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[μ-1,2-Bis(salicyloyl)hydrazine(4−)]-bis[(ethylenediamine)zinc(II)] dimethylformamide disolvate dihydrate

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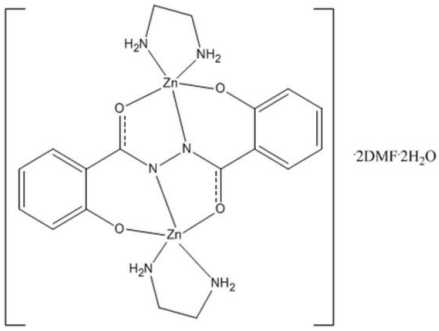
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.110; data-to-parameter ratio = 16.6.

In the title compound, $[Zn_2(C_{14}H_8N_2O_4)(C_2H_8N_2)_2]\cdot 2C_3H_7NO\cdot 2H_2O$, the Zn_2 complex molecule lies on a crystallographic inversion centre. The two Zn atoms are bridged by two diazine N atoms of a 1,2-bis(salicyloyl)hydrazine(4−) ligand (bsh^{4-}); the inversion centre is located at the mid-point of the N—N bond. The coordination geometry of the Zn atom is distorted square-pyramidal. Each water molecule is linked with three surrounding binuclear complexes through four hydrogen bonds, resulting in a two-dimensional network.

Related literature

For related literature, see: Adams *et al.* (2000, 2002); Bazzicalupi *et al.* (1997); Chen & Liu *et al.* (2005); Fletcher & Therien (2000); Gultneh *et al.* (1999); He *et al.* (2007); Hlavinka *et al.* (2006); Khoury *et al.* (1999); Li *et al.* (2003); Liu *et al.* (2001); Mimoun *et al.* (1999); Mo *et al.* (2002); Müller & Robson (2000); Nfor *et al.* (2006); Sousa *et al.* (2000); Wang *et al.* (2004); Wu *et al.* (2003); Xiang *et al.* (2005); Xu *et al.* (2000, 2002); You (2005); Zhang *et al.* (1996); Zhu *et al.* (2003).



Experimental

Crystal data

$[Zn_2(C_{14}H_8N_2O_4)(C_2H_8N_2)_2]\cdot 2C_3H_7NO\cdot 2H_2O$
M_r = 701.40
Monoclinic, $C2/c$
a = 28.715 (14) Å
b = 8.812 (4) Å
c = 13.522 (6) Å
β = 115.606 (18)°
V = 3086 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.05 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: multi-scan (*TEXRAY*; MSC, 1999)
T_{min} = 0.728, T_{max} = 0.917
13504 measured reflections
3191 independent reflections
2537 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.110
S = 1.03
3191 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O3	0.90	2.09	2.956 (5)	162
N3—H3C···O1^{i}	0.90	2.32	3.177 (4)	159
O1W—H01A···O1^{ii}	0.85	1.88	2.716 (3)	171
O1W—H01B···O2^{iii}	0.93	1.90	2.814 (3)	168
N2—H2A···O1W^{iii}	0.90	2.10	2.998 (4)	172
N3—H3B···O1W^{ii}	0.90	2.27	3.064 (4)	146

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *TEXRAY* (MSC, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (MSC, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG3120).

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supplementary materials

Acta Cryst. (2007). E**63**, m3105-m3106 [**doi:10.1107/S1600536807057212**]

[μ-1,2-Bis(salicyloyl)hydrazine(4-)]bis[(ethylenediamine)zinc(II)] dimethylformamide disolvate dihydrate

