

catena-Poly[[[aqua(1,10-phenanthroline)zinc(II)]- μ -3,3'-(*p*-phenylene)diacrylate] hemihydrate]

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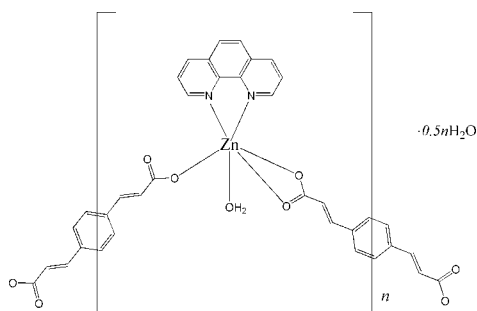
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}–\text{C}) = 0.005$ Å; disorder in solvent or counterion; R factor = 0.036; wR factor = 0.101; data-to-parameter ratio = 12.5.

In the title compound, $\{[\text{Zn}(\text{C}_{12}\text{H}_8\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot 0.5\text{H}_2\text{O}\}_n$, each Zn^{II} atom is six-coordinated by two N atoms from one 1,10-phenanthroline (phen), three carboxylate O atoms from two different L ligands [$\text{H}_2L = 3,3'-(p\text{-phenylene})\text{diacrylate}$] and one water molecule in a distorted octahedral environment. The two L dianions are situated across inversion centres and bridge neighbouring Zn^{II} centres, yielding a chain propagating parallel to $[100]$. $\text{O}–\text{H} \cdots \text{O}$ hydrogen bonds between the coordinated water molecule, the solvent water molecule (half-occupied) and the carboxylate O atoms further stabilize the structure.

Related literature

For general background and related structures see: Wang *et al.* (2008). For related literature, see: Batten & Robson (1998).



Experimental

Crystal data

$[\text{Zn}(\text{C}_{12}\text{H}_8\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot 0.5\text{H}_2\text{O}$
 $M_r = 488.78$
 Triclinic, $P\bar{1}$
 $a = 8.959$ (5) Å
 $b = 11.505$ (5) Å
 $c = 11.691$ (5) Å
 $\alpha = 67.219$ (5)°
 $\beta = 76.434$ (5)°
 $\gamma = 89.555$ (5)°
 $V = 1075.4$ (9) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.18$ mm⁻¹
 $T = 293$ K
 $0.30 \times 0.22 \times 0.19$ mm

Data collection

Bruker APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.701$, $T_{\text{max}} = 0.792$
 6674 measured reflections
 3887 independent reflections
 3193 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.101$
 $S = 0.98$
 3887 reflections
 312 parameters
 6 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.90$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D–H \cdots A$	$D–H$	$H \cdots A$	$D \cdots A$	$D–H \cdots A$
$\text{O1W}–\text{HW12} \cdots \text{O2}^i$	0.85 (3)	1.87 (3)	2.687 (3)	158 (4)
$\text{O1W}–\text{HW11} \cdots \text{O3}^i$	0.86 (2)	1.88 (3)	2.685 (3)	155 (3)
$\text{O2W}–\text{HW21} \cdots \text{O2}$	0.816 (10)	2.044 (14)	2.856 (5)	173 (5)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: AT2836).

References

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 Wang, X.-Y., Wang, J.-J. & Ng, S. W. (2008). *Acta Cryst.* **C64**, m401–m404.

supplementary materials

Acta Cryst. (2009). E65, m944 [doi:10.1107/S1600536809025665]

