Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Di-μ_2-acetato-bis[μ_2-*N*,*N*′-bis(salicylidene)-butane-1,4-diaminato]trimanganese(II)

Ji-Long Ma,[a] Zhong-Lu You[b] and Hai-Liang Zhu[c]*

[a]Department of Chemistry, Fuyang Normal College, Fuyang 236041, People's Republic of China, [b]Department of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China, and [c]Institute of Functional Biomolecules, State Key Laboratory of Pharmaceutical Biotechnology ,Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail:
hailiang_zhu@163.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.088
Data-to-parameter ratio = 13.7

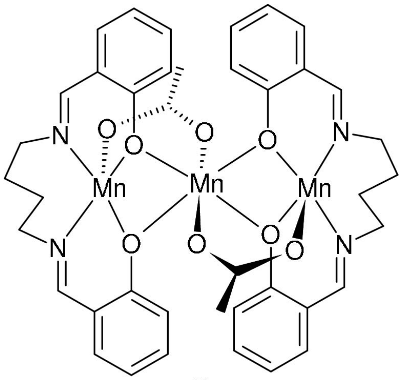
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title trinuclear compound, [$Mn_3(C_{18}H_{18}N_2O_2)_2(C_2H_3O_2)_2$], with a linear array of metal atoms, is isostructural with the cobalt(II) complex reported recently by You, Zhu & Liu [(2004). *Acta Cryst.* E**60**, m1900–m1902]. The central Mn^{II} ion, which is located on an inversion center, has a distorted octahedral geometry. The terminal Mn^{II} ion has an irregular square-pyramidal geometry. The Mn···Mn separation is 3.128 (2) Å.

Received 26 May 2005
Accepted 2 June 2005
Online 10 June 2005

Comment

Recently, we have reported some trinuclear Schiff base complexes (You *et al.*, 2004*a*; You & Zhu, 2004). As an extension of our work on these complexes, the title trinuclear manganese(II) compound, (I), is reported here.



(I)

Compound (I) is a trinuclear manganese(II) complex (Fig. 1), which is isostructural with the trinuclear cobalt(II) complex di-μ-acetato-1:2κ^2*O*,*O*′;2:3κ^2*O*,*O*′-bis{2,2′-[1,4-butanediylbis(nitrilomethylidyne)]diphenolato}-1:2κ^6*O*,*N*,*N*,*O*′:*O*,*O*′;2,3κ^6*O*,*O*′:*O*,*N*,*N*,*O*′-tricobalt(II), (II), which we have reported recently (You *et al.*, 2004*b*). In (I), the bond lengths and angles (Table 1) are comparable to those in (II). The central Mn^{II} ion, which is located on an inversion center, has a distorted octahedral geometry. The terminal Mn^{II} ion has an irregular square-pyramidal geometry. The Mn···Mn separation is 3.128 (2) Å.

In the crystal structure, there are no short contacts between molecules (Fig. 2).

Experimental

1,4-Diaminobutane (0.1 mmol, 8.6 mg) and salicylaldehyde (0.2 mmol, 24.4 mg) were dissolved in MeOH (3 ml). The mixture was stirred for 1 h to give a clear orange solution. To the above solution was added an MeOH solution (2 ml) of $Mn(CH_3COO)_2{\cdot}2H_2O$

doi:10.1107/S1600536805017423

(0.2 mmol, 41.8 mg), with stirring for 10 min. The mixture was transferred to a stainless steel bomb, which was sealed, heated at 423 K for 12 h and cooled gradually to room temperature. Brown block-shaped crystals were formed.

Crystal data

$[Mn_3(C_{18}H_{18}N_2O_2)_2(C_2H_3O_2)_2]$
$M_r = 871.60$
Monoclinic, $P2_1/c$
$a = 9.190$ (5) Å
$b = 16.756$ (9) Å
$c = 12.690$ (7) Å
$\beta = 95.126$ (10)°
$V = 1946.3$ (19) Å^3
$Z = 2$

$D_x = 1.487$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1726 reflections
$\theta = 2.5$–21.1°
$\mu = 1.02$ mm^{-1}
$T = 298$ (2) K
Block, brown
0.25 × 0.18 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.785$, $T_{\max} = 0.897$
10096 measured reflections

