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Triaqua[3-(4-carboxylatophenoxy)propionato-κO](1,10-phenanthroline-$\kappa^2 N,N'$)zinc(II)

Li-Li Kong, Shan Gao* and Li-Hua Huo

School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: shangao67@yahoo.com

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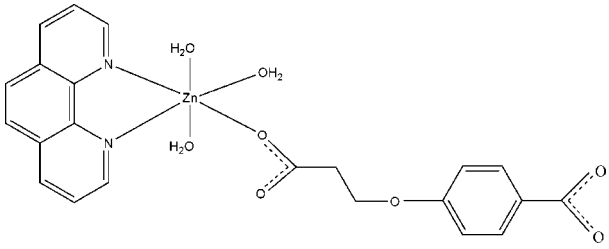
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.101; data-to-parameter ratio = 15.9.

The title compound, $[Zn(C_{10}H_8O_5)(C_{12}H_8N_2)(H_2O)_3]$, is a neutral mononuclear complex. The Zn atom has a distorted octahedral geometry involving one O atom of the 3-(4-carboxylatophenoxy)propionate group, two N atoms of the 1,10-phenanthroline ligand and three water molecules. Extensive hydrogen-bonding and π–π stacking interactions [centroid–centroid distance = 3.656 (3) Å] construct a three-dimensional supramolecular network.

Related literature

The structure of 3-(4-carboxylatophenoxy)propionic acid [3-(p-CPOPH$_2$)] has been reported previously (Gao & Ng, 2006), and the cobalt(II) complex of 3-(p-CPOPH$_2$) was characterized by X-ray crystallography by Kong *et al.* (2007).



Experimental

Crystal data

$[Zn(C_{10}H_8O_5)(C_{12}H_8N_2)(H_2O)_3]$
M_r = 507.79
Triclinic, $P\overline{1}$
a = 7.7101 (15) Å
b = 12.987 (3) Å
c = 13.059 (3) Å
α = 113.31 (3)°
β = 103.62 (3)°
γ = 100.99 (3)°
V = 1106.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 295 (2) K
0.34 × 0.24 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.694, T_{max} = 0.801
10928 measured reflections
5015 independent reflections
4188 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.101
S = 1.16
5015 reflections
316 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1W	2.0443 (19)	Zn1—N2	2.155 (2)
Zn1—O1	2.0598 (16)	Zn1—N1	2.156 (2)
Zn1—O3W	2.135 (2)	Zn1—O2W	2.1848 (19)
O1W—Zn1—O1	95.99 (8)	O3W—Zn1—N1	92.87 (8)
O1W—Zn1—O3W	91.68 (8)	N2—Zn1—N1	77.52 (9)
O1—Zn1—O3W	90.86 (7)	O1W—Zn1—O2W	87.19 (9)
O1W—Zn1—N2	90.54 (9)	O1—Zn1—O2W	86.15 (7)
O1—Zn1—N2	173.43 (8)	O3W—Zn1—O2W	176.67 (7)
O3W—Zn1—N2	89.68 (8)	N2—Zn1—O2W	93.45 (8)
O1W—Zn1—N1	167.19 (8)	N1—Zn1—O2W	88.90 (9)
O1—Zn1—N1	95.91 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O5^{i}	0.847 (10)	1.725 (11)	2.566 (3)	172 (3)
O1W—H1W2···O1^{ii}	0.84 (3)	2.071 (18)	2.834 (3)	150 (3)
O2W—H2W1···O2^{iii}	0.85 (3)	1.93 (3)	2.775 (2)	174 (3)
O2W—H2W2···O5^{iv}	0.84 (3)	2.03 (3)	2.869 (3)	176 (3)
O3W—H3W1···O4^{i}	0.853 (10)	1.835 (11)	2.684 (3)	173 (3)
O3W—H3W2···O2	0.85 (3)	1.89 (3)	2.734 (3)	170 (3)
O3W—H3W2···O1	0.85 (3)	2.56 (3)	2.989 (3)	113 (2)

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

Data collection: *RAPID-AUTO* (Rigaku, 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: BX2110).

  doi:10.1107/S1600536807051318

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supplementary materials

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Triaqua[3-(4-carboxylatophenoxy)propionato-κO](1,10-phenanthroline-$\kappa^2 N,N'$)zinc(II)

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. Thus, 3-(*p*-$CPOPH_2$) may be not only multiple coordination possibilities, but also form regular hydrogen bonds by functioning as both a hydrogen bond donor and acceptor (Gao & Ng, 2006). Recently, we have reported the structures of cobalt(II) complex incorporating 3-(4-carboxylatophenoxy)propionate group, namely $[Co(C_{10}H_9O_5)_2(C_{10}H_{10}O_5)_2(py)_2]$, (Kong *et al.*, 2007).

