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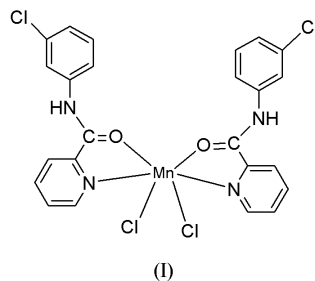
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Key indicatorsSingle-crystal X-ray study
T = 294 K
Mean $\sigma(\text{C}-\text{C})$ = 0.003 Å
R factor = 0.037
wR factor = 0.105
Data-to-parameter ratio = 18.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.***cis*-Dichlorobis[*N*-(3-chlorophenyl)pyridine-2-carboxamide]manganese(II)**

In the title complex, $[\text{MnCl}_2(\text{C}_{12}\text{H}_9\text{ClN}_2\text{O})_2]$, the Mn atom is located on a twofold axis and the asymmetric unit thus contains only one-half of the complex; it is built up from one Cl atom and one 2-pyridinedicarboxamide ligand bonded to the metal through the carbonyl O and pyridine N atoms.

Comment

The selective epoxidation of alkenes by molecular oxygen is a critical technology in organic chemistry because of the low cost and environmentally friendly nature of the oxidant (Bolm *et al.*, 1994; Brink *et al.*, 2000; Neumann & Dahan, 1998). Much effort has been devoted in the past to activate dioxygen by metal complexes (Shilov & Shul'pin, 2000). Recently, we reported that a ruthenium complex containing two Cl atoms and the 2-pyridinedicarboxamide ligand, was an efficient catalyst for the epoxidation of alkenes with dioxygen in the presence of isobutyraldehyde (Qi *et al.*, 2003). In our continuing search for economical and environmentally friendly processes for the production of epoxides, the cheaper and less environmentally damaging manganese complex (I) containing similar ligands was synthesized to replace the expensive ruthenium complex.



The Mn atom of (I), located on a twofold axis, is coordinated by two Cl atoms and two *N*-(3-chlorophenyl)pyridine-2-carboxamide ligands through the pyridine N and carbonyl O atoms, resulting in a distorted octahedral environment. The pyridine-2-carboxamide ligand is planar, the largest deviation from the plane being 0.013 (2) Å for N2, but the chlorophenyl ring is slightly twisted, making a dihedral angle of 5.86 (9)°. This complex is chiral and has a *cis* conformation. Such a conformation may facilitate the attack of reactants or the formation of active intermediates in the catalytic epoxidation of alkenes.

Experimental

The ligand of the complex is synthesized from 2-pyridinecarboxylic acid and 3-chloroaniline by following a published procedure (Ray *et*

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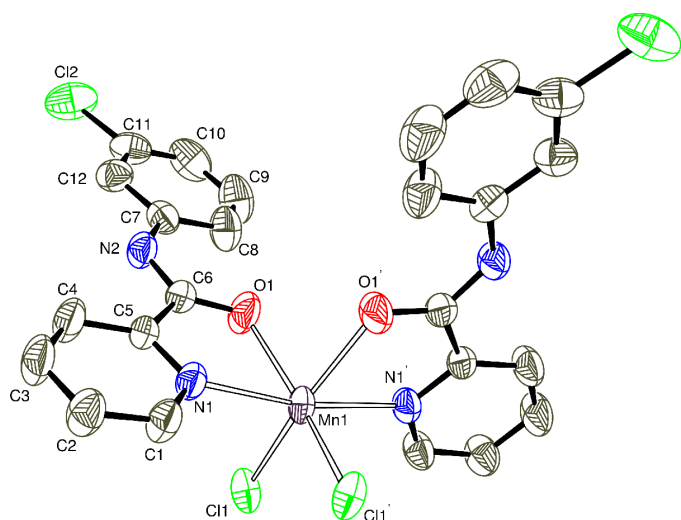


Figure 1
ORTEP-3 (Farrugia, 1997) view of the molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level [symmetry code ('): $-x, y, \frac{1}{2} - z$].

