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## Key indicators

Single-crystal X-ray study  
T = 150 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
R factor = 0.031  
wR factor = 0.080  
Data-to-parameter ratio = 17.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**{2,6-Bis[(4*R*)-(+)-4-isopropyl-4,5-dihydro-1,3-oxazol-2-yl]pyridine- $\kappa^3\text{N}$ }dichlorozinc(II)**

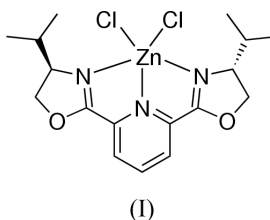
In the title compound,  $[\text{Zn}^{\text{II}}(\text{Cl})_2(\text{C}_{17}\text{H}_{23}\text{N}_3\text{O}_2)]$  or  $[\text{Zn}^{\text{II}}(\text{Cl})_2(\text{pybox})]$ , where pybox is 2,6-bis[(4*R*)-(+)-4-isopropyl-4,5-dihydro-1,3-oxazol-2-yl]pyridine, the coordination geometry is a distorted trigonal bipyramid. The pybox exhibits tridentate coordination to  $\text{Zn}^{\text{II}}$  in a [1:1] ratio, with the apical positions of the bipyramid occupied by the oxazoline N atoms of the ligand. The two Cl atoms and the pyridine N atom form the trigonal base of the bipyramid.

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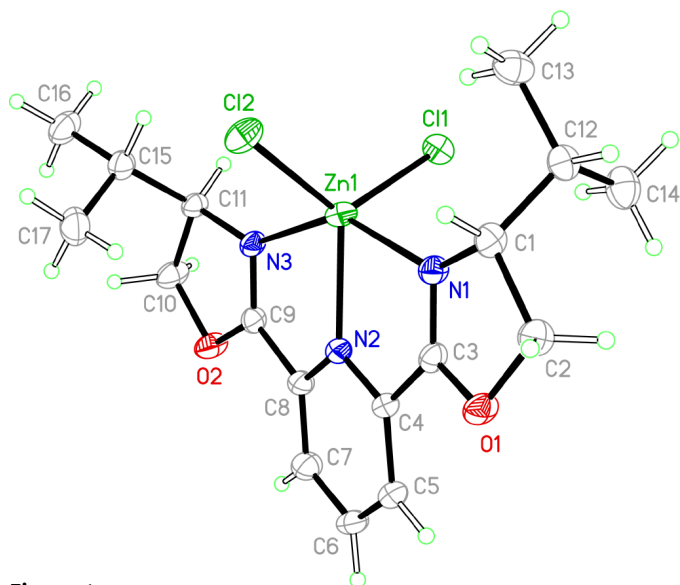
## Comment

Asymmetric catalysis using chiral bis(oxazoline), or box, ligands has attracted considerable interest (Denmark & Stiff, 2000; Evans, Rovis & Johnson, 1999; Gerisch *et al.*, 2001; Johnson & Evans, 2000; Rechavi & Lemaire, 2002). Pyridine-2,6-bis(oxazoline), or pybox, is a unique member of the bisoxazoline family, owing to its ability to form complexes with metal centres in a tridentate manner. Pybox was first introduced as a chiral ligand for the asymmetric hydrosilylation of ketones (Nishiyama *et al.*, 1989). It subsequently proved to be a valuable ligand for a variety of asymmetric reactions (Desimoni *et al.*, 2003; Evans, Barnes *et al.*, 1999; Evans, Burgey *et al.*, 1999; Schaus & Jacobsen, 2000; Yao *et al.*, 1997; Zhao *et al.*, 2001).

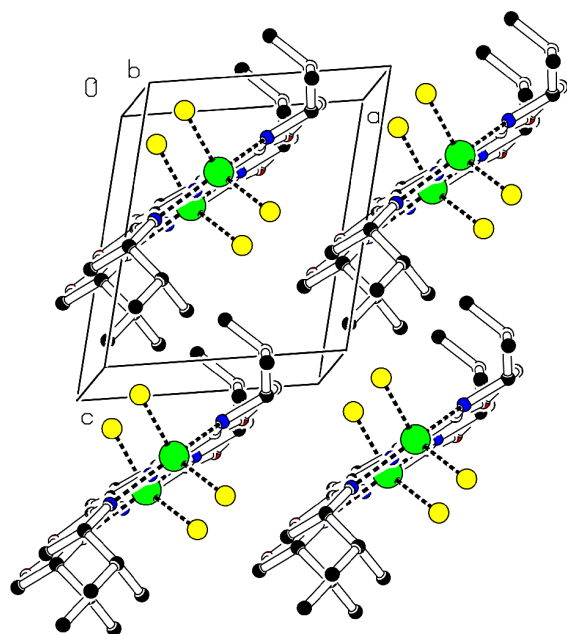
We have been interested in  $C_2$ -symmetric ligands in autocatalytic asymmetric processes using zinc as a Lewis acid (Panosyan & Chin, 2003), and we recently reported the first complex of a pybox coordinated to  $\text{Co}^{\text{III}}$  (Panosyan *et al.*, 2003). Here we report the crystal structure, (I), of 2,6-bis[(4*R*)-(+)-4-isopropyl-4,5-dihydro-1,3-oxazol-2-yl]pyridine complexed to zinc chloride. Although complexes of monodentate and bidentate pybox have been reported (Cuervo *et al.*, 2002; Heard & Jones, 1997; Heard & Tocher, 1998), the tridentate coordination mode of pybox to metals is by far the most common behaviour of the ligand (Evans, Burgey *et al.*, 1999; Evans, Kozłowski *et al.*, 1999; Nishiyama *et al.*, 1996, 1995, 1991, 1989).



