Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[tetrakis(μ-cyclohexane-1,4-dicarboxylato)di-μ-hydroxido-pentazinc(II)]

Jin-Xi Chen* and Wei-Wei Meng

School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, People's Republic of China
Correspondence e-mail: mww_514730@yahoo.com.cn

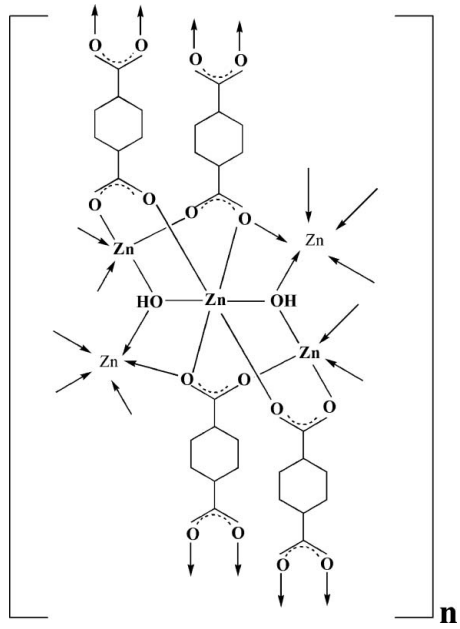
Received 8 November 2009; accepted 1 December 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.008 Å; H-atom completeness 96%; R factor = 0.038; wR factor = 0.095; data-to-parameter ratio = 12.8.

In the title coordination polymer, $[Zn_5(\mu_3\text{-}OH)_2(1,4\text{-}CDC)_4]_n$ (1,4-CDCH$_2$ = 1,4-cyclohexanedicarboxylic acid) or $[Zn_5(C_8H_{10}O_4)_4(OH)_2]_n$, the asymmetric unit comprises one half of an octahedrally coordinated ZnO_6 complex unit (site symmetry $\overline{1}$) and two five-coordinate ZnO_5 complex units, together with two μ_3-bridging hydroxido ligands and four 1,4-CDC ligands (comprising two whole molecules and four inversion-related half-molecules). The ZnO_6 unit consists of four carboxylate O donors (two bridging) and two hydroxido O donors (both bridging three Zn centres) [Zn—O range 2.065 (3)–2.125 (3) Å]. Each of the ZnO_5 units [one capped tetrahedral, the other square-pyrimidal; Zn—O range 1.928 (3)–2.338 (3) Å] has one hydroxido O donor and four carboxyl O donors from three different 1,4-CDC carboxylate O donors (one bridging). Infinite $(ZnO)_n$ inorganic chains run parallel to the a axis and are interconnected by the organic ligands into a three-dimensional structure.

Related literature

For the structures of related complexes of 1,4-cyclohexanedicarboxylic acid, see: Liu, Huang *et al.* (2009); Liu, Zhu *et al.* (2009); Yang *et al.* (2007); Du *et al.* (2005).



Experimental

Crystal data

$[Zn_5(C_8H_{10}O_4)_4(OH)_2]$
M_r = 1039.59
Triclinic, $P\overline{1}$
a = 8.646 (3) Å
b = 10.665 (3) Å
c = 11.804 (3) Å
α = 113.915 (3)°
β = 96.307 (3)°
γ = 106.285 (3)°
V = 923.6 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 3.28 mm^{-1}
T = 295 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
3929 measured reflections
3202 independent reflections
2789 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.095
S = 1.04
3202 reflections
250 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

We gratefully acknowledge financial support by the start-up fund of Southeast University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2020).

References

Du, M., Cai, H. & Zhao, X.-J. (2005). *Inorg. Chim. Acta*, **358**, 4034–4038.
Liu, G.-X., Huang, L.-F., Kong, X.-J., Huang, R.-Y. & Xu, H. (2009). *Inorg. Chim. Acta*, **362**, 1755–1760.
Liu, G.-X., Zhu, K., Chen, H., Huang, R.-Y., Xu, H. & Ren, X.-M. (2009). *Inorg. Chim. Acta*, **362**, 1605–1610.
Rigaku (2005). *CrystalStructure*. Rigaku Americas Corporation, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, E.-C., Zhao, H.-K., Ding, B., Wang, X.-G. & Zhao, X.-J. (2007). *Cryst. Growth Des.* **7**, 2009–2015.

