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Bis[2-(2-naphthyliminomethyl)phenolato-κ^2N,O]zinc(II)

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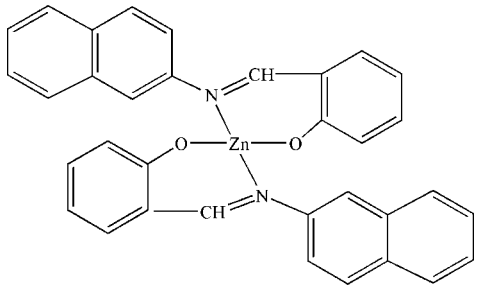
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.017 Å; R factor = 0.123; wR factor = 0.323; data-to-parameter ratio = 12.5.

In the title complex, $[Zn(C_{17}H_{12}NO)_2]$, the Zn^{II} ion is coordinated by two N,O-bidentate ligand molecules in a distorted tetrahedral geometry. The crystal packing may be stabilized by weak C—H$\cdots$*Cg* interactions [*Cg* is a ring centroid; H$\cdots$*Cg* = 2.95 Å].

Related literature

For related literature, see: Hökelek *et al.* (2000); Lipscomb & Strater (1996); Tatar *et al.* (1999).



Experimental

Crystal data

$[Zn(C_{17}H_{12}NO)_2]$
M_r = 557.92
Monoclinic, $P2_1/n$
a = 5.7616 (11) Å
b = 26.912 (3) Å
c = 16.635 (2) Å
β = 90.791 (2)°
V = 2579.0 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 298 (2) K
0.27 × 0.18 × 0.11 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.776, T_{max} = 0.899
12472 measured reflections
4398 independent reflections
2620 reflections with $I > 2\sigma(I)$
R_{int} = 0.109

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.123
$wR(F^2)$ = 0.323
S = 1.01
4398 reflections
352 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.51 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O2	1.884 (8)	Zn1—N1	2.016 (8)
Zn1—O1	1.885 (7)	Zn1—N2	2.049 (8)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2423).

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supplementary materials

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Bis[2-(2-naphthyliminomethyl)phenolato-κ^2N,O]zinc(II)

J.-F. Dong, L.-Z. Li, L.-L. Xu, T. Xu and D.-Q. Wang

Comment

As part of our ongoing studies of Schiff bases, we report here the synthesis and crystal structure of the title compound, (I), (Fig. 1), a new zinc(II) complex with a bidentate Schiff base ligand derived from the condensation of salicylaldehyde and 2-naphthylamine.

The coordination around zinc is a distorted tetrahedon involving two O and N atoms of the ligands (Table 1). These bond lengths and angle values are similar to the reported values for related structures (Hokelek *et al.*, 2000, Tatar *et al.*, 1999).

In the crystal of (I), the relatively short intermolecular distances H17···*Cg*(1)^{i} of 2.945Å and H4···*Cg*(2)^{ii} of 2.947Å (symmetry code: (i) 1/2 + *x*, 1/2 − *y*, −1/2 + *z*; (ii) *x* − 1, *y*, *z*; *Cg*(1) and *Cg*(2) are the centroids of the C25–34 and C29–34 rings, respectively) indicate the presence of weak C—H···π interactions (Fig. 2), which stabilize the crystal packing along with van der Waals forces.

Experimental

2-Naphthylamine (1 mmol, 143.19 mg) was dissolved in hot methanol (10 ml) and added in portions to a methanol solution (3 ml) of salicylaldehyde (1 mmol, 0.11 ml). The mixture was then stirred at 323 K for 2 h. Subsequently, an aqueous solution (2 ml) of zinc acetate dihydrate (1 mmol, 219.5 mg) was added dropwise and stirred for another 5 h. The solution was held at room temperature for ten days, whereupon yellow blocks of (I) were obtained.

