	-0.0129 (14)
O3	0.055 (2)	0.063 (2)	0.063 (2)	-0.0343 (18)	0.0056 (17)	-0.0086 (19)
O4	0.0518 (19)	0.061 (2)	0.059 (2)	-0.0265 (16)	-0.0042 (16)	-0.0263 (18)
O5	0.0587 (19)	0.0331 (16)	0.0444 (19)	-0.0054 (14)	0.0034 (16)	-0.0088 (14)
O6	0.0482 (16)	0.0239 (14)	0.0425 (17)	-0.0089 (12)	-0.0098 (13)	-0.0115 (13)
Mn1	0.0326 (3)	0.0273 (3)	0.0316 (4)	-0.0081 (2)	-0.0036 (3)	-0.0088 (3)
Mn2	0.0341 (4)	0.0253 (4)	0.0306 (5)	-0.0070 (3)	-0.0073 (4)	-0.0067 (4)

Geometric parameters (Å, °)

C1—N1	1.329 (5)	C21—H21A	0.9700
C1—C2	1.383 (6)	C21—H21B	0.9700
C1—H1	0.9300	C22—C23	1.523 (6)
C2—C3	1.379 (6)	C22—H22A	0.9700
C2—H2	0.9300	C22—H22B	0.9700
C3—C4	1.403 (6)	C23—C24	1.520 (5)
C3—H3	0.9300	C23—C25	1.529 (6)
C4—C5	1.396 (5)	C23—H23	0.9800

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C4—C12	1.472 (5)	C24—O3	1.234 (5)
C5—N1	1.351 (5)	C24—O4	1.253 (5)
C5—C6	1.464 (5)	C25—C26	1.526 (6)
C6—N2	1.351 (5)	C25—H25A	0.9700
C6—C10	1.397 (5)	C25—H25B	0.9700
C7—N2	1.337 (5)	C26—H26A	0.9700
C7—C8	1.389 (6)	C26—H26B	0.9700
C7—H7	0.9300	C27—O5	1.243 (5)
C8—C9	1.368 (6)	C27—O6	1.283 (5)
C8—H8	0.9300	C27—C28	1.514 (6)
C9—C10	1.391 (6)	C28—C30	1.500 (6)
C9—H9	0.9300	C28—C29	1.539 (6)
C10—C11	1.461 (5)	C28—H28	0.9800
C11—N4	1.325 (5)	C29—C30 ⁱ	1.533 (6)
C11—C12	1.428 (6)	C29—H29A	0.9700
C12—N3	1.322 (5)	C29—H29B	0.9700
C13—N3	1.365 (5)	C30—C29 ⁱ	1.533 (6)
C13—C18	1.411 (6)	C30—H30A	0.9700
C13—C14	1.414 (6)	C30—H30B	0.9700
C14—C15	1.360 (6)	N1—Mn1	2.356 (3)
C14—H14	0.9300	N2—Mn1	2.303 (3)
C15—C16	1.395 (7)	O1—Mn2	2.102 (3)
C15—H15	0.9300	O2—Mn1	2.107 (3)
C16—C17	1.356 (6)	O3—Mn2 ⁱⁱ	2.165 (3)
C16—H16	0.9300	O3—Mn1 ⁱⁱ	2.495 (4)
C17—C18	1.408 (6)	O4—Mn1 ⁱⁱ	2.200 (3)
C17—H17	0.9300	O5—Mn1	2.312 (3)
C18—N4	1.364 (5)	O6—Mn2	2.218 (3)
C19—O1	1.251 (5)	O6—Mn1	2.314 (3)
C19—O2	1.253 (5)	Mn1—O4 ⁱⁱⁱ	2.200 (3)
C19—C20	1.531 (5)	Mn1—O3 ⁱⁱⁱ	2.495 (4)
C20—C26	1.531 (6)	Mn2—O1 ^{iv}	2.102 (3)
C20—C21	1.536 (6)	Mn2—O3 ^v	2.165 (3)
C20—H20	0.9800	Mn2—O3 ⁱⁱⁱ	2.165 (3)
C21—C22	1.521 (5)	Mn2—O6 ^{iv}	2.218 (3)
N1—C1—C2	123.2 (4)	C23—C25—H25A	109.5
N1—C1—H1	118.4	C26—C25—H25B	109.5
C2—C1—H1	118.4	C23—C25—H25B	109.5
C3—C2—C1	119.0 (4)	H25A—C25—H25B	108.0
C3—C2—H2	120.5	C25—C26—C20	111.9 (3)
C1—C2—H2	120.5	C25—C26—H26A	109.2
C2—C3—C4	119.0 (4)	C20—C26—H26A	109.2
C2—C3—H3	120.5	C25—C26—H26B	109.2
C4—C3—H3	120.5	C20—C26—H26B	109.2
C5—C4—C3	118.0 (4)	H26A—C26—H26B	107.9
C5—C4—C12	120.2 (3)	O5—C27—O6	121.1 (4)