supporting information

Acta Cryst. (2010). E**66**, m16–m17 [doi:10.1107/S1600536809051666]

Poly[tetrakis(μ-cyclohexane-1,4-dicarboxylato)di-μ-hydroxido-pentazinc(II)]

Jin-Xi Chen and Wei-Wei Meng

S1. Comment

In recent years, new coordination compounds formed from reaction of metals with cyclohexane-1,4-dicarboxylic acid [1,4-$CDCH_2$] have attracted much attention (Liu, Huang *et al.*, 2009; Liu, Zhu *et al.*, 2009; Yang *et al.*, 2007; Du *et al.*, 2005). The structure of the title complex from the reaction of this acid with Zn^{II} ion, $[Zn_5(\mu_3\text{-}OH)_2(1,4\text{-}CDC)_4]_n$ (I) has been determined and the structure is reported here.

Compound (I) is a coordination polymer in which the repeating unit lies on a crystallographic inversion centre,the asymmetric unit comprising a half of an octahedraly coordinated Zn atom (Zn1) which lies on the centre, two five-coordinate Zn atoms in (Zn2 and Zn3), general sites, one μ_3-hydroxido ligand (O1) and two cyclohexane-1,4-dicarboxylate ligands (Fig. 1). One of these 1,4-CDC ligands is complete (associated with donor atoms O6, O8, O3, O7) while the other 1,4-CDC ligand consists of two inversion-related halves (associated with O4, O5 and O2, O9). The ZnO_6 coordination sphere about Zn1 consists of four carboxylate O donors (two bridging) and two hydroxido O donors (both bridging three Zn centres), [Zn—O bond length range, 2.065 (3)–2.125 (3) Å]. Both Zn2 and Zn3 are five coordinate, Zn2 having a capped tetrahedral stereochemistry, comprising one bridging hydroxyl O donor and four O donors from three different 1,4-CDC ligands (one bridging) [Zn–O bond length and O–Zn–O bond angle ranges, 1.928 (3)–2.338 (3) Å and 58.85 (11)–145.39 (12)° respectively]. The stereochemistry about Zn3 is tetragonal pyramidal with the four basal coordination sites occupied by O donor atoms from three different 1,4-CDC ligands (one bridging) [Zn—O range, 1.938 (3)–2.207 (3) Å], with the axial site occupied by the bridging hydroxido O donor [Zn–O1, 1.977 (3) Å]. The bond angle range is 86.00 (12)–125.97 (12)°. The repeat units form infinite $(ZnO)_n$ inorganic chains parallel to the *a*-axis which are interconnected by the organic ligands into a three-dimensional structure (Fig. 2).

S2. Experimental

An aqueous mixture of cyclohexane-1,4-dicarboxylic acid (0.086 g, 0.5 mmol) and NaOH (0.040 g, 1 mmol) in 8 ml of water was stirred for half an hour. The pH was adjusted to *ca*. 7 with 1M HNO_3 and (0.147 g, 0.5 mmol) of $Zn(NO_3)_2 \cdot 6H_2O$ was added and the solution was stirred for half an hour. After adding 3 ml of cyclohexanol, the mixture was transferred into a 23 ml Teflon-lined autoclave and heated at 180° for 120 h. After cooling to room temperature, colorless single crystal blocks were obtained, which were washed with water.

S3. Refinement

All H atoms were fixed geometrically and treated as riding, with C—H = 0.97 –0.98 Å and with *U*iso(H) = 1.2*U*eq(C).

