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catena-Poly[[[aqua(1,10-phenanthroline-κ^2N,N')zinc]-μ-acetylenedicarboxylato-$\kappa^2O^1:O^2$] monohydrate]

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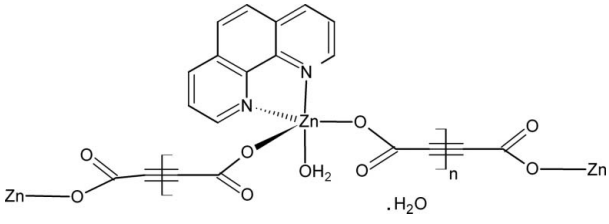
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.111; data-to-parameter ratio = 14.0.

In the title complex, $\{[Zn(C_4O_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O\}_n$, the pentacoordinated Zn^{II} ion is bound to two N atoms of the 1,10-phenanthroline ligand, two O atoms from two bridging acetylenedicarboxylate anions and a water O atom in a distorted trigonal–bipyramidal geometry. The crystal structure is characterized by polymeric zigzag chains running parallel to [2$\bar{1}$0] and is stabilized by O—H···O hydrogen bonds.

Related literature

For background to polymetallic complexes, see: Winpenny (2001); Swiegers & Malefetse (2000). For polymeric complexes based on acetylenedicarboxylate, see: Hermann *et al.* (2011); Lin *et al.* (2011); Zheng *et al.* (2010). For a related six-coordinate octahedral Zn^{II}–pyridine complex with similar hydrogen-bonding interactions, see: Stein & Ruschewitz (2009).



Experimental

Crystal data

$[Zn(C_4O_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O$
M_r = 393.65
Triclinic, $P\bar{1}$
a = 7.9592 (8) Å
b = 7.9598 (8) Å
c = 13.3712 (13) Å
α = 105.062 (2)°
β = 101.287 (2)°
γ = 99.131 (2)°
V = 782.30 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 296 K
0.37 × 0.14 × 0.07 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.588, T_{max} = 0.896
6649 measured reflections
3398 independent reflections
3069 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.111
S = 1.14
3398 reflections
242 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O3^{i}	0.83 (2)	1.91 (2)	2.741 (4)	176 (4)
O5—H2W···O6^{ii}	0.83 (2)	1.93 (2)	2.746 (4)	167 (5)
O6—H3W···O2^{iii}	0.83 (2)	2.04 (3)	2.847 (5)	164 (6)
O6—H4W···O4^{iv}	0.85 (2)	1.97 (2)	2.806 (4)	168 (5)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5933).

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supporting information

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catena-Poly[[[aqua(1,10-phenanthroline-κ^2N,N')zinc]-μ-acetylenedicarboxylato-κ^2O^1:O^2] monohydrate]

Mohammed Fettouhi

S1. Comment

The design and structural control of polymetallic complexes is an area of interest owing to wide potential applications (Winpenny, 2001; Swiegers *et al.*, 2000). In this context, acetylenedicarboxylate is a particularly attracting ligand as a building block of polymeric metal complexes (Hermann *et al.*, 2011; Lin *et al.*, 2011; Zheng *et al.*, 2010). I report herein on a polymeric zinc complex based on 1,10-phenanthroline and the acetylenedicarboxylate anion. The Zn(II) ion is bound to two nitrogen atoms of the 1,10-phenanthroline ligand, two oxygen atoms each belonging to an acetylenedicarboxylate anion and an oxygen atom of a water molecule (Figure 1). The geometry is distorted trigonal bipyramidal where the equatorial positions are occupied by the two carboxylate oxygen atoms and one nitrogen atom. The two acetylenedicarboxylate anions are each located on an inversion center and bridging Zn(II) ions to generate a zigzag chain structure parallel to [2 $\bar{1}$ 0] (Figure 2). The coordinated water molecule belonging to one chain interacts with a carbonyl oxygen of an adjacent chain, giving rise to eight-membered [Zn—(O···H—O)$_2$—Zn] inter-chain rings with a chair configuration. One crystallization water molecule in the lattice has hydrogen bonding interactions connecting three adjacent chains by interacting with two carbonyl oxygen atoms of the first and second chain respectively in addition to a hydrogen atom of the coordinated water molecule of the third chain. A six-coordinate octahedral pyridine complex with similar hydrogen bonding interactions has been reported (Stein *et al.*, 2009).

