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Bis[2-(cyclopropyliminomethyl)phenolato]zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.019 Å
R factor = 0.055
wR factor = 0.159
Data-to-parameter ratio = 13.9

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

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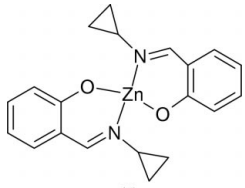
The title compound, $[Zn(C_{10}H_{10}NO)_2]$, contains an enantiomeric pair of molecules in the asymmetric unit of the non-centrosymmetric space group *C*2. In this mononuclear compound, each Zn^{II} atom is coordinated by two N atoms and two O atoms from two Schiff bases in a slightly distorted tetrahedral geometry.

Comment

Transition metal compounds containing Schiff base ligands have been of great interest for many years (Yamada, 1999; Chang *et al.*, 1998; Chaturvedi, 1977; Archer & Wang, 1990). These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). Zinc, the second most abundant transition metal in biology, functions as the active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase, where it is in a hard donor coordination environment of nitrogen and oxygen (Lipscomb & Sträter, 1996; Bertini *et al.*, 1994). Zinc has long been recognized as an important cofactor in biological molecules, either as a structural template in protein folding or as a Lewis acid catalyst that can readily adopt 4-, 5- or 6-coordination (Vallee & Auld, 1993). Recent reports have suggested that zinc is able to play a catalytic role in the activation of thiols as nucleophiles at physiological pH (Matthews & Goulding, 1997; Wilker & Lippard, 1997; Myers *et al.*, 1993). The crystal structure of a mononuclear zinc(II) compound, (I), is reported here.



(I)

The title compound, (I), is an electronically neutral mononuclear Zn^{II} compound. The asymmetric unit contains an enantiomeric pair of molecules in the non-centrosymmetric space group *C*2 (Fig. 1). Both the Zn^{II} atoms in the compound are in a tetrahedral geometry and are four-coordinated by two O atoms and by two N atoms from two Schiff base ligands. This ZnO_2N_2 coordination forms a distorted tetrahedral geometry, as usually observed in the structures of Zn^{II} complexes (McCleverty *et al.*, 1980), with angles subtended at the Zn^{II} atom in the range 96.8 (3)–121.0 (3)° for Zn1 and 96.1 (3)–121.2 (3)° for Zn2. The average Zn—O(phenolate) bond length of 1.898 (8) Å is a little shorter than the value of 1.949 (12) Å observed in the Schiff base Zn^{II} complex

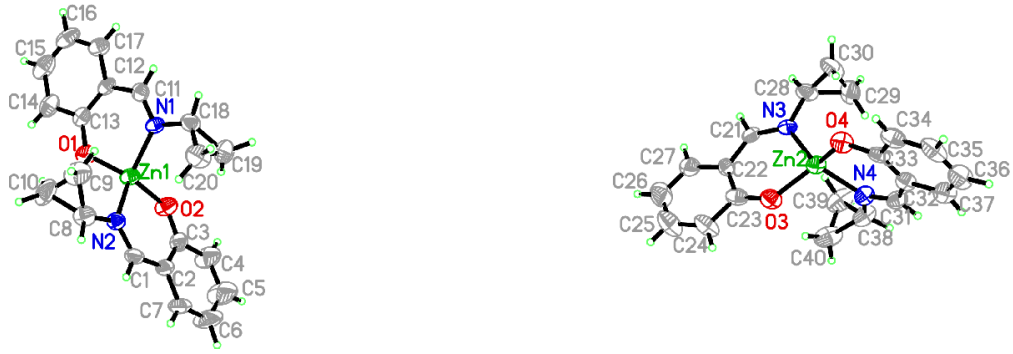


Figure 1
The asymmetric unit of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

reported by us recently (Usman *et al.*, 2003). The mean Zn—N(imine) bond length of 2.004 (8) Å is comparable to the value of 2.0166 (13) Å observed in that complex cited.