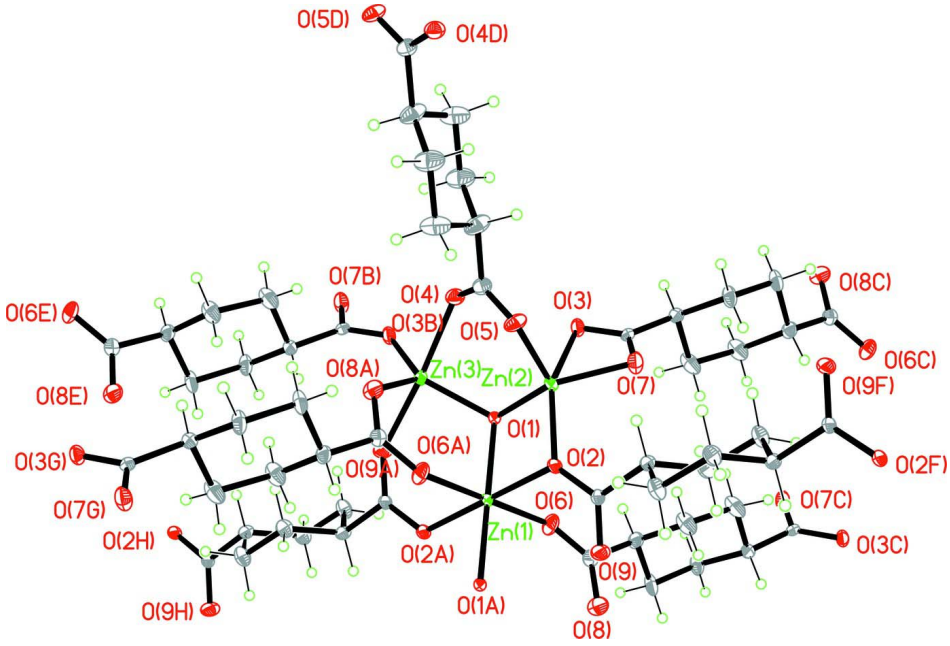


Figure 1

The asymmetric unit of the title compound (I), with displacement ellipsoids drawn at the 30% probability level. For symmetry codes: (A),-*x*+1,-*y*+1,-*z*+1; (B),-*x*,-*y*+1,-*z*+1; (C),-*x*,-*y*,-*z*; (D),-*x*,-*y*+2,-*z*+1; (E), -*x*,-*y*-1,-*z*+1;(F),-*x*+1,-*y*+1,-*z*; (G), *x*+1, *y*+1, *z*+1; (H), *x*, *y*,*z*+1.

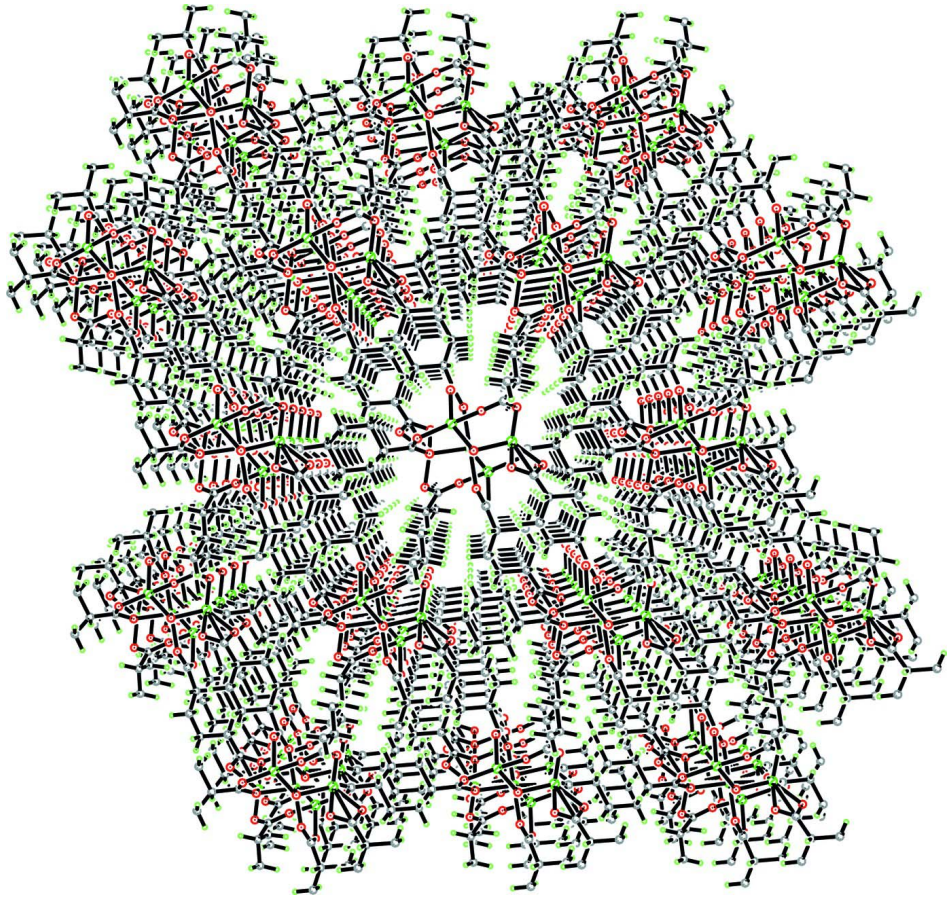


Figure 2

The two-dimensional framework polymer structure of (I).

