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Poly[[μ -aqua-triaqua[μ_6 -1,3,4,6-tetrakis-(carboxylatomethyl)-7,8-diphenylglycoluril]dizinc] monohydrate]

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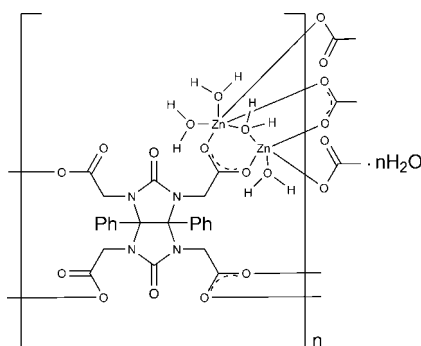
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Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.060; wR factor = 0.151; data-to-parameter ratio = 11.2.

In the crystal structure of the title coordination polymer, $\{[\text{Zn}_2(\text{C}_{24}\text{H}_{18}\text{N}_4\text{O}_{10})(\text{H}_2\text{O})_4]\cdot\text{H}_2\text{O}\}_n$, the molecular building block (MBB), *viz.* $[\text{Zn}_2(\text{CO}_2)_4(\text{H}_2\text{O})_4]$, comprises two Zn^{II} cations, each bridged by three carboxylate groups from different ligand molecules. These two Zn^{II} cations exhibit different coordination environments: a distorted trigonal-pyramidal coordination, as an intermediate, is formed by the two coordinated water molecules and three carboxylate groups, and a distorted octahedral geometry defined by three water molecules and three carboxylate groups, in which two carboxylate groups from the same side of the clip glycoluril ring and one water molecule are bidentate bridging, whereas others are monodentate units. Every ligand molecule connects four MBBs, thus forming a three-dimensional structure. Extensive intra- and intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding is observed.

Related literature

For the use of clip ligands in the generation of coordination frameworks, see: Deshpande *et al.* (2008); Li *et al.* (2008). For the synthesis of the ligand, see: Kang *et al.* (2004).



Experimental

Crystal data

$[\text{Zn}_2(\text{C}_{24}\text{H}_{18}\text{N}_4\text{O}_{10})(\text{H}_2\text{O})_4]\cdot\text{H}_2\text{O}$
 $M_r = 743.24$
 Orthorhombic, $Pbca$
 $a = 18.091$ (4) Å
 $b = 15.245$ (3) Å
 $c = 19.007$ (4) Å
 $V = 5242.0$ (18) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 1.92$ mm⁻¹
 $T = 113$ K
 $0.20 \times 0.18 \times 0.12$ mm

Data collection

Rigaku Saturn CCD diffractometer
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku/MS, 2005)
 $T_{\text{min}} = 0.700$, $T_{\text{max}} = 0.802$
 33644 measured reflections
 4616 independent reflections
 4022 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.086$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.151$
 $S = 1.13$
 4616 reflections
 413 parameters
 3 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.61$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.85$ e Å⁻³

Table 1

Selected bond lengths (Å).

Zn1—O11	2.059 (3)	Zn2—O5 ⁱⁱⁱ	1.960 (3)
Zn1—O1	2.063 (3)	Zn2—O6	2.014 (3)
Zn1—O4 ⁱ	2.063 (4)	Zn2—O10 ^{iv}	2.030 (3)
Zn1—O7 ⁱⁱ	2.091 (3)	Zn2—O13 ^v	2.133 (3)
Zn1—O12	2.116 (4)	Zn2—O14	2.183 (4)
Zn1—O13	2.183 (3)		

Symmetry codes: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (iii) $-x + 1, -y, -z + 2$; (iv) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 2$; (v) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O15—H15B \cdots O1 ^{vi}	0.84 (3)	2.54 (6)	3.108 (6)	126 (6)
O15—H15B \cdots O3 ^{vi}	0.84 (3)	2.29 (6)	2.995 (6)	141 (6)
O15—H15A \cdots O2 ^v	0.83 (3)	2.23 (6)	2.954 (6)	145 (8)
O14—H14A \cdots O3 ^{iv}	0.85	1.99	2.812 (5)	164
O14—H14B \cdots O8	0.85	2.30	3.104 (5)	159
O13—H13B \cdots O2	0.97	1.86	2.684 (5)	142
O13—H13A \cdots O9 ^{vii}	0.97	1.90	2.671 (5)	134
O12—H12B \cdots O15 ^{viii}	0.85	1.91	2.723 (6)	158
O12—H12A \cdots O14 ^{viii}	0.85	2.03	2.827 (5)	156
O11—H11A \cdots O10 ^j	0.85	2.10	2.945 (5)	170
O11—H11B \cdots O8 ⁱ	0.85	1.98	2.749 (5)	150

Symmetry codes: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iv) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 2$; (v) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (vi) $x + \frac{1}{2}, y, -z + \frac{3}{2}$; (vii) $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$; (viii) $x - \frac{1}{2}, y, -z + \frac{3}{2}$.

Data collection: *CrystalClear* (Rigaku/MS, 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2362).

