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Bis(4-methoxybenzaldehyde 2-hydroxybenzoylhydrazonato)pyridinezinc(II) pyridine solvate

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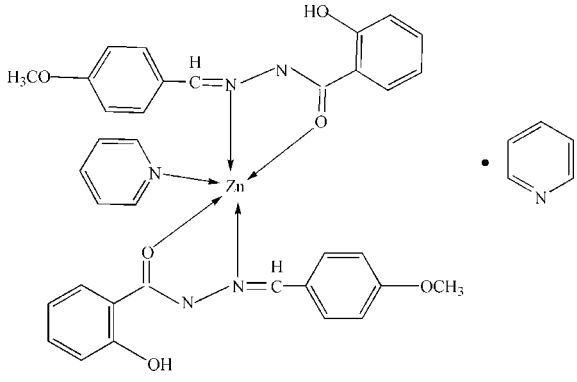
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; disorder in solvent or counterion; R factor = 0.044; wR factor = 0.144; data-to-parameter ratio = 13.2.

In the title compound, $[Zn(C_{15}H_{13}N_2O_3)_2(C_5H_5N)]\cdot C_5H_5N$, a distorted ZnN_3O_2 trigonal–bipyramidal coordination geometry results from the coordination of the two bidentate ligands and one pyridine molecule. A crystallographic twofold rotation axis passes through Zn and the pyridine ligand. The pyridine solvent molecule is disordered over an inversion centre. Intermolecular C—H···O and intramolecular C—H···O and O—H···N hydrogen-bonding interactions help to establish the crystal packing.

Related literature

For related literature, see: Tai *et al.* (2005).



Experimental

Crystal data

$[Zn(C_{15}H_{13}N_2O_3)_2(C_5H_5N)]\cdot C_5H_5N$
M_r = 762.14
Orthorhombic, *Pbcn*
a = 15.447 (2) Å
b = 10.0122 (17) Å
c = 23.598 (3) Å
V = 3649.6 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 298 K
0.43 × 0.32 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.744, T_{max} = 0.874
14274 measured reflections
3183 independent reflections
1794 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.144
S = 1.06
3183 reflections
241 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.988 (3)	Zn1—O1^{i}	1.988 (3)
Zn1—N2	2.195 (3)	Zn1—N2^{i}	2.195 (3)
Zn1—N3	2.065 (5)		
O1—Zn1—N2	78.49 (11)	N2^{i}—Zn1—N3	94.99 (8)
O1—Zn1—N3	124.50 (9)	O1^{i}—Zn1—N2^{i}	78.49 (11)
O1—Zn1—O1^{i}	111.01 (13)	Zn1—O1—C1	113.0 (3)
O1—Zn1—N2^{i}	95.80 (11)	Zn1—N2—N1	107.2 (2)
N2—Zn1—N3	94.99 (8)	Zn1—N2—C8	140.1 (3)
O1^{i}—Zn1—N2	95.80 (11)	Zn1—N3—C16^{i}	120.6 (3)
N2—Zn1—N2^{i}	170.02 (12)	Zn1—N3—C16	120.6 (3)
O1^{i}—Zn1—N3	124.50 (9)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1	0.82	1.80	2.522 (4)	147
C7—H7···O1	0.93	2.51	2.827 (6)	100
C16—H16···O2^{iii}	0.93	2.43	3.190 (6)	139

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 2000); 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: AT2306).

 doi:10.1107/S1600536807028917

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supplementary materials

Acta Cryst. (2007). E**63**, m1927-m1928 [**doi:10.1107/S1600536807028917**]

Bis(4-methoxybenzaldehyde 2-hydroxybenzoylhydrazonato)pyridinezinc(II) pyridine solvate

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Comment

As part of our onging studies of metal coordination complexes with multidentate ligands (Tai *et al.*, 2005), the synthesis and structure of the title compound, (I), is reported.

