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Aqua{6,6-dimethyl-2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}zinc(II) chloroform solvate[1]

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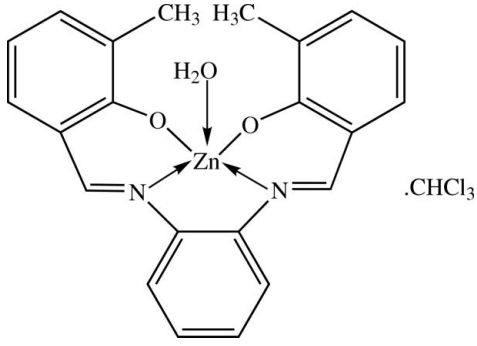
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.076; data-to-parameter ratio = 18.1.

In the title compound, $[Zn(C_{22}H_{18}N_2O_2)(H_2O)]\cdot CHCl_3$, the Zn^{II} centre is in a five-coordinate square-pyramidal N_2O_3 environment, with the N_2O_2 set of atoms from the Schiff base ligand forming the basal plane; the water molecule occupies the apical position. Intermolecular O—H···O hydrogen bonds and weak C—H···O interactions link the molecules into a chain along [100]. The chains form sheets parallel to the *ac* plane.

Related literature

For normal values of bond lengths, see Allen *et al.* (1987). For related structures see, for example, Chaudhuri *et al.* (2007); Eltayeb *et al.* (2007*a*,*b*,*c*). For literature on the biological activities of related compounds, see: Assaf & Chung (1984); Berg & Shi (1996); Tarafder *et al.* (2002).



Experimental

Crystal data

$[Zn(C_{22}H_{18}N_2O_2)(H_2O)]\cdot CHCl_3$
M_r = 545.16
Triclinic, $P\overline{1}$
a = 9.0115 (1) Å
b = 10.7771 (2) Å
c = 12.9018 (2) Å
α = 94.338 (1)°
β = 103.963 (1)°
γ = 109.851 (1)°
V = 1126.55 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.48 mm^{-1}
T = 100.0 (1) K
0.32 × 0.21 × 0.15 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.651, T_{max} = 0.810
19823 measured reflections
5412 independent reflections
4243 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.077
S = 1.03
5412 reflections
299 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H2WA···O1^{i}	0.81 (3)	1.91 (3)	2.646 (2)	151 (3)
O1W—H1WA···O2^{i}	0.81 (4)	1.90 (3)	2.636 (3)	152 (3)
C23—H23A···O1W^{ii}	0.98	2.15	3.132 (3)	174

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

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: NG2303).

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[1] This paper is dedicated to the memory of Professor M. O. Taha.
§ On study leave from International University of Africa, Sudan.

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supplementary materials

Acta Cryst. (2007). E**63**, m2294-m2295 [**doi:10.1107/S1600536807038536**]

Aqua{6,6-dimethyl-2,2'-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}zinc(II) chloroform solvate

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

Comment

Zinc is an essential element for the normal function of most biological systems. Zn^{II} chelate complexes are studied as models for hydrolytically active enzymes. It also 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 Zn^{II} complexes with Schiff bases are biologically active and show very good cytotoxicity against the leukemic cell (Tarafder *et al.*, 2002). The coordination number of Zn^{II} in the catalytic sites is often lower than six, even though water molecule or hydroxide ion is bound to the metal as an additional ligand. Since our previous investigations (Eltayeb *et al.*, 2007*a*,b,c) have shown the possibility of formation of a five coordination environment with tetradentate Schiff base ligand, we have extend our synthesis to the title complex and its crystal structure is reported.

The title complex molecule (Fig. 1) is characterized by an approxmately square pyramidal Zn^{II} coordination, 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 atom is almost in the same plane of this basal plane, as indicated by the displacement of 0.0098 Å out of this basal donor atoms in the direction of the apical water molecule. Bond lengths and angles in this Schiff base ligand are very similar to those reported for the other Zn^{II} complexes with Schiff base ligands (Eltayeb *et al.*, 2007*a*,b,c). The Zn1—N1 and Zn1—N2 distances of 2.0818 (19) Å and 2.0708 (18) Å, respectively lie in the same range as the other five coordination Zn^{II} complexes of Schiff base ligands (Chaudhuri *et al.*, 2007; Eltayeb *et al.*, 2007,b,c). However, the Zn1—O1 and Zn1—O2 distances of 2.0036 (15) Å and 2.0027 (15) Å, respectively, are longer than those observed in other closely related structures (Eltayeb *et al.*, 2007*a*,b,c) where the Zn—O distances are in the range of 1.9326 (17)–1.9798 (13) Å. Bond angles around Zn1 are in agreement with the values found for similar Zn^{II} complexes (Eltayeb *et al.*, 2007*a*,b,c). Evidently, changing the substitutional groups on the Schiff base ligands has no effect on the coordination of the tetradentate Schiff base ligands. Bond lengths and angles observed in the structure are normal (Allen *et al.*, 1987).

