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Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.037
 wR factor = 0.082
Data-to-parameter ratio = 17.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis $\{\mu_2$ -2-[2-(dimethylamino)ethyliminomethyl]-phenolato}bis[chlorozinc(II)]

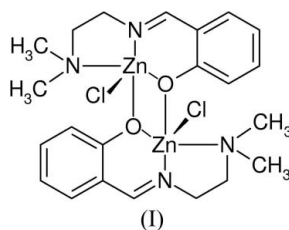
The title complex, $[\text{Zn}_2(\text{C}_{11}\text{H}_{15}\text{N}_2\text{O})_2\text{Cl}_2]$ or $[\text{LZnCl}]_2$, where L is the 2-[2-(dimethylamino)ethyliminomethyl]phenolate anion, is obtained by the reaction of LZnEt with CDCl_3 or by the reaction of LH with ZnCl_2 in refluxing tetrahydrofuran. The Zn atoms in the dimeric complex are bridged by the O atoms of the phenolate anions, and the coordination geometry around each Zn atom is distorted square-based pyramidal. The two Cl atoms lie on the same side of the central Zn_2O_2 plane.

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Comment

Poly(lactide) (PLA) and its copolymers have been studied intensively because of their potential applications in many fields (Jeong *et al.*, 1997; Gref *et al.*, 1994). The major polymerization method used to synthesize these polymers is the ring-opening polymerization (ROP) of lactides. In these processes, undesirable transesterification reactions can be minimized by using bulky ligands coordinated to the active metal centre (Dechy-Cabaret *et al.*, 2004; Wu *et al.*, 2006). Many complexes with sterically bulky ligands have been developed for this purpose, incorporating a single active metal site such as Al (Zhong *et al.*, 2003), Li (Ko & Lin, 2001), Mg (Chisholm *et al.*, 2000), Fe (O'Keefe *et al.*, 2002), Sn (Nimit-siriwat *et al.*, 2004) and Zn (Chamberlain *et al.*, 2001). Zn complexes coordinated by NNO-tridentate ligands have shown excellent activity towards ROP of lactides, giving polymers with narrow polydispersity (Williams *et al.*, 2003). Recently, we have prepared a series of NNO-tridentate Schiff base ligands (Chen *et al.*, 2006) which have shown great activity in the ROP of lactides. During these studies, it has been observed that LZnEt , where L is the 2-[2-(dimethylamino)ethyliminomethyl]phenolate anion ($\text{C}_{11}\text{H}_{15}\text{N}_2\text{O}$), reacts slowly with CDCl_3 in an NMR tube to give $[\text{LZnCl}]_2$, (I). $[\text{LZnCl}]_2$ can also be prepared by the reaction of LH with ZnCl_2 in refluxing tetrahydrofuran. Complex (I) has been widely used as a catalyst for the copolymerization of carbon dioxide and epoxides (Darensbourg, Adams *et al.*, 2003; Darensbourg, Lewis *et al.*, 2003; Darensbourg *et al.*, 2002).



In the solid state, (I) exhibits a dimeric structure in which both Zn atoms are pentacoordinated (Fig. 1). The geometry

around Zn1 and Zn2 is comparable, resembling distorted square-based pyramidal (Table 1). The central Zn₂O₂ core of the complex is close to planar, and the two Cl atoms lie on the same side of that plane. A closely comparable conformation has been observed for the diisothiocyanate complex, {LZn(NCS)}₂ (You & Zhu, 2006).

Experimental

To a suspension of LH (1.92 g, 10 mmol) in tetrahydrofuran (15 ml) was added ZnCl₂ (2.64 g, 20 mmol). After being stirred and refluxed for 2 d, the turbid solution was filtered to remove the excess ZnCl₂. Volatile materials were then removed under a vacuum to yield a light-yellow powder. The powder was washed twice with hexane (30 ml), and a white powder was obtained after filtration. A colourless crystal was selected from this sample.