Z.-Y. Wang and S.-X. Liu

Comment

Diazine ligands can provide four or more donor atoms, its several possible mononucleating and dinucleating coordination modes lead to formation of mononuclear, binuclear and polynuclear complexes. In some cases, six or more donors in this type of ligand coordinated to two metal atoms *M*(II) to get centrosymmetrical binuclear complexes with discrete structure (Zhang *et al.*, 1996; Chen *et al.*, 2005 & Xiang *et al.*, 2005), using multidentate ligand and divalent metal salts. Several polynuclear complexes with one-dimensional structure (Adams *et al.*, 2000), two-dimensional structure (Xu *et al.*, 2000; Xu *et al.*, 2002) and three-dimensional structure (Mo *et al.*, 2002) have been synthesized, respectively, depending on the different types of donor and coordination models in the ligands and the different coordination geometries in different metal atoms. Two fancy 30-MC-10 type of azametallacrowns were obtained, using trianionic pentadentate ligand *N*-phenylsalicylhydrazidate and trivalent metal salts (Liu *et al.*, 2001). The guanidine-based hydrazone ligands with diazine promise a rich coordination chemistry and access to a wide range of oligomers and polymers (Müller *et al.*, 2000). As an extension of our previous work (Chen *et al.*, 2005), we report here the synthesis and crystal structure of the title compound (I) $[Zn_2(bsh)(en)_2]\cdot 2DMF\cdot 2H_2O$ (bsh and en are 1,2-bis(salicyloyl)hydrazine and ethylenediamine, respectively).

The molecular structure of complex (I) is illustrated in Fig. 1. The title binuclear complex molecule (I) is centrosymmetric, with the symmetric center located at the midpoint of the N—N single bond. Every Zn atom is coordinated by three donors (O1, N1 and $O2^i$) of the bsh^{4-} ligand [symmetry code (i): $-x + 1/2, -y + 1/2, -z + 1$] and two N atoms (N2 and N3) of ethylenediamine. Each zinc atom has a distorted ZnN_3O_2 square-pyramid coordination geometry with τ value of 0.08 (some parameters are listed in Table 1), atoms N1/N3/O1/$O2^i$ being in the basal plane, atom N2 being at the top of the pyramid. The bond length of Zn—O(phenol oxygen) (Zn1—O1) in complex (I) is 2.049 (2) Å, while the corresponding values in the known binuclear Zn complexes are between 1.948–2.094Å (Adams *et al.*, 2002; You, 2005). The bond lengths of Zn—*O*(carbonyl oxygen) (Zn1—$O2^i$) in complex (I) is 2.121 (2) Å, and the corresponding values in the known binuclear Zn complexes are between 2.010 and 2.215Å (Nfor *et al.*, 2006; Wu *et al.*, 2003).

Many binuclear zinc complexes have been reported. The two Zn atoms in many binuclear zinc complexes are bridged by two acid liands (You, 2005; Nfor *et al.*, 2006), two μ^2-N_3 ligands (Wang *et al.*, 2004), two μ^2-OH groups (Gultneh *et al.*, 1999) or other two ligands (Li *et al.*, 2003; Mimoun *et al.*, 1999; Sousa *et al.*, 2000). It is found in some binuclear zinc complexes that two Zn atoms are linked by several donors from one ligand, such as $[Zn_2(2)(AN)_2](ClO_4)_4]$ (Zhu *et al.*, 2003), $^{Me}LZn_2(O^iPr)_2$ (Hlavinka *et al.*, 2006), $[Zn_2(C_9H_7NO_4)Cl_2(C_{12}H_8N_2)_2]$ (He *et al.*, 2007), and in (I). Some binuclear zinc complexes with macrocyclic ligand were also synthesized (Bazzicalupi *et al.*, 1997; Khoury *et al.*, 1999; Fletcher *et al.*, 2000). The Zn···Zn interatomic distances in different binuclear complexes are quite different from 2.652–5.354Å (You, 2005; Nfor *et al.*, 2006; Bazzicalupi *et al.*, 1997; Hlavinka *et al.*, 2006), depending on different connecting ways between the two Zn atoms. The two zinc atoms in (I) are linked by N—N single bond of the bsh^{4-} ligand. The ligand bsh^{4-} in (I) is a tetraanionic hexadentate ligand. The bsh4- anion coordinated to one metal atom through its three donors and coordinated to

the other metal atom through its other three donors. The ligand bsh^{4-} is in *trans* configuration. These structural phenomena have been observed in $[Ni_2(bsh)(C_5H_5N)_6]\cdot 2C_5H_5N$ (Chen *et al.*, 2005). The Zn···Zn distance in (I) is 4.783 (2) Å, while the Ni···Ni distance in the nickel complex mentioned above is 4.6883 (4) Å.