Two N,*O*-bidentate ligands and one pyridine molecule are attached to the zinc atom, resulting in a distorted ZnN_3O_2 trigonal bipyramidal co-ordination geometry (Fig. 1). The C1═O1 [1.287 (4) Å] and C8═N2 [1.290 (5) Å] bond lengths implies double bond character. The dihedral angle between the (C2—C7) and (C9—C14) planes is 29.0 (2)°. The geometrical parameters for (I) are normal.

Two molecules of pyridine complete the structure of (I) and the intermolecular C—H···O, and intramolecular C—H···O and O—H···N hydrogen bonding interactions help to establish the crystal packing..

Experimental

1 mmol of Zinc acetate was added to a solution of nisoldehyde-salicyloyl hydrazone (2 mmol) in 10 ml of CH_3OH/pyridine (*v*/*v* 10:1). The mixture was continuously stirred for 6 h at refluxing temperature, evaporating some solvent, then, upon cooling, the solid product was collected by filtration and dried *in vacuo* (yield 58%). Clear blocks of (I) were obtained by evaporation from a methanol solution after two week.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(C_{methyl},$O_{hydroxy}$).

Figures

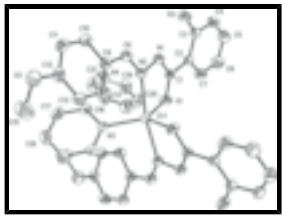


Fig. 1. The complex molecule in (I), with 50% probabiility ellipsoids.

Bis(4-methoxybenzaldehyde 2-hydroxybenzoylhydrazonato)pyridinezinc(II) pyridine solvate

Crystal data

$[Zn(C_{15}H_{13}N_2O_3)_2(C_5H_5N)]\cdot C_5H_5N$ F_{000} = 1584

M_r = 762.14	D_x = 1.387 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 1992 reflections
a = 15.447 (2) Å	θ = 2.4–23.0º
b = 10.0122 (17) Å	μ = 0.73 mm^{-1}
c = 23.598 (3) Å	*T* = 298 K
V = 3649.6 (9) Å^3	Laminar, colourless
Z = 4	0.43 × 0.32 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3183 independent reflections
Radiation source: fine-focus sealed tube	1794 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.068
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −18→16
T_{min} = 0.744, T_{max} = 0.874	*k* = −10→11
14274 measured reflections	*l* = −27→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H-atom parameters constrained
$wR(F^2)$ = 0.144	$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 2.7233P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
3183 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
241 parameters	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating –*R*-factor-obs *etc*. and is not relevant to the choice of reflections for re-