Crystal data

[Zn ₂ (C ₁₁ H ₁₅ N ₂ O) ₂ Cl ₂]	Z = 4
M _r = 584.14	D _x = 1.535 Mg m ⁻³
Monoclinic, P2 ₁ /n	Mo Kα radiation
a = 7.6532 (9) Å	μ = 2.13 mm ⁻¹
b = 24.206 (3) Å	T = 292 (2) K
c = 13.6466 (16) Å	Block, colourless
β = 91.634 (2)°	0.42 × 0.16 × 0.10 mm
V = 2527.0 (5) Å ³	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	14165 measured reflections
φ and ω scans	4992 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3151 reflections with I > 2σ(I)
T _{min} = 0.487, T _{max} = 0.808	R _{int} = 0.061
	θ _{max} = 26.1°

Refinement

Refinement on F ²	H-atom parameters constrained
R[F ² > 2σ(F ²)] = 0.037	w = 1/[σ ² (F _o ²) + (0.03P) ²]
wR(F ²) = 0.082	where P = (F _o ² + 2F _c ²)/3
S = 0.97	(Δ/σ) _{max} < 0.001
4992 reflections	Δρ _{max} = 0.36 e Å ⁻³
289 parameters	Δρ _{min} = -0.40 e Å ⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	2.070 (2)	Zn2—O1	2.024 (2)
Zn1—O2	2.006 (2)	Zn2—O2	2.072 (2)
Zn1—N1	2.173 (3)	Zn2—N3	2.172 (3)
Zn1—N2	2.106 (3)	Zn2—N4	2.101 (3)
Zn1—Cl1	2.2379 (11)	Zn2—Cl2	2.2430 (11)
O2—Zn1—O1	75.18 (9)	O1—Zn2—N4	136.96 (10)
O2—Zn1—N2	138.19 (11)	O2—Zn2—N4	82.03 (11)
O1—Zn1—N2	81.81 (11)	O1—Zn2—N3	96.55 (11)
O2—Zn1—N1	99.35 (10)	O2—Zn2—N3	141.21 (12)
O1—Zn1—N1	144.83 (11)	N4—Zn2—N3	79.48 (13)
N2—Zn1—N1	80.09 (13)	O1—Zn2—Cl2	112.87 (7)
O2—Zn1—Cl1	115.12 (8)	O2—Zn2—Cl2	111.94 (8)
O1—Zn1—Cl1	112.72 (7)	N4—Zn2—Cl2	109.28 (9)
N2—Zn1—Cl1	105.82 (9)	N3—Zn2—Cl2	106.29 (10)
N1—Zn1—Cl1	101.15 (9)	Zn1—O1—Zn2	103.37 (9)
O1—Zn2—O2	74.76 (9)	Zn1—O2—Zn2	103.91 (10)

H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp²,

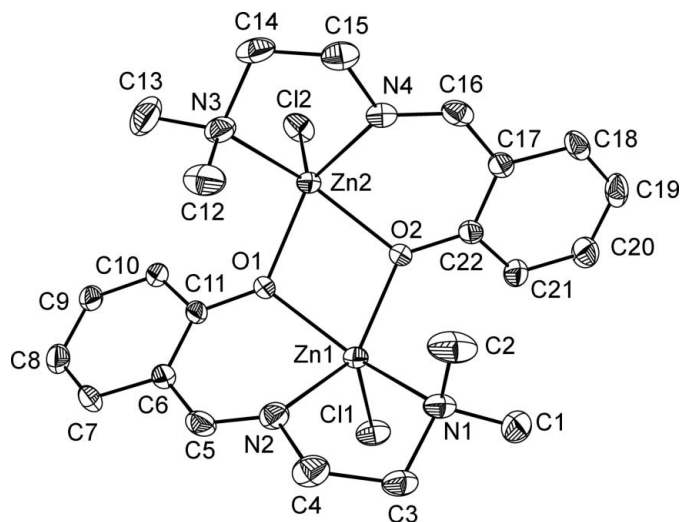


Figure 1

A view of the molecular structure of (I), showing displacement ellipsoids at the 20% probability level. H atoms have been omitted.

C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for the methylene groups, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl groups.

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 1999); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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