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catena-Poly[[[(2,2′-bipyridyl-κ^2N,N')-zinc(II)]-μ_3-(5-hydroxyisophthalato-$\kappa^4O,O':O'':O'''$)] monohydrate]

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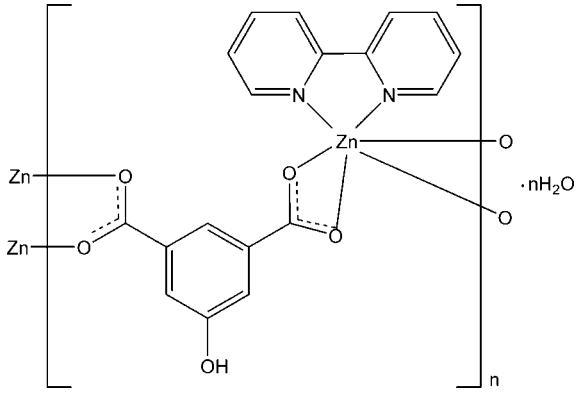
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.111; data-to-parameter ratio = 15.5.

The title compound, $\{[Zn(C_8H_4O_5)(C_{10}H_8N_2)]\cdot H_2O\}_n$, was synthesized by reacting $Zn(NO_3)_2$, 5-hydroxyisophthalic acid and 2,2′-bipyridine under hydrothermal conditions. Self-assembly between the bridging ligands, chelating ligands and metal ions results in a one-dimensional coordination polymer, in which the Zn^{II} atom is six-coordinate and shows a $[ZnN_2O_4]$ octahedral geometry. The ribbons are interconnected by an extensive network of hydrogen bonds involving the water molecule, the hydroxyl group and the carboxylate O atoms, forming a two-dimensional layer. These layers are connected through π–π interactions between the pyridyl rings [centroid-to-centroid distance 3.57 (1) Å].

Related literature

For related literature, see: Amabilino & Stoddart (1995); Inoue *et al.* (2001); Plater *et al.* (2001).



Experimental

Crystal data

$[Zn(C_8H_4O_5)(C_{10}H_8N_2)]\cdot H_2O$
M_r = 419.68
Monoclinic, $P2/n$
a = 8.777 (2) Å
b = 10.9763 (16) Å
c = 17.981 (3) Å
β = 103.650 (14)°
V = 1683.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.50 mm^{-1}
T = 293 (2) K
0.37 × 0.32 × 0.23 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.608, T_{max} = 0.720
5111 measured reflections
3880 independent reflections
2902 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.111
S = 1.02
3880 reflections
250 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O4^{i}	2.0449 (19)	Zn1—N2	2.131 (2)
Zn1—O3^{ii}	2.087 (2)	Zn1—O1	2.135 (2)
Zn1—N1	2.129 (2)	Zn1—O2	2.326 (3)
O4^{i}—Zn1—O3^{ii}	93.05 (8)	N1—Zn1—O1	143.52 (9)
O4^{i}—Zn1—N1	95.83 (9)	N2—Zn1—O1	97.00 (9)
O3^{ii}—Zn1—N1	123.06 (9)	O4^{i}—Zn1—O2	99.15 (9)
O4^{i}—Zn1—N2	165.77 (8)	O3^{ii}—Zn1—O2	147.19 (8)
O3^{ii}—Zn1—N2	82.17 (9)	N1—Zn1—O2	86.00 (9)
N1—Zn1—N2	75.95 (10)	N2—Zn1—O2	91.94 (9)
O4^{i}—Zn1—O1	96.42 (9)	O1—Zn1—O2	58.17 (8)
O3^{ii}—Zn1—O1	90.39 (9)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5B···O1W^{iii}	0.82	1.86	2.646 (4)	161
O1W—H1WA···O4^{iv}	0.85 (3)	2.02 (2)	2.790 (3)	150 (4)
O1W—H1WB···O1^{v}	0.85 (3)	2.25 (3)	2.910 (4)	135 (4)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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, 2001); 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: HY2097).

