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catena-Poly[tris(μ_2-oxalato-$\kappa^4O,O':O''O'''$)-bis(μ_2-4,4′-bipyridyl-κ^2N,N')bis(4,4′-bipyridyl-κN)trimanganese(II)]

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Key indicators

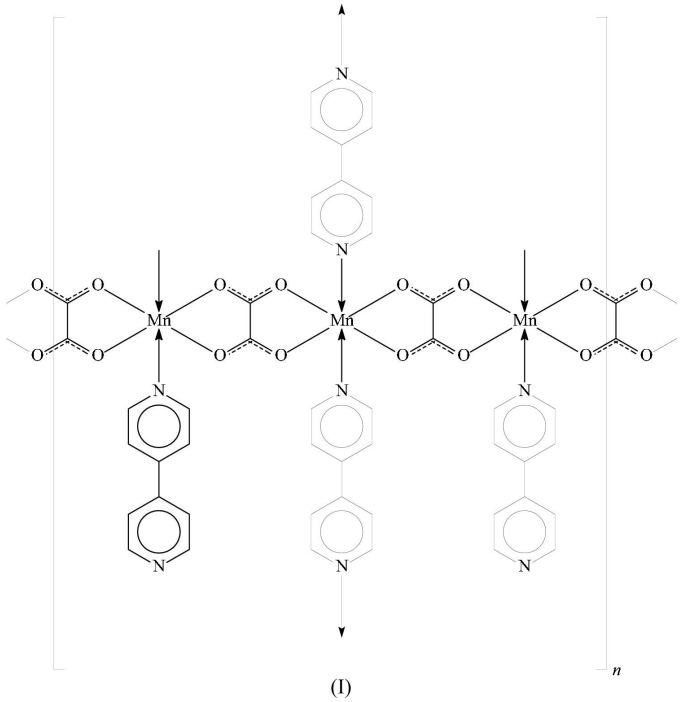
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.031
wR factor = 0.094
Data-to-parameter ratio = 15.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The layer structure of the title compound, $[Mn_3(C_2O_4)_3(C_{10}H_8N_2)_4]$, consists of undulating manganese(II) oxalate chains with terminal and bridging 4,4′-bipyridine ligands stacked alternately along the chains. The compound is isostructural with $[Fe_3(C_2O_4)_3(C_{10}H_8N_2)_4]$, the structure of which has previously been described in detail [Zheng, Fang, Lii, Song, Xin, Fun, Chinnakali & Razak (1999). *J. Chem. Soc. Dalton Trans.* pp. 2311–2316].

Comment

Compounds of the formula $[M(C_2O_4)(C_{10}H_8N_2)]$, where M is Fe^{II}, Co^{II}, Ni^{II} or Zn^{II}, are isostructural and consist of two-dimensional networks (Yu *et al.*, 1999). Another study published at the same time reported the Co^{II} complex, along with an iron(II) complex, $[Fe_3(C_2O_4)_3(C_{10}H_8N_2)_4]$, which exhibits weak antiferromagnetic behaviour (Zheng *et al.*, 1999). That compound features $Fe(C_2O_4)$ chains, as well as terminal and bridging heterocycles stacked alternately along the chains. The title manganese(II) compound, (I) (Fig. 1), is isostructural with the latter iron(II) compound, which has already been described in detail by Zheng *et al.* (1999).



(I)

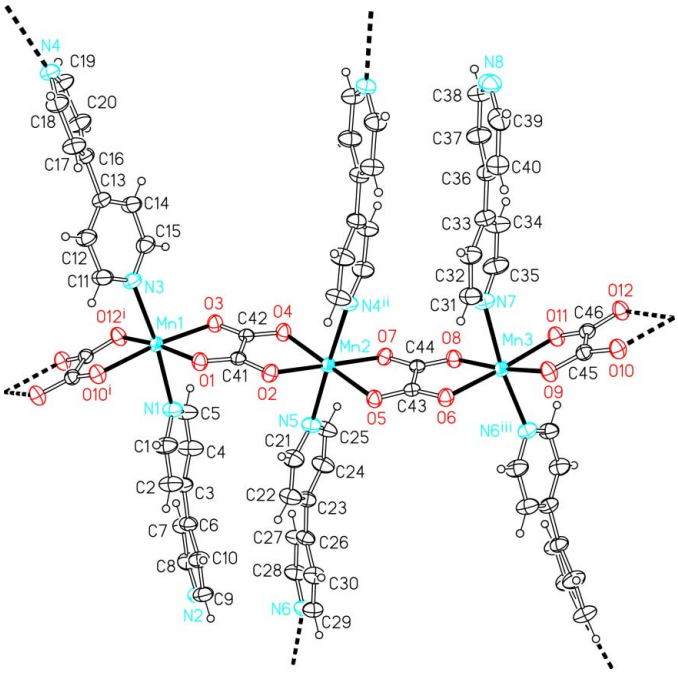


Figure 1
A view of a portion of the layer structure of (I). Displacement ellipsoids are drawn at the 30% probablity level and H atoms are shown as small spheres of arbitrary radii. Symmetry codes are given in Table 1.