The molecular structure of the title complex is shown in Fig. 1. The 3-$(p\text{-CPOP})^{2-}$ ligand coordinates in a monodentate fashion to the Zn atom through the carboxylate group. The Zn atom displays a distorted octahedral geometry involving one O atom of the 3-(4-carboxylatophenoxy)propionate group, two N atoms of 1,10-phenanthroline ligand and three water molecules. Furthermore, a three-dimensional supramolecular network is constructed *via* π-π stacking interactions between the 1,10-phenanthroline rings (centroid-centroid distance being 3.656 Å) and hydrogen-bonding interactions (Table 2).

Experimental

The title complex was prepared by the addition of zinc diacetate dihydrate (10 mmol), 1,10-phenanthroline (10 mmol) to a solution of 3-(*p*-$CPOPH_2$) (15 mmol) in H_2O/MeOH (V/V = 1:1) solution, and the pH value was adjusted to 5 with NaOH (0.2 *M*) solution. Colorless crystals were obtained from the filtered solution at room temperature over several days. CH&N analysis. Calc. for $C_{22}H_{22}N_2O_8Zn$: C 52.04, H 4.37, N 5.52%. Found: C 52.05, H 4.38, N 5.50%.

Refinement

The H atoms were placed in 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. The H atoms of hydroxyl groups 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

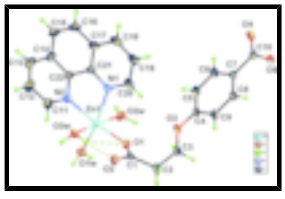


Fig. 1. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

Triaqua[3-(4-carboxylatophenoxy)propionato-κ*O*](1,10-phenanthroline- κ^2N,N')zinc(II)

Crystal data

$[Zn(C_{10}H_8O_5)(C_{12}H_8N_2)(H_2O)_3]$	$Z = 2$
$M_r = 507.79$	$F_{000} = 524$
Triclinic, $P\overline{1}$	$D_x = 1.524$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.7101$ (15) Å	Cell parameters from 9001 reflections
$b = 12.987$ (3) Å	$\theta = 3.1$–27.5º
$c = 13.059$ (3) Å	$\mu = 1.16$ mm^{-1}
$\alpha = 113.31$ (3)º	$T = 295$ (2) K
$\beta = 103.62$ (3)º	Block, colorless
$\gamma = 100.99$ (3)º	0.34 × 0.24 × 0.20 mm
$V = 1106.4$ (4) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	5015 independent reflections
Radiation source: fine-focus sealed tube	4188 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295(2)$ K	$\theta_{min} = 3.1$º
ω scans	$h = -10 \rightarrow 9$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -16 \rightarrow 16$
$T_{min} = 0.694$, $T_{max} = 0.801$	$l = -16 \rightarrow 16$
10928 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
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.6471P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.16$	$(\Delta/\sigma)_{max} < 0.001$
5015 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
316 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
9 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	0.45725 (4)	0.57914 (2)	0.84281 (2)	0.03132 (10)
O1	0.5645 (2)	0.44139 (14)	0.82196 (16)	0.0356 (4)
O1W	0.5203 (3)	0.64632 (17)	1.02239 (16)	0.0399 (4)
H1W1	0.633 (2)	0.684 (2)	1.070 (2)	0.060*
H1W2	0.466 (3)	0.600 (2)	1.044 (3)	0.060*
O2W	0.1961 (2)	0.46005 (17)	0.8234 (2)	0.0456 (5)
H2W1	0.098 (3)	0.478 (3)	0.832 (3)	0.068*
H2W2	0.187 (4)	0.3925 (16)	0.819 (3)	0.068*
O3W	0.7211 (3)	0.68984 (15)	0.86547 (16)	0.0385 (4)
H3W1	0.782 (4)	0.7501 (16)	0.9330 (16)	0.058*
H3W2	0.777 (4)	0.6381 (18)	0.857 (2)	0.058*
O2	0.8616 (2)	0.50571 (15)	0.83328 (17)	0.0398 (4)
O3	0.5297 (2)	0.20884 (15)	0.59373 (16)	0.0397 (4)
O4	−0.0807 (3)	−0.13327 (18)	0.08476 (18)	0.0570 (5)
O5	−0.1526 (3)	−0.23347 (16)	0.18182 (19)	0.0509 (5)
N1	0.3454 (3)	0.52921 (18)	0.65624 (18)	0.0345 (4)
N2	0.3334 (3)	0.71451 (19)	0.84272 (19)	0.0385 (5)
C1	0.7219 (3)	0.4274 (2)	0.81742 (19)	0.0295 (5)
C2	0.7365 (3)	0.3056 (2)	0.7931 (2)	0.0355 (5)
H1	0.8385	0.2951	0.7626	0.043*
H2	0.7678	0.3012	0.8673	0.043*
C3	0.5579 (3)	0.2060 (2)	0.7053 (2)	0.0355 (5)
H3	0.5705	0.1307	0.6976	0.043*
H4	0.4521	0.2173	0.7314	0.043*
C4	0.3857 (3)	0.1200 (2)	0.4968 (2)	0.0344 (5)
C5	0.3654 (4)	0.1241 (2)	0.3900 (2)	0.0402 (6)
H5	0.4480	0.1852	0.3882	0.048*
C6	0.2245 (4)	0.0390 (2)	0.2872 (2)	0.0401 (6)
H7	0.2126	0.0431	0.2165	0.048*
C7	0.0988 (3)	−0.0537 (2)	0.2878 (2)	0.0351 (5)
C8	0.1205 (4)	−0.0569 (2)	0.3944 (2)	0.0387 (6)
H8	0.0388	−0.1184	0.3962	0.046*
C9	0.2617 (4)	0.0295 (2)	0.4990 (2)	0.0402 (6)

