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Bis[4-bromo-2-(cyclohexyliminomethyl)-phenolato]zinc(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.051
wR factor = 0.131
Data-to-parameter ratio = 19.6

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

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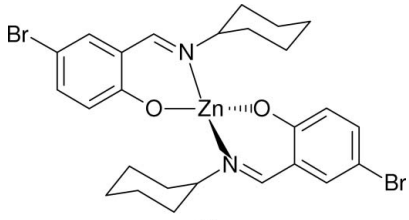
In the mononuclear title compound, $[Zn(C_{13}H_{15}BrNO)_2]$, the Zn^{II} atom is four-coordinated in a distorted tetrahedral configuration by two imine N and two phenolate O atoms from two Schiff base ligands.

Comment

The crystal structures of a few Schiff base zinc(II) compounds have been reported (You, 2005*a*,*b*,*c*). As an extension of the work on these compounds, the title zinc(II) compound, (I), is reported here.



(I)

Complex (I) is a mononuclear zinc(II) compound (Fig. 1), which is structurally similar to bis[2-(cyclopropyliminomethyl)phenolato]zinc(II) [(II); You *et al.*, 2003]. The bond lengths and angles in (I) (Table 1) are comparable to those in (II). The central Zn^{II} atom is four-coordinated by two imine N and two phenolate O atoms from two Schiff base ligands. This ZnN_2O_2 coordination forms a distorted tetrahedral geometry, with angles subtended at the Zn^{II} atom in the range 93.83 (14)–122.59 (15)°. No significant hydrogen-bonding interactions are observed in the crystal structure.

Experimental

Cyclohexylamine (0.1 mmol, 9.9 mg) and 5-bromosalicylaldehyde (0.1 mmol, 20.1 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added a MeOH solution (5 ml) of $Zn(CH_3COO)_2{\cdot}4H_2O$ (0.1 mmol, 25.6 mg), with stirring. The resulting mixture was stirred for another 10 min at room temperature. After keeping the filtrate in air for 7 d, colourless block-shaped crystals were formed at the bottom of the vessel.

Crystal data

$[Zn(C_{13}H_{15}BrNO)_2]$
M_r = 627.71
Orthorhombic, *Pbca*
a = 14.983 (1) Å
b = 13.587 (1) Å
c = 25.143 (2) Å
V = 5118.5 (7) Å^3
Z = 8
D_x = 1.629 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5469 reflections
θ = 2.5–23.7°
μ = 4.11 mm^{-1}
T = 298 (2) K
Block, colourless
0.18 × 0.13 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.525, T_{max} = 0.709
41942 measured reflections
5837 independent reflections
3518 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 27.5°
$h = -19 \rightarrow 19$
$k = -17 \rightarrow 17$
$l = -32 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.131
S = 1.02
5837 reflections
298 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 6.6703P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.918 (3)	Zn1—N1	2.026 (4)
Zn1—O2	1.918 (3)	Zn1—N2	2.032 (4)
O1—Zn1—O2	119.70 (14)	O1—Zn1—N2	113.83 (14)
O1—Zn1—N1	93.83 (14)	O2—Zn1—N2	95.33 (14)
O2—Zn1—N1	113.64 (15)	N1—Zn1—N2	122.59 (15)

H atoms were placed in idealized positions and constrained 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* (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*.

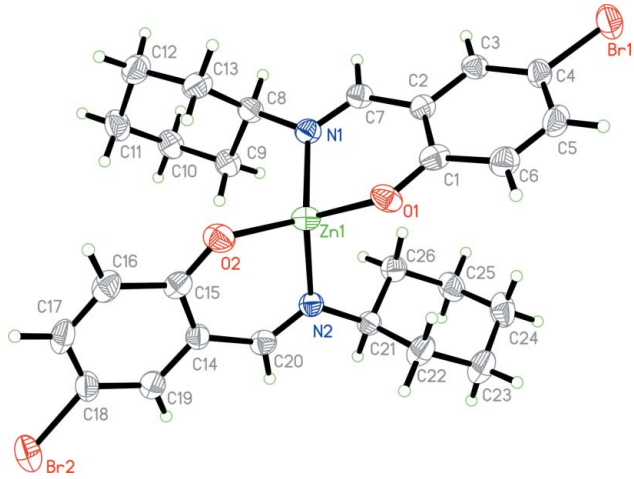


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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