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Kang, J., Ju, H. K. & Jo, J. H. (2004). *Supramol. Chem.* **16**, 175–179.
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supporting information

Acta Cryst. (2011). E67, m1818–m1819 [https://doi.org/10.1107/S1600536811049191]

Poly[[μ -aqua-triaqua[μ_6 -1,3,4,6-tetrakis(carboxylatomethyl)-7,8-diphenylglycoluril]dizinc] monohydrate]

Chuan-Qiang Li, Wen-Ge Qiu, Hong He and Xiuguang Wang

S1. Comment

The clip ligands, such as molecular clips based on concave glycoluril unit or its derivatives, would offer the possibility of the construction of frameworks with novel patterns not easily achievable by planar or linear ligands, which are widely used by chemists in the generation of coordination frameworks (Li *et al.* 2008; Deshpande *et al.* 2008). Herein we chose a multicarboxylate derivative of glycoluril, 1,3,4,6-tetracarboxymethyl-7,8-diphenylglycoluril, as a clip ligand, reacted with zinc nitrate affording a new three-dimensional coordination polymer, (I), $\{[\text{Zn}(\text{II})_2(L)(\text{H}_2\text{O})_4](\text{H}_2\text{O})\}_n$, where $L=1,3,4,6$ -tetracarboxymethyl-7,8-diphenylglycoluril.

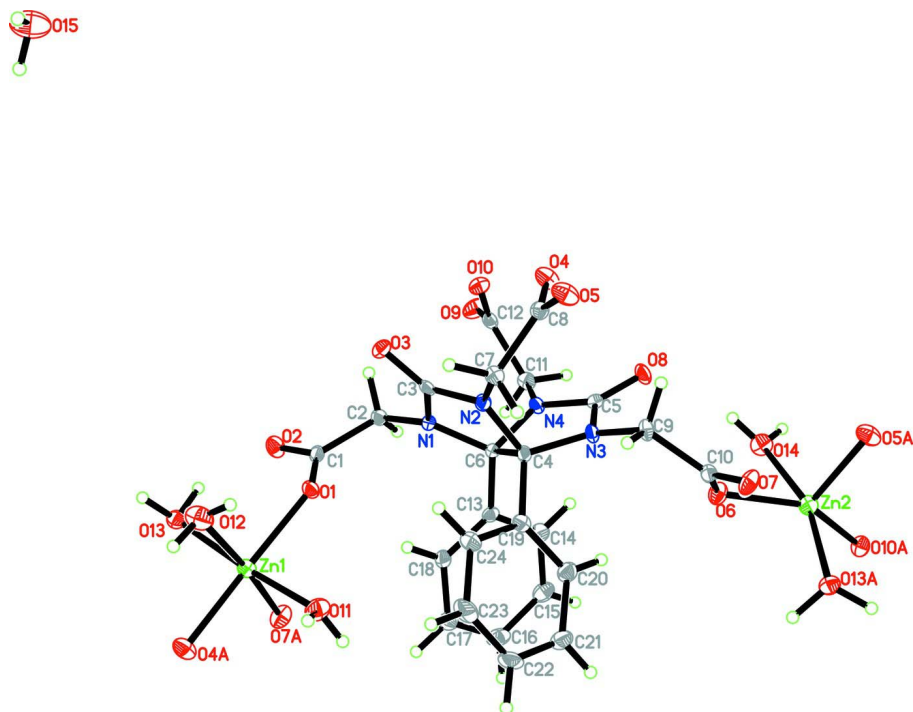
The molecular building blocks (MBBs) comprise two zinc centres, in which the two Zn atoms are five-coordinated and six-coordinated, respectively (Table 1 and Fig. 1). The different coordination environments in the dinuclear zinc cluster reveal that the Zn1 centre coordinated by five oxygen atoms from three L ligands and two water molecules, and Zn2 centre coordinated by six oxygen atoms from three L ligands and three water molecules. Each L ligand molecule connects four MBBs to form a three-dimensional coordination polymer (Fig. 2). A non-coordinated water molecules occupy the interstitial voids within the framework.

S2. Experimental

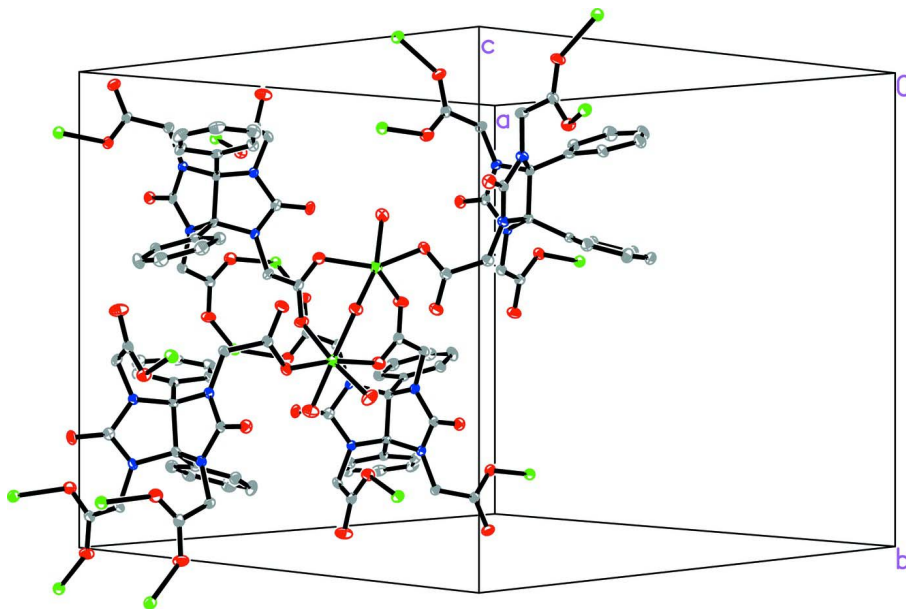
The tetracarboxylic ligand, H_4L was synthesised according to the literature procedure of Kang (2004). A mixture of H_4L (20 mg, 0.0380 mmol) and zinc nitrate hexahydrate (28.28 mg, 0.095 mmol) in water (4 mL) was added to a 5 mL sealed glass vial, and heated at 333 K for a week. Colourless rod-like crystals of the title compound were obtained after cooling to room temperature (yield=34% based on H_4L)

S3. 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.

