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{2,2′-[1,2-Phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}-(pyridine-κN)zinc(II)

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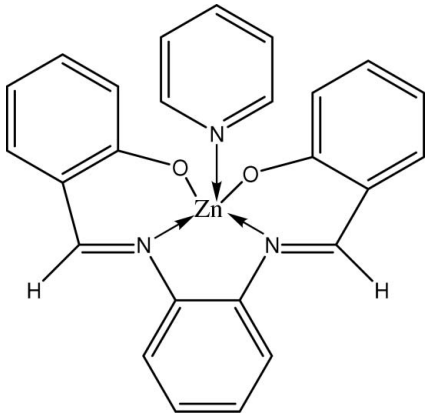
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.104; data-to-parameter ratio = 40.8.

In the title compound, $[Zn(C_{20}H_{14}N_2O_2)(C_5H_5N)]$, the Zn^{II} atom is in a distorted square-pyramidal environment. In the crystal structure, intermolecular C—H···O interactions interconnect the molecules into wave-like chains along the c axis. In addition, the crystal packing is further stabilized by weak C—H···π interactions.

Related literature

For related literature, see: Allen *et al.* (1987); Assaf & Chung (1984); Berg & Shi (1996); Bernstein *et al.* (1995); Tarafder *et al.* (2002).



Experimental

Crystal data

$[Zn(C_{20}H_{14}N_2O_2)(C_5H_5N)]$
M_r = 458.80
Monoclinic, Cc
a = 17.8611 (3) Å
b = 11.9929 (3) Å
c = 9.4946 (2) Å
β = 95.540 (1)°
V = 2024.30 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 100.0 (1) K
0.53 × 0.38 × 0.21 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.588, T_{max} = 0.778
31548 measured reflections
11416 independent reflections
9121 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.104
S = 1.07
11416 reflections
280 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}
Absolute structure: Flack (1983), with 5258 Friedel pairs
Flack parameter: 0.014 (7)

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	1.9637 (14)	Zn1—N1	2.0956 (16)
Zn1—O1	1.9707 (14)	Zn1—N2	2.1092 (15)
Zn1—N3	2.0910 (18)		
O2—Zn1—O1	96.51 (6)	N3—Zn1—N1	102.65 (6)
O2—Zn1—N3	103.55 (7)	O2—Zn1—N2	88.50 (6)
O1—Zn1—N3	98.26 (6)	O1—Zn1—N2	158.38 (7)
O2—Zn1—N1	152.21 (7)	N3—Zn1—N2	100.99 (6)
O1—Zn1—N1	88.75 (6)	N1—Zn1—N2	77.55 (6)

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

*Cg*1 is the centroid of the Zn1/O1/C1/C6/C7/N1 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C25—H25A···O1	0.93	2.58	3.156 (3)	121
C23—H23A···O2^{i}	0.93	2.54	3.211 (3)	129
C18—H18A···*Cg*1^{ii}	0.93	2.87	3.537 (2)	130

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2249).

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supplementary materials

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{2,2'-[1,2-Phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}(pyridine-κN)zinc(II)

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Comment

Zinc, an element of strong interest in biology, medicine, materials and catalysis, plays important roles in various biological systems, such as neurotransmission, signal transduction and gene expression (Assaf & Chung, 1984; Berg & Shi, 1996). It is well known that zinc complexes with Schiff bases show very good activity against the leukaemic cell (Tarafder *et al.*, 2002). Here, we report the crystal structure of the title Zn^{II} complex, (I), with the 2,2'-{1,2-phenylenebis[nitrilomethylylide]}diphenol Schiff base.

The Zn^{II} atom in (I) is five-coordinated by two O atoms and two N atoms in the basal plane, together with the N atom of the pyridine ring in the apical position, giving a distorted square-pyramidal geometry (Fig. 1 and Table 1). The Zn^{II} ion is displaced from the basal plane (N1/N2/O2/O1) by 0.3975 (2) Å. The N3/C21–C25 pyridine ring is attached axially to Zn1 with the torsion angle O1—Zn1—N3—C25 = −3.93 (15)°. The bond lengths and angles in (I) have normal values (Allen *et al.*, 1987).

