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catena-Poly[[[aquazinc(II)]-bis[*μ*-(*p*-phenylenedioxy)diacetato]-zinc(II)-*μ*-1,4-bis(1*H*-imidazol-l-yl)butane] dihydrate]

Ming Lv

Department of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China
Correspondence e-mail: lumingjlsp@yahoo.com.cn

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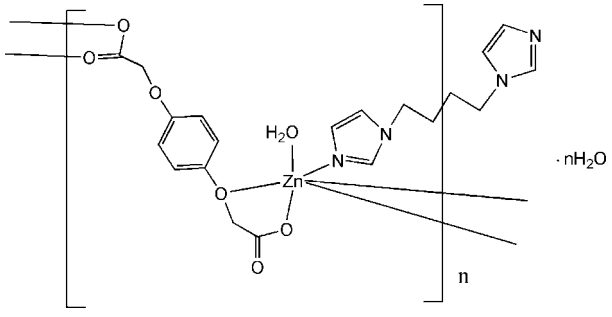
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.107; data-to-parameter ratio = 13.2.

In the title compound, $\{[Zn_2(C_{10}H_8O_6)_2(C_{10}H_{14}N_4)(H_2O)_2]\cdot 2H_2O\}_n$, the Zn^{II} atom is six-coordinated by one N atom from one 1,4-bis(1*H*-imidazol-l-yl)butane ligand and five O atoms from two different (*p*-phenylenedioxy)diacetate ligands and one water molecule in a very distorted $ZnNO_5$ octahedral environment. Two (*p*-phenylenedioxy)diacetate ligands bridge two Zn^{II} atoms to form a dimer. The dimers are further linked by the centrosymmetric 1,4-bis(1*H*-imidazol-l-yl)butane ligands, thus forming a chain structure. O—H···O hydrogen bonds link the chains, forming a three-dimensional supramolecular network.

Related literature

For related literature, see: Chen & Liu (2002); Che *et al.* (2006).



Experimental

Crystal data

$[Zn_2(C_{10}H_8O_6)_2(C_{10}H_{14}N_4)(H_2O)_2]\cdot 2H_2O$
M_r = 420.69
Triclinic, $P\overline{1}$
a = 8.9061 (12) Å
b = 9.8617 (14) Å
c = 10.6066 (15) Å
α = 100.014 (2)°
β = 94.614 (2)°
γ = 111.107 (2)°
V = 845.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.50 mm^{-1}
T = 293 (2) K
0.19 × 0.19 × 0.18 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.745, T_{max} = 0.764
4802 measured reflections
3252 independent reflections
2667 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.107
S = 1.07
3252 reflections
247 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.014 (3)	Zn1—O3	2.446 (3)
Zn1—O1	1.978 (2)	Zn1—O5^{i}	2.099 (3)
Zn1—O1*W*	2.029 (3)	Zn1—O6^{i}	2.351 (3)

Symmetry code: (i) $-x, -y, -z+2$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H*W*22···O5^{ii}	0.83 (4)	2.03 (2)	2.805 (4)	158 (4)
O1*W*—H*W*11···O1^{iii}	0.81 (4)	1.93 (2)	2.727 (4)	168 (4)
O1*W*—H*W*12···O2*W*	0.782 (17)	1.98 (2)	2.632 (4)	140 (3)
O2*W*—H*W*21···O2^{iii}	0.866 (17)	1.99 (2)	2.790 (4)	153 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

The author thanks Jilin Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2591).

References

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Che, G.-B., Liu, H., Liu, C.-B. & Liu, B. (2006). *Acta Cryst.* E**62**, m286–m288.
Chen, X. M. & Liu, G. F. (2002). *Chem. Eur. J.* **8**, 4811–4817.
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supplementary materials

Acta Cryst. (2007). E**63**, m2833 [**doi:10.1107/S1600536807052518**]

catena-Poly[[[aquazinc(II)]-bis[μ-(*p*-phenylenedioxy)diacetato]-zinc(II)-μ-1,4-bis(1*H*-imidazol-l-yl)butane] dihydrate]

M. Lv

Comment

As part of the ongoing effort to create new coordinatiom polymer chain structures (Chen & Liu, 2002; Che *et al.*, 2006), we selected 1,4-benzenedioxydiacetic acid (1,4-H_2bdd) and 1-(4-(1*H*-imidazole-l-yl)butyl)-1*H*-imidazole (ibi) as bridging ligands, in combination with zinc cations, generating a new chain coordination polymer, $[Zn_2(1,4\text{-bdd})_2(ibi)(H_2O)_2]\cdot 2H_2O$, (I), which is reported here.

