Bis(di-2-pyridylmethanediol-$\kappa^3 N,N',O$)-manganese(II) bis(acetate) tetrahydrate

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The Mn atom in the title compound, $[Mn(C_{11}H_{10}N_2O_2)_2](CH_3CO_2)_2 \cdot 4H_2O$, which lies on a centre of inversion, displays a tetragonally distorted octahedral coordination. The compound is isostructural with the analogous copper complex [Reinoso, Vitoria, San Felices, Lezama & Gutiérrez-Zorrilla (2003). *Acta Cryst.* E**59**, m548–m550].

Comment

Di-2-pyridyl ketone, when reacted with metal salts, is sometimes oxidized to di-2-pyridylmethanediol, which chelates to the metal. The diol binds through three donor sites to the metal in the purple copper diacetate adduct, which exists as a tetrahydrate (Reinoso *et al.*, 2003). The title manganese analogue, (I), is isostructural with this complex, and the geometry of the metal centre is again tetragonally distorted octahedral (Fig. 1). The cation interacts with the anion through a pair of hydrogen bonds; the cations, anions and uncoordinated water molecules are linked by hydrogen bonds (Table 2) into a three-dimensional network.

(I)
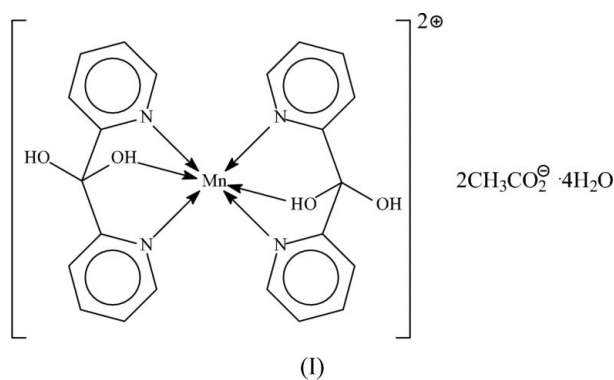
Experimental

The title compound was synthesized according to the literature procedure used for the isostructural copper compound (Reinoso *et al.*, 2003), but with manganese(II) acetate in place of copper(II) acetate. Crystals were grown from ethanol as solvent.

Crystal data

$[Mn(C_{11}H_{10}N_2O_2)_2](C_2H_3O_2)_2 \cdot 4H_2O$	$V = 1560.2$ (2) Å^3
$M_r = 649.51$	$Z = 2$
Monoclinic, $P2_1/n$	$D_x = 1.383$ Mg m^{-3}
$a = 8.6266$ (6) Å	Mo $K\alpha$ radiation
$b = 7.8941$ (5) Å	$\mu = 0.49$ mm^{-1}
$c = 23.137$ (2) Å	$T = 295$ (2) K
$\beta = 98.018$ (1)°	Irregular block, brown–red
	$0.38 \times 0.32 \times 0.23$ mm

metal-organic papers

Table 1
Selected geometric parameters (Å, °).

Mn1—N1	2.025 (2)	Mn1—O1	2.409 (2)
Mn1—N2	2.002 (3)		
N1—Mn1—N2	88.03 (9)	N1—Mn1—O1^i	106.06 (8)
N1—Mn1—N2^i	91.97 (9)	N2—Mn1—O1	75.67 (7)
N1—Mn1—O1	73.94 (8)	N2—Mn1—O1^i	104.33 (8)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1o$\cdots$O3	0.87 (1)	1.73 (1)	2.595 (3)	179 (4)
O2—H2o$\cdots$O4	0.86 (1)	1.76 (2)	2.605 (3)	166 (5)
O1w—H1w1$\cdots$O3	0.85 (1)	1.92 (2)	2.757 (4)	168 (6)
O1w—H1w2$\cdots$O2w	0.85 (1)	1.91 (1)	2.758 (5)	172 (6)
O2w—H2w1$\cdots$O4^{ii}	0.86 (1)	2.01 (3)	2.788 (4)	150 (5)
O2w—H2w2$\cdots$O1w^{iii}	0.85 (1)	1.96 (4)	2.737 (5)	150 (7)

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

Carbon-bound H atoms were placed in calculated positions (C—H = 0.93–0.96 Å) and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2$ or 1.5 times $U_{eq}(C)$. The H atoms of the hydroxy groups and water molecules were located in a difference Fourier map and were refined with distance restraints [O—H = 0.85 (1) Å and H$\cdots$H = 1.39 (1) Å]; their displacement parameters were refined. The largest peak in the final difference Fourier map is about about 1 Å from atom Mn1.
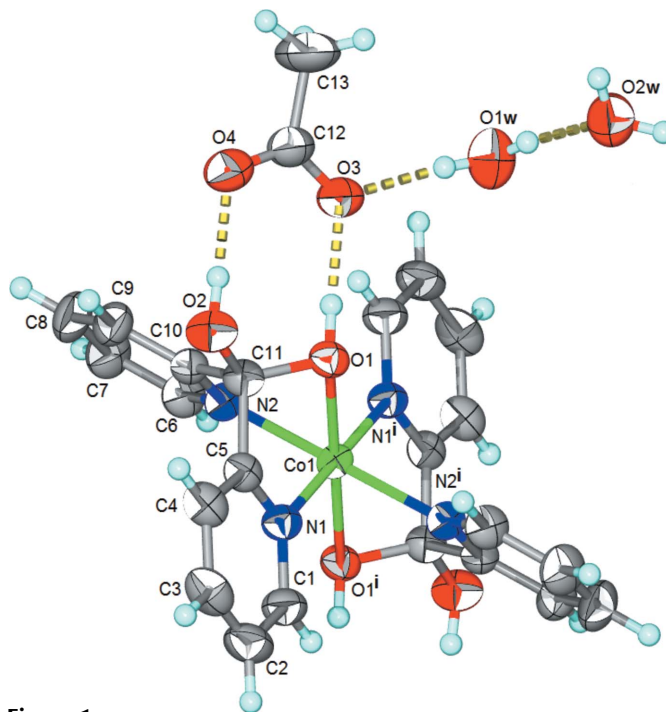

Figure 1
The structural components of (I), with displacement ellipsoids drawn at the 50% probability level and H atoms shown as spheres of arbitrary radii. The dashed lines represent hydrogen bonds. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$].

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; method used to solve structure: atomic coordinates taken from the isostructural Cu analogue (Reinoso *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

References

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