finement. *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}	Occ. (<1)
Zn1	0.00000	0.36156 (7)	0.25000	0.0450 (3)	
O1	0.01587 (16)	0.2491 (3)	0.18135 (13)	0.0527 (10)	
O2	0.26418 (18)	0.0842 (3)	0.15935 (14)	0.0655 (11)	
O3	0.2533 (2)	0.7767 (3)	0.43932 (15)	0.0750 (14)	
N1	0.1609 (2)	0.2463 (3)	0.20545 (15)	0.0461 (13)	
N2	0.14146 (19)	0.3425 (3)	0.24685 (15)	0.0411 (11)	
N3	0.00000	0.5678 (5)	0.25000	0.0460 (16)	
C1	0.0935 (2)	0.2040 (4)	0.17617 (18)	0.0393 (14)	
C2	0.1130 (2)	0.0966 (4)	0.13529 (18)	0.0403 (14)	
C3	0.1957 (3)	0.0397 (4)	0.13005 (19)	0.0443 (16)	
C4	0.2087 (3)	−0.0664 (5)	0.0931 (2)	0.0567 (17)	
C5	0.1428 (3)	−0.1155 (5)	0.0603 (2)	0.069 (2)	
C6	0.0614 (3)	−0.0602 (5)	0.0644 (2)	0.072 (2)	
C7	0.0471 (3)	0.0440 (5)	0.1016 (2)	0.0597 (18)	
C8	0.2098 (3)	0.3930 (4)	0.26981 (19)	0.0500 (16)	
C9	0.2142 (3)	0.4902 (4)	0.31474 (19)	0.0463 (16)	
C10	0.2943 (3)	0.5537 (4)	0.3236 (2)	0.0540 (17)	
C11	0.3043 (3)	0.6484 (5)	0.3644 (2)	0.0600 (19)	
C12	0.2361 (3)	0.6831 (4)	0.3983 (2)	0.0530 (17)	
C13	0.1564 (3)	0.6219 (5)	0.3912 (2)	0.0570 (17)	
C14	0.1464 (3)	0.5250 (5)	0.34936 (19)	0.0543 (16)	
C15	0.1843 (4)	0.8321 (6)	0.4695 (3)	0.097 (3)	
C16	0.0500 (3)	0.6355 (5)	0.2142 (2)	0.0570 (18)	
C17	0.0512 (3)	0.7726 (5)	0.2125 (2)	0.071 (2)	
C18	0.00000	0.8425 (7)	0.25000	0.082 (3)	
N4	0.0692 (4)	0.5482 (7)	0.0272 (3)	0.107 (3)	0.500
C19	0.0303 (4)	0.4354 (6)	0.0459 (3)	0.084 (3)	
C20	−0.0386 (4)	0.3879 (6)	0.0180 (3)	0.089 (3)	
C21	0.0692 (4)	0.5482 (7)	0.0272 (3)	0.107 (3)	0.500
H2	0.24920	0.14630	0.17980	0.0980*	
H4	0.26330	−0.10490	0.09050	0.0680*	
H5	0.15300	−0.18580	0.03540	0.0830*	
H6	0.01630	−0.09280	0.04220	0.0870*	
H7	−0.00820	0.08030	0.10420	0.0720*	
H8	0.26260	0.36300	0.25570	0.0600*	
H10	0.34140	0.53040	0.30120	0.0650*	
H11	0.35770	0.68980	0.36920	0.0720*	
H13	0.10990	0.64530	0.41420	0.0690*	
H14	0.09300	0.48330	0.34480	0.0650*	
H15A	0.14340	0.87010	0.44350	0.1460*	
H15B	0.20560	0.90060	0.49440	0.1460*	
H15C	0.15650	0.76380	0.49150	0.1460*	

H16	0.08540	0.58830	0.18950	0.0680*	
H17	0.08600	0.81740	0.18660	0.0850*	
H18	0.00000	0.93530	0.25000	0.0980*	
H19	0.05130	0.39130	0.07770	0.1000*	
H20	−0.06530	0.30980	0.03030	0.1070*	
H21	0.11750	0.58130	0.04610	0.1290*	0.500