S2. Experimental

Acetylenedicarboxylic acid (0.2 mmol, 0.0228 g) and 1,10-phenanthroline (0.2 mmol, 0.0397 g) were mixed in 2 ml e thanol. A clear solution was obtained upon addition of an aqueous solution (2 ml) of $Zn(NO_3)_2.6H_2O$ (0.2 mmol, 0.0595 g). The pH was then adjusted to 4.4 using NaOH (0.010 *M*) and the solution was filtered. Colorless crystals suitable for X-ray diffraction were obtained after few days by slow evaporation of the filtrate.

S3. Refinement

H atoms of the two water molecules were located on a difference Fourier map and refined isotropically with distance restraints of O—H = 0.84 (2) Å. All other H atoms were placed in calculated positions with a C—H distance of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

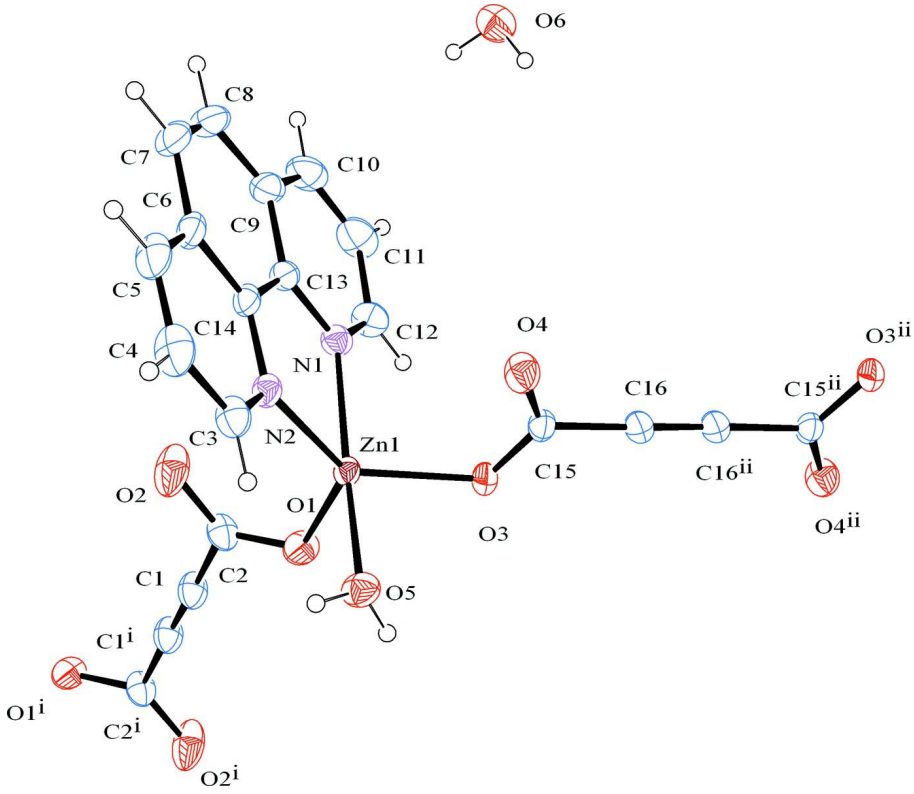

Figure 1

Molecular structure of a fragment of the title compound showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level (Symmetry codes: i = -*x* + 1,-*y* + 2,-*z*; ii = -*x*,-*y*,-*z*).

