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

Hapipah M. Ali, M. I Mohamed Mustafa, Mohd. Razali Rizal and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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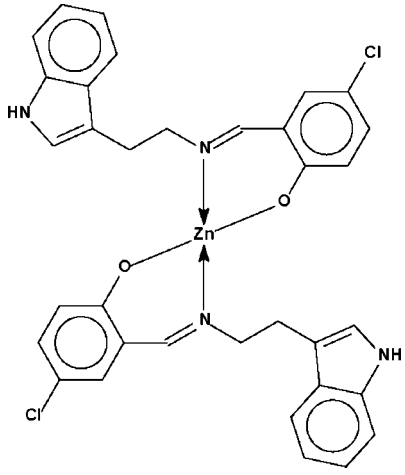
Key indicators: single-crystal X-ray study; T = 128 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.100; data-to-parameter ratio = 13.4.

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).

The authors thank the University of Canterbury, New Zealand, for the diffraction measurements, and the Science Fund (12–02-03–2031) for supporting this study.

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

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supporting information

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)

Hapipah M. Ali, M. I Mohamed Mustafa, Mohd. Razali Rizal and Seik Weng Ng

S1. 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.

S2. 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 dimethyl-formamide.

S3. 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.

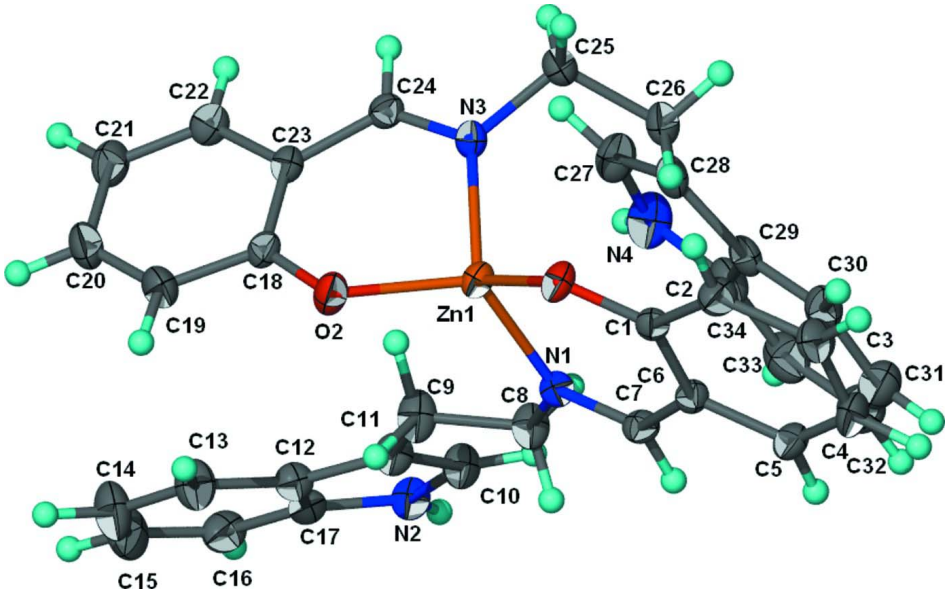

Figure 1

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.

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Crystal data

$[Zn(C_{17}H_{14}ClN_2O)_2]$
$M_r = 660.87$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 25.8989$ (3) Å
$b = 5.4960$ (1) Å
$c = 20.6138$ (3) Å
$\beta = 91.801$ (1)°
$V = 2932.73$ (8) Å^3
$Z = 4$
$F(000) = 1360$
$D_x = 1.497$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9956 reflections
$\theta = 2.5$–$31.2°$
$\mu = 1.06$ mm^{-1}
$T = 128$ K
Block, colorless
0.50 × 0.30 × 0.17 mm

Data collection

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

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.100$
$S = 1.21$
3352 reflections
251 parameters
14 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 1.1156P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ 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 (Å²)

	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, º)

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 code: (i) $-x+1, y, -z+3/2$.