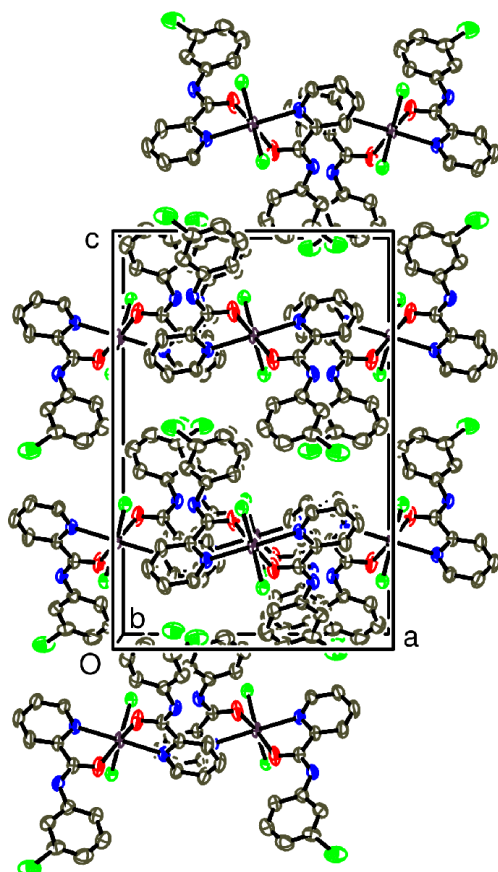


Figure 2
A view of the molecular packing along the *b* axis.

al., 1997). The ligand was dissolved in EtOH, and the manganese dichloride dissolved in EtOH was then added. The resulting pale yellow solution was stirred for 0.5 h. After nearly 35 d, a yellow precipitate appeared. The crystal used for the data collection was obtained by slow evaporation from an ethanol–water saturated solution at room temperature.

Crystal data

[MnCl₂(C₁₂H₉ClN₂O)₂]
M_r = 591.16
 Orthorhombic, *Pbcn*
a = 13.181 (4) Å
b = 9.738 (3) Å
c = 19.707 (6) Å
V = 2529.6 (12) Å³
Z = 4
D_x = 1.552 Mg m⁻³

Mo *K*α radiation
 Cell parameters from 4832 reflections
 θ = 1.5–27.5°
 μ = 0.97 mm⁻¹
T = 294 (2) K
 Block, yellow
 0.28 × 0.24 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 T_{\min} = 0.772, T_{\max} = 0.829
 16055 measured reflections

2924 independent reflections
 2076 reflections with $I > 2\sigma(I)$
 R_{int} = 0.039
 θ_{max} = 27.6°
 h = -17 → 10
 k = -12 → 12
 l = -23 → 25

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)]$ = 0.037
 $wR(F^2)$ = 0.105
 S = 1.04
 2924 reflections
 159 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.46 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Mn1—O1	2.2158 (14)	N1—C1	1.327 (2)
Mn1—N1	2.2821 (15)	N1—C5	1.342 (2)
Mn1—Cl1	2.4598 (7)	N2—C6	1.336 (2)
O1—C6	1.234 (2)	N2—C7	1.423 (2)
O1 ⁱ —Mn1—O1	82.50 (8)	Cl1 ⁱ —Mn1—Cl1	100.44 (4)
O1—Mn1—N1	71.38 (5)	C6—O1—Mn1	119.49 (11)
N1 ⁱ —Mn1—N1	169.84 (7)	C1—N1—C5	118.31 (15)
O1—Mn1—Cl1 ⁱ	160.13 (4)	Cl1—N1—Mn1	124.72 (12)
N1—Mn1—Cl1 ⁱ	91.47 (4)	C5—N1—Mn1	116.26 (11)
O1—Mn1—Cl1	91.24 (5)	C6—N2—C7	127.75 (15)
N1—Mn1—Cl1	95.03 (4)	N1—C1—C2	122.98 (17)

Symmetry code: (i) $1 - x, y, \frac{3}{2} - z$.

The H atoms were placed in their geometrically calculated positions (N—H = 0.86 and C—H = 0.93 Å) and included in the final refinement in the riding-model approximation ($U_{\text{iso}} = 1.2$ times U_{eq} of the parent atom).

Data collection: SMART (Siemens, 1995); cell refinement: SMART; data reduction: SHELXTL-NT (Siemens, 1995); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-NT; software used to prepare material for publication: SHELXTL-NT.

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