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catena-Poly[[[di-μ-acetato-κ^4O:O'-bis[(acetato-κ^2O,O')manganese(II)]]-di-μ-4,4′-bipyridine-κ^4N:N'] monohydrate]

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The title compound, $\{[Mn_2(CH_3CO_2)_4(C_{10}H_8N_2)_2]\cdot H_2O\}_n$, is a one-dimensional coordination polymer with a ladder-like structure. Two Mn^{II} atoms, each coordinated by a chelating acetate ligand, are bridged by two bidentate acetate ligands to form a centrosymmetric $[Mn_2(CH_3CO_2)_4]$ unit. Two 4,4′-bipyridine ligands link the $[Mn_2(CH_3CO_2)_4]$ units through Mn—N bonds to generate a molecular ladder. The water O atom lies on a crystallographic twofold rotation axis.

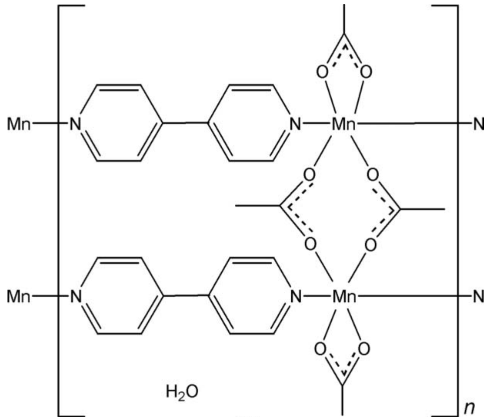
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.118
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.

Comment

Self-assembly based on molecular building blocks has become an effective approach to construct coordination polymers (Kitagawa *et al.*, 2004). 4,4′-Bipyridine (4,4′-bipy) acting as a linear rigid connector between metal atoms is a common building block. Biradha *et al.* (2006) have shown with a search of the Cambridge Structural Database (Version 5.27; Allen, 2002) that 30% of the structures of pyridine-based coordination polymers contain 4,4′-bipy ligands. One-, two- or three-dimensional coordination polymers can be assembled using 4,4′-bipy and transition metals. One-dimensional ladder-like structures are observed when the anion is nitrate (Fletcher *et al.*, 2004; Wagner *et al.*, 2002). It is of interest to examine whether this preference is also found in the structures of 4,4′-bipy/metal complexes with the acetate anion. We report here the structure of $\{[Mn_2(CH_3CO_2)_4(4,4'\text{-bipy})_2]\cdot H_2O\}_n$, (I).



(I)

As shown in Fig. 1, complex (I) contains a dinuclear $[Mn_2(CH_3CO_2)_4]$ unit lying on a centre of inversion, in which two Mn^{II} atoms are bridged by two bidentate acetate ligands [Mn—O = 2.171 (2) and 2.104 (2) Å] and each Mn^{II} atom is also coordinated by a chelating acetate ligand [Mn—O = 2.240 (2) and 2.309 (2) Å]. The coordination geometry of the Mn^{II} atom is severely distorted octahedral as a result of the

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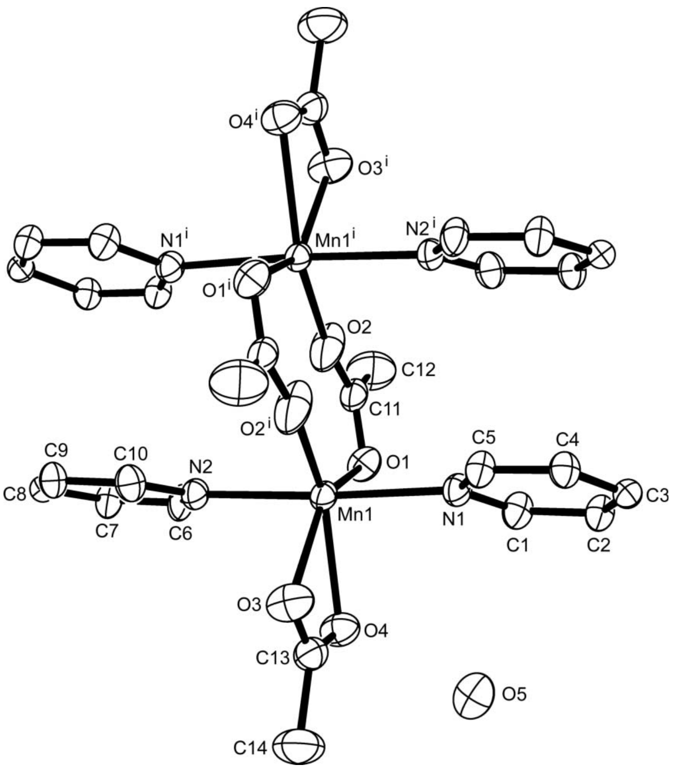

Figure 1
Part of the polymeric structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, 1 - z$.]

