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Aqua{5,5′-dihydroxy-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}zinc(II) trihydrate[1]

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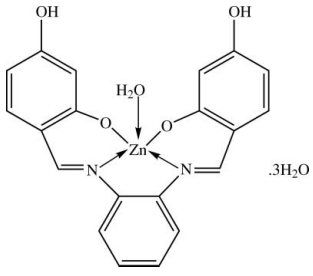
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.088; data-to-parameter ratio = 13.5.

In the title complex, $[Zn(C_{20}H_{14}N_2O_4)(H_2O)]\cdot 3H_2O$, the Zn^{II} center is in an approximately square-pyramidal coordination environment with the two N and two O atoms of the tetradentate Schiff base ligand forming the basal plane and the coordinated water molecule in the apical position. Three solvent water molecules complete the asymmetric unit. The dihedral angles between the two outer benzene rings of the Schiff base and the central benzene ring are 12.64 (14) and 17.25 (14)°. In the crystal structure, intermolecular O—H···O hydrogen bonds link the molecules into sheets parallel to the *ab* plane.

Related literature

For bond-length data, see Allen *et al.* (1987). For related structures, see for example: Chaudhuri *et al.* (2007); Eltayeb *et al.* (2007*a*,*b*,*c*,*d*). For background information on the biological activity of zinc and its complexes, see for example: Assaf & Chung (1984); Berg & Shi (1996); Tarafder *et al.* (2002).



Experimental

Crystal data

$[Zn(C_{20}H_{14}N_2O_4)(H_2O)]\cdot 3H_2O$
M_r = 483.77
Triclinic, $P\overline{1}$
a = 4.7462 (1) Å
b = 13.9290 (2) Å
c = 15.1128 (2) Å
α = 82.147 (1)°
β = 82.367 (1)°
γ = 85.640 (1)°
V = 979.26 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.31 mm^{-1}
T = 100.0 (1) K
0.45 × 0.44 × 0.06 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.591, T_{max} = 0.928
13930 measured reflections
3830 independent reflections
3151 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.088
S = 1.03
3830 reflections
283 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O3W^{i}	0.82	1.87	2.688 (3)	175
O4—H4B···O4^{ii}	0.82	1.93	2.728 (3)	164
O1W—H1W1···O2^{iii}	0.85	2.14	2.879 (3)	146
O2W—H1W2···O1	0.85	2.31	3.066 (3)	149
O2W—H1W2···O1W	0.85	2.36	2.936 (3)	125
O3W—H1W3···O4W^{iv}	0.85 (2)	1.95 (2)	2.788 (3)	169 (3)
O4W—H1W4···O4^{v}	0.85	1.87	2.685 (3)	161
O1W—H2W1···O1^{iii}	0.85	1.91	2.670 (3)	148
O2W—H2W2···O2W^{vi}	0.85	2.42	2.732 (4)	103
O3W—H2W3···O2W	0.85	1.85	2.701 (3)	173
O4W—H2W4···O2	0.85	1.99	2.774 (3)	153

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+2, -y+2, -z+1$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z+1$; (v) $-x+1, -y+2, -z+1$; (vi) $-x, -y+1, -z+1$.

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* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2387).

[1] This paper is dedicated to the memory of Professor M. O. Taha.
§ On study leave from International University of Africa, Sudan.
¶ Additional correspondence author, email: suchada.c@psu.ac.th.

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supplementary materials

Acta Cryst. (2007). E**63**, m2838-m2839 [**doi:10.1107/S1600536807052713**]

Aqua{5,5'-dihydroxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}zinc(II) trihydrate

N. E. Eltayeb, S. G. Teoh, S. Chantrapromma, H.-K. Fun and K. Ibrahim

Comment

Zinc is an element attracting strong interests in biology, medicine, materials, and catalysis. It 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 are biologically active and show very good cytotoxicity against the leukemic cell (Tarafder *et al.*, 2002). Since our previous investigations (Eltayeb *et al.*, 2007*a*, b, c, d) show the possibility of generating five coordinate zinc complexes using tetradentate Schiff base ligands, we have extended our synthesis to the title complex and report its crystal structure here.

