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Chlorido[4,5-dichloro-1,2-bis(2-pyridylcarboxamido)-benzene(2–)](dimethylformamide)manganese(III)

Lei Liang, Yan-Yang Qu, Li Yang and Xiang-Ge Zhou*

Institute of Homogeneous Catalysis, Department of Chemistry, Sichuan University, Chengdu 610064, People's Republic of China

Correspondence e-mail: scuzhouxg@163.com

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In the title compound, [MnCl($C_{18}H_{10}Cl_2N_4O_2$)(C_3H_7NO)], the central atom is within a distorted octahedral geometry defined by a ClN_4O donor set with the bis-picolinamide providing four N atoms and the remaining positions occupied by Cl and O atoms, with the latter provided by a dimethylformamide molecule.

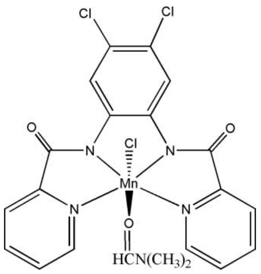
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.044
wR factor = 0.118
Data-to-parameter ratio = 17.9

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

Comment

There has been growing interest in the coordination chemistry of Mn^{III} peptide complexes containing amide ligands as it is assumed that these ligands, after deprotonation, will stabilize high oxidation states of metal ions (Che *et al.*, 1986). Motivation for studies on high-valent Mn species arises owing to interest in catalytic studies for a variety of oxidation systems (Che *et al.*, 1986; Leung *et al.*, 1991). Examples now exist of structurally characterized complexes with coordinated carboxamide N atoms as part of macrocyclic and non-macrocyclic ligand frameworks (Marlin *et al.*, 1999; Collins *et al.*, 1992). As the continuation of our studies on catalytic aspects of N_4 non-porphyrin complexes (Liu *et al.*, 2006; Yan *et al.*, 2006), the title complex, (I), is reported, which contains a bis-picolinamide ligand.



(I)

As shown in Fig. 1, the central Mn atom is six-coordinated within a distorted octahedral geometry. The four N atoms derived from the amido and pyridine groups of the 1,2-bis(2-pyridinecarboxamido)-4,5-dichlorobenzene (bpc) ligand define a square plane. The two axial sites are occupied by a Cl atom and an O atom from the coordinated dimethylformamide (DMF) molecule. Complex (I) has approximate $C2$ symmetry.

The Mn—N(amide) distances of *ca* 1.93 Å are significantly shorter than the Mn—N(pyridine) distances of *ca* 2.07 Å, both of which are appreciably shorter than the Fe—N distances of [Fe^{III}(bpc)Cl(DMF)] (Patra & Mukherjee, 1999) (see Table 1). Similarly, the Mn—N(amide) and Mn—N(pyridine) distances in (I) are both shorter than the Mn—N distances found in related MnN_4 complexes: *cis*-[Mn^{II}(mep)Cl_2] and [Mn^{III}(mpp)Cl$(OH)_2$](ClO_4) [mep is *N*,*N*′-dimethyl-*N*,*N*′-bis(2-pyridylmethyl)ethane-1,2-diamine and mpp is *N*,*N*′-dimethyl-*N*,*N*′-bis(2-pyridylmethyl)propane-1,2-diamine (Hureau *et al.*, 2005)].

The Mn—Cl distance (*ca* 2.45 Å) in (I) is identical with the corresponding Mn—Cl distances in *cis*-[Mn^{II}(mep)Cl_2] and [Mn^{III}(mpp)Cl$(OH)_2$](ClO_4) (Hureau *et al.*, 2005). The remaining bond lengths are in the usual ranges and the structural parameters of the bpc ligand agree with those reported for [Fe(bpc)Cl(DMF)] (Patra & Mukherjee, 1999). Distortions from the regular octahedral geometry are evident (Table 1), particularly for the N(pyridine)—Mn—N(pyridine) and N(amide)—Mn—N(amide) angles. A similar situation pertains in [Fe(bpc)Cl(DMF)] (Patra & Mukherjee, 1999).

Experimental

Complex (I) was prepared in a manner similar to that reported for related systems by the reaction of manganese(III) acetate and H_2bpc in DMF solution in the presence of triethylamine (Ray *et al.*, 1993). Single crystals suitable for X-ray analysis were obtained by slow diffusion of diethyl ether into a DMF solution of (I). Analysis calculated for $C_{21}H_{17}Cl_3MnN_5O_3$: C 45.97, H 3.12, N 12.76%; found: C 45.87, H 3.42, N 12.58%. MS (FAB): 439 ([Mn(bpc)]+).

Crystal data

[MnCl($C_{18}H_{10}Cl_2N_4O_2$)(C_3H_7NO)]
M_r = 548.69
Monoclinic, $P2_1/c$
a = 10.7467 (16) Å
b = 14.308 (2) Å
c = 16.102 (2) Å
β = 108.785 (3)°
V = 2344.1 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 294 (2) K
0.24 × 0.14 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.806, T_{max} = 0.912
15438 measured reflections
5379 independent reflections
3367 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
S = 1.02
5379 reflections
300 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—Cl1	2.4497 (9)	Mn1—N2	2.070 (2)
Mn1—O3	2.273 (2)	Mn1—N3	1.935 (2)
Mn1—N1	1.927 (2)	Mn1—N4	2.077 (2)
Cl1—Mn1—O3	159.45 (6)	N2—Mn1—N3	161.10 (10)
N1—Mn1—N2	80.37 (10)	N2—Mn1—N4	117.35 (9)
N1—Mn1—N3	81.40 (10)	N3—Mn1—N4	80.02 (10)
N1—Mn1—N4	160.22 (10)		

H atoms were positioned geometrically and refined as riding, with C—H = 0.93 and 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C).

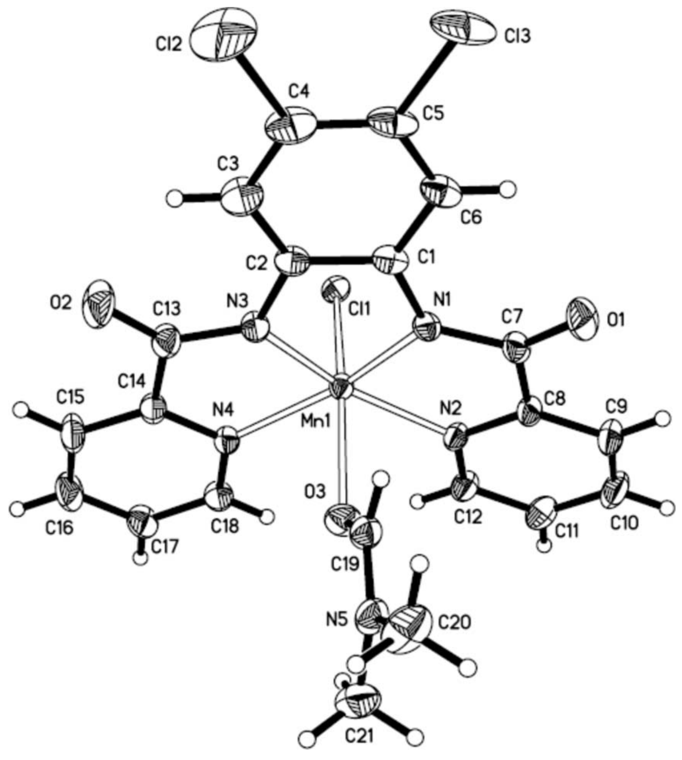


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

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

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