Poly[tetrakis(*μ*-cyclohexane-1,4-dicarboxylato)di-*μ*-hydroxido-pentazinc(II)]

Crystal data

$[Zn_5(OH)_2(C_8H_{10}O_4)_4]$
$M_r = 1039.59$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.646$ (3) Å
$b = 10.665$ (3) Å
$c = 11.804$ (3) Å
$\alpha = 113.915$ (3)°
$\beta = 96.307$ (3)°
$\gamma = 106.285$ (3)°
$V = 923.6$ (5) Å^3
$Z = 1$
$F(000) = 526$
$D_x = 1.869$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 30 reflections
$\theta = 3$–25°
$\mu = 3.28$ mm^{-1}
$T = 295$ K
Block, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
3929 measured reflections
3202 independent reflections
2789 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 9$

$l = -14 \rightarrow 13$
3 standard reflections every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.095$
$S = 1.04$
3202 reflections
250 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 2.2254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.11$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ 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	0.5000	0.5000	0.5000	0.01886 (17)
Zn2	0.23318 (6)	0.53614 (5)	0.33384 (4)	0.02004 (14)
Zn3	0.22931 (6)	0.63639 (5)	0.63471 (4)	0.02095 (15)
O1	0.2545 (3)	0.4858 (3)	0.4786 (2)	0.0165 (6)
O2	0.4649 (3)	0.5325 (3)	0.3351 (3)	0.0227 (6)
O3	−0.0494 (4)	0.3940 (3)	0.2794 (3)	0.0260 (7)
O4	0.0760 (4)	0.7048 (3)	0.5332 (3)	0.0292 (7)
O5	0.2146 (4)	0.7268 (3)	0.3889 (3)	0.0329 (8)
O6	0.4102 (4)	0.2695 (3)	0.3800 (3)	0.0333 (8)
O7	0.1035 (4)	0.4072 (4)	0.1489 (3)	0.0354 (8)
O8	0.5888 (4)	0.1755 (3)	0.2861 (3)	0.0367 (8)
O9	0.6515 (4)	0.4466 (4)	0.2502 (3)	0.0391 (9)
C1	−0.0356 (5)	0.3514 (5)	0.1658 (4)	0.0216 (9)
C2	0.4892 (6)	0.5179 (5)	0.1295 (4)	0.0244 (9)
H2	0.4089	0.5681	0.1453	0.029*
C3	0.5402 (5)	0.4959 (5)	0.2450 (4)	0.0210 (9)
C4	−0.1756 (5)	0.2307 (5)	0.0558 (4)	0.0239 (9)
H4	−0.2808	0.2294	0.0799	0.029*
C5	0.4451 (6)	0.1700 (5)	0.2982 (4)	0.0266 (10)
C6	0.3284 (6)	−0.1108 (5)	0.1772 (4)	0.0340 (11)
H6A	0.3326	−0.1206	0.2556	0.041*
H6B	0.4337	−0.1087	0.1553	0.041*

