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## Key indicators

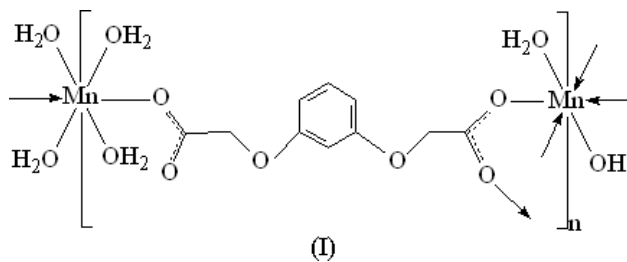
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.133  
Data-to-parameter ratio = 14.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Poly[triaqua( $\mu$ -benzene-1,3-dioxyacetato)-  
manganese(II)]: a two-dimensional manganese(II)  
coordination polymer

In the asymmetric unit of the title compound,  $[\text{Mn}(\text{C}_{10}\text{H}_8\text{O}_6)(\text{H}_2\text{O})_3]_n$ , the two half- $\text{Mn}^{\text{II}}$  atoms lie on inversion centres. One  $\text{Mn}^{\text{II}}$  atom is in an octahedral configuration, defined by two O atoms from two monodentate carboxylate groups and four water molecules, and the other  $\text{Mn}^{\text{II}}$  atom exists in a different octahedral coordination environment, defined by four O atoms from four monodentate carboxylate groups and two water molecules. The  $\text{Mn}^{\text{II}}$  atoms are bridged by a benzene-1,3-dioxyacetate dianion in monodentate and bridging-bidentate modes, forming a two-dimensional layer structure.

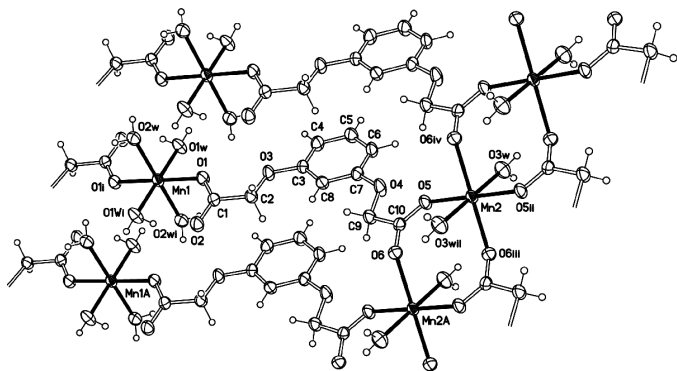
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## Comment

Rational design and construction of supramolecular architectures with specific network structures, and investigation of their properties, have become particularly important and topical subjects (Tao *et al.*, 2000; Choi & Jeon, 2003). The generation of molecular architectures relies on the combination of several factors, such as the coordination geometry of the metals, the bonding of the ligands and the reaction conditions. In relation to the ligands, the judicious choice of a suitable ligand is an important factor which greatly influences the structure of the coordination architecture and the functionality of the complex formed. In this context, phenylene-dioxydiacetic acids ( $\text{bdoaH}_2$ ), especially 1,3- and 1,4- $\text{bdoaH}_2$ , are good candidates for the construction of supramolecular complexes, because they are not only capable of binding to metal centres in versatile binding modes, but can also form regular hydrogen bonds by functioning as either hydrogen-bond donors or acceptors.



Recently, we have reported the structures of some one-dimensional chain  $\text{Cu}^{\text{II}}$ ,  $\text{Zn}^{\text{II}}$ ,  $\text{Co}^{\text{II}}$  and  $\text{Cd}^{\text{II}}$  complexes constructed with 1,3- or 1,4- $\text{bdoa}^{2-}$  ligands (Gao, Li *et al.*, 2004; Gao, Liu, Huo, Zhao & Ng, 2004; Gao, Liu, Huo, Zhao & Zhao, 2004*b,c,d*), but less attention has been paid to complexes with  $\text{Mn}^{\text{II}}$ . In the complexes  $[\text{Mn}(\text{H}_2\text{O})_6](1,4\text{-bdoa})$  (Liu *et al.*, 2004) and  $[\text{MnCl}(\text{phen})_2(\text{H}_2\text{O})]_2(1,4\text{-bdoa})\cdot 2\text{H}_2\text{O}$  (Gao, Liu, Huo, Zhao & Zhao, 2004*a*), the carboxylate acts as