The selected bond lengths and angles are listed in Table 1. In compound (I), the Zn^{II} atom is six-coordinated by one N atom from one ibi ligand, and five O atoms from two different 1,4-bdd ligands and one water molecule in a very distorted octahedral environment (Fig. 1). As shown in Fig. 2, two 1,4-bdd ligands bridge two Zn^{II} atoms to form a dimer. The dimers are further linked by ibi ligands, forming a chain structure (Fig. 2). Furthermore, the O—H···O hydrogen bonds (Table 2) link the chains together, forming a three-dimensional supramolecular network.

Experimental

A mixture of $ZnCl_2\cdot 2H_2O$ (0.5 mmol), 1,4-H_2dbb (0.5 mmol), ibi (0.5 mmol), and H_2O (500 mmol) was adjusted to pH = 6.5 by addition of aqueous NaOH solution, and heated at 448 K for three days. After the mixture was slowly cooled to room temperature, colourless blocks of (I) resulted.

Refinement

All C-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier). The water H-atoms were located in a difference Fourier map, and were freely refined.

Figures

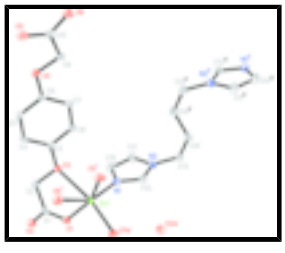

Fig. 1. The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level. (H atoms have been omitted). Symmetry codes: (i) −*x*, −*y*, 2 − *z*; (ii) 1 − *x*, −*y*, 1 − *z*.

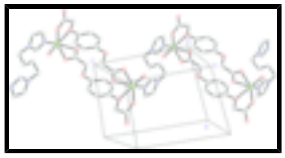

Fig. 2. View of the chain structure of (I).

catena-Poly[[[aquazinc(II)]-bis[μ-(_p_-phenylenedioxy)diacetato]-zinc(II)- μ-1,4-bis(1_H_-imidazol-l-yl)butane] dihydrate]

Crystal data

$[Zn_2(C_{10}H_8O_6)_2(C_{10}H_{14}N_4)(H_2O)_2]\cdot 2H_2O$	$Z = 2$
$M_r = 420.69$	$F_{000} = 434$
Triclinic, $P\bar{1}$	$D_x = 1.653$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.9061$ (12) Å	Cell parameters from 3252 reflections
$b = 9.8617$ (14) Å	$\theta = 2.0$–26.0º
$c = 10.6066$ (15) Å	$\mu = 1.50$ mm^{-1}
$\alpha = 100.014$ (2)º	$T = 293$ (2) K
$\beta = 94.614$ (2)º	Block, colorless
$\gamma = 111.107$ (2)º	0.19 × 0.19 × 0.18 mm
$V = 845.4$ (2) Å^3	

Data collection

Bruker APEX CCD diffractometer	3252 independent reflections
Radiation source: fine-focus sealed tube	2667 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
$T = 293$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -8\rightarrow 10$
$T_{min} = 0.745$, $T_{max} = 0.764$	$k = -11\rightarrow 12$
4802 measured reflections	$l = -13\rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)] = 0.050$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.4041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
3252 reflections	$\Delta\rho_{max} = 0.61$ e Å^{-3}
247 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}