An intramolecular C25—H25A···O1 interaction (Table 2 and Fig. 1) generates S(5) ring motifs (Bernstein *et al.*, 1995). In the crystal structure, the molecules are linked by intermolecular C23—H23A···O2 interactions into wave-like chains along the *c* axis (Fig. 2). In addition, the crystal packing is further stabilized by weak intermolecular C—H···π interactions involving the Zn1/O1/C1/C6/C7/N1 ring (centroid *Cg*1) (Table 2).

Experimental

The title compound was synthesized as follows. To a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol (20 ml) was added 2-hydroxybenzaldehyde (0.4 ml, 4 mmol). The mixture was refluxed with stirring for half an hour. Zinc chloride (0.272 g, 2 mmol) in ethanol (10 ml) was then added, followed by triethylamine (0.5 ml, 3.6 mmol). The mixture was stirred at

room temperature for 2 h, following which the yellow precipitate obtained was washed with ethanol (about 5 ml), dried and then washed in a copious amount of diethyl ether. This precipitate was dissolved in pyridine (15 ml), and after 9 d of slow evaporation of the pyridine at room temperature, yellow crystals of

(I) suitable for X-ray diffraction analysis were formed.

Refinement

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å and the U_{iso}(H) = 1.2U_{eq}(C).

Figures

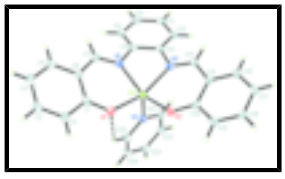

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates the intramolecular hydrogen bond.

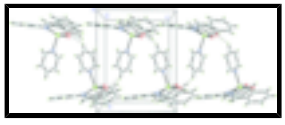

Fig. 2. The crystal packing of (I), viewed down the *a* axis. The intermolecular C—H···O hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

[2,2'-{1,2-Phenylenebis(nitrilomethylylidyne)}diphenolato- κ^4*O*,*N*,*N*',*O*'](pyridine-κ*N*)zinc(II)

Crystal data

$[Zn(C_{20}H_{14}N_2O_2)(C_5H_5N)]$	F_{000} = 944
M_r = 458.80	D_x = 1.505 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 9040 reflections
a = 17.8611 (3) Å	θ = 2.1–40.0º
b = 11.9929 (3) Å	μ = 1.24 mm^{-1}
c = 9.4946 (2) Å	*T* = 100.0 (1) K
β = 95.540 (1)º	Block, yellow
V = 2024.30 (7) Å^3	0.53 × 0.38 × 0.21 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	11416 independent reflections
Radiation source: fine-focus sealed tube	9121 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 40.0º
T = 297(2) K	θ_{min} = 2.1º
ω scans	*h* = −31→31
Absorption correction: multi-scan (SADABS; Bruker, 2005)	*k* = −19→21
T_{min} = 0.588, T_{max} = 0.778	*l* = −17→16
31548 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + 1.0902P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.104$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.87$ e Å^{-3}
11416 reflections	$\Delta\rho_{min} = -0.92$ e Å^{-3}
280 parameters	Extinction correction: none
2 restraints	Absolute structure: Flack (1983), with 5258 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.014 (7)
Secondary atom site location: difference Fourier map	

Special details

Experimental. The data were collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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	0.137941 (15)	0.276624 (17)	0.931457 (18)	0.01513 (4)
O1	0.05548 (8)	0.26576 (14)	1.05451 (15)	0.0210 (3)
O2	0.22018 (8)	0.28305 (14)	1.08423 (15)	0.0213 (3)
N1	0.06264 (9)	0.35148 (15)	0.77673 (16)	0.0166 (3)
N2	0.21070 (8)	0.35007 (15)	0.79573 (15)	0.0161 (3)
C1	−0.01125 (10)	0.30971 (18)	1.04053 (19)	0.0178 (3)
C2	−0.05900 (11)	0.29339 (19)	1.1504 (2)	0.0212 (4)
H2A	−0.0418	0.2502	1.2282	0.025*
C3	−0.12951 (11)	0.3392 (2)	1.1455 (2)	0.0245 (4)
H3A	−0.1587	0.3273	1.2200	0.029*
C4	−0.15823 (12)	0.4040 (2)	1.0294 (2)	0.0258 (4)
H4A	−0.2060	0.4353	1.0265	0.031*
C5	−0.11409 (12)	0.4202 (2)	0.9195 (2)	0.0224 (4)
H5A	−0.1328	0.4630	0.8423	0.027*
C6	−0.04126 (12)	0.3736 (2)	0.9211 (2)	0.0176 (4)
C7	−0.00347 (10)	0.39031 (18)	0.79527 (19)	0.0180 (3)
H7A	−0.0282	0.4318	0.7223	0.022*
C8	0.09499 (10)	0.36759 (17)	0.64817 (18)	0.0167 (3)
C9	0.05405 (11)	0.37665 (18)	0.51553 (19)	0.0189 (3)
H9A	0.0018	0.3751	0.5079	0.023*
C10	0.09183 (12)	0.38795 (18)	0.3952 (2)	0.0197 (3)

