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Bis(2,2′-bipyridine-κ^2N,N')bis(4-hydroxybenzoato-κO)manganese(II)

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Key indicators

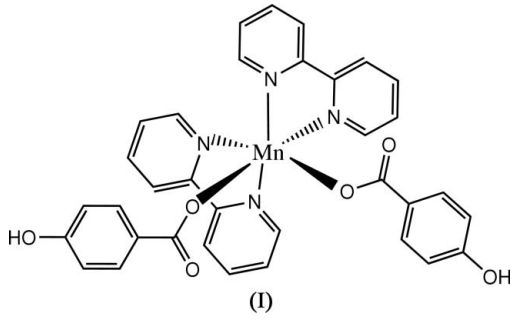
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.072
Data-to-parameter ratio = 16.5

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

The title Mn^{II} complex, $[Mn(C_7H_5O_3)_2(C_{10}H_8N_2)_2]$, has twofold symmetry, with the Mn^{II} atom located on a twofold axis. Two 4-hydroxybenzoate anions and two 2,2′-bipyridine coordinate to the Mn^{II} atom which has a distorted octahedral geometry. Hydrogen bonding between the carboxylate and hydroxyl groups forms a sheet perpendicular to the *a* axis.

Comment

Recently, we have investigated manganese complexes which have shown catalytic activity in industrial and biochemical processes (Kono & Fridovich, 1983; Wu *et al.*, 2001). As part of our work on polymerization catalysed by manganese complexes, we present here the structure of the title Mn^{II} complex, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The Mn^{II} atom sits on a twofold axis and is coordinated by two 2,2′-bipyridine (bipy) and two 4-hydroxybenzoate (hba) anions in a distorted octahedral geometry. The hba anion coordinates in a monodentate manner to the Mn^{II} atom; the Mn—O1 bond distance (Table 1) is comparable to that found in [Mn(hba)-(phen)$_2$(H$_2$O)](hba) (phen is phenanthroline); [2.1054 (17) Å; Su *et al.*, 2005]. The variation in bond angles at the Mn center shows the degree of distortion from a regular octahedral coordination geometry. The O1—Mn—N2 angle is larger than O1—Mn—N2^i by 21.45 (8)° (Table 1) [symmetry code: (i) $1-x, 1-y, z$].

There is an extensive two-dimensional hydrogen-bonding network between the carboxylate and hydroxyl groups, forming a sheet perpendicular to the *a* axis (Fig. 2 and Table 2).

Experimental

$Mn(CH_3COO)_2{\cdot}4H_2O$ (0.25 g, 1 mmol), 4-hydroxybenzoic acid (0.14 g, 1 mmol), bipy (0.20 g, 1 mmol) and Na_2CO_3 (0.05 g, 1 mmol) were dissolved in a water/ethanol solution (20 ml, 1:1 *v*/*v*). The

solution was refluxed for 3 h, then cooled to room temperature and filtered. Yellow single crystals of (I) were obtained from the filtrate after one week.

Crystal data

$[Mn(C_7H_5O_3)_2(C_{10}H_8N_2)_2]$
M_r = 641.53
Orthorhombic, *Aba*2
a = 12.948 (4) Å
b = 21.805 (4) Å
c = 10.470 (2) Å
V = 2956.2 (12) Å^3
Z = 4
D_x = 1.441 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12451 reflections
θ = 3.1–27.0°
μ = 0.50 mm^{-1}
T = 295 (2) K
Block, pale yellow
0.28 × 0.18 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.848, T_{max} = 0.925
14027 measured reflections
3362 independent reflections
2851 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.5°
$h = -16 \rightarrow 16$
$k = -28 \rightarrow 28$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.072
S = 1.01
3362 reflections
204 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), 1577 Friedel pairs
Flack parameter: 0.019 (15)

Table 1
Selected geometric parameters (Å, °).

Mn—O1	2.1111 (14)	Mn—N2	2.2812 (16)
Mn—N1	2.3220 (17)		
O1—Mn—O1^{i}	98.72 (8)	O1—Mn—N2^{i}	87.14 (6)
O1—Mn—N1	92.49 (6)	N1—Mn—N1^{i}	83.96 (8)
O1—Mn—N1^{i}	157.65 (5)	N2—Mn—N2^{i}	156.17 (9)
O1—Mn—N2	108.59 (6)		

Symmetry code: (i) $-x+1, -y+1, z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{ii}	0.86	1.81	2.633 (2)	159

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

The hydroxy H atom was located in a difference Fourier map and refined as riding on O3, with U_{iso}(H) = 1.2U_{eq}(O) and O—H = 0.86 Å. Aromatic H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

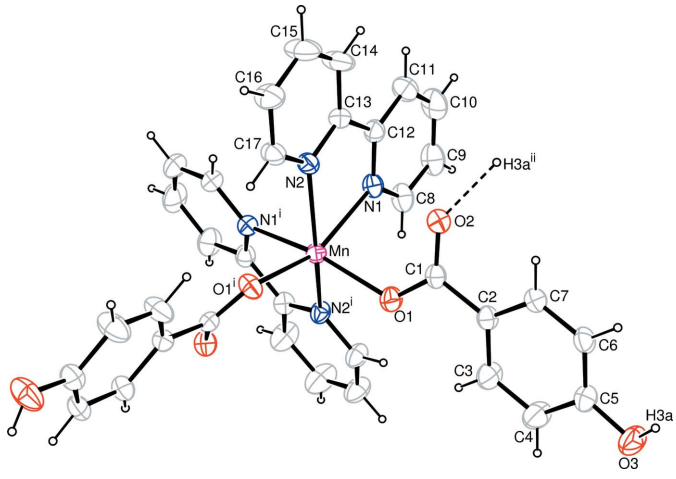


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms), showing a hydrogen bond as a dashed line. [Symmetry codes: (i) $1-x, 1-y, z$; (ii) $1-x, \frac{3}{2}-y, \frac{1}{2}+z$.]

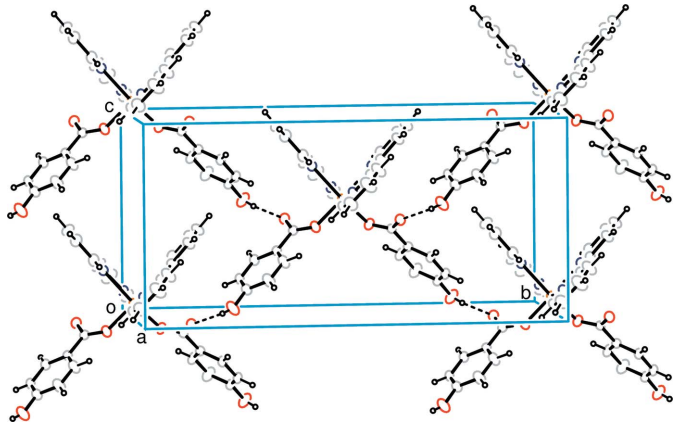


Figure 2
The packing of (I), showing the hydrogen bonds as dashed lines.

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