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catena-Poly[[[aquabis[3-(4-carboxyphenoxy)propionato-κ^2O,O']zinc(II)]-μ-4,4′-bipyridine-$\kappa^2N:N'$] dihydrate]

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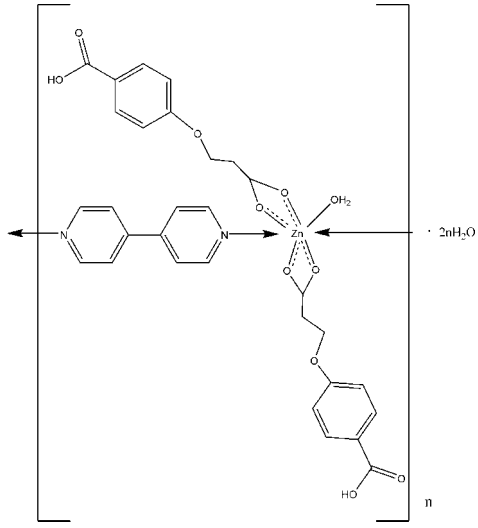
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.118; data-to-parameter ratio = 15.8.

In the title compound, $\{[Zn(C_{10}H_9O_5)_2(C_{10}H_8N_2)(H_2O)]\cdot 2H_2O\}_n$, the Zn atom, which lies on a twofold rotation axis, has a distorted pentagonal–bipyramidal geometry, involving four O atoms from two 3-(4-carboxyphenoxy)propionate groups, two N atoms from two 4,4′-bipyridine ligands and one water molecule, also lying on the symmetry axis. 4,4′-Bipyridine ligands link adjacent Zn atoms, forming a one-dimensional chain structure. Furthermore, a three-dimensional supramolecular network is buildt up *via* hydrogen bonding and π–π stacking interactions [centroid–centroid distance 3.9096 (9) Å].

Related literature

3-(4-Carboxyphenoxy)propionic acid [3-(*p*-cpopH_2)] has been reported previously (Gao & Ng, 2006). In our previous work, the copper(II) and cobalt(II) complexes of 3-(*p*-cpopH_2) have been characterized by X-ray crystallography (Xiao *et al.*, 2007; Kong *et al.*, 2007).



Experimental

Crystal data

$[Zn(C_{10}H_9O_5)_2(C_{10}H_8N_2)(H_2O)]\cdot 2H_2O$
M_r = 693.95
Monoclinic, $P2/c$
a = 11.109 (2) Å
b = 6.0063 (12) Å
c = 22.871 (5) Å
β = 90.54 (3)°
V = 1525.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 295 (2) K
0.28 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.791, T_{max} = 0.858
14159 measured reflections
3498 independent reflections
2191 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.118
S = 1.12
3498 reflections
221 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1*W*	2.052 (3)	Zn1—O2	2.291 (3)
Zn1—N1	2.172 (2)	Zn1—O1	2.298 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{i}	0.846 (10)	1.919 (16)	2.681 (4)	149.3 (14)
O2*W*—H2*W*2···O1^{ii}	0.85 (3)	1.93 (3)	2.782 (3)	177 (4)
O2*W*—H2*W*1···O4^{iii}	0.85 (3)	1.98 (3)	2.826 (3)	173 (4)
O5—H10···O2*W*	0.85 (3)	1.803 (15)	2.632 (3)	164 (4)

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

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Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); 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: BG2117).

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supplementary materials

Acta Cryst. (2007). E**63**, m2791-m2792 [**doi:10.1107/S1600536807050611**]

catena-Poly[[[aquabis[3-(4-carboxyphenoxy)propionato-κ^2O,O']zinc(II)]-μ-4,4'-bipyridine-$\kappa^2N:N'$] dihydrate]

L.-L. Kong, S. Gao and L.-H. Huo

Comment

Our studies have addressed the metal derivatives of carboxyphenoxypropionic acids which are regarded as excellent candidates for the construction of supramolecular architectures. In this line 3-(*p*-CPOPH_2) is not only a multiple coordination ligand, but also may form regular hydrogen bonds by functioning both as a hydrogen bond donor and acceptor(Gao & Ng, 2006). We have recently reported the structures of the cobalt(II) and the copper(II) complexes incorporating the 3-(4-carboxylatophenoxy)propionate group (Kong *et al.*, 2007; Xiao *et al.*, 2007).