In the title complex (Fig. 1), Zn^{II} coordinates with the tetradentate Schiff base ligand in the basal plane (N1, N2, O1 and O2) and a water molecule in the apical site. The Zn^{II} center lies slightly above the N_2O_2 plane in a geometry that is roughly square pyramidal, with the Zn in the Zn—N_2O_2 plane being tilted 0.01190 Å towards the axial water molecule. This geometry has been observed for similar Schiff base ligand Zn^{II} complexes (Eltayeb *et al.*, 2007*a*, b, c, d). The dihedral angles between the two benzene rings (C1–C6) and (C15–C20) and the central benzene ring (C8–C13) are 12.64 (14)° and 17.25 (14) °, respectively. The Zn1—N1 and Zn1—N2 distances of 2.069 (2) Å and 2.075 (2) Å and bond angles around Zn1 are in agreement with the values found for similar Zn^{II} complexes (Eltayeb *et al.*, 2007*a*, b, c, d). However, the Zn1—O1 and Zn1—O2 distances, 1.9905 (19) and 2.001 (2) Å, respectively are slightly shorter than those observed in a closely related structure (Eltayeb ey al., 2007 d) where the Zn—O distances are in the range 2.0027 (15)–2.0036 (15) Å. All water molecules are involved in intermolecular O—H···O hydrogen bonds. Bond lengths and angles observed in the structure are normal (Allen *et al.*, 1987).

In the crystal packing (Fig. 2), O—H···O hydrogen bonds (Table 1) link the molecules into sheets parallel to the *ab* plane.

Experimental

The title compound (I) was synthesized by adding 2,4-dihydroxybenzaldehyde (0.552 g, 4 mmol) to a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol 95% (20 ml). The mixture was refluxed with stirring for an hour. Then zinc chloride (0.272 g, 2 mmol) in ethanol (10 ml) was added, followed by triethylamine (0.5 ml, 3.6 mmol). The mixture was stirred at room temperature for two hours. A yellow precipitate was obtained, washed with about 5 ml e thanol, dried, and then with copious amounts of diethyl ether. This precipitate was dissolved in 20 ml of acetone and, after evaporation of the acetone, the powder obtained was dissolved in diethyl ether. Single crystals of the title compound suitable for *x*-ray structure determination were formed after several days of slow evaporation of the diethyl ether at room temperature.

Refinement

The H atom (H1W3) was located from the difference map and was refined isotropically. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of 0.93 Å and an O—H distance of 0.85 Å and the U_{iso} values were constrained to be $1.2U_{eq}$(C) and $1.5U_{eq}$(O). The highest residual electron density peak is located 0.94 Å from O4W and the deepest hole is located 0.87 Å from Zn1.

Figures

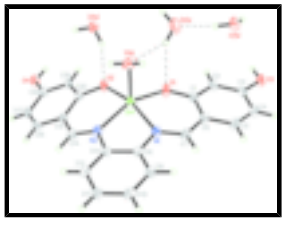

Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen bonds are drawn as dashed lines.

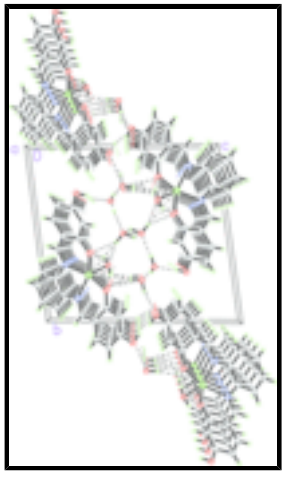

Fig. 2. The crystal packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

Aqua{5,5'-dihydroxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato- κ^4O,N,N',O'}zinc(II) trihydrate

