Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Triaqua(2,2′-bipyridine)(4-sulfonatobenzoato)manganese(II) monohydrate containing seven-coordinate manganese

Li-Ping Zhang and Long-Guan Zhu*

Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China

Correspondence e-mail: chezlg@zju.edu.cn

Received 25 April 2005
Accepted 26 April 2005
Online 7 May 2005

The mononuclear title complex, $[Mn(C_7H_4O_5S)(C_{10}H_8N_2)(H_2O)_3]\cdot H_2O$, was obtained from the hydrothermal reaction of manganese acetate, potassium hydrogen 4-sulfonatobenzoate and 2,2′-bipyridine. The geometry of the seven-coordinate Mn^{II} atom is a monocapped trigonal prismatic. Each 4-sulfonatobenzoate anion chelates to the metal atom *via* its carboxyl O atoms. The crystal structure is stabilized by a three-dimensional O—H···O hydrogen-bond network.

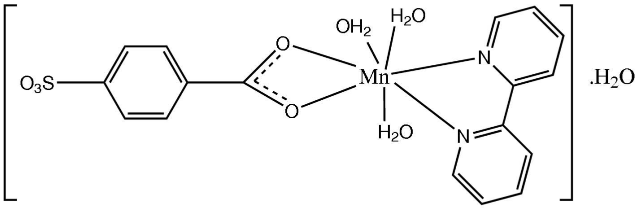
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
Disorder in main residue
R factor = 0.076
wR factor = 0.139
Data-to-parameter ratio = 11.0

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

Comment

Although they are less common than tetrahedral or octahedral complexes, examples of complexes containing seven-coordinate manganese(II) have been known for many years (Richards *et al.*, 1964). Here, we report another example of a seven-coordinate manganese(II) complex, the title complex, (I).



(I)

Compound (I) is a monomeric species. The Mn^{II} cation adopts a monocapped trigonal prismatic geometry consisting of two N donors from one 2,2′-bipyridine ligand, two carboxyl O atoms from one 4-sulfonatobenzoate dianion and three O atoms from water molecules (Fig. 1 and Table 1). The Mn1—O2 distance is significantly longer than the other Mn—O bond lengths but, if it is considered as a bond, then a monocapped

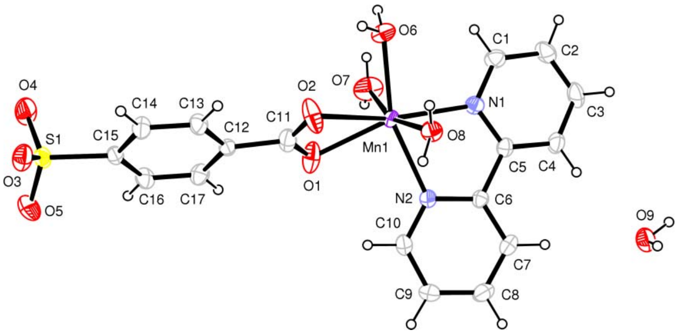


Figure 1
A view of the molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level and H atoms are shown as small spheres of arbitrary radii. The minor disorder component of the sulfonate group has been omitted for clarity.

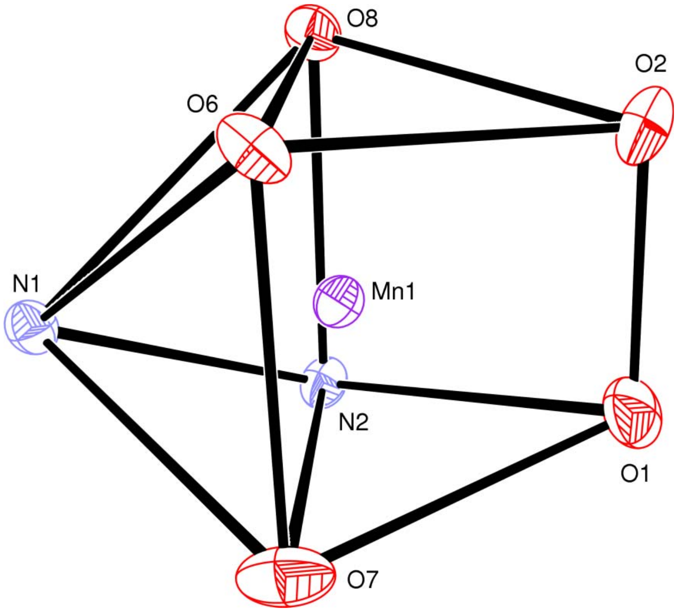


Figure 2
A view of the capped trigonal prismatic coordination polyhedron of the Mn^{II} atom in (I).

trigonal prismatic geometry arises for the Mn^{II} species (Fig. 2). Atom N1 occupies the capping position and the Mn1—N1 bond protrudes through the plane formed by atoms O6, O7, O8 and N2.

The 4-sulfonatobenzoate ligand chelates to the metal atom through its carboxyl group. The partially disordered sulfonate group does not coordinate to the Mn^{II} atom. The S—O bond lengths in (I) fall within the typical range of distances previously reported for the sulfonate anion (Onoda *et al.*, 2001).