**Figure 1**

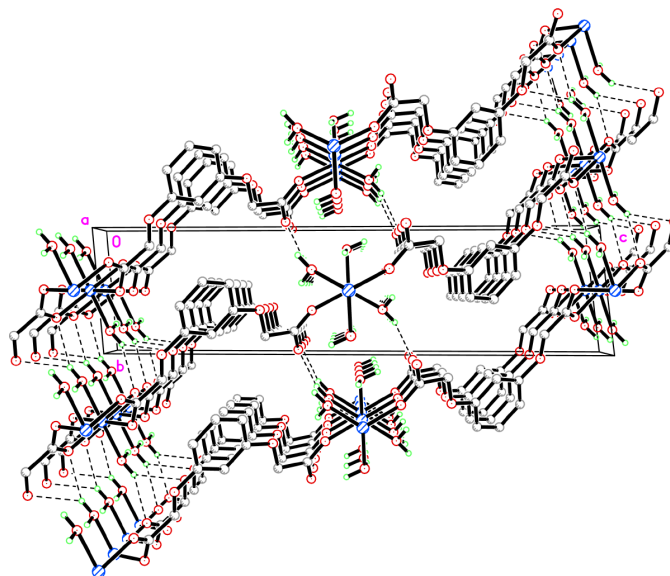
A view of (I), showing the atom-numbering scheme and with 30% probability displacement ellipsoids. [Symmetry codes: (i)  $2 - x, 1 - y, 1 - z$ ; (ii)  $-1 - x, -1 - y, 2 - z$ ; (iii)  $-x, -1 - y, 2 - z$ ; (vi)  $x - 1, y, z$ ; (A)  $x + 1, y, z$ .]

a counter-ion. In the present paper, we report the structure of the title compound, (I),  $[\text{Mn}(\text{1,3-bdoxa})(\text{H}_2\text{O})_3]_n$ .

As shown in Fig. 1, the asymmetric unit of (I) consists of two half- $\text{Mn}^{\text{II}}$  atoms (Mn1 and Mn2), one 1,3-bdoxa<sup>2-</sup> dianion and three coordinated water molecules. Atoms Mn1 and Mn2 occupy inversion centres. The coordination of Mn1 can be described as octahedral, with two O atoms from different monodentate carboxyl groups and four water molecules, while atom Mn2 exists in a different octahedral coordination environment, defined by four O atoms from different monodentate carboxyl groups and two water molecules. All Mn—O<sub>carboxyl</sub> distances (Table 1) are within the previously reported range [2.111 (2)–2.284 (3) Å; Ma *et al.*, 2004].

It is noted that the two C—O bonds of one carboxyl group (O1—C1—O2) are essentially equal, with O1—C1 and O2—C1 distances of 1.256 (4) and 1.255 (4) Å, respectively, suggesting delocalization of electrons throughout. The two C—O bonds of the other carboxyl group (O5—C10—O6) are significantly different, the O6—C10 and O5—C10 distances being 1.267 (4) and 1.246 (4) Å, respectively, in accord with the greater double-bond character of the latter bond. These facts might be the result of hydrogen bonds (Table 2) and different Mn—O bonding interactions.

Adjacent Mn1···Mn2 atoms are connected through 1,3-bdoxa<sup>2-</sup> groups in a bis-monodentate bridging mode, giving rise to a one-dimensional infinite chain running along a diagonal of the *ac* plane. The shortest Mn···Mn separation is 13.861 (4) Å. One pair of Mn atoms (Mn2 and Mn2<sup>iii</sup>) is further connected by carboxyl bridges O5—C10—O6 and O5<sup>iii</sup>—C10<sup>iii</sup>—O6<sup>iii</sup>, to generate an eight-membered ring with a chair conformation [symmetry code: (iii)  $-x, -y - 1, 2 - z$ ]. In Fig. 1, the atom pairs Mn1—Mn1A and Mn2—Mn2A are related by a [100] translation. Consequently, the distance between them is equal to *a*, *i.e.* 4.770 (1) Å. Thus, atoms Mn1, Mn1A, Mn2 and Mn2A define a parallelogram. The resulting architecture can be described as a two-dimensional layer structure. Furthermore, there are intermolecular hydrogen bonds (Table 2) involving the aqua ligands, consolidating the crystal structure and leading to a three-dimensional supramolecular network (Fig. 2).


**Figure 2**

A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

## Experimental

Benzene-1,3-dioxyacetic acid was prepared following the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990).  $\text{MnCl}_2 \cdot 6\text{H}_2\text{O}$  (4.68 g, 20 mmol) and 1,3-bdoxaH<sub>2</sub> (4.52 g, 20 mmol) were dissolved in water (20 ml), and the pH was adjusted to 7 with 0.1 M NaOH. The mixture was sealed in a 25 ml Teflon-lined stainless steel bomb and held at 393 K for 5 d. The bomb was cooled naturally to room temperature, and colourless prismatic crystals of (I) were obtained after several days. Elemental analysis, calculated: C 36.05, H 4.24%; found: C 36.18, H 4.19%.