H9	0.2726	0.0264	0.5701	0.048*
C10	−0.0562 (4)	−0.1477 (2)	0.1751 (2)	0.0398 (6)
C11	0.3223 (5)	0.8017 (3)	0.9337 (3)	0.0589 (8)
H11	0.3635	0.8051	1.0082	0.071*
C12	0.2510 (6)	0.8896 (3)	0.9231 (4)	0.0763 (11)
H12	0.2439	0.9495	0.9895	0.092*
C13	0.1922 (5)	0.8871 (3)	0.8158 (4)	0.0677 (10)
H13	0.1487	0.9468	0.8085	0.081*
C14	0.1975 (4)	0.7939 (3)	0.7155 (3)	0.0494 (7)
C15	0.1320 (4)	0.7806 (3)	0.5974 (3)	0.0577 (9)
H15	0.0866	0.8377	0.5850	0.069*
C16	0.1350 (4)	0.6879 (3)	0.5048 (3)	0.0576 (9)
H16	0.0908	0.6816	0.4292	0.069*
C17	0.2049 (4)	0.5973 (3)	0.5191 (3)	0.0462 (7)
C18	0.2051 (4)	0.4961 (3)	0.4253 (3)	0.0554 (8)
H18	0.1600	0.4845	0.3477	0.066*
C19	0.2713 (4)	0.4148 (3)	0.4477 (3)	0.0528 (7)
H19	0.2698	0.3466	0.3857	0.063*
C20	0.3419 (4)	0.4346 (2)	0.5653 (2)	0.0431 (6)
H20	0.3882	0.3787	0.5798	0.052*
C21	0.2761 (3)	0.6098 (2)	0.6346 (2)	0.0347 (5)
C22	0.2709 (3)	0.7089 (2)	0.7338 (2)	0.0368 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03197 (15)	0.03128 (15)	0.03090 (16)	0.01282 (11)	0.00887 (11)	0.01442 (12)
O1	0.0275 (8)	0.0317 (9)	0.0519 (11)	0.0129 (7)	0.0167 (7)	0.0200 (8)
O1W	0.0366 (9)	0.0456 (10)	0.0323 (9)	0.0045 (8)	0.0085 (7)	0.0186 (8)
O2W	0.0261 (8)	0.0430 (10)	0.0799 (15)	0.0153 (8)	0.0216 (9)	0.0362 (11)
O3W	0.0400 (9)	0.0313 (9)	0.0369 (10)	0.0082 (8)	0.0113 (8)	0.0115 (8)
O2	0.0304 (9)	0.0338 (9)	0.0563 (12)	0.0095 (8)	0.0197 (8)	0.0195 (9)
O3	0.0370 (9)	0.0304 (9)	0.0369 (10)	−0.0007 (7)	0.0087 (8)	0.0090 (8)
O4	0.0700 (14)	0.0369 (10)	0.0395 (11)	0.0023 (10)	0.0031 (10)	0.0098 (9)
O5	0.0393 (10)	0.0349 (10)	0.0579 (13)	−0.0018 (8)	−0.0010 (9)	0.0182 (9)
N1	0.0305 (10)	0.0351 (11)	0.0332 (11)	0.0045 (9)	0.0096 (8)	0.0149 (9)
N2	0.0415 (11)	0.0355 (11)	0.0391 (12)	0.0166 (10)	0.0111 (9)	0.0173 (10)
C1	0.0312 (11)	0.0314 (11)	0.0233 (11)	0.0119 (10)	0.0088 (9)	0.0094 (9)
C2	0.0315 (12)	0.0305 (12)	0.0412 (14)	0.0131 (10)	0.0098 (10)	0.0135 (11)
C3	0.0326 (12)	0.0293 (12)	0.0389 (13)	0.0082 (10)	0.0104 (10)	0.0122 (11)
C4	0.0298 (11)	0.0283 (11)	0.0362 (13)	0.0078 (10)	0.0095 (10)	0.0081 (10)
C5	0.0397 (13)	0.0307 (12)	0.0437 (15)	0.0047 (11)	0.0141 (11)	0.0141 (11)
C6	0.0421 (14)	0.0350 (13)	0.0389 (14)	0.0089 (11)	0.0143 (11)	0.0144 (11)
C7	0.0313 (12)	0.0257 (11)	0.0403 (13)	0.0109 (10)	0.0083 (10)	0.0090 (10)
C8	0.0350 (12)	0.0283 (12)	0.0453 (15)	0.0047 (10)	0.0112 (11)	0.0140 (11)
C9	0.0423 (14)	0.0354 (13)	0.0375 (14)	0.0093 (11)	0.0121 (11)	0.0140 (11)
C10	0.0375 (13)	0.0279 (12)	0.0428 (15)	0.0140 (11)	0.0056 (11)	0.0088 (11)
C11	0.079 (2)	0.0516 (18)	0.0494 (18)	0.0348 (17)	0.0232 (16)	0.0190 (15)