Crystal data

$[Zn(C_{20}H_{14}N_2O_4)(H_2O)]\cdot 3H_2O$	$Z = 2$
$M_r = 483.77$	$F_{000} = 500$
Triclinic, $P\overline{1}$	$D_x = 1.641$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 4.7462$ (1) Å	Cell parameters from 3830 reflections
$b = 13.9290$ (2) Å	$\theta = 1.9$–$26.0°$
$c = 15.1128$ (2) Å	$\mu = 1.31$ mm^{-1}
$\alpha = 82.147$ (1)°	$T = 100.0$ (1) K
$\beta = 82.367$ (1)°	Needle, brown
$\gamma = 85.640$ (1)°	0.45 × 0.44 × 0.06 mm

V = 979.26 (3) Å^3

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	3830 independent reflections
Radiation source: fine-focus sealed tube	3151 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 26.0º
T = 100.0(1) K	θ_{min} = 1.9º
ω scans	h = −5→5
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −17→17
T_{min} = 0.591, T_{max} = 0.928	l = −18→18
13930 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.088	$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 1.1626P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
3830 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
283 parameters	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. The low-temparture data was 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	0.30697 (8)	0.72049 (2)	0.26300 (2)	0.01785 (11)
O1	0.5818 (5)	0.60560 (14)	0.28209 (13)	0.0254 (5)
O2	0.4864 (4)	0.79828 (13)	0.33907 (13)	0.0212 (5)
O3	1.0486 (5)	0.29375 (14)	0.25981 (14)	0.0261 (5)
H3A	1.1055	0.3046	0.3062	0.039*
O4	0.8766 (5)	1.06174 (14)	0.43613 (13)	0.0246 (5)
H4B	0.9353	1.0162	0.4706	0.037*
N1	0.1980 (5)	0.66784 (16)	0.15136 (15)	0.0185 (5)
N2	0.1532 (5)	0.84744 (16)	0.19188 (15)	0.0169 (5)
C1	0.6230 (6)	0.5270 (2)	0.24088 (18)	0.0189 (6)
C2	0.8138 (7)	0.4521 (2)	0.27199 (19)	0.0212 (6)
H2A	0.9083	0.4593	0.3206	0.025*
C3	0.8651 (7)	0.3675 (2)	0.23203 (19)	0.0206 (6)
C4	0.7266 (7)	0.3553 (2)	0.1590 (2)	0.0256 (7)
H4A	0.7608	0.2989	0.1318	0.031*
C5	0.5405 (7)	0.4273 (2)	0.1279 (2)	0.0249 (7)
H5A	0.4477	0.4185	0.0794	0.030*
C6	0.4823 (6)	0.5148 (2)	0.16609 (18)	0.0186 (6)
C7	0.2848 (7)	0.5843 (2)	0.12562 (19)	0.0209 (7)
H7A	0.2113	0.5680	0.0759	0.025*
C8	0.0170 (6)	0.7336 (2)	0.10196 (18)	0.0171 (6)
C9	−0.1341 (7)	0.7108 (2)	0.03546 (19)	0.0212 (7)
H9A	−0.1256	0.6472	0.0226	0.025*
C10	−0.2963 (7)	0.7814 (2)	−0.01161 (19)	0.0229 (7)
H10A	−0.3921	0.7658	−0.0570	0.027*
C11	−0.3156 (7)	0.8755 (2)	0.00914 (19)	0.0226 (7)
H11A	−0.4263	0.9228	−0.0223	0.027*
C12	−0.1730 (7)	0.9001 (2)	0.07570 (18)	0.0210 (6)
H12A	−0.1896	0.9636	0.0891	0.025*
C13	−0.0037 (6)	0.8303 (2)	0.12306 (18)	0.0170 (6)
C14	0.2075 (6)	0.9345 (2)	0.20311 (18)	0.0188 (6)
H14A	0.1272	0.9853	0.1662	0.023*
C15	0.3774 (6)	0.96045 (19)	0.26622 (18)	0.0171 (6)
C16	0.4182 (7)	1.0602 (2)	0.26370 (19)	0.0213 (7)
H16A	0.3286	1.1045	0.2230	0.026*
C17	0.5840 (7)	1.0945 (2)	0.3185 (2)	0.0246 (7)
H17A	0.6095	1.1606	0.3144	0.030*
C18	0.7142 (6)	1.0281 (2)	0.38088 (18)	0.0189 (6)
C19	0.6798 (6)	0.9299 (2)	0.38556 (18)	0.0188 (6)
H19A	0.7697	0.8869	0.4271	0.023*
C20	0.5135 (6)	0.89341 (19)	0.32953 (18)	0.0165 (6)
O1W	−0.0108 (5)	0.67205 (17)	0.35940 (14)	0.0328 (6)
H2W1	−0.1094	0.6304	0.3435	0.049*
H1W1	−0.1175	0.7232	0.3651	0.049*
O2W	0.2688 (6)	0.50060 (16)	0.45460 (16)	0.0441 (7)
H1W2	0.3130	0.5479	0.4146	0.066*
H2W2	0.2341	0.5225	0.5050	0.066*
O3W	0.2523 (5)	0.31908 (15)	0.41217 (14)	0.0268 (5)
H2W3	0.2690	0.3772	0.4216	0.040*