***catena*-Poly[[[aqua(1,10-phenanthroline)zinc(II)]- μ -3,3'-(*p*-phenylene)diacrylato] hemihydrate]**

Y.-P. Li, D.-J. Sun, H. Zang, G.-F. Su and Y.-L. Li

Comment

Recently, chain structures have received much attention in coordination chemistry and medical chemistry (Batten & Robson, 1998). An appropriate bidentate organic acid bridge could be useful in the formation of chains in the presence of secondary ligands, such as 2,2'-bipyridine (bipy) and 1,10-phenanthroline (phen) (Wang *et al.*, 2008). The N atoms from the secondary ligand may occupy two coordination positions of the metal ions. The rest of the coordination positions are available for other carboxylate ligands to allow the formation of a chain. In this regard, 3,3'-(*p*-phenylene)diacrylic acid (H₂L) is a good ligand in coordination chemistry because of its strong coordination ability and versatile coordination modes, so much attention has been paid to it in recent decades. In the present study, we selected H₂L as a linker and phen as a secondary chelating ligand, forming a unique zigzag chain coordination polymer [Zn(phen)(L)(H₂O)]0.5H₂O.

As shown in Fig. 1, each Zn^{II} atom is six-coordinated by two N atoms from one phen, three carboxylate O atoms from two different *L* ligands, and one water molecule in a distorted octahedral sphere. The two *L* dianions are situated across inversion centres. The bpea dianions bridge two neighboring Zn^{II} centres to form a one-dimensional chain (Fig. 2). The O—H \cdots O_{carboxylate} H-bonding interactions further stabilize the structure of the title compound (Table 1).

Experimental

A mixture of 3,3'-(*p*-phenylene)diacrylic acid (0.5 mmol), 1,10-phenanthroline (0.5 mmol), NaOH (1 mmol) and ZnCl₂·2H₂O (0.5 mmol) was suspended in deionized water (12 ml) and sealed in a 20 ml Teflon-lined autoclave. After heating at 438 K for one week, the autoclave was cooled slowly to room temperature. Crystals were collected, washed with deionized water and dried.

Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$. The water H atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.85 Å and H \cdots H = 1.35 Å. The displacement parameters of the H atoms attached to atom O2W were tied to those of the parent atom by a factor of 1.5, while those on O1W were refined freely.

Figures

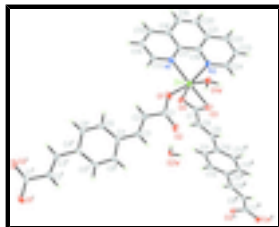


Fig. 1. The asymmetric unit in the polymeric structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 20% probability level [symmetry operations: (i) 1-x, -y, 3-z; (ii) -x-1, 1-y, 2-z].

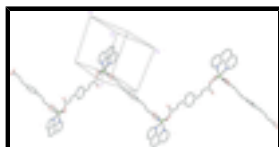


Fig. 2. View of the one-dimensional chain of the title compound.

catena-Poly[[[aqua(1,10-phenanthroline)zinc(II)]- μ -3,3'-(*p*-phenylene)diacrylate] hemihydrate]

Crystal data

[Zn(C₁₂H₈O₄)(C₁₂H₈N₂)(H₂O)]·0.5H₂O

$M_r = 488.78$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.959 (5) \text{ \AA}$

$b = 11.505 (5) \text{ \AA}$

$c = 11.691 (5) \text{ \AA}$

$\alpha = 67.219 (5)^\circ$

$\beta = 76.434 (5)^\circ$

$\gamma = 89.555 (5)^\circ$

$V = 1075.4 (9) \text{ \AA}^3$

$Z = 2$

$F_{000} = 502$

$D_x = 1.509 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3887 reflections

$\theta = 3.0\text{--}25.4^\circ$

$\mu = 1.18 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

$0.30 \times 0.22 \times 0.19 \text{ mm}$

Data collection

Bruker APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293 \text{ K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick 1996)

$T_{\min} = 0.701$, $T_{\max} = 0.792$

6674 measured reflections

3887 independent reflections

3193 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\text{max}} = 25.4^\circ$

