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Bis{4-chloro-2-[2-(1*H*-indol-3-yl)ethyliminomethyl]phenolato-κ^2N,O}zinc(II)

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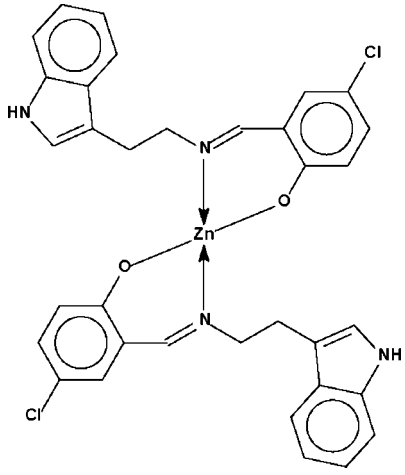
Key indicators: single-crystal X-ray study; T = 128 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.100; data-to-parameter ratio = 13.4.

The Zn atom in the title compound, $[Zn(C_{17}H_{14}ClN_2O)_2]$, is N,O-chelated by two deprotonated Schiff base monoanionic ligands in a tetrahedral coordination geometry. The Zn atom lies on a special position of site symmetry 2.

Related literature

For the structure of the unsubstituted $[(C_{17}H_{15}N_2O)_2Zn]$, see Chen *et al.* (2007); Ng (2008).



Experimental

Crystal data

$[Zn(C_{17}H_{14}ClN_2O)_2]$
M_r = 660.87
Monoclinic, $C2/c$
a = 25.8989 (3) Å
b = 5.4960 (1) Å
c = 20.6138 (3) Å
β = 91.801 (1)°
V = 2932.73 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 128 (2) K
0.50 × 0.30 × 0.17 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.714, T_{max} = 0.840
17664 measured reflections
3352 independent reflections
3023 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.100
S = 1.21
3352 reflections
251 parameters
14 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.907 (1)	Zn1—N1	2.016 (1)
O1—Zn1—O1^{i}	116.62 (8)	O1—Zn1—N1^{i}	125.55 (6)
O1—Zn1—N1	95.57 (5)	N1—Zn1—N1^{i}	99.56 (8)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2370).

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supplementary materials

Acta Cryst. (2008). E**64**, m421 [**doi:10.1107/S1600536808002213**]

Bis{4-chloro-2-[2-(1*H*-indol-3-yl)ethyliminomethyl]phenolato-κ^2N,O}zinc(II)

H. M. Ali, M. I. Mohamed Mustafa, M. R. Rizal and S. W. Ng

Comment

We have recently reported the low-temperature structure of the zinc derivative of the ligand without any substituent, $[C_{17}H_{15}N_2O)_2Zn]$ (Ng, 2008); the low-temperature structure is identical to the room-temperature structure (Chen *et al.*, 2007). The present compound has a chlorine substituent but this does not lead to significant changes to the bond dimensions of the central metal.

Experimental

The Schiff base ligand was synthesized by the reaction of tryptamine (0.32 g, 2 mmol), 5-chlorosalicylaldehyde (0.24 g, 2 mmol) and zinc acetate (0.19 g, 1 mmol) in ethanol. There organic reagents were first heated for an hour. Zinc acetate was then added followed by excess of triethylamine (1 ml). Crystals were obtained by recrystallization from dimethylformamide.

Refinement

All H atoms were located in a difference Fourier map, and were refined with distance restraints of C–H 1.00 Å and N–H 0.88 Å; their temperature factors were freely refined.

Figures

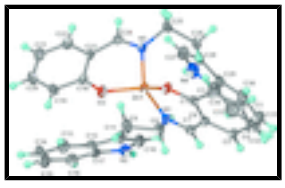


Fig. 1. Thermal ellipsoid plot of $Zn(C_{17}H_{14}ClN_2O)$. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radii.