H10A	0.0646	0.3950	0.3071	0.024*
C11	0.17024 (12)	0.38874 (18)	0.4054 (2)	0.0200 (3)
H11A	0.1950	0.3963	0.3240	0.024*
C12	0.21155 (11)	0.37828 (18)	0.53604 (19)	0.0190 (3)
H12A	0.2638	0.3784	0.5423	0.023*
C13	0.17443 (10)	0.36752 (16)	0.65840 (17)	0.0157 (3)
C14	0.27789 (10)	0.38710 (17)	0.83114 (18)	0.0174 (3)
H14A	0.3015	0.4257	0.7629	0.021*
C15	0.31893 (12)	0.3730 (2)	0.9683 (2)	0.0175 (4)
C16	0.39295 (12)	0.4161 (2)	0.9850 (2)	0.0232 (4)
H16A	0.4121	0.4504	0.9084	0.028*
C17	0.43724 (12)	0.4087 (2)	1.1108 (2)	0.0246 (4)
H17A	0.4859	0.4373	1.1193	0.030*
C18	0.40826 (11)	0.35744 (19)	1.2266 (2)	0.0207 (3)
H18A	0.4380	0.3516	1.3123	0.025*
C19	0.33618 (11)	0.31565 (19)	1.21453 (19)	0.0201 (3)
H19A	0.3183	0.2822	1.2930	0.024*
C20	0.28810 (10)	0.32175 (17)	1.08643 (18)	0.0172 (3)
N3	0.13875 (8)	0.11047 (15)	0.86487 (16)	0.0172 (3)
C21	0.18650 (11)	0.07344 (18)	0.7742 (2)	0.0197 (3)
H21A	0.2177	0.1247	0.7351	0.024*
C22	0.19123 (11)	−0.03757 (19)	0.7364 (2)	0.0218 (3)
H22A	0.2259	−0.0603	0.6752	0.026*
C23	0.14410 (12)	−0.11397 (18)	0.7905 (2)	0.0213 (3)
H23A	0.1456	−0.1888	0.7653	0.026*
C24	0.09411 (12)	−0.0766 (2)	0.8840 (2)	0.0230 (4)
H24A	0.0619	−0.1263	0.9231	0.028*
C25	0.09292 (11)	0.03505 (19)	0.9177 (2)	0.0201 (3)
H25A	0.0591	0.0595	0.9796	0.024*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01612 (7)	0.01586 (9)	0.01368 (7)	0.00019 (10)	0.00283 (5)	0.00089 (9)
O1	0.0196 (6)	0.0259 (8)	0.0182 (6)	0.0050 (5)	0.0054 (5)	0.0034 (5)
O2	0.0199 (6)	0.0276 (8)	0.0164 (5)	−0.0057 (5)	0.0021 (4)	0.0040 (5)
N1	0.0186 (6)	0.0166 (8)	0.0149 (6)	−0.0004 (5)	0.0034 (5)	0.0002 (5)
N2	0.0184 (6)	0.0164 (7)	0.0134 (6)	−0.0002 (5)	0.0017 (4)	0.0011 (5)
C1	0.0175 (7)	0.0189 (9)	0.0174 (7)	−0.0007 (6)	0.0035 (5)	−0.0024 (6)
C2	0.0207 (8)	0.0237 (10)	0.0197 (7)	−0.0006 (7)	0.0040 (6)	−0.0008 (7)
C3	0.0212 (8)	0.0305 (12)	0.0228 (8)	−0.0017 (7)	0.0073 (6)	−0.0043 (8)
C4	0.0187 (8)	0.0315 (12)	0.0278 (9)	0.0040 (7)	0.0049 (7)	−0.0042 (8)
C5	0.0192 (8)	0.0251 (11)	0.0229 (9)	0.0024 (7)	0.0016 (7)	−0.0014 (8)
C6	0.0171 (8)	0.0171 (9)	0.0189 (8)	−0.0002 (6)	0.0025 (6)	−0.0029 (7)
C7	0.0192 (7)	0.0178 (9)	0.0169 (7)	0.0003 (6)	0.0012 (6)	0.0003 (6)
C8	0.0204 (7)	0.0148 (8)	0.0147 (7)	0.0003 (6)	0.0013 (5)	0.0002 (6)
C9	0.0218 (8)	0.0180 (9)	0.0164 (7)	0.0023 (6)	−0.0004 (6)	0.0000 (6)
C10	0.0289 (9)	0.0161 (9)	0.0140 (7)	0.0012 (7)	0.0012 (6)	0.0013 (6)

