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Tris[2-(cyclopropyliminomethyl)phenolato]-manganese(III)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.011 Å
R factor = 0.069
wR factor = 0.184
Data-to-parameter ratio = 13.9

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

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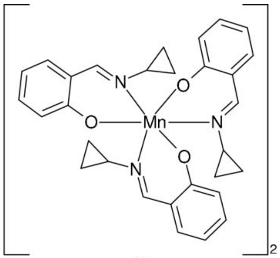
The title compound, $[Mn(C_{10}H_{10}NO)_3]$, contains two molecules in the asymmetric unit of the centrosymmetric space group *Pbcn*. In this mononuclear compound, each Mn^{III} atom is coordinated by three O atoms and three N atoms from three Schiff bases, in a slightly distorted octahedral geometry.

Comment

Transition metal compounds containing Schiff base ligands have been of great interest for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). Manganese plays an important role in biological redox-active systems (Larson & Pecoraro, 1991; Gohdes & Armstrong, 1992). Recently, we have reported the crystal structures of a few Schiff base complexes (Usman *et al.*, 2003; You, Lin *et al.*, 2003; You, Qu *et al.*, 2003; You *et al.*, 2004). As an extension of our work on the structural characterization of Schiff base complexes, the crystal structure of a mononuclear manganese(III) complex, (I), is reported here.



(I)

The title compound, (I), is an electronically neutral mononuclear manganese(III) compound (Fig. 1). The asymmetric unit contains two molecules. In both of the molecules, the

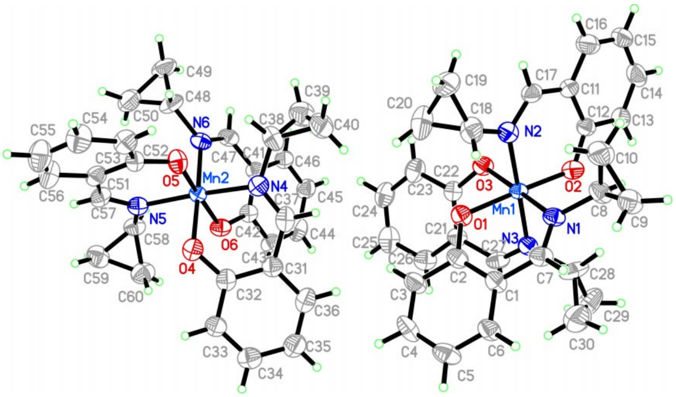


Figure 1
The structure of the asymmetric unit of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

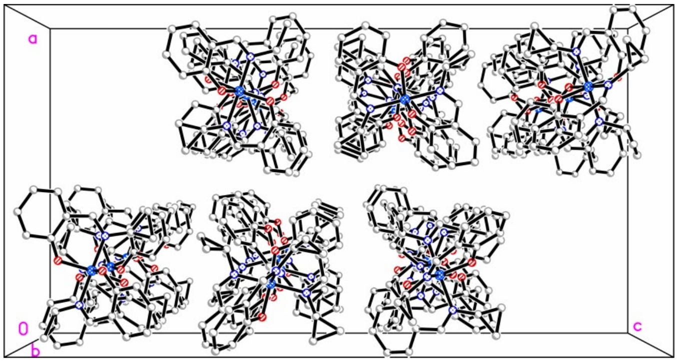


Figure 2
The crystal packing of (I), viewed along the *b* axis.

Mn^{III} atoms are in an octahedral geometry and are six-coordinated by three O atoms and by three N atoms from three Schiff base ligands. This MnO_3N_3 coordination forms a slightly distorted octahedral geometry, as usually observed in the structures of manganese(III) complexes (Gohdes & Armstrong, 1992). The *trans* angles for the manganese(III) octahedron are all close to 180° (Table 1) and the other angles subtended at the Mn^{III} atom are in the range 85.2 (2)–94.2 (2)° for Mn1 and 85.7 (2)–94.4 (2)° for Mn2. The average Mn—O(phenolate) bond lengths [1.889 (4) Å for Mn1 and 1.890 (4) Å for Mn2] are a little longer than the value of 1.873 (2) Å observed in another Schiff base manganese(III) complex (Korendovych & Rybak-Akimova, 2004). The mean Mn—N(imine) bond distances [1.929 (5) Å for Mn1 and 1.939 (5) Å for Mn2] are a little shorter than the value of 1.989 (2) Å observed in the complex cited above.

