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# Poly[[aqua-$\mu_6$-benzene-1,2,3-tricarboxylato-$\mu_3$-hydroxido-dizinc] hemihydrate]

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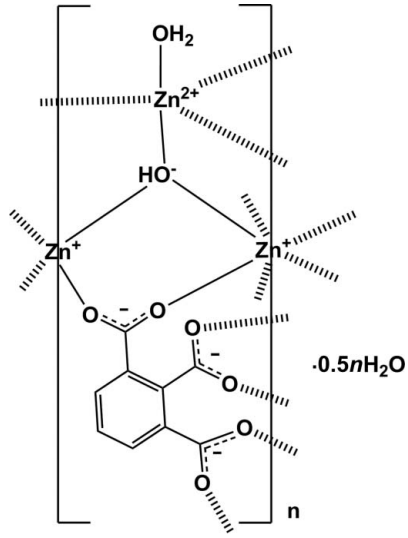
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.008 Å; disorder in solvent or counterion; $R$ factor = 0.035; $wR$ factor = 0.090; data-to-parameter ratio = 10.3.

In the title compound, $\{[Zn_2(C_9H_3O_6)(OH)(H_2O)]\cdot 0.5H_2O\}_n$, there are three independent $Zn^{II}$ atoms present; two are located on special positions, *viz* a twofold rotation axis and an inversion centre, and the third is located in a general position. The $Zn^{II}$ atom on the inversion centre is six-coordinated by four O atoms from four different benzene-1,2,3-tricarboxylate anions and two $OH^-$ anions. The $Zn^{II}$ atom located on a twofold axis is four coordinated by two O atoms from two different benzene-1,2,3-tricarboxylate anions and two $OH^-$ anions. The third $Zn^{II}$ atom, located in a general position, is five coordinated by three O atoms from three different benzene-1,2,3-tricarboxylate anions, one $OH^-$ anion and one water molecule. Each benzene-1,2,3-tricarboxylate anion bridges six $Zn^{II}$ atoms, and the $OH^-$ anion bridges three $Zn^{II}$ atoms, resulting in the formation of a three-dimensional framework. A series of O—H···O hydrogen bonds involving the benzene-1,2,3-tricarboxylate anions, the $OH^-$ anion and the coordinating and the two water solvent molecules further stablize the crystal structure. The two solvent water molecules show occupancies of 0.5 and 0.25.

## Related literature

For complexes of benzene tricarboxylic acids, see: Chui *et al.* (1999); Majumder *et al.* (2005). For related structures, see: Wu *et al.* (2009).




## Experimental

### Crystal data

$[Zn_2(C_9H_3O_6)(OH)(H_2O)]\cdot 0.5H_2O$
$M_r$ = 381.89
Tetragonal, $I4_1/a$
$a$ = 12.8412 (2) Å
$c$ = 27.2647 (7) Å
$V$ = 4495.85 (15) Å$^3$
$Z$ = 16
Mo $K\alpha$ radiation
$\mu$ = 4.31 mm$^{-1}$
$T$ = 293 K
0.28 × 0.23 × 0.21 mm

### Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.312, $T_{max}$ = 0.399
9288 measured reflections
2048 independent reflections
1402 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
$S$ = 0.94
2048 reflections
198 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.80 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.53 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$WA$···O2$W$ | 0.86 (2) | 2.37 (4) | 3.121 (7) | 146 (6) |
| O1$W$—H1$WB$···O2$^{i}$ | 0.86 (2) | 2.28 (5) | 2.981 (6) | 139 (6) |
| O1$W$—H1$WB$···O5$^{ii}$ | 0.86 (2) | 2.40 (4) | 3.084 (6) | 137 (5) |
| O7—H7$O$···O3$^{iii}$ | 0.79 (2) | 2.38 (2) | 3.174 (5) | 179 (5) |
| O2$W$—H2$WA$···O3$W^{iv}$ | 0.64 | 2.30 | 2.776 (18) | 134 |
| O3$W$—H3$WA$···O2$W^{v}$ | 0.86 | 1.94 | 2.776 (18) | 164 |
| O3$W$—H3$WB$···O4$^{vi}$ | 0.90 | 2.24 | 2.811 (15) | 121 |