The crystal structure of (I) is consolidated by an extensive network of O—H···O hydrogen bonds (Table 2) which gives rise to the formation of a three-dimensional architecture.

Experimental

A mixture of manganese acetate tetrahydrate (0.123 g, 0.50 mmol), potassium hydrogen 4-sulfonatobenzoate (0.121 g, 0.5 mmol), 2,2′-bipyridine (0.079 g, 0.5 mmol) and water (15 ml) was heated at 423 K for 3 h in a 30 ml Teflon-lined stainless steel autoclave. After cooling, a yellow solution was obtained. This solution was set aside and the solvent allowed to evaporate at room temperature. After 10 d, pale yellow block-shaped crystals of (I) were obtained.

Crystal data

$[Mn(C_7H_4O_5S)(C_{10}H_8N_2)(H_2O)_3]\cdot H_2O$
$M_r = 483.35$
Monoclinic, $P2_1/c$
$a = 10.3822\ (6)$ Å
$b = 17.6359\ (10)$ Å
$c = 11.4516\ (7)$ Å
$\beta = 105.191\ (1)^\circ$
$V = 2023.5\ (2)$ Å^3
$Z = 4$

$D_x = 1.587$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4074 reflections
$\theta = 2.3$–27.7°
$\mu = 0.81$ mm^{-1}
$T = 295\ (2)$ K
Block, pale yellow
0.32 × 0.26 × 0.22 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.782$, $T_{max} = 0.842$
10 472 measured reflections

3560 independent reflections
3452 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0^\circ$
$h = -12 \rightarrow 12$
$k = -20 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.077$
$wR(F^2) = 0.139$
$S = 1.30$
3560 reflections
323 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0204P)^2 + 6.1194P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.252 (4)	Mn1—O8	2.222 (3)
Mn1—O2	2.545 (5)	Mn1—N1	2.291 (4)
Mn1—O6	2.222 (4)	Mn1—N2	2.280 (4)
Mn1—O7	2.214 (4)		
O1—Mn1—O2	52.41 (15)	O7—Mn1—O6	82.17 (16)
O6—Mn1—O1	111.27 (16)	O8—Mn1—O6	86.88 (14)
O7—Mn1—O1	80.93 (18)	O6—Mn1—N1	90.92 (14)
O8—Mn1—O1	114.25 (15)	O6—Mn1—N2	160.19 (15)
O1—Mn1—N1	151.43 (16)	O7—Mn1—O8	163.86 (17)
O1—Mn1—N2	88.18 (16)	O7—Mn1—N1	84.74 (18)
O6—Mn1—O2	75.03 (16)	O7—Mn1—N2	105.48 (17)
O7—Mn1—O2	112.26 (19)	O8—Mn1—N1	83.61 (14)
O8—Mn1—O2	75.93 (14)	O8—Mn1—N2	81.42 (14)
N1—Mn1—O2	155.61 (15)	N2—Mn1—N1	72.00 (14)
N2—Mn1—O2	116.96 (17)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8*A*···O3′^{i}	0.85 (4)	1.96 (4)	2.67 (3)	141 (4)
O8—H8*A*···O3^{i}	0.85 (4)	2.02 (1)	2.862 (5)	174 (4)
O6—H6*B*···O5^{ii}	0.85 (4)	1.97 (2)	2.808 (5)	169 (5)
O6—H6*B*···O5′^{ii}	0.85 (4)	2.27 (4)	2.95 (3)	137 (4)
O8—H8*B*···O9^{iii}	0.85 (1)	1.87 (1)	2.721 (6)	177 (5)
O9—H9*B*···O3′^{iv}	0.85 (4)	1.78 (4)	2.53 (2)	148 (5)
O9—H9*B*···O5^{iv}	0.85 (4)	2.12 (1)	2.948 (6)	167 (4)
O6—H6*A*···O4^{v}	0.85 (1)	1.93 (2)	2.738 (5)	159 (5)
O9—H9*A*···O2^{i}	0.85 (3)	1.93 (4)	2.776 (6)	172 (4)
O7—H7*B*···O1^{vi}	0.85 (1)	1.89 (2)	2.717 (6)	166 (4)
O7—H7*A*···O4′^{v}	0.85 (3)	1.84 (3)	2.67 (2)	167 (5)
O7—H7*A*···O4^{v}	0.85 (3)	1.97 (2)	2.775 (7)	159 (4)

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y-\frac{1}{2}, z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x, y+1, z$; (v) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (vi) $-x, -y, -z+1$.

Aromatic H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in a difference Fourier map and refined with a distance restraint of O—H = 0.85 (1) Å and a fixed isotropic displacement parameter of $U_{iso}(H) = 0.05$ Å^2. The sulfonate O atoms are disordered over two positions in the ratio 0.889 (8):0.111 (8), for atoms O3/O4/O5 and O3′/O4′/O5′, respectively.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the National Natural Science Foundation of China (grant No. 50073019) for supporting this study.

References

Bruker (2002). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Onoda, A., Yamada, Y., Doi, M., Okamura, T. & Ueyama, N. (2001). *Inorg. Chem.* **40**, 516–521.

Richards, S., Pederson, B., Silverton, J. V. & Hoard, J. L. (1964). *Inorg. Chem.* **3**, 27–33.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.