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References

Amabilino, D. B. & Stoddart, J. F. (1995). *Chem. Rev.* **95**, 2725–2828.
Bruker (2001). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Inoue, K., Imai, H., Ghalsasi, P. S., Kikuchi, K., Ohba, M., Okawa, H. & Yakhmi, J. V. (2001). *Angew. Chem. Int. Ed.* **40**, 4242–4245.
Plater, M., Foreman, M., Howie, R., Skakle, J., McWilliam, S. & Coronado, E. (2001). *Polyhedron*, **18**, 2293–2303.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

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catena-Poly[[[(2,2'-bipyridyl-κ^2N,N')zinc(II)]-μ_3-(5-hydroxyisophthalato-$\kappa^4O,O':O'':O'''$)] monohydrate]

X.-F. Li, Y. An and Y.-S. Yin

Comment

The design and construction of coordination polymers has attracted much attention owing to their intriguing topologies and potential applications as functional materials (Inoue *et al.*, 2001). Many networks with various structural motifs have been documented in the past decade (Amabilino & Stoddart, 1995). Unlike pyridine-2,4-, 3,4- 2,5- and 2,6-dicarboxylic acids, which have been widely used as bridging ligands to assemble various coordination polymers, 5-hydroxyisophthalic acid (H_2hip) as a member of the multicarboxylate ligands has been rarely reported (Plater *et al.*, 2001). We report here the synthesis and structure of a zinc(II) coordination polymer constructed from 5-hydroxyisophthalic acid and 2,2'-bipyridine (bpy).

In the title compound, the asymmetric unit contains one Zn^{II} atom, one hip ligand, one bpy ligand and one lattice water molecule. Each Zn^{II} atom is coordinated by four O atoms from three hip ligands (Table 1) and two N atoms from a chelating bpy ligand in a distorted octahedral geometry (Fig. 1). Each pair of adjacent Zn^{II} atoms are bridged by two hip ligands to form a binuclear Zn subunit. The adjacent binuclear subunits are further interconnected by two hip ligands to form a one-dimensional ribbon running along the $a + c$ direction (Fig. 2). These ribbons are decorated with bpy ligands alternately at two sides.

The ribbons are interconnected by an extensive network of hydrogen bonds involving water molecule, hydroxyl group and carboxylate O atoms (Table 2), forming a two-dimensional layer. The layers are connected through π–π interactions between the pyridyl rings with a centroid-to-centroid distance of 3.57 (1) Å.

Experimental

A mixture of $Zn(NO_3)_2{\cdot}2H_2O$ (0.120 g, 0.5 mmol), 5-hydroxyisophthalic acid (0.091 g, 0.5 mmol), 2,2'-bipyridine (0.078 g, 0.5 mmol), NaOH (0.04 g, 1 mmol) and water (10 ml) was sealed in a 23 ml Teflon-lined reactor, which was heated at 453 K for 6 d and then cooled to room temperature at a rate of 5 K h^{-1} (yield 58%). Analysis calculated for $C_{18}H_{14}N_2O_6Zn$: C 51.51, H 3.36, N 6.67%; found: C 51.68, H 3.64, N 6.73%.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of water molecule were located in a difference Fourier map and refined with a distance restrain of O—H = 0.85 (1) and $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

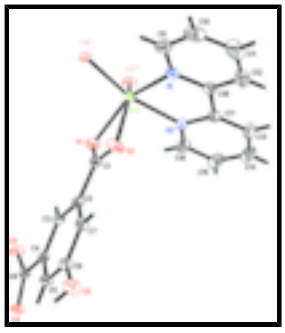

Fig. 1. Part of the polymeric structure of the title compound with symmetric equivalent atoms to complete the Zn coordination. Displacement ellipsoids are drawn at the 30% probability level. Lattice water molecule has been omitted. [Symmetry codes: (i) $x + 1/2, -y + 2, z + 1/2$; (ii) $-x, -y + 2, -z$.]