Symmetry codes: (i) $-y+\frac{3}{4}, x-\frac{3}{4}, z+\frac{1}{4}$; (ii) $-x+1, -y, -z+1$; (iii) $y+\frac{1}{4}, -x+\frac{1}{4}, z+\frac{1}{4}$; (iv) $-y+\frac{3}{4}, x-\frac{1}{4}, -z+\frac{3}{4}$; (v) $y+\frac{1}{4}, -x+\frac{3}{4}, -z+\frac{3}{4}$; (vi) $-x+\frac{1}{2}, -y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97*

(Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL* and *publCIF (*Westrip, 2010).

We thank Jilin Agricultural Science and Technology College for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2346).

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# supporting information

*Acta Cryst.* (2012). E**68**, m103–m104 [doi:10.1107/S1600536811055358]

## Poly[[aqua-$\mu_6$-benzene-1,2,3-tricarboxylato-$\mu_3$-hydroxido-dizinc] hemihydrate]

**Chao-Hong Ma, Qiang Liu, Xiu-Yan Wang, Xian-Wu Dong and Yu-Jie Li**

### S1. Comment

The title compound consists of three crystallographically unique $Zn^{II}$ cations, two of which are located on special positions, one benzene-1,2,3-tricarboxylate anion, an $OH^-$ anion (O7), a coordinated water molecule (O1W), and two disordered solvent water molecules (Fig. 1).

Atom Zn1 is located on an inversion center and is six coordinated by four oxygen atoms from four symmetry related 1,2,3-tricarboxybenzene anions and two symmetry related $OH^-$ anions. The Zn1—*O*(carboxylate) distances are 2.022 (4) and 2.199 (3) Å. The Zn1—O7($OH^-$) distance is 2.089 (3) Å. Atom Zn2, also located on a 2-fold axis, is four coordinated by two oxygen atoms from two symmetry related 1,2,3-tricarboxybenzene anions and two symmetry related $OH^-$ anions. The Zn2—O (carboxylate) and Zn2—O7 distances are 1.943 (4) Å and 1.948 (3) Å, respectively. Atom Zn3, locate in a general position, is five coordinated by three oxygen atoms from three different 1,2,3-tricarboxybenzene anions, one $OH^-$ anion and one water molecule (O1W). The Zn3—*O*(carboxylate) distances are 1.935 (4), 1.984 (3) and 2.008 (4) Å. The Zn3—O7 distance is 2.069 (4) Å, and the Zn3—O1W distance is 2.136 (5) Å. The Zn—O (carboxylate) distances are similar to those observed in related structures (Wu *et al.*, 2009).

Each benzene-1,2,3-tricarboxylate anion bridges six $Zn^{II}$ centers, and the $OH^-$ anion bridges three $Zn^{II}$ centers, leading to the formation of an infinite three-dimensional framework (Fig. 2). A series of O—H···O hydrogen bonds (Table 1) involving the tricarboxybenzene anions, the $OH^-$ anion and the coordinating and two solvent water molecules (both of which are only partially occupied), further stabilize the crystal structure (Table 1).

### S2. Experimental

A mixture of benzene-1,2,3-tricarboxylic acid (0.063 g, 0.3 mmol), NaOH (0.036 g, 0.9 mmol), and $Zn(Ac)_2$ (0.066 g, 0.3 mmol), in 10 ml $H_2O$ was sealed in 18 ml Teflon-lined stainless steel container. The container was heated to 433 K and held at that temperature for 72 h. It was then cooled to room temperature at a rate of 10 K per hour and block-like colourless crystals of the title compound were isolated.

### S3. Refinement

C-bound H-atoms were included in calculated positions and were refined as riding atoms: C—H = 0.93 Å, with $U_{iso}$ = 1.2$U_{eq}$ (C). The $OH^-$ and water H atoms were located in difference Fourier maps and were refined with distance restraints of 0.86 (2) Å, or treated as riding atoms, all with $U_{iso}$(H) = 1.2$U_{eq}$(O). Water molecule O2W located on a 2-fold axis is 0.5 occupied, while water O3W is located in a general position is 0.25 occupied.