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0366 (4)	0.0443 (4)	0.0541 (5)	0.0000	0.0067 (4)	0.0000
O1	0.0335 (15)	0.0647 (19)	0.060 (2)	0.0082 (14)	−0.0031 (14)	−0.0111 (16)
O2	0.0406 (17)	0.074 (2)	0.082 (2)	0.0109 (15)	−0.0115 (16)	−0.0238 (19)
O3	0.068 (2)	0.078 (2)	0.079 (3)	−0.0053 (19)	−0.0110 (19)	−0.025 (2)
N1	0.0343 (18)	0.048 (2)	0.056 (3)	0.0005 (16)	0.0005 (17)	−0.0103 (19)
N2	0.0333 (17)	0.0440 (19)	0.046 (2)	−0.0009 (14)	0.0023 (17)	−0.003 (2)
N3	0.030 (2)	0.048 (3)	0.060 (3)	0.0000	0.009 (3)	0.0000
C1	0.032 (2)	0.044 (2)	0.042 (3)	0.0010 (18)	−0.0018 (19)	0.006 (2)
C2	0.036 (2)	0.041 (2)	0.044 (3)	0.0001 (18)	−0.0008 (19)	0.000 (2)
C3	0.040 (2)	0.045 (3)	0.048 (3)	0.0008 (19)	−0.001 (2)	0.000 (2)
C4	0.051 (3)	0.055 (3)	0.064 (3)	0.009 (2)	0.005 (2)	−0.009 (3)
C5	0.071 (3)	0.063 (4)	0.073 (4)	−0.001 (3)	0.006 (3)	−0.025 (3)
C6	0.056 (3)	0.077 (4)	0.083 (4)	−0.005 (3)	−0.014 (3)	−0.028 (3)
C7	0.042 (2)	0.068 (3)	0.069 (4)	0.004 (2)	−0.005 (2)	−0.013 (3)
C8	0.040 (2)	0.052 (3)	0.058 (3)	0.001 (2)	0.002 (2)	−0.005 (2)
C9	0.041 (2)	0.049 (3)	0.049 (3)	−0.002 (2)	−0.002 (2)	−0.001 (2)
C10	0.043 (3)	0.058 (3)	0.061 (3)	−0.003 (2)	0.005 (2)	−0.004 (3)
C11	0.043 (3)	0.064 (3)	0.073 (4)	−0.011 (2)	−0.001 (2)	−0.011 (3)
C12	0.056 (3)	0.046 (3)	0.057 (3)	−0.003 (2)	−0.016 (2)	−0.004 (2)
C13	0.048 (3)	0.063 (3)	0.060 (3)	0.002 (2)	0.004 (2)	−0.006 (3)
C14	0.042 (2)	0.067 (3)	0.054 (3)	−0.007 (2)	−0.001 (2)	−0.008 (3)
C15	0.094 (4)	0.105 (5)	0.093 (5)	0.018 (4)	0.000 (4)	−0.042 (4)
C16	0.041 (2)	0.057 (3)	0.073 (4)	−0.001 (2)	0.013 (2)	0.004 (3)
C17	0.055 (3)	0.064 (4)	0.094 (5)	−0.013 (3)	0.000 (3)	0.026 (3)
C18	0.070 (5)	0.042 (4)	0.134 (8)	0.0000	−0.011 (6)	0.0000
N4	0.087 (4)	0.104 (5)	0.131 (6)	−0.011 (4)	−0.016 (4)	−0.002 (5)
C19	0.091 (4)	0.070 (4)	0.090 (5)	0.005 (3)	0.004 (4)	0.014 (4)
C20	0.084 (4)	0.068 (4)	0.115 (6)	−0.022 (3)	0.009 (4)	0.016 (4)
C21	0.087 (4)	0.104 (5)	0.131 (6)	−0.011 (4)	−0.016 (4)	−0.002 (5)

Geometric parameters (Å, °)

Zn1—O1	1.988 (3)	C9—C10	1.407 (6)
Zn1—N2	2.195 (3)	C10—C11	1.360 (7)
Zn1—N3	2.065 (5)	C11—C12	1.368 (7)
Zn1—O1^{i}	1.988 (3)	C12—C13	1.385 (7)
Zn1—N2^{i}	2.195 (3)	C13—C14	1.393 (7)
O1—C1	1.287 (4)	C16—C17	1.373 (7)