The molecular structure of the title complex $[Zn(C_{10}H_8N_2)(C_{10}H_9O_5)_2(H_2O)]_n.2n(H_2O)$is shown in Fig. 1. The 3-(*p*-CPOP)$^{2-}$ ligand coordinates in a chelating fashion to the Zn atom through the deprotonated carboxylate group while the remaining protonated carboxyl group forms a hydrogen bond with an uncoordinated water molecule. The Zn atom, which lies on a two fold axis displays a distorted pentagonal bipyramid geometry involving four O atoms of the two 3-(4-carboxylatophenoxy)propionic acid groups, two N atom from two 4,4'-bipyridine ligands and one water molecule also lying on the two fold axis. The 4,4'-bipyridine ligands act in a bis-monodentate bridging mode to link two Zn atoms, giving rise to a one-dimensional chain running along the *c* axis. Furthermore, a three-dimensional supramolecular network is constructed *via* π-π stacking interactions between the adjacent 3-(*p*-CPOP)$^{2-}$ ligand rings (centroid-centroid distance being 3.910 Å) and hydrogen-bonding interactions (Fig 2, Table 2).

Experimental

The title complex was prepared by the addition of zinc diacetate dihydrate (10 mmol), 4,4'-bipyridine (10 mmol) to a solution of 3-(*p*-CPOPH_2) (15 mmol) in H_2O/EtOH (V/V = 1:1), and the pH value was adjusted to 5 with a NaOH (0.2 *M*) solution. Colorless crystals were obtained from the filtered solution at room temperature over several days. CH&N analysis. Calc. for $C_{30}H_{32}N_2O_{13}Zn$: C 52.01, H 4.66, N 4.05%. Found: C 52.00, H 4.68, N 4.04%.

Refinement

H atoms attached to carbon were placed at calculated positions with C—H = 0.93 or 0.97Å and U_{iso}(H) = 1.2U_{eq} (C) and were included in the refinement in the riding model approximation. Those bound to oxygen were located in difference Fourier maps and refined with the O—H distance restrained to 0.85 (1)Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

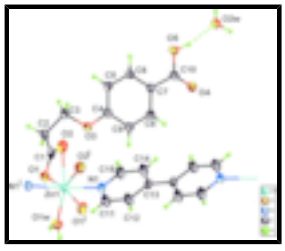

Fig. 1. Molecular structure of the title complex with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

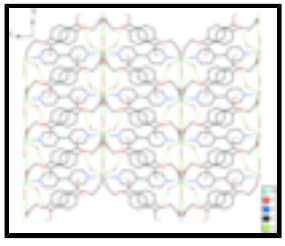

Fig. 2. The packing diagram of the title complex. Dashed lines indicate O—H···O hydrogen bonds.

catena-Poly[[[aquabis[3-(4-carboxyphenoxy)propionato- κ^2O,O']zinc(II)]-μ-4,4'-bipyridine-$\kappa^2N:N'$] dihydrate]

Crystal data

$[Zn(C_{10}H_9O_5)_2(C_{10}H_8N_2)(H_2O)]\cdot 2H_2O$	F_{000} = 720
M_r = 693.95	D_x = 1.510 Mg m^{-3}
Monoclinic, *P*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yc	Cell parameters from 9291 reflections
a = 11.109 (2) Å	θ = 3.4–27.5º
b = 6.0063 (12) Å	μ = 0.88 mm^{-1}
c = 22.871 (5) Å	*T* = 295 (2) K
β = 90.54 (3)º	Block, colorless
V = 1525.9 (5) Å^3	0.28 × 0.24 × 0.18 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	3498 independent reflections
Radiation source: fine-focus sealed tube	2191 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.052
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 3.4º
ω scans	*h* = −14→14
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*k* = −7→7
T_{min} = 0.791, T_{max} = 0.858	*l* = −29→28
14159 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
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.3569P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} < 0.001$
3498 reflections	$\Delta\rho_{max} = 0.78$ e Å^{-3}
221 parameters	$\Delta\rho_{min} = -0.73$ 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}
Zn1	0.5000	0.44267 (8)	0.7500	0.03760 (17)
O1W	0.5000	0.1010 (5)	0.7500	0.0547 (8)
O1	0.2947 (2)	0.3990 (4)	0.74492 (10)	0.0635 (7)
O2	0.3670 (2)	0.7310 (4)	0.73806 (10)	0.0644 (7)
O2W	0.1267 (3)	1.7261 (4)	0.32819 (10)	0.0668 (7)
O3	0.1899 (2)	0.7907 (4)	0.62824 (9)	0.0560 (6)
O4	0.1688 (2)	1.1631 (4)	0.36930 (9)	0.0604 (6)
O5	0.1102 (3)	1.4599 (4)	0.41913 (9)	0.0631 (7)
N1	0.5053 (2)	0.4529 (4)	0.65511 (9)	0.0400 (5)
C1	0.2792 (3)	0.6033 (6)	0.73615 (11)	0.0454 (7)
C2	0.1545 (3)	0.6905 (5)	0.72592 (13)	0.0445 (7)
H1	0.1222	0.7403	0.7629	0.053*
H2	0.1040	0.5698	0.7118	0.053*
C3	0.1476 (3)	0.8794 (6)	0.68294 (12)	0.0525 (8)
H4	0.0654	0.9321	0.6789	0.063*
H3	0.1980	1.0023	0.6957	0.063*