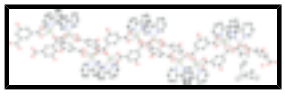

Fig. 2. A view of the one-dimensional ribbon structure. H atoms and lattice water molecule have been omitted for clarity.

catena-Poly[[(2,2'-bipyridyl-κ^2N,N')zinc(II)]-μ_3– (5-hydroxyisophthalato-$\kappa^4O,O':O'':O'''$) monohydrate]

Crystal data

$[Zn(C_8H_4O_5)(C_{10}H_8N_2)]\cdot H_2O$	$F_{000} = 856$
$M_r = 419.68$	$D_x = 1.656$ Mg m^{-3}
Monoclinic, $P2/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yac	Cell parameters from 3685 reflections
$a = 8.777$ (2) Å	$\theta = 2.5$–22.4º
$b = 10.9763$ (16) Å	$\mu = 1.50$ mm^{-1}
$c = 17.981$ (3) Å	$T = 293$ (2) K
$\beta = 103.650$ (14)º	Block, colourless
$V = 1683.4$ (5) Å^3	0.37 × 0.32 × 0.23 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3880 independent reflections
Radiation source: fine-focus sealed tube	2902 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
$T = 293(2)$ K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 1$
$T_{min} = 0.608$, $T_{max} = 0.720$	$k = -1 \rightarrow 14$
5111 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.111$

$S = 1.02$

3880 reflections

250 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.43$ e Å^{-3}

$\Delta\rho_{min} = -0.72$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.04335 (4)	0.79387 (3)	0.171663 (16)	0.02547 (12)
C1	−0.1934 (4)	0.8493 (3)	0.06332 (15)	0.0333 (7)
C2	−0.3194 (3)	0.8800 (3)	−0.00631 (14)	0.0266 (6)
C3	−0.2932 (3)	0.9639 (3)	−0.06037 (14)	0.0265 (6)
H3A	−0.1974	1.0041	−0.0529	0.032*
C4	−0.4116 (3)	0.9871 (2)	−0.12579 (14)	0.0252 (6)
C5	−0.5553 (3)	0.9282 (3)	−0.13638 (15)	0.0294 (6)
H5A	−0.6339	0.9437	−0.1800	0.035*
C6	−0.5818 (3)	0.8457 (3)	−0.08168 (16)	0.0290 (6)
C7	−0.4635 (4)	0.8226 (3)	−0.01715 (15)	0.0297 (6)
H7A	−0.4811	0.7678	0.0194	0.036*
C8	−0.3810 (3)	1.0759 (3)	−0.18412 (14)	0.0260 (6)
C9	−0.0538 (4)	0.6455 (3)	0.29853 (17)	0.0422 (8)
H9A	−0.0723	0.7214	0.3176	0.051*
C10	−0.0911 (5)	0.5421 (4)	0.33393 (19)	0.0558 (10)
H10A	−0.1345	0.5484	0.3762	0.067*
C11	−0.0640 (5)	0.4309 (4)	0.3066 (2)	0.0634 (12)
H11A	−0.0877	0.3604	0.3303	0.076*
C12	−0.0003 (5)	0.4235 (3)	0.2430 (2)	0.0509 (9)
H12A	0.0187	0.3482	0.2232	0.061*
C13	0.1464 (4)	0.4292 (3)	0.1073 (2)	0.0473 (8)
H13A	0.1391	0.3524	0.1280	0.057*
C14	0.2047 (4)	0.4431 (4)	0.0426 (2)	0.0546 (10)
H14A	0.2353	0.3751	0.0188	0.066*
C15	0.2171 (4)	0.5564 (4)	0.0140 (2)	0.0510 (9)