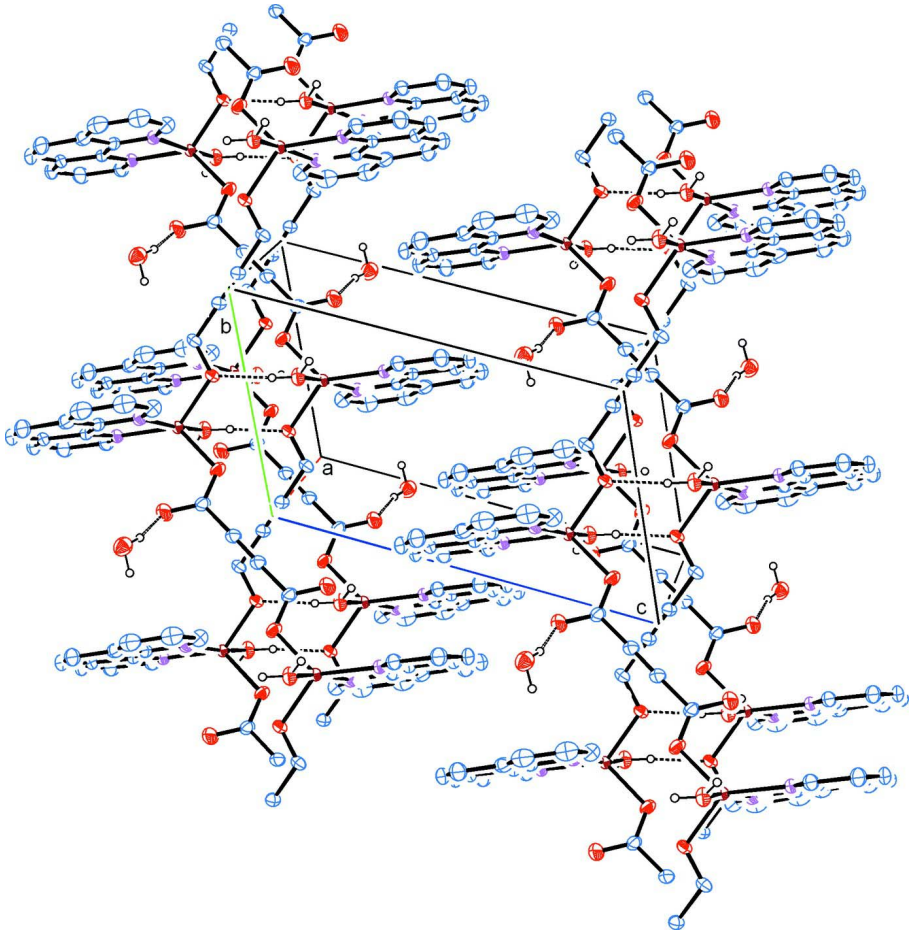

Figure 2

Packing diagram of the title complex showing the H-bonding interactions.

***catena*-Poly[[[aqua(1,10-phenanthroline-κ^2N,N')zinc]- μ-acetylenedicarboxylato-κ^2O^1:O^2] monohydrate]**

Crystal data

$[Zn(C_4O_4)(C_{12}H_8N_2)(H_2O)]\cdot H_2O$
$M_r = 393.65$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.9592$ (8) Å
$b = 7.9598$ (8) Å
$c = 13.3712$ (13) Å
$\alpha = 105.062$ (2)°
$\beta = 101.287$ (2)°
$\gamma = 99.131$ (2)°
$V = 782.30$ (13) Å^3
$Z = 2$
$F(000) = 400$
$D_x = 1.671$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6941 reflections
$\theta = 1.6$–28.3°
$\mu = 1.61$ mm^{-1}
$T = 296$ K
Parallelepiped, yellow
0.37 × 0.14 × 0.07 mm

Data collection

Bruker Smart Apex area detector diffractometer
Radiation source: normal-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan *SADABS*; Sheldrick, 1996
$T_{min} = 0.588$, $T_{max} = 0.896$
6649 measured reflections
3398 independent reflections