7 restraints
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}
C1	0.2172 (5)	0.6757 (4)	0.8133 (4)	0.0243 (9)
C2	0.2508 (5)	0.6119 (4)	0.9271 (4)	0.0283 (9)
H2A	0.3512	0.6809	0.9819	0.034*
H2B	0.1631	0.5985	0.9783	0.034*
C3	0.2504 (4)	0.3788 (4)	0.9701 (3)	0.0219 (8)
C4	0.1930 (5)	0.3990 (4)	1.0865 (3)	0.0239 (9)
H4	0.1710	0.4835	1.1153	0.029*
C5	0.1686 (5)	0.2912 (4)	1.1597 (4)	0.0235 (8)
H5	0.1291	0.3035	1.2376	0.028*
C6	0.2024 (5)	0.1649 (4)	1.1181 (3)	0.0225 (8)
C7	0.2670 (5)	0.1497 (4)	1.0044 (4)	0.0260 (9)
H7	0.2949	0.0682	0.9777	0.031*
C8	0.2900 (5)	0.2567 (4)	0.9304 (4)	0.0257 (9)
H8	0.3323	0.2460	0.8537	0.031*
C9	0.1705 (5)	−0.0791 (4)	1.1446 (4)	0.0252 (9)
H9A	0.2825	−0.0712	1.1469	0.030*
H9B	0.1173	−0.1140	1.0551	0.030*
C10	0.4694 (5)	0.4290 (5)	0.6597 (4)	0.0338 (10)
H10	0.5053	0.5092	0.7305	0.041*
C11	0.5664 (5)	0.3722 (5)	0.5957 (4)	0.0349 (10)
H11	0.6792	0.4049	0.6140	0.042*
C12	0.3132 (5)	0.2476 (4)	0.5073 (4)	0.0274 (9)
H12	0.2210	0.1777	0.4522	0.033*
C13	0.5125 (5)	0.1560 (4)	0.4063 (4)	0.0308 (10)
H13A	0.6299	0.1973	0.4099	0.037*
H13B	0.4630	0.1487	0.3192	0.037*
C14	0.4608 (5)	0.0011 (4)	0.4346 (4)	0.0299 (9)
H14A	0.3434	−0.0399	0.4303	0.036*
H14B	0.4886	−0.0625	0.3679	0.036*
C15	0.0841 (5)	−0.1884 (4)	1.2237 (4)	0.0278 (9)