Experimental

Cyclopropylamine and salicylaldehyde were available commercially and were used without further purification. Cyclopropylamine (2.0 mmol, 114 mg) and salicylaldehyde (2.0 mmol, 244 mg) were dissolved in methanol (30 ml). The mixture was stirred for 1 h to give a clear yellow solution of *L* (2.0 mmol), where *L* is 2-[(cyclopropylamino)methyl]phenol. To the methanol solution of *L* was added a methanol solution (30 ml) of $Mn(CH_3COO)_2{\cdot}4H_2O$ (1.0 mmol, 245 mg), with stirring. After keeping the resulting solution at room temperature in air for 8 d, brown block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using P_4O_{10} (yield 73.2%). Analysis found: C 67.17, H 5.72, N 7.79%; calculated for $C_{30}H_{30}MnN_3O_3$: C 67.28, H 5.65, N 7.85%. IR data: 3438 (*m*), 1612 (*s*), 1537 (*m*), 1466 (*s*), 1445 (*m*), 1410 (*m*), 1181 (*m*), 1153 (*m*), 603 (*w*) cm^{-1}.

Crystal data

$[Mn(C_{10}H_{10}NO)_3]$
$M_r = 535.51$
Orthorhombic, *Pbcn*
$a = 19.227$ (4) Å
$b = 14.948$ (3) Å
$c = 36.427$ (7) Å
$V = 10469$ (4) $Å^3$
$Z = 16$
$D_x = 1.359$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 2923 reflections
$\theta = 2.4$–17.0°
$\mu = 0.54$ mm^{-1}
$T = 293$ (2) K
Block, brown
0.23 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.886$, $T_{max} = 0.918$
51 009 measured reflections

9247 independent reflections
3755 reflections with $I > 2\sigma(I)$
$R_{int} = 0.157$
$\theta_{max} = 25.0°$
$h = -22 \rightarrow 22$
$k = -16 \rightarrow 17$
$l = -36 \rightarrow 43$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.184$
$S = 0.90$
9247 reflections
667 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.18$ e $Å^{-3}$
$\Delta\rho_{min} = -0.29$ e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	1.871 (4)	Mn2—O6	1.864 (4)
Mn1—O2	1.883 (4)	Mn2—O4	1.899 (4)
Mn1—O3	1.912 (4)	Mn2—O5	1.907 (4)
Mn1—N3	1.922 (5)	Mn2—N4	1.927 (6)
Mn1—N2	1.926 (5)	Mn2—N6	1.943 (5)
Mn1—N1	1.940 (5)	Mn2—N5	1.947 (5)
O1—Mn1—O2	173.53 (19)	O6—Mn2—O4	86.71 (18)
O1—Mn1—O3	86.22 (19)	O6—Mn2—O5	173.46 (18)
O2—Mn1—O3	89.75 (19)	O4—Mn2—O5	88.6 (2)
O1—Mn1—N3	89.7 (2)	O6—Mn2—N4	89.7 (2)
O2—Mn1—N3	85.2 (2)	O4—Mn2—N4	89.9 (2)
O3—Mn1—N3	90.3 (2)	O5—Mn2—N4	85.7 (2)
O1—Mn1—N2	90.7 (2)	O6—Mn2—N6	91.6 (2)
O2—Mn1—N2	94.2 (2)	O4—Mn2—N6	176.9 (2)
O3—Mn1—N2	87.3 (2)	O5—Mn2—N6	93.2 (2)
N3—Mn1—N2	177.5 (2)	N4—Mn2—N6	92.7 (2)
O1—Mn1—N1	91.0 (2)	O6—Mn2—N5	89.9 (2)
O2—Mn1—N1	93.3 (2)	O4—Mn2—N5	86.5 (2)
O3—Mn1—N1	176.3 (2)	O5—Mn2—N5	94.4 (2)
N3—Mn1—N1	92.0 (2)	N4—Mn2—N5	176.3 (2)
N2—Mn1—N1	90.4 (2)	N6—Mn2—N5	91.0 (2)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) values fixed at $1.2U_{eq}$(C). An unassigned maximum residual density was observed 0.7 Å from atom H45*A*. The minimum residual density was observed 1.1 Å from atom C2. The R_{int} value and the low ratio of observed to unique reflections (0.41) were the result of weak high-angle data.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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