C11	0.0299 (9)	0.0172 (9)	0.0131 (7)	0.0001 (7)	0.0030 (6)	0.0010 (6)
C12	0.0233 (8)	0.0182 (9)	0.0164 (7)	−0.0006 (6)	0.0057 (6)	0.0026 (6)
C13	0.0190 (7)	0.0145 (8)	0.0138 (6)	−0.0011 (6)	0.0026 (5)	0.0008 (5)
C14	0.0196 (7)	0.0179 (9)	0.0153 (7)	−0.0011 (6)	0.0043 (5)	0.0019 (6)
C15	0.0192 (8)	0.0180 (10)	0.0154 (7)	−0.0004 (7)	0.0016 (6)	0.0025 (6)
C16	0.0202 (8)	0.0297 (12)	0.0196 (8)	−0.0042 (7)	0.0010 (7)	0.0049 (8)
C17	0.0198 (8)	0.0306 (12)	0.0228 (8)	−0.0050 (7)	−0.0005 (6)	0.0050 (8)
C18	0.0215 (8)	0.0213 (10)	0.0186 (7)	0.0003 (7)	−0.0018 (6)	0.0016 (7)
C19	0.0218 (8)	0.0216 (10)	0.0166 (7)	−0.0018 (7)	0.0012 (6)	0.0025 (7)
C20	0.0203 (7)	0.0162 (9)	0.0150 (7)	−0.0005 (6)	0.0020 (5)	0.0004 (6)
N3	0.0151 (6)	0.0192 (8)	0.0174 (6)	−0.0001 (5)	0.0023 (5)	0.0010 (5)
C21	0.0201 (7)	0.0184 (9)	0.0213 (8)	−0.0015 (6)	0.0059 (6)	−0.0017 (7)
C22	0.0239 (8)	0.0214 (10)	0.0208 (8)	0.0011 (7)	0.0059 (6)	−0.0013 (7)
C23	0.0292 (9)	0.0160 (9)	0.0187 (7)	−0.0009 (7)	0.0020 (6)	−0.0022 (6)
C24	0.0262 (9)	0.0214 (10)	0.0222 (8)	−0.0056 (7)	0.0062 (7)	−0.0007 (7)
C25	0.0204 (8)	0.0217 (10)	0.0188 (7)	−0.0025 (6)	0.0052 (6)	0.0003 (7)

Geometric parameters (Å, °)