### Crystal data

$[\text{Mn}(\text{C}_{10}\text{H}_8\text{O}_6)(\text{H}_2\text{O})_3]$   
 $M_r = 333.15$   
 Triclinic, *P*1  
 $a = 4.770$  (1) Å  
 $b = 5.797$  (2) Å  
 $c = 22.923$  (7) Å  
 $\alpha = 83.65$  (2)°  
 $\beta = 84.16$  (1)°  
 $\gamma = 84.92$  (1)°  
 $V = 624.8$  (3) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.771$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 5921 reflections  
 $\theta = 3.7$ – $27.5^\circ$   
 $\mu = 1.10$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Prism, colourless  
 $0.38 \times 0.25 \times 0.19$  mm

### Data collection

Rigaku R-AXIS RAPID diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\text{min}} = 0.679, T_{\text{max}} = 0.818$   
 6030 measured reflections

2841 independent reflections  
 2278 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -6 \rightarrow 5$   
 $k = -7 \rightarrow 7$   
 $l = -29 \rightarrow 29$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.133$   
 $S = 1.04$   
 2841 reflections  
 202 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 1.0201P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.48$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.55$  e Å<sup>-3</sup>

**Table 1**  
Selected geometric parameters (Å, °).

Mn1—O1	2.187 (2)	Mn2—O3W	2.182 (2)
Mn1—O1W	2.138 (2)	O1—C1	1.256 (4)
Mn1—O2W	2.204 (3)	O2—C1	1.255 (4)
Mn2—O5	2.152 (2)	O5—C10	1.246 (4)
Mn2—O6 <sup>i</sup>	2.238 (2)	O6—C10	1.267 (4)
O1—Mn1—O2W	90.86 (10)	O1W—Mn1—O1	91.86 (9)
O1 <sup>ii</sup> —Mn1—O2W	89.14 (10)	O1W <sup>iii</sup> —Mn1—O1	88.14 (9)
O5—Mn2—O6 <sup>iii</sup>	88.04 (9)	O1W—Mn1—O2W	91.24 (10)
O5—Mn2—O6 <sup>i</sup>	91.96 (9)	O1W <sup>iii</sup> —Mn1—O2W	88.76 (10)
O5 <sup>iv</sup> —Mn2—O3W	89.87 (9)	O3W—Mn2—O6 <sup>i</sup>	85.10 (9)
O5—Mn2—O3W	90.13 (9)	O3W—Mn2—O6 <sup>iii</sup>	94.90 (9)
C3—O3—C2—C1	−179.7 (3)	C7—O4—C9—C10	−173.5 (3)

Symmetry codes: (i)  $x-1, y, z$ ; (ii)  $2-x, 1-y, 1-z$ ; (iii)  $-x, -1-y, 2-z$ ; (iv)  $-1-x, -1-y, 2-z$ .

**Table 2**  
Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H10 <sup>..</sup> —O2 <sup>ii</sup>	0.85 (3)	1.89 (3)	2.706 (3)	159 (4)
O1W—H11 <sup>..</sup> —O1 <sup>v</sup>	0.85 (3)	2.57 (3)	3.161 (4)	128 (3)
O1W—H11 <sup>..</sup> —O2W <sup>w</sup>	0.85 (3)	2.13 (2)	2.849 (4)	143 (3)
O2W—H12 <sup>..</sup> —O1 <sup>v</sup>	0.85 (3)	2.08 (2)	2.795 (3)	142 (3)
O2W—H12 <sup>..</sup> —O3 <sup>v</sup>	0.85 (3)	2.30 (3)	3.025 (3)	144 (3)
O2W—H13 <sup>..</sup> —O2 <sup>vi</sup>	0.85 (3)	1.94 (3)	2.765 (3)	162 (4)
O3W—H14 <sup>..</sup> —O6 <sup>iv</sup>	0.85 (3)	2.11 (2)	2.903 (4)	155 (4)
O3W—H15 <sup>..</sup> —O4 <sup>viii</sup>	0.85 (4)	2.35 (3)	2.952 (4)	129 (3)
O3W—H15 <sup>..</sup> —O5 <sup>vii</sup>	0.85 (4)	2.23 (3)	2.983 (4)	147 (4)

Symmetry codes: (iv)  $-1-x, -1-y, 2-z$ ; (ii)  $2-x, 1-y, 1-z$ ; (v)  $1-x, 1-y, 1-z$ ; (vi)  $2-x, -y, 1-z$ ; (vii)  $-1-x, -y, 2-z$ .

C-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ , and were refined in the riding-model approximation. Water H atoms were located in difference maps and refined with O—H and H<sup>..</sup>H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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