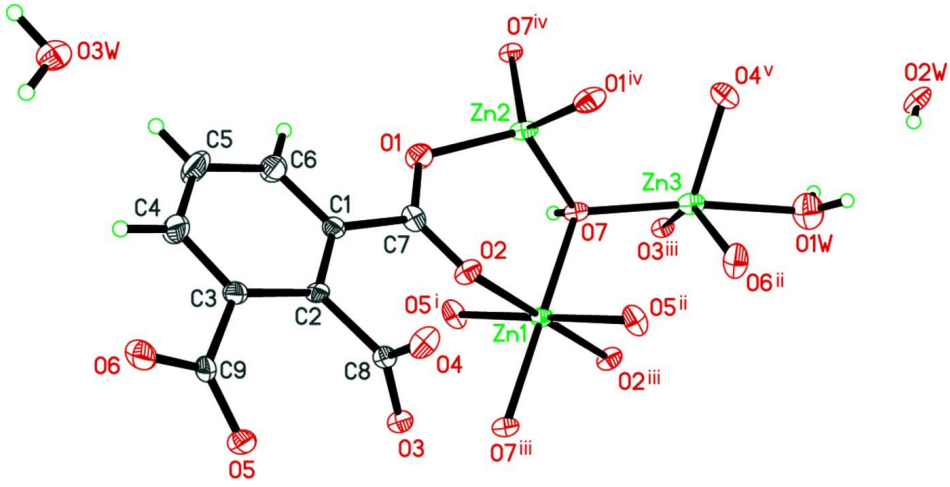


**Figure 1**

A view of the asymmetric unit of the title compound, showing the coordination environments of the three $Zn^{II}$ centers and the 30% probability displacement ellipsoids [symmetry codes: (i) $y + 1/4$, $-x + 1/4$, $z + 1/4$; (ii) $-y + 3/4$, $x - 1/4$,$- z + 3/4$; (iii) $-x + 1$, $-y$, $-z + 1$; (iv) $-x + 1$, $-y - 1/2$, $z$; (v) $-y + 3/4$, $x - 3/4$, $z + 1/4$].

