

Ying Liu,* Jian-Min Dou, Da-Qi Wang, Xian-Xi Zhang and Lei Zhou

College of Chemistry and Chemical Engineering,
 Liaocheng University, Liaocheng 252059,
 People's Republic of China

Correspondence e-mail: yingliu@lctu.edu.cn

Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
 R factor = 0.043
 wR factor = 0.105
 Data-to-parameter ratio = 11.2

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

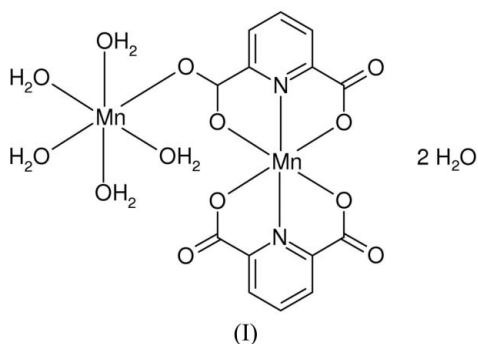
Pentaaqua- $1\kappa^5\text{O}$ -(μ -pyridine-2,6-dicarboxylato- $1\kappa\text{O}^2:2\kappa^3\text{O}^{2'},\text{N},\text{O}^6$)(pyridine-2,6-dicarboxylato- $2\kappa^3\text{O}^2,\text{N},\text{O}^6$)dimanganese(II) dihydrate

The title compound, $[\text{Mn}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{H}_2\text{O})_5]\cdot 2\text{H}_2\text{O}$, has been prepared from the hydrothermal reaction of manganese(II) chloride tetrahydrate and pyridine-2,6-dicarboxylic acid. It is isostructural with the analogous Co^{II} , Ni^{II} , Cu^{II} and Zn^{II} compounds.

Received 17 August 2006
 Accepted 5 September 2006

Comment

The title compound, (I), is isostructural with its Co^{II} , Ni^{II} , Cu^{II} and Zn^{II} analogues (Jiang *et al.*, 2004; Qi *et al.*, 2004; Wang, Duan, Xiao, *et al.*, 2004; Wang, Duan, Wang *et al.*, 2004; Wen *et al.*, 2002; Yang *et al.*, 2002; Nathan & Mai, 2000; Hakansson *et al.*, 1993).



Atom Mn1 is hexacoordinated in an approximately octahedral geometry, chelated by four O atoms and two N atoms from two pyridine-2,6-dicarboxylate ligands (Fig. 1). Atom Mn2 is bound to one O atom of a pyridine-2,6-dicarboxylate

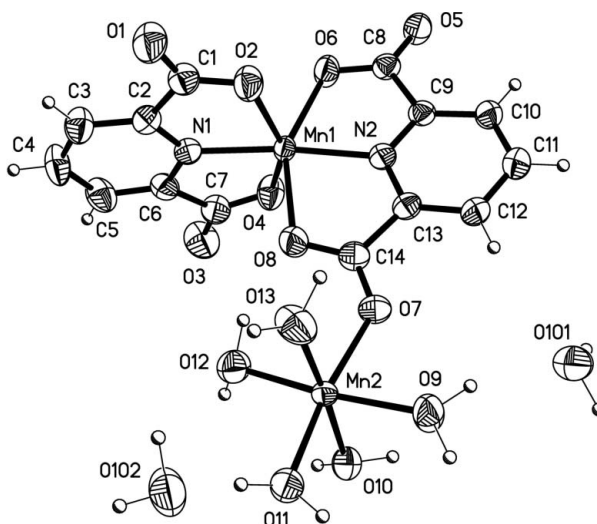


Figure 1
 The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level for non-H atoms.

ligand, with five water molecules completing the octahedral coordination.

Hydrogen bonds between the water molecules and the O atoms of the carboxylate groups (Table 1) link the molecules into a three-dimensional network (Fig. 2).

Experimental

A mixture of manganese(II) chloride tetrahydrate (0.5 mmol), pyridine-2,6-dicarboxylic acid (0.5 mmol) and H₂O (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was heated at 413 K for 2 d, and then cooled to room temperature. Colourless block-shaped crystals of (I) were obtained with a yield of 25%. Elemental analysis found: C 29.56, H 3.51, N 4.99, O 42.21, Mn 19.32%; calculated: C 29.67, H 3.53, N 4.95, O 42.39, Mn 19.43%.

Crystal data

[Mn ₂ (C ₇ H ₃ NO ₄) ₂ (H ₂ O) ₅]-2H ₂ O	Z = 4
<i>M_r</i> = 566.20	<i>D_x</i> = 1.713 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 8.4001 (4) Å	<i>μ</i> = 1.23 mm ⁻¹
<i>b</i> = 27.4340 (14) Å	<i>T</i> = 293 (2) K
<i>c</i> = 9.6260 (5) Å	Block, colourless
<i>β</i> = 98.240 (1)°	0.40 × 0.37 × 0.33 mm
<i>V</i> = 2195.39 (19) Å ³	

Data collection

Bruker SMART CCD diffractometer	7587 measured reflections
<i>φ</i> and <i>ω</i> scans	3831 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3087 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T_{min}</i> = 0.610, <i>T_{max}</i> = 0.667	<i>R_{int}</i> = 0.031
	<i>θ_{max}</i> = 25.0°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 2.7531P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.105$	(Δ/σ) _{max} = 0.001
<i>S</i> = 1.12	$\Delta\rho_{max} = 0.43 \text{ e \AA}^{-3}$
3831 reflections	$\Delta\rho_{min} = -0.39 \text{ e \AA}^{-3}$
341 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

