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Bis[2,4-dibromo-6-(cyclopropylimino-methyl)phenolato]zinc(II)

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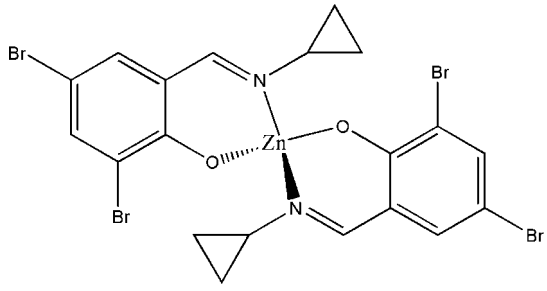
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.037; wR factor = 0.086; data-to-parameter ratio = 18.9.

The title complex, $[Zn(C_{10}H_8Br_2NO)_2]$, is a mononuclear zinc(II) compound. The Zn^{II} ion is four-coordinated by two N and two O atoms from two Schiff base ligands, forming a tetrahedral coordination.

Related literature

For related literature, see: You (2005*a*,*b*); Yuan & Zhang (2005).



Experimental

Crystal data

$[Zn(C_{10}H_8Br_2NO)_2]$
M_r = 701.36
Triclinic, $P\overline{1}$
a = 7.5490 (15) Å
b = 9.883 (2) Å
c = 15.814 (3) Å
α = 78.34 (3)°
β = 82.49 (2)°
γ = 72.24 (3)°
V = 1097.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.42 mm^{-1}
T = 298 (2) K
0.21 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.182, T_{max} = 0.187
12652 measured reflections
4962 independent reflections
3772 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.086
S = 1.04
4962 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2029).

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supplementary materials

Acta Cryst. (2007). E**63**, m1702 [**doi:10.1107/S1600536807023136**]

Bis[2,4-dibromo-6-(cyclopropyliminomethyl)phenolato]zinc(II)

W.-B. Yuan, H.-W. Xu, J.-X. Li, M. Liu and Q. Zhang

Comment

Recently, we have reported the structure of a Schiff base copper(II) complex (Yuan & Zhang, 2005). As an extension of our investigations in this area, we report here the title compound, a new mononuclear Schiff base zinc(II) complex, (I).

In (I), the Zn atom is four-coordinated by two N and two O atoms from two Schiff base ligands, forming a tetrahedral coordination (Fig. 1). The bond lengths and angles are comparable to the values observed in the similar Schiff base zinc(II) complexes (You, 2005*a*,b).

Experimental

3,5-Dibromo-2-hydroxybenzaldehyde (1.0 mmol, 280.0 mg), cyclopropylamine (1.0 mmol, 57.0 mg) and zinc dichloride (0.5 mmol, 68.1 mg) were dissolved in a methanol solution (50 ml). The mixture was stirred at room temperature for 30 min and filtered. After keeping the filtrate in air for 8 days, colorless block-shaped crystals were formed.

Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2 times U_{eq}(C). The maximum residual electron density peak is observed 1.91 Å from Br3. The minimum residual electron density peak is observed 0.86 Å from Br1.

Figures

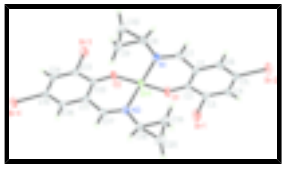


Fig. 1. The structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

Bis[2,4-dibromo-6-(cyclopropyliminomethyl)phenolato]zinc(II)

Crystal data

$[Zn(C_{10}H_8Br_2NO)_2]$	$Z = 2$
$M_r = 701.36$	$F_{000} = 672$
Triclinic, $P\overline{1}$	$D_x = 2.122$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.5490$ (15) Å	Cell parameters from 3389 reflections

b = 9.883 (2) Å	θ = 2.2–26.0º
c = 15.814 (3) Å	μ = 8.42 mm^{-1}
α = 78.34 (3)º	T = 298 (2) K
β = 82.49 (2)º	Block, colorless
γ = 72.24 (3)º	0.21 × 0.20 × 0.20 mm
V = 1097.4 (4) Å^3	