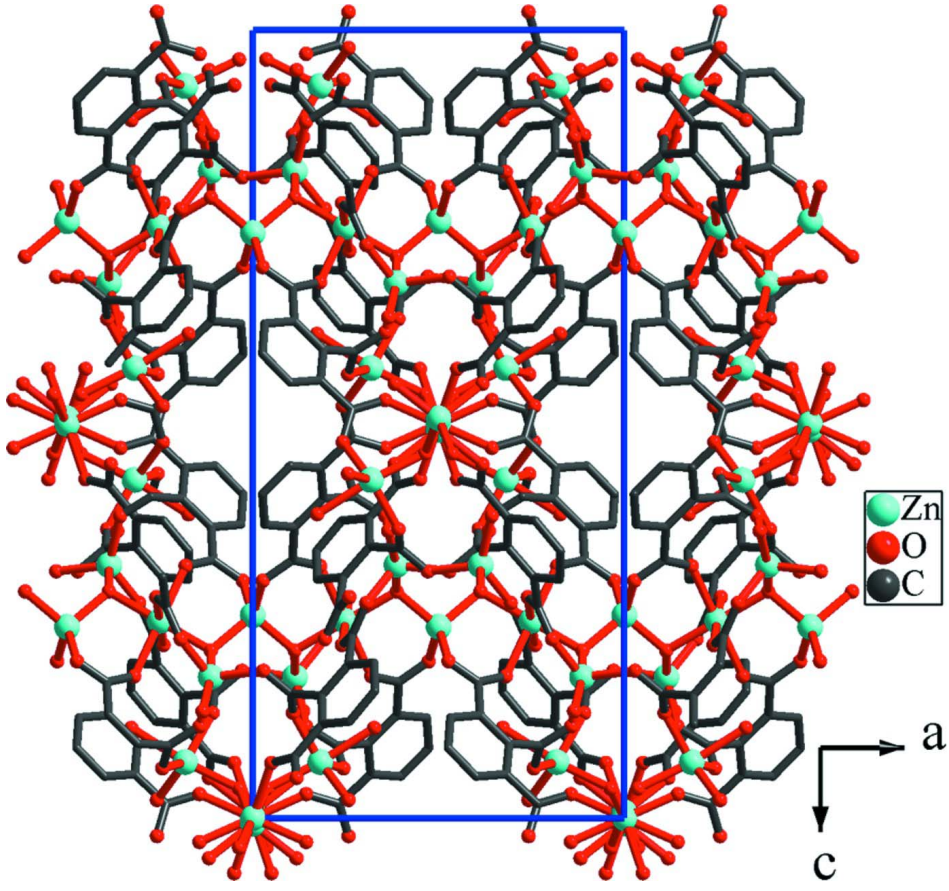


**Figure 2**

A view along the *b* axis of the three-dimensional structure of the title compound [the solvent water molecules and the H atoms have been omitted for clarity].

**Poly[[aqua-$\mu_6$-benzene-1,2,3-tricarboxylato-$\mu_3$-hydroxido-dizinc] hemihydrate]**

*Crystal data*

$[Zn_2(C_9H_3O_6)(OH)(H_2O)]\cdot 0.5H_2O$
$M_r = 381.89$
Tetragonal, $I4_1/a$
Hall symbol: -I 4ad
$a = 12.8412$ (2) Å
$c = 27.2647$ (7) Å
$V = 4495.85$ (15) Å$^3$
$Z = 16$
$F(000) = 3024$
$D_x = 2.257$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2048 reflections
$\theta = 2.8$–$25.3°$
$\mu = 4.31$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.28 × 0.23 × 0.21 mm

*Data collection*

Oxford Diffraction Gemini R Ultra diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.312$, $T_{max} = 0.399$
9288 measured reflections
2048 independent reflections
1402 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.8°$
$h = -15\rightarrow15$
$k = -15\rightarrow15$
$l = -22\rightarrow32$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.090$
$S = 0.94$
2048 reflections
198 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.80$ e Å$^{-3}$
$\Delta\rho_{min} = -0.53$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Zn1 | 0.5000 | 0.0000 | 0.5000 | 0.0208 (2) | |
| Zn2 | 0.5000 | −0.2500 | 0.49263 (3) | 0.0250 (3) | |
| Zn3 | 0.68168 (5) | −0.13663 (5) | 0.57097 (2) | 0.0274 (2) | |
| O1 | 0.3829 (3) | −0.2239 (3) | 0.44919 (13) | 0.0350 (10) | |

