

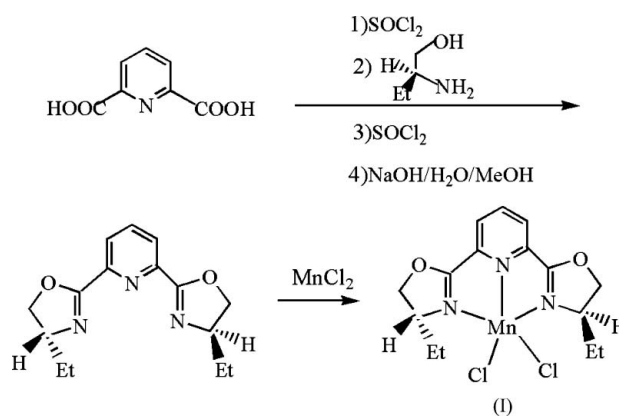
**[2,6-Bis[(4*R*)-4-ethoxyoxazolin-2-yl]pyridine]-  
dichloromanganese(II)****Jian-Ping Li and Jian-She Zhao\***Department of Chemistry, Shaanxi Key  
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The title compound,  $[\text{MnCl}_2(\text{C}_{15}\text{H}_{19}\text{N}_3\text{O}_2)]$ , was synthesized from the chiral ligand (*R,R*)-*et*-pybox {(*R,R*)-*et*-pybox is 2,6-bis[(4*R*)-4-ethoxyoxazolin-2-yl]pyridine}. The complex is mononuclear and its Mn atom has a distorted trigonal-bipyramidal coordination environment. In the complex, (*R,R*)-*et*-pybox is coordinated in a tridentate fashion to the Mn atom *via* three N atoms, having a pybox–cation ratio of 1:1.

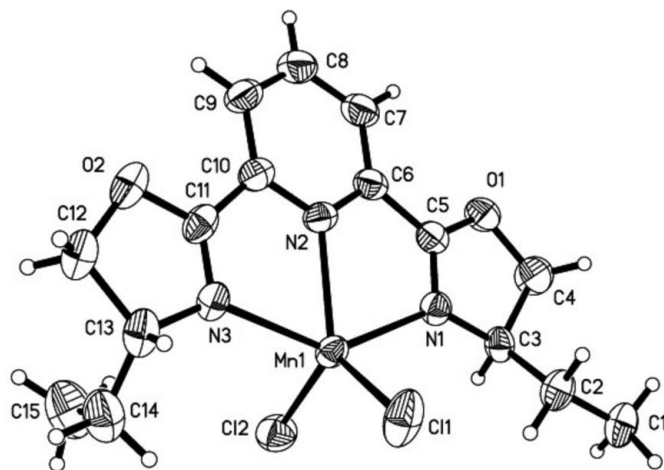
Received 6 March 2006  
Accepted 13 March 2006**Key indicators**Single-crystal X-ray study  
 $T = 296 \text{ K}$   
Mean  $\sigma(\text{C}–\text{C}) = 0.007 \text{ \AA}$   
 $R$  factor = 0.032  
 $wR$  factor = 0.085  
Data-to-parameter ratio = 14.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**Comment**

In 1989, Nishiyama first synthesized box [bis(oxazolin-2-yl)] ligands with a pyridine (py) ring as a spacer (Nishiyama *et al.*, 1989); this was a small revolution in the field, because an originally bidentate ligand was converted to the widely adopted tridentate pybox [2,6-bis(oxazolin-2-yl)pyridine] ligand, this being due to the presence of the felicitously placed pyridine N atom (Desimoni *et al.*, 2003). Normally, pyboxes behave as tridentate ligands, but a few examples of pyboxes as mono- (through one oxazoline N atom) (Cuervo *et al.*, 2002) and bidentate (involving pyridine and only one oxazoline N atom) (Heard *et al.*, 1998) ligands have been reported. Besides these exceptions, pybox behaves as a tridentate ligand (Jensen *et al.*, 1999; Lu *et al.*, 2005; Abul *et al.*, 2005) in several metal complexes which are by far the most studied. In these cases, pybox complexes can be divided into two main classes, those having pybox–cation ratios of either 1:1 or 2:1.



As part of our ongoing research, in the present study we report the synthesis and crystal structure of the title manganese(II) complex, (I), with 2,6-bis[(4*R*)-4-ethoxyoxazolin-2-yl]pyridine.

