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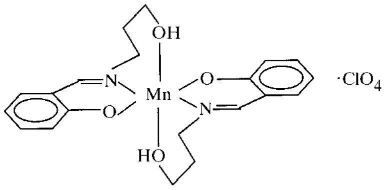
In the complex $[Mn(C_{10}H_{12}NO_2)_2]ClO_4$, the Mn atom lies on an inversion centre and the Cl of the perchlorate is on a twofold axis. In the cation, the Mn atom has distorted octahedral coordination with Mn—N 2.206 (3), Mn—O(phenolato) 1.871 (2) and Mn—O(propanolato) 2.300 (2) Å. In the crystal structure, the ions are linked by O—H···O hydrogen bonds [O···O 2.826 (4) Å] between the propanolato O—H group and a perchlorate O atom to form infinite chains. This is not what was proposed from a previous spectroscopic study.

Comment

It is well established that manganese plays an important role in several biological systems, *e.g.* in manganese superoxide dismutase, manganese catalase, manganese peroxidase, manganese ribonucleotide reductase, and the oxygen-evolving complex (OEC) (Gohdes & Armstrong, 1992; Hoganson & Babcock, 1997; Tommos & Babcock, 1998). Of these, the most important is undoubtly the oxygen-evolving complex of photosystem II (PSII) found in green plants. However, their precise configuration is not yet known. In order to understand the interaction between Mn atoms, it is important to study a number of model complexes with a wide range of ligand environment. In this paper, we report a monomeric six-coordinate manganese complex, bis[3-(salicylideneamino)-propanolato]manganese(III) perchlorate, (I).



(I)

The title compound forms centrosymmetric mononuclear molecules with a Schiff base ligand, *i.e.* the salicylideneamino-3-propanolate anion, acting as a tridentate ligand. The Mn atom is six-coordinated. The octahedral geometry is distorted. The equatorial approximate square plane involving the Mn atoms at its center is formed by two imino N atoms and two phenolic O atoms of the Hvanpa ligands. The Mn—O1 [1.871 (2) Å] and Mn—N1 [2.026 (3) Å] are normal for the in-plane bonds of manganese complexes (Xu *et al.*, 1997; Zhang *et al.*, 1999). The bond angles around the manganese atoms vary from 83 to 97°. The axial Mn—O distance [2.300 (2) Å] are considerably longer than the in-plane Mn—O distances. Thus, the coordination geometry around the Mn atom deviates significantly from a regular octahedron and this tetragonal elongation is attributed to a Jahn—Teller distortion at the d^4 manganese center. Each bond length in the Schiff base ligand has a normal value.

In the crystal structure, the ions are linked by O—H···O hydrogen bonds [O2···O4 2.826 (4) Å] to form infinite chains. A previous report (Torihara *et al.*, 1980) suggested that the perchlorate ion coordinates to Mn atom as a bidentate ligand because the Cl—O stretching frequency of perchlorate ion splits into three (1130, 1080 and 1040 cm^{-1}).

Experimental

A deep green solution of the complex was generated by the addition of $Mn(ClO_4)_2.6H_2O$ (3.60 g, 10 mmol) to a solution of salicylaldehyde (1.56 g, 10 mmol) and 3-amino-1-propanol (0.75 g, 10 mmol). Green prismatic crystals were obtained after the solution was filtered and left to stand for a week (overall yield: 75%).

Crystal data

$[Mn(C_{10}H_{12}NO_2)_2]ClO_4$
$M_r = 510.81$
Monoclinic, $C2/c$
$a = 18.359$ (4) Å
$b = 6.898$ (1) Å
$c = 18.256$ (4) Å
$\beta = 110.62$ (2)°
$V = 2163.8$ (9) $Å^3$
$Z = 4$
$D_x = 1.568$ Mg m^{-3}
$D_m = 1.57$ Mg m^{-3}
D_m measured by flotation in 1,2-dibromoethane and *cyclo*hexane
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
$\theta = 13.34$–19.58°
$\mu = 0.784$ mm^{-1}
$T = 293$ (2) K
Prismatic, green
0.30 × 0.20 × 0.20 mm

Data collection

Rigaku AFC-7*R* diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical azimuthal scans (*TEXSAN*; Molecular Structure Corporation, 1985)
$T_{min} = 0.804$, $T_{max} = 0.855$
2604 measured reflections
2604 independent reflections
1598 reflections with $I > 3\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$
$h = -23 \rightarrow 23$
$k = -8 \rightarrow 8$
$l = -23 \rightarrow 23$
3 standard reflections every 200 reflections intensity decay: 0.02%

Refinement

Refinement on F
$R = 0.039$
R = missing
$wR = 0.048$
$S = 1.52$
1598 reflections
147 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o)]$
$(\Delta/\sigma)_{max} = 0.028$
$\Delta\rho_{max} = 0.41$ e $Å^{-3}$
$\Delta\rho_{min} = -0.27$ e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Mn—O1	1.871 (2)	N—C7	1.293 (4)
Mn—O2	2.300 (2)	N—C8	1.480 (4)
Mn—N	2.026 (3)		
O1—Mn—O2	92.65 (9)	Mn—O2—C10	118.1 (2)
O1—Mn—N	89.17 (10)	Mn—N—C7	122.4 (2)
O2—Mn—N	82.63 (10)	Mn—N—C8	119.5 (2)
Mn—O1—C1	125.2 (2)		

All H atoms were created using a riding mode. We try to collect reflections up to 27.5° until no one can be observed.

Data collection: MSC/AFC Diffractometer Control Software (Molecular Structure Corporation, 1992); cell refinement: MSC/AFC Diffractometer Control Software; data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1985); program(s) used to solve structure: *SAPI*91 (Fan, 1991); program(s) used to refine structure: *TEXSAN* LS (Molecular Structure Corporation, 1985); software used to prepare material for publication: *TEXSAN FINISH* (Molecular Structure Corporation, 1985).

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