O2—C3	1.340 (5)	C17—C18	1.378 (6)
O3—C12	1.373 (5)	C4—H4	0.9300
O3—C15	1.397 (7)	C5—H5	0.9300
O2—H2	0.8200	C6—H6	0.9300
N1—C1	1.319 (5)	C7—H7	0.9300
N1—N2	1.404 (5)	C8—H8	0.9300
N2—C8	1.290 (5)	C10—H10	0.9300
N3—C16^{i}	1.330 (5)	C11—H11	0.9300
N3—C16	1.330 (5)	C13—H13	0.9300
N4—C19	1.353 (9)	C14—H14	0.9300
N4—C20^{ii}	1.331 (10)	C15—H15B	0.9600
N4—H21	0.9300	C15—H15C	0.9600
C1—C2	1.476 (6)	C15—H15A	0.9600
C2—C3	1.404 (6)	C16—H16	0.9300
C2—C7	1.395 (6)	C17—H17	0.9300
C3—C4	1.389 (6)	C18—H18	0.9300
C4—C5	1.370 (7)	C19—C20	1.339 (9)
C5—C6	1.377 (7)	C19—C21	1.353 (9)
C6—C7	1.381 (7)	C19—H19	0.9300
C8—C9	1.441 (6)	C20—H20	0.9300
C9—C14	1.373 (6)	C21—H21	0.9300
Zn1···C14	3.646 (5)	C13···H15C	2.7600
Zn1···C14^{i}	3.646 (5)	C13···H15A	2.7800
Zn1···H14	2.9200	C15···H13	2.5500
Zn1···H14^{i}	2.9200	C16···H14^{i}	3.0200
O1···N1	2.312 (4)	C19···H15C^{ix}	3.0700
O1···N2	2.651 (4)	C20···H5^{x}	2.9700
O1···N2^{i}	3.107 (4)	C21···H5^{xi}	2.9700
O2···C16^{iii}	3.190 (6)	H2···N1	1.8000
O2···N1	2.522 (4)	H2···C1	2.4700
O2···C8^{iii}	3.259 (5)	H5···C21^{viii}	2.9700
O1···H7	2.5100	H5···H21^{viii}	2.4100
O1···H19	2.8800	H5···H20^{x}	2.4000
O1···H11^{iv}	2.7800	H5···C20^{x}	2.9700
O2···H16^{iii}	2.4300	H5···O3^{xii}	2.8400
O3···H5^{v}	2.8400	H6···H15A^{xiii}	2.5200
O3···H20^{vi}	2.9100	H7···C11^{iv}	3.0700
N1···O1	2.312 (4)	H7···O1	2.5100
N1···O2	2.522 (4)	H7···H11^{iv}	2.4300
N2···O1^{i}	3.107 (4)	H8···H10	2.3300
N2···O1	2.651 (4)	H10···H8	2.3300
N2···N3	3.142 (5)	H11···O1^{vi}	2.7800
N2···C1	2.292 (5)	H11···H7^{vi}	2.4300
N2···C16	3.346 (6)	H13···H15A	2.4100
N3···C14^{i}	3.286 (5)	H13···C15	2.5500