Bis{4-chloro-2-[2-(1*H*-indol-3-yl)ethyliminomethyl]phenolato- κ^2N,O}zinc(II)

Crystal data

$[Zn(C_{17}H_{14}ClN_2O)_2]$	$F(000) = 1360$
$M_r = 660.87$	$D_x = 1.497$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 9956 reflections
$a = 25.8989$ (3) Å	$\theta = 2.5$–$31.2°$
$b = 5.4960$ (1) Å	$\mu = 1.06$ mm^{-1}
$c = 20.6138$ (3) Å	$T = 128$ K
$\beta = 91.801$ (1)°	Block, colorless

V = 2932.73 (8) Å^3	0.50 × 0.30 × 0.17 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	3352 independent reflections
Radiation source: medium-focus sealed tube	3023 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.025
φ and ω scans	θ_{max} = 27.5°, θ_{min} = 1.6°
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −33→33
T_{min} = 0.714, T_{max} = 0.840	k = −6→7
17664 measured reflections	l = −26→26

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.025	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.100	All H-atom parameters refined
S = 1.21	$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 1.1156P]$ where $P = (F_o^2 + 2F_c^2)/3$
3352 reflections	$(\Delta/\sigma)_{max}$ = 0.001
251 parameters	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
14 restraints	$\Delta\rho_{min}$ = −0.56 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.5000	0.49480 (5)	0.7500	0.01823 (11)
Cl1	0.39490 (2)	0.33657 (10)	0.42675 (2)	0.03469 (14)
O1	0.46240 (5)	0.6771 (2)	0.68555 (6)	0.0256 (3)
N1	0.53085 (5)	0.2579 (3)	0.68736 (6)	0.0167 (3)
C1	0.45075 (6)	0.5975 (3)	0.62688 (7)	0.0175 (3)
N2	0.71557 (6)	−0.2875 (3)	0.76815 (7)	0.0235 (3)
C2	0.41428 (7)	0.7308 (3)	0.58836 (8)	0.0226 (3)
C3	0.39787 (7)	0.6548 (3)	0.52766 (8)	0.0230 (3)
C4	0.41765 (7)	0.4409 (4)	0.50234 (8)	0.0216 (3)
C5	0.45433 (7)	0.3096 (3)	0.53648 (8)	0.0206 (3)
C6	0.47188 (6)	0.3836 (3)	0.59882 (7)	0.0167 (3)
C7	0.51092 (6)	0.2301 (3)	0.63013 (8)	0.0181 (3)
C8	0.56967 (6)	0.0809 (3)	0.71064 (8)	0.0186 (3)
C9	0.62386 (7)	0.1885 (4)	0.70984 (11)	0.0305 (4)
C10	0.66211 (7)	0.0247 (3)	0.74448 (10)	0.0233 (4)
C11	0.68435 (7)	−0.1805 (3)	0.72056 (9)	0.0245 (4)