As shown in Fig. 2 and Table 2, every water molecule is linked with three surrounding binuclear structure units $[Zn_2(C_{14}H_8N_2O_4)\ (C_2H_8N_2)_2]$ through four hydrogen bonds. These hydrogen bonds are O1W—H01A···O2^{ii}, O1W—H01B···O1, N2^{iii}—H2A^{iii}···O1W and N3—H3B···O1W [symmetry codes: (ii) $x, -y+1, z+1/2$; (iii) $x, -y, z+1/2$]. Therefore, an extended two-dimensional structure paralleled the *bc* plane is formed.

Experimental

To a mixed solution of H_4bsh dissolved by DMF (1 ml), methanol (4 ml) and CH_2Cl_2 (6 ml), $Zn(acac)_2\cdot H_2O$ (0.028 g, 0.1 mmol) was added (acac is short for acetylacetone). Then add two drops of ethylenediamine, and the white suspended solution turned to light yellow mixture. After stirring for 3 h at ambient temperature, the mixture was filtrated to obtain a light yellow solution. The filtrate was left to stand and evaporate at room temperature and yellow crystals of suitable size were obtained after 10 days.

Refinement

The water H atoms and the H atom bonded to C10 in DMF were located in difference Fourier maps and their positional parameters were refined. The remaining H atoms were placed in calculated positions and treated using a riding model with C—H = 0.93–0.97 Å, N—H = 0.90Å and U_{iso}(H) = 1.2–1.5 U_{eq}(C/N).

Figures

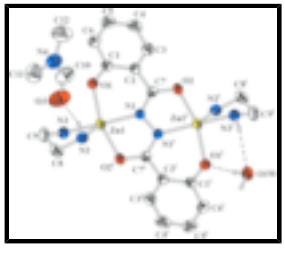


Fig. 1. The molecular structure of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. The intermolecular hydrogen bond is shown as a dashed line [symmetry code (i) $-x+1/2,-y+1/2,-z+1$].

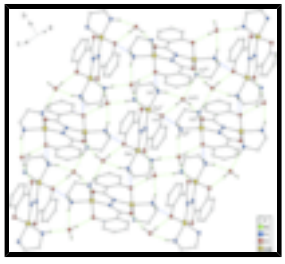


Fig. 2. The hydrogen-bonding interactions involving solvent water molecules. Dashed lines represent hydrogen bonds. [Symmetry codes: (i) $1/2-x, 1/2-y, 1-z$; (ii) $x, 1-y, 1/2+z$; (iii) $x, -y, 1/2+z$.].

[μ-1,2-Bis(salicyloyl)hydrazine(4-)]bis[(ethylenediamine)zinc(II)] bis(dimethylformamide) solvate dihydrate

Crystal data

$[Zn_2(C_{14}H_8N_2O_4)(C_2H_8N_2)_2]\cdot 2C_3H_7NO\cdot 2H_2O$	$F_{000} = 1464$
$M_r = 701.40$	$D_x = 1.510$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 13504 reflections
$a = 28.715$ (14) Å	$\theta = 3.0$–26.5°
$b = 8.812$ (4) Å	$\mu = 1.61$ mm^{-1}
$c = 13.522$ (6) Å	$T = 293$ (2) K
$\beta = 115.606$ (18)°	Block, yellow
$V = 3086$ (2) Å^3	0.20 × 0.20 × 0.05 mm
$Z = 4$	