C12	0.099 (3)	0.056 (2)	0.079 (3)	0.052 (2)	0.034 (2)	0.0220 (19)
C13	0.065 (2)	0.0548 (19)	0.094 (3)	0.0352 (17)	0.022 (2)	0.040 (2)
C14	0.0349 (13)	0.0506 (16)	0.072 (2)	0.0144 (13)	0.0125 (13)	0.0403 (16)
C15	0.0395 (15)	0.066 (2)	0.083 (2)	0.0134 (15)	0.0094 (15)	0.057 (2)
C16	0.0354 (14)	0.086 (2)	0.066 (2)	0.0094 (15)	0.0071 (14)	0.059 (2)
C17	0.0311 (12)	0.0660 (18)	0.0423 (15)	0.0023 (13)	0.0079 (11)	0.0344 (15)
C18	0.0416 (15)	0.079 (2)	0.0339 (15)	−0.0026 (15)	0.0082 (12)	0.0269 (16)
C19	0.0420 (15)	0.0608 (19)	0.0356 (15)	0.0008 (14)	0.0143 (12)	0.0098 (14)
C20	0.0377 (13)	0.0421 (14)	0.0410 (15)	0.0057 (12)	0.0150 (11)	0.0135 (12)
C21	0.0259 (11)	0.0418 (13)	0.0376 (13)	0.0058 (10)	0.0072 (9)	0.0237 (11)
C22	0.0274 (11)	0.0388 (13)	0.0466 (15)	0.0093 (10)	0.0081 (10)	0.0250 (12)

Geometric parameters (Å, °)