H1W3	0.400 (6)	0.289 (2)	0.429 (2)	0.040*
O4W	0.2536 (5)	0.75935 (14)	0.51765 (13)	0.0250 (5)
H1W4	0.2389	0.8198	0.5220	0.037*
H2W4	0.3054	0.7527	0.4627	0.037*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0192 (2)	0.01691 (18)	0.01923 (18)	−0.00110 (14)	−0.00642 (14)	−0.00494 (12)
O1	0.0318 (13)	0.0187 (10)	0.0301 (11)	0.0039 (10)	−0.0159 (10)	−0.0103 (9)
O2	0.0263 (12)	0.0143 (10)	0.0257 (10)	−0.0019 (9)	−0.0108 (10)	−0.0045 (8)
O3	0.0284 (13)	0.0196 (11)	0.0317 (11)	0.0047 (10)	−0.0092 (10)	−0.0064 (9)
O4	0.0263 (13)	0.0205 (11)	0.0310 (11)	−0.0017 (10)	−0.0142 (10)	−0.0074 (9)
N1	0.0186 (14)	0.0172 (12)	0.0208 (12)	−0.0036 (11)	−0.0041 (11)	−0.0035 (10)
N2	0.0152 (13)	0.0186 (12)	0.0192 (12)	−0.0008 (10)	−0.0063 (10)	−0.0064 (9)
C1	0.0182 (16)	0.0177 (14)	0.0208 (14)	−0.0032 (13)	−0.0006 (13)	−0.0033 (11)
C2	0.0222 (17)	0.0214 (15)	0.0218 (14)	−0.0029 (13)	−0.0070 (13)	−0.0045 (12)
C3	0.0193 (16)	0.0156 (14)	0.0250 (15)	−0.0007 (13)	0.0023 (13)	−0.0010 (11)
C4	0.0306 (19)	0.0208 (15)	0.0277 (16)	−0.0002 (14)	−0.0037 (15)	−0.0116 (12)
C5	0.0272 (18)	0.0268 (16)	0.0234 (15)	−0.0002 (14)	−0.0074 (14)	−0.0088 (13)
C6	0.0175 (16)	0.0190 (14)	0.0200 (14)	−0.0028 (13)	−0.0022 (13)	−0.0041 (11)
C7	0.0224 (17)	0.0219 (15)	0.0211 (14)	−0.0056 (13)	−0.0060 (13)	−0.0070 (12)
C8	0.0141 (15)	0.0207 (14)	0.0169 (13)	−0.0032 (12)	−0.0020 (12)	−0.0022 (11)
C9	0.0227 (17)	0.0186 (14)	0.0236 (15)	−0.0048 (13)	−0.0046 (13)	−0.0037 (12)
C10	0.0211 (17)	0.0291 (16)	0.0204 (14)	−0.0040 (14)	−0.0068 (13)	−0.0047 (12)
C11	0.0216 (17)	0.0257 (16)	0.0204 (14)	0.0006 (14)	−0.0051 (13)	−0.0017 (12)
C12	0.0203 (17)	0.0226 (15)	0.0206 (14)	−0.0014 (13)	−0.0021 (13)	−0.0047 (12)
C13	0.0140 (15)	0.0211 (14)	0.0160 (13)	−0.0038 (12)	−0.0009 (12)	−0.0027 (11)
C14	0.0176 (16)	0.0192 (14)	0.0192 (14)	0.0015 (13)	−0.0028 (13)	−0.0023 (11)
C15	0.0167 (16)	0.0174 (14)	0.0175 (13)	−0.0021 (12)	−0.0002 (12)	−0.0042 (11)
C16	0.0245 (17)	0.0172 (14)	0.0228 (15)	0.0003 (13)	−0.0086 (13)	−0.0005 (12)
C17	0.0326 (19)	0.0144 (14)	0.0294 (16)	−0.0029 (14)	−0.0104 (15)	−0.0043 (12)
C18	0.0169 (16)	0.0195 (14)	0.0221 (14)	−0.0038 (13)	−0.0040 (13)	−0.0066 (12)
C19	0.0185 (16)	0.0177 (14)	0.0215 (14)	0.0010 (13)	−0.0069 (13)	−0.0033 (11)
C20	0.0152 (15)	0.0145 (13)	0.0206 (14)	−0.0002 (12)	−0.0013 (12)	−0.0060 (11)
O1W	0.0326 (14)	0.0409 (13)	0.0280 (12)	−0.0171 (11)	0.0019 (11)	−0.0126 (10)
O2W	0.070 (2)	0.0225 (12)	0.0439 (14)	0.0046 (13)	−0.0254 (14)	−0.0063 (10)
O3W	0.0268 (13)	0.0195 (11)	0.0361 (12)	0.0014 (10)	−0.0103 (11)	−0.0053 (9)
O4W	0.0329 (13)	0.0201 (10)	0.0241 (11)	−0.0022 (10)	−0.0083 (10)	−0.0053 (8)