Refinement

All the H atoms were geometrically placed (C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

Figures

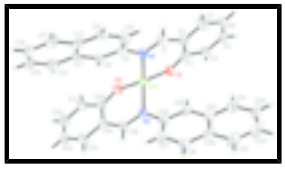

Fig. 1. The structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

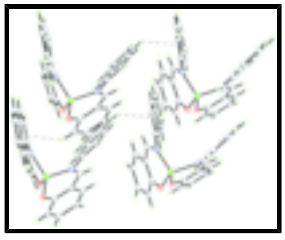

Fig. 2. The C—H···π interactions (dashed lines) in the crystal structure of (I).

Bis[2-(2-naphthyliminomethyl)phenolato-κ^2*N*,*O*]zinc(II)

Crystal data

$[Zn(C_{17}H_{12}NO)_2]$	F_{000} = 1152
M_r = 557.92	D_x = 1.437 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2565 reflections
a = 5.7616 (11) Å	θ = 2.6–19.3º
b = 26.912 (3) Å	μ = 0.99 mm^{-1}
c = 16.635 (2) Å	T = 298 (2) K
β = 90.791 (2)º	Block, yellow
V = 2579.0 (6) Å^3	0.27 × 0.18 × 0.11 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	4398 independent reflections
Radiation source: fine-focus sealed tube	2620 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.109
T = 298(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −6→6
T_{min} = 0.776, T_{max} = 0.899	k = −28→32
12472 measured reflections	l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.123	H-atom parameters constrained
$wR(F^2)$ = 0.323	$w = 1/[\sigma^2(F_o^2) + (0.1741P)^2 + 8.9475P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.002
4398 reflections	$\Delta\rho_{max}$ = 1.51 e Å^{-3}
352 parameters	$\Delta\rho_{min}$ = −1.04 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 $F^2 > \sigma(F^2)$ 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	0.3650 (2)	0.23346 (4)	0.67332 (7)	0.0501 (5)
N1	0.5696 (14)	0.2282 (3)	0.5763 (5)	0.0467 (19)
N2	0.5939 (14)	0.2372 (3)	0.7685 (4)	0.0414 (18)
O1	0.1839 (13)	0.1768 (3)	0.6500 (5)	0.0590 (19)
O2	0.1955 (14)	0.2908 (3)	0.7000 (4)	0.063 (2)
C1	0.5715 (19)	0.1862 (5)	0.5369 (7)	0.060 (3)
H1	0.6808	0.1837	0.4965	0.072*
C2	0.4265 (19)	0.1437 (4)	0.5480 (6)	0.053 (3)
C3	0.241 (2)	0.1414 (4)	0.6000 (7)	0.057 (3)
C4	0.113 (3)	0.0972 (4)	0.5990 (7)	0.078 (4)
H4	−0.0140	0.0947	0.6325	0.094*
C5	0.166 (3)	0.0577 (5)	0.5514 (9)	0.093 (5)
H5	0.0776	0.0289	0.5535	0.112*
C6	0.351 (3)	0.0606 (5)	0.5001 (9)	0.092 (5)
H6	0.3887	0.0338	0.4676	0.111*
C7	0.477 (2)	0.1028 (5)	0.4975 (8)	0.077 (4)
H7	0.5996	0.1050	0.4619	0.092*
C8	0.6637 (17)	0.3146 (4)	0.5780 (6)	0.049 (2)
H8	0.5256	0.3200	0.6049	0.058*
C9	0.7230 (17)	0.2665 (4)	0.5553 (6)	0.048 (2)
C10	0.9323 (19)	0.2581 (4)	0.5148 (8)	0.062 (3)
H10	0.9727	0.2263	0.4984	0.074*
C11	1.0722 (18)	0.2967 (4)	0.5005 (6)	0.052 (3)
H11	1.2127	0.2906	0.4755	0.062*
C12	1.0190 (17)	0.3456 (4)	0.5209 (6)	0.051 (3)
C13	0.8093 (17)	0.3550 (3)	0.5608 (5)	0.042 (2)
C14	0.750 (2)	0.4042 (4)	0.5842 (7)	0.066 (3)
H14	0.6116	0.4102	0.6108	0.079*
C15	0.895 (2)	0.4423 (4)	0.5673 (7)	0.065 (3)
H15	0.8556	0.4746	0.5817	0.078*
C16	1.103 (2)	0.4333 (5)	0.5287 (7)	0.069 (3)
H16	1.2050	0.4595	0.5193	0.083*
C17	1.160 (2)	0.3868 (5)	0.5046 (8)	0.067 (3)

