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# Bis[2-(cyclohexyliminomethyl)phenolato]zinc(II)

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**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.039
*wR* factor = 0.105
Data-to-parameter ratio = 17.6

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



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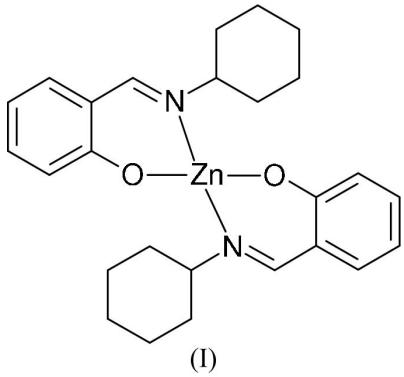
The title compound, $[Zn(C_{13}H_{16}NO)_2]$, is a mononuclear zinc(II) complex. The central $Zn^{II}$ ion, lying on an inversion centre, is coordinated by two N atoms and two O atoms from two Schiff base 2-cyclohexyliminomethylphenolate anions, resulting in a square-planar geometry.

## Comment

Schiff base complexes have been studied extensively because of their interesting structures and varied applications (Bhaduri, *et al.*, 2003; You, 2005). Zinc(II) has long been recognized 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; Lipscomb & Sträter, 1996). As part of an investigation of the structures of Schiff base zinc(II) compounds, the title compound, (I) (Fig. 1), a mononuclear zinc(II) complex, is reported here.




(I)

The central $Zn^{II}$ ion, lying on an inversion centre, is in a square-planar geometry and is four-coordinated by two N atoms and two O atoms from two Schiff base molecules. Both the Zn—O bond length of 1.891 (2) Å and the Zn—N bond length of 2.015 (2) Å are comparable with the corresponding values observed in other Schiff base zinc(II) complexes (Kratochvíl *et al.*, 1991; Tatar *et al.*, 1999). As expected, the cyclohexyl group adopts a chair conformation to minimize steric effects. There are no short intermolecular contacts in the crystal structure of (I) (Fig. 2).

## Experimental

Salicylaldehyde (0.1 mmol, 12.1 mg), cyclohexylamine (0.1 mmol, 10.1 mg) and $Zn(CH_3COO)_2{\cdot}2H_2O$ (0.1 mmol, 22.0 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 1 h to give a clear yellow solution. After the solution had been kept in air for 3 d, yellow block-shaped crystals of (I) were formed.

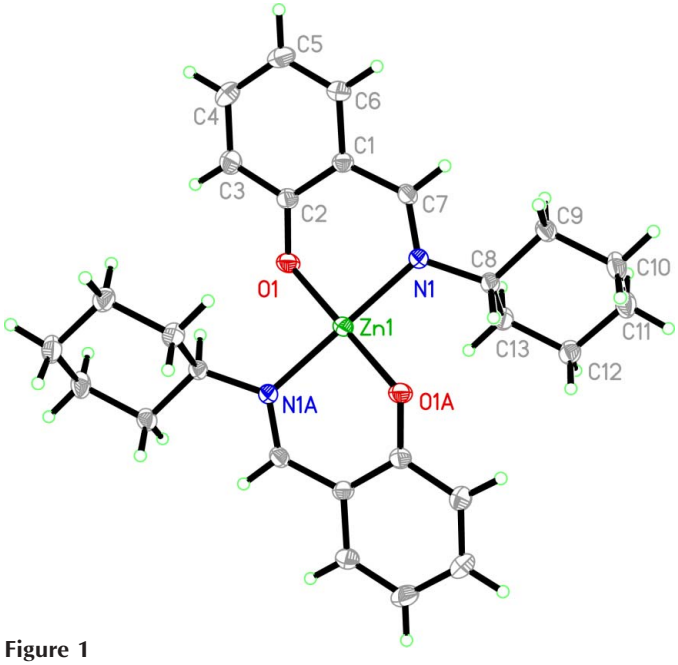



**Figure 1**
The structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). Atoms labelled with the suffix *A* are generated by the symmetry operation $(-x, 2-y, 2-z)$.

*Crystal data*

$[Zn(C_{13}H_{16}NO)_2]$
$M_r$ = 469.91
Triclinic, $P\overline{1}$
$a$ = 6.470 (2) Å
$b$ = 7.814 (2) Å
$c$ = 12.035 (2) Å
$\alpha$ = 97.70 (3)°
$\beta$ = 101.90 (3)°
$\gamma$ = 104.88 (3)°
$V$ = 564.1 (3) Å$^3$
$Z$ = 1
$D_x$ = 1.383 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3750 reflections
$\theta$ = 2.8–28.3°
$\mu$ = 1.11 mm$^{-1}$
$T$ = 298 (2) K
Block, yellow
0.28 × 0.25 × 0.21 mm

*Data collection*

Bruker SMART CCD diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.746, $T_{max}$ = 0.800
5204 measured reflections
2502 independent reflections
2457 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056
$\theta_{max}$ = 27.5°
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -15 \rightarrow 15$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
$S$ = 1.14
2502 reflections
142 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.3104P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.49 e Å$^{-3}$

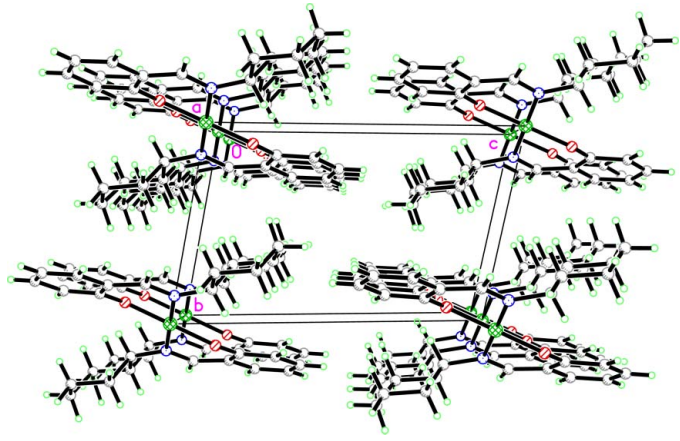



**Figure 2**
The crystal packing in (I), viewed along the *a* axis.

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—O1 | 1.891 (2) | Zn1—N1 | 2.015 (2) |
| O1$^{i}$—Zn1—N1 | 89.54 (8) | O1—Zn1—N1 | 90.46 (8) |

Symmetry code: (i) $-x, -y+2, -z+2$.

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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