

# Poly[[tetraqua( $\mu_6$ -2,2'-diiodobiphenyl-4,4',5,5'-tetracarboxylato)dizinc(II)] dihydrate]

Yan Wang, Yue-Qin Li and Ying-Zhong Shen\*

Applied Chemistry Department, School of Material Science & Engineering, Nanjing University of Aeronautics & Astronautics, Nanjing 210016, People's Republic of China

Correspondence e-mail: yz\_shen@nuaa.edu.cn

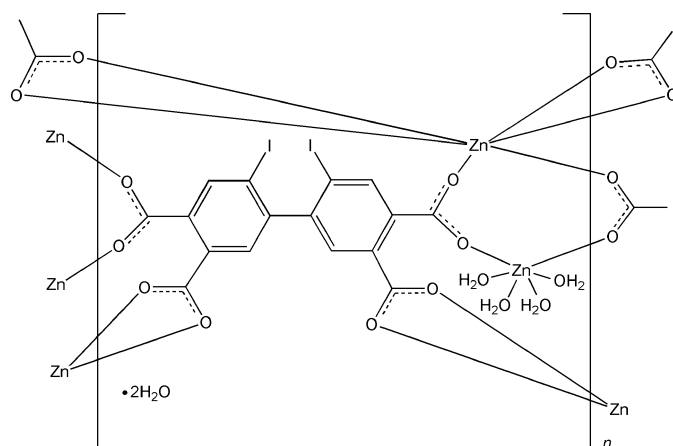
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Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.013$  Å;  $R$  factor = 0.053;  $wR$  factor = 0.088; data-to-parameter ratio = 13.7.

In the title compound,  $\{[\text{Zn}_2(\text{C}_{16}\text{H}_4\text{I}_2\text{O}_8)(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}\}_n$ , two crystallographically independent  $\text{Zn}^{\text{II}}$  atoms are each located on a twofold rotation axis. Both  $\text{Zn}^{\text{II}}$  atoms are in distorted octahedral coordination geometries: one is coordinated by six O atoms from four carboxylate groups, while the other is coordinated by two carboxylate groups and four water molecules. The tetracarboxylate ligand molecules connect the  $\text{Zn}^{\text{II}}$  atoms, completing a three-dimensional metal-organic framework.  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds link the metal-organic framework with the uncoordinated water molecules.

## Related literature

For related literature, see: Beringer *et al.* (1953); Cordes *et al.* (2006); Garay *et al.* (2007); Noro *et al.* (2007); Qiu *et al.* (2007); Wang *et al.* (2007); Weng *et al.* (2007); Williams *et al.* (2005).



## Experimental

### Crystal data

$[\text{Zn}_2(\text{C}_{16}\text{H}_4\text{I}_2\text{O}_8)(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$	$V = 1204.4$ (3) Å <sup>3</sup>
$M_r = 816.83$	$Z = 2$
Monoclinic, $C2$	Mo $K\alpha$ radiation
$a = 10.9466$ (16) Å	$\mu = 4.62$ mm <sup>-1</sup>
$b = 9.8135$ (14) Å	$T = 295$ (2) K
$c = 11.3913$ (17) Å	$0.40 \times 0.30 \times 0.20$ mm
$\beta = 100.187$ (3)°	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	3279 measured reflections
Absorption correction: numerical (SADABS; Bruker, 2000)	2126 independent reflections
$T_{\text{min}} = 0.20$ , $T_{\text{max}} = 0.39$	1767 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.040$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.088$	$\Delta\rho_{\text{max}} = 1.07$ e Å <sup>-3</sup>
$S = 0.97$	$\Delta\rho_{\text{min}} = -1.01$ e Å <sup>-3</sup>
2126 reflections	Absolute structure: Flack (1983),
155 parameters	870 Friedel pairs
1 restraint	Flack parameter: 0.00 (4)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O5}-\text{H5A}\cdots\text{O3}^{\text{i}}$	0.85	2.35	3.074 (9)	144
$\text{O5}-\text{H5A}\cdots\text{O1}^{\text{ii}}$	0.85	2.30	2.967 (9)	136
$\text{O5}-\text{H5B}\cdots\text{O7}^{\text{iii}}$	0.85	1.97	2.807 (15)	169
$\text{O6}-\text{H6A}\cdots\text{O3}^{\text{iv}}$	0.85	2.01	2.772 (10)	148
$\text{O6}-\text{H6B}\cdots\text{O7}$	0.85	2.50	3.113 (16)	129
$\text{O7}-\text{H7B}\cdots\text{O4}$	0.85	2.23	2.910 (16)	137

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); 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: IS2308).