H15A	0.2572	0.5670	−0.0290	0.061*
C16	0.1694 (4)	0.6549 (3)	0.04976 (17)	0.0393 (7)
H16A	0.1782	0.7325	0.0303	0.047*
C17	0.0992 (3)	0.5322 (3)	0.14052 (17)	0.0320 (6)
C18	0.0340 (4)	0.5299 (3)	0.20978 (17)	0.0333 (7)
N1	0.0082 (3)	0.6396 (2)	0.23741 (13)	0.0313 (5)
N2	0.1105 (3)	0.6432 (2)	0.11174 (13)	0.0297 (5)
O1	−0.0610 (3)	0.9002 (2)	0.07345 (12)	0.0420 (5)
O2	−0.2190 (3)	0.7718 (2)	0.10882 (12)	0.0491 (6)
O3	−0.2652 (2)	1.1432 (2)	−0.16680 (11)	0.0359 (5)
O4	−0.4802 (2)	1.07902 (19)	−0.24867 (10)	0.0329 (5)
O5	−0.7167 (3)	0.7825 (2)	−0.08941 (13)	0.0432 (6)
H5B	−0.7905	0.8242	−0.1123	0.065*
O1W	0.9935 (4)	0.1276 (2)	0.15885 (16)	0.0578 (7)
H1WA	1.003 (6)	0.086 (3)	0.1992 (13)	0.087*
H1WB	1.014 (6)	0.085 (3)	0.1235 (15)	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03291 (19)	0.02413 (18)	0.01813 (16)	0.00019 (14)	0.00356 (12)	−0.00048 (12)
C1	0.0404 (17)	0.0369 (16)	0.0210 (12)	0.0125 (14)	0.0042 (12)	−0.0026 (12)
C2	0.0306 (14)	0.0297 (14)	0.0193 (11)	0.0034 (12)	0.0058 (10)	−0.0008 (11)
C3	0.0263 (13)	0.0314 (14)	0.0206 (11)	−0.0006 (12)	0.0027 (10)	−0.0018 (11)
C4	0.0296 (14)	0.0262 (13)	0.0195 (11)	−0.0015 (12)	0.0053 (10)	0.0002 (10)
C5	0.0307 (14)	0.0337 (15)	0.0216 (12)	0.0005 (13)	0.0018 (11)	0.0021 (11)
C6	0.0276 (14)	0.0304 (15)	0.0292 (13)	−0.0018 (12)	0.0071 (11)	0.0015 (12)
C7	0.0371 (16)	0.0284 (14)	0.0246 (12)	0.0024 (13)	0.0090 (12)	0.0044 (11)
C8	0.0298 (14)	0.0274 (14)	0.0209 (12)	−0.0011 (12)	0.0066 (11)	0.0001 (10)
C9	0.0488 (19)	0.050 (2)	0.0289 (14)	−0.0088 (17)	0.0105 (14)	−0.0011 (14)
C10	0.064 (2)	0.071 (3)	0.0339 (17)	−0.015 (2)	0.0151 (17)	0.0118 (18)
C11	0.077 (3)	0.054 (2)	0.060 (2)	−0.018 (2)	0.019 (2)	0.023 (2)
C12	0.060 (2)	0.0345 (18)	0.056 (2)	−0.0060 (17)	0.0090 (18)	0.0107 (16)
C13	0.054 (2)	0.0302 (16)	0.055 (2)	0.0049 (16)	0.0071 (17)	−0.0062 (15)
C14	0.053 (2)	0.052 (2)	0.061 (2)	0.0072 (19)	0.0178 (19)	−0.0225 (19)
C15	0.051 (2)	0.063 (2)	0.0433 (19)	−0.0040 (19)	0.0198 (17)	−0.0173 (18)
C16	0.0465 (19)	0.0411 (18)	0.0344 (15)	−0.0047 (16)	0.0175 (14)	−0.0064 (14)
C17	0.0290 (15)	0.0302 (15)	0.0338 (15)	−0.0015 (13)	0.0014 (12)	−0.0023 (12)
C18	0.0325 (15)	0.0300 (15)	0.0336 (15)	−0.0038 (13)	0.0002 (12)	0.0010 (12)
N1	0.0349 (13)	0.0339 (13)	0.0235 (11)	−0.0032 (11)	0.0038 (10)	0.0042 (10)
N2	0.0314 (13)	0.0285 (12)	0.0296 (12)	−0.0034 (11)	0.0083 (10)	−0.0056 (10)
O1	0.0365 (12)	0.0500 (14)	0.0333 (11)	0.0009 (11)	−0.0044 (9)	0.0020 (10)
O2	0.0505 (15)	0.0616 (16)	0.0317 (11)	0.0056 (13)	0.0029 (10)	0.0201 (11)
O3	0.0363 (11)	0.0440 (12)	0.0266 (10)	−0.0162 (10)	0.0062 (9)	0.0010 (9)
O4	0.0380 (11)	0.0356 (11)	0.0211 (9)	−0.0060 (9)	−0.0009 (8)	0.0071 (8)
O5	0.0322 (12)	0.0487 (14)	0.0468 (13)	−0.0086 (11)	0.0057 (10)	0.0143 (11)
O1W	0.0690 (18)	0.0398 (14)	0.0631 (17)	0.0135 (14)	0.0125 (15)	0.0079 (13)

