

# catena-Poly[(aquadimethanolzinc)- $\mu$ -furan-2,5-dicarboxylato- $\kappa^3 O^2:O^2,O^2'$ ]

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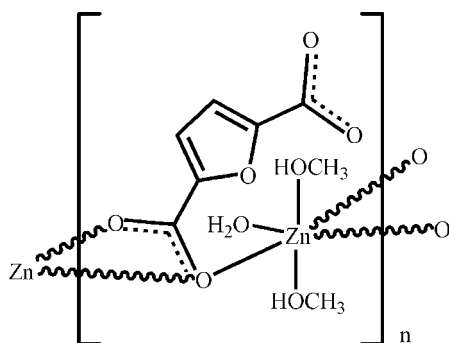
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.007$  Å;  $R$  factor = 0.062;  $wR$  factor = 0.142; data-to-parameter ratio = 15.5.

In the crystal structure of the title compound,  $[Zn(C_6H_2O_5)(CH_3OH)_2(H_2O)]_n$ , an infinite chain is formed along the  $b$  axis by linking of the  $Zn(OH_2)(CH_3OH)_2$  unit with one carboxylate group of the furan-2,5-dicarboxylate ligand. The  $Zn^{II}$  ion is in a distorted octahedral environment with one weak coordination [ $Zn-O_{\text{carboxylate}} = 2.565$  (3) Å] and two methanol molecules located in axial positions. In the chain,  $O_{\text{water}}-H \cdots O$  hydrogen bonds are present, while adjacent chains are linked by  $O_{\text{methanol}}-H \cdots O$  hydrogen bonds into a layer parallel to (102).

## Related literature

For applications and structures of metal-organic framework materials, see: Chui *et al.* (1999); Corma *et al.* (2010); Ferey (2008); Li *et al.* (1999, 2012a,b); Ma *et al.* (2009); Murray *et al.* (2009); Tranchemontagne *et al.* (2009).



## Experimental

### Crystal data

$[Zn(C_6H_2O_5)(CH_3O)_2(H_2O)]_n$	$b = 8.1235$ (16) Å
$M_r = 301.57$	$c = 17.101$ (3) Å
Monoclinic, $P2_1/c$	$\beta = 124.86$ (3)°
$a = 10.077$ (2) Å	$V = 1148.7$ (6) Å <sup>3</sup>

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 2.17$  mm<sup>-1</sup>

$T = 293$  K  
 $0.10 \times 0.10 \times 0.10$  mm

### Data collection

Rigaku R-Axis RAPID diffractometer  
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.813$ ,  $T_{\max} = 0.813$

10467 measured reflections  
2605 independent reflections  
1593 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.119$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.142$   
 $S = 1.01$   
2605 reflections  
168 parameters  
5 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.61$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.71$  e Å<sup>-3</sup>

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1W-H1A \cdots O1^i$	0.83 (2)	1.92 (2)	2.745 (5)	171 (5)
$O1W-H1B \cdots O5^{ii}$	0.83 (2)	1.76 (2)	2.571 (5)	165 (5)
$O7-H7 \cdots O4^{iii}$	0.82 (2)	1.86 (3)	2.639 (5)	158 (6)
$O8-H8 \cdots O4^{iv}$	0.82 (2)	1.88 (3)	2.682 (5)	163 (6)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); 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: IS5106).

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## supporting information

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**catena-Poly[(aquadimethanolzinc)- $\mu$ -furan-2,5-dicarboxylato- $\kappa^3 O^2:O^2,O^2'$ ]**

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**S1. Comment**

During past decades, more efforts have made to construct the metal organic framework (MOF) materials due to the potential applications including gas absorption and catalyst reactions (Ma *et al.*, 2009; Murray *et al.*, 2009; Corma *et al.*, 2010). The more attentions have been focused on the MOF based on the phenyl ring with carboxylate groups (Chui *et al.*, 1999; Li *et al.*, 1999; Ferey, 2008; Tranchemontagne *et al.*, 2009). Compared with phenyl ring with carboxylate groups, the 5-membered rings with carboxylate groups as the ligand are rarely studied. Recently, we utilize furan-2,5-dicarboxyl acid as the ligand to constructed the MOFs (Li *et al.*, 2012*a,b*). In this work, a novel chainlike compound,  $[Zn(C_6H_2O_5)(H_2O)(CH_3OH)_2]_n$ , (I), is structurally determined.