3069 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.1°$, $\theta_{min} = 1.6°$

$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.111$
$S = 1.14$
3398 reflections
242 parameters
4 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 1.0051P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.23205 (5)	0.62227 (5)	0.17319 (3)	0.02899 (13)
N1	0.4701 (4)	0.5448 (4)	0.2254 (2)	0.0364 (6)
N2	0.2790 (4)	0.7239 (4)	0.3405 (2)	0.0339 (6)
O1	0.3084 (3)	0.7402 (4)	0.0701 (2)	0.0472 (7)
O2	0.5273 (5)	0.9248 (5)	0.1989 (2)	0.0753 (11)
O3	0.1288 (3)	0.3764 (3)	0.06832 (19)	0.0386 (5)
O4	0.0871 (4)	0.2719 (3)	0.2021 (2)	0.0481 (6)
O5	−0.0117 (4)	0.6855 (4)	0.1476 (2)	0.0440 (6)
O6	0.9009 (5)	−0.0096 (5)	0.2544 (3)	0.0570 (8)
C1	0.4810 (5)	0.9623 (5)	0.0304 (3)	0.0432 (8)
C2	0.4356 (5)	0.8714 (5)	0.1069 (3)	0.0417 (8)
C3	0.1800 (6)	0.8060 (5)	0.3967 (3)	0.0439 (8)
H3	0.0747	0.8234	0.3609	0.053*
C4	0.2293 (7)	0.8677 (6)	0.5091 (3)	0.0588 (12)
H4	0.1567	0.9244	0.5464	0.071*
C5	0.3816 (7)	0.8450 (6)	0.5629 (3)	0.0622 (13)
H5	0.4151	0.8868	0.6371	0.075*
C6	0.4893 (6)	0.7575 (5)	0.5058 (3)	0.0488 (10)
C7	0.6539 (7)	0.7268 (7)	0.5552 (4)	0.0673 (15)
H7	0.6943	0.7677	0.6293	0.081*
C8	0.7501 (6)	0.6408 (7)	0.4972 (4)	0.0674 (14)