C4	0.1775 (3)	0.9169 (5)	0.57937 (12)	0.0431 (7)
C5	0.1268 (3)	1.1283 (5)	0.57735 (13)	0.0461 (7)
H5	0.1000	1.1966	0.6113	0.055*
C6	0.1166 (3)	1.2357 (5)	0.52392 (13)	0.0455 (7)
H6	0.0826	1.3771	0.5224	0.055*
C7	0.1560 (3)	1.1377 (5)	0.47271 (12)	0.0389 (6)
C8	0.2079 (3)	0.9277 (5)	0.47588 (12)	0.0440 (7)
H8	0.2356	0.8604	0.4420	0.053*
C9	0.2191 (3)	0.8180 (5)	0.52833 (12)	0.0444 (7)
H9	0.2544	0.6777	0.5298	0.053*
C10	0.1456 (3)	1.2510 (5)	0.41552 (13)	0.0444 (7)
C11	0.4569 (4)	0.2967 (6)	0.62145 (13)	0.0592 (9)
H11	0.4239	0.1722	0.6394	0.071*
C12	0.4531 (3)	0.3088 (6)	0.56117 (13)	0.0573 (9)
H12	0.4175	0.1945	0.5397	0.069*
C13	0.5017 (2)	0.4896 (5)	0.53254 (11)	0.0380 (6)
C14	0.5498 (3)	0.6531 (6)	0.56790 (13)	0.0560 (9)
H14	0.5819	0.7809	0.5512	0.067*
C15	0.5506 (3)	0.6288 (6)	0.62788 (13)	0.0577 (9)
H15	0.5847	0.7417	0.6504	0.069*
H1W1	0.4378 (6)	0.021 (3)	0.7461 (18)	0.087*
H2W2	0.178 (3)	1.692 (5)	0.3021 (14)	0.087*
H2W1	0.145 (3)	1.854 (4)	0.3420 (15)	0.087*
H10	0.119 (4)	1.523 (6)	0.3861 (9)	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0430 (3)	0.0433 (3)	0.0264 (2)	0.000	−0.00367 (18)	0.000
O1W	0.0471 (18)	0.0484 (18)	0.069 (2)	0.000	−0.0052 (17)	0.000
O1	0.0719 (17)	0.0668 (16)	0.0520 (13)	0.0202 (13)	0.0076 (12)	0.0169 (12)
O2	0.0479 (14)	0.0886 (18)	0.0567 (14)	−0.0157 (13)	−0.0051 (12)	−0.0120 (12)
O2W	0.107 (2)	0.0466 (13)	0.0470 (14)	0.0085 (14)	0.0125 (14)	−0.0026 (11)
O3	0.0745 (16)	0.0593 (13)	0.0341 (11)	0.0200 (12)	0.0034 (11)	0.0097 (10)
O4	0.100 (2)	0.0482 (12)	0.0331 (11)	0.0059 (13)	0.0030 (12)	−0.0029 (10)
O5	0.108 (2)	0.0446 (13)	0.0374 (11)	0.0164 (13)	0.0074 (13)	0.0050 (10)
N1	0.0436 (14)	0.0492 (14)	0.0272 (11)	−0.0028 (12)	−0.0038 (10)	−0.0012 (11)
C1	0.0460 (18)	0.068 (2)	0.0223 (13)	−0.0034 (16)	−0.0011 (12)	0.0004 (13)
C2	0.0369 (16)	0.0593 (18)	0.0372 (15)	0.0018 (14)	−0.0029 (13)	0.0077 (14)
C3	0.060 (2)	0.062 (2)	0.0360 (15)	0.0146 (17)	0.0026 (15)	0.0030 (14)
C4	0.0448 (17)	0.0488 (17)	0.0356 (14)	0.0033 (14)	−0.0041 (12)	0.0058 (13)
C5	0.0548 (19)	0.0484 (17)	0.0353 (15)	0.0104 (15)	0.0031 (14)	−0.0007 (13)
C6	0.0528 (19)	0.0436 (16)	0.0402 (16)	0.0070 (14)	−0.0010 (14)	0.0006 (13)
C7	0.0431 (17)	0.0396 (15)	0.0340 (14)	−0.0010 (13)	−0.0036 (12)	0.0000 (12)
C8	0.0525 (18)	0.0436 (16)	0.0358 (14)	0.0018 (14)	−0.0009 (13)	−0.0045 (13)
C9	0.0485 (18)	0.0421 (16)	0.0426 (16)	0.0078 (14)	−0.0046 (14)	0.0008 (14)
C10	0.0548 (19)	0.0389 (16)	0.0396 (16)	−0.0011 (14)	−0.0036 (14)	−0.0023 (13)
C11	0.088 (3)	0.056 (2)	0.0339 (16)	−0.0196 (19)	−0.0054 (17)	0.0003 (15)