The asymmetric unit of (I) contains one  $Zn^{II}$  cation, one furan-2,5-dicarboxylate anion, one water and two methanol molecules (Fig. 1). The  $Zn^{II}$  cation is coordinated by three carboxylate O atoms, one water molecule and two methanol molecules which locate at the axial positions, exhibiting a distorted octahedron. The oxygen of carboxylate  $[Zn-O_{\text{carboxylate}} = 2.565(2) \text{ \AA}]$  is very weakly ligated to the Zn cation. If excluding this oxygen, the  $Zn^{II}$  ion displays a distorted trigonal bipyramid geometry but the chain property may not be changed. Only one carboxyl of furan-2,5-dicarboxylate involves in the formation of infinite chain. The carboxyl shows a  $\mu_2:\eta^1,\eta^2$  coordinated mode.

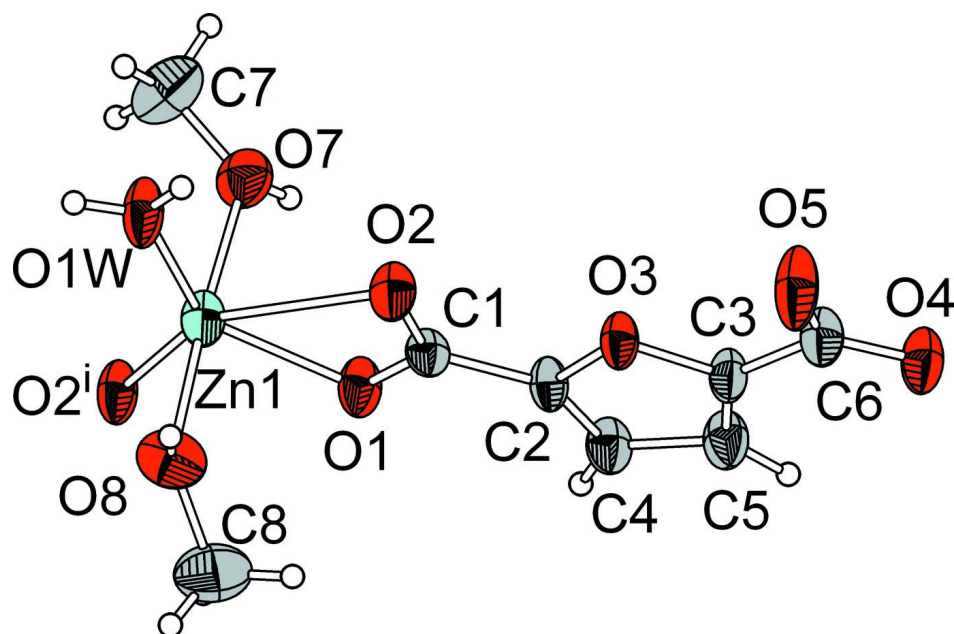
The  $Zn^{II}$  cations are linked by one carboxylate of furan-2,5-dicarboxylate to give rise to an infinite chain (Fig. 2).  $O_{\text{water}}-H\cdots O$  hydrogen bonds are intra-chain interactions, while  $O_{\text{methanol}}-H\cdots O$  hydrogen bonds inter-chain interactions which are responsible to link the adjacent chains into a layer parallel to the  $(10\bar{2})$  plane (Fig. 3).