H17	1.2959	0.3820	0.4764	0.080*
C18	0.6095 (19)	0.2797 (4)	0.8069 (6)	0.054 (3)
H18	0.7286	0.2820	0.8450	0.065*
C19	0.4681 (19)	0.3230 (4)	0.7979 (6)	0.054 (3)
C20	0.2714 (19)	0.3266 (4)	0.7466 (6)	0.052 (3)
C21	0.148 (2)	0.3713 (4)	0.7471 (7)	0.067 (3)
H21	0.0154	0.3746	0.7152	0.080*
C22	0.221 (3)	0.4108 (5)	0.7944 (9)	0.087 (4)
H22	0.1343	0.4399	0.7943	0.104*
C23	0.415 (3)	0.4082 (4)	0.8406 (8)	0.078 (4)
H23	0.4631	0.4359	0.8699	0.094*
C24	0.542 (2)	0.3650 (5)	0.8446 (8)	0.076 (4)
H24	0.6739	0.3631	0.8773	0.091*
C25	0.6688 (18)	0.1505 (4)	0.7680 (6)	0.051 (2)
H25	0.5266	0.1467	0.7416	0.061*
C26	0.7456 (16)	0.1970 (4)	0.7892 (6)	0.047 (2)
C27	0.9610 (18)	0.2040 (4)	0.8274 (6)	0.054 (3)
H27	1.0126	0.2359	0.8398	0.065*
C28	1.0951 (19)	0.1636 (5)	0.8463 (6)	0.058 (3)
H28	1.2370	0.1679	0.8727	0.069*
C29	1.018 (2)	0.1153 (5)	0.8255 (6)	0.062 (3)
C30	0.8047 (19)	0.1086 (4)	0.7862 (7)	0.056 (3)
C31	0.734 (2)	0.0605 (5)	0.7634 (8)	0.072 (3)
H31	0.5922	0.0563	0.7368	0.086*
C32	0.869 (3)	0.0196 (5)	0.7795 (9)	0.084 (4)
H32	0.8206	−0.0118	0.7634	0.100*
C33	1.084 (3)	0.0262 (6)	0.8213 (10)	0.098 (5)
H33	1.1775	−0.0011	0.8337	0.118*
C34	1.151 (2)	0.0726 (6)	0.8427 (9)	0.083 (4)
H34	1.2920	0.0766	0.8700	0.099*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0603 (8)	0.0492 (7)	0.0408 (6)	−0.0029 (6)	0.0011 (5)	−0.0036 (5)
N1	0.047 (5)	0.042 (5)	0.051 (5)	0.002 (4)	0.004 (4)	0.001 (4)
N2	0.055 (5)	0.037 (4)	0.032 (4)	0.001 (4)	0.003 (3)	−0.004 (3)
O1	0.066 (5)	0.043 (4)	0.068 (5)	−0.007 (4)	0.009 (4)	−0.012 (4)
O2	0.079 (5)	0.055 (5)	0.054 (4)	0.008 (4)	−0.009 (4)	−0.009 (4)
C1	0.046 (6)	0.072 (8)	0.064 (7)	0.002 (6)	0.005 (5)	−0.002 (6)
C2	0.057 (7)	0.050 (6)	0.053 (6)	0.006 (5)	−0.004 (5)	−0.002 (5)
C3	0.058 (7)	0.046 (6)	0.066 (7)	−0.007 (5)	−0.011 (5)	0.011 (5)
C4	0.121 (12)	0.055 (7)	0.060 (7)	−0.033 (7)	0.009 (7)	−0.003 (6)
C5	0.167 (16)	0.040 (7)	0.073 (9)	−0.028 (8)	−0.003 (10)	0.009 (6)
C6	0.148 (15)	0.043 (7)	0.086 (10)	0.014 (8)	−0.024 (10)	−0.020 (7)
C7	0.079 (9)	0.073 (9)	0.078 (8)	0.007 (7)	0.000 (7)	−0.014 (7)
C8	0.046 (6)	0.057 (6)	0.044 (5)	0.014 (5)	0.007 (4)	−0.007 (5)
C9	0.037 (5)	0.057 (6)	0.049 (5)	−0.009 (5)	−0.002 (4)	0.003 (5)

