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## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.036  
 $wR$  factor = 0.097  
Data-to-parameter ratio = 14.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Tetraaquabis[4-(4-pyridyl)benzoato- $\kappa$ N]-manganese(II)

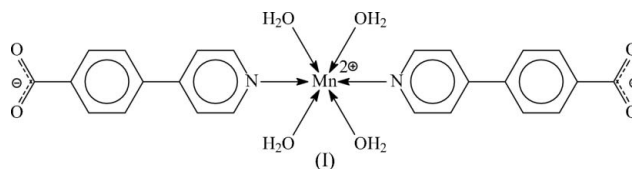
The Mn atom in the title compound,  $[\text{Mn}(\text{C}_{12}\text{H}_8\text{NO}_2)_2(\text{H}_2\text{O})_4]$ , lies on a centre of inversion in an all-*trans*- $\text{N}_2\text{O}_4\text{Mn}$  octahedron; as the 4-(4-pyridyl)benzoate ligands bind to Mn through the pyridyl N atom, the compound is formally a zwitterion. Hydrogen bonds link adjacent zwitterions into a three-dimensional network.

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## Comment

A number of metal derivatives of 4-pyridylcarboxylic acid have been crystallographically authenticated; among the tetraaqua transition metal compounds, the carboxylate binds datively through the neutral nitrogen and not through the negatively charged carboxylate oxygen (Cambridge Structural Database, Version 5.27 of December 2005; Allen, 2002). The studies on tetraaqua(4-pyridylcarboxylato)copper (Lin *et al.*, 2002; Ng, 2003; Okabe *et al.*, 1993; Waizumi *et al.*, 1998) have been extended to an investigation of the copper derivatives of the larger 4-(4-pyridyl)benzoate anion. An anhydrous and a diaqua compound are formed, depending on the conditions of the synthesis; both feature covalent copper–oxygen bonds in their crystal structures (Lu & Luck, 2003). The manganese(II) derivative exists as a tetrahydrate complex, (I) (Fig. 1); the metal lies on a centre of inversion and is datively coordinated by four water molecules and also through the N atoms of the anions. The compound is formally a zwitterion; adjacent zwitterions are linked through hydrogen bonds (Table 2) into a three-dimensional network.



## Experimental

4-(4-Pyridyl)benzoic acid was synthesized from the cross-coupling of 4-carboxybenzeneboronic acid with 4-bromopyridine (Gong & Pauls,

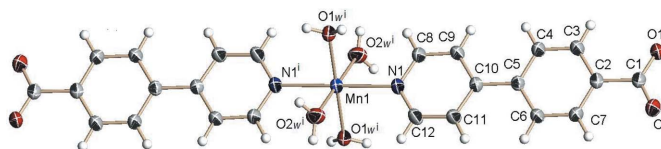


Figure 1

Plot of the structure of (I). Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. [Symmetry code (i) as in Table 1.]

2000). Manganese acetate (0.245 g, 1 mmol), 4-(4-pyridyl)benzoic acid (0.218 g, 2 mmol), triethylamine (0.3 ml, 2 mmol) and water (14 ml) were sealed in a 25 ml Teflon-lined Parr bomb. The bomb was heated at 423 K for 3 d. Light-yellow plates were isolated when the bomb was cooled slowly to room temperature in about 50% yield.

Crystal data

[Mn(C<sub>12</sub>H<sub>8</sub>NO<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>]  
*M<sub>r</sub>* = 523.39  
 Triclinic, *P* $\bar{1}$   
*a* = 6.3442 (3) Å  
*b* = 7.1089 (3) Å  
*c* = 13.2655 (6) Å  
 $\alpha$  = 95.201 (2)°  
 $\beta$  = 96.001 (3)°  
 $\gamma$  = 112.042 (1)°  
*V* = 546.01 (4) Å<sup>3</sup>  
*Z* = 1  
*D<sub>x</sub>* = 1.592 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 1591 reflections  
 $\theta$  = 3.5–28.0°  
 $\mu$  = 0.66 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Plate, yellow  
 0.50 × 0.17 × 0.09 mm

Data collection

Bruker APEX-II area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.828, *T<sub>max</sub>* = 0.943  
 4291 measured reflections  
 2694 independent reflections  
 2103 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.020  
 $\theta_{max}$  = 28.5°  
*h* = -8 → 7  
*k* = -8 → 9  
*l* = -17 → 16

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.036  
*wR* (*F*<sup>2</sup>) = 0.097  
*S* = 1.03  
 2694 reflections  
 176 parameters  
 H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.1086P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.33 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{min} = -0.35 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Mn1—O1 <i>w</i>	2.174 (1)	Mn1—N1	2.272 (2)
Mn1—O2 <i>w</i>	2.208 (2)		
O1 <i>w</i> —Mn1—O1 <i>w</i> <sup>i</sup>	180	O2 <i>w</i> —Mn1—O2 <i>w</i> <sup>i</sup>	180
O1 <i>w</i> —Mn1—O2 <i>w</i> <sup>i</sup>	85.66 (6)	O2 <i>w</i> —Mn1—N1	87.44 (6)
O1 <i>w</i> —Mn1—O2 <i>w</i>	94.34 (6)	O2 <i>w</i> —Mn1—N1 <sup>i</sup>	92.56 (6)
O1 <i>w</i> —Mn1—N1	87.15 (5)	N1—Mn1—N1 <sup>i</sup>	180
O1 <i>w</i> —Mn1—N1 <sup>i</sup>	92.85 (5)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1 <i>w</i> —H1 <i>w</i> 1···O1 <sup>ii</sup>	0.85 (1)	1.81 (1)	2.657 (2)	174 (3)
O1 <i>w</i> —H1 <i>w</i> 2···O2 <sup>iii</sup>	0.85 (1)	1.93 (1)	2.779 (2)	174 (3)
O2 <i>w</i> —H2 <i>w</i> 1···O1 <sup>iv</sup>	0.85 (1)	1.90 (1)	2.757 (2)	179 (3)
O2 <i>w</i> —H2 <i>w</i> 2···O2 <sup>v</sup>	0.85 (1)	2.02 (1)	2.852 (2)	168 (3)

Symmetry codes: (ii) *x* + 1, *y*, *z* + 1; (iii) -*x*, -*y*, -*z*; (iv) -*x* + 1, -*y* + 1, -*z*; (v) -*x*, -*y* + 1, -*z*.

The carbon-bound H atoms were positioned geometrically [C—H = 0.93 Å and *U*(H) = 1.2*U*<sub>eq</sub>(C)], and were included in the refinement in the riding-model approximation. The water H atoms were located in a difference Fourier map and were refined with a distance restraint of O—H = 0.85 (1) Å; their displacement parameters were freely refined.

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; method used to solve structure: difference Fourier with Mn1 at (1/2, 1/2, 1/2); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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