$\theta_{\text{min}} = 4.2^\circ$

$h = -10 \rightarrow 9$

$k = -11 \rightarrow 13$

$l = -12 \rightarrow 14$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.036$$

$$wR(F^2) = 0.101$$

$$S = 0.98$$

3887 reflections

312 parameters

6 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

$$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.90 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Zn1	0.22324 (4)	0.16358 (3)	0.84090 (3)	0.02776 (13)	
O1W	0.1608 (2)	-0.02160 (18)	0.87917 (19)	0.0326 (4)	
O2	0.1060 (3)	0.0767 (2)	1.1643 (2)	0.0512 (6)	
O3	-0.0271 (2)	0.20043 (17)	0.88909 (18)	0.0391 (5)	
O4	0.1579 (2)	0.3439 (2)	0.8484 (2)	0.0469 (5)	
O1	0.3082 (3)	0.1033 (2)	0.99979 (18)	0.0429 (5)	
N2	0.1984 (3)	0.2138 (2)	0.6449 (2)	0.0311 (5)	
N1	0.4515 (3)	0.2360 (2)	0.7226 (2)	0.0310 (5)	
C24	0.0755 (4)	0.1957 (3)	0.6072 (3)	0.0397 (7)	
H24	-0.0132	0.1519	0.6694	0.048*	
C4	0.4100 (3)	0.0176 (2)	1.4115 (3)	0.0312 (6)	
C12	-0.4743 (3)	0.6175 (2)	0.9997 (3)	0.0302 (6)	
H12	-0.4565	0.6976	0.9986	0.036*	
C18	0.3274 (3)	0.2775 (2)	0.5531 (2)	0.0293 (6)	
C16	0.5967 (4)	0.3587 (3)	0.5039 (3)	0.0398 (7)	
C21	0.3323 (4)	0.3264 (3)	0.4225 (3)	0.0385 (7)	
C10	-0.3744 (3)	0.4296 (2)	0.9805 (2)	0.0262 (6)	
C14	0.7138 (4)	0.3119 (3)	0.6779 (4)	0.0529 (9)	
H14	0.7988	0.3171	0.7092	0.064*	
C3	0.3115 (4)	0.0349 (3)	1.3225 (3)	0.0338 (6)	