N3···C14	3.286 (5)	H13···H15C	2.2900
N3···N2	3.142 (5)	H14···Zn1	2.9200
N3···N2^{i}	3.142 (5)	H14···N2	2.8100
N1···H2	1.8000	H14···C16^{i}	3.0200
N2···H16	2.9400	H14···N3	2.7900
N2···H14	2.8100	H15A···H6^{xiv}	2.5200
N3···H14	2.7900	H15A···H13	2.4100
N3···H14^{i}	2.7900	H15A···C13	2.7800
C8···O2^{vii}	3.259 (5)	H15B···C4^{xv}	2.8600
C8···C11^{iii}	3.321 (6)	H15B···C5^{xv}	2.8300
C11···C8^{vii}	3.321 (6)	H15C···C13	2.7600
C14···N3	3.286 (5)	H15C···H13	2.2900
C14···C16^{i}	3.561 (7)	H15C···C19^{xv}	3.0700
C14···Zn1	3.646 (5)	H16···O2^{vii}	2.4300
C16···C14^{i}	3.561 (7)	H16···N2	2.9400
C16···O2^{vii}	3.190 (6)	H17···C2^{xi}	3.0700
C1···H19	3.0600	H17···C3^{xi}	3.1000
C1···H2	2.4700	H17···C7^{xi}	3.0900
C2···H17^{viii}	3.0700	H19···O1	2.8800
C3···H17^{viii}	3.1000	H19···C1	3.0600
C4···H15B^{ix}	2.8600	H20···H5^{x}	2.4000
C5···H21^{viii}	3.0800	H20···O3^{iv}	2.9100
C5···H15B^{ix}	2.8300	H21···C5^{xi}	3.0800
C7···H17^{viii}	3.0900	H21···H5^{xi}	2.4100
C11···H7^{vi}	3.0700		
O1—Zn1—N2	78.49 (11)	C9—C14—C13	120.9 (4)
O1—Zn1—N3	124.50 (9)	N3—C16—C17	122.4 (4)
O1—Zn1—O1^{i}	111.01 (13)	C16—C17—C18	118.8 (5)
O1—Zn1—N2^{i}	95.80 (11)	C17—C18—C17^{i}	119.0 (6)
N2—Zn1—N3	94.99 (8)	C5—C4—H4	119.00
O1^{i}—Zn1—N2	95.80 (11)	C3—C4—H4	119.00
N2—Zn1—N2^{i}	170.02 (12)	C6—C5—H5	120.00
O1^{i}—Zn1—N3	124.50 (9)	C4—C5—H5	120.00
N2^{i}—Zn1—N3	94.99 (8)	C7—C6—H6	120.00
O1^{i}—Zn1—N2^{i}	78.49 (11)	C5—C6—H6	120.00
Zn1—O1—C1	113.0 (3)	C6—C7—H7	119.00
C12—O3—C15	118.9 (4)	C2—C7—H7	119.00
C3—O2—H2	109.00	C9—C8—H8	116.00
N2—N1—C1	114.6 (3)	N2—C8—H8	116.00
Zn1—N2—N1	107.2 (2)	C9—C10—H10	119.00
Zn1—N2—C8	140.1 (3)	C11—C10—H10	119.00
N1—N2—C8	112.7 (3)	C10—C11—H11	120.00
Zn1—N3—C16^{i}	120.6 (3)	C12—C11—H11	120.00