**Figure 1**

Crystal structure of (I) with the atom labeling and displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (A) $-x + 1/2, -y, z + 1/2$; (B) $-x, y + 1/2, -z + 1/2$; (C) $x + 1/2, -y + 1/2, -z$.]

**Figure 2**

A view of the polymeric structure of (I). The hydrogen atoms and the water molecules in the channels have been omitted for clarity.

Poly[[μ -aqua-triaqua[μ_6 -1,3,4,6-tetrakis(carboxylatomethyl)-7,8-diphenylglycoluril]dizinc] monohydrate]

Crystal data

[Zn₂(C₂₄H₁₈N₄O₁₀)(H₂O)₄] \cdot H₂O $M_r = 743.24$ Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

 $a = 18.091$ (4) Å $b = 15.245$ (3) Å $c = 19.007$ (4) Å $V = 5242.0$ (18) Å³ $Z = 8$ $F(000) = 3040$ $D_x = 1.884$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 11423 reflections

 $\theta = 2.4$ – 27.9° $\mu = 1.92$ mm⁻¹ $T = 113$ K

Rod, colourless

 $0.20 \times 0.18 \times 0.12$ mm

Data collection

Rigaku Saturn 70CCD

diffractometer

Radiation source: rotating anode

Multilayer monochromator

Detector resolution: 7.31 pixels mm⁻¹ ω scans

Absorption correction: multi-scan

(CrystalClear; Rigaku/MSC, 2005)

 $T_{\min} = 0.700$, $T_{\max} = 0.802$

33644 measured reflections

4616 independent reflections

4022 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.086$ $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.4^\circ$ $h = -21 \rightarrow 21$ $k = -18 \rightarrow 18$ $l = -14 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.060$ $wR(F^2) = 0.151$ $S = 1.13$

4616 reflections

413 parameters

3 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

 $w = 1/[\sigma^2(F_o^2) + (0.0772P)^2 + 11.5013P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.61$ e Å⁻³ $\Delta\rho_{\min} = -0.85$ e Å⁻³

Extinction correction: SHELXL97 (Sheldrick,

2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0169 (7)

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	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.31740 (3)	0.38833 (3)	0.58277 (3)	0.0244 (2)
Zn2	0.72087 (3)	0.09336 (4)	0.98785 (3)	0.0257 (2)
O1	0.31600 (17)	0.3726 (2)	0.69057 (16)	0.0236 (7)

O2	0.2850 (2)	0.5068 (2)	0.72587 (18)	0.0309 (8)
O3	0.25130 (17)	0.2574 (2)	0.83197 (17)	0.0245 (7)
O4	0.3152 (2)	0.1190 (2)	0.97441 (18)	0.0328 (9)
O5	0.3015 (2)	-0.0169 (2)	0.93205 (19)	0.0328 (8)
O6	0.62798 (18)	0.1136 (2)	0.93178 (19)	0.0286 (8)
O7	0.59177 (18)	-0.0269 (2)	0.9208 (2)	0.0310 (8)
O8	0.51124 (19)	0.2312 (2)	1.00804 (16)	0.0279 (8)
O9	0.3748 (2)	0.4990 (2)	1.0069 (2)	0.0381 (9)
O10	0.32546 (18)	0.3666 (2)	0.99074 (18)	0.0268 (8)
O11	0.3804 (2)	0.2759 (2)	0.58136 (19)	0.0363 (9)
H11B	0.4266	0.2785	0.5737	0.054*
H11A	0.3657	0.2307	0.5593	0.054*
O12	0.2201 (2)	0.3113 (3)	0.5791 (2)	0.0416 (10)
H12A	0.2128	0.2941	0.5371	0.062*
H12B	0.2266	0.2647	0.6028	0.062*
O13	0.24415 (19)	0.5017 (2)	0.59018 (17)	0.0272 (7)
H13A	0.1933	0.4842	0.5818	0.033*
H13B	0.2473	0.5278	0.6366	0.033*
O14	0.67873 (19)	0.2110 (2)	1.03965 (19)	0.0342 (8)
H14B	0.6329	0.2227	1.0421	0.041*
H14A	0.6971	0.2307	1.0776	0.041*
N1	0.36573 (19)	0.3234 (2)	0.82313 (18)	0.0166 (8)
N2	0.3603 (2)	0.1803 (2)	0.84462 (19)	0.0185 (8)
N3	0.4826 (2)	0.1711 (2)	0.89992 (19)	0.0199 (8)
N4	0.4545 (2)	0.3105 (2)	0.91913 (18)	0.0184 (8)
C1	0.3114 (2)	0.4320 (3)	0.7363 (2)	0.0204 (10)
C2	0.3388 (3)	0.4123 (3)	0.8108 (2)	0.0209 (10)
H2A	0.3783	0.4530	0.8218	0.025*
H2B	0.2986	0.4236	0.8434	0.025*
C3	0.3197 (2)	0.2545 (3)	0.8337 (2)	0.0178 (9)
C4	0.4399 (2)	0.1956 (3)	0.8382 (2)	0.0172 (9)
C5	0.4854 (2)	0.2371 (3)	0.9482 (2)	0.0212 (10)
C6	0.4411 (2)	0.3008 (3)	0.8433 (2)	0.0159 (9)
C7	0.3268 (3)	0.0946 (3)	0.8513 (2)	0.0212 (10)
H7A	0.3583	0.0521	0.8279	0.025*
H7B	0.2798	0.0952	0.8269	0.025*
C8	0.3140 (2)	0.0645 (3)	0.9261 (2)	0.0218 (10)
C9	0.4996 (3)	0.0798 (3)	0.9173 (2)	0.0239 (10)
H9A	0.4768	0.0428	0.8819	0.029*
H9B	0.4762	0.0663	0.9619	0.029*
C10	0.5807 (3)	0.0544 (3)	0.9226 (2)	0.0223 (10)
C11	0.4525 (3)	0.3943 (3)	0.9552 (2)	0.0231 (10)
H11C	0.4686	0.4393	0.9225	0.028*
H11D	0.4883	0.3926	0.9932	0.028*
C12	0.3774 (3)	0.4225 (3)	0.9862 (2)	0.0224 (10)
C13	0.4999 (2)	0.3428 (3)	0.7982 (2)	0.0191 (9)
C14	0.5696 (3)	0.3608 (3)	0.8253 (3)	0.0265 (10)
H14	0.5774	0.3570	0.8735	0.032*