C12	0.087 (3)	0.0542 (19)	0.0307 (15)	−0.0229 (18)	−0.0090 (16)	−0.0016 (14)
C13	0.0366 (15)	0.0492 (16)	0.0283 (13)	0.0007 (12)	−0.0026 (12)	−0.0028 (12)
C14	0.073 (2)	0.063 (2)	0.0324 (15)	−0.0270 (18)	−0.0031 (15)	0.0010 (15)
C15	0.075 (2)	0.067 (2)	0.0309 (15)	−0.0289 (19)	−0.0075 (15)	−0.0049 (15)

Geometric parameters (Å, °)

Zn1—O1W	2.052 (3)	C3—H4	0.9700
Zn1—N1	2.172 (2)	C3—H3	0.9700
Zn1—O2	2.291 (3)	C4—C5	1.390 (4)
Zn1—O1	2.298 (3)	C4—C9	1.392 (4)
Zn1—O1^{i}	2.298 (3)	C5—C6	1.385 (4)
Zn1—N1^{i}	2.172 (2)	C5—H5	0.9300
Zn1—O2^{i}	2.291 (3)	C6—C7	1.385 (4)
O1W—H1W1	0.846 (10)	C6—H6	0.9300
O1—C1	1.255 (4)	C7—C8	1.388 (4)
O2—C1	1.241 (4)	C7—C10	1.478 (4)
O2W—H2W2	0.85 (3)	C8—C9	1.373 (4)
O2W—H2W1	0.85 (3)	C8—H8	0.9300
O3—C4	1.357 (3)	C9—H9	0.9300
O3—C3	1.442 (3)	C11—C12	1.381 (4)
O4—C10	1.212 (3)	C11—H11	0.9300
O5—C10	1.317 (4)	C12—C13	1.381 (4)
O5—H10	0.85 (3)	C12—H12	0.9300
N1—C11	1.324 (4)	C13—C14	1.376 (4)
N1—C15	1.328 (4)	C13—C13^{ii}	1.494 (5)
C1—C2	1.497 (4)	C14—C15	1.379 (4)
C2—C3	1.503 (4)	C14—H14	0.9300
C2—H1	0.9700	C15—H15	0.9300
C2—H2	0.9700		
O1W—Zn1—N1	91.62 (7)	C2—C3—H4	110.6
O1W—Zn1—N1^{i}	91.62 (7)	O3—C3—H3	110.6
N1—Zn1—N1^{i}	176.76 (13)	C2—C3—H3	110.6
O1W—Zn1—O2^{i}	139.10 (6)	H4—C3—H3	108.7
N1—Zn1—O2^{i}	94.27 (9)	O3—C4—C5	125.2 (3)
N1^{i}—Zn1—O2^{i}	83.28 (9)	O3—C4—C9	114.9 (3)
O1W—Zn1—O2	139.10 (6)	C5—C4—C9	120.0 (3)
N1—Zn1—O2	83.28 (9)	C6—C5—C4	119.0 (3)
N1^{i}—Zn1—O2	94.27 (9)	C6—C5—H5	120.5
O2^{i}—Zn1—O2	81.80 (12)	C4—C5—H5	120.5
O1W—Zn1—O1	83.44 (6)	C7—C6—C5	121.6 (3)
N1—Zn1—O1	89.35 (9)	C7—C6—H6	119.2
N1^{i}—Zn1—O1	91.02 (9)	C5—C6—H6	119.2
O2^{i}—Zn1—O1	136.98 (9)	C6—C7—C8	118.4 (3)
O2—Zn1—O1	56.05 (8)	C6—C7—C10	122.0 (3)
O1W—Zn1—O1^{i}	83.44 (6)	C8—C7—C10	119.6 (2)