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H3	0.2058	0.0276	1.3575	0.041*	
C2	0.3556 (4)	0.0593 (3)	1.1999 (3)	0.0350 (7)	
H2	0.4604	0.0638	1.1629	0.042*	
C9	-0.2477 (3)	0.3549 (2)	0.9552 (3)	0.0298 (6)	
H9	-0.2753	0.2706	0.9736	0.036*	
C5	0.5685 (4)	0.0473 (3)	1.3708 (3)	0.0398 (7)	
H5	0.6161	0.0793	1.2835	0.048*	
C6	0.6565 (4)	0.0305 (3)	1.4563 (3)	0.0387 (7)	
H6	0.7624	0.0515	1.4259	0.046*	
C11	-0.3509 (3)	0.5488 (2)	0.9820 (2)	0.0303 (6)	
H11	-0.2517	0.5818	0.9709	0.036*	
C17	0.4611 (3)	0.2916 (2)	0.5953 (2)	0.0297 (6)	
C15	0.7236 (4)	0.3696 (3)	0.5503 (4)	0.0506 (9)	
H15	0.8145	0.4161	0.4941	0.061*	
C8	-0.0978 (3)	0.3927 (3)	0.9090 (3)	0.0333 (6)	
H8	-0.0641	0.4748	0.8939	0.040*	
C22	0.2003 (4)	0.3045 (3)	0.3869 (3)	0.0466 (8)	
H22	0.1996	0.3345	0.3009	0.056*	
C23	0.0726 (4)	0.2386 (3)	0.4800 (3)	0.0467 (8)	
H23	-0.0160	0.2227	0.4578	0.056*	
C1	0.2466 (4)	0.0804 (2)	1.1161 (3)	0.0345 (7)	
C7	0.0161 (3)	0.3079 (3)	0.8811 (3)	0.0335 (6)	
C19	0.5968 (4)	0.4111 (3)	0.3712 (3)	0.0491 (9)	
H19	0.6851	0.4579	0.3107	0.059*	
C20	0.4736 (4)	0.3944 (3)	0.3323 (3)	0.0499 (9)	
H20	0.4788	0.4273	0.2450	0.060*	
C13	0.5761 (4)	0.2450 (3)	0.7616 (3)	0.0412 (7)	
H13	0.5717	0.2052	0.8486	0.049*	
O2W	-0.0410 (4)	0.2769 (3)	1.2193 (3)	0.0270 (8)	0.50
HW22	-0.121 (4)	0.275 (5)	1.198 (6)	0.040*	0.50
HW21	0.008 (5)	0.223 (4)	1.202 (6)	0.040*	0.50
HW12	0.073 (4)	-0.019 (4)	0.863 (4)	0.090 (16)*	
HW11	0.144 (4)	-0.074 (3)	0.958 (2)	0.057 (11)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0284 (2)	0.03257 (19)	0.02057 (18)	0.00310 (12)	-0.00688 (12)	-0.00830 (13)
O1W	0.0300 (12)	0.0337 (10)	0.0290 (11)	-0.0016 (8)	-0.0075 (9)	-0.0067 (9)
O2	0.0353 (13)	0.0729 (15)	0.0441 (13)	-0.0072 (11)	-0.0161 (10)	-0.0180 (11)
O3	0.0455 (13)	0.0329 (11)	0.0309 (10)	0.0078 (9)	0.0001 (9)	-0.0098 (8)
O4	0.0272 (12)	0.0614 (13)	0.0518 (13)	0.0078 (10)	-0.0054 (10)	-0.0248 (11)
O1	0.0513 (14)	0.0539 (12)	0.0247 (10)	0.0023 (10)	-0.0200 (9)	-0.0108 (9)
N2	0.0305 (13)	0.0360 (12)	0.0228 (11)	-0.0001 (10)	-0.0064 (9)	-0.0075 (10)
N1	0.0310 (13)	0.0360 (12)	0.0299 (12)	0.0063 (10)	-0.0095 (10)	-0.0163 (10)
C24	0.0337 (17)	0.0485 (17)	0.0344 (16)	0.0003 (13)	-0.0104 (13)	-0.0127 (14)
C4	0.0380 (16)	0.0340 (14)	0.0255 (14)	0.0037 (12)	-0.0135 (12)	-0.0127 (11)
C12	0.0329 (15)	0.0255 (13)	0.0314 (14)	0.0005 (11)	-0.0048 (12)	-0.0121 (11)