C10	0.046 (6)	0.061 (7)	0.079 (8)	−0.003 (5)	0.018 (5)	−0.014 (6)
C11	0.045 (6)	0.073 (8)	0.038 (5)	0.009 (6)	0.003 (4)	−0.003 (5)
C12	0.039 (6)	0.063 (7)	0.050 (6)	−0.006 (5)	0.000 (4)	0.017 (5)
C13	0.054 (6)	0.037 (5)	0.034 (5)	0.000 (4)	−0.006 (4)	−0.001 (4)
C14	0.060 (7)	0.069 (8)	0.070 (8)	0.006 (6)	−0.002 (6)	−0.013 (6)
C15	0.084 (9)	0.039 (6)	0.073 (8)	0.001 (6)	−0.008 (7)	0.004 (5)
C16	0.080 (9)	0.061 (8)	0.066 (7)	−0.015 (7)	−0.007 (6)	0.020 (6)
C17	0.053 (7)	0.070 (8)	0.079 (8)	−0.014 (6)	0.003 (6)	0.017 (6)
C18	0.057 (7)	0.059 (7)	0.047 (6)	−0.011 (5)	−0.012 (5)	−0.004 (5)
C19	0.060 (7)	0.058 (6)	0.045 (6)	−0.002 (5)	−0.001 (5)	−0.009 (5)
C20	0.061 (7)	0.048 (6)	0.046 (6)	0.000 (5)	0.013 (5)	0.003 (5)
C21	0.074 (8)	0.064 (8)	0.062 (7)	0.017 (6)	−0.001 (6)	−0.002 (6)
C22	0.124 (13)	0.050 (8)	0.086 (10)	0.015 (8)	0.008 (9)	−0.006 (7)
C23	0.113 (12)	0.037 (6)	0.084 (9)	−0.001 (7)	−0.008 (8)	−0.015 (6)
C24	0.084 (9)	0.061 (8)	0.082 (9)	−0.003 (7)	−0.008 (7)	−0.027 (6)
C25	0.046 (6)	0.049 (6)	0.057 (6)	−0.001 (5)	0.006 (5)	0.010 (5)
C26	0.039 (6)	0.060 (7)	0.043 (5)	0.003 (5)	0.006 (4)	0.007 (5)
C27	0.043 (6)	0.062 (7)	0.058 (6)	−0.002 (5)	0.014 (5)	0.006 (5)
C28	0.049 (7)	0.085 (9)	0.039 (5)	0.000 (6)	0.002 (4)	−0.001 (5)
C29	0.066 (8)	0.073 (8)	0.046 (6)	0.017 (6)	0.009 (5)	0.018 (5)
C30	0.042 (6)	0.058 (7)	0.070 (7)	0.001 (5)	0.011 (5)	0.002 (5)
C31	0.078 (9)	0.066 (8)	0.071 (8)	−0.005 (7)	0.017 (6)	0.006 (6)
C32	0.094 (11)	0.046 (7)	0.112 (11)	0.009 (7)	0.022 (9)	0.021 (7)
C33	0.101 (12)	0.087 (11)	0.108 (12)	0.033 (9)	0.015 (10)	0.042 (9)
C34	0.066 (9)	0.091 (11)	0.091 (10)	0.018 (8)	−0.002 (7)	0.028 (8)

Geometric parameters (Å, °)