Data collection

Rigaku Weissenberg IP diffractometer	3191 independent reflections
Radiation source: rotor target	2537 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.056$
$T = 293(2)$ K	$\theta_{max} = 26.5^\circ$
ω scans	$\theta_{min} = 3.0^\circ$
Absorption correction: ψ scan (TEXRAY; MSC, 1999)	$h = -36\rightarrow 36$
$T_{min} = 0.728$, $T_{max} = 0.917$	$k = -11\rightarrow 10$
13504 measured reflections	$l = -16\rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 3.1677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3191 reflections	$\Delta\rho_{max} = 0.84$ e Å^{-3}
192 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Zn1	0.283933 (14)	0.09578 (4)	0.66136 (3)	0.03147 (14)
N1	0.27204 (10)	0.2583 (3)	0.54944 (18)	0.0303 (6)
N2	0.33371 (11)	−0.0796 (3)	0.6755 (2)	0.0356 (6)
H2A	0.3282	−0.1145	0.6088	0.043*
H2B	0.3667	−0.0484	0.7105	0.043*
N3	0.26794 (10)	−0.0216 (3)	0.7784 (2)	0.0349 (6)
H3B	0.2667	0.0422	0.8292	0.042*
H3C	0.2378	−0.0719	0.7465	0.042*
O1	0.32649 (9)	0.2536 (2)	0.77614 (16)	0.0390 (5)
O2	0.28689 (9)	0.4695 (3)	0.46998 (17)	0.0389 (5)
C1	0.35718 (12)	0.3510 (4)	0.7583 (2)	0.0324 (7)
C2	0.34744 (12)	0.4106 (3)	0.6532 (2)	0.0300 (6)
C3	0.38339 (13)	0.5084 (4)	0.6438 (3)	0.0393 (7)
H3A	0.3776	0.5434	0.5746	0.047*
C4	0.42691 (15)	0.5551 (4)	0.7325 (3)	0.0490 (9)
H4A	0.4504	0.6198	0.7236	0.059*
C5	0.43535 (14)	0.5043 (4)	0.8359 (3)	0.0491 (9)
H5A	0.4643	0.5369	0.8971	0.059*
C6	0.40102 (15)	0.4058 (4)	0.8483 (3)	0.0435 (8)
H6A	0.4070	0.3745	0.9185	0.052*
C7	0.29969 (12)	0.3788 (3)	0.5520 (2)	0.0287 (6)
C8	0.32285 (14)	−0.1992 (4)	0.7391 (3)	0.0432 (8)
H8A	0.3524	−0.2664	0.7718	0.052*
H8B	0.2934	−0.2588	0.6909	0.052*
C9	0.31175 (14)	−0.1279 (4)	0.8275 (3)	0.0439 (8)
H9A	0.3035	−0.2062	0.8678	0.053*
H9B	0.3421	−0.0739	0.8784	0.053*
O1W	0.19090 (11)	0.2778 (3)	0.04279 (18)	0.0487 (6)
H01A	0.1825	0.2636	0.0948	0.073*
H01B	0.1972	0.1785	0.0279	0.073*
N4	0.52553 (14)	0.0566 (4)	0.8992 (3)	0.0605 (9)
O3	0.44552 (14)	−0.0441 (5)	0.8158 (3)	0.0913 (12)
C10	0.4743 (2)	0.0630 (7)	0.8429 (4)	0.0735 (14)

H10A	0.4630	0.1761	0.8218	0.088*
C11	0.5515 (2)	−0.0861 (6)	0.9321 (4)	0.0772 (14)
H11A	0.5265	−0.1662	0.9137	0.116*
H11B	0.5726	−0.0856	1.0098	0.116*
H11C	0.5730	−0.1022	0.8947	0.116*
C12	0.5555 (2)	0.1936 (7)	0.9292 (5)	0.1004 (19)
H12A	0.5332	0.2793	0.8992	0.151*
H12B	0.5809	0.1910	0.9009	0.151*
H12C	0.5724	0.2020	1.0077	0.151*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0396 (2)	0.0271 (2)	0.02645 (19)	−0.00065 (16)	0.01315 (16)	0.00291 (13)
N1	0.0334 (14)	0.0287 (14)	0.0246 (11)	−0.0044 (11)	0.0085 (10)	0.0009 (9)
N2	0.0362 (15)	0.0356 (15)	0.0336 (13)	−0.0013 (12)	0.0139 (12)	−0.0032 (11)
N3	0.0359 (15)	0.0367 (15)	0.0321 (12)	−0.0038 (12)	0.0146 (12)	0.0004 (11)
O1	0.0534 (15)	0.0357 (13)	0.0272 (10)	−0.0105 (11)	0.0168 (10)	−0.0020 (9)
O2	0.0453 (14)	0.0337 (12)	0.0315 (11)	−0.0107 (11)	0.0107 (10)	0.0072 (9)
C1	0.0371 (18)	0.0246 (15)	0.0328 (14)	0.0026 (13)	0.0125 (13)	−0.0031 (12)
C2	0.0311 (16)	0.0262 (15)	0.0310 (14)	0.0028 (13)	0.0117 (13)	0.0007 (11)
C3	0.0365 (19)	0.0367 (19)	0.0430 (17)	−0.0018 (15)	0.0155 (15)	0.0036 (14)
C4	0.040 (2)	0.044 (2)	0.060 (2)	−0.0159 (17)	0.0179 (17)	−0.0031 (17)
C5	0.037 (2)	0.044 (2)	0.0475 (19)	−0.0014 (17)	0.0006 (16)	−0.0040 (15)
C6	0.046 (2)	0.040 (2)	0.0344 (16)	−0.0013 (16)	0.0077 (15)	−0.0013 (13)
C7	0.0313 (16)	0.0302 (16)	0.0259 (13)	−0.0001 (13)	0.0134 (12)	−0.0007 (11)
C8	0.044 (2)	0.0284 (18)	0.055 (2)	0.0038 (15)	0.0195 (17)	0.0048 (14)
C9	0.044 (2)	0.048 (2)	0.0367 (16)	0.0013 (16)	0.0144 (15)	0.0159 (15)
O1W	0.0784 (19)	0.0356 (13)	0.0357 (12)	0.0049 (13)	0.0280 (13)	−0.0001 (10)
N4	0.050 (2)	0.066 (2)	0.060 (2)	−0.0007 (18)	0.0177 (17)	−0.0060 (17)
O3	0.055 (2)	0.123 (3)	0.089 (3)	−0.025 (2)	0.0244 (19)	−0.027 (2)
C10	0.057 (3)	0.093 (4)	0.064 (3)	0.004 (3)	0.019 (2)	−0.011 (3)
C11	0.080 (4)	0.076 (4)	0.074 (3)	0.018 (3)	0.032 (3)	0.007 (2)
C12	0.087 (4)	0.081 (4)	0.107 (4)	−0.026 (3)	0.018 (3)	−0.007 (3)