Geometric parameters (Å, °)

Zn1—O4^{i}	2.0449 (19)	C9—H9A	0.9300
Zn1—O3^{ii}	2.087 (2)	C10—C11	1.357 (6)
Zn1—N1	2.129 (2)	C10—H10A	0.9300
Zn1—N2	2.131 (2)	C11—C12	1.390 (6)
Zn1—O1	2.135 (2)	C11—H11A	0.9300
Zn1—O2	2.326 (3)	C12—C18	1.377 (4)
C1—O2	1.237 (4)	C12—H12A	0.9300
C1—O1	1.263 (4)	C13—C17	1.387 (4)
C1—C2	1.500 (4)	C13—C14	1.386 (5)
C2—C7	1.385 (4)	C13—H13A	0.9300
C2—C3	1.397 (4)	C14—C15	1.360 (6)
C3—C4	1.397 (4)	C14—H14A	0.9300
C3—H3A	0.9300	C15—C16	1.373 (5)
C4—C5	1.390 (4)	C15—H15A	0.9300
C4—C8	1.502 (4)	C16—N2	1.341 (4)
C5—C6	1.396 (4)	C16—H16A	0.9300
C5—H5A	0.9300	C17—N2	1.337 (4)
C6—O5	1.351 (4)	C17—C18	1.489 (4)
C6—C7	1.386 (4)	C18—N1	1.342 (4)
C7—H7A	0.9300	O3—Zn1^{ii}	2.087 (2)
C8—O3	1.235 (3)	O4—Zn1^{iii}	2.0449 (19)
C8—O4	1.277 (3)	O5—H5B	0.8200
C9—N1	1.338 (4)	O1W—H1WA	0.85 (3)
C9—C10	1.378 (5)	O1W—H1WB	0.85 (3)
O4^{i}—Zn1—O3^{ii}	93.05 (8)	O3—C8—O4	123.9 (3)
O4^{i}—Zn1—N1	95.83 (9)	O3—C8—C4	118.9 (2)
O3^{ii}—Zn1—N1	123.06 (9)	O4—C8—C4	117.2 (2)
O4^{i}—Zn1—N2	165.77 (8)	N1—C9—C10	121.7 (3)
O3^{ii}—Zn1—N2	82.17 (9)	N1—C9—H9A	119.1
N1—Zn1—N2	75.95 (10)	C10—C9—H9A	119.1
O4^{i}—Zn1—O1	96.42 (9)	C11—C10—C9	119.5 (3)
O3^{ii}—Zn1—O1	90.39 (9)	C11—C10—H10A	120.2
N1—Zn1—O1	143.52 (9)	C9—C10—H10A	120.2
N2—Zn1—O1	97.00 (9)	C10—C11—C12	119.3 (3)
O4^{i}—Zn1—O2	99.15 (9)	C10—C11—H11A	120.4
O3^{ii}—Zn1—O2	147.19 (8)	C12—C11—H11A	120.4
N1—Zn1—O2	86.00 (9)	C18—C12—C11	118.6 (4)
N2—Zn1—O2	91.94 (9)	C18—C12—H12A	120.7
O1—Zn1—O2	58.17 (8)	C11—C12—H12A	120.7
O4^{i}—Zn1—C1	99.93 (9)	C17—C13—C14	118.6 (3)
O3^{ii}—Zn1—C1	119.10 (9)	C17—C13—H13A	120.7
N1—Zn1—C1	114.40 (10)	C14—C13—H13A	120.7
N2—Zn1—C1	94.09 (9)	C15—C14—C13	119.7 (3)