Zn1—O2	1.884 (8)	C15—C16	1.390 (17)
Zn1—O1	1.885 (7)	C15—H15	0.9300
Zn1—N1	2.016 (8)	C16—C17	1.355 (17)
Zn1—N2	2.049 (8)	C16—H16	0.9300
N1—C1	1.307 (14)	C17—H17	0.9300
N1—C9	1.404 (12)	C18—C19	1.428 (15)
N2—C18	1.314 (13)	C18—H18	0.9300
N2—C26	1.429 (12)	C19—C20	1.413 (15)
O1—C3	1.309 (13)	C19—C24	1.433 (15)
O2—C20	1.308 (13)	C20—C21	1.396 (14)
C1—C2	1.431 (15)	C21—C22	1.382 (18)
C1—H1	0.9300	C21—H21	0.9300
C2—C3	1.385 (15)	C22—C23	1.347 (19)
C2—C7	1.418 (16)	C22—H22	0.9300
C3—C4	1.398 (15)	C23—C24	1.374 (17)
C4—C5	1.364 (18)	C23—H23	0.9300
C4—H4	0.9300	C24—H24	0.9300
C5—C6	1.38 (2)	C25—C26	1.373 (14)
C5—H5	0.9300	C25—C30	1.403 (14)
C6—C7	1.347 (19)	C25—H25	0.9300
C6—H6	0.9300	C26—C27	1.399 (14)

C7—H7	0.9300	C27—C28	1.367 (15)
C8—C9	1.392 (13)	C27—H27	0.9300
C8—C13	1.406 (13)	C28—C29	1.417 (17)
C8—H8	0.9300	C28—H28	0.9300
C9—C10	1.408 (14)	C29—C30	1.393 (16)
C10—C11	1.338 (15)	C29—C34	1.409 (17)
C10—H10	0.9300	C30—C31	1.408 (16)
C11—C12	1.393 (14)	C31—C32	1.370 (17)
C11—H11	0.9300	C31—H31	0.9300
C12—C13	1.410 (14)	C32—C33	1.43 (2)
C12—C17	1.402 (15)	C32—H32	0.9300
C13—C14	1.424 (14)	C33—C34	1.35 (2)
C14—C15	1.355 (16)	C33—H33	0.9300
C14—H14	0.9300	C34—H34	0.9300
O2—Zn1—O1	115.1 (3)	C16—C15—H15	119.8
O2—Zn1—N1	123.8 (3)	C17—C16—C15	120.5 (11)
O1—Zn1—N1	96.1 (3)	C17—C16—H16	119.7
O2—Zn1—N2	96.2 (3)	C15—C16—H16	119.7
O1—Zn1—N2	123.2 (3)	C16—C17—C12	122.3 (12)
N1—Zn1—N2	104.2 (3)	C16—C17—H17	118.9
C1—N1—C9	119.9 (9)	C12—C17—H17	118.9
C1—N1—Zn1	118.1 (7)	N2—C18—C19	128.7 (9)
C9—N1—Zn1	121.7 (6)	N2—C18—H18	115.7
C18—N2—C26	120.3 (9)	C19—C18—H18	115.7
C18—N2—Zn1	117.2 (7)	C20—C19—C18	124.8 (9)
C26—N2—Zn1	122.3 (6)	C20—C19—C24	120.2 (11)
C3—O1—Zn1	125.2 (7)	C18—C19—C24	115.0 (10)
C20—O2—Zn1	125.0 (7)	O2—C20—C21	118.2 (10)
N1—C1—C2	128.2 (10)	O2—C20—C19	124.5 (10)
N1—C1—H1	115.9	C21—C20—C19	117.3 (10)
C2—C1—H1	115.9	C22—C21—C20	120.9 (12)
C3—C2—C1	125.0 (10)	C22—C21—H21	119.5
C3—C2—C7	120.1 (11)	C20—C21—H21	119.5
C1—C2—C7	114.8 (11)	C23—C22—C21	121.9 (13)
O1—C3—C2	124.5 (10)	C23—C22—H22	119.1
O1—C3—C4	119.3 (11)	C21—C22—H22	119.1
C2—C3—C4	116.2 (11)	C22—C23—C24	120.4 (12)
C5—C4—C3	123.2 (13)	C22—C23—H23	119.8
C5—C4—H4	118.4	C24—C23—H23	119.8
C3—C4—H4	118.4	C23—C24—C19	119.1 (12)
C6—C5—C4	119.8 (13)	C23—C24—H24	120.4
C6—C5—H5	120.1	C19—C24—H24	120.4
C4—C5—H5	120.1	C26—C25—C30	120.0 (10)
C7—C6—C5	119.4 (12)	C26—C25—H25	120.0
C7—C6—H6	120.3	C30—C25—H25	120.0
C5—C6—H6	120.3	C25—C26—C27	121.3 (10)
C6—C7—C2	121.3 (13)	C25—C26—N2	115.7 (9)
C6—C7—H7	119.4	C27—C26—N2	122.9 (9)
C2—C7—H7	119.4	C28—C27—C26	119.5 (10)