Geometric parameters (Å, °)

Zn1—N1	2.003 (2)	C4—H4A	0.9300
Zn1—N2	2.057 (3)	C5—C6	1.378 (5)
Zn1—N3	2.101 (3)	C5—H5A	0.9300
Zn1—O1	2.049 (2)	C6—H6A	0.9300
Zn1—O2^{i}	2.121 (2)	C8—C9	1.500 (5)
N1—C7	1.317 (4)	C8—H8A	0.9700
N1—N1^{i}	1.396 (5)	C8—H8B	0.9700
N2—C8	1.477 (4)	C9—H9A	0.9700
N2—H2A	0.9000	C9—H9B	0.9700
N2—H2B	0.9000	O1W—H01A	0.8457
N3—C9	1.476 (4)	O1W—H01B	0.9335

N3—H3B	0.9000	N4—C10	1.335 (6)
N3—H3C	0.9000	N4—C11	1.432 (6)
O1—C1	1.325 (4)	N4—C12	1.435 (6)
O2—C7	1.286 (4)	O3—C10	1.202 (6)
O2—Zn1^{i}	2.121 (2)	C10—H10A	1.0485
C1—C6	1.405 (5)	C11—H11A	0.9600
C1—C2	1.424 (4)	C11—H11B	0.9600
C2—C3	1.392 (4)	C11—H11C	0.9600
C2—C7	1.486 (4)	C12—H12A	0.9600
C3—C4	1.369 (5)	C12—H12B	0.9600
C3—H3A	0.9300	C12—H12C	0.9600
C4—C5	1.386 (5)		
N1—Zn1—O1	86.46 (10)	C6—C5—H5A	119.9
N1—Zn1—N2	119.46 (11)	C4—C5—H5A	119.9
O1—Zn1—N2	106.06 (11)	C5—C6—C1	122.1 (3)
N1—Zn1—N3	154.15 (11)	C5—C6—H6A	119.0
O1—Zn1—N3	90.96 (10)	C1—C6—H6A	119.0
N2—Zn1—N3	85.97 (11)	O2—C7—N1	122.3 (3)
N1—Zn1—O2^{i}	76.84 (9)	O2—C7—C2	118.9 (3)
O1—Zn1—O2^{i}	149.38 (10)	N1—C7—C2	118.8 (3)
N2—Zn1—O2^{i}	104.49 (11)	N2—C8—C9	109.7 (3)
N3—Zn1—O2^{i}	93.13 (10)	N2—C8—H8A	109.7
C7—N1—N1^{i}	113.3 (3)	C9—C8—H8A	109.7
C7—N1—Zn1	130.7 (2)	N2—C8—H8B	109.7
N1^{i}—N1—Zn1	115.9 (2)	C9—C8—H8B	109.7
C8—N2—Zn1	106.1 (2)	H8A—C8—H8B	108.2
C8—N2—H2A	110.5	N3—C9—C8	109.9 (3)
Zn1—N2—H2A	110.5	N3—C9—H9A	109.7
C8—N2—H2B	110.5	C8—C9—H9A	109.7
Zn1—N2—H2B	110.5	N3—C9—H9B	109.7
H2A—N2—H2B	108.7	C8—C9—H9B	109.7
C9—N3—Zn1	103.29 (19)	H9A—C9—H9B	108.2
C9—N3—H3B	111.1	H01A—O1W—H01B	101.0
Zn1—N3—H3B	111.1	C10—N4—C11	120.9 (5)
C9—N3—H3C	111.1	C10—N4—C12	120.3 (5)
Zn1—N3—H3C	111.1	C11—N4—C12	118.8 (4)
H3B—N3—H3C	109.1	O3—C10—N4	125.7 (6)
C1—O1—Zn1	121.85 (17)	O3—C10—H10A	124.9
C7—O2—Zn1^{i}	111.55 (19)	N4—C10—H10A	109.3
O1—C1—C6	118.8 (3)	N4—C11—H11A	109.5
O1—C1—C2	124.1 (3)	N4—C11—H11B	109.5
C6—C1—C2	117.0 (3)	H11A—C11—H11B	109.5
C3—C2—C1	119.0 (3)	N4—C11—H11C	109.5
C3—C2—C7	117.3 (3)	H11A—C11—H11C	109.5
C1—C2—C7	123.6 (3)	H11B—C11—H11C	109.5
C4—C3—C2	122.6 (3)	N4—C12—H12A	109.5
C4—C3—H3A	118.7	N4—C12—H12B	109.5