C18	0.0350 (16)	0.0266 (13)	0.0222 (13)	0.0042 (11)	-0.0046 (11)	-0.0068 (11)
C16	0.0352 (17)	0.0350 (15)	0.0423 (17)	-0.0020 (13)	0.0037 (13)	-0.0156 (13)
C21	0.0473 (19)	0.0384 (15)	0.0242 (14)	0.0083 (13)	-0.0073 (13)	-0.0076 (12)
C10	0.0280 (14)	0.0278 (13)	0.0205 (12)	0.0010 (11)	-0.0044 (11)	-0.0080 (10)
C14	0.0295 (17)	0.077 (2)	0.068 (2)	0.0018 (16)	-0.0132 (16)	-0.044 (2)
C3	0.0356 (16)	0.0383 (15)	0.0292 (15)	0.0011 (12)	-0.0137 (12)	-0.0120 (12)
C2	0.0378 (17)	0.0386 (15)	0.0290 (15)	0.0000 (13)	-0.0164 (13)	-0.0093 (12)
C9	0.0318 (15)	0.0277 (13)	0.0287 (14)	0.0045 (11)	-0.0086 (12)	-0.0091 (11)
C5	0.0402 (18)	0.0584 (18)	0.0192 (13)	0.0004 (14)	-0.0079 (12)	-0.0131 (13)
C6	0.0285 (15)	0.0572 (18)	0.0306 (15)	0.0006 (13)	-0.0088 (12)	-0.0168 (14)
C11	0.0246 (14)	0.0360 (14)	0.0287 (14)	-0.0022 (11)	-0.0028 (11)	-0.0133 (12)
C17	0.0324 (15)	0.0270 (13)	0.0272 (14)	0.0011 (11)	-0.0030 (12)	-0.0105 (11)
C15	0.0322 (18)	0.0564 (19)	0.061 (2)	-0.0060 (15)	0.0019 (15)	-0.0283 (17)
C8	0.0313 (16)	0.0324 (14)	0.0348 (15)	0.0032 (12)	-0.0077 (12)	-0.0121 (12)
C22	0.057 (2)	0.0567 (19)	0.0252 (15)	0.0122 (16)	-0.0152 (15)	-0.0119 (14)
C23	0.046 (2)	0.065 (2)	0.0369 (17)	0.0091 (16)	-0.0225 (15)	-0.0210 (15)
C1	0.0420 (19)	0.0300 (14)	0.0300 (15)	-0.0061 (12)	-0.0169 (13)	-0.0056 (12)
C7	0.0347 (17)	0.0369 (16)	0.0229 (14)	0.0073 (12)	-0.0059 (12)	-0.0065 (12)
C19	0.044 (2)	0.0462 (18)	0.0369 (17)	-0.0047 (15)	0.0089 (15)	-0.0064 (14)
C20	0.059 (2)	0.0505 (18)	0.0210 (14)	0.0018 (16)	0.0035 (15)	-0.0014 (13)
C13	0.0371 (17)	0.0548 (18)	0.0437 (17)	0.0104 (14)	-0.0172 (14)	-0.0282 (15)
O2W	0.029 (2)	0.0325 (19)	0.0288 (19)	0.0005 (15)	-0.0180 (16)	-0.0163 (16)

Geometric parameters (Å, °)

Zn1—O1	2.041 (2)	C21—C20	1.442 (5)
Zn1—O1W	2.053 (2)	C10—C11	1.396 (4)
Zn1—N1	2.144 (3)	C10—C12 ⁱⁱ	1.397 (4)
Zn1—O4	2.180 (2)	C10—C9	1.462 (4)
Zn1—N2	2.202 (2)	C14—C15	1.359 (5)
Zn1—O3	2.260 (2)	C14—C13	1.392 (5)
Zn1—C7	2.563 (3)	C14—H14	0.9300
O1W—HW12	0.85 (3)	C3—C2	1.309 (4)
O1W—HW11	0.86 (2)	C3—H3	0.9300
O2—C1	1.246 (4)	C2—C1	1.494 (4)
O3—C7	1.260 (4)	C2—H2	0.9300
O4—C7	1.261 (4)	C9—C8	1.331 (4)
O1—C1	1.263 (4)	C9—H9	0.9300
N2—C24	1.324 (4)	C5—C6	1.369 (4)
N2—C18	1.360 (4)	C5—H5	0.9300
N1—C13	1.320 (4)	C6—C4 ⁱ	1.401 (4)
N1—C17	1.355 (4)	C6—H6	0.9300
C24—C23	1.380 (4)	C11—H11	0.9300
C24—H24	0.9300	C15—H15	0.9300
C4—C5	1.388 (4)	C8—C7	1.475 (4)
C4—C6 ⁱ	1.401 (4)	C8—H8	0.9300
C4—C3	1.472 (4)	C22—C23	1.363 (5)
C12—C11	1.378 (4)	C22—H22	0.9300

