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Bis[2-(2-hydroxyethyliminomethyl)-6-methoxyphenolato-κ^2N,O^1]zinc(II)

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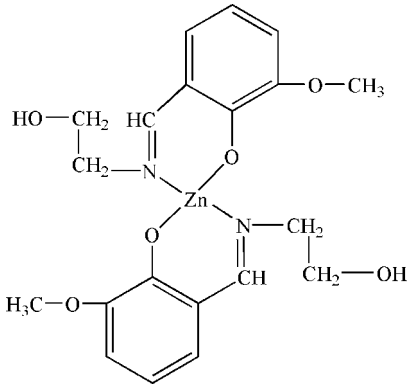
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; disorder in main residue; R factor = 0.078; wR factor = 0.170; data-to-parameter ratio = 14.7.

In the title complex, $[Zn(C_{10}H_{12}NO_3)_2]$, the Zn^{II} ion is coordinated by two N,O-bidentate ligands in a distorted tetrahedral geometry. The crystal packing is stabilized by intermolecular O—H···O hydrogen bonds and C—H···*Cg* interactions (*Cg* is an aromatic ring centroid). The hydroxy substituent of one ethanolamine group is disordered over two sites with the ratio of refined occupancies being 0.844 (4): 0.156 (4).

Related literature

The bond lengths and angles in the title structure are similar to those in related structures (Hökelek *et al.*, 2000; Tatar *et al.*, 1999; Dong, *et al.*, 2007).



Experimental

Crystal data

$[Zn(C_{10}H_{12}NO_3)_2]$
M_r = 453.78
Orthorhombic, *Pbca*
a = 17.624 (2) Å
b = 7.2013 (14) Å
c = 34.853 (3) Å
V = 4423.3 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 298 (2) K
0.59 × 0.26 × 0.24 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.551, T_{max} = 0.770
20138 measured reflections
3904 independent reflections
2485 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.170
S = 1.08
3904 reflections
266 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O4	1.913 (4)	Zn1—N1	1.985 (5)
Zn1—O1	1.921 (4)	Zn1—N2	1.990 (6)
O4—Zn1—O1	124.7 (2)	O4—Zn1—N2	95.3 (2)
O4—Zn1—N1	110.8 (2)	O1—Zn1—N2	108.1 (2)
O1—Zn1—N1	97.2 (2)	N1—Zn1—N2	123.1 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1^{i}	0.82	2.07	2.799 (7)	148
O3—H3···O2^{i}	0.82	2.28	2.954 (8)	139
C—H···*Cg*		2.962		

Symmetry code: (i) $x, y-1, z$.

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: LH2415).

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supplementary materials

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Bis[2-(2-hydroxyethyliminomethyl)-6-methoxyphenolato-κ^2N,O^1]zinc(II)

J.-F. Dong, L.-Z. Li, W.-J. Yu, H. Cui and D.-Q. Wang

Comment

As part of our ongoing studies of Schiff bases, we reported here the synthesis and crystal structure of the title compound (Fig. 1), a new zinc(II) complex with a bidentate Schiff base ligand derived from the condensation of *o*-vanillin and ethanolamine.

The coordination around zinc is a distored tetrahedral involving two O and N atoms of the ligands. These bond lengths and angles values are similar to the reported values for related structures (Hokelek *et al.*, 2000, Tatar *et al.*, 1999, Dong *et al.*, 2007).

In the crystal structure, the intermolecular hydrogen bonds of O3—H3···O1^{i} and O3—H3···O2^{i}(symmetry code: (i) *x*, *y* − 1, *Z*) (Fig. 2) and the relatively short intermolecular distances H18*a*···*Cg*^{ii} of 2.962Å (symmetry code: 0.5 − *x*, 1/2 + *y*, *Z*; *Cg* is the centroid of the C12—17 ring) indicating the prescence of weak C—H···π interaction, stabilize the crystal packing along with van der Waals forces.