C15	0.6269 (3)	0.3841 (3)	0.7820 (3)	0.0331 (12)
H15	0.6731	0.3968	0.8008	0.040*
C16	0.6152 (3)	0.3886 (3)	0.7088 (3)	0.0353 (13)
H16	0.6545	0.4012	0.6789	0.042*
C17	0.5468 (3)	0.3745 (3)	0.6818 (3)	0.0328 (12)
H17	0.5389	0.3803	0.6337	0.039*
C18	0.4879 (3)	0.3512 (3)	0.7261 (2)	0.0251 (10)
H18	0.4411	0.3413	0.7074	0.030*
C19	0.4733 (3)	0.1581 (3)	0.7713 (2)	0.0203 (9)
C20	0.5502 (3)	0.1551 (3)	0.7646 (3)	0.0277 (11)
H20	0.5799	0.1687	0.8031	0.033*
C21	0.5826 (3)	0.1320 (3)	0.7011 (3)	0.0330 (12)
H21	0.6338	0.1330	0.6963	0.040*
C22	0.5384 (3)	0.1072 (3)	0.6447 (3)	0.0354 (13)
H22	0.5599	0.0916	0.6020	0.042*
C23	0.4627 (3)	0.1059 (3)	0.6521 (3)	0.0366 (13)
H23	0.4333	0.0866	0.6151	0.044*
C24	0.4298 (3)	0.1333 (3)	0.7148 (2)	0.0257 (10)
H24	0.3785	0.1349	0.7185	0.031*
O15	0.7371 (3)	0.1916 (3)	0.8159 (3)	0.0617 (13)
H15A	0.713 (4)	0.150 (4)	0.799 (4)	0.093*
H15B	0.757 (4)	0.224 (4)	0.786 (3)	0.093*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0274 (4)	0.0245 (3)	0.0212 (3)	−0.0003 (2)	0.0003 (2)	0.0001 (2)
Zn2	0.0249 (4)	0.0253 (3)	0.0271 (4)	−0.0041 (2)	−0.0018 (2)	0.0009 (2)
O1	0.0285 (18)	0.0260 (16)	0.0163 (16)	0.0054 (14)	−0.0012 (13)	−0.0012 (14)
O2	0.043 (2)	0.0228 (17)	0.0272 (18)	0.0090 (15)	−0.0027 (15)	0.0014 (14)
O3	0.0157 (16)	0.0287 (17)	0.0289 (17)	0.0010 (13)	0.0010 (14)	−0.0010 (14)
O4	0.048 (2)	0.0281 (18)	0.0225 (18)	−0.0025 (16)	0.0010 (16)	0.0011 (15)
O5	0.048 (2)	0.0211 (17)	0.0290 (18)	−0.0078 (16)	0.0056 (17)	0.0021 (15)
O6	0.0238 (18)	0.0242 (17)	0.038 (2)	−0.0003 (14)	−0.0037 (16)	0.0008 (15)
O7	0.0240 (18)	0.0201 (16)	0.049 (2)	0.0055 (14)	−0.0008 (16)	−0.0012 (15)
O8	0.0345 (19)	0.0334 (19)	0.0157 (16)	0.0041 (15)	−0.0071 (14)	0.0027 (14)
O9	0.034 (2)	0.0239 (18)	0.056 (2)	0.0008 (16)	0.0126 (18)	−0.0084 (17)
O10	0.0241 (18)	0.0259 (17)	0.0303 (18)	0.0014 (14)	0.0053 (14)	−0.0036 (15)
O11	0.037 (2)	0.0284 (19)	0.044 (2)	0.0042 (16)	0.0063 (17)	−0.0023 (16)
O12	0.046 (2)	0.046 (2)	0.033 (2)	−0.0173 (19)	0.0009 (17)	−0.0060 (17)
O13	0.0264 (17)	0.0277 (17)	0.0276 (17)	−0.0007 (14)	0.0025 (14)	0.0041 (14)
O14	0.035 (2)	0.0332 (19)	0.035 (2)	−0.0018 (16)	−0.0008 (16)	−0.0056 (16)
N1	0.0154 (18)	0.0180 (17)	0.0164 (18)	0.0013 (14)	−0.0004 (14)	0.0008 (14)
N2	0.0170 (18)	0.0179 (18)	0.0206 (19)	−0.0010 (14)	−0.0007 (15)	0.0038 (15)
N3	0.024 (2)	0.0194 (18)	0.0167 (18)	0.0047 (16)	−0.0055 (15)	0.0016 (15)
N4	0.023 (2)	0.0175 (18)	0.0144 (18)	0.0019 (15)	−0.0023 (15)	−0.0001 (14)
C1	0.016 (2)	0.022 (2)	0.023 (2)	0.0018 (18)	−0.0008 (18)	0.0038 (19)
C2	0.024 (2)	0.021 (2)	0.018 (2)	0.0030 (18)	0.0006 (19)	0.0003 (18)