C3—C4—C12	121.8 (4)	O5—C27—C28	122.5 (4)
N1—C5—C4	122.5 (4)	O6—C27—C28	116.3 (4)
N1—C5—C6	116.7 (3)	C30—C28—C27	114.1 (4)
C4—C5—C6	120.8 (3)	C30—C28—C29	111.5 (3)
N2—C6—C10	122.6 (4)	C27—C28—C29	108.7 (4)
N2—C6—C5	117.5 (3)	C30—C28—H28	107.4
C10—C6—C5	119.9 (3)	C27—C28—H28	107.4
N2—C7—C8	122.9 (4)	C29—C28—H28	107.4
N2—C7—H7	118.5	C30 ⁱ —C29—C28	110.7 (4)
C8—C7—H7	118.5	C30 ⁱ —C29—H29A	109.5
C9—C8—C7	119.5 (4)	C28—C29—H29A	109.5
C9—C8—H8	120.3	C30 ⁱ —C29—H29B	109.5
C7—C8—H8	120.3	C28—C29—H29B	109.5
C8—C9—C10	118.8 (4)	H29A—C29—H29B	108.1
C8—C9—H9	120.6	C28—C30—C29 ⁱ	111.0 (4)
C10—C9—H9	120.6	C28—C30—H30A	109.4
C9—C10—C6	118.5 (4)	C29 ⁱ —C30—H30A	109.4
C9—C10—C11	121.6 (4)	C28—C30—H30B	109.4
C6—C10—C11	119.9 (3)	C29 ⁱ —C30—H30B	109.4
N4—C11—C12	121.9 (4)	H30A—C30—H30B	108.0
N4—C11—C10	117.4 (4)	C1—N1—C5	118.2 (4)
C12—C11—C10	120.6 (3)	C1—N1—Mn1	125.1 (3)
N3—C12—C11	122.4 (3)	C5—N1—Mn1	116.4 (2)
N3—C12—C4	119.1 (4)	C7—N2—C6	117.6 (3)
C11—C12—C4	118.5 (3)	C7—N2—Mn1	124.1 (3)
N3—C13—C18	121.2 (4)	C6—N2—Mn1	117.8 (3)
N3—C13—C14	120.0 (4)	C12—N3—C13	116.4 (3)
C18—C13—C14	118.8 (4)	C11—N4—C18	116.3 (3)
C15—C14—C13	119.8 (4)	C19—O1—Mn2	137.6 (3)
C15—C14—H14	120.1	C19—O2—Mn1	130.2 (3)
C13—C14—H14	120.1	C24—O3—Mn2 ⁱⁱ	158.1 (3)
C14—C15—C16	121.5 (4)	C24—O3—Mn1 ⁱⁱ	86.0 (3)
C14—C15—H15	119.3	Mn2 ⁱⁱ —O3—Mn1 ⁱⁱ	93.87 (12)
C16—C15—H15	119.3	C24—O4—Mn1 ⁱⁱ	99.5 (3)
C17—C16—C15	120.0 (4)	C27—O5—Mn1	91.5 (2)
C17—C16—H16	120.0	C27—O6—Mn2	124.5 (3)
C15—C16—H16	120.0	C27—O6—Mn1	90.3 (2)
C16—C17—C18	120.5 (4)	Mn2—O6—Mn1	97.62 (11)
C16—C17—H17	119.8	O2—Mn1—O4 ⁱⁱⁱ	95.86 (12)
C18—C17—H17	119.8	O2—Mn1—N2	120.52 (12)
N4—C18—C17	118.7 (4)	O4 ⁱⁱⁱ —Mn1—N2	82.87 (12)
N4—C18—C13	121.8 (4)	O2—Mn1—O5	147.38 (12)
C17—C18—C13	119.5 (4)	O4 ⁱⁱⁱ —Mn1—O5	108.96 (13)
O1—C19—O2	124.9 (4)	N2—Mn1—O5	84.24 (12)
O1—C19—C20	116.1 (3)	O2—Mn1—O6	91.43 (11)
O2—C19—C20	118.9 (4)	O4 ⁱⁱⁱ —Mn1—O6	127.44 (12)