H8	0.8569	0.6246	0.5319	0.081*
C9	0.6940 (5)	0.5727 (6)	0.3829 (4)	0.0519 (10)
C10	0.7835 (6)	0.4750 (6)	0.3164 (5)	0.0639 (13)
H10	0.8896	0.4513	0.3461	0.077*
C11	0.7161 (6)	0.4151 (6)	0.2092 (5)	0.0620 (12)
H11	0.7741	0.3486	0.1650	0.074*
C12	0.5598 (5)	0.4544 (5)	0.1665 (3)	0.0469 (9)
H12	0.5159	0.4152	0.0926	0.056*
C13	0.5344 (4)	0.6041 (5)	0.3325 (3)	0.0366 (7)
C14	0.4315 (5)	0.6990 (4)	0.3941 (3)	0.0366 (8)
C15	0.0839 (4)	0.2526 (4)	0.1076 (3)	0.0341 (7)
C16	0.0234 (5)	0.0720 (4)	0.0302 (3)	0.0356 (7)
H1W	−0.051 (5)	0.662 (6)	0.0818 (16)	0.045 (12)*
H2W	−0.029 (6)	0.775 (4)	0.188 (3)	0.066 (15)*
H3W	0.795 (3)	−0.030 (8)	0.226 (4)	0.079 (19)*
H4W	0.946 (6)	0.084 (4)	0.242 (4)	0.067 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0351 (2)	0.0266 (2)	0.02205 (19)	0.00242 (14)	0.00536 (14)	0.00573 (13)
N1	0.0358 (15)	0.0368 (15)	0.0382 (15)	0.0069 (12)	0.0095 (12)	0.0146 (12)
N2	0.0412 (15)	0.0308 (14)	0.0261 (13)	0.0017 (12)	0.0073 (11)	0.0071 (11)
O1	0.0449 (15)	0.0527 (16)	0.0448 (15)	−0.0046 (12)	0.0066 (12)	0.0288 (13)
O2	0.108 (3)	0.063 (2)	0.0341 (16)	−0.0223 (19)	0.0131 (16)	0.0070 (14)
O3	0.0461 (14)	0.0252 (11)	0.0342 (12)	−0.0001 (10)	−0.0009 (10)	0.0041 (9)
O4	0.0627 (17)	0.0410 (14)	0.0359 (14)	0.0072 (12)	0.0133 (12)	0.0057 (11)
O5	0.0486 (15)	0.0492 (16)	0.0330 (14)	0.0156 (12)	0.0073 (12)	0.0096 (12)
O6	0.068 (2)	0.057 (2)	0.0536 (18)	0.0196 (17)	0.0231 (17)	0.0201 (15)
C1	0.048 (2)	0.0378 (19)	0.040 (2)	−0.0027 (16)	0.0129 (16)	0.0109 (15)
C2	0.057 (2)	0.0356 (19)	0.0361 (19)	0.0063 (16)	0.0198 (17)	0.0130 (15)
C3	0.057 (2)	0.0379 (19)	0.0354 (19)	0.0064 (16)	0.0171 (17)	0.0071 (15)
C4	0.089 (3)	0.050 (2)	0.037 (2)	0.007 (2)	0.029 (2)	0.0050 (18)
C5	0.104 (4)	0.046 (2)	0.0228 (18)	−0.006 (2)	0.006 (2)	0.0065 (16)
C6	0.068 (3)	0.0359 (19)	0.0285 (18)	−0.0112 (18)	−0.0038 (17)	0.0108 (15)
C7	0.081 (3)	0.056 (3)	0.042 (2)	−0.015 (2)	−0.022 (2)	0.021 (2)
C8	0.053 (3)	0.066 (3)	0.068 (3)	−0.003 (2)	−0.022 (2)	0.032 (3)
C9	0.037 (2)	0.049 (2)	0.066 (3)	−0.0021 (17)	−0.0050 (18)	0.031 (2)
C10	0.037 (2)	0.061 (3)	0.100 (4)	0.015 (2)	0.006 (2)	0.040 (3)
C11	0.046 (2)	0.060 (3)	0.091 (4)	0.021 (2)	0.026 (2)	0.030 (3)
C12	0.048 (2)	0.049 (2)	0.049 (2)	0.0166 (18)	0.0177 (18)	0.0167 (18)
C13	0.0350 (17)	0.0340 (17)	0.0381 (18)	−0.0008 (14)	0.0018 (14)	0.0166 (14)
C14	0.0439 (19)	0.0299 (16)	0.0289 (16)	−0.0066 (14)	0.0013 (14)	0.0115 (13)
C15	0.0310 (16)	0.0267 (16)	0.0371 (18)	0.0055 (13)	0.0023 (13)	0.0017 (13)
C16	0.0385 (18)	0.0290 (15)	0.0378 (18)	0.0061 (13)	0.0084 (14)	0.0091 (13)

Geometric parameters (Å, º)

Zn1—O1	1.992 (2)	C4—C5	1.347 (7)
Zn1—O3	2.021 (2)	C4—H4	0.9300
Zn1—O5	2.067 (3)	C5—C6	1.404 (7)
Zn1—N2	2.106 (3)	C5—H5	0.9300
Zn1—N1	2.129 (3)	C6—C14	1.400 (5)
N1—C12	1.318 (5)	C6—C7	1.435 (7)
N1—C13	1.349 (4)	C7—C8	1.335 (8)
N2—C3	1.324 (5)	C7—H7	0.9300
N2—C14	1.354 (4)	C8—C9	1.433 (7)
O1—C2	1.249 (4)	C8—H8	0.9300
O2—C2	1.227 (5)	C9—C10	1.403 (7)
O3—C15	1.267 (4)	C9—C13	1.408 (5)
O4—C15	1.227 (4)	C10—C11	1.353 (7)
O5—H1W	0.834 (19)	C10—H10	0.9300
O5—H2W	0.829 (19)	C11—C12	1.382 (6)
O6—H3W	0.826 (19)	C11—H11	0.9300
O6—H4W	0.849 (19)	C12—H12	0.9300
C1—C1^{i}	1.185 (7)	C13—C14	1.435 (5)
C1—C2	1.465 (5)	C15—C16	1.477 (4)
C3—C4	1.406 (5)	C16—C16^{ii}	1.171 (7)
C3—H3	0.9300		