C7	0.4060 (6)	0.3693 (5)	0.0104 (4)	0.0293 (10)
H7A	0.4817	0.3156	−0.0022	0.035*
H7B	0.3068	0.3126	0.0236	0.035*
C8	0.3027 (5)	0.0317 (5)	0.1984 (4)	0.0274 (10)
H8	0.1995	0.0306	0.2258	0.033*
C9	0.6414 (6)	0.6136 (5)	0.1087 (4)	0.0330 (11)
H9A	0.6883	0.7096	0.1827	0.040*
H9B	0.7258	0.5689	0.1000	0.040*
C10	−0.1861 (6)	0.2424 (5)	−0.0691 (4)	0.0330 (11)
H10A	−0.0815	0.2467	−0.0928	0.040*
H10B	−0.2041	0.3323	−0.0568	0.040*
C11	0.1180 (6)	0.7593 (5)	0.4592 (4)	0.0281 (10)
C12	0.0494 (7)	0.8716 (6)	0.4494 (6)	0.0441 (13)
H12	0.0263	0.8499	0.3590	0.053*
C13	−0.1518 (7)	0.0883 (5)	0.0363 (5)	0.0425 (13)
H13A	−0.1540	0.0779	0.1141	0.051*
H13B	−0.0434	0.0922	0.0200	0.051*
C14	0.2867 (7)	0.0456 (5)	0.0755 (5)	0.0396 (12)
H14A	0.3928	0.0582	0.0533	0.047*
H14B	0.2606	0.1326	0.0894	0.047*
C15	0.1774 (7)	1.0209 (7)	0.5214 (7)	0.0554 (16)
H15A	0.2750	1.0237	0.4876	0.066*
H15B	0.2105	1.0432	0.6107	0.066*
C16	−0.1133 (7)	0.8624 (6)	0.4875 (7)	0.0518 (15)
H16A	−0.0976	0.8752	0.5746	0.062*
H16B	−0.1962	0.7657	0.4319	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0198 (3)	0.0240 (4)	0.0140 (3)	0.0118 (3)	0.0024 (3)	0.0077 (3)
Zn2	0.0223 (3)	0.0226 (3)	0.0165 (3)	0.0107 (2)	0.00190 (19)	0.0092 (2)
Zn3	0.0198 (3)	0.0234 (3)	0.0170 (3)	0.0083 (2)	0.00536 (19)	0.0062 (2)
O1	0.0185 (13)	0.0181 (14)	0.0134 (13)	0.0092 (11)	0.0029 (11)	0.0062 (11)
O2	0.0255 (15)	0.0346 (17)	0.0163 (14)	0.0167 (13)	0.0072 (12)	0.0150 (13)
O3	0.0235 (15)	0.0329 (17)	0.0157 (15)	0.0074 (13)	0.0038 (12)	0.0077 (13)
O4	0.0330 (17)	0.0306 (17)	0.0320 (18)	0.0168 (14)	0.0109 (14)	0.0175 (15)
O5	0.0436 (19)	0.0259 (17)	0.045 (2)	0.0222 (15)	0.0220 (16)	0.0213 (15)
O6	0.0372 (19)	0.0199 (16)	0.0304 (18)	0.0063 (14)	0.0105 (15)	0.0020 (14)
O7	0.0249 (17)	0.046 (2)	0.0211 (17)	0.0037 (15)	0.0056 (13)	0.0077 (15)
O8	0.0246 (17)	0.0229 (17)	0.045 (2)	0.0037 (13)	0.0040 (15)	0.0030 (15)
O9	0.051 (2)	0.069 (2)	0.0274 (18)	0.046 (2)	0.0192 (16)	0.0314 (18)
C1	0.019 (2)	0.027 (2)	0.020 (2)	0.0133 (18)	0.0068 (17)	0.0076 (18)
C2	0.036 (2)	0.035 (3)	0.020 (2)	0.024 (2)	0.0138 (19)	0.020 (2)
C3	0.023 (2)	0.029 (2)	0.015 (2)	0.0126 (18)	0.0066 (16)	0.0118 (18)
C4	0.021 (2)	0.026 (2)	0.021 (2)	0.0091 (18)	0.0035 (17)	0.0071 (18)
C5	0.027 (2)	0.025 (2)	0.024 (2)	0.0082 (19)	0.0048 (18)	0.009 (2)
C6	0.047 (3)	0.026 (2)	0.017 (2)	0.005 (2)	−0.004 (2)	0.006 (2)

C7	0.033 (2)	0.032 (3)	0.028 (2)	0.011 (2)	0.0070 (19)	0.018 (2)
C8	0.023 (2)	0.023 (2)	0.025 (2)	0.0057 (18)	0.0033 (18)	0.0029 (19)
C9	0.036 (3)	0.037 (3)	0.024 (2)	0.009 (2)	0.002 (2)	0.017 (2)
C10	0.046 (3)	0.020 (2)	0.020 (2)	0.006 (2)	−0.002 (2)	0.0038 (19)
C11	0.030 (2)	0.024 (2)	0.033 (3)	0.0117 (19)	0.010 (2)	0.014 (2)
C12	0.062 (4)	0.038 (3)	0.059 (4)	0.033 (3)	0.034 (3)	0.032 (3)
C13	0.047 (3)	0.031 (3)	0.038 (3)	0.006 (2)	−0.011 (2)	0.016 (2)
C14	0.043 (3)	0.020 (2)	0.040 (3)	−0.001 (2)	−0.009 (2)	0.012 (2)
C15	0.042 (3)	0.056 (4)	0.084 (5)	0.029 (3)	0.019 (3)	0.038 (4)
C16	0.044 (3)	0.039 (3)	0.080 (4)	0.018 (3)	0.017 (3)	0.032 (3)