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**supplementary materials**

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## Poly[[tetraaqua( $\mu_6$ -2,2'-diiodobiphenyl-4,4',5,5'-tetracarboxylato)dizinc(II)] dihydrate]

Y. Wang, Y.-Q. Li and Y.-Z. Shen

### Comment

Interest in the self-assembled construction of coordination polymers is rapidly increasing not only owing to their potential applications in gas storage, ion-exchange, catalysis, electrical conductivity, nonlinear optics and magnetism, but also because of their fascinating diversified architectures and topologies (Cordes *et al.*, 2006; Garay *et al.*, 2007). Multicarboxylate ligands, such as 1,4-benzenedicarboxylate (Williams *et al.*, 2005), 1,3,5-benzenetricarboxylate (Noro *et al.*, 2007) and biphenyl-3,3',4,4'-tetracarboxylate (Weng *et al.*, 2007), have been extensively employed in the construction of novel metal-organic complexes with multidimensional networks and interesting properties. In view of the excellent coordination capability of multicarboxylate anions and the solubility of diaryliodonium salts, we employed 2,2'-diiodobiphenyl-4,4',5,5'-tetracarboxylic acid ( $H_4L$ ), as an organic building unit to generate three dimensional metal-organic framework. In this paper, we describe the synthesis of a novel zinc(II) complexes, namely,  $[Zn_2(L)(H_2O)_4 \cdot 2H_2O]_n$ , by reaction of  $Zn(NO_3)_2 \cdot 6H_2O$  and  $H_4L$  via hydrothermal method, which was characterized by IR, elemental analysis and X-ray single-crystal analysis. To the best of our knowledge, transition metal coordination polymers based on diiodobiphenyl tetracarboxylate has never been reported before. This work may provide useful information for the further design of metal-organic frameworks with interesting architectures using diiodobiphenyl tetracarboxylate as versatile multidentate ligands.

The title complex crystallizes in the monoclinic system, space group  $C2$ , with two crystallographically independent  $Zn^{II}$  atoms each located on a twofold axis. As shown in Fig. 1, both  $Zn^{II}$  atoms are in distorted octahedral configurations and are connected by carboxylate groups. The Zn1 center is coordinated by four carboxylate groups, that is, 4(4')- $COO^-$  from two different  $L^{4-}$  ligands in a monodentate fashion (O1 and O1<sup>ii</sup>) and 5(5')- $COO^-$  from other two  $L^{4-}$  ligands in a bichelating fashion (O3<sup>i</sup>, O4<sup>i</sup>, O3<sup>iii</sup> and O4<sup>iii</sup>). In contrast, the Zn2 center is coordinated by four O atoms of water (O5, O6, O5<sup>ii</sup> and O6<sup>ii</sup>) and two carboxylate groups: 4(4')- $COO^-$  from two different  $L^{4-}$  ligands in a monodentate fashion (O2 and O2<sup>ii</sup>). The Zn–O bond lengths fall in the range of 1.953 (6)–2.368 (7) Å, similar to those in other zinc-tetracarboxylate coordination polymers (Wang *et al.*, 2007). Hence, the  $L^{4-}$  ligand acts as a octadentate ligand, linking six different  $Zn^{II}$  atoms to form a three-dimensional metal–organic framework (Fig. 2); the 5,5'-carboxyl groups adopt a bidentate bridging mode, while the 4,4'-carboxyl groups exhibit a bis(monodentate) bridging mode. Within the  $L^{4-}$  ligand, the two phenyl rings are almost perpendicular to each other with the dihedral angle of 88.6 (1)°, and the dihedral angles between 4,5(4',5')-carboxylate groups and the plane of correspondingly linked phenyl rings are respectively 72.0 (1) and 27.3 (1)°.

There are various O—H $\cdots$ O hydrogen bonds associated with the coordinated water molecules, uncoordinated water molecules and carboxylate O atoms in the title complex, linking the metal-organic framework with the uncoordinated water molecules.