Zn1—O2	1.9637 (14)	C10—H10A	0.9300
Zn1—O1	1.9707 (14)	C11—C12	1.387 (3)
Zn1—N3	2.0910 (18)	C11—H11A	0.9300
Zn1—N1	2.0956 (16)	C12—C13	1.398 (2)
Zn1—N2	2.1092 (15)	C12—H12A	0.9300
O1—C1	1.298 (2)	C14—C15	1.441 (3)
O2—C20	1.297 (2)	C14—H14A	0.9300
N1—C7	1.297 (2)	C15—C16	1.414 (3)
N1—C8	1.413 (2)	C15—C20	1.435 (3)
N2—C14	1.293 (2)	C16—C17	1.371 (3)
N2—C13	1.414 (2)	C16—H16A	0.9300
C1—C2	1.423 (3)	C17—C18	1.402 (3)
C1—C6	1.429 (3)	C17—H17A	0.9300
C2—C3	1.371 (3)	C18—C19	1.376 (3)
C2—H2A	0.9300	C18—H18A	0.9300
C3—C4	1.405 (3)	C19—C20	1.421 (3)
C3—H3A	0.9300	C19—H19A	0.9300
C4—C5	1.380 (3)	N3—C21	1.345 (2)
C4—H4A	0.9300	N3—C25	1.349 (3)
C5—C6	1.414 (3)	C21—C22	1.383 (3)
C5—H5A	0.9300	C21—H21A	0.9300
C6—C7	1.442 (3)	C22—C23	1.377 (3)
C7—H7A	0.9300	C22—H22A	0.9300
C8—C9	1.398 (3)	C23—C24	1.392 (3)
C8—C13	1.413 (2)	C23—H23A	0.9300
C9—C10	1.388 (3)	C24—C25	1.377 (3)
C9—H9A	0.9300	C24—H24A	0.9300
C10—C11	1.395 (3)	C25—H25A	0.9300
O2—Zn1—O1	96.51 (6)	C12—C11—C10	120.33 (18)
O2—Zn1—N3	103.55 (7)	C12—C11—H11A	119.8

O1—Zn1—N3	98.26 (6)	C10—C11—H11A	119.8
O2—Zn1—N1	152.21 (7)	C11—C12—C13	119.86 (18)
O1—Zn1—N1	88.75 (6)	C11—C12—H12A	120.1
N3—Zn1—N1	102.65 (6)	C13—C12—H12A	120.1
O2—Zn1—N2	88.50 (6)	C12—C13—C8	119.77 (16)
O1—Zn1—N2	158.38 (7)	C12—C13—N2	124.61 (16)
N3—Zn1—N2	100.99 (6)	C8—C13—N2	115.54 (14)
N1—Zn1—N2	77.55 (6)	N2—C14—C15	124.96 (17)
C1—O1—Zn1	130.08 (13)	N2—C14—H14A	117.5
C20—O2—Zn1	131.12 (12)	C15—C14—H14A	117.5
C7—N1—C8	121.44 (16)	C16—C15—C20	119.59 (18)
C7—N1—Zn1	126.14 (12)	C16—C15—C14	116.58 (18)
C8—N1—Zn1	112.07 (12)	C20—C15—C14	123.80 (19)
C14—N2—C13	121.32 (15)	C17—C16—C15	121.96 (19)
C14—N2—Zn1	126.56 (12)	C17—C16—H16A	119.0
C13—N2—Zn1	111.75 (11)	C15—C16—H16A	119.0
O1—C1—C2	118.57 (18)	C16—C17—C18	119.09 (19)
O1—C1—C6	124.69 (17)	C16—C17—H17A	120.5
C2—C1—C6	116.73 (18)	C18—C17—H17A	120.5
C3—C2—C1	122.2 (2)	C19—C18—C17	120.51 (18)
C3—C2—H2A	118.9	C19—C18—H18A	119.7
C1—C2—H2A	118.9	C17—C18—H18A	119.7
C2—C3—C4	120.89 (18)	C18—C19—C20	122.40 (17)
C2—C3—H3A	119.6	C18—C19—H19A	118.8
C4—C3—H3A	119.6	C20—C19—H19A	118.8
C5—C4—C3	118.62 (19)	O2—C20—C19	118.83 (16)
C5—C4—H4A	120.7	O2—C20—C15	124.72 (17)
C3—C4—H4A	120.7	C19—C20—C15	116.44 (17)
C4—C5—C6	121.9 (2)	C21—N3—C25	117.51 (18)
C4—C5—H5A	119.1	C21—N3—Zn1	122.12 (14)
C6—C5—H5A	119.1	C25—N3—Zn1	120.30 (13)
C5—C6—C1	119.63 (18)	N3—C21—C22	122.83 (19)
C5—C6—C7	116.1 (2)	N3—C21—H21A	118.6
C1—C6—C7	124.18 (18)	C22—C21—H21A	118.6
N1—C7—C6	124.60 (18)	C23—C22—C21	119.27 (18)
N1—C7—H7A	117.7	C23—C22—H22A	120.4
C6—C7—H7A	117.7	C21—C22—H22A	120.4
C9—C8—C13	119.77 (16)	C22—C23—C24	118.4 (2)
C9—C8—N1	124.52 (16)	C22—C23—H23A	120.8
C13—C8—N1	115.61 (15)	C24—C23—H23A	120.8
C10—C9—C8	119.68 (18)	C25—C24—C23	119.12 (19)
C10—C9—H9A	120.2	C25—C24—H24A	120.4
C8—C9—H9A	120.2	C23—C24—H24A	120.4
C9—C10—C11	120.59 (19)	N3—C25—C24	122.81 (17)
C9—C10—H10A	119.7	N3—C25—H25A	118.6
C11—C10—H10A	119.7	C24—C25—H25A	118.6
O2—Zn1—O1—C1	142.18 (19)	C8—C9—C10—C11	0.9 (3)
N3—Zn1—O1—C1	−113.06 (19)	C9—C10—C11—C12	0.0 (3)
N1—Zn1—O1—C1	−10.46 (19)	C10—C11—C12—C13	−0.4 (3)