3432 independent reflections
2059 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$
$\theta_{\max} = 25.0°$
$h = -10 \rightarrow 10$
$k = -17 \rightarrow 19$
$l = -9 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.088$
$S = 0.84$
3432 reflections
250 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O2	2.080 (2)	Mn1—N2	2.176 (3)
Mn1—O3	2.083 (2)	Mn2—O1	2.165 (2)
Mn1—O1	2.102 (2)	Mn2—O4	2.194 (2)
Mn1—N1	2.160 (3)	Mn2—O2	2.215 (2)
O2—Mn1—O3	108.73 (10)	O1—Mn2—O1$^{\rm i}$	180
O2—Mn1—O1	81.20 (10)	O1—Mn2—O4$^{\rm i}$	92.14 (9)
O3—Mn1—O1	94.15 (10)	O1—Mn2—O4	87.86 (9)
O2—Mn1—N1	133.74 (10)	O4$^{\rm i}$—Mn2—O4	180
O3—Mn1—N1	116.55 (11)	O1—Mn2—O2	76.83 (9)
O1—Mn1—N1	86.49 (10)	O1$^{\rm i}$—Mn2—O2	103.17 (9)
O2—Mn1—N2	85.34 (11)	O4$^{\rm i}$—Mn2—O2	92.64 (9)
O3—Mn1—N2	102.24 (11)	O4—Mn2—O2	87.36 (9)
O1—Mn1—N2	161.46 (10)	O2—Mn2—O2$^{\rm i}$	180
N1—Mn1—N2	93.76 (12)		

Symmetry code: (i) $-x+1, -y, -z+1$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, People's Republic of China, for research grant No. 2004kj300zd.

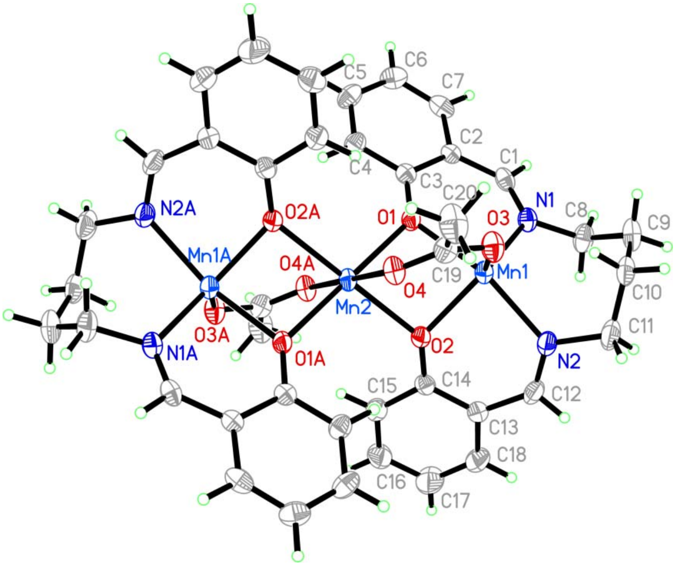


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Atoms labeled with the suffix *A* are related by the symmetry operator $(1 - x, -y, 1 - z)$.

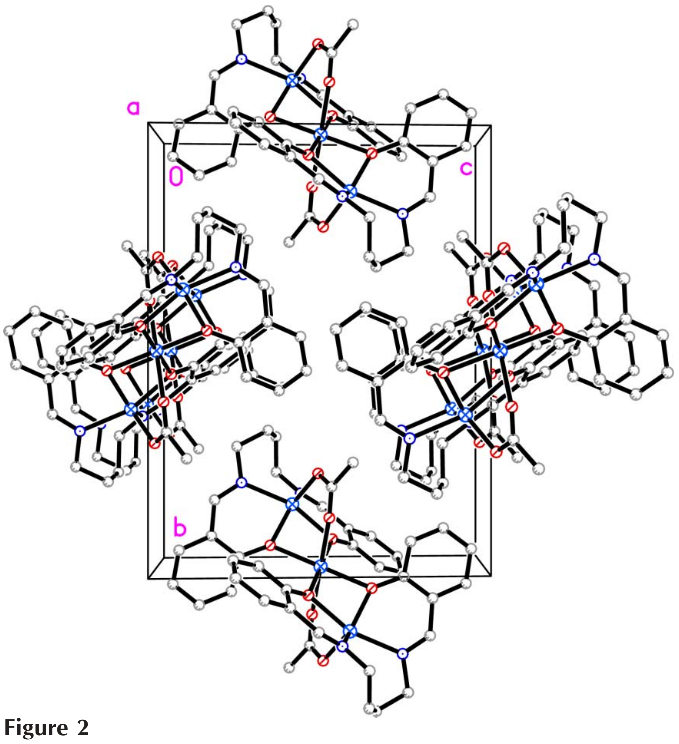


Figure 2
The crystal packing of (I), viewed along the *a* axis. H atoms have been omitted.

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