C12	0.68028 (6)	0.0477 (3)	0.81090 (9)	0.0209 (3)
C13	0.67219 (7)	0.2182 (4)	0.86012 (10)	0.0296 (4)
C15	0.69689 (9)	0.1852 (4)	0.91969 (10)	0.0359 (5)
C16	0.72995 (9)	−0.0135 (4)	0.93160 (11)	0.0344 (5)
C17	0.73904 (7)	−0.1845 (4)	0.88415 (9)	0.0279 (4)
C18	0.71359 (6)	−0.1517 (3)	0.82397 (8)	0.0205 (3)
H2N	0.7331 (9)	−0.421 (3)	0.7639 (13)	0.042 (7)*
H2	0.3996 (9)	0.884 (3)	0.6056 (11)	0.036 (6)*
H3	0.3712 (7)	0.753 (4)	0.5031 (10)	0.033 (6)*
H5	0.4670 (8)	0.155 (3)	0.5170 (11)	0.036 (6)*
H7	0.5240 (7)	0.097 (3)	0.6024 (8)	0.017 (5)*
H81	0.5617 (8)	0.033 (3)	0.7554 (6)	0.018 (5)*
H82	0.5676 (9)	−0.067 (3)	0.6831 (10)	0.028 (5)*
H91	0.6237 (11)	0.351 (3)	0.7316 (12)	0.052 (8)*
H92	0.6344 (10)	0.217 (5)	0.6640 (6)	0.048 (8)*
H11	0.6818 (9)	−0.251 (4)	0.6764 (6)	0.034 (6)*
H13	0.6501 (8)	0.365 (3)	0.8521 (11)	0.038 (6)*
H15	0.6893 (9)	0.299 (4)	0.9553 (9)	0.037 (6)*
H16	0.7477 (10)	−0.026 (5)	0.9748 (8)	0.045 (8)*
H17	0.7634 (8)	−0.323 (3)	0.8917 (12)	0.041 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02395 (17)	0.01667 (17)	0.01391 (15)	0.000	−0.00209 (10)	0.000
Cl1	0.0418 (3)	0.0423 (3)	0.0191 (2)	0.0051 (2)	−0.01249 (18)	−0.00457 (18)
O1	0.0394 (7)	0.0195 (6)	0.0173 (6)	0.0091 (5)	−0.0061 (5)	−0.0035 (5)
N1	0.0163 (6)	0.0165 (7)	0.0174 (6)	0.0011 (5)	−0.0005 (5)	0.0026 (5)
C1	0.0215 (7)	0.0158 (8)	0.0153 (7)	0.0005 (6)	−0.0003 (6)	0.0006 (6)
N2	0.0211 (7)	0.0231 (8)	0.0262 (7)	0.0056 (6)	−0.0016 (6)	−0.0016 (6)
C2	0.0264 (9)	0.0193 (8)	0.0222 (8)	0.0065 (7)	0.0000 (6)	0.0018 (6)
C3	0.0227 (8)	0.0247 (9)	0.0212 (8)	0.0039 (7)	−0.0029 (6)	0.0072 (7)
C4	0.0236 (8)	0.0268 (8)	0.0142 (7)	−0.0009 (7)	−0.0026 (6)	−0.0005 (6)
C5	0.0231 (8)	0.0214 (8)	0.0172 (7)	0.0029 (6)	−0.0001 (6)	−0.0021 (6)
C6	0.0185 (7)	0.0168 (8)	0.0148 (7)	0.0013 (6)	−0.0005 (5)	0.0007 (6)
C7	0.0186 (7)	0.0173 (8)	0.0186 (7)	0.0030 (6)	0.0006 (6)	−0.0001 (6)
C8	0.0183 (7)	0.0173 (8)	0.0201 (7)	0.0020 (6)	−0.0025 (6)	0.0032 (6)
C9	0.0186 (8)	0.0281 (10)	0.0444 (11)	−0.0022 (7)	−0.0044 (7)	0.0164 (9)
C10	0.0154 (7)	0.0226 (9)	0.0319 (10)	−0.0029 (6)	−0.0015 (7)	0.0075 (7)
C11	0.0206 (8)	0.0281 (9)	0.0246 (8)	−0.0026 (7)	−0.0040 (6)	0.0022 (7)
C12	0.0152 (7)	0.0179 (8)	0.0298 (9)	−0.0013 (6)	0.0030 (6)	0.0036 (7)
C13	0.0264 (9)	0.0199 (9)	0.0431 (11)	−0.0029 (7)	0.0094 (8)	−0.0036 (8)
C15	0.0408 (11)	0.0315 (11)	0.0359 (10)	−0.0118 (9)	0.0098 (8)	−0.0126 (9)
C16	0.0399 (11)	0.0382 (12)	0.0249 (10)	−0.0122 (8)	−0.0022 (8)	0.0001 (8)
C17	0.0265 (9)	0.0293 (10)	0.0275 (9)	−0.0020 (7)	−0.0043 (7)	0.0047 (7)
C18	0.0179 (7)	0.0194 (8)	0.0241 (8)	−0.0010 (6)	0.0010 (6)	0.0018 (6)

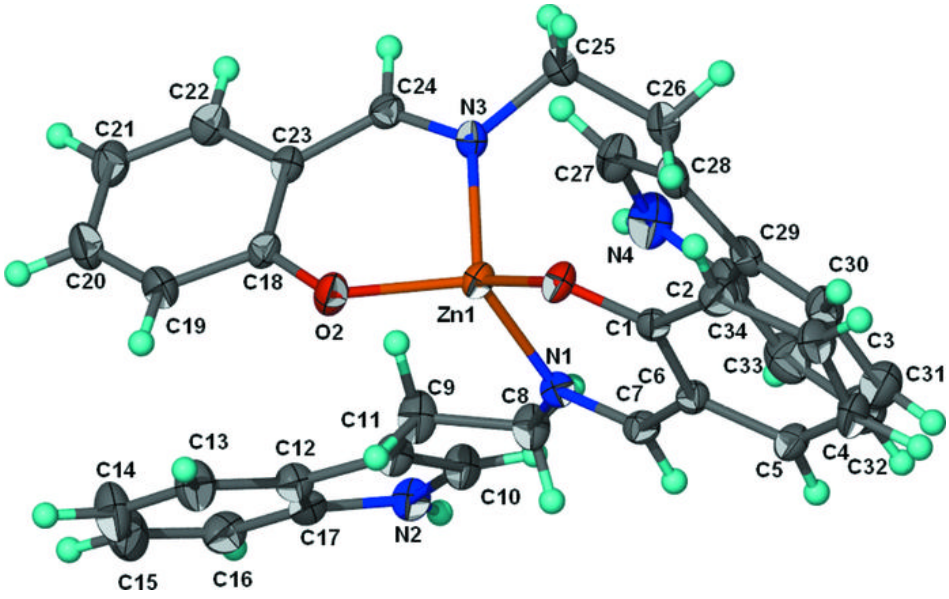
Geometric parameters (Å, °)

