Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

μ-Acetato-*O*:*O*′-bis{[bis(salicylidene)-ethylenediaminato]manganese(III)} perchlorate

Yoshiyuki Kani,[a] Shigeru Ohba[a]* and Yuzo Nishida[b]

[a]Department of Chemistry, Faculty of Science and Technology, Keio University, Hiyoshi 3-14-1, Kohoku-ku, Yokohama 223-8522, Japan, and [b]Institute for Molecular Science, Myodaijimachi, Okazaki 444-8585, Japan
Correspondence e-mail: ohba@chem.keio.ac.jp

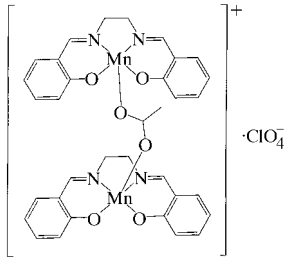
Received 31 March 2000
Accepted 11 April 2000

Data validation number: IUC0000105

In the title complex, $[Mn_2(C_{16}H_{14}N_2O_2)_2(C_2H_3O_2)]ClO_4$, two [Mn(salen)] moieties [salen is bis(salicylidene)ethylenediamine] are connected through a μ-acetate bridge in a *syn–anti* fashion. The Mn···Mn distance is 5.365 (1) Å.

Comment

The X-ray structure analysis of $[Mn_2(7\text{-Me-salen})_2(CH_3COO)]ClO_4$ gave an unsatisfactory *R* value of 0.140 due to the



(I)

poor crystalinity (Suzuki *et al.*, 1997). The structure of $[Mn_2(salen)_2(CH_3COO)]ClO_4$, (I), is presented here.

Experimental

The title compound, $[Mn_2(salen)_2(CH_3COO)]ClO_4$, was synthesized as described previously by Suzuki *et al.* (1997).

Crystal data

$[Mn_2(C_{16}H_{14}N_2O_2)_2(C_2H_3O_2)]ClO_4$
M_r = 800.97
Triclinic, $P\overline{1}$
a = 11.990 (4) Å
b = 12.988 (4) Å
c = 11.296 (5) Å
α = 106.52 (3)°
β = 94.31 (3)°
γ = 90.79 (3)°
V = 1680.5 (9) Å^3
Z = 2
D_x = 1.583 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–15°
μ = 0.896 mm^{-1}
T = 298 K
Prism, black
0.5 × 0.5 × 0.3 mm

Data collection

Rigaku AFC-5*S* diffractometer
θ–2θ scans
Absorption correction: by integration (Coppens *et al.*, 1965)
T_{min} = 0.670, T_{max} = 0.789
8092 measured reflections
7723 independent reflections
6237 reflections with $I > 2\sigma(I)$
R_{int} = 0.011
θ_{max} = 27.5°
$h = 0 \rightarrow 16$
$k = -17 \rightarrow 17$
$l = -15 \rightarrow 15$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.039
$wR(F^2)$ = 0.106
S = 1.37
7723 reflections
460 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + \{0.05(F_o^2 + 2F_c^2)/3\}^2]$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	1.924 (2)	Mn2—O3	1.897 (1)
Mn1—O2	1.873 (2)	Mn2—O4	1.878 (2)
Mn1—O5	2.129 (2)	Mn2—O6	2.113 (2)
Mn1—N1	1.987 (2)	Mn2—N3	1.984 (2)
Mn1—N2	1.989 (2)	Mn2—N4	1.975 (2)
Mn1—O5—C33	155.9 (2)	Mn2—O6—C33	140.1 (1)
Mn1—O5—C33—O6	−148.6 (3)	Mn2—O6—C33—O5	0.9 (4)

The positional parameters of all the H atoms were calculated geometrically and fixed with U(H) = 1.2U_{eq}(parent atom).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *DIRDIF*94 (Beurskens *et al.*, 1994); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

References

Beurskens, P. T., Admiraal, G., Beurskens, G., Bosman, W. P., de Gelder, R., Israel, R. & Smits, J. M. M. (1994). *The DIRDIF*94 *Program System*. Technical Report, Crystallography Laboratory, University of Nijmegen, The Netherlands.
Coppens, P., Leiserowitz, L. & Rabinovich, D. (1965). *Acta Cryst.* **18**, 1035–1038.
Molecular Structure Corporation (1993). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1999). *TEXSAN*. Version 1.10. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Suzuki, M., Ishikawa, T., Harada, A., Ohba, S., Sakamoto, M. & Nishida, Y. (1997). *Polyhedron*, **16**, 2553–2561.