C16—N3—C16^{i}	118.7 (5)	C14—C13—H13	120.00
Zn1—N3—C16	120.6 (3)	C12—C13—H13	120.00
C19—N4—C20^{ii}	120.3 (6)	C13—C14—H14	120.00
C20^{ii}—N4—H21	120.00	C9—C14—H14	120.00
C19—N4—H21	120.00	O3—C15—H15B	110.00
O1—C1—N1	125.0 (4)	O3—C15—H15A	110.00
N1—C1—C2	114.5 (3)	H15A—C15—H15C	109.00
O1—C1—C2	120.5 (3)	H15B—C15—H15C	109.00
C1—C2—C7	119.9 (3)	O3—C15—H15C	110.00
C1—C2—C3	122.6 (3)	H15A—C15—H15B	109.00
C3—C2—C7	117.4 (4)	N3—C16—H16	119.00
O2—C3—C4	117.7 (4)	C17—C16—H16	119.00
C2—C3—C4	119.8 (4)	C16—C17—H17	121.00
O2—C3—C2	122.5 (4)	C18—C17—H17	121.00
C3—C4—C5	121.5 (4)	C17—C18—H18	121.00
C4—C5—C6	119.6 (5)	C17^{i}—C18—H18	121.00
C5—C6—C7	119.6 (4)	N4—C19—C20	119.3 (6)
C2—C7—C6	122.1 (4)	C20—C19—C21	119.3 (6)
N2—C8—C9	127.8 (4)	N4^{ii}—C20—C19	120.4 (6)
C10—C9—C14	117.9 (4)	C19—C21—C20^{ii}	120.3 (6)
C8—C9—C14	125.0 (4)	N4—C19—H19	120.00
C8—C9—C10	117.1 (4)	C20—C19—H19	120.00
C9—C10—C11	121.3 (4)	C21—C19—H19	120.00
C10—C11—C12	120.2 (4)	C19—C20—H20	120.00
O3—C12—C11	115.9 (4)	N4^{ii}—C20—H20	120.00
O3—C12—C13	124.0 (4)	C19—C21—H21	120.00
C11—C12—C13	120.1 (4)	C20^{ii}—C21—H21	120.00
C12—C13—C14	119.5 (4)		
N2—Zn1—O1—C1	11.7 (3)	O1—C1—C2—C7	0.5 (6)
N3—Zn1—O1—C1	99.8 (3)	N1—C1—C2—C3	3.0 (6)
O1^{i}—Zn1—O1—C1	−80.2 (3)	O1—C1—C2—C3	−176.8 (4)
N2^{i}—Zn1—O1—C1	−160.1 (3)	C1—C2—C3—C4	176.3 (4)
O1—Zn1—N2—N1	−9.7 (2)	C7—C2—C3—O2	178.5 (4)
O1—Zn1—N2—C8	168.4 (5)	C1—C2—C3—O2	−4.1 (6)
N3—Zn1—N2—N1	−133.9 (2)	C1—C2—C7—C6	−177.3 (4)
N3—Zn1—N2—C8	44.2 (4)	C3—C2—C7—C6	0.2 (7)
O1^{i}—Zn1—N2—N1	100.6 (2)	C7—C2—C3—C4	−1.2 (6)
O1^{i}—Zn1—N2—C8	−81.3 (5)	C2—C3—C4—C5	1.6 (7)
O1—Zn1—N3—C16	−33.8 (2)	O2—C3—C4—C5	−178.1 (4)
O1—Zn1—N3—C16^{i}	146.2 (2)	C3—C4—C5—C6	−0.9 (7)
N2—Zn1—N3—C16	45.6 (3)	C4—C5—C6—C7	−0.1 (7)
N2—Zn1—N3—C16^{i}	−134.4 (3)	C5—C6—C7—C2	0.5 (7)
O1^{i}—Zn1—N3—C16	146.2 (2)	N2—C8—C9—C14	14.9 (7)
N2^{i}—Zn1—N3—C16	−134.4 (3)	N2—C8—C9—C10	−165.2 (4)
Zn1—O1—C1—N1	−13.0 (5)	C10—C9—C14—C13	1.2 (7)

Zn1—O1—C1—C2	166.8 (3)	C8—C9—C14—C13	−178.9 (4)
C15—O3—C12—C11	170.1 (5)	C8—C9—C10—C11	178.9 (4)
C15—O3—C12—C13	−11.8 (7)	C14—C9—C10—C11	−1.2 (7)
C1—N1—N2—Zn1	6.5 (4)	C9—C10—C11—C12	0.6 (7)
N2—N1—C1—C2	−176.2 (3)	C10—C11—C12—C13	0.0 (7)
N2—N1—C1—O1	3.6 (6)	C10—C11—C12—O3	178.1 (4)
C1—N1—N2—C8	−172.2 (4)	C11—C12—C13—C14	0.0 (7)
Zn1—N2—C8—C9	4.2 (8)	O3—C12—C13—C14	−178.0 (4)
N1—N2—C8—C9	−177.7 (4)	C12—C13—C14—C9	−0.6 (7)
C16^{i}—N3—C16—C17	−0.7 (6)	N3—C16—C17—C18	1.3 (7)
Zn1—N3—C16—C17	179.3 (3)	C16—C17—C18—C17^{i}	−0.6 (5)
C19—N4—C20^{ii}—C19^{ii}	−0.9 (10)	N4—C19—C20—N4^{ii}	−0.9 (10)
C20^{ii}—N4—C19—C20	0.9 (10)	C21—C19—C20—N4^{ii}	−0.9 (10)
N1—C1—C2—C7	−179.7 (4)	C20—C19—C21—C20^{ii}	0.9 (10)