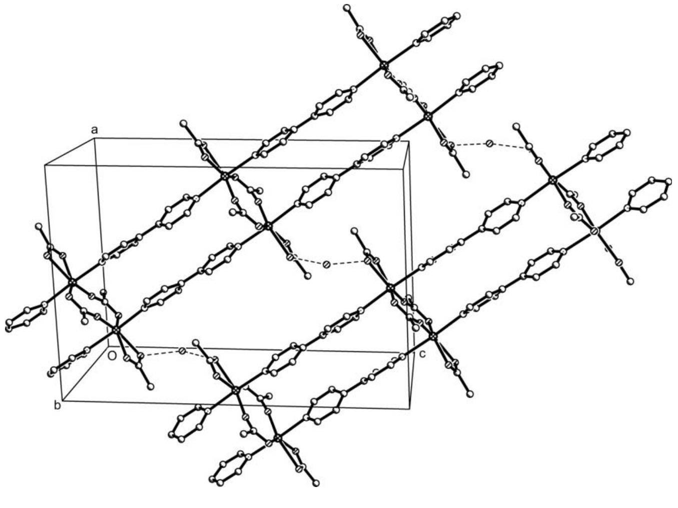

Figure 2
A view of the one-dimensional ladder structure in (I). H atoms have been omitted. Dashed lines denote hydrogen bonds.

presence of the chelating ligand, with the equatorial plane formed by the carboxylate O atoms. The 4,4′-bipy ligands occupy the two axial positions, with Mn—N bond lengths of 2.270 (2) and 2.273 (2) Å, generating a molecular ladder (Fig. 2). The ladders are connected by hydrogen bonds through water molecules (Table 1). The ladder structure is somewhat different from those found in the complexes of 4,4′-bipy with nickel nitrate (Fletcher *et al.*, 2004) and zinc nitrate (Wagner *et al.*, 2002). In those complexes, three coordination sites of the metal are occupied by 4,4′-bipy ligands in a 'T-shaped' fashion and the nitrate anions bind to the metal in either monodentate or chelating modes. Therefore, the coordination mode of the anion is also an important factor that influences these structural motifs. The water O atom lies on a crystallographic twofold rotation axis.

Experimental

A solution of 4,4′-bipy (0.038 g, 0.2 mmol) in ethanol (10 ml) and a solution of $Mn(CH_3CO_2)_2{\cdot}4H_2O$ (0.049 g, 0.2 mmol) in water (5 ml) were mixed. The resulting solution was set aside to crystallize at room temperature and yellow needle crystals of (I) were obtained after two weeks (yield 41%).

Crystal data

$[Mn_2(C_2H_3O_2)_4(C_{10}H_8N_2)_2]{\cdot}H_2O$
$M_r = 676.44$
Monoclinic, $C2/c$
$a = 13.385$ (4) Å
$b = 11.664$ (4) Å
$c = 19.470$ (6) Å
$\beta = 92.071$ (5)°
$V = 3037.6$ (16) Å^3
$Z = 4$
$D_x = 1.479$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.89$ mm^{-1}
$T = 293$ (2) K
Needle, yellow
0.41 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.711$, $T_{max} = 0.919$
8397 measured reflections
2970 independent reflections
2304 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.118$
$S = 1.02$
2970 reflections
197 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 1.7367P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O4	0.92	1.92	2.829 (2)	171

All C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic H) or 0.96 Å (CH_3), and with $U_{iso}(H) = 1.2U_{eq}(C)$. The unique H atom on the water molecule was included in the location determined from a difference Fourier map and allowed to ride on O5 during subsequent refinement with $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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