Zn1—O1W	2.0443 (19)	C5—C6	1.373 (4)
Zn1—O1	2.0598 (16)	C5—H5	0.9300
Zn1—O3W	2.135 (2)	C6—C7	1.398 (4)
Zn1—N2	2.155 (2)	C6—H7	0.9300
Zn1—N1	2.156 (2)	C7—C8	1.381 (4)
Zn1—O2W	2.1848 (19)	C7—C10	1.509 (4)
O1—C1	1.272 (3)	C8—C9	1.390 (4)
O1W—H1W1	0.847 (10)	C8—H8	0.9300
O1W—H1W2	0.84 (3)	C9—H9	0.9300
O2W—H2W1	0.85 (3)	C11—C12	1.397 (4)
O2W—H2W2	0.84 (3)	C11—H11	0.9300
O3W—H3W1	0.853 (10)	C12—C13	1.353 (5)
O3W—H3W2	0.85 (3)	C12—H12	0.9300
O2—C1	1.244 (3)	C13—C14	1.404 (5)
O3—C4	1.364 (3)	C13—H13	0.9300
O3—C3	1.437 (3)	C14—C22	1.408 (4)
O4—C10	1.244 (3)	C14—C15	1.432 (4)
O5—C10	1.262 (3)	C15—C16	1.336 (5)
N1—C20	1.319 (3)	C15—H15	0.9300
N1—C21	1.355 (3)	C16—C17	1.441 (4)
N2—C11	1.312 (4)	C16—H16	0.9300
N2—C22	1.357 (3)	C17—C18	1.399 (5)
C1—C2	1.517 (3)	C17—C21	1.409 (3)
C2—C3	1.512 (3)	C18—C19	1.357 (5)
C2—H1	0.9700	C18—H18	0.9300
C2—H2	0.9700	C19—C20	1.399 (4)
C3—H3	0.9700	C19—H19	0.9300
C3—H4	0.9700	C20—H20	0.9300
C4—C9	1.381 (4)	C21—C22	1.435 (4)
C4—C5	1.390 (4)		
O1W—Zn1—O1	95.99 (8)	C4—C5—H5	119.7
O1W—Zn1—O3W	91.68 (8)	C5—C6—C7	120.7 (3)
O1—Zn1—O3W	90.86 (7)	C5—C6—H7	119.7
O1W—Zn1—N2	90.54 (9)	C7—C6—H7	119.7
O1—Zn1—N2	173.43 (8)	C8—C7—C6	118.1 (2)

O3W—Zn1—N2	89.68 (8)	C8—C7—C10	120.8 (2)
O1W—Zn1—N1	167.19 (8)	C6—C7—C10	121.0 (2)
O1—Zn1—N1	95.91 (8)	C7—C8—C9	121.6 (2)
O3W—Zn1—N1	92.87 (8)	C7—C8—H8	119.2
N2—Zn1—N1	77.52 (9)	C9—C8—H8	119.2
O1W—Zn1—O2W	87.19 (9)	C4—C9—C8	119.6 (3)
O1—Zn1—O2W	86.15 (7)	C4—C9—H9	120.2
O3W—Zn1—O2W	176.67 (7)	C8—C9—H9	120.2
N2—Zn1—O2W	93.45 (8)	O4—C10—O5	125.6 (3)
N1—Zn1—O2W	88.90 (9)	O4—C10—C7	117.7 (2)
C1—O1—Zn1	133.85 (16)	O5—C10—C7	116.7 (2)
Zn1—O1W—H1W1	121 (2)	N2—C11—C12	122.7 (3)
Zn1—O1W—H1W2	115 (2)	N2—C11—H11	118.7
H1W1—O1W—H1W2	110.3 (16)	C12—C11—H11	118.7
Zn1—O2W—H2W1	126 (2)	C13—C12—C11	119.7 (3)
Zn1—O2W—H2W2	123 (2)	C13—C12—H12	120.2
H2W1—O2W—H2W2	110 (4)	C11—C12—H12	120.2
Zn1—O3W—H3W1	118 (2)	C12—C13—C14	119.6 (3)
Zn1—O3W—H3W2	96 (2)	C12—C13—H13	120.2
H3W1—O3W—H3W2	109.1 (16)	C14—C13—H13	120.2
C4—O3—C3	117.65 (19)	C13—C14—C22	117.1 (3)
C20—N1—C21	118.5 (2)	C13—C14—C15	124.0 (3)
C20—N1—Zn1	128.33 (19)	C22—C14—C15	119.0 (3)
C21—N1—Zn1	113.14 (17)	C16—C15—C14	121.3 (3)
C11—N2—C22	118.5 (2)	C16—C15—H15	119.4
C11—N2—Zn1	128.2 (2)	C14—C15—H15	119.4
C22—N2—Zn1	113.17 (17)	C15—C16—C17	121.6 (3)
O2—C1—O1	124.9 (2)	C15—C16—H16	119.2
O2—C1—C2	119.1 (2)	C17—C16—H16	119.2
O1—C1—C2	116.0 (2)	C18—C17—C21	117.2 (3)
C3—C2—C1	113.5 (2)	C18—C17—C16	124.3 (3)
C3—C2—H1	108.9	C21—C17—C16	118.5 (3)
C1—C2—H1	108.9	C19—C18—C17	119.9 (3)
C3—C2—H2	108.9	C19—C18—H18	120.0
C1—C2—H2	108.9	C17—C18—H18	120.0
H1—C2—H2	107.7	C18—C19—C20	119.3 (3)
O3—C3—C2	106.5 (2)	C18—C19—H19	120.3
O3—C3—H3	110.4	C20—C19—H19	120.3
C2—C3—H3	110.4	N1—C20—C19	122.7 (3)
O3—C3—H4	110.4	N1—C20—H20	118.7
C2—C3—H4	110.4	C19—C20—H20	118.7
H3—C3—H4	108.6	N1—C21—C17	122.4 (3)
O3—C4—C9	124.6 (2)	N1—C21—C22	117.9 (2)
O3—C4—C5	116.0 (2)	C17—C21—C22	119.8 (2)
C9—C4—C5	119.4 (2)	N2—C22—C14	122.4 (3)
C6—C5—C4	120.7 (2)	N2—C22—C21	117.7 (2)
C6—C5—H5	119.7	C14—C22—C21	119.9 (2)
O1W—Zn1—O1—C1	−95.5 (2)	C6—C7—C10—O4	−7.4 (4)
O3W—Zn1—O1—C1	−3.7 (2)	C8—C7—C10—O5	−5.9 (4)