Data collection

Bruker SMART 1000 CCD area detector diffractometer	4962 independent reflections
Radiation source: fine-focus sealed tube	3772 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
T_{min} = 0.182, T_{max} = 0.187	$k = -12 \rightarrow 12$
12652 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H-atom parameters constrained
$wR(F^2)$ = 0.086	$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.0662P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
4962 reflections	$\Delta\rho_{max}$ = 0.65 e Å^{-3}
262 parameters	$\Delta\rho_{min}$ = −0.73 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.63891 (6)	0.71541 (4)	0.74530 (2)	0.03400 (12)
Br1	0.26207 (8)	0.94742 (6)	0.97427 (3)	0.07098 (18)
Br2	0.68209 (6)	0.50762 (5)	1.21708 (2)	0.05179 (13)
Br3	0.27136 (7)	0.65425 (6)	0.53715 (3)	0.05651 (14)
Br4	0.68691 (6)	0.92573 (4)	0.27077 (2)	0.04488 (12)
O1	0.5050 (4)	0.7705 (3)	0.84927 (15)	0.0408 (6)
O2	0.5105 (3)	0.7210 (3)	0.64830 (14)	0.0390 (6)
N1	0.7902 (4)	0.5186 (3)	0.80191 (18)	0.0315 (7)
N2	0.7973 (4)	0.8430 (3)	0.68016 (18)	0.0346 (7)
C1	0.6930 (5)	0.5771 (4)	0.9477 (2)	0.0305 (8)
C2	0.5521 (5)	0.7084 (4)	0.9267 (2)	0.0313 (8)
C3	0.4576 (5)	0.7739 (4)	0.9983 (2)	0.0383 (9)
C4	0.4982 (5)	0.7182 (4)	1.0822 (2)	0.0395 (9)
H4	0.4330	0.7660	1.1268	0.047*
C5	0.6371 (5)	0.5904 (4)	1.1000 (2)	0.0367 (9)
C6	0.7302 (5)	0.5184 (4)	1.0352 (2)	0.0366 (9)
H6	0.8191	0.4298	1.0485	0.044*
C7	0.7958 (5)	0.4884 (4)	0.8844 (2)	0.0354 (8)
H7	0.8751	0.3992	0.9063	0.042*
C8	0.9041 (5)	0.4100 (4)	0.7528 (2)	0.0381 (9)
H8	0.9931	0.3281	0.7853	0.046*
C9	0.9640 (6)	0.4547 (4)	0.6611 (2)	0.0478 (11)
H9A	0.9240	0.5566	0.6368	0.057*
H9B	1.0871	0.4028	0.6393	0.057*
C10	0.8206 (6)	0.3770 (5)	0.6822 (3)	0.0512 (11)
H10A	0.8559	0.2776	0.6735	0.061*
H10B	0.6928	0.4314	0.6709	0.061*
C11	0.6953 (5)	0.8382 (4)	0.5393 (2)	0.0306 (8)
C12	0.5560 (5)	0.7659 (4)	0.5682 (2)	0.0313 (8)
C13	0.4627 (5)	0.7448 (4)	0.5020 (2)	0.0353 (8)
C14	0.5031 (5)	0.7891 (4)	0.4152 (2)	0.0355 (8)
H14	0.4384	0.7728	0.3739	0.043*
C15	0.6398 (5)	0.8575 (4)	0.3902 (2)	0.0344 (8)
C16	0.7330 (5)	0.8838 (4)	0.4509 (2)	0.0344 (8)
H16	0.8226	0.9328	0.4332	0.041*
C17	0.7993 (5)	0.8760 (4)	0.5980 (2)	0.0361 (8)
H17	0.8776	0.9316	0.5719	0.043*
C18	0.9148 (6)	0.8962 (4)	0.7221 (2)	0.0419 (9)
H18	1.0079	0.9340	0.6837	0.050*
C19	0.9688 (7)	0.8296 (5)	0.8106 (3)	0.0531 (11)