| | | | | | |
|---|---|---|---|---|---|
| O1W | 0.8258 (4) | −0.1142 (4) | 0.61415 (16) | 0.0569 (13) | |
| O2 | 0.4505 (3) | −0.0690 (3) | 0.42997 (12) | 0.0275 (9) | |
| O3 | 0.3919 (3) | 0.1070 (3) | 0.36657 (11) | 0.0224 (8) | |
| O4 | 0.4706 (3) | 0.0068 (3) | 0.31306 (13) | 0.0326 (10) | |
| O5 | 0.2600 (3) | 0.1066 (3) | 0.28024 (12) | 0.0312 (9) | |
| O6 | 0.1945 (3) | −0.0076 (3) | 0.22700 (13) | 0.0411 (11) | |
| O7 | 0.5375 (3) | −0.1373 (3) | 0.53706 (12) | 0.0209 (8) | |
| C1 | 0.3132 (4) | −0.1383 (4) | 0.38044 (18) | 0.0250 (13) | |
| C2 | 0.3150 (4) | −0.0597 (4) | 0.34414 (17) | 0.0201 (12) | |
| C3 | 0.2429 (4) | −0.0677 (4) | 0.30533 (19) | 0.0273 (13) | |
| C4 | 0.1747 (5) | −0.1498 (5) | 0.3023 (2) | 0.0485 (18) | |
| H4 | 0.1296 | −0.1543 | 0.2757 | 0.058* | |
| C5 | 0.1720 (6) | −0.2254 (5) | 0.3380 (3) | 0.061 (2) | |
| H5 | 0.1251 | −0.2803 | 0.3357 | 0.074* | |
| C6 | 0.2400 (5) | −0.2187 (5) | 0.3774 (2) | 0.0439 (17) | |
| H6 | 0.2370 | −0.2685 | 0.4022 | 0.053* | |
| C7 | 0.3880 (4) | −0.1430 (4) | 0.42282 (17) | 0.0239 (12) | |
| C8 | 0.3973 (4) | 0.0242 (4) | 0.34212 (17) | 0.0197 (12) | |
| C9 | 0.2329 (4) | 0.0172 (4) | 0.26799 (19) | 0.0246 (12) | |
| O2W | 1.0000 | −0.2500 | 0.5664 (4) | 0.038 (3) | 0.50 |
| H2WA | 0.9977 | −0.2203 | 0.5475 | 0.057* | 0.50 |
| O3W | 0.0743 (12) | −0.3649 (12) | 0.2625 (5) | 0.038 (4) | 0.25 |
| H3WA | 0.0608 | −0.3205 | 0.2396 | 0.057* | 0.25 |
| H3WB | 0.0318 | −0.4194 | 0.2582 | 0.057* | 0.25 |
| H1WA | 0.885 (3) | −0.124 (5) | 0.6006 (18) | 0.057* | |
| H1WB | 0.825 (4) | −0.141 (5) | 0.6431 (11) | 0.057* | |
| H7O | 0.493 (3) | −0.139 (4) | 0.5572 (14) | 0.019 (16)* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0265 (5) | 0.0185 (5) | 0.0174 (4) | −0.0003 (4) | 0.0020 (4) | 0.0024 (3) |
| Zn2 | 0.0434 (6) | 0.0173 (5) | 0.0143 (4) | −0.0014 (4) | 0.000 | 0.000 |
| Zn3 | 0.0421 (5) | 0.0242 (4) | 0.0159 (3) | −0.0009 (3) | 0.0057 (3) | 0.0027 (3) |
| O1 | 0.047 (3) | 0.030 (2) | 0.028 (2) | −0.007 (2) | −0.0119 (19) | 0.0136 (18) |
| O1W | 0.054 (3) | 0.073 (4) | 0.043 (3) | 0.000 (3) | −0.003 (2) | 0.007 (3) |
| O2 | 0.040 (2) | 0.028 (2) | 0.0146 (18) | −0.0088 (19) | −0.0061 (16) | 0.0001 (15) |
| O3 | 0.031 (2) | 0.021 (2) | 0.0149 (18) | −0.0029 (17) | −0.0013 (15) | 0.0002 (15) |
| O4 | 0.036 (2) | 0.037 (2) | 0.024 (2) | −0.0105 (19) | 0.0064 (18) | −0.0061 (17) |
| O5 | 0.047 (3) | 0.024 (2) | 0.0218 (19) | −0.0069 (19) | −0.0138 (18) | 0.0090 (16) |
| O6 | 0.062 (3) | 0.033 (2) | 0.028 (2) | 0.010 (2) | −0.025 (2) | −0.0059 (18) |
| O7 | 0.034 (2) | 0.018 (2) | 0.0101 (18) | −0.0017 (17) | 0.0051 (17) | 0.0005 (15) |
| C1 | 0.029 (3) | 0.021 (3) | 0.025 (3) | 0.003 (3) | −0.006 (2) | 0.000 (2) |
| C2 | 0.028 (3) | 0.016 (3) | 0.016 (3) | 0.001 (2) | −0.002 (2) | −0.005 (2) |
| C3 | 0.033 (3) | 0.021 (3) | 0.028 (3) | 0.002 (3) | −0.009 (3) | −0.002 (2) |
| C4 | 0.059 (5) | 0.035 (4) | 0.052 (4) | −0.009 (3) | −0.035 (4) | 0.008 (3) |
| C5 | 0.065 (5) | 0.041 (4) | 0.078 (5) | −0.029 (4) | −0.037 (4) | 0.020 (4) |
| C6 | 0.051 (4) | 0.032 (4) | 0.049 (4) | −0.009 (3) | −0.024 (3) | 0.016 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.025 (3) | 0.033 (3) | 0.013 (3) | 0.005 (3) | 0.003 (2) | 0.000 (2) |
| C8 | 0.027 (3) | 0.021 (3) | 0.011 (2) | −0.001 (2) | −0.003 (2) | 0.004 (2) |
| C9 | 0.023 (3) | 0.026 (3) | 0.025 (3) | 0.001 (3) | −0.008 (2) | −0.001 (2) |
| O2W | 0.039 (7) | 0.030 (7) | 0.044 (7) | −0.018 (5) | 0.000 | 0.000 |
| O3W | 0.044 (11) | 0.037 (10) | 0.033 (9) | 0.004 (8) | 0.010 (8) | −0.014 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—O5$^{i}$ | 2.022 (4) | O4—Zn3$^{vi}$ | 2.008 (4) |
| Zn1—O5$^{ii}$ | 2.022 (4) | O5—C9 | 1.245 (6) |
| Zn1—O7$^{iii}$ | 2.089 (3) | O5—Zn1$^{vii}$ | 2.022 (3) |
| Zn1—O7 | 2.089 (3) | O6—C9 | 1.263 (6) |
| Zn1—O2 | 2.199 (3) | O6—Zn3$^{viii}$ | 1.935 (4) |
| Zn1—O2$^{iii}$ | 2.199 (3) | O7—H7O | 0.79 (2) |
| Zn2—O1$^{iv}$ | 1.943 (4) | C1—C6 | 1.399 (8) |
| Zn2—O1 | 1.943 (4) | C1—C2 | 1.413 (7) |
| Zn2—O7 | 1.948 (3) | C1—C7 | 1.504 (7) |
| Zn2—O7$^{iv}$ | 1.948 (3) | C2—C3 | 1.410 (7) |
| Zn3—O6$^{i}$ | 1.935 (4) | C2—C8 | 1.511 (7) |
| Zn3—O3$^{iii}$ | 1.984 (3) | C3—C4 | 1.373 (8) |
| Zn3—O4$^{v}$ | 2.008 (4) | C3—C9 | 1.497 (7) |
| Zn3—O7 | 2.069 (4) | C4—C5 | 1.374 (9) |
| Zn3—O1W | 2.213 (5) | C4—H4 | 0.9300 |
| O1—C7 | 1.265 (6) | C5—C6 | 1.388 (9) |
| O1W—H1WA | 0.86 (2) | C5—H5 | 0.9300 |
| O1W—H1WB | 0.86 (2) | C6—H6 | 0.9300 |
| O2—C7 | 1.259 (6) | O2W—H2WA | 0.6405 |
| O3—C8 | 1.257 (6) | O3W—H3WA | 0.8614 |
| O3—Zn3$^{iii}$ | 1.984 (3) | O3W—H3WB | 0.8960 |
| O4—C8 | 1.250 (6) | | |