In the crystal packing (Fig. 2), the water molecule is involved in intermolecular O—H···O hydrogen bonds [O1W—H2WA···O1 and O1W—H1WA···O2; symmetry code *1 − x*, *-y*, *2 − z*] and the chloroform molecule is involved in a weak C—H···O intermolecular interaction [C23—H23···O1W; symmetry code 1 − *x*, −*y*, 2 − *z*] (Table 2). The molcecules are linked into one-dimension chains along the *a* axis. These chains form molecular sheets parallel to the *ac* plane. The crystal is stabilized by intermolecular O—H···O hydrogen bonds and weak C—H···O interaction.

Experimental

The title compound (I) was synthesized by adding 3-methyl-2-hydroxybenzaldehyde (0.544 g, 4 mmol) into a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol 95% (20 ml). The mixture was refluxed with stirring for half an hour. 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, which was washed by about 5 ml e thanol, dried, and then washed by copious amounts of diethyl ether. The precipitate was dissolved in 20 ml of chloroform and single crystals of the title compound were formed after one day of slow evaporation of chloroform at room temperature.

Refinement

The water H atoms were located in a difference map and isotropically refined. The remainning H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

Figures

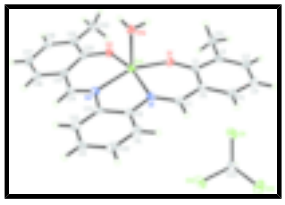

Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering.

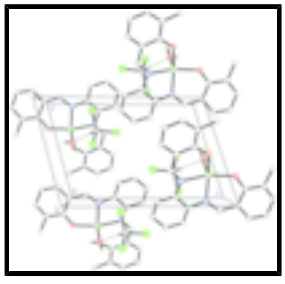

Fig. 2. The crystal packing of the title compound, viewed along the *b* axis. Only water and chloroform H atoms were drawn for clarify. Hydrogen bonds are shown as dash lines.

Aqua{6,6-dimethyl-2,2'-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}zinc(II) chloroform solvate

Crystal data

$[Zn(C_{22}H_{18}N_2O_2)(H_2O)]\cdot CHCl_3$	$Z = 2$
$M_r = 545.16$	$F_{000} = 556$
Triclinic, $P\overline{1}$	$D_x = 1.607$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.0115$ (1) Å	Cell parameters from 5412 reflections
$b = 10.7771$ (2) Å	$\theta = 2.4$–$28.0°$
$c = 12.9018$ (2) Å	$\mu = 1.48$ mm^{-1}
$\alpha = 94.338$ (1)°	$T = 100.0$ (1) K
$\beta = 103.963$ (1)°	Block, yellow
$\gamma = 109.851$ (1)°	0.32 × 0.21 × 0.15 mm
$V = 1126.55$ (3) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	5412 independent reflections
Radiation source: fine-focus sealed tube	4243 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.043$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 28.0°$
$T = 100.0(1)$ K	$\theta_{min} = 2.4°$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -14 \rightarrow 13$
$T_{min} = 0.651$, $T_{max} = 0.810$	$l = -16 \rightarrow 17$
19823 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
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 0.4583P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
5412 reflections	$\Delta\rho_{max} = 0.38$ e $Å^{-3}$
299 parameters	$\Delta\rho_{min} = -0.41$ e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.27559 (3)	−0.00780 (3)	0.88420 (2)	0.01584 (8)
O1	0.46560 (18)	0.16671 (15)	0.91153 (12)	0.0174 (3)