H19A	0.9238	0.7485	0.8390	0.064*
H19B	1.0926	0.8241	0.8242	0.064*
C20	0.8322 (7)	0.9723 (5)	0.7968 (3)	0.0592 (12)
H20A	0.8720	1.0547	0.8017	0.071*
H20B	0.7031	0.9790	0.8165	0.071*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0398 (3)	0.0374 (2)	0.0239 (2)	−0.01177 (19)	−0.00172 (17)	−0.00263 (17)
Br1	0.0755 (4)	0.0668 (3)	0.0449 (3)	0.0230 (3)	−0.0076 (2)	−0.0167 (2)
Br2	0.0531 (3)	0.0735 (3)	0.0269 (2)	−0.0183 (2)	−0.00901 (17)	−0.00014 (19)
Br3	0.0553 (3)	0.0854 (4)	0.0435 (2)	−0.0439 (3)	−0.0016 (2)	−0.0088 (2)
Br4	0.0519 (3)	0.0523 (3)	0.02541 (19)	−0.0129 (2)	−0.00125 (16)	0.00065 (16)
O1	0.0453 (16)	0.0445 (16)	0.0227 (12)	−0.0010 (13)	−0.0005 (11)	−0.0030 (11)
O2	0.0416 (15)	0.0552 (17)	0.0236 (13)	−0.0246 (13)	−0.0013 (11)	0.0014 (11)
N1	0.0328 (17)	0.0344 (16)	0.0269 (15)	−0.0097 (13)	0.0008 (12)	−0.0064 (12)
N2	0.0398 (18)	0.0368 (17)	0.0291 (16)	−0.0136 (14)	−0.0036 (13)	−0.0052 (13)
C1	0.0296 (19)	0.0345 (19)	0.0263 (17)	−0.0088 (15)	−0.0002 (14)	−0.0045 (14)
C2	0.0309 (19)	0.040 (2)	0.0248 (17)	−0.0131 (16)	−0.0010 (14)	−0.0050 (15)
C3	0.035 (2)	0.040 (2)	0.035 (2)	−0.0048 (17)	−0.0021 (16)	−0.0050 (16)
C4	0.045 (2)	0.053 (2)	0.0255 (18)	−0.019 (2)	0.0018 (16)	−0.0116 (17)
C5	0.040 (2)	0.050 (2)	0.0258 (18)	−0.0207 (19)	−0.0097 (16)	−0.0008 (16)
C6	0.038 (2)	0.039 (2)	0.033 (2)	−0.0118 (17)	−0.0072 (16)	−0.0022 (16)
C7	0.035 (2)	0.032 (2)	0.037 (2)	−0.0090 (16)	−0.0040 (16)	−0.0038 (16)
C8	0.038 (2)	0.038 (2)	0.037 (2)	−0.0055 (17)	−0.0017 (16)	−0.0115 (16)
C9	0.054 (3)	0.045 (2)	0.041 (2)	−0.009 (2)	0.0113 (19)	−0.0154 (18)
C10	0.052 (3)	0.056 (3)	0.054 (3)	−0.015 (2)	−0.005 (2)	−0.027 (2)
C11	0.031 (2)	0.0312 (19)	0.0289 (18)	−0.0081 (15)	−0.0053 (15)	−0.0036 (14)
C12	0.032 (2)	0.033 (2)	0.0257 (17)	−0.0060 (16)	−0.0009 (14)	−0.0047 (15)
C13	0.034 (2)	0.037 (2)	0.036 (2)	−0.0121 (17)	0.0001 (16)	−0.0066 (16)
C14	0.039 (2)	0.039 (2)	0.0295 (19)	−0.0097 (17)	−0.0057 (16)	−0.0087 (16)
C15	0.035 (2)	0.036 (2)	0.0261 (18)	−0.0037 (16)	0.0023 (15)	−0.0046 (15)
C16	0.037 (2)	0.034 (2)	0.034 (2)	−0.0146 (17)	0.0007 (16)	−0.0047 (16)
C17	0.037 (2)	0.040 (2)	0.035 (2)	−0.0172 (17)	−0.0014 (16)	−0.0058 (16)
C18	0.047 (2)	0.051 (2)	0.035 (2)	−0.024 (2)	−0.0004 (17)	−0.0103 (17)
C19	0.064 (3)	0.058 (3)	0.047 (2)	−0.030 (2)	−0.021 (2)	−0.001 (2)
C20	0.062 (3)	0.065 (3)	0.059 (3)	−0.018 (3)	−0.011 (2)	−0.028 (2)