## Experimental

All chemicals were of analytical grade and used without further purification. According to the reported procedure (Beringer *et al.*, 1953; Qiu *et al.*, 2007), H<sub>4</sub>L was prepared by iodine substitution of the *N*-methyl protected 3,3',4,4'-biphenyltetracarboxylicdianhydride, hydrolysis by 3M KOH and acidification by 6.5 M HCl to pH 1.0. The hydrothermal reaction was performed in a 25 ml Teflon-lined stainless steel autoclave under autogenous pressure. An solution of H<sub>4</sub>L (58 mg, 0.1 mmol), Zn(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (59 mg, 0.2 mmol), 2 ml EtOH and 8 ml H<sub>2</sub>O was adjusted to pH 7 with 1 M NaOH solution and then heated at 140 °C for 3 days. After the sample was cooled slowly to room temperature, colourless crystals were obtained and air-dried by filtration *ca* 60% yield based on Zn. Anal. calcd for C<sub>8</sub>H<sub>8</sub>O<sub>7</sub>I<sub>2</sub>Zn: C 23.53, H 1.97%; Found: C 23.48, H 2.02%. IR (KBr discs,  $\nu_{\max}/\text{cm}^{-1}$ ): 3379(*vs*), 1599(*s*), 1562(*s*), 1539(*s*), 1472(*w*), 1401(*vs*), 1318(*w*), 1254(*m*), 1163(*w*), 1098(*m*), 953(*w*), 915(*w*), 873(*m*), 846(*m*), 802(*m*), 678(*w*), 605(*w*), 543(*w*).

## Refinement

O-bound H atoms were located in a difference Fourier map and then constrained to ride on their parent atoms, with O—H = 0.85 Å and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ . Other H atoms were positioned geometrically (C—H = 0.93 Å) and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The highest peak and the deepest hole are 0.34 and 0.97 Å, respectively, from II.

## Figures

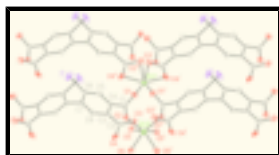


Fig. 1. A view of the title complex, depicting the Zn<sup>II</sup> coordination environment. Displacement ellipsoids are drawn at the 30% probability level. The solvent water molecules and H atoms have been omitted for clarity [symmetry codes: (i)  $-x + 1/2, y - 1/2, -z + 1$ ; (ii)  $-x, y, -z + 1$ ; (iii)  $x - 1/2, y - 1/2, z$ ].

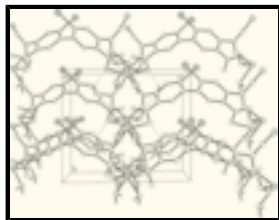


Fig. 2. Packing diagram of the title complex viewed along the *a* axis, showing a three-dimensional metal-organic framework. The dashed lines indicate hydrogen bonds.

## Poly[[tetraqua(μ<sub>6</sub>-2,2'-diiodobiphenyl-4,4',5,5'-tetracarboxylato)dizinc(II)] dihydrate]

### Crystal data

[Zn<sub>2</sub>(C<sub>16</sub>H<sub>4</sub>I<sub>2</sub>O<sub>8</sub>)(H<sub>2</sub>O)<sub>4</sub>]·2H<sub>2</sub>O

$M_r = 816.83$

Monoclinic, C2

Hall symbol: C 2y

$a = 10.9466$  (16) Å

$F_{000} = 780$

$D_x = 2.252$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71069$  Å

Cell parameters from 762 reflections

$\theta = 2.8\text{--}18.3^\circ$

$b = 9.8135 (14) \text{ \AA}$   
 $c = 11.3913 (17) \text{ \AA}$   
 $\beta = 100.187 (3)^\circ$   
 $V = 1204.4 (3) \text{ \AA}^3$   
 $Z = 2$

$\mu = 4.62 \text{ mm}^{-1}$   
 $T = 295 (2) \text{ K}$   
 Block, colourless  
 $0.40 \times 0.30 \times 0.20 \text{ mm}$

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	2126 independent reflections
Radiation source: fine-focus sealed tube	1767 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.040$
$T = 295(2) \text{ K}$	$\theta_{\text{max}} = 26.0^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 2.8^\circ$
Absorption correction: numerical (SADABS; Bruker, 2000)	$h = -9 \rightarrow 13$
$T_{\text{min}} = 0.20, T_{\text{max}} = 0.39$	$k = -11 \rightarrow 12$
3279 measured reflections	$l = -14 \rightarrow 14$

### Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.052$	$w = 1/[\sigma^2(F_o^2) + (0.0207P)^2]$
$wR(F^2) = 0.088$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2126 reflections	$\Delta\rho_{\text{max}} = 1.07 \text{ e \AA}^{-3}$
155 parameters	$\Delta\rho_{\text{min}} = -1.01 \text{ e \AA}^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 870 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.00 (4)