N1—Zn1—O1—C1	89.3 (2)	C6—C7—C10—O5	174.0 (2)
O2W—Zn1—O1—C1	177.8 (2)	C22—N2—C11—C12	−0.8 (5)
O1W—Zn1—N1—C20	−153.9 (3)	Zn1—N2—C11—C12	174.9 (3)
O1—Zn1—N1—C20	4.3 (2)	N2—C11—C12—C13	−0.8 (6)
O3W—Zn1—N1—C20	95.5 (2)	C11—C12—C13—C14	2.2 (6)
N2—Zn1—N1—C20	−175.5 (2)	C12—C13—C14—C22	−2.1 (5)
O2W—Zn1—N1—C20	−81.7 (2)	C12—C13—C14—C15	177.5 (3)
O1W—Zn1—N1—C21	28.0 (4)	C13—C14—C15—C16	−177.8 (3)
O1—Zn1—N1—C21	−173.77 (16)	C22—C14—C15—C16	1.8 (4)
O3W—Zn1—N1—C21	−82.61 (17)	C14—C15—C16—C17	−0.4 (5)
N2—Zn1—N1—C21	6.43 (16)	C15—C16—C17—C18	177.5 (3)
O2W—Zn1—N1—C21	100.21 (16)	C15—C16—C17—C21	−1.7 (4)
O1W—Zn1—N2—C11	1.9 (3)	C21—C17—C18—C19	0.3 (4)
O3W—Zn1—N2—C11	−89.8 (3)	C16—C17—C18—C19	−178.9 (3)
N1—Zn1—N2—C11	177.2 (3)	C17—C18—C19—C20	−1.2 (4)
O2W—Zn1—N2—C11	89.1 (3)	C21—N1—C20—C19	0.7 (4)
O1W—Zn1—N2—C22	177.79 (18)	Zn1—N1—C20—C19	−177.37 (19)
O3W—Zn1—N2—C22	86.11 (18)	C18—C19—C20—N1	0.7 (4)
N1—Zn1—N2—C22	−6.89 (17)	C20—N1—C21—C17	−1.5 (4)
O2W—Zn1—N2—C22	−95.00 (19)	Zn1—N1—C21—C17	176.77 (19)
Zn1—O1—C1—O2	4.9 (4)	C20—N1—C21—C22	176.5 (2)
Zn1—O1—C1—C2	−176.39 (16)	Zn1—N1—C21—C22	−5.2 (3)
O2—C1—C2—C3	−143.6 (2)	C18—C17—C21—N1	1.1 (4)
O1—C1—C2—C3	37.6 (3)	C16—C17—C21—N1	−179.7 (2)
C4—O3—C3—C2	174.05 (19)	C18—C17—C21—C22	−176.9 (2)
C1—C2—C3—O3	64.8 (3)	C16—C17—C21—C22	2.4 (4)
C3—O3—C4—C9	2.0 (3)	C11—N2—C22—C14	0.9 (4)
C3—O3—C4—C5	−178.6 (2)	Zn1—N2—C22—C14	−175.4 (2)
O3—C4—C5—C6	−179.8 (2)	C11—N2—C22—C21	−177.1 (3)
C9—C4—C5—C6	−0.4 (4)	Zn1—N2—C22—C21	6.5 (3)
C4—C5—C6—C7	−0.1 (4)	C13—C14—C22—N2	0.5 (4)
C5—C6—C7—C8	0.0 (4)	C15—C14—C22—N2	−179.1 (2)
C5—C6—C7—C10	−179.9 (2)	C13—C14—C22—C21	178.5 (3)
C6—C7—C8—C9	0.5 (4)	C15—C14—C22—C21	−1.1 (4)
C10—C7—C8—C9	−179.5 (2)	N1—C21—C22—N2	−0.9 (3)
O3—C4—C9—C8	−179.6 (2)	C17—C21—C22—N2	177.2 (2)
C5—C4—C9—C8	1.0 (4)	N1—C21—C22—C14	−179.0 (2)
C7—C8—C9—C4	−1.1 (4)	C17—C21—C22—C14	−1.0 (4)
C8—C7—C10—O4	172.6 (2)		