C3	0.021 (2)	0.022 (2)	0.0096 (19)	-0.0013 (18)	-0.0010 (17)	0.0011 (17)
C4	0.016 (2)	0.018 (2)	0.018 (2)	0.0002 (16)	-0.0008 (17)	0.0041 (17)
C5	0.016 (2)	0.026 (2)	0.021 (2)	0.0006 (18)	0.0044 (18)	0.0013 (19)
C6	0.015 (2)	0.017 (2)	0.016 (2)	0.0012 (16)	-0.0001 (17)	0.0006 (17)
C7	0.022 (2)	0.019 (2)	0.022 (2)	-0.0054 (18)	-0.0019 (19)	0.0009 (18)
C8	0.019 (2)	0.025 (2)	0.022 (2)	-0.0014 (19)	-0.0011 (19)	-0.001 (2)
C9	0.027 (3)	0.020 (2)	0.025 (2)	0.0024 (19)	-0.005 (2)	0.0055 (19)
C10	0.025 (2)	0.023 (2)	0.019 (2)	0.005 (2)	-0.0012 (19)	0.0016 (19)
C11	0.025 (2)	0.024 (2)	0.020 (2)	-0.0045 (19)	-0.003 (2)	-0.0044 (19)
C12	0.029 (3)	0.024 (2)	0.014 (2)	0.004 (2)	-0.0019 (19)	0.0000 (18)
C13	0.019 (2)	0.016 (2)	0.023 (2)	0.0018 (17)	0.0044 (18)	0.0001 (18)
C14	0.025 (3)	0.027 (2)	0.027 (2)	-0.001 (2)	-0.001 (2)	-0.003 (2)
C15	0.021 (3)	0.036 (3)	0.042 (3)	-0.005 (2)	0.002 (2)	-0.002 (2)
C16	0.034 (3)	0.027 (3)	0.045 (3)	0.001 (2)	0.018 (3)	0.008 (2)
C17	0.035 (3)	0.034 (3)	0.030 (3)	0.007 (2)	0.009 (2)	0.010 (2)
C18	0.022 (2)	0.027 (2)	0.026 (2)	0.004 (2)	0.0000 (19)	0.007 (2)
C19	0.027 (2)	0.0133 (19)	0.020 (2)	0.0019 (18)	0.0013 (19)	0.0003 (17)
C20	0.026 (3)	0.027 (2)	0.029 (3)	0.005 (2)	0.001 (2)	-0.003 (2)
C21	0.030 (3)	0.034 (3)	0.035 (3)	0.008 (2)	0.008 (2)	0.000 (2)
C22	0.051 (3)	0.035 (3)	0.020 (3)	0.011 (2)	0.011 (2)	-0.006 (2)
C23	0.050 (3)	0.040 (3)	0.019 (2)	-0.001 (3)	-0.007 (2)	-0.010 (2)
C24	0.030 (3)	0.027 (2)	0.020 (2)	-0.003 (2)	0.000 (2)	-0.001 (2)
O15	0.078 (4)	0.044 (3)	0.063 (3)	-0.014 (2)	0.023 (3)	-0.002 (2)

Geometric parameters (Å, °)

Zn1—O11	2.059 (3)	N4—C5	1.367 (6)
Zn1—O1	2.063 (3)	N4—C11	1.452 (5)
Zn1—O4 ⁱ	2.063 (4)	N4—C6	1.469 (5)
Zn1—O7 ⁱⁱ	2.091 (3)	C1—C2	1.529 (6)
Zn1—O12	2.116 (4)	C2—H2A	0.9700
Zn1—O13	2.183 (3)	C2—H2B	0.9700
Zn2—O5 ⁱⁱⁱ	1.960 (3)	C4—C19	1.519 (6)
Zn2—O6	2.014 (3)	C4—C6	1.607 (6)
Zn2—O10 ^{iv}	2.030 (3)	C6—C13	1.507 (6)
Zn2—O13 ^v	2.133 (3)	C7—C8	1.513 (6)
Zn2—O14	2.183 (4)	C7—H7A	0.9700
O1—C1	1.259 (6)	C7—H7B	0.9700
O2—C1	1.252 (5)	C9—C10	1.521 (7)
O3—C3	1.238 (5)	C9—H9A	0.9700
O4—C8	1.238 (6)	C9—H9B	0.9700
O4—Zn1 ^{vi}	2.063 (4)	C11—C12	1.543 (7)
O5—C8	1.266 (6)	C11—H11C	0.9700
O5—Zn2 ⁱⁱⁱ	1.960 (3)	C11—H11D	0.9700
O6—C10	1.256 (6)	C13—C14	1.389 (6)
O7—C10	1.256 (6)	C13—C18	1.394 (6)
O7—Zn1 ^v	2.091 (3)	C14—C15	1.371 (7)
O8—C5	1.233 (5)	C14—H14	0.9300

