

A second C-centered monoclinic polymorph of poly[[aquamanganese(II)]-di- $\mu$ -(4-pyridylthioacetato)- $\kappa^6$ O,O':N,N:O,O']Yong-Qing Huang,<sup>a</sup> Hui Zhang,<sup>a</sup>  
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## Key indicators

Single-crystal X-ray study

T = 293 K

Mean  $\sigma$ (C–C) = 0.002 Å

R factor = 0.029

wR factor = 0.084

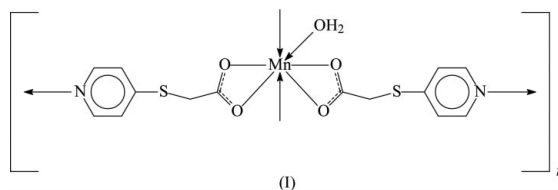
Data-to-parameter ratio = 12.4

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

The water-coordinated Mn atom in the title compound,  $[\text{Mn}(\text{C}_7\text{H}_6\text{NO}_2\text{S})_2(\text{H}_2\text{O})]_n$ , is chelated by two carboxylate groups; it is also linked to the N atoms of two other carboxylate anions in a pentagonal bipyramidal environment. The compound adopts a chain architecture. The Mn and the water O atom lie on a twofold rotation axis.

## Comment

The reaction of divalent transition metal salts with pyridyl-4-thiolyacetic acid gives rise to compounds having different formulations, depending on the synthetic conditions. Two monoaquabis(pyridyl-4-thiolyacetato)nickel complexes have been isolated that differ in the binding mode of the carboxylate anion (Huang *et al.*, 2004*a,b*). The structural motif in these complexes is different from that in monoaquabis(pyridyl-4-thiolyacetato)manganese (Zhang *et al.*, 2004); the latter crystallizes in a C-centered monoclinic cell that is more conveniently converted to an I-centered cell having dimensions of  $a = 15.880$  (3) Å,  $b = 6.490$  (1) Å,  $c = 15.611$  (2) Å and  $\beta = 93.414$  (1)°. Curiously, the present investigation features a C-centered cell of nearly identical dimensions. Compound (I) (Fig. 1) has the Mn atom in a pentagonal bipyramidal environment; the two pairs of chelating carboxyl O atoms and the water O atom comprise the pentagonal plane. The Mn and the water O atom lie on a twofold rotation axis. The compound is isostructural with the cobalt(II) analog, whose structure has been described in detail (Qin *et al.*, 2004).



## Experimental

Manganese acetate (98 mg, 0.4 mmol), 4-pyridylthioacetic acid (68 mg, 0.4 mmol) and sodium hydroxide (16 mg, 0.4 mmol) were dissolved in a water–ethanol (12:5 v/v) mixture (17 ml). The solution was placed in a Teflon-lined stainless-steel bomb (23 ml). The bomb was heated at 393 K for 12 h and then cooled to room temperature.

## Crystal data

 $[\text{Mn}(\text{C}_7\text{H}_6\text{NO}_2\text{S})_2(\text{H}_2\text{O})]$  $M_r = 409.33$ Monoclinic,  $C2/c$  $a = 15.8338$  (10) Å $b = 6.3209$  (4) Å $c = 15.5019$  (10) Å $\beta = 93.703$  (1)° $V = 1548.25$  (17) Å<sup>3</sup> $Z = 4$  $D_x = 1.756$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation

Cell parameters from 3081

reflections

 $\theta = 2.6$ – $28.4$ ° $\mu = 1.15$  mm<sup>-1</sup>

T = 293 (2) K

Prism, colorless

0.40 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2001)  
 $T_{\min} = 0.513$ ,  $T_{\max} = 0.846$   
 4450 measured reflections

1729 independent reflections  
 1645 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.016$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -20 \rightarrow 15$   
 $k = -8 \rightarrow 7$   
 $l = -18 \rightarrow 19$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.084$   
 $S = 1.08$   
 1729 reflections  
 139 parameters  
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.9837P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.37 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.26 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.0052 (7)

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Mn1—O1w	2.1926 (18)	Mn1—O2 <sup>i</sup>	2.3042 (13)
Mn1—O1	2.2724 (13)	Mn1—N1 <sup>ii</sup>	2.2546 (15)
Mn1—O1 <sup>i</sup>	2.2724 (13)	Mn1—N1 <sup>iii</sup>	2.2546 (15)
Mn1—O2	2.3042 (13)		
O1w—Mn1—O1	84.89 (3)	O1—Mn1—N1 <sup>ii</sup>	92.45 (5)
O1w—Mn1—O2	141.21 (3)	O1—Mn1—N1 <sup>iii</sup>	87.75 (5)
O1w—Mn1—N1 <sup>ii</sup>	91.09 (4)	O2—Mn1—O2 <sup>i</sup>	77.57 (6)
O1—Mn1—O1 <sup>i</sup>	169.78 (6)	O2—Mn1—N1 <sup>ii</sup>	87.76 (5)
O1—Mn1—O2	56.46 (4)	O2—Mn1—N1 <sup>iii</sup>	90.54 (5)
O1—Mn1—O2 <sup>i</sup>	133.74 (4)	N1 <sup>ii</sup> —Mn1—N1 <sup>iii</sup>	177.83 (7)

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

The water H atom was located in a difference map and was refined freely. As the diffraction measurements were of a high quality, the carbon-bound H atoms were located and they were refined with a distance restraint of C—H = 0.95  $\text{\AA}$ .

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; method used to solve structure: atomic coordinates taken from published Co structure; 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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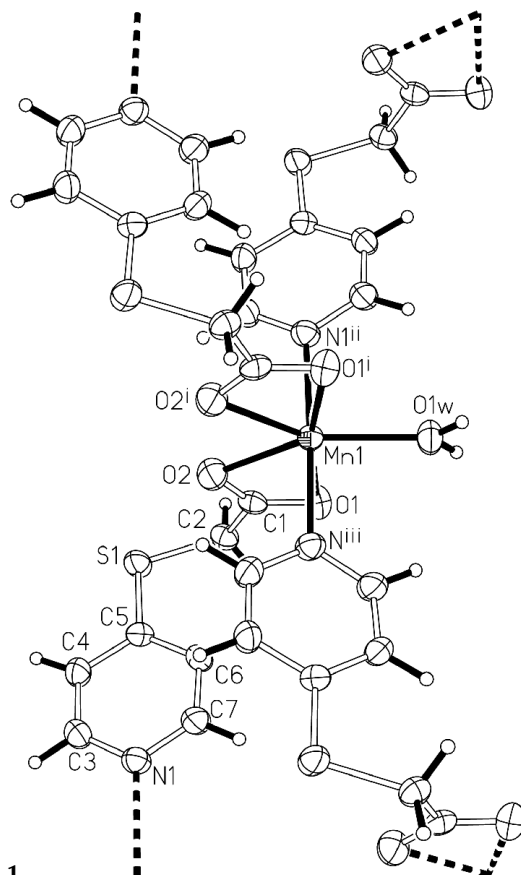


Figure 1

ORTEPII (Johnson, 1976) plot illustrating a portion of the layer structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. Symmetry codes are as in Table 2.

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