Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquamanganese(II) benzene-1,4-dioxyacetate

Ji-Wei Liu,[a] Shan Gao,[a]* Li-Hua Huo,[a] Hui Zhao[a] and Seik Weng Ng[b]

[a]College of Chemistry and Chemical Technology, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: shangao67@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.050
wR factor = 0.169
Data-to-parameter ratio = 14.2

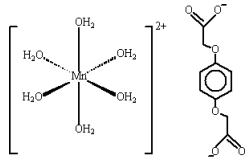
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 25 March 2004
Accepted 29 March 2004
Online 9 April 2004

The cation and anion of the title compound, $[Mn(H_2O)_6](C_{10}H_8O_6)$, lie on inversion centres. The Mn^{II} atom is coordinated by six water molecules to form an octahedral coordination geometry [Mn—O = 2.143 (3)—2.228 (3) Å]. The cations and anions are linked by hydrogen bonds into a three-dimensional network.

Comment

Recently, we have reported the crystal structure of hexaaquacobalt(II) benzene-1,4-dioxyacetate (Liu *et al.*, 2004). In the present work, the structure of the title hexaaquamanganese(II) complex, (I), is reported.



(I)

The structure of (I) (Fig. 1) is similar to that of the hexaaquacobalt(II) complex (Liu *et al.*, 2004). The Mn^{II} atom is six-coordinate in an octahedral environment. The cation and anion both lie on inversion centres and they are linked by O—H···O hydrogen bonds, to give a three-dimensional network structure (for details, see Table 2 and Fig. 2).

Experimental

Benzene-1,4-dioxyacetic acid was prepared following the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990). Manganese dichloride hexahydrate (4.68 g, 20 mmol),

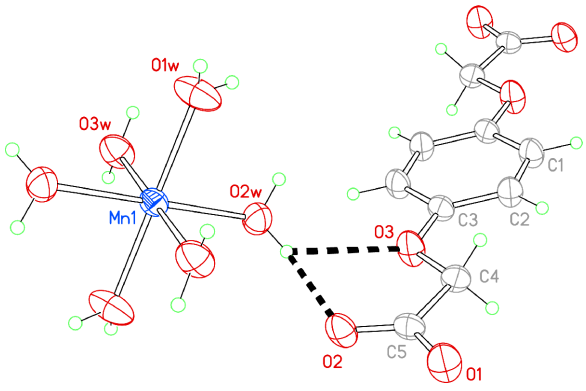


Figure 1
*ORTEP*II (Johnson, 1976) drawing of $[Mn(H_2O)_6](C_{10}H_8O_6)$, showing 30% probability displacement ellipsoids and atom-numbering scheme for the contents of the asymmetric unit. Hydrogen bonds are indicated by dashed lines.

benzene-1,4-dioxyacetic acid (9.04 g, 40 mmol) and quinoline (2 ml) were dissolved in a 1:1 water–ethanol solution (20 ml) and the pH was adjusted to 6 with 0.1 *M* sodium hydroxide. Colourless crystals separated from the filtered solution after several days. Analysis calculated for $C_{10}H_{20}MnO_{12}$: C 31.02, H 5.21%; found: C 30.85, H 5.39%.

Crystal data

$[Mn(H_2O)_6](C_{10}H_8O_6)$
M_r = 387.20
Triclinic, $P\overline{1}$
a = 5.6556 (6) Å
b = 6.3747 (7) Å
c = 11.637 (2) Å
α = 101.809 (6)°
β = 96.159 (8)°
γ = 106.986 (5)°
V = 386.45 (9) Å^3
Z = 1
D_x = 1.664 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1753 reflections
θ = 3.9–27.3°
μ = 0.92 mm^{-1}
T = 293 (2) K
Plate, colourless
0.36 × 0.21 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.734, T_{max} = 0.867
3748 measured reflections
1759 independent reflections
1678 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.5°
$h = -6 \rightarrow 7$
$k = -8 \rightarrow 7$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.169
S = 1.10
1759 reflections
124 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2 + 1.0889P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1*W*	2.143 (3)	Mn1—O3*W*	2.187 (3)
Mn1—O2*W*	2.228 (3)		
O1*W*^{i}—Mn1—O1*W*	180	O2*W*^{i}—Mn1—O2*W*	180
O1*W*—Mn1—O2*W*^{i}	93.1 (1)	O3*W*—Mn1—O2*W*	85.7 (1)
O1*W*—Mn1—O2*W*	86.9 (1)	O3*W*—Mn1—O2*W*^{i}	94.3 (1)
O1*W*—Mn1—O3*W*	87.0 (1)	O3*W*—Mn1—O3*W*^{i}	180
O1*W*—Mn1—O3*W*^{i}	93.0 (1)		