| | | | |
|---|---|---|---|
| O5$^{i}$—Zn1—O5$^{ii}$ | 180.000 (1) | C8—O4—Zn3$^{vi}$ | 123.3 (3) |
| O5$^{i}$—Zn1—O7$^{iii}$ | 87.68 (15) | C9—O5—Zn1$^{vii}$ | 135.5 (3) |
| O5$^{ii}$—Zn1—O7$^{iii}$ | 92.32 (14) | C9—O6—Zn3$^{viii}$ | 133.0 (4) |
| O5$^{i}$—Zn1—O7 | 92.32 (14) | Zn2—O7—Zn3 | 120.15 (18) |
| O5$^{ii}$—Zn1—O7 | 87.68 (15) | Zn2—O7—Zn1 | 105.62 (15) |
| O7$^{iii}$—Zn1—O7 | 180.00 (15) | Zn3—O7—Zn1 | 114.77 (16) |
| O5$^{i}$—Zn1—O2 | 86.24 (15) | Zn2—O7—H7O | 104 (4) |
| O5$^{ii}$—Zn1—O2 | 93.76 (15) | Zn3—O7—H7O | 110 (4) |
| O7$^{iii}$—Zn1—O2 | 81.58 (13) | Zn1—O7—H7O | 101 (4) |
| O7—Zn1—O2 | 98.42 (13) | C6—C1—C2 | 119.8 (5) |
| O5$^{i}$—Zn1—O2$^{iii}$ | 93.76 (15) | C6—C1—C7 | 116.4 (5) |
| O5$^{ii}$—Zn1—O2$^{iii}$ | 86.24 (15) | C2—C1—C7 | 123.8 (5) |
| O7$^{iii}$—Zn1—O2$^{iii}$ | 98.42 (13) | C3—C2—C1 | 117.6 (5) |
| O7—Zn1—O2$^{iii}$ | 81.58 (13) | C3—C2—C8 | 118.9 (4) |
| O2—Zn1—O2$^{iii}$ | 180.000 (1) | C1—C2—C8 | 123.1 (4) |
| O1$^{iv}$—Zn2—O1 | 104.9 (2) | C4—C3—C2 | 121.3 (5) |
| O1$^{iv}$—Zn2—O7 | 108.41 (15) | C4—C3—C9 | 117.7 (5) |