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C12—C10 ⁱⁱ	1.397 (4)	C23—H23	0.9300
C12—H12	0.9300	C19—C20	1.329 (5)
C18—C21	1.398 (4)	C19—H19	0.9300
C18—C17	1.431 (4)	C20—H20	0.9300
C16—C15	1.395 (5)	C13—H13	0.9300
C16—C17	1.407 (4)	O2W—HW22	0.815 (10)
C16—C19	1.431 (5)	O2W—HW21	0.816 (10)
C21—C22	1.396 (5)		
O1—Zn1—O1W	89.22 (9)	C15—C14—H14	120.1
O1—Zn1—N1	89.76 (9)	C13—C14—H14	120.1
O1W—Zn1—N1	115.47 (8)	C2—C3—C4	127.5 (3)
O1—Zn1—O4	96.13 (9)	C2—C3—H3	116.2
O1W—Zn1—O4	149.07 (9)	C4—C3—H3	116.2
N1—Zn1—O4	95.05 (8)	C3—C2—C1	123.6 (3)
O1—Zn1—N2	162.97 (9)	C3—C2—H2	118.2
O1W—Zn1—N2	88.25 (8)	C1—C2—H2	118.2
N1—Zn1—N2	76.20 (9)	C8—C9—C10	128.0 (3)
O4—Zn1—N2	94.67 (9)	C8—C9—H9	116.0
O1—Zn1—O3	111.13 (9)	C10—C9—H9	116.0
O1W—Zn1—O3	90.77 (8)	C6—C5—C4	121.4 (3)
N1—Zn1—O3	147.13 (8)	C6—C5—H5	119.3
O4—Zn1—O3	58.87 (8)	C4—C5—H5	119.3
N2—Zn1—O3	85.75 (8)	C5—C6—C4 ⁱ	121.3 (3)
O1—Zn1—C7	104.70 (9)	C5—C6—H6	119.3
O1W—Zn1—C7	119.90 (9)	C4 ⁱ —C6—H6	119.3
N1—Zn1—C7	122.57 (9)	C12—C11—C10	120.2 (3)
O4—Zn1—C7	29.45 (9)	C12—C11—H11	119.9
N2—Zn1—C7	91.12 (9)	C10—C11—H11	119.9
O3—Zn1—C7	29.44 (8)	N1—C17—C16	123.0 (3)
Zn1—O1W—HW12	104 (3)	N1—C17—C18	117.7 (2)
Zn1—O1W—HW11	116 (2)	C16—C17—C18	119.2 (3)
HW12—O1W—HW11	104 (3)	C14—C15—C16	119.7 (3)
C7—O3—Zn1	88.74 (18)	C14—C15—H15	120.1
C7—O4—Zn1	92.34 (18)	C16—C15—H15	120.1
C1—O1—Zn1	132.4 (2)	C9—C8—C7	121.7 (3)
C24—N2—C18	117.9 (2)	C9—C8—H8	119.1
C24—N2—Zn1	128.96 (19)	C7—C8—H8	119.1
C18—N2—Zn1	113.08 (18)	C23—C22—C21	119.1 (3)
C13—N1—C17	118.0 (3)	C23—C22—H22	120.4
C13—N1—Zn1	126.8 (2)	C21—C22—H22	120.4
C17—N1—Zn1	114.67 (18)	C22—C23—C24	119.6 (3)
N2—C24—C23	123.2 (3)	C22—C23—H23	120.2
N2—C24—H24	118.4	C24—C23—H23	120.2
C23—C24—H24	118.4	O2—C1—O1	125.7 (3)
C5—C4—C6 ⁱ	117.2 (3)	O2—C1—C2	118.7 (3)
C5—C4—C3	123.0 (3)	O1—C1—C2	115.5 (3)
C6 ⁱ —C4—C3	119.8 (3)	O3—C7—O4	120.0 (3)