### 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.

## supplementary materials

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### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
I1	0.31728 (8)	0.46912 (8)	1.05780 (7)	0.0770 (3)
Zn1	0.0000	0.52673 (14)	0.5000	0.0296 (4)
Zn2	0.0000	0.94976 (18)	0.5000	0.0373 (4)
O1	0.1541 (6)	0.6253 (7)	0.5567 (6)	0.0404 (17)
O2	0.1099 (7)	0.8284 (7)	0.6272 (6)	0.0399 (18)
O3	0.3711 (6)	0.8475 (7)	0.5451 (6)	0.0454 (19)
O4	0.4839 (6)	0.9757 (8)	0.6747 (6)	0.0543 (19)
O5	-0.1277 (5)	0.9419 (7)	0.6112 (5)	0.0454 (18)
H5A	-0.2029	0.9518	0.5787	0.054*
H5B	-0.1254	0.8743	0.6577	0.054*
O6	0.1005 (8)	1.1179 (7)	0.5892 (7)	0.057 (2)
H6A	0.1232	1.1982	0.5746	0.068*
H6B	0.1538	1.0920	0.6488	0.068*
O7	0.3492 (12)	1.2077 (15)	0.7470 (11)	0.116 (4)
H7A	0.3346	1.2367	0.8145	0.139*
H7B	0.4010	1.1431	0.7670	0.139*
C1	0.1734 (8)	0.7220 (12)	0.6301 (8)	0.032 (2)
C2	0.4137 (9)	0.8752 (11)	0.6505 (9)	0.038 (3)
C3	0.3828 (10)	0.7879 (9)	0.7465 (9)	0.030 (2)
C4	0.2774 (9)	0.7090 (10)	0.7331 (8)	0.027 (2)
C5	0.2594 (9)	0.6187 (9)	0.8224 (9)	0.036 (2)
H5	0.1881	0.5652	0.8124	0.043*
C6	0.3468 (9)	0.6073 (9)	0.9266 (8)	0.033 (2)
C7	0.4536 (8)	0.6899 (9)	0.9425 (7)	0.028 (2)
C8	0.4700 (9)	0.7767 (9)	0.8536 (9)	0.031 (2)
H8	0.5411	0.8305	0.8636	0.038*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
I1	0.0650 (6)	0.0980 (7)	0.0621 (5)	-0.0337 (6)	-0.0053 (4)	0.0436 (5)
Zn1	0.0288 (9)	0.0325 (9)	0.0269 (8)	0.000	0.0029 (7)	0.000
Zn2	0.0294 (8)	0.0396 (10)	0.0414 (9)	0.000	0.0021 (7)	0.000
O1	0.030 (4)	0.042 (4)	0.047 (5)	0.000 (4)	0.000 (3)	-0.011 (3)
O2	0.037 (4)	0.049 (5)	0.032 (4)	0.015 (4)	-0.001 (3)	0.001 (3)
O3	0.049 (5)	0.050 (5)	0.040 (4)	0.009 (4)	0.015 (4)	0.004 (4)
O4	0.041 (4)	0.054 (5)	0.062 (5)	-0.014 (4)	-0.006 (3)	0.032 (4)
O5	0.027 (3)	0.057 (5)	0.053 (4)	0.012 (4)	0.009 (3)	0.009 (4)
O6	0.079 (6)	0.035 (4)	0.048 (5)	-0.012 (4)	-0.010 (4)	0.010 (3)
O7	0.118 (10)	0.116 (9)	0.124 (10)	0.014 (8)	0.049 (8)	0.031 (8)
C1	0.028 (5)	0.039 (6)	0.029 (5)	-0.006 (5)	0.008 (4)	0.009 (5)
C2	0.027 (6)	0.041 (7)	0.043 (7)	0.004 (5)	-0.003 (5)	0.008 (5)
C3	0.035 (6)	0.021 (5)	0.033 (6)	-0.005 (4)	0.006 (5)	-0.002 (4)
C4	0.035 (6)	0.029 (5)	0.017 (5)	0.006 (5)	0.000 (4)	0.008 (4)

C5	0.026 (6)	0.035 (6)	0.047 (7)	-0.004 (5)	0.009 (5)	0.001 (5)
C6	0.039 (6)	0.028 (5)	0.028 (6)	0.007 (5)	-0.002 (5)	0.003 (4)
C7	0.023 (5)	0.042 (6)	0.022 (5)	0.007 (4)	0.007 (4)	-0.006 (4)
C8	0.021 (5)	0.030 (6)	0.043 (6)	-0.008 (4)	0.006 (5)	0.001 (4)