O1—Zn1—O3	97.23 (11)	C4—C5—H5	120.3
O1—Zn1—O5	92.99 (11)	C6—C5—H5	120.3
O3—Zn1—O5	90.36 (11)	C14—C6—C5	117.3 (4)
O1—Zn1—N2	129.20 (11)	C14—C6—C7	118.9 (4)
O3—Zn1—N2	133.15 (10)	C5—C6—C7	123.8 (4)
O5—Zn1—N2	92.75 (11)	C8—C7—C6	121.4 (4)
O1—Zn1—N1	97.80 (11)	C8—C7—H7	119.3
O3—Zn1—N1	90.77 (11)	C6—C7—H7	119.3
O5—Zn1—N1	168.92 (11)	C7—C8—C9	122.0 (4)
N2—Zn1—N1	78.48 (11)	C7—C8—H8	119.0
C12—N1—C13	118.7 (3)	C9—C8—H8	119.0
C12—N1—Zn1	128.1 (3)	C10—C9—C13	116.8 (4)
C13—N1—Zn1	113.2 (2)	C10—C9—C8	125.6 (4)
C3—N2—C14	118.2 (3)	C13—C9—C8	117.6 (4)
C3—N2—Zn1	128.4 (3)	C11—C10—C9	120.3 (4)
C14—N2—Zn1	113.4 (2)	C11—C10—H10	119.9
C2—O1—Zn1	117.2 (2)	C9—C10—H10	119.9
C15—O3—Zn1	116.4 (2)	C10—C11—C12	119.0 (4)
Zn1—O5—H1W	108 (3)	C10—C11—H11	120.5
Zn1—O5—H2W	120 (4)	C12—C11—H11	120.5
H1W—O5—H2W	119 (5)	N1—C12—C11	123.1 (4)
H3W—O6—H4W	105 (5)	N1—C12—H12	118.4
C1^{i}—C1—C2	179.1 (5)	C11—C12—H12	118.4
O2—C2—O1	125.8 (3)	N1—C13—C9	122.1 (4)

O2—C2—C1	118.4 (3)	N1—C13—C14	117.1 (3)
O1—C2—C1	115.8 (3)	C9—C13—C14	120.8 (4)
N2—C3—C4	121.9 (4)	N2—C14—C6	123.0 (4)
N2—C3—H3	119.0	N2—C14—C13	117.8 (3)
C4—C3—H3	119.0	C6—C14—C13	119.3 (3)
C5—C4—C3	120.1 (4)	O4—C15—O3	125.6 (3)
C5—C4—H4	119.9	O4—C15—C16	119.3 (3)
C3—C4—H4	119.9	O3—C15—C16	115.2 (3)
C4—C5—C6	119.4 (4)	C16^{ii}—C16—C15	179.1 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1*W*···O3^{iii}	0.83 (2)	1.91 (2)	2.741 (4)	176 (4)
O5—H2*W*···O6^{iv}	0.83 (2)	1.93 (2)	2.746 (4)	167 (5)
O6—H3*W*···O2^{v}	0.83 (2)	2.04 (3)	2.847 (5)	164 (6)
O6—H4*W*···O4^{vi}	0.85 (2)	1.97 (2)	2.806 (4)	168 (5)

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