O2	0.26547 (18)	−0.00680 (15)	1.03761 (12)	0.0177 (3)
O1W	0.4145 (2)	−0.12826 (17)	0.89043 (14)	0.0170 (4)
N1	0.2252 (2)	−0.00472 (18)	0.71842 (15)	0.0168 (4)
N2	0.0356 (2)	−0.14449 (18)	0.83007 (15)	0.0159 (4)
C1	0.5332 (3)	0.2309 (2)	0.84187 (18)	0.0161 (5)
C2	0.6815 (3)	0.3463 (2)	0.88245 (19)	0.0176 (5)
C3	0.7567 (3)	0.4130 (2)	0.81148 (19)	0.0207 (5)
H3A	0.8538	0.4873	0.8393	0.025*
C4	0.6930 (3)	0.3738 (2)	0.6991 (2)	0.0220 (5)
H4A	0.7474	0.4201	0.6529	0.026*
C5	0.5491 (3)	0.2659 (2)	0.65847 (19)	0.0198 (5)
H5A	0.5049	0.2399	0.5837	0.024*
C6	0.4655 (3)	0.1926 (2)	0.72707 (18)	0.0172 (5)
C7	0.3160 (3)	0.0813 (2)	0.67323 (19)	0.0172 (5)
H7A	0.2809	0.0700	0.5980	0.021*
C8	0.0777 (3)	−0.1091 (2)	0.65642 (18)	0.0166 (5)
C9	0.0306 (3)	−0.1450 (2)	0.54369 (19)	0.0213 (5)
H9A	0.0992	−0.0992	0.5043	0.026*
C10	−0.1162 (3)	−0.2473 (2)	0.4902 (2)	0.0224 (5)
H10A	−0.1463	−0.2702	0.4151	0.027*
C11	−0.2193 (3)	−0.3164 (2)	0.54805 (19)	0.0207 (5)
H11A	−0.3190	−0.3848	0.5117	0.025*
C12	−0.1739 (3)	−0.2836 (2)	0.65921 (19)	0.0194 (5)
H12A	−0.2434	−0.3308	0.6975	0.023*
C13	−0.0256 (3)	−0.1810 (2)	0.71564 (18)	0.0153 (5)
C14	−0.0571 (3)	−0.1917 (2)	0.89165 (19)	0.0179 (5)
H14A	−0.1656	−0.2469	0.8568	0.022*
C15	−0.0096 (3)	−0.1677 (2)	1.00789 (18)	0.0171 (5)
C16	−0.1320 (3)	−0.2383 (2)	1.0558 (2)	0.0217 (5)
H16A	−0.2348	−0.2944	1.0112	0.026*
C17	−0.1034 (3)	−0.2266 (2)	1.1652 (2)	0.0224 (5)
H17A	−0.1839	−0.2762	1.1951	0.027*
C18	0.0503 (3)	−0.1379 (2)	1.2319 (2)	0.0222 (5)
H18A	0.0701	−0.1288	1.3068	0.027*
C19	0.1727 (3)	−0.0639 (2)	1.19001 (18)	0.0181 (5)
C20	0.1462 (3)	−0.0785 (2)	1.07590 (18)	0.0161 (5)
C21	0.7545 (3)	0.3909 (2)	1.00306 (19)	0.0225 (5)
H21A	0.8440	0.4758	1.0177	0.034*
H21B	0.7945	0.3258	1.0336	0.034*
H21C	0.6718	0.3995	1.0348	0.034*
C22	0.3308 (3)	0.0367 (2)	1.26331 (19)	0.0216 (5)
H22A	0.3276	0.0380	1.3372	0.032*
H22B	0.3450	0.1238	1.2449	0.032*
H22C	0.4210	0.0127	1.2548	0.032*
H2WA	0.417 (3)	−0.158 (3)	0.946 (2)	0.027 (8)*
H1WA	0.507 (4)	−0.083 (3)	0.891 (2)	0.036 (9)*
C23	0.3000 (3)	0.6266 (2)	0.7042 (2)	0.0232 (5)
H23A	0.3319	0.7066	0.7586	0.028*
Cl1	0.43406 (7)	0.54081 (6)	0.74705 (6)	0.03189 (16)