N1	0.3108 (4)	0.3507 (3)	0.6041 (3)	0.0252 (7)
N2	0.4651 (4)	0.2568 (4)	0.4986 (3)	0.0271 (8)
O1	0.1532 (3)	0.5861 (3)	0.7026 (2)	0.0276 (6)
O2	0.2463 (4)	0.8100 (3)	0.8349 (3)	0.0329 (7)
O1W	−0.0434 (4)	0.3118 (3)	0.4941 (3)	0.0366 (7)
O3	0.2645 (3)	0.4722 (3)	0.8831 (2)	0.0249 (6)
O2W	−0.1611 (4)	0.0431 (3)	0.3437 (3)	0.0366 (7)
O4	0.1672 (3)	0.0630 (3)	1.1958 (2)	0.0271 (6)
O5	0.0000 (3)	−0.1547 (3)	1.3035 (3)	0.0333 (7)
O6	0.0941 (4)	−0.3126 (3)	1.2033 (3)	0.0379 (7)
Zn1	0.10926 (6)	0.37051 (5)	0.66421 (4)	0.02388 (15)
HW22	−0.096 (4)	0.004 (5)	0.324 (3)	0.036*
HW11	−0.062 (5)	0.351 (4)	0.437 (3)	0.036*
HW12	−0.047 (5)	0.230 (2)	0.476 (3)	0.036*
HW21	−0.199 (4)	0.060 (4)	0.273 (2)	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.027 (2)	0.023 (2)	0.028 (2)	0.0116 (17)	0.0094 (17)	0.0114 (17)
C2	0.041 (3)	0.020 (2)	0.026 (2)	0.0142 (19)	0.0033 (19)	0.0082 (17)
C3	0.022 (2)	0.022 (2)	0.0196 (19)	0.0063 (16)	−0.0022 (16)	0.0060 (15)
C4	0.029 (2)	0.0182 (19)	0.026 (2)	0.0116 (17)	0.0010 (17)	0.0054 (16)
C5	0.026 (2)	0.023 (2)	0.0182 (19)	0.0062 (17)	0.0024 (16)	0.0037 (16)
C6	0.024 (2)	0.0195 (19)	0.0220 (19)	0.0052 (16)	0.0001 (16)	0.0074 (16)
C7	0.035 (2)	0.021 (2)	0.025 (2)	0.0141 (18)	0.0036 (18)	0.0048 (16)
C8	0.029 (2)	0.024 (2)	0.025 (2)	0.0105 (18)	0.0057 (17)	0.0056 (17)
C9	0.031 (2)	0.019 (2)	0.026 (2)	0.0103 (17)	0.0023 (17)	0.0066 (16)
C10	0.029 (2)	0.033 (2)	0.030 (2)	0.004 (2)	0.0019 (19)	0.0000 (19)
C11	0.020 (2)	0.035 (2)	0.038 (3)	0.0015 (19)	−0.0010 (19)	0.000 (2)
C12	0.025 (2)	0.024 (2)	0.028 (2)	0.0057 (18)	−0.0022 (18)	0.0039 (17)
C13	0.026 (2)	0.036 (2)	0.030 (2)	0.0119 (19)	0.0072 (19)	0.0049 (19)
C14	0.025 (2)	0.030 (2)	0.033 (2)	0.0119 (19)	0.0037 (18)	−0.0003 (19)
C15	0.027 (2)	0.027 (2)	0.023 (2)	0.0045 (18)	−0.0080 (18)	0.0062 (17)
N1	0.0223 (19)	0.0219 (17)	0.0276 (18)	0.0042 (14)	0.0014 (15)	0.0066 (14)
N2	0.0255 (19)	0.0277 (18)	0.0302 (18)	0.0115 (15)	0.0054 (15)	0.0085 (15)
O1	0.0394 (17)	0.0201 (14)	0.0247 (14)	0.0135 (13)	−0.0002 (13)	0.0059 (12)
O2	0.0494 (19)	0.0215 (15)	0.0299 (15)	0.0157 (14)	0.0034 (14)	0.0076 (12)
O1W	0.050 (2)	0.0254 (16)	0.0323 (17)	0.0146 (15)	−0.0113 (15)	0.0101 (13)
O3	0.0352 (16)	0.0227 (14)	0.0213 (14)	0.0146 (13)	0.0040 (12)	0.0082 (11)
O2W	0.049 (2)	0.0356 (18)	0.0308 (16)	0.0239 (15)	0.0037 (15)	0.0070 (14)
O4	0.0420 (18)	0.0209 (14)	0.0210 (14)	0.0127 (13)	0.0065 (12)	0.0084 (11)
O5	0.0312 (17)	0.0387 (17)	0.0392 (17)	0.0166 (14)	0.0096 (14)	0.0229 (14)
O6	0.057 (2)	0.0206 (15)	0.0327 (16)	0.0112 (14)	−0.0009 (15)	0.0096 (13)
Zn1	0.0267 (3)	0.0210 (2)	0.0249 (3)	0.00896 (19)	0.00287 (19)	0.00807 (18)

Geometric parameters (Å, °)

C1—O2	1.230 (4)	C11—N2	1.368 (5)