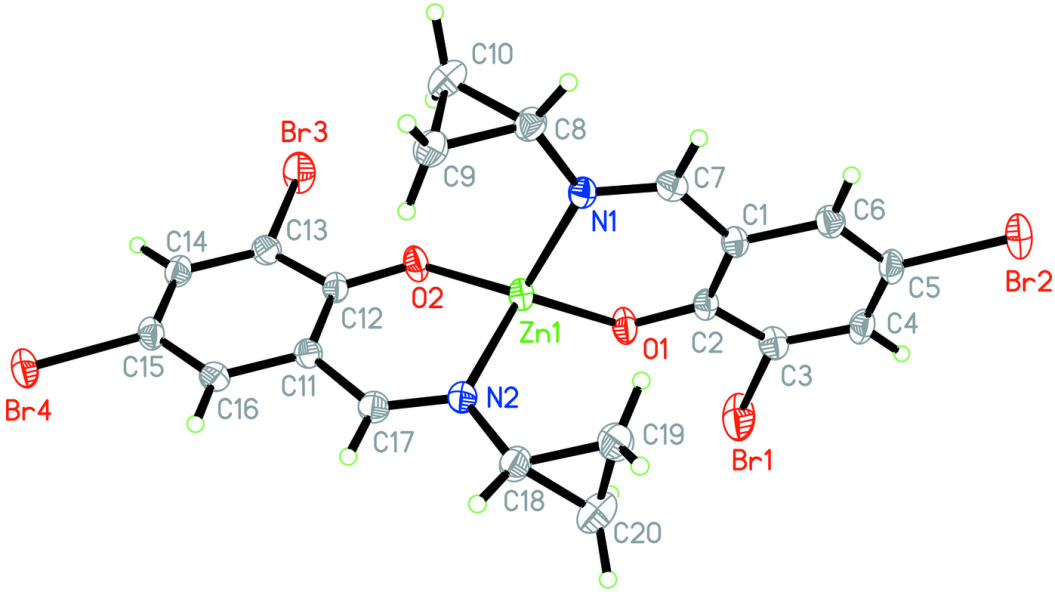
Geometric parameters (Å, °)

Zn1—O1	1.901 (2)	C8—C10	1.486 (5)
Zn1—O2	1.902 (2)	C8—H8	0.9800
Zn1—N1	2.024 (3)	C9—C10	1.477 (6)
Zn1—N2	2.038 (3)	C9—H9A	0.9700
Br1—C3	1.898 (4)	C9—H9B	0.9700
Br2—C5	1.897 (3)	C10—H10A	0.9700
Br3—C13	1.890 (4)	C10—H10B	0.9700
Br4—C15	1.898 (3)	C11—C16	1.399 (5)
O1—C2	1.296 (4)	C11—C12	1.423 (5)
O2—C12	1.293 (4)	C11—C17	1.459 (5)
N1—C7	1.281 (4)	C12—C13	1.416 (5)
N1—C8	1.447 (4)	C13—C14	1.378 (5)
N2—C17	1.274 (4)	C14—C15	1.375 (5)

