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Bis[4-bromo-2-(cyclopropyliminomethyl)-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 = 0.043
wR factor = 0.102
Data-to-parameter ratio = 18.9

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

In the mononuclear title complex, $[Zn(C_{10}H_9BrNO)_2]$, the Zn^{II} atom is four-coordinated by two imine N and two phenolate O atoms from two Schiff base ligands in a distorted tetrahedral geometry.

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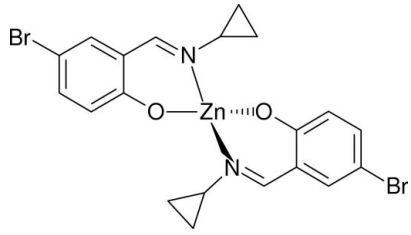
Comment

As an extension of the work on the structural characterization of Schiff base zinc(II) compounds (You, 2005*a*,*b*,*c*), the title Schiff base zinc(II) complex, (I), is reported.



(I)

Complex (I) is a mononuclear zinc(II) compound (Fig. 1). The bond lengths and angles (Table 1) are comparable to those observed in bis[2-(cyclopropyliminomethyl)phenolato]-zinc(II) (You *et al.*, 2003). The Zn^{II} atom is coordinated by two N and two 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 96.69 (12)–120.01 (14)°. C—H···O intermolecular hydrogen bonds (Table 2) link symmetry-related molecules into a three-dimensional network.

Experimental

Cyclopropylamine (0.1 mmol, 5.7 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

$[Zn(C_{10}H_9BrNO)_2]$
M_r = 543.55
Orthorhombic, *Pbca*
a = 23.260 (2) Å
b = 13.305 (2) Å
c = 13.119 (3) Å
V = 4060.0 (12) Å^3
Z = 8
D_x = 1.779 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4849 reflections
θ = 2.3–23.6°
μ = 5.16 mm^{-1}
T = 298 (2) K
Block, colourless
0.24 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.346, T_{max} = 0.538
21839 measured reflections
4619 independent reflections
2693 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 27.5°
$h = -29 \rightarrow 28$
$k = -16 \rightarrow 17$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.102
S = 1.01
4619 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 2.1967P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	1.904 (3)	Zn1—N1	2.002 (3)
Zn1—O1	1.916 (3)	Zn1—N2	2.013 (3)
O2—Zn1—O1	113.95 (12)	O2—Zn1—N2	97.50 (12)
O2—Zn1—N1	116.46 (13)	O1—Zn1—N2	113.33 (13)
O1—Zn1—N1	96.69 (12)	N1—Zn1—N2	120.01 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.98	2.54	3.488 (5)	162
C18—H18···O1^{ii}	0.98	2.49	3.442 (5)	163
C20—H20B···O1	0.97	2.55	3.419 (7)	149

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

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

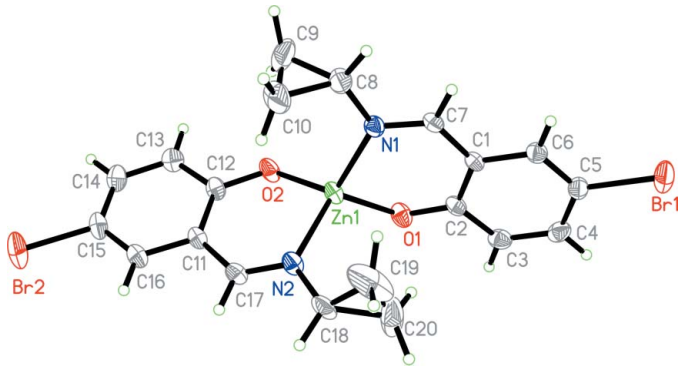


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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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