Cl2	0.09640 (7)	0.52333 (7)	0.69353 (6)	0.03265 (16)
Cl3	0.31570 (9)	0.67676 (7)	0.57947 (5)	0.03654 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01532 (13)	0.01675 (14)	0.01440 (15)	0.00447 (10)	0.00455 (10)	0.00246 (11)
O1	0.0177 (8)	0.0168 (8)	0.0156 (8)	0.0039 (6)	0.0044 (7)	0.0038 (7)
O2	0.0170 (8)	0.0203 (8)	0.0161 (8)	0.0057 (7)	0.0068 (7)	0.0034 (7)
O1W	0.0169 (9)	0.0177 (9)	0.0154 (9)	0.0046 (7)	0.0049 (7)	0.0034 (7)
N1	0.0147 (9)	0.0157 (10)	0.0186 (10)	0.0043 (8)	0.0043 (8)	0.0029 (8)
N2	0.0165 (9)	0.0163 (10)	0.0154 (10)	0.0071 (8)	0.0039 (8)	0.0022 (8)
C1	0.0155 (11)	0.0156 (11)	0.0203 (12)	0.0088 (9)	0.0051 (9)	0.0059 (10)
C2	0.0157 (11)	0.0166 (12)	0.0213 (13)	0.0074 (9)	0.0044 (10)	0.0030 (10)
C3	0.0167 (11)	0.0167 (12)	0.0262 (14)	0.0040 (9)	0.0051 (10)	0.0033 (10)
C4	0.0214 (12)	0.0215 (13)	0.0241 (14)	0.0056 (10)	0.0100 (11)	0.0094 (11)
C5	0.0236 (12)	0.0228 (13)	0.0154 (12)	0.0099 (10)	0.0070 (10)	0.0065 (10)
C6	0.0165 (11)	0.0172 (12)	0.0190 (12)	0.0076 (9)	0.0048 (10)	0.0050 (10)
C7	0.0186 (11)	0.0192 (12)	0.0149 (12)	0.0088 (10)	0.0039 (9)	0.0035 (10)
C8	0.0160 (11)	0.0169 (12)	0.0168 (12)	0.0075 (9)	0.0025 (9)	0.0020 (10)
C9	0.0244 (12)	0.0208 (13)	0.0190 (13)	0.0072 (10)	0.0080 (10)	0.0051 (10)
C10	0.0276 (13)	0.0216 (13)	0.0161 (13)	0.0107 (11)	0.0014 (10)	−0.0004 (10)
C11	0.0156 (11)	0.0177 (12)	0.0225 (13)	0.0043 (9)	−0.0014 (10)	−0.0023 (10)
C12	0.0191 (11)	0.0178 (12)	0.0213 (13)	0.0072 (10)	0.0057 (10)	0.0025 (10)
C13	0.0165 (11)	0.0153 (11)	0.0155 (12)	0.0090 (9)	0.0027 (9)	0.0030 (9)
C14	0.0154 (11)	0.0156 (12)	0.0225 (13)	0.0056 (9)	0.0048 (10)	0.0034 (10)
C15	0.0185 (11)	0.0182 (12)	0.0180 (12)	0.0091 (9)	0.0067 (10)	0.0060 (10)
C16	0.0203 (12)	0.0201 (12)	0.0277 (14)	0.0081 (10)	0.0098 (11)	0.0076 (11)
C17	0.0264 (13)	0.0220 (13)	0.0246 (14)	0.0092 (11)	0.0153 (11)	0.0104 (11)
C18	0.0313 (13)	0.0251 (13)	0.0162 (13)	0.0143 (11)	0.0109 (11)	0.0060 (10)
C19	0.0223 (12)	0.0182 (12)	0.0180 (12)	0.0117 (10)	0.0068 (10)	0.0047 (10)
C20	0.0173 (11)	0.0147 (11)	0.0212 (13)	0.0101 (9)	0.0076 (10)	0.0047 (10)
C21	0.0217 (12)	0.0178 (12)	0.0220 (13)	0.0021 (10)	0.0040 (10)	0.0005 (10)
C22	0.0252 (13)	0.0257 (13)	0.0166 (13)	0.0115 (11)	0.0077 (10)	0.0036 (10)
C23	0.0235 (12)	0.0231 (13)	0.0229 (14)	0.0086 (10)	0.0078 (11)	0.0006 (11)
Cl1	0.0218 (3)	0.0304 (4)	0.0445 (4)	0.0107 (3)	0.0100 (3)	0.0058 (3)
Cl2	0.0204 (3)	0.0332 (4)	0.0433 (4)	0.0078 (3)	0.0118 (3)	0.0018 (3)
Cl3	0.0461 (4)	0.0358 (4)	0.0268 (4)	0.0111 (3)	0.0145 (3)	0.0053 (3)

Geometric parameters (Å, °)