Geometric parameters (Å, °)

Zn1—O2	1.9905 (19)	C9—C10	1.380 (4)
Zn1—O1	2.001 (2)	C9—H9A	0.9300
Zn1—O1W	2.038 (2)	C10—C11	1.382 (4)
Zn1—N1	2.069 (2)	C10—H10A	0.9300
Zn1—N2	2.075 (2)	C11—C12	1.378 (4)
O1—C1	1.322 (3)	C11—H11A	0.9300
O2—C20	1.327 (3)	C12—C13	1.396 (4)

O3—C3	1.354 (3)	C12—H12A	0.9300
O3—H3A	0.8200	C14—C15	1.426 (4)
O4—C18	1.358 (3)	C14—H14A	0.9300
O4—H4B	0.8200	C15—C16	1.412 (4)
N1—C7	1.298 (3)	C15—C20	1.426 (4)
N1—C8	1.414 (4)	C16—C17	1.368 (4)
N2—C14	1.296 (3)	C16—H16A	0.9300
N2—C13	1.412 (3)	C17—C18	1.398 (4)
C1—C2	1.402 (4)	C17—H17A	0.9300
C1—C6	1.422 (4)	C18—C19	1.381 (4)
C2—C3	1.387 (4)	C19—C20	1.399 (4)
C2—H2A	0.9300	C19—H19A	0.9300
C3—C4	1.393 (4)	O1W—H2W1	0.8501
C4—C5	1.361 (4)	O1W—H1W1	0.8500
C4—H4A	0.9300	O2W—H1W2	0.8498
C5—C6	1.411 (4)	O2W—H2W2	0.8499
C5—H5A	0.9300	O3W—H2W3	0.8516
C6—C7	1.429 (4)	O3W—H1W3	0.838 (18)
C7—H7A	0.9300	O4W—H1W4	0.8499
C8—C9	1.392 (4)	O4W—H2W4	0.8499
C8—C13	1.419 (4)		