Geometric parameters (Å, º)

Zn1—O1	2.065 (3)	C5—C8	1.528 (6)
Zn1—O1^{i}	2.065 (3)	C6—C8	1.521 (6)
Zn1—O2^{i}	2.116 (3)	C6—C10^{iii}	1.532 (6)
Zn1—O2	2.116 (3)	C6—H6A	0.9700
Zn1—O6	2.125 (3)	C6—H6B	0.9700
Zn1—O6^{i}	2.125 (3)	C7—C9^{iv}	1.517 (6)
Zn2—O5	1.928 (3)	C7—H7A	0.9700
Zn2—O1	1.993 (3)	C7—H7B	0.9700
Zn2—O2	2.013 (3)	C8—C14	1.513 (7)
Zn2—O7	2.019 (3)	C8—H8	0.9800
Zn2—O3	2.338 (3)	C9—C7^{iv}	1.517 (6)
Zn3—O8^{i}	1.939 (3)	C9—H9A	0.9700
Zn3—O3^{ii}	1.971 (3)	C9—H9B	0.9700
Zn3—O1	1.977 (3)	C10—C6^{iii}	1.532 (6)
Zn3—O4	2.151 (3)	C10—H10A	0.9700
Zn3—O9^{i}	2.207 (3)	C10—H10B	0.9700
O2—C3	1.290 (5)	C11—C12	1.516 (6)
O3—C1	1.261 (5)	C12—C15	1.480 (8)
O4—C11	1.263 (5)	C12—C16	1.513 (8)
O5—C11	1.260 (5)	C12—H12	0.9800
O6—C5	1.250 (5)	C13—C14^{iii}	1.530 (6)
O7—C1	1.261 (5)	C13—H13A	0.9700
O8—C5	1.254 (5)	C13—H13B	0.9700
O9—C3	1.226 (5)	C14—C13^{iii}	1.530 (6)
C1—C4	1.495 (6)	C14—H14A	0.9700
C2—C3	1.514 (5)	C14—H14B	0.9700
C2—C7	1.529 (6)	C15—C16^{v}	1.532 (7)
C2—C9	1.535 (6)	C15—H15A	0.9700
C2—H2	0.9800	C15—H15B	0.9700
C4—C13	1.518 (6)	C16—C15^{v}	1.532 (7)
C4—C10	1.524 (6)	C16—H16A	0.9700
C4—H4	0.9800	C16—H16B	0.9700
O1—Zn1—O2	80.38 (10)	O8—C5—C8	115.7 (4)
O1—Zn1—O6	87.49 (11)	C8—C6—C10^{iii}	110.4 (4)