Experimental

Ethanolamine(1 mmol, 0.059 ml) was dissolved in hot methanol (10 ml) and added in portions to a methanol solution(3 ml) of *o*-vanillin (1 mmol, 152.14 mg). 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, where upon yellow blocks were obtained.

Refinement

Difference Fourier maps revealed that the hydroxy substituent of one ethanolamine group is disordered over two sites. The subsequent refinement of their occupancies gave the values of 0.844 (4) and 0.156 (4), respectively. All the H atoms were placed in geometrically calculated positions (C—H = 0.93 − 0.97Å and O—H = 0.82 Å) and allowed to ride on their respective parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

In the crystal structure, there are solvent accesible voids of 121.0 Å^3. These voids may initially have contained solvent, but this has been lost without degradation of the structure. There is no significant residual electron density to suggest the presence of solvent of crystallization.

Figures

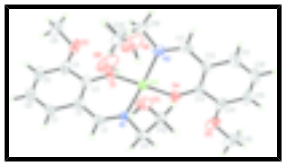

Fig. 1. The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Open bonds indicate the minor component of disorder.

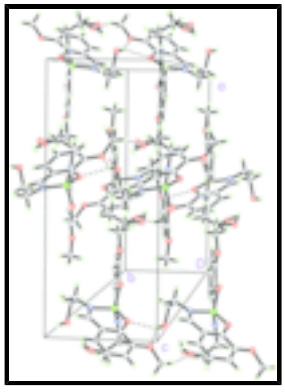

Fig. 2. The packing of the title compound. Hydrogen bond are shown as dashed lines.

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Crystal data

$[Zn(C_{10}H_{12}NO_3)_2]$	F_{000} = 1888
M_r = 453.78	D_x = 1.363 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3930 reflections
a = 17.624 (2) Å	θ = 2.3–23.2º
b = 7.2013 (14) Å	μ = 1.15 mm^{-1}
c = 34.853 (3) Å	*T* = 298 (2) K
V = 4423.3 (11) Å^3	Block, yellow
Z = 8	0.59 × 0.26 × 0.24 mm

Data collection

Bruker SMART CCD diffractometer	3904 independent reflections
Radiation source: fine-focus sealed tube	2485 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.059
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −15→20
T_{min} = 0.551, T_{max} = 0.770	*k* = −8→6
20138 measured reflections	*l* = −40→41

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.078$	H-atom parameters constrained
$wR(F^2) = 0.170$	$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 21.0111P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.002$
3904 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
266 parameters	$\Delta\rho_{min} = -1.04$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
Zn1	0.50272 (4)	0.33878 (10)	0.12373 (2)	0.0460 (3)	
N1	0.4934 (3)	0.1249 (6)	0.15934 (15)	0.0429 (13)	
N2	0.5700 (3)	0.3369 (8)	0.07788 (17)	0.0514 (14)	
O1	0.5436 (3)	0.5126 (6)	0.16004 (13)	0.0561 (13)	
O2	0.6315 (3)	0.7510 (7)	0.19242 (18)	0.0809 (19)	
O3	0.5677 (3)	−0.1683 (7)	0.11585 (15)	0.0645 (14)	
H3	0.5721	−0.2384	0.1343	0.097*	
O4	0.4108 (2)	0.3744 (6)	0.09550 (13)	0.0514 (12)	
O5	0.2730 (3)	0.3516 (8)	0.07015 (18)	0.0788 (17)	
O6	0.6846 (4)	0.0466 (11)	0.0930 (3)	0.112 (3)	0.844 (10)
H6	0.6437	−0.0027	0.0977	0.168*	0.844 (10)
O6'	0.658 (2)	0.109 (5)	0.1366 (9)	0.112 (3)	0.156 (10)
H6'	0.6377	0.0179	0.1272	0.168*	0.156 (10)
C1	0.5196 (3)	0.1339 (10)	0.1936 (2)	0.0490 (18)	
H1	0.5110	0.0311	0.2091	0.059*	
C2	0.5610 (4)	0.2867 (10)	0.21073 (19)	0.0481 (17)	
C3	0.5730 (4)	0.4594 (10)	0.1931 (2)	0.0490 (17)	