O9—C12	1.230 (6)	C15—C16	1.408 (8)
O10—C12	1.272 (6)	C15—H15	0.9300
O10—Zn2 ^{vii}	2.030 (3)	C16—C17	1.357 (8)
O11—H11B	0.8500	C16—H16	0.9300
O11—H11A	0.8499	C17—C18	1.404 (7)
O12—H12A	0.8500	C17—H17	0.9300
O12—H12B	0.8501	C18—H18	0.9300
O13—Zn2 ⁱⁱ	2.133 (3)	C19—C24	1.384 (6)
O13—H13A	0.9700	C19—C20	1.399 (7)
O13—H13B	0.9700	C20—C21	1.388 (7)
O14—H14B	0.8500	C20—H20	0.9300
O14—H14A	0.8500	C21—C22	1.390 (8)
N1—C3	1.357 (5)	C21—H21	0.9300
N1—C6	1.458 (5)	C22—C23	1.377 (8)
N1—C2	1.459 (5)	C22—H22	0.9300
N2—C3	1.365 (6)	C23—C24	1.395 (7)
N2—C7	1.444 (5)	C23—H23	0.9300
N2—C4	1.463 (5)	C24—H24	0.9300
N3—C5	1.363 (6)	O15—H15A	0.83 (3)
N3—C4	1.454 (5)	O15—H15B	0.84 (3)
N3—C9	1.463 (5)		
O11—Zn1—O1	85.56 (13)	C19—C4—C6	114.9 (3)
O11—Zn1—O4 ⁱ	87.28 (14)	O8—C5—N3	125.5 (4)
O1—Zn1—O4 ⁱ	170.01 (13)	O8—C5—N4	126.0 (4)
O11—Zn1—O7 ⁱⁱ	94.52 (14)	N3—C5—N4	108.5 (4)
O1—Zn1—O7 ⁱⁱ	96.54 (14)	N1—C6—N4	112.9 (3)
O4 ⁱ —Zn1—O7 ⁱⁱ	90.95 (15)	N1—C6—C13	114.2 (3)
O11—Zn1—O12	89.89 (16)	N4—C6—C13	113.5 (3)
O1—Zn1—O12	87.59 (14)	N1—C6—C4	102.0 (3)
O4 ⁱ —Zn1—O12	85.44 (15)	N4—C6—C4	99.3 (3)
O7 ⁱⁱ —Zn1—O12	174.17 (15)	C13—C6—C4	113.5 (3)
O11—Zn1—O13	175.16 (13)	N2—C7—C8	114.9 (4)
O1—Zn1—O13	91.19 (12)	N2—C7—H7A	108.5
O4 ⁱ —Zn1—O13	95.49 (13)	C8—C7—H7A	108.5
O7 ⁱⁱ —Zn1—O13	89.42 (13)	N2—C7—H7B	108.5
O12—Zn1—O13	86.37 (15)	C8—C7—H7B	108.5
O5 ⁱⁱⁱ —Zn2—O6	109.28 (15)	H7A—C7—H7B	107.5
O5 ⁱⁱⁱ —Zn2—O10 ^{iv}	102.44 (15)	O4—C8—O5	126.5 (4)
O6—Zn2—O10 ^{iv}	146.94 (14)	O4—C8—C7	119.3 (4)
O5 ⁱⁱⁱ —Zn2—O13 ^v	102.22 (14)	O5—C8—C7	114.1 (4)
O6—Zn2—O13 ^v	88.84 (14)	N3—C9—C10	117.4 (4)
O10 ^{iv} —Zn2—O13 ^v	93.43 (13)	N3—C9—H9A	107.9
O5 ⁱⁱⁱ —Zn2—O14	93.81 (14)	C10—C9—H9A	107.9
O6—Zn2—O14	79.72 (13)	N3—C9—H9B	107.9
O10 ^{iv} —Zn2—O14	89.30 (13)	C10—C9—H9B	107.9
O13 ^v —Zn2—O14	162.73 (13)	H9A—C9—H9B	107.2
C1—O1—Zn1	127.1 (3)	O7—C10—O6	127.2 (4)