N2—Zn1—O1—C1	39.7 (3)	C11—C12—C13—C8	−0.1 (3)
O1—Zn1—O2—C20	−157.39 (19)	C11—C12—C13—N2	176.26 (19)
N3—Zn1—O2—C20	102.47 (19)	C9—C8—C13—C12	1.0 (3)
N1—Zn1—O2—C20	−57.7 (3)	N1—C8—C13—C12	177.39 (18)
N2—Zn1—O2—C20	1.53 (19)	C9—C8—C13—N2	−175.69 (18)
O2—Zn1—N1—C7	−88.4 (2)	N1—C8—C13—N2	0.7 (3)
O1—Zn1—N1—C7	13.18 (18)	C14—N2—C13—C12	29.3 (3)
N3—Zn1—N1—C7	111.36 (18)	Zn1—N2—C13—C12	−157.32 (16)
N2—Zn1—N1—C7	−149.98 (19)	C14—N2—C13—C8	−154.23 (19)
O2—Zn1—N1—C8	84.83 (18)	Zn1—N2—C13—C8	19.2 (2)
O1—Zn1—N1—C8	−173.55 (13)	C13—N2—C14—C15	−180.0 (2)
N3—Zn1—N1—C8	−75.36 (14)	Zn1—N2—C14—C15	7.7 (3)
N2—Zn1—N1—C8	23.29 (13)	N2—C14—C15—C16	177.8 (2)
O2—Zn1—N2—C14	−5.67 (18)	N2—C14—C15—C20	−4.2 (4)
O1—Zn1—N2—C14	98.3 (2)	C20—C15—C16—C17	1.2 (4)
N3—Zn1—N2—C14	−109.17 (18)	C14—C15—C16—C17	179.4 (2)
N1—Zn1—N2—C14	150.13 (19)	C15—C16—C17—C18	−0.3 (4)
O2—Zn1—N2—C13	−178.67 (14)	C16—C17—C18—C19	−0.4 (4)
O1—Zn1—N2—C13	−74.7 (2)	C17—C18—C19—C20	0.2 (3)
N3—Zn1—N2—C13	77.82 (13)	Zn1—O2—C20—C19	179.71 (15)
N1—Zn1—N2—C13	−22.88 (13)	Zn1—O2—C20—C15	0.8 (3)
Zn1—O1—C1—C2	−176.48 (15)	C18—C19—C20—O2	−178.2 (2)
Zn1—O1—C1—C6	4.0 (3)	C18—C19—C20—C15	0.7 (3)
O1—C1—C2—C3	178.4 (2)	C16—C15—C20—O2	177.5 (2)
C6—C1—C2—C3	−2.0 (3)	C14—C15—C20—O2	−0.5 (4)
C1—C2—C3—C4	0.8 (4)	C16—C15—C20—C19	−1.4 (3)
C2—C3—C4—C5	0.3 (4)	C14—C15—C20—C19	−179.4 (2)
C3—C4—C5—C6	0.0 (4)	O2—Zn1—N3—C21	−82.04 (15)
C4—C5—C6—C1	−1.3 (4)	O1—Zn1—N3—C21	179.17 (15)
C4—C5—C6—C7	175.6 (2)	N1—Zn1—N3—C21	88.61 (15)
O1—C1—C6—C5	−178.2 (2)	N2—Zn1—N3—C21	9.07 (16)
C2—C1—C6—C5	2.3 (3)	O2—Zn1—N3—C25	94.86 (15)
O1—C1—C6—C7	5.1 (4)	O1—Zn1—N3—C25	−3.93 (15)
C2—C1—C6—C7	−174.4 (2)	N1—Zn1—N3—C25	−94.50 (15)
C8—N1—C7—C6	177.53 (19)	N2—Zn1—N3—C25	−174.04 (14)
Zn1—N1—C7—C6	−9.8 (3)	C25—N3—C21—C22	−1.4 (3)
C5—C6—C7—N1	−178.3 (2)	Zn1—N3—C21—C22	175.55 (16)
C1—C6—C7—N1	−1.5 (4)	N3—C21—C22—C23	1.6 (3)
C7—N1—C8—C9	−30.6 (3)	C21—C22—C23—C24	−1.2 (3)
Zn1—N1—C8—C9	155.77 (17)	C22—C23—C24—C25	0.7 (3)
C7—N1—C8—C13	153.21 (19)	C21—N3—C25—C24	0.9 (3)
Zn1—N1—C8—C13	−20.4 (2)	Zn1—N3—C25—C24	−176.16 (16)
C13—C8—C9—C10	−1.4 (3)	C23—C24—C25—N3	−0.5 (3)
N1—C8—C9—C10	−177.44 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C25—H25A···O1	0.93	2.58	3.156 (3)	121