Zn1—O1	1.907 (1)	C7—H7	0.994 (9)
Zn1—O1^{i}	1.907 (1)	C8—C9	1.523 (2)
Zn1—N1	2.016 (1)	C8—H81	0.989 (9)
Zn1—N1^{i}	2.016 (1)	C8—H82	0.994 (10)
Cl1—C4	1.745 (2)	C9—C10	1.502 (2)
O1—C1	1.312 (2)	C9—H91	0.998 (10)
N1—C7	1.282 (2)	C9—H92	1.004 (10)
N1—C8	1.469 (2)	C10—C11	1.366 (3)
C1—C2	1.419 (2)	C10—C12	1.439 (3)
C1—C6	1.427 (2)	C11—H11	0.990 (10)
N2—C18	1.374 (2)	C12—C13	1.402 (3)
N2—C11	1.383 (2)	C12—C18	1.415 (2)
N2—H2N	0.870 (10)	C13—C15	1.379 (3)
C2—C3	1.374 (2)	C13—H13	0.998 (10)
C2—H2	0.994 (10)	C15—C16	1.405 (3)
C3—C4	1.391 (3)	C15—H15	0.990 (10)
C3—H3	1.001 (10)	C16—C17	1.382 (3)
C4—C5	1.370 (2)	C16—H16	0.992 (10)
C5—C6	1.410 (2)	C17—C18	1.398 (2)
C5—H5	0.999 (10)	C17—H17	0.996 (10)
C6—C7	1.453 (2)		
O1—Zn1—O1^{i}	116.62 (8)	N1—C8—H81	108.7 (12)
O1—Zn1—N1	95.57 (5)	C9—C8—H81	109.5 (12)
O1—Zn1—N1^{i}	125.55 (6)	N1—C8—H82	109.4 (14)
O1^{i}—Zn1—N1	125.55 (6)	C9—C8—H82	110.3 (13)
O1^{i}—Zn1—N1^{i}	95.57 (5)	H81—C8—H82	107.8 (18)
N1—Zn1—N1^{i}	99.56 (8)	C10—C9—C8	110.87 (15)
C1—O1—Zn1	124.38 (11)	C10—C9—H91	109.5 (17)
C7—N1—C8	118.25 (14)	C8—C9—H91	109.0 (16)
C7—N1—Zn1	120.68 (11)	C10—C9—H92	110.3 (16)
C8—N1—Zn1	119.96 (10)	C8—C9—H92	110.3 (15)
O1—C1—C2	118.25 (15)	H91—C9—H92	107 (2)
O1—C1—C6	124.63 (15)	C11—C10—C12	106.68 (16)
C2—C1—C6	117.12 (14)	C11—C10—C9	127.04 (19)
C18—N2—C11	109.06 (15)	C12—C10—C9	126.20 (17)
C18—N2—H2N	125.3 (18)	C10—C11—N2	109.81 (16)
C11—N2—H2N	125.7 (18)	C10—C11—H11	129.7 (14)
C3—C2—C1	122.28 (16)	N2—C11—H11	120.4 (14)
C3—C2—H2	118.2 (14)	C13—C12—C18	118.94 (17)
C1—C2—H2	119.6 (14)	C13—C12—C10	134.06 (17)
C2—C3—C4	119.47 (15)	C18—C12—C10	106.99 (15)
C2—C3—H3	119.0 (14)	C15—C13—C12	118.76 (19)
C4—C3—H3	121.5 (14)	C15—C13—H13	120.0 (14)
C5—C4—C3	120.68 (16)	C12—C13—H13	121.2 (14)