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| O1—Zn2—O7 | 116.25 (16) | C2—C3—C9 | 120.9 (5) |
| O1$^{iv}$—Zn2—O7$^{iv}$ | 116.25 (16) | C3—C4—C5 | 121.1 (6) |
| O1—Zn2—O7$^{iv}$ | 108.41 (15) | C3—C4—H4 | 119.5 |
| O7—Zn2—O7$^{iv}$ | 103.1 (2) | C5—C4—H4 | 119.5 |
| O6$^{i}$—Zn3—O3$^{iii}$ | 135.77 (17) | C4—C5—C6 | 119.3 (6) |
| O6$^{i}$—Zn3—O4$^{v}$ | 102.75 (17) | C4—C5—H5 | 120.4 |
| O3$^{iii}$—Zn3—O4$^{v}$ | 117.03 (14) | C6—C5—H5 | 120.4 |
| O6$^{i}$—Zn3—O7 | 98.68 (14) | C5—C6—C1 | 120.9 (6) |
| O3$^{iii}$—Zn3—O7 | 87.62 (14) | C5—C6—H6 | 119.5 |
| O4$^{v}$—Zn3—O7 | 107.46 (15) | C1—C6—H6 | 119.5 |
| O6$^{i}$—Zn3—O1W | 82.42 (17) | O2—C7—O1 | 124.3 (5) |
| O3$^{iii}$—Zn3—O1W | 85.21 (16) | O2—C7—C1 | 119.8 (5) |
| O4$^{v}$—Zn3—O1W | 81.20 (18) | O1—C7—C1 | 115.9 (5) |
| O7—Zn3—O1W | 170.65 (17) | O4—C8—O3 | 122.0 (5) |
| C7—O1—Zn2 | 116.6 (3) | O4—C8—C2 | 115.0 (4) |
| Zn3—O1W—H1WA | 120 (4) | O3—C8—C2 | 123.0 (5) |
| Zn3—O1W—H1WB | 116 (4) | O5—C9—O6 | 125.4 (5) |
| H1WA—O1W—H1WB | 110 (3) | O5—C9—C3 | 117.7 (4) |
| C7—O2—Zn1 | 128.5 (3) | O6—C9—C3 | 116.8 (5) |
| C8—O3—Zn3$^{iii}$ | 130.1 (3) | H3WA—O3W—H3WB | 107.3 |