C4	0.6204 (4)	0.5901 (11)	0.2130 (2)	0.057 (2)	
C5	0.6516 (4)	0.5473 (14)	0.2473 (2)	0.069 (2)	
H5	0.6826	0.6340	0.2594	0.083*	
C6	0.6389 (5)	0.3790 (15)	0.2649 (2)	0.070 (2)	
H6A	0.6611	0.3525	0.2885	0.084*	
C7	0.5936 (4)	0.2518 (12)	0.2473 (2)	0.058 (2)	
H7A	0.5836	0.1396	0.2595	0.070*	
C8	0.6948 (5)	0.8650 (12)	0.2030 (3)	0.090 (3)	
H8A	0.6881	0.9091	0.2287	0.135*	
H8B	0.6981	0.9689	0.1858	0.135*	
H8C	0.7407	0.7934	0.2015	0.135*	
C9	0.4568 (4)	−0.0470 (9)	0.14736 (19)	0.0507 (18)	
H9A	0.4031	−0.0245	0.1432	0.061*	
H9B	0.4617	−0.1390	0.1675	0.061*	
C10	0.4916 (4)	−0.1202 (8)	0.11123 (18)	0.0482 (18)	
H10A	0.4635	−0.2287	0.1029	0.058*	
H10B	0.4875	−0.0267	0.0913	0.058*	
C11	0.5428 (4)	0.3142 (10)	0.0441 (2)	0.0559 (19)	
H11	0.5779	0.3098	0.0241	0.067*	
C12	0.4643 (4)	0.2946 (9)	0.03341 (18)	0.0465 (17)	
C13	0.4036 (4)	0.3298 (8)	0.05885 (19)	0.0421 (15)	
C14	0.3285 (4)	0.3176 (10)	0.0440 (2)	0.0535 (19)	
C15	0.3167 (6)	0.2739 (12)	0.0058 (3)	0.077 (3)	
H15	0.2674	0.2674	−0.0036	0.093*	
C16	0.3767 (6)	0.2399 (13)	−0.0186 (2)	0.082 (3)	
H16	0.3677	0.2088	−0.0441	0.099*	
C17	0.4493 (5)	0.2520 (12)	−0.0053 (2)	0.074 (2)	
H17	0.4895	0.2317	−0.0220	0.088*	
C18	0.1962 (4)	0.3283 (14)	0.0591 (3)	0.107 (4)	
H18A	0.1813	0.4291	0.0427	0.160*	
H18B	0.1647	0.3269	0.0815	0.160*	
H18C	0.1907	0.2130	0.0455	0.160*	
C19	0.6518 (3)	0.3659 (11)	0.0824 (2)	0.068 (2)	
H19A	0.6609	0.4877	0.0933	0.081*	
H19B	0.6761	0.3613	0.0574	0.081*	
C20	0.6857 (5)	0.2195 (11)	0.1080 (3)	0.091 (3)	
H20A	0.7378	0.2531	0.1137	0.109*	0.844 (10)
H20B	0.6580	0.2184	0.1321	0.109*	0.844 (10)
H20C	0.7024	0.1211	0.0910	0.109*	0.156 (10)
H20D	0.7317	0.2751	0.1181	0.109*	0.156 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0508 (4)	0.0403 (4)	0.0471 (4)	−0.0061 (4)	−0.0087 (4)	0.0018 (4)
N1	0.045 (3)	0.031 (3)	0.053 (3)	−0.009 (3)	0.007 (3)	0.000 (2)
N2	0.041 (3)	0.053 (4)	0.060 (4)	−0.009 (3)	0.003 (3)	0.011 (3)
O1	0.071 (3)	0.034 (3)	0.063 (3)	0.000 (2)	−0.025 (3)	−0.002 (2)