N1—Zn1—O1^{i}	91.02 (9)	C9—C8—C7	121.0 (3)
N1^{i}—Zn1—O1^{i}	89.35 (9)	C9—C8—H8	119.5
O2^{i}—Zn1—O1^{i}	56.05 (8)	C7—C8—H8	119.5
O2—Zn1—O1^{i}	136.98 (9)	C8—C9—C4	120.0 (3)
O1—Zn1—O1^{i}	166.88 (12)	C8—C9—H9	120.0
Zn1—O1W—H1W1	124.6 (11)	C4—C9—H9	120.0
C1—O1—Zn1	91.8 (2)	O4—C10—O5	122.4 (3)
C1—O2—Zn1	92.5 (2)	O4—C10—C7	123.8 (3)
H2W2—O2W—H2W1	108.5 (16)	O5—C10—C7	113.8 (2)
C4—O3—C3	118.5 (2)	N1—C11—C12	123.5 (3)
C10—O5—H10	109 (3)	N1—C11—H11	118.2
C11—N1—C15	116.4 (2)	C12—C11—H11	118.2
C11—N1—Zn1	123.1 (2)	C11—C12—C13	120.4 (3)
C15—N1—Zn1	120.32 (19)	C11—C12—H12	119.8
O2—C1—O1	119.4 (3)	C13—C12—H12	119.8
O2—C1—C2	121.0 (3)	C14—C13—C12	115.7 (3)
O1—C1—C2	119.5 (3)	C14—C13—C13^{ii}	122.2 (3)
C1—C2—C3	114.1 (3)	C12—C13—C13^{ii}	122.1 (3)
C1—C2—H1	108.7	C13—C14—C15	120.5 (3)
C3—C2—H1	108.7	C13—C14—H14	119.7
C1—C2—H2	108.7	C15—C14—H14	119.7
C3—C2—H2	108.7	N1—C15—C14	123.5 (3)
H1—C2—H2	107.6	N1—C15—H15	118.3
O3—C3—C2	105.9 (2)	C14—C15—H15	118.3
O3—C3—H4	110.6		
O1W—Zn1—O1—C1	−171.21 (17)	C4—O3—C3—C2	170.9 (3)
N1—Zn1—O1—C1	−79.51 (17)	C1—C2—C3—O3	61.9 (3)
N1^{i}—Zn1—O1—C1	97.28 (17)	C3—O3—C4—C5	0.0 (5)
O2^{i}—Zn1—O1—C1	16.1 (2)	C3—O3—C4—C9	−179.2 (3)
O2—Zn1—O1—C1	2.82 (16)	O3—C4—C5—C6	−178.1 (3)
O1^{i}—Zn1—O1—C1	−171.21 (17)	C9—C4—C5—C6	1.1 (5)
O1W—Zn1—O2—C1	6.2 (2)	C4—C5—C6—C7	−0.1 (5)
N1—Zn1—O2—C1	90.92 (18)	C5—C6—C7—C8	−0.8 (5)
N1^{i}—Zn1—O2—C1	−91.20 (18)	C5—C6—C7—C10	−180.0 (3)
O2^{i}—Zn1—O2—C1	−173.8 (2)	C6—C7—C8—C9	0.7 (5)
O1—Zn1—O2—C1	−2.85 (16)	C10—C7—C8—C9	179.9 (3)
O1^{i}—Zn1—O2—C1	175.17 (15)	C7—C8—C9—C4	0.3 (5)
O1W—Zn1—N1—C11	30.2 (3)	O3—C4—C9—C8	178.1 (3)
O2^{i}—Zn1—N1—C11	169.7 (3)	C5—C4—C9—C8	−1.2 (5)
O2—Zn1—N1—C11	−109.1 (3)	C6—C7—C10—O4	−173.1 (3)
O1—Zn1—N1—C11	−53.3 (3)	C8—C7—C10—O4	7.8 (5)
O1^{i}—Zn1—N1—C11	113.6 (3)	C6—C7—C10—O5	8.0 (4)
O1W—Zn1—N1—C15	−154.9 (3)	C8—C7—C10—O5	−171.2 (3)
O2^{i}—Zn1—N1—C15	−15.4 (3)	C15—N1—C11—C12	0.6 (5)
O2—Zn1—N1—C15	65.8 (3)	Zn1—N1—C11—C12	175.7 (3)

