A two-dimensional manganese coordination polymer: poly[bis(μ-3,5-dimethylbenzoato)-(μ-4,4'-pyridine)manganese(II)]

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In the title compound, $[Mn(C_9H_9O_2)_2(C_{10}H_8N_2)]_n$, the Mn atom lies on a twofold axis and is octahedrally coordinated by two N atoms of two bipyridine ligands and four O atoms of four dimethylbenzoate ligands. The carboxylate O atoms coordinate two symmetry-related Mn^{II} ions in the bidentate bridging mode. This manganese complex exhibits a two-dimensional layer structure.

Comment

In recent decades, there has been considerable interest in the design and synthesis of manganese(II) complexes with carboxylate ligands. They can be used for the investigation of exchange coupling interactions between metal ions *via* organic bridging ligands since they have provided a great variety of molecular-based magnetic materials (Khan, 1993). Furthermore, 4,4'-bipy is an excellent bridging ligand, and many one-, two- and three-dimensional infinite metal-4,4'-bipy frameworks have already been generated. Of the above-mentioned frameworks, most are generated directly by coordination bonds; the others show the formation of one-dimensional coordination chains further extended into higher-dimensional networks by hydrogen-bonding or π–π interactions (Rowsell & Yaghi, 2004).

(I)
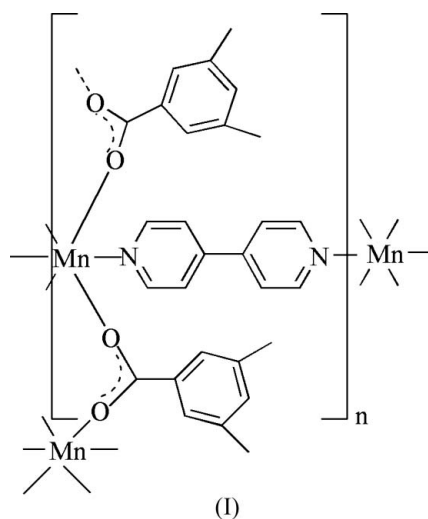
In the title compound, $[Mn(C_9H_9O_2)_2(C_{10}H_8N_2)]_n$, (I) (Fig. 1), the Mn^{II} ion lies on the twofold axis that runs longitudinally through the bipyridine ligands. Each Mn^{II} ion has a slightly distorted octahedral geometry, being coordinated by two N atoms of two bipyridine ligands in the axial positions and four O atoms from four dimethylbenzoate ligands in the

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equatorial positions (Table 1). Each dimethylbenzoate ligand bridges two symmetry-related Mn^{II} ions in a *syn–syn* conformation, forming a chain along the *c* axis. These chains are cross-linked by the bipyridine ligands along the *b* axis. Thus, the structure of this complex consists of a two-dimensional rectangular grid (Fig. 2) extending in the *bc* plane with the organic ligands acting as bidentate bridges within each layer.

Experimental

An aqueous solution (5 ml) of $Mn(ClO_4)_2 \cdot 6H_2O$ (1 mmol, 0.382 g) was added dropwise to a methanol solution (10 ml) of NaOH (2 mmol, 0.081 g), 4,4'-bipyridine (1 mmol, 0.156 g) and 3,5-dimethylbenzoic acid (2 mmol, 0.301 g). The reaction mixture was refluxed for 6 h and filtered; the filtrate was kept in a $CaCl_2$ desiccator. After a few days, colorless block crystals suitable for X-ray analysis were obtained. Analysis calculated: C 65.95, H 5.10, N 5.49%; found: C 65.71, H 4.97, N 5.58%

Crystal data

$[Mn(C_9H_9O_2)_2(C_{10}H_8N_2)]$	$Z = 4$
$M_r = 509.45$	$D_x = 1.457$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 20.996$ (8) Å	$\mu = 0.61$ mm^{-1}
$b = 11.835$ (5) Å	$T = 294$ (2) K
$c = 9.958$ (4) Å	Block, colorless
$\beta = 110.161$ (5)°	$0.20 \times 0.18 \times 0.10$ mm
$V = 2322.9$ (16) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4687 measured reflections
φ and ω scans	1988 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1680 reflections with $I > 2\sigma(I)$
$T_{min} = 0.655$, $T_{max} = 1.000$	$R_{int} = 0.057$
(expected range = 0.616–0.941)	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$+ 0.9512P]$
$wR(F^2) = 0.113$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
1988 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
163 parameters	$\Delta\rho_{min} = -0.45$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Mn1—O2^i	2.1466 (18)	Mn1—N2^{ii}	2.307 (2)
Mn1—O1	2.1710 (15)	Mn1—N1	2.400 (2)
O2^i—Mn1—O2^{iii}	170.67 (8)	O1—Mn1—N2^{ii}	87.78 (4)
O2^i—Mn1—O1	87.62 (7)	O2^i—Mn1—N1	85.33 (4)
O2^{iii}—Mn1—O1	92.74 (7)	O1—Mn1—N1	92.22 (4)
O1—Mn1—O1^{iv}	175.57 (9)	N2^{ii}—Mn1—N1	180.
O2^i—Mn1—N2^{ii}	94.67 (4)		

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

H atoms were positioned geometrically and treated as riding with C—H distances of 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$ [C—H =
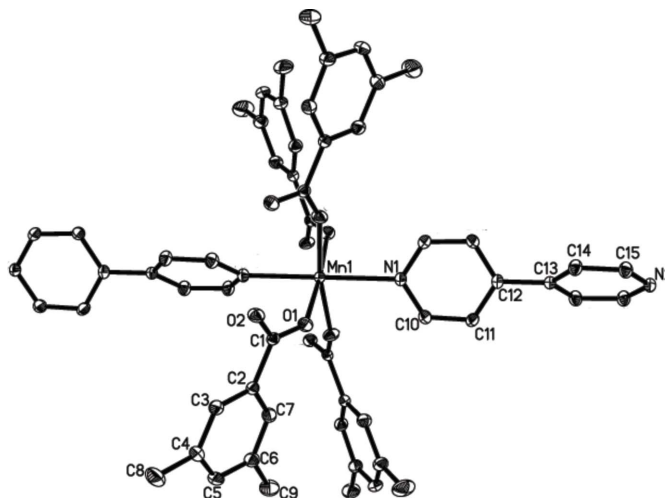
Figure 1
Part of the polymeric structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. Unlabeled atoms are related to labeled atoms by the various symmetry codes in Table 1.
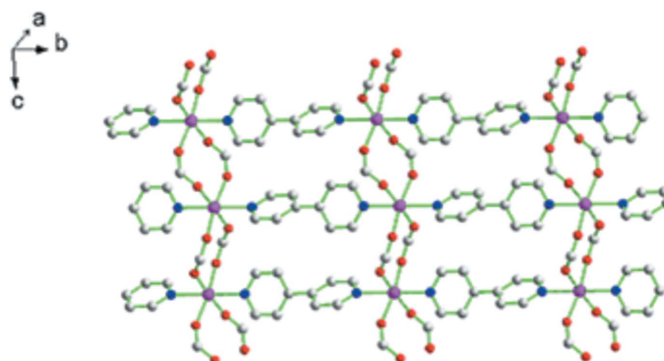
Figure 2
The two-dimensional layer structure of (I). For clarity, all H atoms have been omitted and only the carboxylate groups of the dimethylbenzoate molecules are shown.

0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for C8 and C9].

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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