O1—Zn1—C1	29.40 (9)	C15—C14—H14A	120.1
O2—Zn1—C1	28.80 (9)	C13—C14—H14A	120.1
O2—C1—O1	120.9 (3)	C14—C15—C16	118.9 (3)
O2—C1—C2	119.5 (3)	C14—C15—H15A	120.5
O1—C1—C2	119.6 (3)	C16—C15—H15A	120.5
O2—C1—Zn1	64.87 (17)	N2—C16—C15	122.2 (3)
O1—C1—Zn1	56.11 (15)	N2—C16—H16A	118.9
C2—C1—Zn1	173.3 (2)	C15—C16—H16A	118.9
C7—C2—C3	119.8 (2)	N2—C17—C13	121.3 (3)
C7—C2—C1	119.0 (3)	N2—C17—C18	114.7 (3)
C3—C2—C1	121.2 (3)	C13—C17—C18	124.0 (3)
C4—C3—C2	119.6 (3)	N1—C18—C12	121.8 (3)
C4—C3—H3A	120.2	N1—C18—C17	115.2 (3)
C2—C3—H3A	120.2	C12—C18—C17	123.0 (3)
C5—C4—C3	120.1 (2)	C9—N1—C18	119.0 (3)
C5—C4—C8	120.8 (2)	C9—N1—Zn1	123.9 (2)
C3—C4—C8	119.1 (2)	C18—N1—Zn1	116.67 (19)
C4—C5—C6	120.1 (2)	C17—N2—C16	119.2 (3)
C4—C5—H5A	119.9	C17—N2—Zn1	117.20 (19)
C6—C5—H5A	119.9	C16—N2—Zn1	123.5 (2)
O5—C6—C7	117.2 (3)	C1—O1—Zn1	94.49 (18)
O5—C6—C5	123.3 (3)	C1—O2—Zn1	86.3 (2)
C7—C6—C5	119.5 (3)	C8—O3—Zn1^{ii}	155.2 (2)
C2—C7—C6	120.9 (3)	C8—O4—Zn1^{iii}	119.67 (18)
C2—C7—H7A	119.5	C6—O5—H5B	109.5
C6—C7—H7A	119.5	H1WA—O1W—H1WB	111 (3)
O4^{i}—Zn1—C1—O2	−90.96 (19)	C17—C18—N1—Zn1	5.8 (3)
O3^{ii}—Zn1—C1—O2	169.88 (17)	O4^{i}—Zn1—N1—C9	16.1 (3)
N1—Zn1—C1—O2	10.2 (2)	O3^{ii}—Zn1—N1—C9	113.6 (2)
N2—Zn1—C1—O2	86.58 (19)	N2—Zn1—N1—C9	−175.7 (3)
O1—Zn1—C1—O2	−176.4 (3)	O1—Zn1—N1—C9	−93.0 (3)
O4^{i}—Zn1—C1—O1	85.45 (18)	O2—Zn1—N1—C9	−82.7 (3)
O3^{ii}—Zn1—C1—O1	−13.7 (2)	C1—Zn1—N1—C9	−87.6 (3)
N1—Zn1—C1—O1	−173.44 (17)	O4^{i}—Zn1—N1—C18	−171.7 (2)
N2—Zn1—C1—O1	−97.02 (18)	O3^{ii}—Zn1—N1—C18	−74.2 (2)
O2—Zn1—C1—O1	176.4 (3)	N2—Zn1—N1—C18	−3.5 (2)
O2—C1—C2—C7	1.5 (4)	O1—Zn1—N1—C18	79.2 (3)
O1—C1—C2—C7	179.3 (3)	O2—Zn1—N1—C18	89.5 (2)
O2—C1—C2—C3	−177.8 (3)	C1—Zn1—N1—C18	84.6 (2)
O1—C1—C2—C3	0.1 (4)	C13—C17—N2—C16	−0.4 (4)
C7—C2—C3—C4	−1.4 (4)	C18—C17—N2—C16	179.3 (3)
C1—C2—C3—C4	177.8 (2)	C13—C17—N2—Zn1	−177.3 (2)
C2—C3—C4—C5	0.9 (4)	C18—C17—N2—Zn1	2.4 (3)
C2—C3—C4—C8	−179.0 (2)	C15—C16—N2—C17	0.8 (5)
C3—C4—C5—C6	0.0 (4)	C15—C16—N2—Zn1	177.5 (3)
C8—C4—C5—C6	179.9 (3)	O4^{i}—Zn1—N2—C17	56.3 (5)

