

**Hong Li, Jia-Geng Liu and
Duan-Jun Xu***Department of Chemistry, Zhejiang University,
People's Republic of China

Correspondence e-mail: xudj@mail.hz.zj.cn

Key indicators

Single-crystal X-ray study

 $T = 295$ KMean $\sigma(\text{C}-\text{C}) = 0.002$ Å R factor = 0.027 wR factor = 0.075

Data-to-parameter ratio = 15.3

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Poly[[bis(1*H*-benzimidazole- κ N³)manganese(II)]-
 μ -aqua- μ -succinato- κ^2 O:O']**

In the title polymeric compound, $[\text{Mn}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_7\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})]_n$, the Mn^{II} atom is located on an inversion center and is coordinated by succinate dianions and benzimidazole and water molecules with an elongated octahedral coordination geometry. The long $\text{Mn}-\text{O}(\text{water})$ bond distance of $2.4982(3)$ Å shows the rather weak nature of this bond. The succinate dianion and water molecule are located on an inversion center and a twofold axis, respectively; they bridge the Mn^{II} atoms to form a polymeric structure.

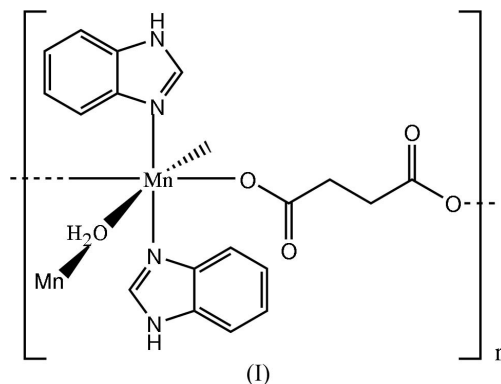
Received 21 March 2005

Accepted 22 March 2005

Online 31 March 2005

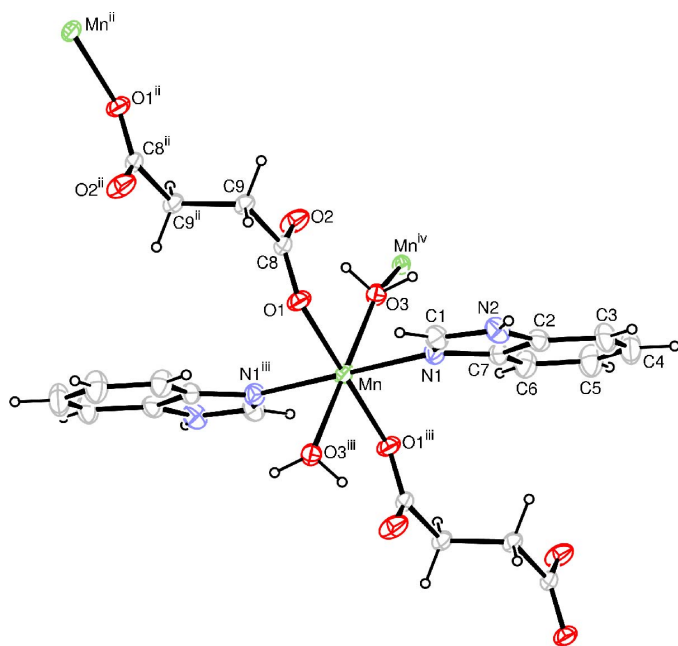
Comment

As coordination of water to Mn is an important step in the photosynthesis process (Vincent & Christou, 1989), we have been interested in the coordination properties of manganese for several years (Nie *et al.*, 2001). The large $\text{Mn}-\text{O}(\text{water})-\text{Mn}$ bond angle and long $\text{Mn}-\text{O}(\text{water})$ bond distance observed in the title compound, (I), show the rather weak nature of the bond from water to the Mn^{II} atom.

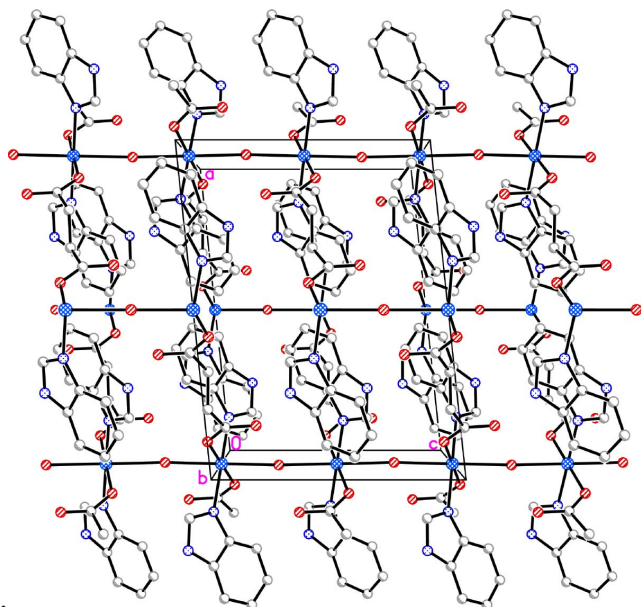


A segment of the polymeric structure of (I) is illustrated in Fig. 1. The repeat unit of the polymeric complex consists of one Mn^{II} atom, one succinate dianion, two benzimidazole ligands and one coordinated water molecule. The Mn^{II} atom lies at an inversion center and is coordinated by succinate dianions, benzimidazole and water molecules with an elongated octahedral geometry (Table 1), similar to the situation in the Cd^{II} analog (Liu & Xu, 2004).