C8—O4—Zn1 ^{vi}	134.7 (3)	O7—C10—C9	113.8 (4)
C8—O5—Zn2 ⁱⁱⁱ	133.5 (3)	O6—C10—C9	118.9 (4)
C10—O6—Zn2	122.1 (3)	N4—C11—C12	116.6 (4)
C10—O7—Zn1 ^v	137.4 (3)	N4—C11—H11C	108.1
C12—O10—Zn2 ^{vii}	120.0 (3)	C12—C11—H11C	108.1
Zn1—O11—H11B	120.6	N4—C11—H11D	108.1
Zn1—O11—H11A	120.6	C12—C11—H11D	108.1
H11B—O11—H11A	105.1	H11C—C11—H11D	107.3
Zn1—O12—H12A	109.4	O9—C12—O10	125.8 (5)
Zn1—O12—H12B	109.4	O9—C12—C11	114.8 (4)
H12A—O12—H12B	105.1	O10—C12—C11	119.3 (4)
Zn2 ⁱⁱ —O13—Zn1	107.08 (14)	C14—C13—C18	119.1 (4)
Zn2 ⁱⁱ —O13—H13A	110.3	C14—C13—C6	120.9 (4)
Zn1—O13—H13A	110.3	C18—C13—C6	119.2 (4)
Zn2 ⁱⁱ —O13—H13B	110.3	C15—C14—C13	121.0 (5)
Zn1—O13—H13B	110.3	C15—C14—H14	119.5
H13A—O13—H13B	108.6	C13—C14—H14	119.5
Zn2—O14—H14B	122.5	C14—C15—C16	119.4 (5)
Zn2—O14—H14A	122.4	C14—C15—H15	120.3
H14B—O14—H14A	105.2	C16—C15—H15	120.3
C3—N1—C6	110.6 (3)	C17—C16—C15	120.2 (5)
C3—N1—C2	122.5 (4)	C17—C16—H16	119.9
C6—N1—C2	125.1 (3)	C15—C16—H16	119.9
C3—N2—C7	122.4 (4)	C16—C17—C18	120.3 (5)
C3—N2—C4	112.6 (3)	C16—C17—H17	119.8
C7—N2—C4	124.3 (3)	C18—C17—H17	119.8
C5—N3—C4	111.9 (3)	C13—C18—C17	119.7 (5)
C5—N3—C9	122.9 (4)	C13—C18—H18	120.1
C4—N3—C9	122.5 (4)	C17—C18—H18	120.1
C5—N4—C11	122.7 (4)	C24—C19—C20	119.1 (4)
C5—N4—C6	112.5 (3)	C24—C19—C4	121.8 (4)
C11—N4—C6	123.2 (3)	C20—C19—C4	118.9 (4)
O2—C1—O1	124.9 (4)	C21—C20—C19	120.5 (5)
O2—C1—C2	116.7 (4)	C21—C20—H20	119.8
O1—C1—C2	118.4 (4)	C19—C20—H20	119.8
N1—C2—C1	116.1 (4)	C20—C21—C22	119.8 (5)
N1—C2—H2A	108.3	C20—C21—H21	120.1
C1—C2—H2A	108.3	C22—C21—H21	120.1
N1—C2—H2B	108.3	C23—C22—C21	119.8 (5)
C1—C2—H2B	108.3	C23—C22—H22	120.1
H2A—C2—H2B	107.4	C21—C22—H22	120.1
O3—C3—N1	125.6 (4)	C22—C23—C24	120.5 (5)
O3—C3—N2	124.9 (4)	C22—C23—H23	119.7
N1—C3—N2	109.5 (4)	C24—C23—H23	119.7
N3—C4—N2	114.5 (3)	C19—C24—C23	120.1 (5)
N3—C4—C19	111.6 (3)	C19—C24—H24	120.0
N2—C4—C19	113.6 (3)	C23—C24—H24	120.0
N3—C4—C6	101.5 (3)	H15A—O15—H15B	114 (4)

N2—C4—C6	99.7 (3)		
O11—Zn1—O1—C1	150.5 (4)	N3—C4—C6—N1	-139.5 (3)
O4 ⁱ —Zn1—O1—C1	-165.2 (7)	N2—C4—C6—N1	-21.9 (4)
O7 ⁱⁱ —Zn1—O1—C1	56.4 (4)	C19—C4—C6—N1	100.0 (4)
O12—Zn1—O1—C1	-119.4 (4)	N3—C4—C6—N4	-23.5 (4)
O13—Zn1—O1—C1	-33.1 (4)	N2—C4—C6—N4	94.1 (3)
O5 ⁱⁱⁱ —Zn2—O6—C10	-37.3 (4)	C19—C4—C6—N4	-144.1 (4)
O10 ^{iv} —Zn2—O6—C10	159.8 (3)	N3—C4—C6—C13	97.2 (4)
O13 ^v —Zn2—O6—C10	65.2 (4)	N2—C4—C6—C13	-145.1 (3)
O14—Zn2—O6—C10	-127.8 (4)	C19—C4—C6—C13	-23.3 (5)
O11—Zn1—O13—Zn2 ⁱⁱ	-169.0 (16)	C3—N2—C7—C8	-96.5 (5)
O1—Zn1—O13—Zn2 ⁱⁱ	143.10 (15)	C4—N2—C7—C8	93.1 (5)
O4 ⁱ —Zn1—O13—Zn2 ⁱⁱ	-44.33 (17)	Zn1 ^{vi} —O4—C8—O5	12.9 (8)
O7 ⁱⁱ —Zn1—O13—Zn2 ⁱⁱ	46.57 (16)	Zn1 ^{vi} —O4—C8—C7	-168.7 (3)
O12—Zn1—O13—Zn2 ⁱⁱ	-129.39 (16)	Zn2 ⁱⁱⁱ —O5—C8—O4	0.0 (8)
Zn1—O1—C1—O2	22.7 (6)	Zn2 ⁱⁱⁱ —O5—C8—C7	-178.5 (3)
Zn1—O1—C1—C2	-158.1 (3)	N2—C7—C8—O4	17.2 (6)
C3—N1—C2—C1	-78.8 (5)	N2—C7—C8—O5	-164.2 (4)
C6—N1—C2—C1	117.6 (4)	C5—N3—C9—C10	-79.0 (6)
O2—C1—C2—N1	176.9 (4)	C4—N3—C9—C10	120.9 (4)
O1—C1—C2—N1	-2.4 (6)	Zn1 ^v —O7—C10—O6	-9.9 (8)
C6—N1—C3—O3	168.1 (4)	Zn1 ^v —O7—C10—C9	174.1 (3)
C2—N1—C3—O3	2.4 (6)	Zn2—O6—C10—O7	-28.8 (6)
C6—N1—C3—N2	-13.5 (5)	Zn2—O6—C10—C9	147.1 (3)
C2—N1—C3—N2	-179.3 (4)	N3—C9—C10—O7	-163.9 (4)
C7—N2—C3—O3	3.9 (6)	N3—C9—C10—O6	19.7 (6)
C4—N2—C3—O3	175.3 (4)	C5—N4—C11—C12	-104.8 (5)
C7—N2—C3—N1	-174.4 (4)	C6—N4—C11—C12	90.9 (5)
C4—N2—C3—N1	-3.0 (5)	Zn2 ^{vii} —O10—C12—O9	15.3 (6)
C5—N3—C4—N2	-86.1 (4)	Zn2 ^{vii} —O10—C12—C11	-167.5 (3)
C9—N3—C4—N2	75.9 (5)	N4—C11—C12—O9	-169.6 (4)
C5—N3—C4—C19	143.1 (4)	N4—C11—C12—O10	12.9 (6)
C9—N3—C4—C19	-54.9 (5)	N1—C6—C13—C14	151.7 (4)
C5—N3—C4—C6	20.2 (4)	N4—C6—C13—C14	20.4 (6)
C9—N3—C4—C6	-177.8 (4)	C4—C6—C13—C14	-92.0 (5)
C3—N2—C4—N3	123.4 (4)	N1—C6—C13—C18	-38.2 (5)
C7—N2—C4—N3	-65.4 (5)	N4—C6—C13—C18	-169.5 (4)
C3—N2—C4—C19	-106.8 (4)	C4—C6—C13—C18	78.1 (5)
C7—N2—C4—C19	64.5 (5)	C18—C13—C14—C15	-1.9 (7)
C3—N2—C4—C6	15.9 (4)	C6—C13—C14—C15	168.2 (4)
C7—N2—C4—C6	-172.8 (4)	C13—C14—C15—C16	-0.9 (7)
C4—N3—C5—O8	172.1 (4)	C14—C15—C16—C17	3.5 (8)
C9—N3—C5—O8	10.2 (7)	C15—C16—C17—C18	-3.1 (7)
C4—N3—C5—N4	-7.7 (5)	C14—C13—C18—C17	2.3 (7)
C9—N3—C5—N4	-169.6 (4)	C6—C13—C18—C17	-168.0 (4)
C11—N4—C5—O8	3.9 (7)	C16—C17—C18—C13	0.3 (7)
C6—N4—C5—O8	169.8 (4)	N3—C4—C19—C24	147.2 (4)