**S2. Experimental**

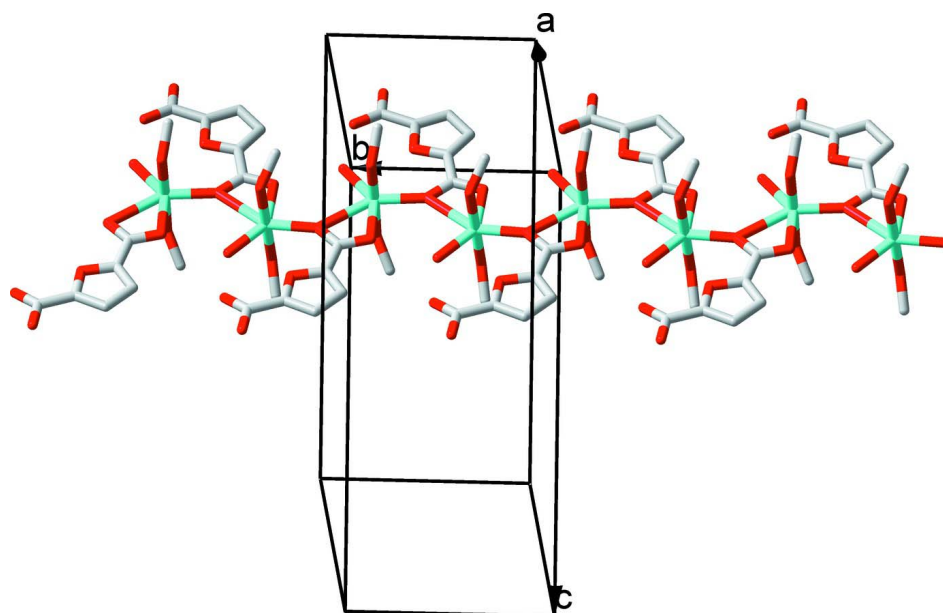
In a typically synthesized route of (I), furan-2,5-dicarboxyl acid (0.312 g, 2.0 mmol) and  $Zn(NO_3)_2 \cdot 6H_2O$  (0.592 g, 2.0 mmol) were dissolved in DMF (7.8 ml, 0.1 mol) under stirring. Then, 72 ml methanol and  $N(\text{et})_3$  (0.29 ml, 2.0 mmol) were successively added. The mixture with molar ratio of 1 (furan-2,5-dicarboxyl acid): 1 ( $Zn(NO_3)_2 \cdot 6H_2O$ ): 1 ( $N(\text{et})_3$ ) was laid under room temperature for 4 days. The colorless block product was collected as a single phase.

**S3. Refinement**

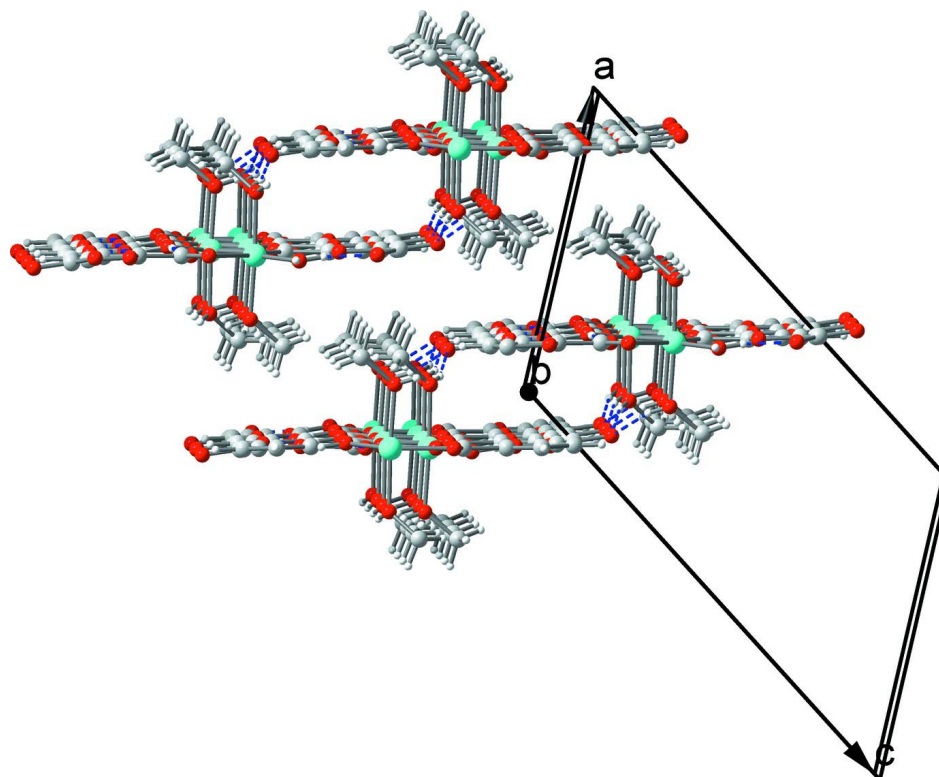
Water H atoms were located in a difference Fourier map and refined with distance restraints of  $O-H = 0.82(2) \text{ \AA}$  and  $H\cdots H = 1.37(2) \text{ \AA}$ , and with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(O)$ . Hydroxyl H atoms were located in a difference Fourier map and refined with a restraint of  $O-H = 0.82(2) \text{ \AA}$ , and with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(O)$ . The carbon H-atoms were placed in calculated positions [ $C-H$  (furan ring) =  $0.93 \text{ \AA}$  and  $C-H$  (methyl) =  $0.96 \text{ \AA}$ ] and were included in the refinement in the riding-model approximation, with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ .