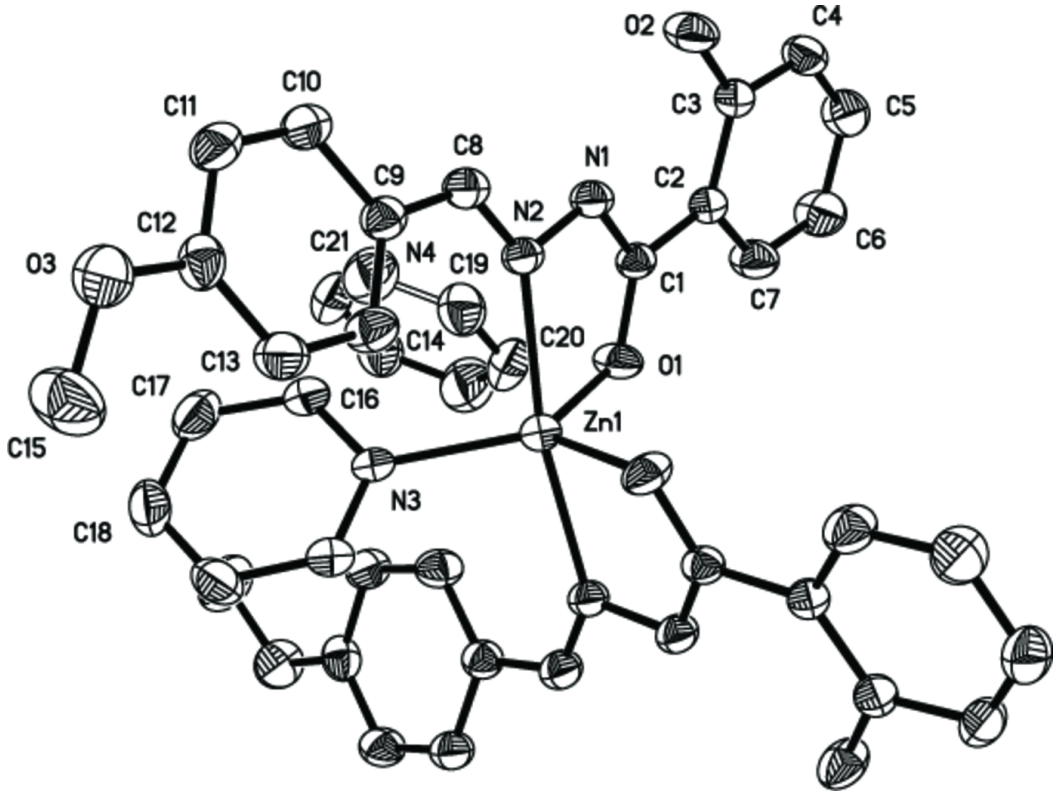
Symmetry codes: (i) −*x*, *y*, −*z*+1/2; (ii) −*x*, −*y*+1, −*z*; (iii) −*x*+1/2, *y*−1/2, *z*; (iv) *x*−1/2, *y*−1/2, −*z*+1/2; (v) −*x*+1/2, −*y*+1/2, *z*+1/2; (vi) *x*+1/2, *y*+1/2, −*z*+1/2; (vii) −*x*+1/2, *y*+1/2, *z*; (viii) *x*, *y*−1, *z*; (ix) *x*, −*y*+1, *z*−1/2; (x) −*x*, −*y*, −*z*; (xi) *x*, *y*+1, *z*; (xii) −*x*+1/2, −*y*+1/2, *z*−1/2; (xiii) −*x*, *y*−1, −*z*+1/2; (xiv) −*x*, *y*+1, −*z*+1/2; (xv) *x*, −*y*+1, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1	0.82	1.80	2.522 (4)	147
C7—H7···O1	0.93	2.51	2.827 (6)	100
C16—H16···O2^{vii}	0.93	2.43	3.190 (6)	139

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

Fig. 1


O2
C4
C10
C11
C3
C5
C8
N1
C9
C2
N2
C12
C21
N4
C19
C6
O3
C1
C7
C14
C20
C13
O1
C17
C16
Zn1
C15
N3
C18