O2	0.083 (4)	0.048 (3)	0.112 (5)	−0.007 (3)	−0.060 (4)	−0.005 (3)
O3	0.062 (3)	0.052 (3)	0.079 (4)	−0.002 (3)	0.010 (3)	0.002 (3)
O4	0.043 (3)	0.059 (3)	0.052 (3)	0.002 (2)	−0.001 (2)	−0.006 (2)
O5	0.038 (3)	0.085 (4)	0.113 (5)	−0.004 (3)	−0.009 (3)	−0.003 (4)
O6	0.056 (4)	0.081 (6)	0.200 (10)	0.003 (4)	0.010 (5)	−0.025 (6)
O6'	0.056 (4)	0.081 (6)	0.200 (10)	0.003 (4)	0.010 (5)	−0.025 (6)
C1	0.043 (4)	0.049 (4)	0.056 (4)	0.005 (3)	0.010 (3)	0.007 (4)
C2	0.041 (4)	0.058 (5)	0.046 (4)	0.005 (3)	0.006 (3)	0.001 (4)
C3	0.047 (4)	0.050 (4)	0.050 (4)	0.013 (3)	−0.009 (3)	−0.014 (4)
C4	0.049 (4)	0.067 (5)	0.055 (5)	0.015 (4)	−0.013 (4)	−0.022 (4)
C5	0.050 (5)	0.100 (7)	0.056 (5)	0.015 (5)	−0.014 (4)	−0.037 (5)
C6	0.057 (5)	0.108 (8)	0.045 (4)	0.014 (5)	−0.002 (4)	−0.013 (5)
C7	0.055 (4)	0.081 (6)	0.038 (4)	0.009 (4)	0.009 (4)	0.007 (4)
C8	0.077 (6)	0.054 (5)	0.139 (9)	−0.013 (5)	−0.042 (6)	−0.015 (6)
C9	0.051 (4)	0.036 (4)	0.065 (5)	−0.010 (3)	0.006 (4)	0.001 (4)
C10	0.073 (5)	0.026 (3)	0.046 (4)	−0.009 (3)	−0.009 (4)	−0.008 (3)
C11	0.055 (5)	0.057 (5)	0.056 (5)	0.007 (4)	0.018 (4)	0.009 (4)
C12	0.059 (4)	0.044 (4)	0.037 (4)	−0.003 (3)	0.001 (3)	0.002 (3)
C13	0.049 (4)	0.029 (3)	0.049 (4)	−0.007 (3)	−0.008 (3)	−0.001 (3)
C14	0.051 (4)	0.038 (4)	0.072 (5)	−0.004 (4)	−0.020 (4)	0.003 (4)
C15	0.090 (7)	0.069 (6)	0.073 (6)	−0.011 (5)	−0.044 (5)	0.000 (5)
C16	0.119 (8)	0.084 (7)	0.044 (5)	−0.015 (6)	−0.025 (5)	−0.009 (5)
C17	0.090 (6)	0.085 (7)	0.046 (5)	−0.007 (5)	0.004 (5)	−0.002 (4)
C18	0.040 (5)	0.090 (7)	0.189 (11)	−0.007 (5)	−0.026 (6)	0.020 (8)
C19	0.042 (4)	0.063 (5)	0.098 (6)	−0.007 (4)	0.009 (4)	0.018 (5)
C20	0.044 (5)	0.070 (6)	0.157 (10)	0.006 (4)	−0.031 (6)	−0.003 (7)

Geometric parameters (Å, °)