**Figure 1**

The asymmetric unit of the title compound, showing the atomic labelling scheme and displacement ellipsoids at the 50% probability level. [Symmetry code: (i)  $1 - x, -1/2 + y, 1/2 - z$ .]

**Figure 2**

The stick plot of the title compound, displaying the infinite chain along the [010] direction formed by linking the Zn<sup>II</sup> ion with one carboxyl of furan-2,5-dicarboxylate.

**Figure 3**

The ball-stick packing diagram of the title compound. The adjacent chains are held together by the  $O_{\text{methanol}}\text{-H}\cdots\text{O}$  hydrogen bonds into layers.

**catena-Poly[(aquadimethanolzinc)- $\mu$ -furan-2,5- dicarboxylato- $\kappa^3 O^2:O^2,O^2$ ]**

*Crystal data*

$[\text{Zn}(\text{C}_6\text{H}_2\text{O}_5)(\text{CH}_4\text{O})_2(\text{H}_2\text{O})]$

$M_r = 301.57$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 10.077\ (2)\ \text{\AA}$

$b = 8.1235\ (16)\ \text{\AA}$

$c = 17.101\ (3)\ \text{\AA}$

$\beta = 124.86\ (3)^\circ$

$V = 1148.7\ (6)\ \text{\AA}^3$

$Z = 4$

$F(000) = 616$

$D_x = 1.744\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2000 reflections

$\theta = 3.2\text{--}27.5^\circ$

$\mu = 2.17\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, colorless

$0.10 \times 0.10 \times 0.10\ \text{mm}$

*Data collection*

Rigaku R-AXIS RAPID  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution:  $10.00\ \text{pixels mm}^{-1}$

$\omega$  scans

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\text{min}} = 0.813$ ,  $T_{\text{max}} = 0.813$

10467 measured reflections

2605 independent reflections

1593 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.119$

$\theta_{\text{max}} = 27.5^\circ$ ,  $\theta_{\text{min}} = 3.2^\circ$

$h = -13 \rightarrow 13$

$k = -10 \rightarrow 10$

$l = -22 \rightarrow 22$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.142$   
 $S = 1.01$   
 2605 reflections  
 168 parameters  
 5 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  
 $w = 1/[\sigma^2(F_o^2) + (0.057P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.61 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.71 \text{ e } \text{\AA}^{-3}$