O2—Zn1—O1	93.81 (8)	N1—C8—C13	115.4 (2)
O2—Zn1—O1W	96.57 (8)	C10—C9—C8	120.9 (3)
O1—Zn1—O1W	97.05 (10)	C10—C9—H9A	119.6
O2—Zn1—N1	161.27 (9)	C8—C9—H9A	119.6
O1—Zn1—N1	89.57 (8)	C9—C10—C11	119.6 (3)
O1W—Zn1—N1	101.29 (9)	C9—C10—H10A	120.2
O2—Zn1—N2	90.02 (8)	C11—C10—H10A	120.2
O1—Zn1—N2	154.17 (9)	C12—C11—C10	120.9 (3)
O1W—Zn1—N2	107.88 (10)	C12—C11—H11A	119.5
N1—Zn1—N2	79.23 (9)	C10—C11—H11A	119.5
C1—O1—Zn1	129.69 (18)	C11—C12—C13	120.4 (3)
C20—O2—Zn1	129.08 (17)	C11—C12—H12A	119.8
C3—O3—H3A	109.5	C13—C12—H12A	119.8
C18—O4—H4B	109.5	C12—C13—N2	125.2 (3)
C7—N1—C8	121.3 (2)	C12—C13—C8	118.9 (3)
C7—N1—Zn1	125.6 (2)	N2—C13—C8	115.9 (2)
C8—N1—Zn1	113.17 (17)	N2—C14—C15	126.8 (3)
C14—N2—C13	121.7 (2)	N2—C14—H14A	116.6
C14—N2—Zn1	125.19 (19)	C15—C14—H14A	116.6
C13—N2—Zn1	112.96 (17)	C16—C15—C20	118.0 (3)
O1—C1—C2	118.8 (2)	C16—C15—C14	117.0 (3)
O1—C1—C6	122.9 (3)	C20—C15—C14	125.0 (3)
C2—C1—C6	118.3 (2)	C17—C16—C15	122.8 (3)
C3—C2—C1	121.6 (3)	C17—C16—H16A	118.6
C3—C2—H2A	119.2	C15—C16—H16A	118.6
C1—C2—H2A	119.2	C16—C17—C18	118.6 (3)
O3—C3—C2	123.4 (3)	C16—C17—H17A	120.7
O3—C3—C4	116.5 (2)	C18—C17—H17A	120.7