C9—C8—C13	121.0 (9)	C28—C27—H27	120.3
C9—C8—H8	119.5	C26—C27—H27	120.3
C13—C8—H8	119.5	C27—C28—C29	119.9 (11)
C8—C9—N1	117.2 (9)	C27—C28—H28	120.0
C8—C9—C10	119.6 (9)	C29—C28—H28	120.0
N1—C9—C10	123.2 (9)	C30—C29—C28	120.3 (10)
C11—C10—C9	118.9 (10)	C30—C29—C34	117.7 (12)
C11—C10—H10	120.5	C28—C29—C34	121.9 (12)
C9—C10—H10	120.5	C25—C30—C29	118.8 (10)
C10—C11—C12	123.6 (10)	C25—C30—C31	121.5 (11)
C10—C11—H11	118.2	C29—C30—C31	119.7 (11)
C12—C11—H11	118.2	C32—C31—C30	121.6 (14)
C11—C12—C13	118.5 (9)	C32—C31—H31	119.2
C11—C12—C17	124.8 (10)	C30—C31—H31	119.2
C13—C12—C17	116.7 (10)	C31—C32—C33	119.0 (14)
C8—C13—C12	118.3 (9)	C31—C32—H32	120.5
C8—C13—C14	121.1 (9)	C33—C32—H32	120.5
C12—C13—C14	120.6 (10)	C34—C33—C32	119.0 (13)
C15—C14—C13	119.6 (11)	C34—C33—H33	120.5
C15—C14—H14	120.2	C32—C33—H33	120.5
C13—C14—H14	120.2	C33—C34—C29	123.1 (14)
C14—C15—C16	120.3 (11)	C33—C34—H34	118.5
C14—C15—H15	119.8	C29—C34—H34	118.5

Fig. 1

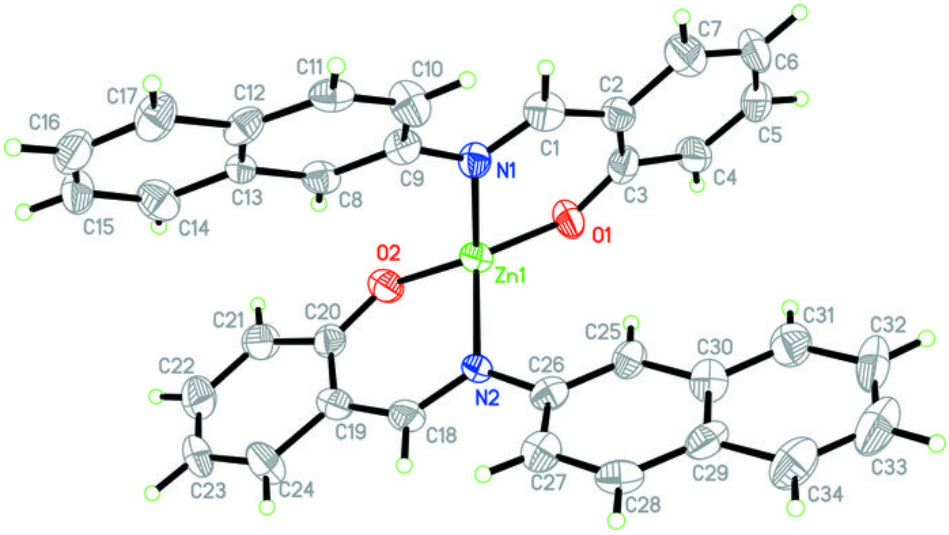
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Fig. 2