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>
O9—H91...O5 ⁱ	1.00 (2)	1.652 (18)	2.648 (4)	174 (5)
O9—H92...O101	1.00 (2)	2.04 (2)	2.991 (4)	159 (3)
O10—H101...O5 ⁱⁱ	1.00 (2)	1.687 (17)	2.691 (4)	178 (4)
O10—H102...O2 ⁱⁱⁱ	1.00 (2)	1.809 (19)	2.796 (4)	168 (3)
O11—H112...O6 ⁱ	1.00 (2)	1.783 (19)	2.775 (4)	171 (4)
O11—H111...O102	1.00 (2)	1.672 (19)	2.659 (4)	170 (3)
O12—H122...O1 ⁱⁱⁱ	1.00 (2)	1.721 (19)	2.707 (4)	167 (4)
O12—H121...O8	1.00 (2)	1.89 (2)	2.836 (4)	156 (4)
O13—H131...O3 ^{iv}	1.00 (2)	1.732 (18)	2.731 (4)	174 (4)
O13—H132...O101 ^v	1.00 (2)	1.84 (2)	2.830 (4)	168 (4)
O101—H2...O10 ^{vi}	1.00 (2)	2.00 (2)	2.945 (4)	159 (4)
O101—H1...O4 ⁱⁱ	1.00 (2)	2.16 (3)	3.063 (4)	150 (4)
O101—H1...O6 ⁱⁱ	1.00 (2)	2.47 (4)	3.217 (4)	131 (4)
O102—H4...O3 ^{iv}	1.00 (2)	1.83 (2)	2.777 (5)	157 (4)
O102—H3...O1 ^{vii}	1.00 (2)	1.784 (18)	2.785 (4)	178 (6)

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

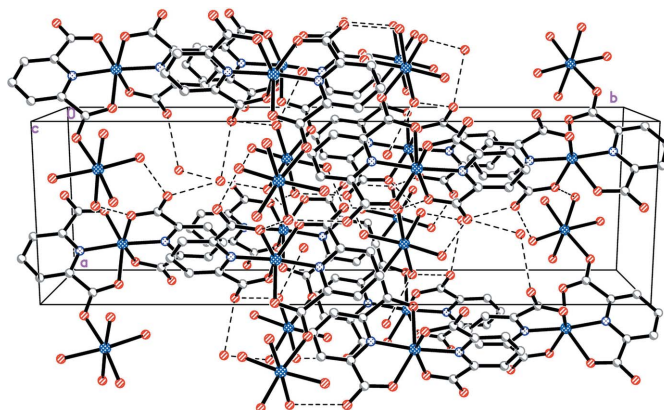


Figure 2

View of (I), approximately along *c*, showing the three-dimensional network of O—H...O hydrogen bonds (dashed lines). H atoms have been omitted.

H atoms bound to C atoms were placed in calculated positions and allowed to ride during subsequent refinement, with C—H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C). H atoms of the water molecules were located in difference Fourier maps and refined with all O—H distances restrained to be equal, all H...H distances restrained to be 1.58 times the O—H distance, and *U*_{iso}(H) = 1.5*U*_{eq}(O). The refined O—H distance is 1.00 (2) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Chinese Natural Science Foundation (grant No. 20501011) and Liaocheng University (grant No. 31801) for financial support. In addition, we thank Professor Jianmin Dou for assistance.

References

- Bruker (1998). *SMART*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1999). *SAINTE* and *SHELXTL*. Versions 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Hakansson, K., Lindahl, M., Svensson, G. & Albertsson, J. (1993). *Acta Chem. Scand.* **47**, 449–452.
- Jiang, Y. M., Wang, X. L. & Yin, X. J. (2004). *Chin. J. Inorg. Chem.*, **20**, 175–178.
- Nathan, L. C. & Mai, T. D. (2000). *J. Chem. Crystallogr.* **30**, 509–518.
- Qi, Y. J., Wang, Y. H., Fan, H. L., Cao, M. H., Mao, L., Hu, C. W., Wang, E. & Hu, N. H. (2004). *J. Mol. Struct.* **694**, 73–78.
- Sheldrick, G. M. (1996). *SADABS*. Version 2.05. University of Göttingen, Germany.
- Wang, L., Duan, L. Y., Wang, E. B., Xiao, D. R., Li, Y. G., Lan, Y., Xu, L. & Hu, C. W. (2004). *Transition Met. Chem.* **29**, 212–215.
- Wang, L., Duan, L. Y., Xiao, D. R., Wang, E. B. & Hu, C. W. (2004). *J. Coord. Chem.* **57**, 1079–1082.
- Wen, Y.-H., Li, Z.-J., Qin, Y.-Y., Kang, Y., Chen, Y.-B., Cheng, J.-K. & Yao, Y.-G. (2002). *Acta Cryst.* **E58**, m762–m764.
- Yang, L. Q., Crans, D. C., Miller, S. M., la Cour, A., Anderson, O. P., Kaszynski, P. M., Godzala, M. E. III, Austin, L. D. & Willsky, G. R. (2002). *Inorg. Chem.* **41**, 859–863.