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.44202 (7)	0.83143 (7)	0.20225 (4)	0.0346 (2)
O1	0.6292 (4)	0.8216 (4)	0.3472 (2)	0.0380 (9)
O2	0.5778 (4)	1.0836 (4)	0.3099 (2)	0.0389 (9)
O4	1.1259 (4)	1.3677 (4)	0.7066 (2)	0.0438 (10)
O5	0.9191 (5)	1.4792 (4)	0.5739 (3)	0.0589 (13)
O1W	0.3262 (4)	0.9960 (4)	0.1007 (3)	0.0475 (11)
H1A	0.334 (6)	1.097 (3)	0.110 (3)	0.057*
H1B	0.244 (4)	0.976 (5)	0.047 (2)	0.057*
C1	0.6580 (5)	0.9708 (5)	0.3707 (3)	0.0294 (12)
C2	0.7857 (5)	1.0133 (5)	0.4697 (3)	0.0297 (11)
O3	0.8150 (4)	1.1781 (3)	0.4901 (2)	0.0329 (8)
C3	0.9431 (6)	1.1887 (6)	0.5841 (3)	0.0334 (12)
C5	0.9904 (6)	1.0374 (6)	0.6215 (4)	0.0401 (14)
H5	1.0737	1.0123	0.6841	0.048*
C4	0.8892 (6)	0.9213 (6)	0.5474 (3)	0.0365 (13)
H4	0.8937	0.8071	0.5519	0.044*
C6	0.9997 (6)	1.3588 (6)	0.6231 (4)	0.0382 (13)
O7	0.6257 (4)	0.8255 (5)	0.1789 (3)	0.0463 (10)
H7	0.708 (5)	0.785 (7)	0.224 (3)	0.056*
C7	0.5999 (8)	0.8006 (8)	0.0889 (4)	0.066 (2)
H7A	0.5788	0.6861	0.0722	0.080*
H7B	0.6945	0.8338	0.0923	0.080*
H7C	0.5089	0.8649	0.0414	0.080*
O8	0.2706 (5)	0.8407 (4)	0.2328 (3)	0.0519 (10)

H8	0.225 (6)	0.931 (4)	0.214 (4)	0.062*
C8	0.2859 (9)	0.7722 (8)	0.3147 (5)	0.0660 (19)
H8A	0.3299	0.6631	0.3258	0.079*
H8B	0.1814	0.7675	0.3038	0.079*
H8C	0.3566	0.8399	0.3692	0.079*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn1	0.0342 (4)	0.0245 (3)	0.0305 (3)	0.0015 (2)	0.0098 (3)	0.0008 (3)
O1	0.043 (2)	0.0227 (16)	0.0330 (18)	−0.0025 (15)	0.0124 (16)	−0.0055 (15)
O2	0.040 (2)	0.0242 (17)	0.0311 (19)	0.0018 (15)	0.0075 (17)	0.0067 (15)
O4	0.037 (2)	0.0347 (19)	0.0316 (19)	0.0007 (16)	0.0034 (16)	−0.0017 (16)
O5	0.055 (2)	0.0290 (19)	0.042 (2)	0.0009 (18)	−0.0027 (19)	−0.0061 (18)
O1W	0.050 (2)	0.0228 (17)	0.0315 (19)	−0.0047 (17)	0.0005 (17)	−0.0004 (16)
C1	0.031 (3)	0.020 (2)	0.031 (3)	−0.0002 (19)	0.015 (2)	0.000 (2)
C2	0.029 (3)	0.023 (2)	0.030 (3)	−0.003 (2)	0.012 (2)	−0.009 (2)
O3	0.0324 (18)	0.0215 (15)	0.0272 (16)	−0.0021 (14)	0.0068 (14)	−0.0041 (14)
C3	0.028 (2)	0.032 (3)	0.025 (2)	−0.004 (2)	0.006 (2)	−0.002 (2)
C5	0.033 (3)	0.036 (3)	0.032 (3)	0.000 (2)	0.007 (2)	0.004 (2)
C4	0.036 (3)	0.025 (2)	0.035 (3)	−0.001 (2)	0.013 (2)	0.000 (2)
C6	0.036 (3)	0.034 (3)	0.033 (3)	−0.003 (2)	0.012 (2)	−0.006 (2)
O7	0.041 (2)	0.051 (2)	0.038 (2)	0.0064 (18)	0.0175 (18)	0.0070 (19)
C7	0.071 (5)	0.081 (5)	0.047 (4)	0.019 (4)	0.033 (3)	0.010 (3)
O8	0.048 (2)	0.041 (2)	0.067 (3)	0.0144 (18)	0.033 (2)	0.019 (2)
C8	0.084 (5)	0.054 (4)	0.071 (5)	0.008 (4)	0.051 (4)	0.018 (4)