supplementary materials

C19—C20—C26	110.3 (4)	N2—Mn1—O6	135.18 (11)
C19—C20—C21	114.4 (3)	O5—Mn1—O6	56.78 (10)
C26—C20—C21	110.8 (3)	O2—Mn1—N1	84.36 (11)
C19—C20—H20	107.0	O4 ⁱⁱⁱ —Mn1—N1	148.93 (13)
C26—C20—H20	107.0	N2—Mn1—N1	70.66 (12)
C21—C20—H20	107.0	O5—Mn1—N1	84.83 (12)
C22—C21—C20	112.2 (3)	O6—Mn1—N1	83.54 (12)
C22—C21—H21A	109.2	O2—Mn1—O3 ⁱⁱⁱ	91.42 (12)
C20—C21—H21A	109.2	O4 ⁱⁱⁱ —Mn1—O3 ⁱⁱⁱ	54.17 (12)
C22—C21—H21B	109.2	N2—Mn1—O3 ⁱⁱⁱ	129.79 (12)
C20—C21—H21B	109.2	O5—Mn1—O3 ⁱⁱⁱ	86.59 (12)
H21A—C21—H21B	107.9	O6—Mn1—O3 ⁱⁱⁱ	73.72 (11)
C21—C22—C23	111.7 (3)	N1—Mn1—O3 ⁱⁱⁱ	156.77 (12)
C21—C22—H22A	109.3	O1 ^{iv} —Mn2—O1	180.00 (17)
C23—C22—H22A	109.3	O1 ^{iv} —Mn2—O3 ^v	89.57 (15)
C21—C22—H22B	109.3	O1—Mn2—O3 ^v	90.43 (15)
C23—C22—H22B	109.3	O1 ^{iv} —Mn2—O3 ⁱⁱⁱ	90.43 (15)
H22A—C22—H22B	107.9	O1—Mn2—O3 ⁱⁱⁱ	89.57 (15)
C24—C23—C22	112.7 (3)	O3 ^v —Mn2—O3 ⁱⁱⁱ	180.0 (2)
C24—C23—C25	112.4 (4)	O1 ^{iv} —Mn2—O6	89.89 (11)
C22—C23—C25	110.7 (3)	O1—Mn2—O6	90.11 (11)
C24—C23—H23	106.9	O3 ^v —Mn2—O6	97.56 (12)
C22—C23—H23	106.9	O3 ⁱⁱⁱ —Mn2—O6	82.44 (12)
C25—C23—H23	106.9	O1 ^{iv} —Mn2—O6 ^{iv}	90.11 (11)
O3—C24—O4	120.0 (4)	O1—Mn2—O6 ^{iv}	89.89 (11)
O3—C24—C23	120.7 (4)	O3 ^v —Mn2—O6 ^{iv}	82.44 (12)
O4—C24—C23	119.2 (4)	O3 ⁱⁱⁱ —Mn2—O6 ^{iv}	97.56 (12)
C26—C25—C23	110.9 (4)	O6—Mn2—O6 ^{iv}	180.00 (11)
C26—C25—H25A	109.5		

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

Fig. 1

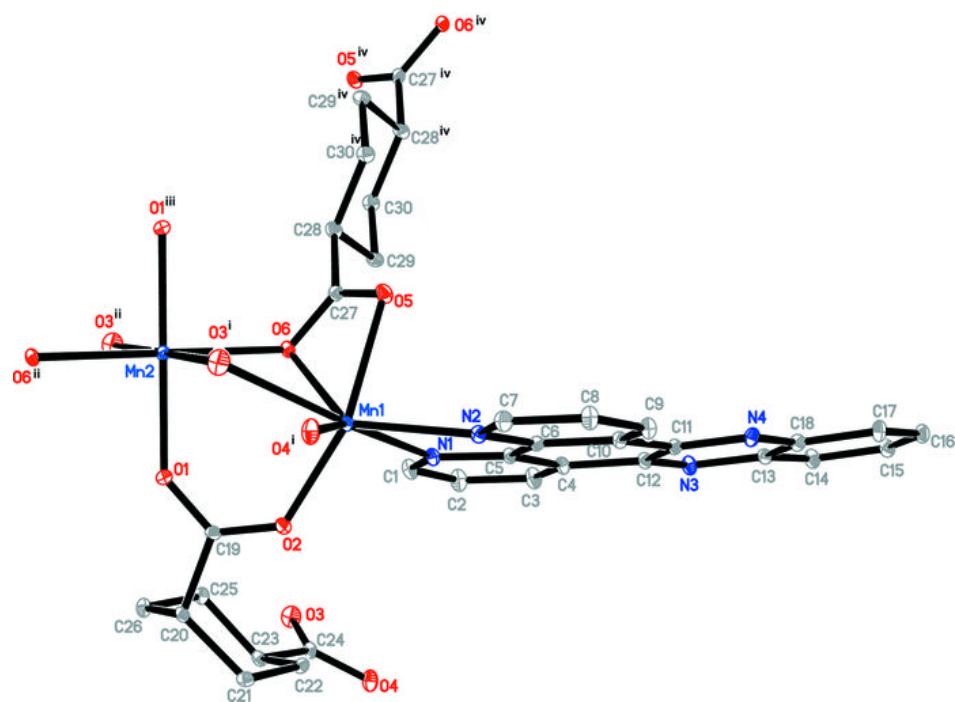


Fig. 2