C11—N4—C5—N3	-176.3 (4)	N2—C4—C19—C24	16.0 (6)
C6—N4—C5—N3	-10.4 (5)	C6—C4—C19—C24	-97.9 (5)
C3—N1—C6—N4	-83.2 (4)	N3—C4—C19—C20	-37.9 (5)
C2—N1—C6—N4	82.1 (5)	N2—C4—C19—C20	-169.1 (4)
C3—N1—C6—C13	145.3 (4)	C6—C4—C19—C20	77.0 (5)
C2—N1—C6—C13	-49.4 (5)	C24—C19—C20—C21	3.4 (7)
C3—N1—C6—C4	22.4 (4)	C4—C19—C20—C21	-171.7 (4)
C2—N1—C6—C4	-172.3 (4)	C19—C20—C21—C22	-3.3 (8)
C5—N4—C6—N1	128.8 (4)	C20—C21—C22—C23	0.1 (8)
C11—N4—C6—N1	-65.4 (5)	C21—C22—C23—C24	3.2 (8)
C5—N4—C6—C13	-99.3 (4)	C20—C19—C24—C23	-0.1 (7)
C11—N4—C6—C13	66.5 (5)	C4—C19—C24—C23	174.7 (4)
C5—N4—C6—C4	21.5 (4)	C22—C23—C24—C19	-3.1 (8)
C11—N4—C6—C4	-172.7 (4)		

Symmetry codes: (i) $x, -y+1/2, z-1/2$; (ii) $-x+1, y+1/2, -z+3/2$; (iii) $-x+1, -y, -z+2$; (iv) $x+1/2, -y+1/2, -z+2$; (v) $-x+1, y-1/2, -z+3/2$; (vi) $x, -y+1/2, z+1/2$; (vii) $x-1/2, -y+1/2, -z+2$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O15—H15B \cdots O1 ^{viii}	0.84 (3)	2.54 (6)	3.108 (6)	126 (6)
O15—H15B \cdots O3 ^{viii}	0.84 (3)	2.29 (6)	2.995 (6)	141 (6)
O15—H15A \cdots O2 ^v	0.83 (3)	2.23 (6)	2.954 (6)	145 (8)
O14—H14A \cdots O3 ^{iv}	0.85	1.99	2.812 (5)	164
O14—H14B \cdots O8	0.85	2.30	3.104 (5)	159
O13—H13B \cdots O2	0.97	1.86	2.684 (5)	142
O13—H13A \cdots O9 ^{ix}	0.97	1.90	2.671 (5)	134
O12—H12B \cdots O15 ^x	0.85	1.91	2.723 (6)	158
O12—H12A \cdots O14 ^x	0.85	2.03	2.827 (5)	156
O11—H11A \cdots O10 ⁱ	0.85	2.10	2.945 (5)	170
O11—H11B \cdots O8 ⁱ	0.85	1.98	2.749 (5)	150

Symmetry codes: (i) $x, -y+1/2, z-1/2$; (iv) $x+1/2, -y+1/2, -z+2$; (v) $-x+1, y-1/2, -z+3/2$; (viii) $x+1/2, y, -z+3/2$; (ix) $-x+1/2, -y+1, z-1/2$; (x) $x-1/2, y, -z+3/2$.