Zn1—O4	1.913 (4)	C7—H7A	0.9300
Zn1—O1	1.921 (4)	C8—H8A	0.9600
Zn1—N1	1.985 (5)	C8—H8B	0.9600
Zn1—N2	1.990 (6)	C8—H8C	0.9600
N1—C1	1.281 (8)	C9—C10	1.497 (8)
N1—C9	1.458 (7)	C9—H9A	0.9700
N2—C11	1.283 (9)	C9—H9B	0.9700
N2—C19	1.465 (7)	C10—H10A	0.9700
O1—C3	1.319 (8)	C10—H10B	0.9700
O2—C4	1.378 (9)	C11—C12	1.440 (10)
O2—C8	1.433 (8)	C11—H11	0.9300
O3—C10	1.394 (7)	C12—C17	1.408 (10)
O3—H3	0.8200	C12—C13	1.412 (9)
O4—C13	1.323 (7)	C13—C14	1.425 (9)
O5—C14	1.358 (9)	C14—C15	1.383 (11)
O5—C18	1.417 (8)	C15—C16	1.379 (12)
O6—C20	1.352 (8)	C15—H15	0.9300
O6—H6	0.8200	C16—C17	1.362 (12)
O6—H20C	0.6256	C16—H16	0.9300
O6'—C20	1.361 (11)	C17—H17	0.9300

O6'—H6'	0.8200	C18—H18A	0.9600
C1—C2	1.450 (10)	C18—H18B	0.9600
C1—H1	0.9300	C18—H18C	0.9600
C2—C3	1.404 (10)	C19—C20	1.506 (9)
C2—C7	1.421 (9)	C19—H19A	0.9700
C3—C4	1.437 (9)	C19—H19B	0.9700
C4—C5	1.351 (10)	C20—H20A	0.9700
C5—C6	1.376 (11)	C20—H20B	0.9700
C5—H5	0.9300	C20—H20C	0.9700
C6—C7	1.362 (11)	C20—H20D	0.9700
C6—H6A	0.9300		
O4—Zn1—O1	124.7 (2)	C9—C10—H10A	109.1
O4—Zn1—N1	110.8 (2)	O3—C10—H10B	109.1
O1—Zn1—N1	97.2 (2)	C9—C10—H10B	109.1
O4—Zn1—N2	95.3 (2)	H10A—C10—H10B	107.8
O1—Zn1—N2	108.1 (2)	N2—C11—C12	127.4 (6)
N1—Zn1—N2	123.1 (2)	N2—C11—H11	116.3
C1—N1—C9	118.0 (6)	C12—C11—H11	116.3
C1—N1—Zn1	120.9 (4)	C17—C12—C13	119.9 (7)
C9—N1—Zn1	121.1 (4)	C17—C12—C11	116.7 (7)
C11—N2—C19	118.9 (6)	C13—C12—C11	123.3 (6)
C11—N2—Zn1	121.1 (5)	O4—C13—C12	125.3 (6)
C19—N2—Zn1	120.0 (5)	O4—C13—C14	117.0 (6)
C3—O1—Zn1	122.2 (4)	C12—C13—C14	117.7 (6)
C4—O2—C8	117.4 (6)	O5—C14—C15	125.3 (7)
C10—O3—H3	109.5	O5—C14—C13	114.5 (6)
C13—O4—Zn1	123.0 (4)	C15—C14—C13	120.2 (8)
C14—O5—C18	118.9 (7)	C16—C15—C14	121.3 (8)
C20—O6—H6	109.5	C16—C15—H15	119.4
H6—O6—H20C	146.5	C14—C15—H15	119.4
C20—O6'—H6'	109.5	C17—C16—C15	119.9 (8)
N1—C1—C2	127.2 (6)	C17—C16—H16	120.1
N1—C1—H1	116.4	C15—C16—H16	120.1
C2—C1—H1	116.4	C16—C17—C12	121.1 (8)
C3—C2—C7	119.3 (7)	C16—C17—H17	119.4
C3—C2—C1	124.6 (6)	C12—C17—H17	119.4
C7—C2—C1	116.1 (7)	O5—C18—H18A	109.5
O1—C3—C2	125.5 (6)	O5—C18—H18B	109.5
O1—C3—C4	117.4 (7)	H18A—C18—H18B	109.5
C2—C3—C4	117.1 (7)	O5—C18—H18C	109.5
C5—C4—O2	126.5 (8)	H18A—C18—H18C	109.5
C5—C4—C3	121.0 (8)	H18B—C18—H18C	109.5
O2—C4—C3	112.4 (6)	N2—C19—C20	110.7 (6)
C4—C5—C6	121.9 (8)	N2—C19—H19A	109.5
C4—C5—H5	119.1	C20—C19—H19A	109.5
C6—C5—H5	119.1	N2—C19—H19B	109.5
C7—C6—C5	119.2 (8)	C20—C19—H19B	109.5
C7—C6—H6A	120.4	H19A—C19—H19B	108.1
C5—C6—H6A	120.4	O6—C20—O6'	75.0 (19)

