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Bis{2-[(2-oxidoethyl)iminomethyl]phenolato-κ^3O,N,O'}manganese(IV) hemihydrate

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.030
wR factor = 0.090
Data-to-parameter ratio = 16.7

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

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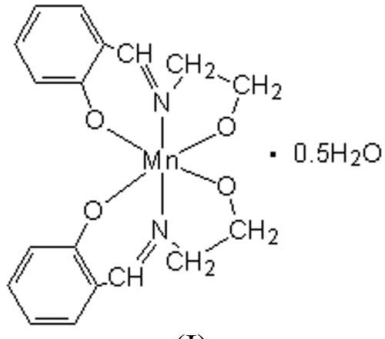
The crystal structure of the title complex, $[Mn(C_9H_9NO_2)_2]\cdot 0.5H_2O$, contains two Mn^{IV} units related by a twofold rotation axis and linked by intermolecular hydrogen bonds to a water molecule lying on this twofold axis.

Comment

Manganese(II) centres coordinated by an *O*,*N*,*N*-tridentate Schiff base can form a variety of compounds which have been found to function as molecular nanomagnets (Aliaga *et al.*, 2001; Soler *et al.*, 2001; Yang *et al.*, 2003). Such molecules have been called single-molecule magnets (SMMs). Interest in SMMs has grown considerably since it was found that a reversal of the direction of magnetization can occur *via* quantum mechanical tunnelling. Recently, an Fe_4 SMM was synthesized by treating $FeCl_2\cdot 4H_2O$ with a Schiff base ligand generated from the condensation of *o*-vanillin with 3-aminopropanol (Madhu *et al.*, 2005). We present here the structure of a new Mn^{IV} complex, (I) (Fig. 1).



(I)

The Mn^{IV} atom is coordinated by two N and four O atoms of the Schiff base ligands. The Mn—O bond lengths range from 1.8569 (12) to 1.9166 (11) Å and the Mn—N distances are 1.9682 (12) and 1.9771 (13) Å. The structure contains two Mn^{IV} units related by a twofold rotation axis and linked by intermolecular hydrogen bonds to a water molecule lying on this twofold axis.

Experimental

A solution of salicylaldehyde (10 mmol) in methanol (10 ml) was added to a solution of ethanolamine (10 mmol) in methanol (20 ml). The mixture was refluxed for 1 h before the addition of $MnCl_2\cdot H_2O$ (10 mmol) and $K_2S_2O_8$ (20 mmol) dissolved in a minimum of water. After filtration, the solution was left to stand for several days, leading to the formation of yellow crystals (yield 65%). Crystals of (I)

suitable for single-crystal X-ray diffraction were selected directly from the sample as prepared.

Crystal data

$[Mn(C_9H_9NO_2)_2]\cdot 0.5H_2O$
$M_r = 390.29$
Orthorhombic, *Pbcn*
$a = 27.6765\ (16)$ Å
$b = 10.6137\ (6)$ Å
$c = 11.6820\ (7)$ Å
$V = 3431.6\ (3)$ Å^3
$Z = 8$
$D_x = 1.511$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.80$ mm^{-1}
$T = 291\ (2)$ K
Block, yellow
0.39 × 0.28 × 0.21 mm

Data collection

Bruker SMART APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.745$, $T_{max} = 0.850$
19518 measured reflections
3929 independent reflections
3255 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.090$
$S = 1.02$
3929 reflections
235 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.8471P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O3	0.884 (9)	1.897 (10)	2.7666 (16)	168 (2)

H atoms were placed in calculated positions (N—H = 0.89 Å and C—H = 0.97 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C,N)$. the water H atom was restrained, with H—O = 0.83 Å.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1995); software used to prepare material for publication: *SHELXTL*.

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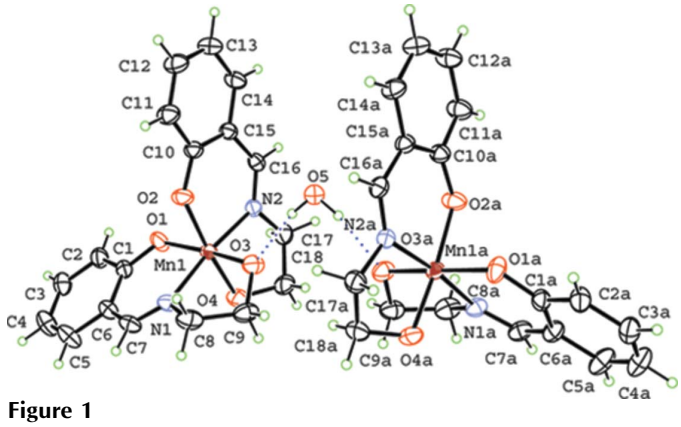

Figure 1
Two complex molecules linked by hydrogen bonds (dashed lines) to a water molecule. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (a) $1-x, y, \frac{1}{2}-z$.]

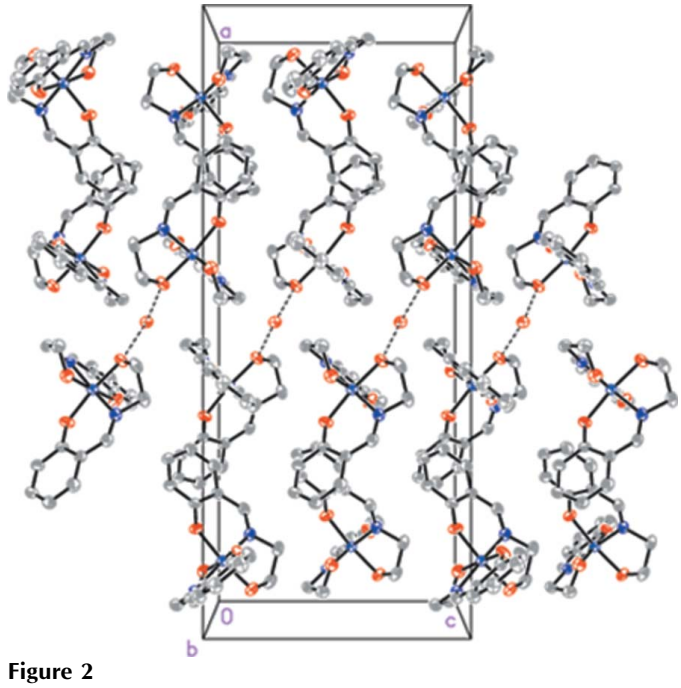

Figure 2
View along the *b* axis of the packing of the title compound. Dashed lines indicate hydrogen bonds.

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