Complex (I) includes the known chiral ligand (*R,R*)-*et*-pybox, which was prepared according to the literature method (Nishiyama *et al.*, 1991). The crystal structure of (I) has a mononuclear skeleton; the Mn atom exists in a distorted



**Figure 1**  
Perspective view of the title complex, showing 30% probability displacement ellipsoids and the atom-labelling scheme.

trigonal–bipyramidal coordination environment, as shown in Fig. 1. In the complex, (*R,R*)-*et*-pybox is coordinated in a tridentate fashion to Mn via three N atoms, the trigonal–bipyramidal coordination of Mn being completed by two Cl atoms. The average values of the Mn–N and Mn–Cl bond distances are 2.253 (5) and 2.2248 (18) Å, respectively (Table 1). Atoms N2, Cl1, Cl2 and Mn1 are approximately coplanar, the mean deviation from the plane being 0.0146 Å. Atoms N1 and N3 are axial, their displacements from the mean plane defined by atoms N2, Cl1, Cl2 and Mn1 being –2.215 (6) Å and 2.217 (3) Å, respectively; the *trans* angle N1–Mn1–N3 is 146.81 (19)°.

## Experimental

All manipulations of air- and/or moisture-sensitive compounds were carried out under an atmosphere of dry nitrogen using Schlenk and cannula techniques. All solvents except *n*-pentane were deoxygenated and distilled under nitrogen before use. A mixture of MnCl<sub>2</sub> (38 mg, 0.3 mmol, in 6 ml CH<sub>3</sub>OH) and 2,6-bis[(4*R*)-4-ethoxyoxazolin-2-yl]pyridine (82 mg, 0.3 mmol, in 4 ml CH<sub>2</sub>Cl<sub>2</sub>) was stirred at room temperature for 24 h. Upon subsequent removal of the volatiles under reduced pressure, the crude product was taken up in a mixture of CH<sub>2</sub>Cl<sub>2</sub> and CHCl<sub>3</sub> (1:1 *v/v*) and then filtered. Single crystals of (I) suitable for X-ray analysis were grown by direct diffusion of *n*-pentane into the solution. Elemental analysis calculated for C<sub>15</sub>H<sub>19</sub>Cl<sub>2</sub>MnN<sub>3</sub>O<sub>2</sub>: C 45.13, H 4.80, N 10.53%. found: C 44.89, H 5.22, N 10.09%;

### Crystal data

[MnCl<sub>2</sub>(C<sub>15</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>)]  
*M<sub>r</sub>* = 399.17  
 Monoclinic, *P*2<sub>1</sub>  
*a* = 8.063 (3) Å  
*b* = 14.231 (4) Å  
*c* = 9.027 (3) Å  
 $\beta$  = 116.382 (5)°  
*V* = 928.0 (5) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 1.429 Mg m<sup>–3</sup>  
 Mo *K*α radiation  
 Cell parameters from 1749 reflections  
 $\theta$  = 2.5–21.7°  
 $\mu$  = 1.01 mm<sup>–1</sup>  
*T* = 296 (2) K  
 Block, yellow  
 0.33 × 0.21 × 0.18 mm

### Data collection

Bruker SMART CCD area-detector  
 diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)  
 $T_{\min}$  = 0.732,  $T_{\max}$  = 0.841  
 4771 measured reflections

2934 independent reflections  
 2478 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}}$  = 0.019  
 $\theta_{\text{max}}$  = 25.1°  
 $h$  = –9 → 9  
 $k$  = –16 → 16  
 $l$  = –10 → 7

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)]$  = 0.032  
 $wR(F^2)$  = 0.085  
 $S$  = 1.00  
 2934 reflections  
 210 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$   
 Absolute structure: Flack (1983),  
 with 1207 Freidel pairs  
 Flack parameter: 0.01 (2)

**Table 1**

Selected geometric parameters (Å, °).

Mn1–N2	2.263 (3)	Mn1–Cl1	2.3353 (12)
Mn1–N1	2.309 (3)	Mn1–Cl2	2.3502 (13)
Mn1–N3	2.315 (3)		
N2–Mn1–N1	70.34 (11)	N3–Mn1–Cl1	99.05 (9)
N2–Mn1–N3	70.82 (11)	N2–Mn1–Cl2	116.09 (8)
N1–Mn1–N3	141.11 (11)	N1–Mn1–Cl2	96.55 (9)
N2–Mn1–Cl1	126.11 (8)	N3–Mn1–Cl2	102.04 (8)
N1–Mn1–Cl1	101.98 (8)	Cl1–Mn1–Cl2	117.78 (5)

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C–H = 0.93–0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2$  or 1.5 (methyl) times  $U_{\text{eq}}(\text{C})$ .

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1995); software used to prepare material for publication: *SHELXTL*.

We are grateful to the National Science Foundation of China (grant No. 20371039), the National Basic Research Programme (the ‘973’ Programme, grant No. 2003CB214600) and the Natural Science Foundation of Shaanxi Education Section (grant No. 04JK143) for support.

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