C6—C7—C2	121.5 (8)	O6—C20—C19	114.2 (9)
C6—C7—H7A	119.3	O6'—C20—C19	134.6 (18)
C2—C7—H7A	119.3	O6—C20—H20A	108.7
O2—C8—H8A	109.5	O6'—C20—H20A	109.4
O2—C8—H8B	109.5	C19—C20—H20A	108.7
H8A—C8—H8B	109.5	O6—C20—H20B	108.7
O2—C8—H8C	109.5	C19—C20—H20B	108.7
H8A—C8—H8C	109.5	H20A—C20—H20B	107.6
H8B—C8—H8C	109.5	O6'—C20—H20C	97.4
N1—C9—C10	111.0 (5)	C19—C20—H20C	105.6
N1—C9—H9A	109.4	H20A—C20—H20C	91.0
C10—C9—H9A	109.4	H20B—C20—H20C	132.5
N1—C9—H9B	109.4	O6—C20—H20D	122.1
C10—C9—H9B	109.4	O6'—C20—H20D	105.8
H9A—C9—H9B	108.0	C19—C20—H20D	104.9
O3—C10—C9	112.7 (5)	H20B—C20—H20D	96.3
O3—C10—H10A	109.1	H20C—C20—H20D	105.5
O4—Zn1—N1—C1	−137.9 (5)	C3—C4—C5—C6	−0.9 (11)
O1—Zn1—N1—C1	−6.4 (5)	C4—C5—C6—C7	0.0 (12)
N2—Zn1—N1—C1	110.7 (5)	C5—C6—C7—C2	2.0 (11)
O4—Zn1—N1—C9	42.2 (5)	C3—C2—C7—C6	−3.0 (10)
O1—Zn1—N1—C9	173.7 (5)	C1—C2—C7—C6	174.5 (6)
N2—Zn1—N1—C9	−69.3 (5)	C1—N1—C9—C10	−126.1 (6)
O4—Zn1—N2—C11	−16.0 (6)	Zn1—N1—C9—C10	53.9 (7)
O1—Zn1—N2—C11	−145.2 (6)	N1—C9—C10—O3	63.3 (7)
N1—Zn1—N2—C11	103.1 (6)	C19—N2—C11—C12	−176.1 (7)
O4—Zn1—N2—C19	162.6 (5)	Zn1—N2—C11—C12	2.5 (11)
O1—Zn1—N2—C19	33.4 (6)	N2—C11—C12—C17	−173.6 (8)
N1—Zn1—N2—C19	−78.3 (6)	N2—C11—C12—C13	11.3 (12)
O4—Zn1—O1—C3	138.0 (5)	Zn1—O4—C13—C12	−16.3 (9)
N1—Zn1—O1—C3	16.4 (5)	Zn1—O4—C13—C14	164.1 (4)
N2—Zn1—O1—C3	−111.9 (5)	C17—C12—C13—O4	−178.7 (7)
O1—Zn1—O4—C13	139.0 (5)	C11—C12—C13—O4	−3.8 (11)
N1—Zn1—O4—C13	−105.8 (5)	C17—C12—C13—C14	0.9 (10)
N2—Zn1—O4—C13	22.6 (5)	C11—C12—C13—C14	175.8 (7)
C9—N1—C1—C2	176.8 (6)	C18—O5—C14—C15	5.0 (12)
Zn1—N1—C1—C2	−3.1 (9)	C18—O5—C14—C13	−174.9 (7)
N1—C1—C2—C3	6.4 (11)	O4—C13—C14—O5	−0.9 (9)
N1—C1—C2—C7	−171.1 (6)	C12—C13—C14—O5	179.5 (6)
Zn1—O1—C3—C2	−18.0 (9)	O4—C13—C14—C15	179.2 (7)
Zn1—O1—C3—C4	163.0 (5)	C12—C13—C14—C15	−0.5 (10)
C7—C2—C3—O1	−177.0 (6)	O5—C14—C15—C16	−179.4 (8)
C1—C2—C3—O1	5.6 (11)	C13—C14—C15—C16	0.5 (12)
C7—C2—C3—C4	2.0 (9)	C14—C15—C16—C17	−1.0 (14)
C1—C2—C3—C4	−175.3 (6)	C15—C16—C17—C12	1.5 (14)
C8—O2—C4—C5	15.9 (11)	C13—C12—C17—C16	−1.4 (12)
C8—O2—C4—C3	−161.0 (7)	C11—C12—C17—C16	−176.7 (8)
O1—C3—C4—C5	179.0 (6)	C11—N2—C19—C20	−122.0 (8)
C2—C3—C4—C5	−0.1 (10)	Zn1—N2—C19—C20	59.4 (9)