Symmetry code: (i) $-x, -y, -z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O1^{i}	0.85 (5)	1.87 (5)	2.710 (4)	169 (6)
O1*W*—H1*W*2···O2^{ii}	0.85 (5)	2.01 (5)	2.817 (4)	161 (7)
O2*W*—H2*W*1···O1^{i}	0.85 (5)	2.05 (4)	2.857 (4)	160 (4)
O2*W*—H2*W*2···O2	0.85 (2)	1.88 (3)	2.723 (4)	169 (5)
O2*W*—H2*W*2···O3	0.85 (2)	2.53 (4)	3.053 (4)	120 (4)
O3*W*—H3*W*1···O2*W*^{iii}	0.85 (5)	2.12 (4)	2.944 (5)	164 (4)
O3*W*—H3*W*2···O2^{i}	0.85 (5)	1.93 (3)	2.730 (4)	156 (6)

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

C-bound H atoms were placed in calculated positions [C—H = 0.93 (aromatic) and 0.97 Å (aliphatic), and U_{iso}(H) = 1.2U_{eq}(C)] in the riding-model approximation. The H atoms of water molecules were located in a difference map and refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and U_{iso}(H) = 1.5U_{eq}(O). The largest peak in the final difference Fourier map is 1.34 Å from atom Mn1.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

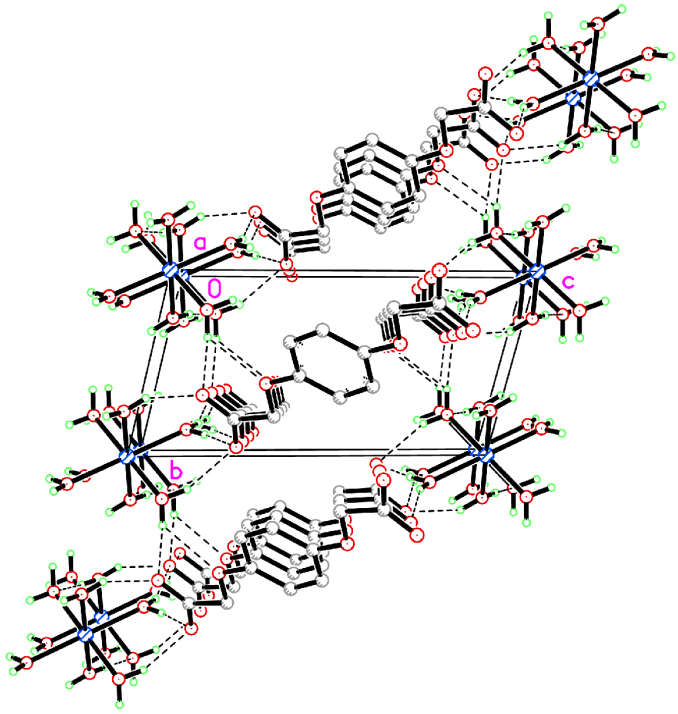


Figure 2
A packing diagram of $[Mn(H_2O)_6](C_{10}H_8O_6)$. Hydrogen bonds are indicated by dashed lines.

The authors thank the National Natural Science Foundation of China (grant No. 20101003), Heilongjiang Province Natural Science Foundation (grant No. B0007), the Educational Committee Foundation of Heilongjiang Province, Heilongjiang University and University of Malaya.

References

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Liu, J.-W., Huo, L.-H., Gao, S. & Ng, S. W. (2004). *Acta Cryst.* E**60**, m439–m440.
Mirci, L. E. (1990). Rom. Patent No. 07 43 205.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381, USA.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.