Zn1—O2	2.0027 (15)	C10—C11	1.387 (3)
Zn1—O1	2.0036 (15)	C10—H10A	0.9300
Zn1—N2	2.0708 (18)	C11—C12	1.375 (3)
Zn1—O1W	2.0810 (16)	C11—H11A	0.9300
Zn1—N1	2.0818 (19)	C12—C13	1.394 (3)
O1—C1	1.315 (3)	C12—H12A	0.9300
O2—C20	1.322 (2)	C14—C15	1.434 (3)
O1W—H2WA	0.80 (3)	C14—H14A	0.9300

O1W—H1WA	0.81 (3)	C15—C16	1.417 (3)
N1—C7	1.291 (3)	C15—C20	1.423 (3)
N1—C8	1.417 (3)	C16—C17	1.360 (3)
N2—C14	1.296 (3)	C16—H16A	0.9300
N2—C13	1.418 (3)	C17—C18	1.405 (3)
C1—C6	1.427 (3)	C17—H17A	0.9300
C1—C2	1.429 (3)	C18—C19	1.379 (3)
C2—C3	1.372 (3)	C18—H18A	0.9300
C2—C21	1.504 (3)	C19—C20	1.421 (3)
C3—C4	1.397 (3)	C19—C22	1.498 (3)
C3—H3A	0.9300	C21—H21A	0.9600
C4—C5	1.365 (3)	C21—H21B	0.9600
C4—H4A	0.9300	C21—H21C	0.9600
C5—C6	1.413 (3)	C22—H22A	0.9600
C5—H5A	0.9300	C22—H22B	0.9600
C6—C7	1.436 (3)	C22—H22C	0.9600
C7—H7A	0.9300	C23—Cl2	1.758 (2)
C8—C9	1.397 (3)	C23—Cl3	1.759 (2)
C8—C13	1.412 (3)	C23—Cl1	1.771 (2)
C9—C10	1.377 (3)	C23—H23A	0.9800
C9—H9A	0.9300		
O2—Zn1—O1	96.84 (6)	C11—C10—H10A	119.9
O2—Zn1—N2	89.99 (7)	C12—C11—C10	119.9 (2)
O1—Zn1—N2	158.92 (7)	C12—C11—H11A	120.1
O2—Zn1—O1W	95.73 (7)	C10—C11—H11A	120.1
O1—Zn1—O1W	95.93 (7)	C11—C12—C13	121.2 (2)
N2—Zn1—O1W	103.23 (7)	C11—C12—H12A	119.4
O2—Zn1—N1	164.74 (7)	C13—C12—H12A	119.4
O1—Zn1—N1	89.63 (7)	C12—C13—C8	118.8 (2)
N2—Zn1—N1	79.38 (7)	C12—C13—N2	125.3 (2)
O1W—Zn1—N1	97.34 (7)	C8—C13—N2	115.88 (19)
C1—O1—Zn1	129.18 (14)	N2—C14—C15	126.8 (2)
C20—O2—Zn1	129.59 (14)	N2—C14—H14A	116.6
Zn1—O1W—H2WA	107.6 (19)	C15—C14—H14A	116.6
Zn1—O1W—H1WA	109 (2)	C16—C15—C20	119.2 (2)
H2WA—O1W—H1WA	109 (3)	C16—C15—C14	115.5 (2)
C7—N1—C8	121.5 (2)	C20—C15—C14	125.2 (2)
C7—N1—Zn1	125.23 (16)	C17—C16—C15	121.9 (2)
C8—N1—Zn1	113.26 (14)	C17—C16—H16A	119.1
C14—N2—C13	120.93 (19)	C15—C16—H16A	119.1
C14—N2—Zn1	125.15 (16)	C16—C17—C18	118.6 (2)
C13—N2—Zn1	113.89 (13)	C16—C17—H17A	120.7
O1—C1—C6	123.6 (2)	C18—C17—H17A	120.7
O1—C1—C2	118.7 (2)	C19—C18—C17	122.1 (2)
C6—C1—C2	117.7 (2)	C19—C18—H18A	118.9
C3—C2—C1	119.8 (2)	C17—C18—H18A	118.9
C3—C2—C21	121.1 (2)	C18—C19—C20	119.8 (2)
C1—C2—C21	119.1 (2)	C18—C19—C22	120.7 (2)
C2—C3—C4	122.6 (2)	C20—C19—C22	119.5 (2)