C1—O1	1.285 (5)	C11—H11	0.9300
C1—C2	1.511 (5)	C12—N1	1.321 (5)
C2—O3	1.427 (4)	C12—N2	1.335 (5)
C2—H2A	0.9700	C12—H12	0.9300
C2—H2B	0.9700	C13—N2	1.469 (5)
C3—C8	1.380 (5)	C13—C14	1.520 (5)
C3—C4	1.384 (5)	C13—H13A	0.9700
C3—O3	1.396 (4)	C13—H13B	0.9700
C4—C5	1.388 (5)	C14—C14^{i}	1.510 (8)
C4—H4	0.9300	C14—H14A	0.9700
C5—C6	1.391 (5)	C14—H14B	0.9700
C5—H5	0.9300	C15—O6	1.244 (5)
C6—O4	1.375 (4)	C15—O5	1.253 (5)
C6—C7	1.385 (5)	Zn1—N1	2.014 (3)
C7—C8	1.388 (5)	Zn1—O1	1.978 (2)
C7—H7	0.9300	Zn1—O1W	2.029 (3)
C8—H8	0.9300	Zn1—O3	2.446 (3)
C9—O4	1.423 (4)	Zn1—O5^{ii}	2.099 (3)
C9—C15	1.510 (5)	Zn1—O6^{ii}	2.351 (3)
C9—H9A	0.9700	O1W—HW11	0.81 (4)
C9—H9B	0.9700	O1W—HW12	0.782 (17)
C10—C11	1.354 (6)	O2W—HW22	0.83 (4)
C10—N1	1.364 (5)	O2W—HW21	0.866 (17)
C10—H10	0.9300		
O2—C1—O1	124.4 (4)	N2—C13—H13B	109.2
O2—C1—C2	117.1 (3)	C14—C13—H13B	109.2
O1—C1—C2	118.5 (3)	H13A—C13—H13B	107.9
O3—C2—C1	110.4 (3)	C14^{i}—C14—C13	113.5 (4)
O3—C2—H2A	109.6	C14^{i}—C14—H14A	108.9
C1—C2—H2A	109.6	C13—C14—H14A	108.9
O3—C2—H2B	109.6	C14^{i}—C14—H14B	108.9
C1—C2—H2B	109.6	C13—C14—H14B	108.9
H2A—C2—H2B	108.1	H14A—C14—H14B	107.7
C8—C3—C4	120.4 (3)	O6—C15—O5	121.9 (4)
C8—C3—O3	115.7 (3)	O6—C15—C9	118.1 (4)
C4—C3—O3	123.8 (3)	O5—C15—C9	119.9 (3)
C3—C4—C5	119.0 (3)	C12—N1—C10	105.8 (3)
C3—C4—H4	120.5	C12—N1—Zn1	125.7 (3)
C5—C4—H4	120.5	C10—N1—Zn1	128.3 (3)
C4—C5—C6	121.0 (3)	C12—N2—C11	107.3 (3)
C4—C5—H5	119.5	C12—N2—C13	126.0 (3)
C6—C5—H5	119.5	C11—N2—C13	126.7 (3)
O4—C6—C7	124.9 (3)	C1—O1—Zn1	125.2 (2)
O4—C6—C5	115.8 (3)	Zn1—O1W—HW11	138 (3)
C7—C6—C5	119.3 (3)	Zn1—O1W—HW12	96 (2)
C6—C7—C8	119.8 (3)	HW11—O1W—HW12	119 (3)
C6—C7—H7	120.1	C3—O3—C2	118.0 (3)

C8—C7—H7	120.1	C3—O3—Zn1	119.5 (2)
C3—C8—C7	120.5 (3)	C2—O3—Zn1	106.5 (2)
C3—C8—H8	119.8	HW22—O2W—HW21	106 (3)
C7—C8—H8	119.8	C6—O4—C9	117.2 (3)
O4—C9—C15	109.6 (3)	C15—O5—Zn1^{ii}	95.1 (2)
O4—C9—H9A	109.7	C15—O6—Zn1^{ii}	83.9 (2)
C15—C9—H9A	109.7	O1—Zn1—N1	106.17 (12)
O4—C9—H9B	109.7	O1—Zn1—O1W	98.11 (11)
C15—C9—H9B	109.7	N1—Zn1—O1W	101.77 (13)
H9A—C9—H9B	108.2	O1—Zn1—O5^{ii}	152.24 (11)
C11—C10—N1	109.5 (4)	N1—Zn1—O5^{ii}	97.67 (12)
C11—C10—H10	125.2	O1W—Zn1—O5^{ii}	90.59 (12)
N1—C10—H10	125.2	O1—Zn1—O6^{ii}	94.26 (10)
C10—C11—N2	106.2 (4)	N1—Zn1—O6^{ii}	150.08 (11)
C10—C11—H11	126.9	O1W—Zn1—O6^{ii}	96.58 (12)
N2—C11—H11	126.9	O5^{ii}—Zn1—O6^{ii}	58.43 (10)
N1—C12—N2	111.2 (3)	O1—Zn1—O3	73.53 (9)
N1—C12—H12	124.4	N1—Zn1—O3	87.89 (11)
N2—C12—H12	124.4	O1W—Zn1—O3	168.82 (10)
N2—C13—C14	112.2 (3)	O5^{ii}—Zn1—O3	93.70 (10)
N2—C13—H13A	109.2	O6^{ii}—Zn1—O3	77.02 (9)
C14—C13—H13A	109.2		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2W—HW22···O5^{iii}	0.83 (4)	2.03 (2)	2.805 (4)	158 (4)
O1W—HW11···O1^{iv}	0.81 (4)	1.93 (2)	2.727 (4)	168 (4)
O1W—HW12···O2W	0.782 (17)	1.98 (2)	2.632 (4)	140 (3)
O2W—HW21···O2^{iv}	0.866 (17)	1.99 (2)	2.790 (4)	153 (3)