C2—C3—C4	120.1 (3)	O4—C18—C19	120.6 (3)
C5—C4—C3	119.1 (3)	O4—C18—C17	118.9 (2)
C5—C4—H4A	120.5	C19—C18—C17	120.4 (3)
C3—C4—H4A	120.5	C18—C19—C20	121.8 (3)
C4—C5—C6	122.8 (3)	C18—C19—H19A	119.1
C4—C5—H5A	118.6	C20—C19—H19A	119.1
C6—C5—H5A	118.6	O2—C20—C19	118.3 (2)
C5—C6—C1	118.1 (3)	O2—C20—C15	123.4 (2)
C5—C6—C7	116.6 (2)	C19—C20—C15	118.3 (2)
C1—C6—C7	125.3 (3)	Zn1—O1W—H2W1	113.9
N1—C7—C6	126.4 (3)	Zn1—O1W—H1W1	102.4
N1—C7—H7A	116.8	H2W1—O1W—H1W1	107.7
C6—C7—H7A	116.8	H1W2—O2W—H2W2	107.7
C9—C8—N1	125.3 (3)	H2W3—O3W—H1W3	103.5
C9—C8—C13	119.2 (3)	H1W4—O4W—H2W4	107.7
O2—Zn1—O1—C1	−169.1 (2)	C5—C6—C7—N1	178.5 (3)
O1W—Zn1—O1—C1	93.8 (3)	C1—C6—C7—N1	−1.6 (5)
N1—Zn1—O1—C1	−7.6 (3)	C7—N1—C8—C9	14.6 (4)
N2—Zn1—O1—C1	−71.2 (3)	Zn1—N1—C8—C9	−166.5 (2)
O1—Zn1—O2—C20	146.0 (2)	C7—N1—C8—C13	−164.6 (3)
O1W—Zn1—O2—C20	−116.5 (2)	Zn1—N1—C8—C13	14.4 (3)
N1—Zn1—O2—C20	46.0 (4)	N1—C8—C9—C10	−177.3 (3)
N2—Zn1—O2—C20	−8.5 (2)	C13—C8—C9—C10	1.8 (4)
O2—Zn1—N1—C7	107.0 (3)	C8—C9—C10—C11	−1.8 (5)
O1—Zn1—N1—C7	6.4 (3)	C9—C10—C11—C12	0.6 (5)
O1W—Zn1—N1—C7	−90.7 (3)	C10—C11—C12—C13	0.6 (5)
N2—Zn1—N1—C7	163.0 (3)	C11—C12—C13—N2	179.5 (3)
O2—Zn1—N1—C8	−71.9 (4)	C11—C12—C13—C8	−0.5 (4)
O1—Zn1—N1—C8	−172.57 (19)	C14—N2—C13—C12	−16.6 (4)
O1W—Zn1—N1—C8	90.3 (2)	Zn1—N2—C13—C12	167.9 (2)
N2—Zn1—N1—C8	−15.98 (19)	C14—N2—C13—C8	163.4 (3)
O2—Zn1—N2—C14	4.4 (2)	Zn1—N2—C13—C8	−12.1 (3)
O1—Zn1—N2—C14	−94.4 (3)	C9—C8—C13—C12	−0.7 (4)
O1W—Zn1—N2—C14	101.3 (2)	N1—C8—C13—C12	178.5 (3)
N1—Zn1—N2—C14	−160.2 (3)	C9—C8—C13—N2	179.3 (3)
O2—Zn1—N2—C13	179.72 (19)	N1—C8—C13—N2	−1.5 (4)
O1—Zn1—N2—C13	80.9 (3)	C13—N2—C14—C15	−175.9 (3)
O1W—Zn1—N2—C13	−83.36 (19)	Zn1—N2—C14—C15	−0.9 (4)
N1—Zn1—N2—C13	15.15 (19)	N2—C14—C15—C16	177.1 (3)
Zn1—O1—C1—C2	−174.6 (2)	N2—C14—C15—C20	−1.2 (5)
Zn1—O1—C1—C6	5.5 (4)	C20—C15—C16—C17	0.7 (5)
O1—C1—C2—C3	179.6 (3)	C14—C15—C16—C17	−177.8 (3)
C6—C1—C2—C3	−0.4 (4)	C15—C16—C17—C18	−1.2 (5)
C1—C2—C3—O3	179.7 (3)	C16—C17—C18—O4	−179.3 (3)
C1—C2—C3—C4	0.2 (5)	C16—C17—C18—C19	1.2 (5)
O3—C3—C4—C5	−179.7 (3)	O4—C18—C19—C20	179.9 (3)
C2—C3—C4—C5	−0.2 (5)	C17—C18—C19—C20	−0.6 (5)
C3—C4—C5—C6	0.5 (5)	Zn1—O2—C20—C19	−172.2 (2)
C4—C5—C6—C1	−0.7 (5)	Zn1—O2—C20—C15	9.0 (4)