N2—C18	1.443 (5)	C14—H14	0.9300
C1—C2	1.415 (5)	C15—C16	1.369 (5)
C1—C6	1.416 (5)	C16—H16	0.9300
C1—C7	1.453 (5)	C17—H17	0.9300
C2—C3	1.419 (5)	C18—C19	1.473 (5)
C3—C4	1.366 (5)	C18—C20	1.493 (5)
C4—C5	1.378 (5)	C18—H18	0.9800
C4—H4	0.9300	C19—C20	1.465 (6)
C5—C6	1.360 (5)	C19—H19A	0.9700
C6—H6	0.9300	C19—H19B	0.9700
C7—H7	0.9300	C20—H20A	0.9700
C8—C9	1.483 (5)	C20—H20B	0.9700
O1—Zn1—O2	120.70 (11)	H9A—C9—H9B	114.9
O1—Zn1—N1	95.56 (11)	C9—C10—C8	60.0 (3)
O2—Zn1—N1	116.58 (12)	C9—C10—H10A	117.8
O1—Zn1—N2	116.16 (12)	C8—C10—H10A	117.8
O2—Zn1—N2	95.52 (11)	C9—C10—H10B	117.8
N1—Zn1—N2	113.73 (12)	C8—C10—H10B	117.8
C2—O1—Zn1	125.0 (2)	H10A—C10—H10B	114.9
C12—O2—Zn1	126.1 (2)	C16—C11—C12	120.7 (3)
C7—N1—C8	117.0 (3)	C16—C11—C17	116.0 (3)
C7—N1—Zn1	120.1 (2)	C12—C11—C17	123.3 (3)
C8—N1—Zn1	122.8 (2)	O2—C12—C13	119.5 (3)
C17—N2—C18	116.9 (3)	O2—C12—C11	125.0 (3)
C17—N2—Zn1	119.8 (3)	C13—C12—C11	115.4 (3)
C18—N2—Zn1	123.3 (2)	C14—C13—C12	123.2 (3)
C2—C1—C6	120.4 (3)	C14—C13—Br3	119.7 (3)
C2—C1—C7	123.5 (3)	C12—C13—Br3	117.1 (3)
C6—C1—C7	115.8 (3)	C15—C14—C13	119.5 (3)
O1—C2—C1	125.5 (3)	C15—C14—H14	120.3
O1—C2—C3	119.2 (3)	C13—C14—H14	120.3
C1—C2—C3	115.2 (3)	C16—C15—C14	120.4 (3)
C4—C3—C2	123.8 (3)	C16—C15—Br4	120.3 (3)
C4—C3—Br1	119.1 (3)	C14—C15—Br4	119.2 (3)
C2—C3—Br1	117.1 (3)	C15—C16—C11	120.9 (3)
C3—C4—C5	119.2 (3)	C15—C16—H16	119.5
C3—C4—H4	120.4	C11—C16—H16	119.5
C5—C4—H4	120.4	N2—C17—C11	128.7 (3)
C6—C5—C4	120.7 (3)	N2—C17—H17	115.7
C6—C5—Br2	120.2 (3)	C11—C17—H17	115.7
C4—C5—Br2	118.9 (3)	N2—C18—C19	120.8 (3)
C5—C6—C1	120.6 (3)	N2—C18—C20	118.8 (4)
C5—C6—H6	119.7	C19—C18—C20	59.2 (3)
C1—C6—H6	119.7	N2—C18—H18	115.5
N1—C7—C1	127.7 (3)	C19—C18—H18	115.5
N1—C7—H7	116.1	C20—C18—H18	115.5
C1—C7—H7	116.1	C20—C19—C18	61.1 (3)
N1—C8—C9	119.1 (3)	C20—C19—H19A	117.7
N1—C8—C10	118.5 (3)	C18—C19—H19A	117.7

C9—C8—C10	59.7 (3)	C20—C19—H19B	117.7
N1—C8—H8	115.9	C18—C19—H19B	117.7
C9—C8—H8	115.9	H19A—C19—H19B	114.8
C10—C8—H8	115.9	C19—C20—C18	59.7 (3)
C10—C9—C8	60.2 (3)	C19—C20—H20A	117.8
C10—C9—H9A	117.7	C18—C20—H20A	117.8
C8—C9—H9A	117.7	C19—C20—H20B	117.8
C10—C9—H9B	117.7	C18—C20—H20B	117.8
C8—C9—H9B	117.7	H20A—C20—H20B	114.9

Fig. 1


C10
Br3
C8
C9
C7
N1
C1
C6
C14
C13
O2
C5
Br2
C12
Zn1
O1
C2
C4
C15
C11
N2
C3
Br4
C16
C17
C19
Br1
C18
C20