*Geometric parameters (Å, °)*

I1—C6	2.085 (9)	O5—H5A	0.85
Zn1—O1	1.953 (6)	O5—H5B	0.85
Zn1—O1 <sup>i</sup>	1.953 (6)	O6—H6A	0.85
Zn1—O4 <sup>ii</sup>	2.090 (6)	O6—H6B	0.85
Zn1—O4 <sup>iii</sup>	2.090 (6)	O7—H7A	0.85
Zn1—O3 <sup>iii</sup>	2.368 (7)	O7—H7B	0.85
Zn1—O3 <sup>ii</sup>	2.368 (7)	C1—C4	1.488 (12)
Zn2—O5	2.047 (5)	C2—C3	1.475 (13)
Zn2—O5 <sup>i</sup>	2.047 (5)	C3—C4	1.375 (13)
Zn2—O2 <sup>i</sup>	2.085 (7)	C3—C8	1.415 (14)
Zn2—O2	2.085 (7)	C4—C5	1.389 (12)
Zn2—O6	2.138 (8)	C5—C6	1.391 (13)
Zn2—O6 <sup>i</sup>	2.138 (7)	C5—H5	0.9300
O1—C1	1.258 (12)	C6—C7	1.408 (12)
O2—C1	1.251 (12)	C7—C8	1.359 (12)
O3—C2	1.239 (11)	C7—C7 <sup>iv</sup>	1.509 (17)
O4—C2	1.251 (11)	C8—H8	0.9300
O1—Zn1—O1 <sup>i</sup>	120.6 (4)	C1—O2—Zn2	138.1 (6)
O1—Zn1—O4 <sup>ii</sup>	102.7 (3)	C2—O3—Zn1 <sup>v</sup>	84.9 (6)
O1 <sup>i</sup> —Zn1—O4 <sup>ii</sup>	91.0 (3)	C2—O4—Zn1 <sup>v</sup>	97.5 (6)
O1—Zn1—O4 <sup>iii</sup>	91.0 (3)	H5A—O5—H5B	106.00
O1 <sup>i</sup> —Zn1—O4 <sup>iii</sup>	102.7 (3)	H6A—O6—H6B	104.00
O4 <sup>ii</sup> —Zn1—O4 <sup>iii</sup>	152.3 (5)	H7A—O7—H7B	103.00
O1—Zn1—O3 <sup>iii</sup>	144.0 (3)	O2—C1—O1	125.7 (9)
O1 <sup>i</sup> —Zn1—O3 <sup>iii</sup>	85.8 (2)	O2—C1—C4	115.9 (9)
O4 <sup>ii</sup> —Zn1—O3 <sup>iii</sup>	100.5 (3)	O1—C1—C4	118.3 (10)
O4 <sup>iii</sup> —Zn1—O3 <sup>iii</sup>	57.4 (3)	O3—C2—O4	119.9 (10)
O1—Zn1—O3 <sup>ii</sup>	85.8 (2)	O3—C2—C3	119.6 (9)
O1 <sup>i</sup> —Zn1—O3 <sup>ii</sup>	144.0 (3)	O4—C2—C3	120.5 (9)
O4 <sup>ii</sup> —Zn1—O3 <sup>ii</sup>	57.4 (3)	C4—C3—C8	118.5 (8)
O4 <sup>iii</sup> —Zn1—O3 <sup>ii</sup>	100.5 (3)	C4—C3—C2	122.9 (9)
O3 <sup>iii</sup> —Zn1—O3 <sup>ii</sup>	84.1 (3)	C8—C3—C2	118.4 (9)
O5—Zn2—O5 <sup>i</sup>	175.7 (4)	C3—C4—C5	120.2 (9)
O5—Zn2—O2 <sup>i</sup>	92.0 (3)	C3—C4—C1	123.3 (8)
O5 <sup>i</sup> —Zn2—O2 <sup>i</sup>	85.5 (3)	C5—C4—C1	116.3 (9)
O5—Zn2—O2	85.5 (3)	C4—C5—C6	120.7 (9)