Experimental

Cyclopropylamine and salicylaldehyde were available commercially and were used without further purification. Cyclopropylamine (2.0 mmol, 114 mg) and salicylaldehyde (2.0 mmol, 244 mg) were dissolved in methanol (10 ml). The mixture was stirred for 1 h to give a clear yellow solution of *L* (2.0 mmol), where *L* is 2-[(cyclopropylamino)methyl]phenol. To the solution of *L* was added a solution of $Zn(CH_3COO)_2.2H_2O$ (1.0 mmol, 220 mg) in methanol (10 ml), with stirring. After keeping the resulting solution at room temperature in air for 12 d, colorless crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using P_4O_{10} (yield 82.7%). Analysis found: C 62.40, H 5.27, N 7.18%; calculated for $C_{20}H_{20}N_2O_2Zn$: C 62.27, H 5.23, N 7.26%. IR data: 3446.9 (*m*); 3001.4 (*w*); 1613.7 (*s*); 1536.8 (*m*); 1465.2 (*s*); 1444.7 (*m*); 1408.8 (*m*); 1347.4 (*w*); 1311.5 (*w*); 1183.5 (*m*); 1152.8 (*m*); 927.5 (*w*); 748.2 (*w*); 604.8 (*w*) cm^{-1}.

Crystal data

$[Zn(C_{10}H_{10}NO)_2]$
M_r = 385.75
Monoclinic, *C*2
a = 26.99 (2) Å
b = 9.862 (9) Å
c = 19.276 (17) Å
β = 133.473 (10)°
V = 3723 (6) $Å^3$
Z = 8
D_x = 1.376 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2380 reflections
θ = 2.3–19.0°
μ = 1.33 mm^{-1}
T = 293 (2) K
Block, colorless
0.32 × 0.27 × 0.19 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.675, T_{max} = 0.786
9558 measured reflections
6279 independent reflections
3750 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 25.0°
h = −32 → 30
k = −11 → 11
l = −15 → 22

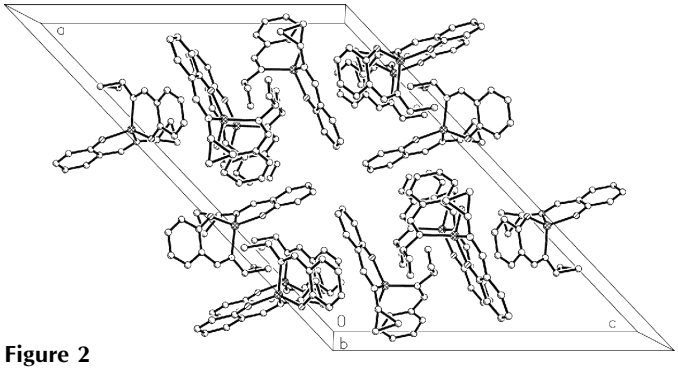


Figure 2
The crystal packing of (I), viewed along the *b* axis.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.159
S = 0.88
6279 reflections
451 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.69 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.36 e $Å^{-3}$
Absolute structure: Flack (1983); 786 Friedel pairs
Flack parameter = 0.00 (2)

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.892 (6)	Zn2—O3	1.899 (6)
Zn1—O2	1.901 (7)	Zn2—O4	1.898 (6)
Zn1—N1	1.996 (6)	Zn2—N3	2.005 (7)
Zn1—N2	2.006 (7)	Zn2—N4	2.006 (7)
O1—Zn1—O2	115.5 (3)	O3—Zn2—O4	115.6 (3)
O1—Zn1—N1	97.2 (3)	O3—Zn2—N3	96.1 (3)
O2—Zn1—N1	111.2 (3)	O4—Zn2—N3	117.3 (3)
O1—Zn1—N2	116.2 (3)	O3—Zn2—N4	111.5 (3)
O2—Zn1—N2	96.8 (3)	O4—Zn2—N4	96.4 (3)
N1—Zn1—N2	121.0 (3)	N3—Zn2—N4	121.2 (3)

H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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