C5—C4—Cl1	119.65 (14)	C13—C15—C16	121.40 (19)
C3—C4—Cl1	119.66 (13)	C13—C15—H15	118.7 (15)
C4—C5—C6	120.98 (16)	C16—C15—H15	119.8 (15)
C4—C5—H5	118.2 (14)	C17—C16—C15	121.4 (2)
C6—C5—H5	120.8 (14)	C17—C16—H16	120.4 (16)
C5—C6—C1	119.38 (14)	C15—C16—H16	118.2 (16)
C5—C6—C7	115.93 (14)	C16—C17—C18	117.02 (18)
C1—C6—C7	124.69 (14)	C16—C17—H17	121.9 (15)
N1—C7—C6	126.44 (15)	C18—C17—H17	121.1 (15)
N1—C7—H7	118.8 (12)	N2—C18—C17	130.10 (17)
C6—C7—H7	114.6 (12)	N2—C18—C12	107.45 (15)
N1—C8—C9	111.15 (14)	C17—C18—C12	122.43 (17)
$O1^{i}$—Zn1—O1—C1	153.77 (15)	C1—C6—C7—N1	2.3 (3)
N1—Zn1—O1—C1	19.16 (14)	C7—N1—C8—C9	104.80 (18)
$N1^{i}$—Zn1—O1—C1	−86.78 (15)	Zn1—N1—C8—C9	−87.15 (16)
O1—Zn1—N1—C7	−18.84 (14)	N1—C8—C9—C10	169.91 (16)
$O1^{i}$—Zn1—N1—C7	−147.38 (12)	C8—C9—C10—C11	79.8 (2)
$N1^{i}$—Zn1—N1—C7	108.67 (14)	C8—C9—C10—C12	−96.6 (2)
O1—Zn1—N1—C8	173.41 (12)	C12—C10—C11—N2	−0.1 (2)
$O1^{i}$—Zn1—N1—C8	44.87 (14)	C9—C10—C11—N2	−177.12 (16)
$N1^{i}$—Zn1—N1—C8	−59.09 (10)	C18—N2—C11—C10	0.3 (2)
Zn1—O1—C1—C2	167.80 (12)	C11—C10—C12—C13	178.99 (19)
Zn1—O1—C1—C6	−11.6 (2)	C9—C10—C12—C13	−4.0 (3)
O1—C1—C2—C3	−176.76 (17)	C11—C10—C12—C18	−0.05 (19)
C6—C1—C2—C3	2.7 (3)	C9—C10—C12—C18	176.96 (16)
C1—C2—C3—C4	−0.4 (3)	C18—C12—C13—C15	−0.2 (3)
C2—C3—C4—C5	−1.9 (3)	C10—C12—C13—C15	−179.14 (19)
C2—C3—C4—Cl1	177.25 (14)	C12—C13—C15—C16	0.4 (3)
C3—C4—C5—C6	1.8 (3)	C13—C15—C16—C17	−0.1 (3)
Cl1—C4—C5—C6	−177.31 (13)	C15—C16—C17—C18	−0.4 (3)
C4—C5—C6—C1	0.5 (3)	C11—N2—C18—C17	−178.80 (18)
C4—C5—C6—C7	−179.84 (16)	C11—N2—C18—C12	−0.31 (19)
O1—C1—C6—C5	176.72 (16)	C16—C17—C18—N2	178.95 (18)
C2—C1—C6—C5	−2.7 (2)	C16—C17—C18—C12	0.7 (3)
O1—C1—C6—C7	−2.9 (3)	C13—C12—C18—N2	−178.99 (16)
C2—C1—C6—C7	177.69 (15)	C10—C12—C18—N2	0.22 (19)
C8—N1—C7—C6	179.43 (15)	C13—C12—C18—C17	−0.4 (3)
Zn1—N1—C7—C6	11.5 (2)	C10—C12—C18—C17	178.85 (16)
C5—C6—C7—N1	−177.31 (16)		

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Fig. 1


C25
C22
C24
N3
C26
C21
C23
C27
C28
N4
C29
C30
C20
C18
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C1
C34
C3
C19
O2
N1
C33
C31
C9
C8
C6
C7
C11
C13
C12
C4
C14
C5
C32
C10
C17
N2
C15
C16