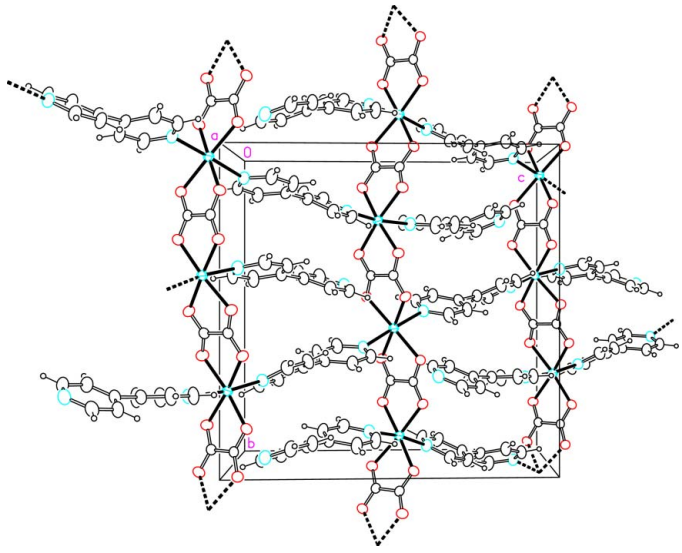


Figure 2
A plot of the layer structure of (I).

Experimental

The title compound was obtained as the main phase (in *ca* 30% yield, based on Mn) from the hydrothermal reaction of potassium oxalate (0.08 g, 0.5 mmol), manganese dichloride tetrahydrate (0.10 g, 0.5 mmol), 4,4′-bipyridine (0.08 g, 0.5 mmol) and water (10 ml) at 413 K for 120 h. The reactants were placed in a Teflon-lined stainless steel Parr bomb and heated. After cooling of the bomb to room temperature at 10 K h^{-1}, pale yellow crystals of (I) were obtained.

Crystal data

$[Mn_3(C_2O_4)_3(C_{10}H_8N_2)_4]$
M_r = 1053.62
Monoclinic, $P2_1/c$
a = 16.289 (2) Å
b = 16.220 (2) Å
c = 16.452 (2) Å
β = 94.981 (2)°
V = 4330.1 (9) Å^3
Z = 4
D_x = 1.616 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 976 reflections
θ = 3.0–26.7°
μ = 0.94 mm^{-1}
T = 295 (2) K
Block, pale yellow
0.32 × 0.16 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.766, T_{max} = 0.896
35 776 measured reflections
9421 independent reflections
7912 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.0°
$h = -20 \rightarrow 20$
$k = -20 \rightarrow 20$
$l = -21 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.094
S = 1.01
9421 reflections
622 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.9427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.144 (1)	Mn2—O7	2.155 (1)
Mn1—O3	2.139 (1)	Mn2—N4^{ii}	2.328 (1)
Mn1—O10^{i}	2.160 (1)	Mn2—N5	2.307 (1)
Mn1—O12^{i}	2.151 (1)	Mn3—O6	2.133 (1)
Mn1—N1	2.374 (1)	Mn3—O8	2.157 (1)
Mn1—N3	2.286 (1)	Mn3—O9	2.163 (1)
Mn2—O2	2.151 (1)	Mn3—O11	2.165 (1)
Mn2—O4	2.160 (1)	Mn3—N6^{iii}	2.268 (1)
Mn2—O5	2.162 (1)	Mn3—N7	2.332 (1)
O1—Mn1—O3	78.38 (4)	O4—Mn2—N5	88.43 (5)
O1—Mn1—O10^{i}	102.53 (4)	O5—Mn2—O7	78.65 (4)
O1—Mn1—O12^{i}	170.80 (5)	O5—Mn2—N4^{ii}	86.25 (5)
O1—Mn1—N1	86.73 (5)	O5—Mn2—N5	92.28 (5)
O1—Mn1—N3	99.08 (5)	O7—Mn2—N4^{ii}	86.12 (5)
O3—Mn1—O10^{i}	171.66 (4)	O7—Mn2—N5	92.34 (5)
O3—Mn1—O12^{i}	99.76 (4)	N4^{ii}—Mn2—N5	178.05 (5)
O3—Mn1—N1	86.58 (5)	O6—Mn3—O8	78.22 (4)
O3—Mn1—N3	98.51 (5)	O6—Mn3—O9	100.94 (4)
O10^{i}—Mn1—O12^{i}	78.00 (4)	O6—Mn3—O11	175.91 (5)
O10^{i}—Mn1—N1	85.20 (5)	O6—Mn3—N6^{iii}	95.13 (5)
O10^{i}—Mn1—N3	89.57 (5)	O6—Mn3—N7	90.83 (5)
O12^{i}—Mn1—N1	84.16 (5)	O8—Mn3—O9	172.57 (5)
O12^{i}—Mn1—N3	90.10 (5)	O8—Mn3—O11	102.57 (4)
N1—Mn1—N3	172.92 (5)	O8—Mn3—N6^{iii}	97.03 (5)
O2—Mn2—O4	78.60 (4)	O8—Mn3—N7	88.49 (5)
O2—Mn2—O5	100.77 (4)	O9—Mn3—O11	77.76 (4)
O2—Mn2—O7	178.76 (4)	O9—Mn3—N6^{iii}	90.39 (5)
O2—Mn2—N4^{ii}	92.75 (5)	O9—Mn3—N7	84.13 (5)
O2—Mn2—N5	88.78 (5)	O11—Mn3—N6^{iii}	88.77 (5)
O4—Mn2—O5	179.04 (4)	O11—Mn3—N7	85.18 (5)
O4—Mn2—O7	101.97 (4)	N6^{iii}—Mn3—N7	172.58 (5)
O4—Mn2—N4^{ii}	93.06 (5)		

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

The structure was solved using atomic coordinates taken from the Fe analogue (Zheng *et al.*, 1999). The H atoms were positioned geometrically and refined with a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; method used to solve structure: atomic coordinates taken from the Fe analogue (Zheng *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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