C4—C5—C6—O5	−177.8 (3)	O3^{ii}—Zn1—N2—C17	127.4 (2)
C4—C5—C6—C7	−0.4 (4)	N1—Zn1—N2—C17	0.4 (2)
C3—C2—C7—C6	1.0 (4)	O1—Zn1—N2—C17	−143.2 (2)
C1—C2—C7—C6	−178.3 (3)	O2—Zn1—N2—C17	−85.0 (2)
O5—C6—C7—C2	177.5 (3)	C1—Zn1—N2—C17	−113.8 (2)
C5—C6—C7—C2	−0.1 (4)	O4^{i}—Zn1—N2—C16	−120.5 (4)
C5—C4—C8—O3	166.5 (3)	O3^{ii}—Zn1—N2—C16	−49.4 (2)
C3—C4—C8—O3	−13.6 (4)	N1—Zn1—N2—C16	−176.4 (3)
C5—C4—C8—O4	−11.8 (4)	O1—Zn1—N2—C16	40.1 (3)
C3—C4—C8—O4	168.1 (3)	O2—Zn1—N2—C16	98.2 (2)
N1—C9—C10—C11	0.3 (6)	C1—Zn1—N2—C16	69.5 (3)
C9—C10—C11—C12	−0.6 (6)	O2—C1—O1—Zn1	3.8 (3)
C10—C11—C12—C18	0.3 (6)	C2—C1—O1—Zn1	−174.0 (2)
C17—C13—C14—C15	1.2 (6)	O4^{i}—Zn1—O1—C1	−98.84 (18)
C13—C14—C15—C16	−0.8 (6)	O3^{ii}—Zn1—O1—C1	168.04 (18)
C14—C15—C16—N2	−0.2 (6)	N1—Zn1—O1—C1	10.1 (3)
C14—C13—C17—N2	−0.6 (5)	N2—Zn1—O1—C1	85.89 (18)
C14—C13—C17—C18	179.7 (3)	O2—Zn1—O1—C1	−2.04 (17)
C11—C12—C18—N1	0.3 (5)	O1—C1—O2—Zn1	−3.5 (3)
C11—C12—C18—C17	−178.7 (3)	C2—C1—O2—Zn1	174.3 (2)
N2—C17—C18—N1	−5.4 (4)	O4^{i}—Zn1—O2—C1	93.99 (18)
C13—C17—C18—N1	174.3 (3)	O3^{ii}—Zn1—O2—C1	−16.5 (3)
N2—C17—C18—C12	173.6 (3)	N1—Zn1—O2—C1	−170.74 (19)
C13—C17—C18—C12	−6.7 (5)	N2—Zn1—O2—C1	−94.97 (19)
C10—C9—N1—C18	0.3 (5)	O1—Zn1—O2—C1	2.08 (17)
C10—C9—N1—Zn1	172.4 (3)	O4—C8—O3—Zn1^{ii}	−71.6 (6)
C12—C18—N1—C9	−0.6 (5)	C4—C8—O3—Zn1^{ii}	110.2 (4)
C17—C18—N1—C9	178.4 (3)	O3—C8—O4—Zn1^{iii}	−2.8 (4)
C12—C18—N1—Zn1	−173.2 (3)	C4—C8—O4—Zn1^{iii}	175.39 (17)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5B···O1W^{iv}	0.82	1.86	2.646 (4)	161
O1W—H1WA···O4^{v}	0.85 (3)	2.02 (2)	2.790 (3)	150 (4)
O1W—H1WB···O1^{vi}	0.85 (3)	2.25 (3)	2.910 (4)	135 (4)

Symmetry codes: (iv) −*x*, −*y*+1, −*z*; (v) *x*+3/2, −*y*+1, *z*+1/2; (vi) *x*+1, *y*−1, *z*.