The coordination geometry of (I) is a distorted trigonal bipyramid around the zinc metal centre. The Cl atoms and the pyridine N atoms form the trigonal base of the bipyramid and



**Figure 1**  
View of the molecule of (I), with the crystallographic labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.



**Figure 2**  
Packing diagram (Spek, 2002) of (I), viewed approximately along the *b* axis. Colour codes: green Zn, yellow Cl, blue N, red O, black C.

the oxazoline N atoms of the pybox ligand occupy the apical positions. The main distortion of the bipyramid is due to the  $N_{ox}-Zn-N_{ox}$  ( $ox = \text{oxazoline}$ ) angle of  $147.60(8)^\circ$ , which is significantly smaller than the ideal  $180^\circ$ . These parameters are similar to those reported for another zinc complex of a pybox molecule  $[Zn^{II}(Cl)_2(C_{25}H_{19}N_3O_2)]$  (Jiang *et al.*, 2001). The  $Cl1-Zn-Cl2$  angle of  $121.28(3)^\circ$  in (I) is, on the other hand, significantly larger than the previously reported corresponding angle of  $112.79(7)^\circ$  (Jiang *et al.*, 2001). This increase is presumably due to the smaller steric interactions of the isopropyl groups, which would allow the  $Cl1-Zn-Cl2$  angle

to approach the ideal trigonal angle of  $120^\circ$ . Interestingly, although one of the isopropyl groups (C15/C16/C17) on the ligand is positioned with both methyl groups facing away from the Cl atoms, the methyl groups of the opposing isopropyl group (C12/C13/C14) are facing toward the Cl atoms. This is further proof of the smaller steric demand around the metal centre in (I), compared to larger substituents on the chiral centre of pybox.

## Experimental

2,6-Bis(4*R*-(+)-4-isopropyl-4,5-dihydro-1,3-oxazol-2-yl)pyridine (28.0 mg, 92.9  $\mu\text{mol}$ ) dissolved in (3.0 ml) diethyl ether was added to zinc dichloride (0.107 g, 0.78 mmol) in 1.5 ml  $\text{H}_2\text{O}$ . Upon mixing the biphasic solution, the complex precipitated out as white powder. The product was filtered, washed with  $\text{H}_2\text{O}$  and diethyl ether to afford the product (39.9 mg, 98%).  $^1\text{H-NMR}$ , 300 MHz ( $\text{CDCl}_3$ ): 8.26 (*t*,  $J = 7.7$  Hz, 1H), 8.05 (*d*,  $J = 7.7$  Hz, 2H), 4.77 (*m*, 2H), 4.54 (*m*, 4H), 2.33 (*m*, 2H), 1.12 (*d*,  $J = 6.6$  Hz, 6H), 1.01 (*d*,  $J = 6.6$  Hz, 6H). Crystals suitable for X-ray analysis were obtained by dissolving the complex in hot ethanol, followed by slow evaporation of the solvent at room temperature.

## Crystal data

$[\text{Zn}(\text{C}_{17}\text{H}_{23}\text{N}_3\text{O}_2)\text{Cl}_2]$

$M_r = 437.65$

Triclinic, *P1*

$a = 7.4392(1) \text{ \AA}$

$b = 8.4408(1) \text{ \AA}$

$c = 8.7411(2) \text{ \AA}$

$\alpha = 113.027(1)^\circ$

$\beta = 97.040(1)^\circ$

$\gamma = 101.818(1)^\circ$

$V = 481.76(2) \text{ \AA}^3$

$Z = 1$

$D_x = 1.509 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

Cell parameters from 10216 reflections

$\theta = 2.6\text{--}27.5^\circ$

$\mu = 1.57 \text{ mm}^{-1}$

$T = 150(1) \text{ K}$

Needle, colourless

$0.46 \times 0.16 \times 0.14 \text{ mm}$

## Data collection

Nonius KappaCCD diffractometer

$\varphi$  scans and  $\omega$  scans with  $\kappa$  offsets

Absorption correction: multi-scan

(SORTAV; Blessing, 1995)

$T_{\min} = 0.710$ ,  $T_{\max} = 0.800$

7172 measured reflections

3959 independent reflections

3899 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 27.6^\circ$

$h = -9 \rightarrow 9$

$k = -10 \rightarrow 10$

$l = -11 \rightarrow 11$

## Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.080$

$S = 1.05$

3959 reflections

227 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2$

$+ 0.1173P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.47 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.54 \text{ e \AA}^{-3}$

Extinction correction: *SHELXTL* (Sheldrick, 2001)

Extinction coefficient: 0.035 (5)

Absolute structure: (Flack, 1983);

1455 Friedel pairs

Flack parameter = 0.006 (7)

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Zn1—N2	2.117 (2)	Zn1—N1	2.271 (2)
Zn1—Cl2	2.2283 (7)	Zn1—N3	2.362 (2)
Zn1—Cl1	2.2316 (6)		
N2—Zn1—Cl2	124.58 (6)	Cl1—Zn1—N1	99.43 (6)
N2—Zn1—Cl1	114.03 (6)	N2—Zn1—N3	72.71 (8)
Cl2—Zn1—Cl1	121.28 (3)	Cl2—Zn1—N3	99.09 (6)
N2—Zn1—N1	74.90 (9)	Cl1—Zn1—N3	94.34 (6)
Cl2—Zn1—N1	98.50 (6)	N1—Zn1—N3	147.60 (8)

All H atoms bonded to C atoms were placed in calculated positions, with C–H distances ranging from 0.95 to 1.00 Å, and included in the refinement in riding motion approximation, with  $U_{\text{iso}} = 1.2$  (1.5 for methyl) times  $U_{\text{eq}}$  of the carrier atom.

Data collection: *COLLECT* (Nonius, 1997–2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2001); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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