C2—C3—H3A	118.7	H12A—C12—H12B	109.5
C3—C4—C5	118.8 (3)	N4—C12—H12C	109.5
C3—C4—H4A	120.6	H12A—C12—H12C	109.5
C5—C4—H4A	120.6	H12B—C12—H12C	109.5
C6—C5—C4	120.3 (3)		
O1—Zn1—N1—C7	25.5 (3)	O1—C1—C2—C7	4.5 (5)
N2—Zn1—N1—C7	−80.9 (3)	C6—C1—C2—C7	−172.4 (3)
N3—Zn1—N1—C7	110.4 (3)	C1—C2—C3—C4	−2.8 (5)
O2^{i}—Zn1—N1—C7	179.7 (3)	C7—C2—C3—C4	175.0 (3)
O1—Zn1—N1—N1^{i}	−156.1 (3)	C2—C3—C4—C5	−0.6 (6)
N2—Zn1—N1—N1^{i}	97.5 (3)	C3—C4—C5—C6	1.5 (6)
N3—Zn1—N1—N1^{i}	−71.2 (4)	C4—C5—C6—C1	1.2 (6)
O2^{i}—Zn1—N1—N1^{i}	−1.9 (3)	O1—C1—C6—C5	178.4 (3)
N1—Zn1—N2—C8	−164.09 (19)	C2—C1—C6—C5	−4.5 (5)
O1—Zn1—N2—C8	100.8 (2)	Zn1^{i}—O2—C7—N1	2.5 (4)
N3—Zn1—N2—C8	11.0 (2)	Zn1^{i}—O2—C7—C2	−177.8 (2)
O2^{i}—Zn1—N2—C8	−81.2 (2)	N1^{i}—N1—C7—O2	−0.9 (5)
N1—Zn1—N3—C9	−172.2 (2)	Zn1—N1—C7—O2	177.5 (2)
O1—Zn1—N3—C9	−88.4 (2)	N1^{i}—N1—C7—C2	179.4 (3)
N2—Zn1—N3—C9	17.6 (2)	Zn1—N1—C7—C2	−2.2 (4)
O2^{i}—Zn1—N3—C9	122.0 (2)	C3—C2—C7—O2	−18.4 (4)
N1—Zn1—O1—C1	−39.0 (2)	C1—C2—C7—O2	159.3 (3)
N2—Zn1—O1—C1	80.7 (2)	C3—C2—C7—N1	161.4 (3)
N3—Zn1—O1—C1	166.7 (2)	C1—C2—C7—N1	−20.9 (4)
O2^{i}—Zn1—O1—C1	−95.5 (3)	Zn1—N2—C8—C9	−38.1 (3)
Zn1—O1—C1—C6	−151.3 (2)	Zn1—N3—C9—C8	−43.6 (3)
Zn1—O1—C1—C2	31.8 (4)	N2—C8—C9—N3	57.5 (4)
O1—C1—C2—C3	−177.8 (3)	C11—N4—C10—O3	0.9 (8)
C6—C1—C2—C3	5.2 (4)	C12—N4—C10—O3	−178.3 (5)

