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Bis{2-[1-(adamantan-1-yl)ethyliminomethyl]-phenolato-κO}dichloromanganese(II)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.130
Data-to-parameter ratio = 20.0

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

In the title compound, $[MnCl_2(C_{19}H_{25}NO)_2]$, each Mn^{II} ion is coordinated by two Cl^- ions and two O atoms from two 2-[1-(adamantan-1-yl)ethyliminomethyl]phenolate ligands in a distorted tetrahedral geometry. The Mn atom lies on a twofold rotation axis. There are intramolecular hydrogen-bonding interactions between the imino N and phenolate O atoms.

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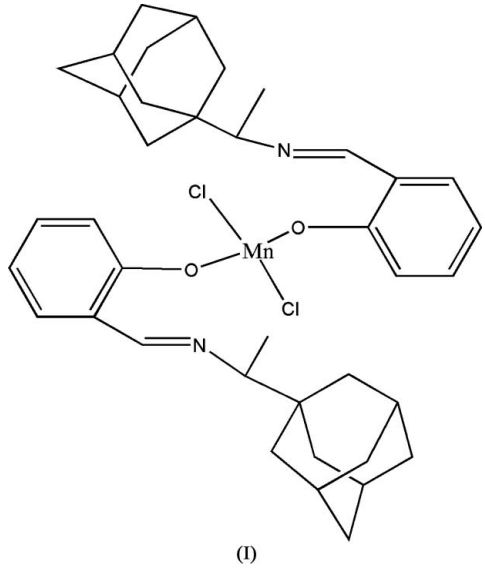
Comment

In the past few years, manganese chemistry has developed rapidly to provide model complexes of biological systems. Model complexes with one, two, or more manganese centers in oxidation states ranging from +2 to +5 have provided information on the mechanisms of some oxygen-transfer reactions and on the role of manganese-containing enzymes (Gupta *et al.*, 1999). 1-(1-Adamant-1-yl)ethylamine has been largely used to prevent or treat some kinds of flu virus, such as Asian A2 type flu virus and bird flu virus (Bright *et al.*, 2005). In the present paper, we report the synthesis and crystal structure of a mononuclear manganese(II) complex, (I).



(I)

The crystallographic analysis of (I) shows that the Mn atom lies on a twofold rotation axis and is four-coordinated by two Cl ligands and two O atoms from the Schiff base ligands, forming a distorted tetrahedral geometry (Fig. 1 and Table 1). Its structure is similar to the reported complexes $MnCl_2(C_{18}H_{15}PO)_2$ (Tomita, 1985) and $MnCl_2(C_{18}H_{15}AsO)_2$ (El-Sayrafi *et al.*, 1993). In the title complex, the two benzene rings are approximately perpendicular to each other, with a

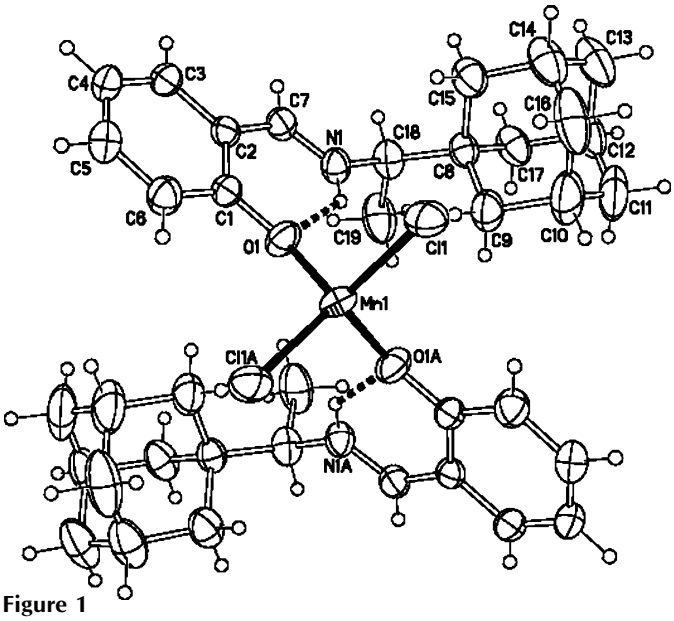


Figure 1
The molecular structure of (I), with displacement ellipsoids shown at the 30% probability level. Intramolecular hydrogen bonds are indicated by dashed lines. [Symmetry code: (A) $-x, y, -z+\frac{1}{2}$].

dihedral angle of 98.7 (3)°. The crystal structure involves N—H···O intramolecular hydrogen bonds, which help stabilize the complex.

Experimental

The Schiff base ligand was prepared by refluxing a mixture of 1-(1-adamantyl)ethylamine hydrochloride, KOH (1 mmol) and salicylidene (1 mmol) in ethanol for an hour. A solution of $MnCl_2$ (0.13 g, 1 mmol) in ethanol (10 ml) was added slowly to a solution of 2-[1-(adamantan-1-yl)ethyliminomethyl]phenolate (1.13 g, 2 mmol) in ethanol (15 ml), with refluxing for an hour. After seven days, yellow crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$[MnCl_2(C_{19}H_{25}NO)_2]$
M_r = 692.64
Orthorhombic, *Pbcn*
a = 14.440 (3) Å
b = 10.753 (2) Å
c = 23.222 (5) Å
V = 3605.9 (13) Å^3
Z = 4
D_x = 1.276 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 21347 reflections
θ = 3.5–27.5°
μ = 0.55 mm^{-1}
T = 296 (2) K
Prism, yellow
0.40 × 0.32 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.810, T_{max} = 0.921
31203 measured reflections
4106 independent reflections
2967 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°
$h = -18 \rightarrow 18$
$k = -13 \rightarrow 13$
$l = -29 \rightarrow 30$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.130
S = 1.06
4106 reflections
205 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.4209P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.0301 (14)	Mn1—Cl1	2.3372 (7)
O1—Mn1—O1^{i}	93.91 (9)	O1^{i}—Mn1—Cl1	112.74 (5)
O1—Mn1—Cl1	109.87 (5)		

Symmetry code: (i) $-x, y, -z+\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	1.93	2.604 (2)	135

The methyl groups were allowed to rotate to fit the electron density [C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C)]; the other H atoms were positioned geometrically [aromatic C—H = 0.93 Å and aliphatic C—H = 0.97 Å, U_{iso}(H) = 1.2U_{eq}(C)]. H atoms bonded to N were placed in calculated positions [N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N)] and refined using the riding-model approximation.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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