*Geometric parameters (Å, °)*

Zn1—O1W	1.962 (3)	O3—C3	1.372 (5)
Zn1—O2 <sup>i</sup>	2.022 (3)	C3—C5	1.341 (6)
Zn1—O8	2.072 (4)	C3—C6	1.499 (6)
Zn1—O1	2.090 (4)	C5—C4	1.435 (6)
Zn1—O7	2.105 (4)	C5—H5	0.9300
Zn1—O2	2.565 (3)	C4—H4	0.9300
O1—C1	1.257 (5)	O7—C7	1.421 (7)
O2—C1	1.270 (5)	O7—H7	0.817 (19)
O2—Zn1 <sup>ii</sup>	2.022 (3)	C7—H7A	0.9600
O4—C6	1.259 (5)	C7—H7B	0.9600
O5—C6	1.243 (6)	C7—H7C	0.9600
O1W—H1A	0.828 (19)	O8—C8	1.430 (7)
O1W—H1B	0.828 (19)	O8—H8	0.82 (2)
C1—C2	1.467 (6)	C8—H8A	0.9600
C2—C4	1.352 (6)	C8—H8B	0.9600
C2—O3	1.372 (5)	C8—H8C	0.9600
O1W—Zn1—O2 <sup>i</sup>	127.86 (14)	C5—C3—C6	133.7 (4)
O1W—Zn1—O8	92.21 (17)	O3—C3—C6	116.3 (4)