O1—C3—C4—O2	−4.0 (9)	N2—C19—C20—O6	67.2 (11)
C2—C3—C4—O2	176.9 (6)	N2—C19—C20—O6'	−25 (3)
O2—C4—C5—C6	−177.5 (7)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1^{i}	0.82	2.07	2.799 (7)	148
O3—H3···O2^{i}	0.82	2.28	2.954 (8)	139

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1

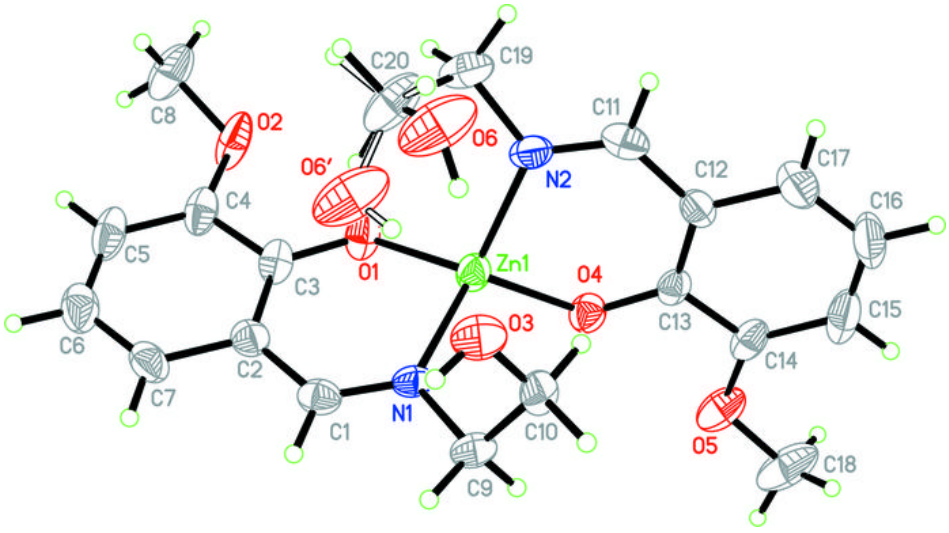
C20
C19
C8
O2
O6
C11
O6'
N2
C12
C17
C4
C16
C5
O1
Zn1
O4
C3
C15
O3
C13
C6
C14
C2
C7
N1
C10
C1
O5
C18
C9

Fig. 2