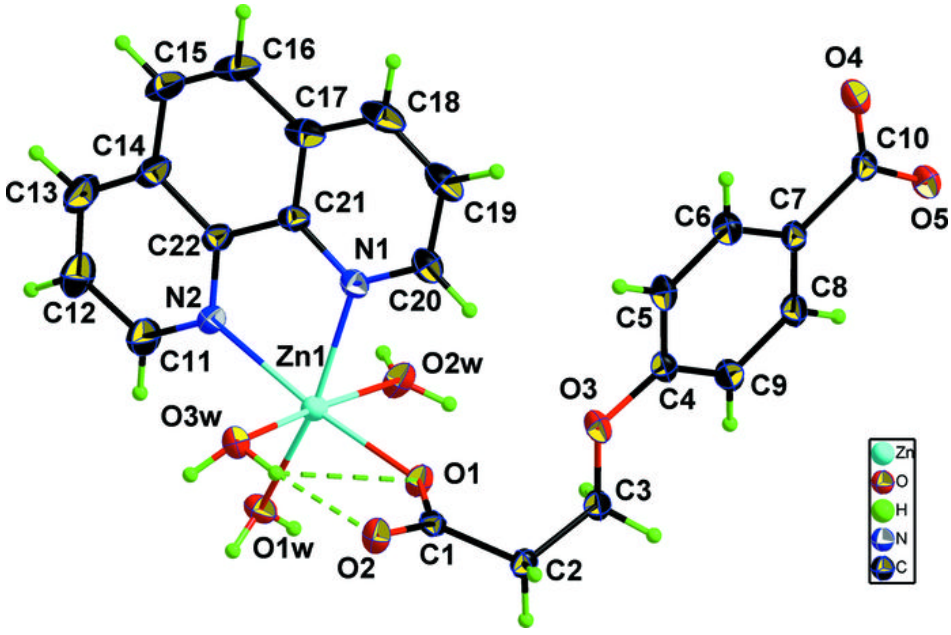
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O5^{i}	0.847 (10)	1.725 (11)	2.566 (3)	172 (3)
O1W—H1W2···O1^{ii}	0.84 (3)	2.071 (18)	2.834 (3)	150 (3)
O2W—H2W1···O2^{iii}	0.85 (3)	1.93 (3)	2.775 (2)	174 (3)
O2W—H2W2···O5^{iv}	0.84 (3)	2.03 (3)	2.869 (3)	176 (3)
O3W—H3W1···O4^{i}	0.853 (10)	1.835 (11)	2.684 (3)	173 (3)

O3W—H3W2···O2	0.85 (3)	1.89 (3)	2.734 (3)	170 (3)
O3W—H3W2···O1	0.85 (3)	2.56 (3)	2.989 (3)	113 (2)

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

Fig. 1


C15
C16
C17
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C6
C7
C8
C9
C10
O4
O5
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