The water molecule (O3) is located on a twofold axis and links neighboring Mn^{II} atoms to form the 'water-bridged' polymeric chain (Fig. 2). The $\text{Mn}-\text{O3}$ bond distance is longer than the $\text{Mn}-\text{O1}$ bond distance in the equatorial plane by $0.377(9)$ Å. The $\text{Mn}-\text{O3}-\text{Mn}^{\text{IV}}$ bond angle of $152.31(6)^\circ$ [symmetry code: (iv) $1-x, y, -z+\frac{1}{2}$] is much larger than the value of 109° expected for a normal sp^3 -hybridized O atom, corresponding to the longer $\text{Mn}-\text{O3}$ bond. These observa-


Figure 1

A segment of the polymeric structure of (I) with 40% probability displacement ellipsoids (arbitrary spheres for the H atoms) [symmetry codes: (ii) $-x + \frac{1}{2}$, $-y + \frac{1}{2}$, $1 - z$; (iii) $1 - x$, $-y$, $1 - z$; (iv) $1 - x$, $-z + \frac{1}{2}$].


Figure 2

The crystal packing. H atoms have been omitted.

tions indicate the weaker coordination interaction between the Mn^{II} atom and water molecule.

The succinate dianion is located on another inversion center and thus displays a planar carbon skeleton. The succinate dianions bridge neighboring Mn^{II} atoms and thus displays a planar carbon skeleton. The succinate dianions bridge neighboring Mn^{II} atoms through terminal carboxyl groups to form a 'succinate-bridged' polymeric chain; the chains are nearly perpendicular to the 'water-bridged' polymeric chains shown in Fig. 2.

O—H...O hydrogen bonding between carboxylate ligands and coordinated water molecules and N—H...O hydrogen

bonding between carboxylate and benzimidazole (Table 2) stabilize the polymeric structure.

π – π stacking interactions are usually found in the structures of metal complexes with benzimidazole (Li *et al.*, 2005); however, no such π – π stacking between benzimidazole rings is observed in (I).

Experimental

MnCl₂·4H₂O (0.20 g, 1 mmol) was added to an aqueous solution (20 ml) containing succinic acid (0.12 g, 1 mmol) and NaOH (0.08 g, 2 mmol). After the solution was refluxed for 2 h, an aqueous solution (10 ml) of benzimidazole (0.12 g, 1 mmol) was added to the above solution. The solution was refluxed for a further 3 h and filtered. After cooling to room temperature, the solution was filtered once more. Single crystals of (I) were obtained from the filtrate after two weeks.

Crystal data

[Mn(C₄H₄O₄)(C₇H₆N₂)₂(H₂O)]
 $M_r = 425.30$
 Monoclinic, C2/c
 $a = 13.0071$ (5) Å
 $b = 13.9756$ (6) Å
 $c = 9.7024$ (4) Å
 $\beta = 96.042$ (2)°
 $V = 1753.92$ (12) Å³
 $Z = 4$

$D_x = 1.611$ Mg m⁻³
 Mo K α radiation
 Cell parameters from 5996 reflections
 $\theta = 2.1$ – 27.2°
 $\mu = 0.79$ mm⁻¹
 $T = 295$ (2) K
 Chunk, colorless
 $0.41 \times 0.35 \times 0.20$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.745$, $T_{\max} = 0.850$
 7988 measured reflections

1994 independent reflections
 1859 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$
 $\theta_{\max} = 27.4^\circ$
 $h = -16 \rightarrow 16$
 $k = -18 \rightarrow 18$
 $l = -11 \rightarrow 12$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.075$
 $S = 1.11$
 1994 reflections
 130 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 1.0253P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.25$ e Å⁻³
 $\Delta\rho_{\min} = -0.30$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Mn—O1	2.1217 (9)	Mn—O3	2.4982 (3)
Mn—N1	2.2295 (11)		
O1—Mn—N1	87.60 (4)	N1—Mn—O3	89.28 (3)
O1—Mn—O3	90.82 (4)		

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H2...O2 ⁱ	0.86	1.96	2.7992 (16)	163
O3—H3A...O2	0.90	1.82	2.6845 (14)	160

Symmetry code: (i) $\frac{1}{2} + x$, $\frac{1}{2} - y$, $\frac{1}{2} + z$.

The water H atoms were located in a difference Fourier map and isotropically refined by riding in their as-found positions relative to

the atom O3. Other H atoms were placed in calculated positions with C–H = 0.93 (aromatic) or 0.97 Å (methylene) and N–H = 0.86 Å, and included in the final cycles of refinement in the riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ of the carrier atom.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *XP* (Siemens, 1994); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The project was supported by the National Natural Science Foundation of China (grant No. 20443003).

References

- Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Li, H., Yin, K.-L. & Xu, D.-J. (2005). *Acta Cryst.* **C61**, m19–m21.
- Liu, B.-X. & Xu, D.-J. (2004). *Acta Cryst.* **C60**, m39–m41.
- Nie, J.-J., Liu, L.-J., Luo, Y. & Xu, D.-J. (2001). *J. Coord. Chem.* **53**, 365–371.
- Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MS (2002). *CrystalStructure*. Version 3.00. Rigaku/MS, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Siemens (1994). *XP*. Version 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Vincent, J. B. & Christou, G. (1989). *Adv. Inorg. Chem.* **28**, 197–206.