O2 <sup>i</sup> —Zn1—O8	90.81 (15)	C3—C5—C4	107.5 (4)
O1W—Zn1—O1	138.87 (13)	C3—C5—H5	126.2
O2 <sup>i</sup> —Zn1—O1	93.05 (12)	C4—C5—H5	126.2
O8—Zn1—O1	91.10 (16)	C2—C4—C5	105.3 (4)
O1W—Zn1—O7	89.45 (17)	C2—C4—H4	127.3
O2 <sup>i</sup> —Zn1—O7	90.23 (15)	C5—C4—H4	127.3
O8—Zn1—O7	176.90 (15)	O5—C6—O4	124.6 (4)
O1—Zn1—O7	85.93 (15)	O5—C6—C3	119.3 (4)
O1W—Zn1—O2	83.95 (13)	O4—C6—C3	116.0 (4)
O2 <sup>i</sup> —Zn1—O2	148.19 (7)	C7—O7—Zn1	124.9 (4)
O8—Zn1—O2	88.27 (15)	C7—O7—H7	116 (4)
O1—Zn1—O2	55.19 (11)	Zn1—O7—H7	111 (4)
O7—Zn1—O2	89.31 (13)	O7—C7—H7A	109.5
C1—O1—Zn1	103.2 (3)	O7—C7—H7B	109.5
C1—O2—Zn1 <sup>ii</sup>	141.4 (3)	H7A—C7—H7B	109.5
C1—O2—Zn1	80.8 (3)	O7—C7—H7C	109.5
Zn1 <sup>ii</sup> —O2—Zn1	137.77 (14)	H7A—C7—H7C	109.5
Zn1—O1W—H1A	124 (3)	H7B—C7—H7C	109.5
Zn1—O1W—H1B	124 (3)	C8—O8—Zn1	126.4 (4)
H1A—O1W—H1B	110 (3)	C8—O8—H8	117 (5)
O1—C1—O2	120.8 (4)	Zn1—O8—H8	107 (4)
O1—C1—C2	119.0 (4)	O8—C8—H8A	109.5
O2—C1—C2	120.2 (4)	O8—C8—H8B	109.5
C4—C2—O3	110.9 (4)	H8A—C8—H8B	109.5
C4—C2—C1	132.8 (4)	O8—C8—H8C	109.5
O3—C2—C1	116.3 (4)	H8A—C8—H8C	109.5
C3—O3—C2	106.3 (3)	H8B—C8—H8C	109.5
C5—C3—O3	110.0 (4)		
O1W—Zn1—O1—C1	7.3 (5)	O1—C1—C2—O3	177.9 (4)
O2 <sup>i</sup> —Zn1—O1—C1	-178.2 (3)	O2—C1—C2—O3	-2.3 (7)
O8—Zn1—O1—C1	-87.3 (3)	C4—C2—O3—C3	0.7 (6)
O7—Zn1—O1—C1	91.8 (3)	C1—C2—O3—C3	-176.8 (4)
O2—Zn1—O1—C1	-0.2 (3)	C2—O3—C3—C5	-1.1 (6)
O1W—Zn1—O2—C1	-174.9 (3)	C2—O3—C3—C6	179.2 (4)
O2 <sup>i</sup> —Zn1—O2—C1	4.0 (3)	O3—C3—C5—C4	1.0 (6)
O8—Zn1—O2—C1	92.7 (3)	C6—C3—C5—C4	-179.3 (6)
O1—Zn1—O2—C1	0.2 (3)	O3—C2—C4—C5	-0.1 (6)
O7—Zn1—O2—C1	-85.3 (3)	C1—C2—C4—C5	176.8 (5)
O1W—Zn1—O2—Zn1 <sup>ii</sup>	5.4 (3)	C3—C5—C4—C2	-0.5 (6)
O2 <sup>i</sup> —Zn1—O2—Zn1 <sup>ii</sup>	-175.7 (3)	C5—C3—C6—O5	-171.4 (6)
O8—Zn1—O2—Zn1 <sup>ii</sup>	-87.0 (3)	O3—C3—C6—O5	8.3 (8)
O1—Zn1—O2—Zn1 <sup>ii</sup>	-179.5 (3)	C5—C3—C6—O4	6.4 (10)
O7—Zn1—O2—Zn1 <sup>ii</sup>	95.0 (3)	O3—C3—C6—O4	-174.0 (5)
Zn1—O1—C1—O2	0.4 (6)	O1W—Zn1—O7—C7	-52.1 (4)
Zn1—O1—C1—C2	-179.9 (4)	O2 <sup>i</sup> —Zn1—O7—C7	75.8 (4)
Zn1 <sup>ii</sup> —O2—C1—O1	179.4 (4)	O1—Zn1—O7—C7	168.8 (4)
Zn1—O2—C1—O1	-0.3 (5)	O2—Zn1—O7—C7	-136.1 (4)

Zn1 <sup>ii</sup> —O2—C1—C2	-0.4 (8)	O1W—Zn1—O8—C8	-167.6 (5)
Zn1—O2—C1—C2	179.9 (5)	O2 <sup>i</sup> —Zn1—O8—C8	64.5 (5)
O1—C1—C2—C4	1.1 (9)	O1—Zn1—O8—C8	-28.6 (5)
O2—C1—C2—C4	-179.1 (5)	O2—Zn1—O8—C8	-83.7 (5)

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

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O1W—H1A...O1 <sup>ii</sup>	0.83 (2)	1.92 (2)	2.745 (5)	171 (5)
O1W—H1B...O5 <sup>i</sup>	0.83 (2)	1.76 (2)	2.571 (5)	165 (5)
O7—H7...O4 <sup>iii</sup>	0.82 (2)	1.86 (3)	2.639 (5)	158 (6)
O8—H8...O4 <sup>iv</sup>	0.82 (2)	1.88 (3)	2.682 (5)	163 (6)

Symmetry codes: (i)  $-x+1, y-1/2, -z+1/2$ ; (ii)  $-x+1, y+1/2, -z+1/2$ ; (iii)  $-x+2, -y+2, -z+1$ ; (iv)  $x-1, -y+5/2, z-1/2$ .