Fig. 1

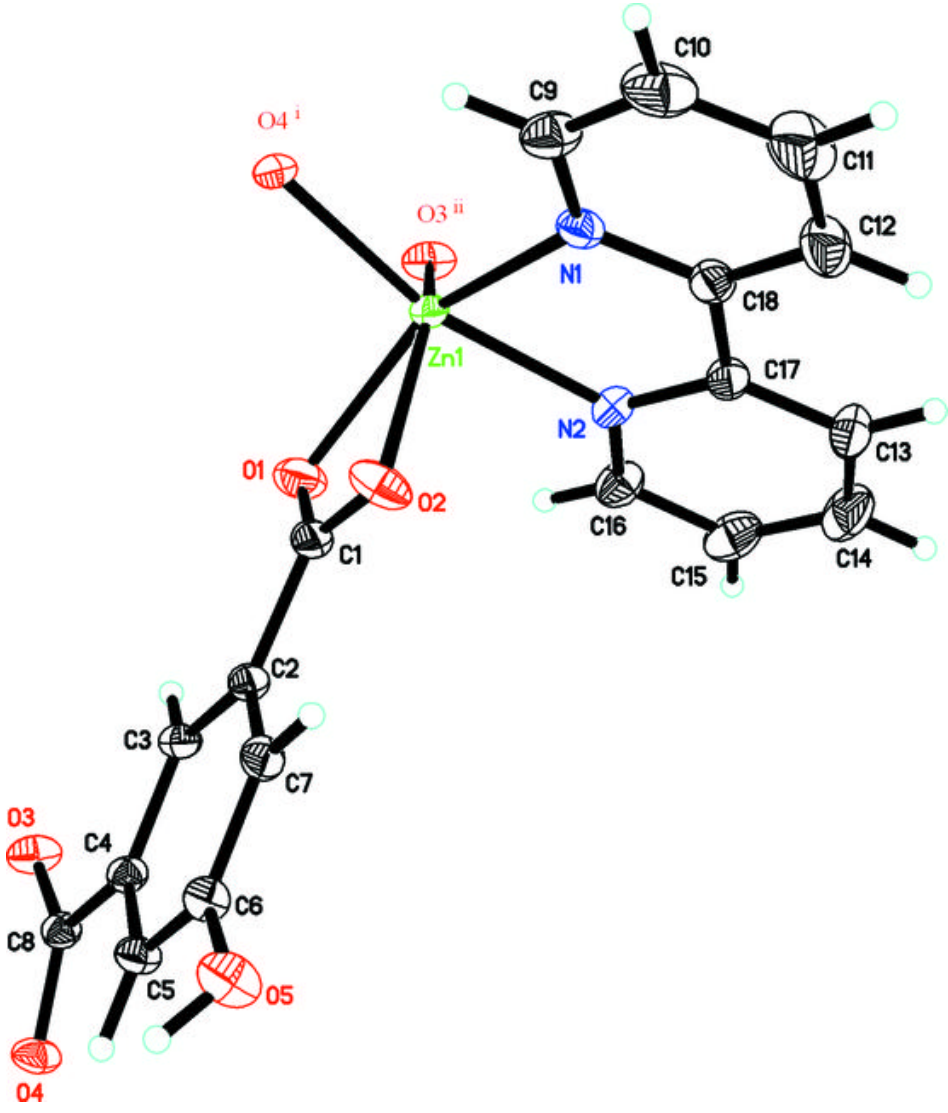
C10
C9
O4 i
C11
O3 ii
C12
N1
C18
Zn1
C17
N2
C13
O1
O2
C16
C1
C15
C14
C2
C3
C7
O3
C4
C6
C8
C5
O5
O4

Fig. 2