## supplementary materials

O5 <sup>i</sup> —Zn2—O2	92.0 (3)	C4—C5—H5	120
O2 <sup>i</sup> —Zn2—O2	110.3 (4)	C6—C5—H5	120
O5—Zn2—O6	94.9 (3)	C5—C6—C7	119.6 (9)
O5 <sup>i</sup> —Zn2—O6	88.4 (3)	C5—C6—I1	119.6 (7)
O2 <sup>i</sup> —Zn2—O6	163.0 (3)	C7—C6—I1	120.8 (7)
O2—Zn2—O6	85.7 (3)	C8—C7—C6	118.8 (9)
O5—Zn2—O6 <sup>i</sup>	88.4 (3)	C8—C7—C7 <sup>iv</sup>	119.3 (9)
O5 <sup>i</sup> —Zn2—O6 <sup>i</sup>	94.9 (3)	C6—C7—C7 <sup>iv</sup>	121.9 (8)
O2 <sup>i</sup> —Zn2—O6 <sup>i</sup>	85.7 (3)	C7—C8—C3	122.2 (9)
O2—Zn2—O6 <sup>i</sup>	163.0 (3)	C7—C8—H8	119
O6—Zn2—O6 <sup>i</sup>	79.0 (4)	C3—C8—H8	119
C1—O1—Zn1	128.9 (6)		
O1 <sup>i</sup> —Zn1—O1—C1	49.0 (8)	O3—C2—C3—C8	150.4 (9)
O4 <sup>ii</sup> —Zn1—O1—C1	147.9 (8)	O4—C2—C3—C8	-28.7 (14)
O4 <sup>iii</sup> —Zn1—O1—C1	-56.4 (9)	C8—C3—C4—C5	-1.3 (16)
O3 <sup>iii</sup> —Zn1—O1—C1	-83.0 (9)	C2—C3—C4—C5	173.6 (8)
O3 <sup>ii</sup> —Zn1—O1—C1	-156.9 (8)	C8—C3—C4—C1	173.6 (9)
C2 <sup>iii</sup> —Zn1—O1—C1	-67.9 (9)	C2—C3—C4—C1	-11.5 (17)
C2 <sup>ii</sup> —Zn1—O1—C1	176.4 (8)	O2—C1—C4—C3	-70.1 (13)
O5—Zn2—O2—C1	132.2 (10)	O1—C1—C4—C3	112.1 (12)
O5 <sup>i</sup> —Zn2—O2—C1	-44.3 (10)	O2—C1—C4—C5	105.0 (11)
O2 <sup>i</sup> —Zn2—O2—C1	41.7 (9)	O1—C1—C4—C5	-72.8 (12)
O6—Zn2—O2—C1	-132.6 (11)	C3—C4—C5—C6	0.4 (15)
O6 <sup>i</sup> —Zn2—O2—C1	-158.2 (10)	C1—C4—C5—C6	-174.8 (9)
Zn2—O2—C1—O1	-28.8 (16)	C4—C5—C6—C7	1.1 (14)
Zn2—O2—C1—C4	153.7 (7)	C4—C5—C6—I1	-179.4 (7)
Zn1—O1—C1—O2	-50.1 (14)	C5—C6—C7—C8	-1.7 (13)
Zn1—O1—C1—C4	127.4 (8)	I1—C6—C7—C8	178.8 (6)
Zn1 <sup>v</sup> —O3—C2—O4	5.3 (9)	C5—C6—C7—C7 <sup>iv</sup>	175.1 (8)
Zn1 <sup>v</sup> —O3—C2—C3	-173.8 (9)	I1—C6—C7—C7 <sup>iv</sup>	-4.4 (11)
Zn1 <sup>v</sup> —O4—C2—O3	-6.1 (10)	C6—C7—C8—C3	0.8 (13)
Zn1 <sup>v</sup> —O4—C2—C3	173.0 (8)	C7 <sup>iv</sup> —C7—C8—C3	-176.1 (9)
O3—C2—C3—C4	-24.4 (15)	C4—C3—C8—C7	0.7 (16)
O4—C2—C3—C4	156.5 (10)	C2—C3—C8—C7	-174.4 (8)

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

### 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>
O5—H5A $\cdots$ O3 <sup>i</sup>	0.85	2.35	3.074 (9)	144
O5—H5A $\cdots$ O1 <sup>vi</sup>	0.85	2.30	2.967 (9)	136
O5—H5B $\cdots$ O7 <sup>iii</sup>	0.85	1.97	2.807 (15)	169
O6—H6A $\cdots$ O3 <sup>vii</sup>	0.85	2.01	2.772 (10)	148

O6—H6B···O7	0.85	2.50	3.113 (16)	129
O7—H7B···O4	0.85	2.23	2.910 (16)	137

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



Fig. 2