O1—Zn1—N1—C15	121.7 (3)	N1—C11—C12—C13	0.4 (6)
O1^{i}—Zn1—N1—C15	−71.4 (3)	C11—C12—C13—C14	−1.6 (5)
Zn1—O2—C1—O1	5.0 (3)	C11—C12—C13—C13^{ii}	−179.3 (4)
Zn1—O2—C1—C2	−177.5 (2)	C12—C13—C14—C15	1.7 (5)
Zn1—O1—C1—O2	−5.0 (3)	C13^{ii}—C13—C14—C15	179.5 (4)
Zn1—O1—C1—C2	177.5 (2)	C11—N1—C15—C14	−0.4 (5)
O2—C1—C2—C3	37.8 (4)	Zn1—N1—C15—C14	−175.7 (3)
O1—C1—C2—C3	−144.6 (3)	C13—C14—C15—N1	−0.8 (6)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O2^{iii}	0.846 (10)	1.919 (16)	2.681 (4)	149.3 (14)
O2W—H2W2···O1^{iv}	0.85 (3)	1.93 (3)	2.782 (3)	177 (4)
O2W—H2W1···O4^{v}	0.85 (3)	1.98 (3)	2.826 (3)	173 (4)
O5—H10···O2W	0.85 (3)	1.803 (15)	2.632 (3)	164 (4)

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

Fig. 1

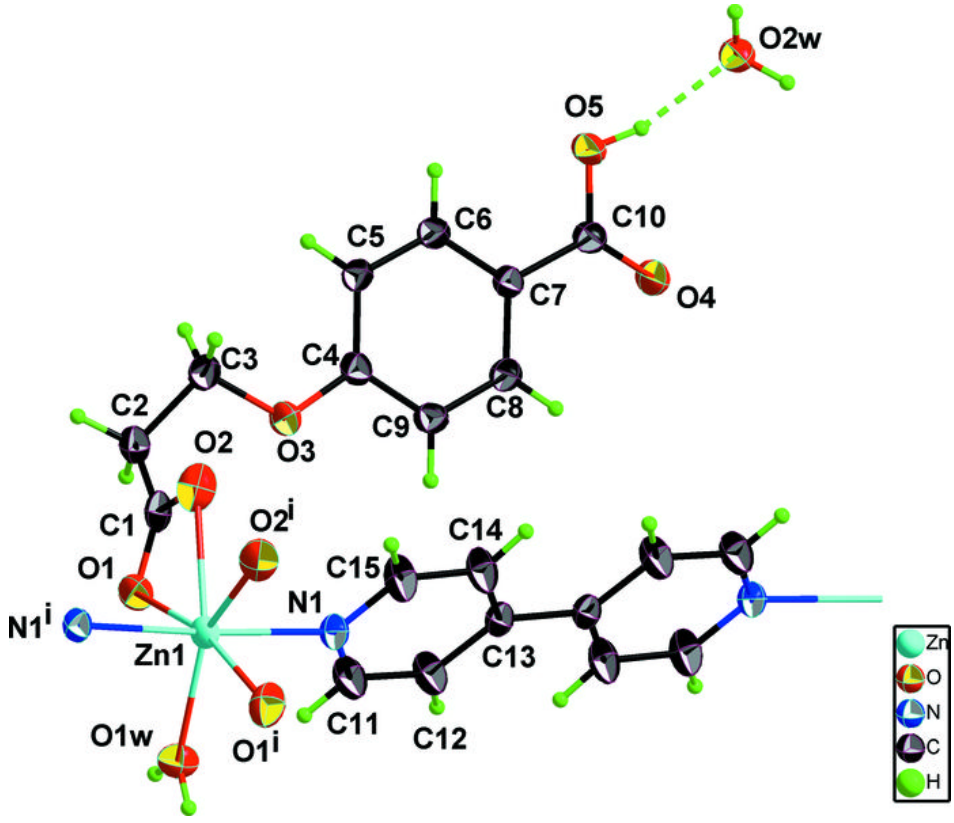
O2w
O5
C10
C6
C5
C7
O4
C3
C4
C2
C8
O2
O3
C9
C1
O2i
C14
O1
C15
N1
N1i
Zn1
C13
O1w
O1i
C11
C12
Zn
O
N
C
H

Fig. 2