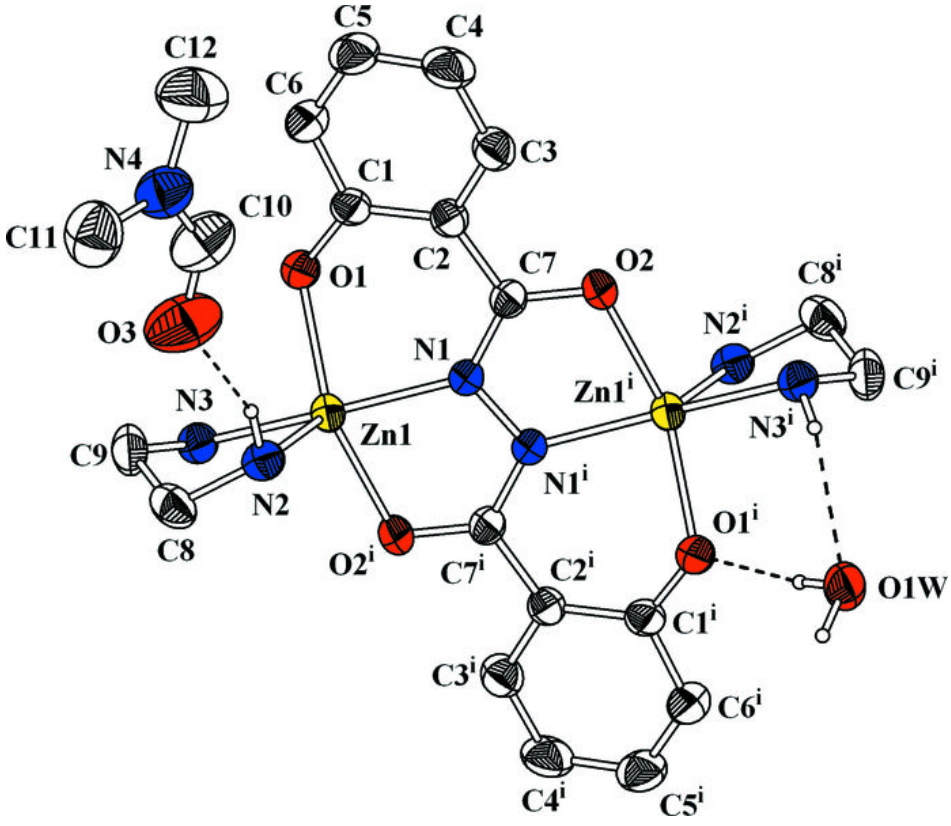
Symmetry codes: (i) −*x*+1/2, −*y*+1/2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···O3	0.90	2.09	2.956 (5)	162
N3—H3C···O1^{ii}	0.90	2.32	3.177 (4)	159
O1W—H01A···O1^{i}	0.85	1.88	2.716 (3)	171
O1W—H01B···O2^{iii}	0.93	1.90	2.814 (3)	168
N2—H2A···O1W^{iii}	0.90	2.10	2.998 (4)	172
N3—H3B···O1W^{i}	0.90	2.27	3.064 (4)	146

Symmetry codes: (ii) −*x*+1/2, *y*−1/2, −*z*+3/2; (i) −*x*+1/2, −*y*+1/2, −*z*+1; (iii) −*x*+1/2, *y*−1/2, −*z*+1/2.

Fig. 1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C4
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C6
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N4
C1
C10
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O1
C2
C7
O2
C8i
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N1
C9i
Zn1i
N3
Zn1
N3i
C9
N1i
N2
O1i
C8
O2i
C7i
C2i
O1W
C1i
C3i
C6i
C4i
C5i

Fig. 2