C2—C3—H3A	118.7	O2—C20—C19	118.7 (2)
C4—C3—H3A	118.7	O2—C20—C15	123.0 (2)
C5—C4—C3	118.6 (2)	C19—C20—C15	118.3 (2)
C5—C4—H4A	120.7	C2—C21—H21A	109.5
C3—C4—H4A	120.7	C2—C21—H21B	109.5
C4—C5—C6	121.7 (2)	H21A—C21—H21B	109.5
C4—C5—H5A	119.1	C2—C21—H21C	109.5
C6—C5—H5A	119.1	H21A—C21—H21C	109.5
C5—C6—C1	119.5 (2)	H21B—C21—H21C	109.5
C5—C6—C7	115.7 (2)	C19—C22—H22A	109.5
C1—C6—C7	124.8 (2)	C19—C22—H22B	109.5
N1—C7—C6	126.7 (2)	H22A—C22—H22B	109.5
N1—C7—H7A	116.6	C19—C22—H22C	109.5
C6—C7—H7A	116.6	H22A—C22—H22C	109.5
C9—C8—C13	119.2 (2)	H22B—C22—H22C	109.5
C9—C8—N1	124.8 (2)	Cl2—C23—Cl3	110.58 (13)
C13—C8—N1	115.96 (19)	Cl2—C23—Cl1	109.94 (13)
C10—C9—C8	120.7 (2)	Cl3—C23—Cl1	110.28 (12)
C10—C9—H9A	119.7	Cl2—C23—H23A	108.7
C8—C9—H9A	119.7	Cl3—C23—H23A	108.7
C9—C10—C11	120.2 (2)	Cl1—C23—H23A	108.7
C9—C10—H10A	119.9		
O2—Zn1—O1—C1	−176.55 (17)	C5—C6—C7—N1	175.1 (2)
N2—Zn1—O1—C1	−68.4 (3)	C1—C6—C7—N1	−4.0 (4)
O1W—Zn1—O1—C1	86.93 (17)	C7—N1—C8—C9	12.0 (3)
N1—Zn1—O1—C1	−10.41 (17)	Zn1—N1—C8—C9	−167.72 (18)
O1—Zn1—O2—C20	163.81 (17)	C7—N1—C8—C13	−168.7 (2)
N2—Zn1—O2—C20	3.80 (18)	Zn1—N1—C8—C13	11.6 (2)
O1W—Zn1—O2—C20	−99.50 (18)	C13—C8—C9—C10	1.3 (3)
N1—Zn1—O2—C20	49.3 (3)	N1—C8—C9—C10	−179.4 (2)
O2—Zn1—N1—C7	122.3 (3)	C8—C9—C10—C11	−0.1 (4)
O1—Zn1—N1—C7	6.87 (18)	C9—C10—C11—C12	−0.8 (4)
N2—Zn1—N1—C7	168.79 (19)	C10—C11—C12—C13	0.4 (3)
O1W—Zn1—N1—C7	−89.06 (18)	C11—C12—C13—C8	0.8 (3)
O2—Zn1—N1—C8	−58.0 (3)	C11—C12—C13—N2	−176.6 (2)
O1—Zn1—N1—C8	−173.39 (15)	C9—C8—C13—C12	−1.7 (3)
N2—Zn1—N1—C8	−11.48 (14)	N1—C8—C13—C12	179.02 (19)
O1W—Zn1—N1—C8	90.68 (15)	C9—C8—C13—N2	176.00 (19)
O2—Zn1—N2—C14	1.06 (18)	N1—C8—C13—N2	−3.3 (3)
O1—Zn1—N2—C14	−108.3 (2)	C14—N2—C13—C12	−11.3 (3)
O1W—Zn1—N2—C14	96.94 (18)	Zn1—N2—C13—C12	170.87 (17)
N1—Zn1—N2—C14	−167.93 (19)	C14—N2—C13—C8	171.2 (2)
O2—Zn1—N2—C13	178.78 (14)	Zn1—N2—C13—C8	−6.6 (2)
O1—Zn1—N2—C13	69.5 (2)	C13—N2—C14—C15	177.3 (2)
O1W—Zn1—N2—C13	−85.34 (15)	Zn1—N2—C14—C15	−5.1 (3)
N1—Zn1—N2—C13	9.79 (14)	N2—C14—C15—C16	−176.2 (2)
Zn1—O1—C1—C6	8.5 (3)	N2—C14—C15—C20	5.1 (4)
Zn1—O1—C1—C2	−172.26 (14)	C20—C15—C16—C17	−2.0 (3)
O1—C1—C2—C3	178.4 (2)	C14—C15—C16—C17	179.1 (2)