C4—C5—C6—C7	179.2 (3)	C18—C19—C20—O2	−178.8 (3)
O1—C1—C6—C5	−179.4 (3)	C18—C19—C20—C15	0.0 (4)
C2—C1—C6—C5	0.6 (4)	C16—C15—C20—O2	178.8 (3)
O1—C1—C6—C7	0.7 (5)	C14—C15—C20—O2	−2.9 (5)
C2—C1—C6—C7	−179.3 (3)	C16—C15—C20—C19	0.0 (4)
C8—N1—C7—C6	175.4 (3)	C14—C15—C20—C19	178.3 (3)
Zn1—N1—C7—C6	−3.4 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···O3W^{i}	0.82	1.87	2.688 (3)	175
O4—H4B···O4^{ii}	0.82	1.93	2.728 (3)	164
O1W—H1W1···O2^{iii}	0.85	2.14	2.879 (3)	146
O2W—H1W2···O1	0.85	2.31	3.066 (3)	149
O2W—H1W2···O1W	0.85	2.36	2.936 (3)	125
O3W—H1W3···O4W^{iv}	0.85 (2)	1.95 (2)	2.788 (3)	169 (3)
O4W—H1W4···O4^{v}	0.85	1.87	2.685 (3)	161
O1W—H2W1···O1^{iii}	0.85	1.91	2.670 (3)	148
O2W—H2W2···O2W^{vi}	0.85	2.42	2.732 (4)	103
O3W—H2W3···O2W	0.85	1.85	2.701 (3)	173
O4W—H2W4···O2	0.85	1.99	2.774 (3)	153

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+2, −*y*+2, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*+1, −*y*+2, −*z*+1; (vi) −*x*, −*y*+1, −*z*+1.

Fig. 1

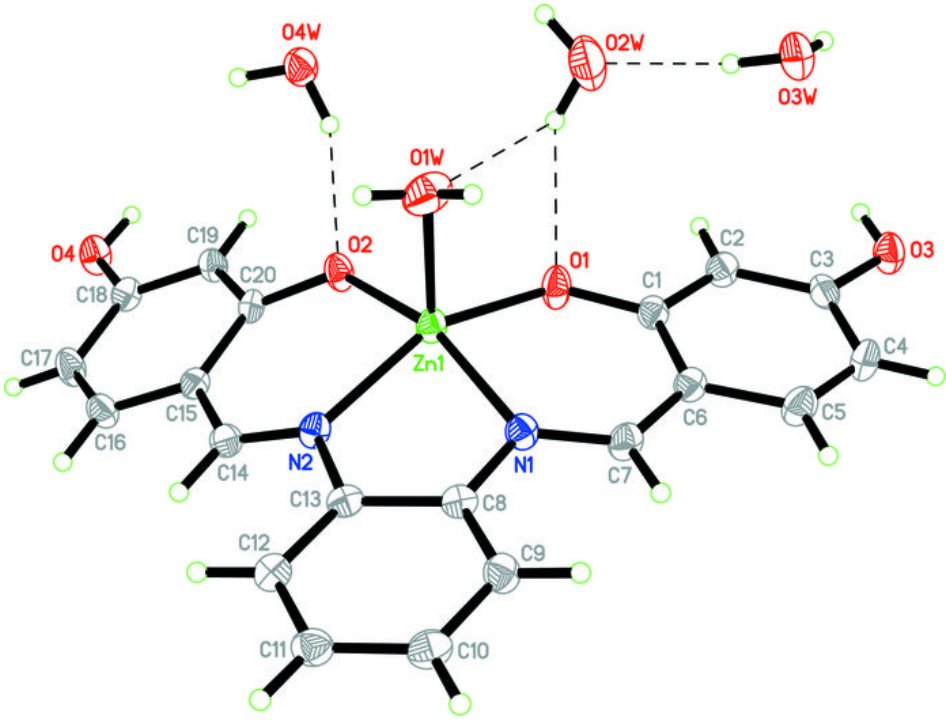
O4W
O2W
O3W
O1W
O4
C19
O2
C20
O1
C1
C2
C3
O3
C18
Zn1
C4
C17
C15
C6
C5
C16
C14
N2
N1
C7
C13
C8
C12
C9
C11
C10

Fig. 2