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

Fig. 1

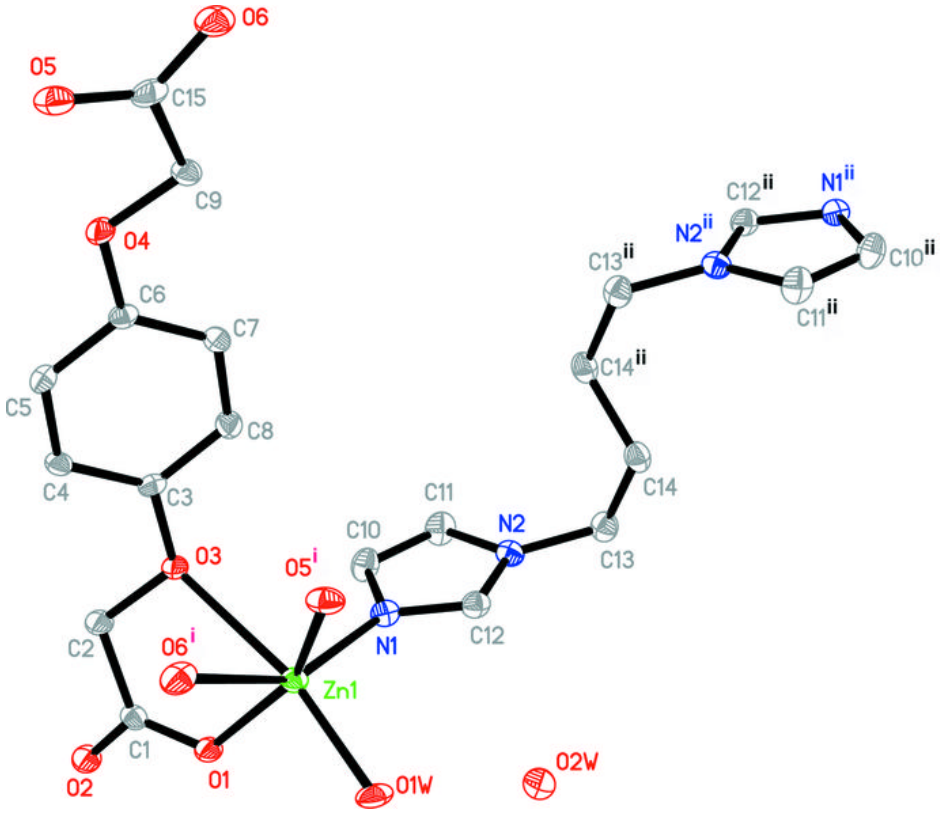
O6
O5
C15
C9
O4
C6
C7
C5
C8
C4
C3
O3
C2
O6i
C1
O2
O1
Zn1
O5i
N1
C10
C11
N2
C12
C13
C14
O1W
O2W
C12ii
N1ii
N2ii
C13ii
C10ii
C11ii
C14ii

Fig. 2