C6—C1—C2—C3	−2.3 (3)	C15—C16—C17—C18	2.3 (4)
O1—C1—C2—C21	−0.4 (3)	C16—C17—C18—C19	−0.6 (4)
C6—C1—C2—C21	178.9 (2)	C17—C18—C19—C20	−1.3 (3)
C1—C2—C3—C4	0.8 (3)	C17—C18—C19—C22	175.7 (2)
C21—C2—C3—C4	179.5 (2)	Zn1—O2—C20—C19	176.74 (14)
C2—C3—C4—C5	1.0 (4)	Zn1—O2—C20—C15	−4.8 (3)
C3—C4—C5—C6	−1.0 (3)	C18—C19—C20—O2	−179.9 (2)
C4—C5—C6—C1	−0.6 (3)	C22—C19—C20—O2	3.1 (3)
C4—C5—C6—C7	−179.8 (2)	C18—C19—C20—C15	1.6 (3)
O1—C1—C6—C5	−178.50 (19)	C22—C19—C20—C15	−175.5 (2)
C2—C1—C6—C5	2.3 (3)	C16—C15—C20—O2	−178.5 (2)
O1—C1—C6—C7	0.6 (3)	C14—C15—C20—O2	0.3 (3)
C2—C1—C6—C7	−178.7 (2)	C16—C15—C20—C19	0.0 (3)
C8—N1—C7—C6	178.6 (2)	C14—C15—C20—C19	178.7 (2)
Zn1—N1—C7—C6	−1.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H2WA···O1^{i}	0.81 (3)	1.91 (3)	2.646 (2)	151 (3)
O1W—H1WA···O2^{i}	0.81 (4)	1.90 (3)	2.636 (3)	152 (3)
C23—H23A···O1W^{ii}	0.98	2.16	3.132 (3)	174

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

Fig. 1

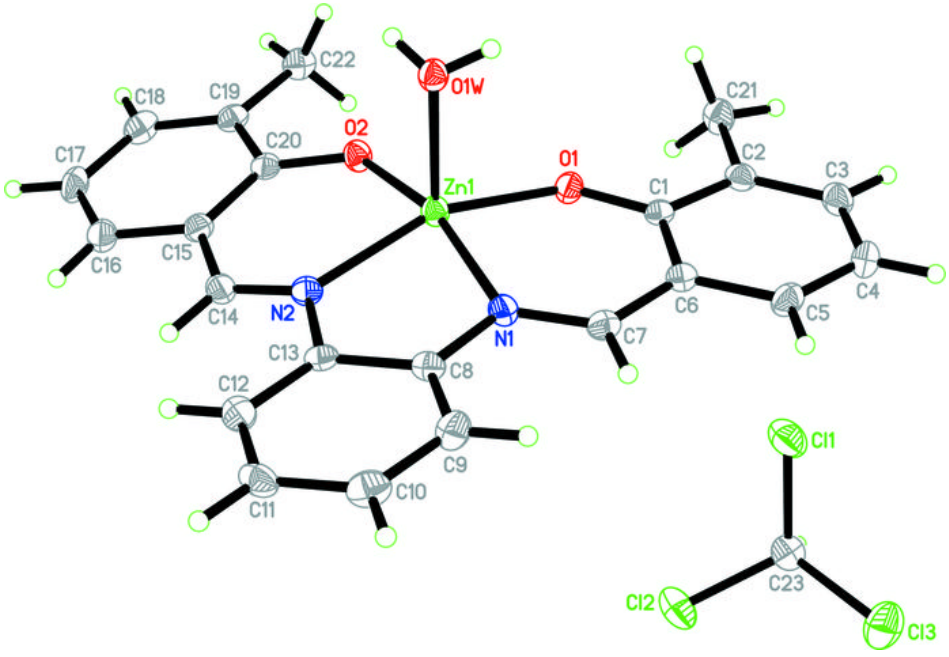
O1W
C22
C18
C19
C21
O2
C20
C17
O1
Zn1
C2
C3
C1
C16
C15
C6
C4
C14
N2
N1
C5
C7
C13
C8
C12
Cl1
C9
C10
C11
C23
Cl2
Cl3

Fig. 2