O2—Zn1—O6	89.32 (12)	C8—C6—H6A	109.6
O1—Zn1—O6^{i}	92.51 (11)	C10^{iii}—C6—H6A	109.6
O2—Zn1—O6^{i}	90.68 (12)	C8—C6—H6B	109.6
O6—Zn1—O6^{i}	180.00 (12)	C10^{iii}—C6—H6B	109.6
O1—Zn1—Zn2^{i}	140.05 (7)	H6A—C6—H6B	108.1
O2—Zn1—Zn2^{i}	139.33 (8)	C9^{iv}—C7—C2	111.9 (4)
O6—Zn1—Zn2^{i}	88.74 (9)	C9^{iv}—C7—H7A	109.2
O5—Zn2—O1	111.19 (13)	C2—C7—H7A	109.2
O5—Zn2—O2	115.65 (13)	C9^{iv}—C7—H7B	109.2
O1—Zn2—O2	84.68 (11)	C2—C7—H7B	109.2
O5—Zn2—O7	108.81 (15)	H7A—C7—H7B	107.9
O1—Zn2—O7	129.58 (13)	C14—C8—C6	110.5 (4)
O2—Zn2—O7	104.36 (12)	C14—C8—C5	106.2 (4)
O5—Zn2—O3	98.81 (13)	C6—C8—C5	114.1 (4)
O1—Zn2—O3	85.57 (11)	C14—C8—H8	108.6
O2—Zn2—O3	145.41 (12)	C6—C8—H8	108.6
O7—Zn2—O3	58.86 (11)	C5—C8—H8	108.6
O8^{i}—Zn3—O3^{ii}	118.92 (13)	C7^{iv}—C9—C2	111.0 (4)
O8^{i}—Zn3—O1	114.91 (13)	C7^{iv}—C9—H9A	109.4
O3^{ii}—Zn3—O1	125.97 (12)	C2—C9—H9A	109.4
O8^{i}—Zn3—O4	93.78 (14)	C7^{iv}—C9—H9B	109.4
O3^{ii}—Zn3—O4	86.00 (12)	C2—C9—H9B	109.4
O1—Zn3—O4	94.98 (11)	H9A—C9—H9B	108.0
O8^{i}—Zn3—O9^{i}	92.49 (15)	C4—C10—C6^{iii}	111.1 (4)
O3^{ii}—Zn3—O9^{i}	84.37 (13)	C4—C10—H10A	109.4
O1—Zn3—O9^{i}	89.19 (12)	C6^{iii}—C10—H10A	109.4
O4—Zn3—O9^{i}	170.20 (13)	C4—C10—H10B	109.4
Zn3—O1—Zn2	111.16 (13)	C6^{iii}—C10—H10B	109.4
Zn3—O1—Zn1	110.07 (12)	H10A—C10—H10B	108.0
Zn2—O1—Zn1	98.36 (11)	O5—C11—O4	124.9 (4)
C3—O2—Zn2	132.3 (3)	O5—C11—C12	115.1 (4)
C3—O2—Zn1	125.5 (3)	O4—C11—C12	120.0 (4)
Zn2—O2—Zn1	96.09 (11)	C15—C12—C16	112.4 (5)
C1—O3—Zn3^{ii}	137.0 (3)	C15—C12—C11	110.3 (5)
C1—O3—Zn2	84.3 (2)	C16—C12—C11	113.4 (4)
Zn3^{ii}—O3—Zn2	138.63 (14)	C15—C12—H12	106.8
C11—O4—Zn3	125.9 (3)	C16—C12—H12	106.8
C11—O5—Zn2	118.8 (3)	C11—C12—H12	106.8
C5—O6—Zn1	142.7 (3)	C4—C13—C14^{iii}	112.1 (4)
C1—O7—Zn2	99.0 (3)	C4—C13—H13A	109.2
C5—O8—Zn3^{i}	119.7 (3)	C14^{iii}—C13—H13A	109.2
C3—O9—Zn3^{i}	140.7 (3)	C4—C13—H13B	109.2
O7—C1—O3	117.8 (4)	C14^{iii}—C13—H13B	109.2
O7—C1—C4	121.1 (4)	H13A—C13—H13B	107.9
O3—C1—C4	121.0 (4)	C8—C14—C13^{iii}	112.6 (4)
C3—C2—C7	110.1 (3)	C8—C14—H14A	109.1
C3—C2—C9	110.3 (4)	C13^{iii}—C14—H14A	109.1
C7—C2—C9	110.4 (4)	C8—C14—H14B	109.1

C3—C2—H2	108.6	C13^{iii}—C14—H14B	109.1
C7—C2—H2	108.6	H14A—C14—H14B	107.8
C9—C2—H2	108.6	C12—C15—C16^{v}	111.8 (5)
O9—C3—O2	122.9 (4)	C12—C15—H15A	109.2
O9—C3—C2	119.3 (4)	C16^{v}—C15—H15A	109.2
O2—C3—C2	117.8 (4)	C12—C15—H15B	109.2
C1—C4—C13	106.4 (4)	C16^{v}—C15—H15B	109.2
C1—C4—C10	115.0 (4)	H15A—C15—H15B	107.9
C13—C4—C10	109.7 (4)	C12—C16—C15^{v}	112.0 (5)
C1—C4—H4	108.5	C12—C16—H16A	109.2
C13—C4—H4	108.5	C15^{v}—C16—H16A	109.2
C10—C4—H4	108.5	C12—C16—H16B	109.2
O6—C5—O8	125.7 (4)	C15^{v}—C16—H16B	109.2
O6—C5—C8	118.6 (4)	H16A—C16—H16B	107.9

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