C11—C12—C10 ⁱⁱ	121.8 (2)	O3—C7—C8	120.6 (3)
C11—C12—H12	119.1	O4—C7—C8	119.4 (3)
C10 ⁱⁱ —C12—H12	119.1	O3—C7—Zn1	61.82 (15)
N2—C18—C21	122.3 (3)	O4—C7—Zn1	58.21 (16)
N2—C18—C17	117.1 (2)	C8—C7—Zn1	176.5 (2)
C21—C18—C17	120.6 (3)	C20—C19—C16	121.5 (3)
C15—C16—C17	116.9 (3)	C20—C19—H19	119.2
C15—C16—C19	124.2 (3)	C16—C19—H19	119.2
C17—C16—C19	118.9 (3)	C19—C20—C21	121.4 (3)
C22—C21—C18	117.9 (3)	C19—C20—H20	119.3
C22—C21—C20	123.8 (3)	C21—C20—H20	119.3
C18—C21—C20	118.3 (3)	N1—C13—C14	122.6 (3)
C11—C10—C12 ⁱⁱ	118.0 (2)	N1—C13—H13	118.7
C11—C10—C9	122.8 (2)	C14—C13—H13	118.7
C12 ⁱⁱ —C10—C9	119.1 (2)	HW22—O2W—HW21	105.6 (18)
C15—C14—C13	119.8 (3)		

Symmetry codes: (i) $-x+1, -y, -z+3$; (ii) $-x-1, -y+1, -z+2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1W—HW12 \cdots O2 ⁱⁱⁱ	0.85 (3)	1.87 (3)	2.687 (3)	158 (4)
O1W—HW11 \cdots O3 ⁱⁱⁱ	0.86 (2)	1.88 (3)	2.685 (3)	155 (3)
O2W—HW21 \cdots O2	0.816 (10)	2.044 (14)	2.856 (5)	173 (5)

Symmetry codes: (iii) $-x, -y, -z+2$.

Fig. 1

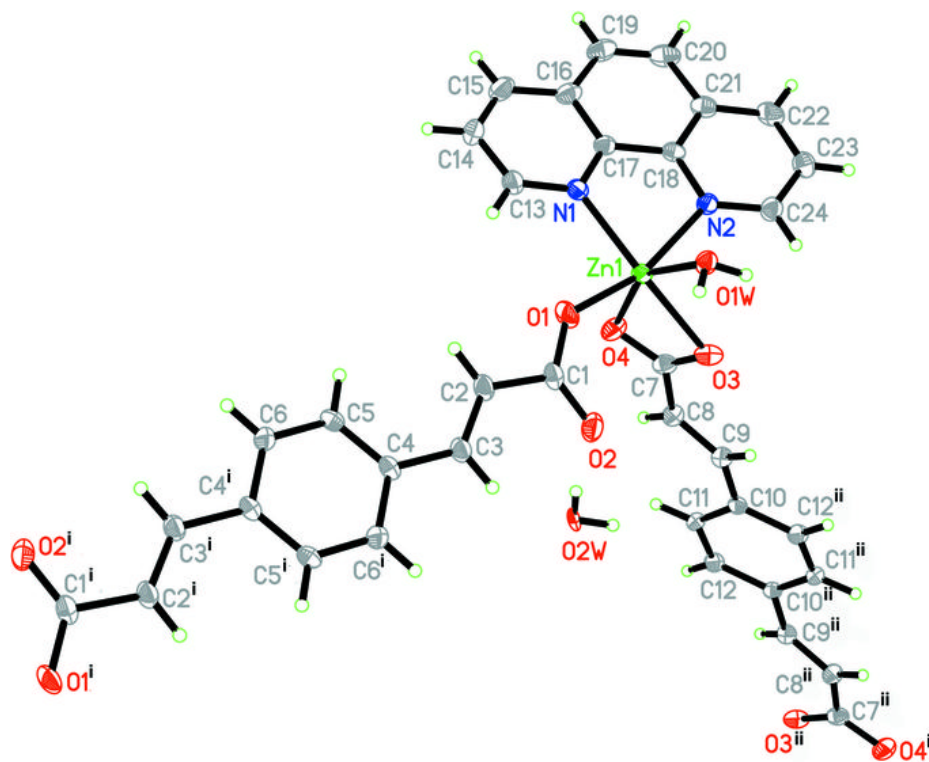


Fig. 2