C23—H23A···O2^{i}	0.93	2.54	3.211 (3)	129
C18—H18A···Cg1^{ii}	0.93	2.87	3.537 (2)	130

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

Fig. 1

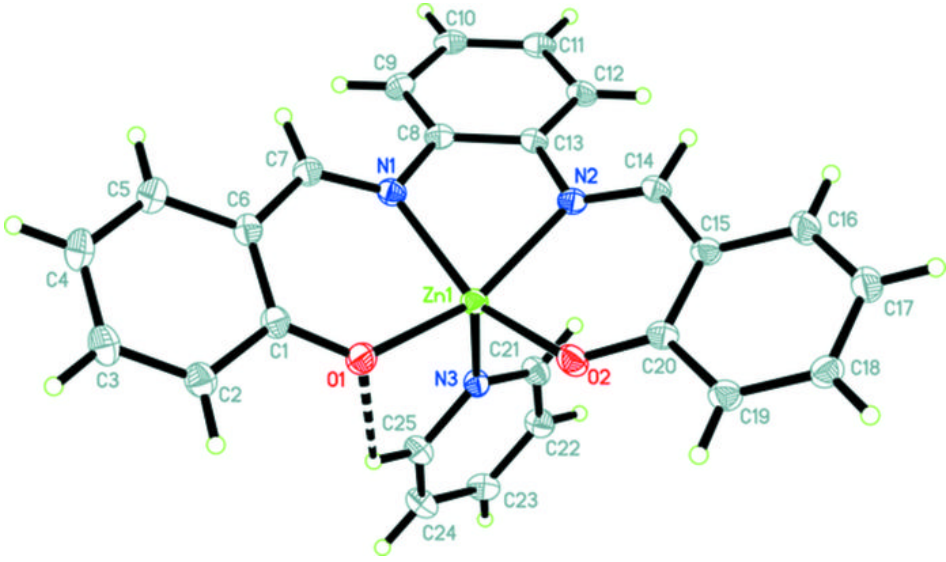
C10
C11
C9
C12
C8
C13
C7
N1
N2
C14
C5
C6
C15
C16
C4
Zn1
C17
C1
C21
O1
N3
O2
C20
C18
C3
C2
C25
C22
C19
C23
C24

Fig. 2