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| O1$^{iv}$—Zn2—O1—C7 | −65.4 (4) | C7—C1—C2—C8 | 4.3 (8) |
| O7—Zn2—O1—C7 | 54.3 (4) | C1—C2—C3—C4 | −1.2 (9) |
| O7$^{iv}$—Zn2—O1—C7 | 169.8 (4) | C8—C2—C3—C4 | 172.1 (6) |
| O5$^{i}$—Zn1—O2—C7 | 141.0 (4) | C1—C2—C3—C9 | 174.2 (5) |
| O5$^{ii}$—Zn1—O2—C7 | −39.0 (4) | C8—C2—C3—C9 | −12.5 (8) |
| O7$^{iii}$—Zn1—O2—C7 | −130.8 (5) | C2—C3—C4—C5 | 2.2 (11) |
| O7—Zn1—O2—C7 | 49.2 (5) | C9—C3—C4—C5 | −173.4 (7) |
| O2$^{iii}$—Zn1—O2—C7 | −117 (100) | C3—C4—C5—C6 | −0.5 (12) |
| O1$^{iv}$—Zn2—O7—Zn3 | −45.2 (2) | C4—C5—C6—C1 | −2.0 (12) |
| O1—Zn2—O7—Zn3 | −163.02 (17) | C2—C1—C6—C5 | 2.9 (10) |
| O7$^{iv}$—Zn2—O7—Zn3 | 78.55 (17) | C7—C1—C6—C5 | −175.8 (6) |
| O1$^{iv}$—Zn2—O7—Zn1 | 86.51 (19) | Zn1—O2—C7—O1 | −39.5 (7) |
| O1—Zn2—O7—Zn1 | −31.3 (2) | Zn1—O2—C7—C1 | 140.8 (4) |
| O7$^{iv}$—Zn2—O7—Zn1 | −149.7 (2) | Zn2—O1—C7—O2 | −15.6 (7) |
| O6$^{i}$—Zn3—O7—Zn2 | 91.9 (2) | Zn2—O1—C7—C1 | 164.2 (3) |
| O3$^{iii}$—Zn3—O7—Zn2 | −132.1 (2) | C6—C1—C7—O2 | −174.5 (5) |
| O4$^{v}$—Zn3—O7—Zn2 | −14.5 (2) | C2—C1—C7—O2 | 6.8 (8) |
| O1W—Zn3—O7—Zn2 | −172.0 (9) | C6—C1—C7—O1 | 5.7 (8) |
| O6$^{i}$—Zn3—O7—Zn1 | −35.8 (2) | C2—C1—C7—O1 | −172.9 (5) |
| O3$^{iii}$—Zn3—O7—Zn1 | 100.22 (18) | Zn3$^{vi}$—O4—C8—O3 | 27.5 (7) |
| O4$^{v}$—Zn3—O7—Zn1 | −142.15 (16) | Zn3$^{vi}$—O4—C8—C2 | −154.5 (3) |
| O1W—Zn3—O7—Zn1 | 60.3 (10) | Zn3$^{iii}$—O3—C8—O4 | −156.6 (4) |
| O5$^{i}$—Zn1—O7—Zn2 | −90.46 (18) | Zn3$^{iii}$—O3—C8—C2 | 25.5 (7) |
| O5$^{ii}$—Zn1—O7—Zn2 | 89.54 (18) | C3—C2—C8—O4 | −75.5 (6) |
| O7$^{iii}$—Zn1—O7—Zn2 | 118.7 (5) | C1—C2—C8—O4 | 97.4 (6) |
| O2—Zn1—O7—Zn2 | −3.92 (19) | C3—C2—C8—O3 | 102.5 (6) |
| O2$^{iii}$—Zn1—O7—Zn2 | 176.08 (19) | C1—C2—C8—O3 | −84.5 (7) |

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| O5$^{i}$—Zn1—O7—Zn3 | 44.24 (18) | Zn1$^{vii}$—O5—C9—O6 | 5.9 (9) |
| O5$^{ii}$—Zn1—O7—Zn3 | −135.76 (18) | Zn1$^{vii}$—O5—C9—C3 | −171.8 (4) |
| O7$^{iii}$—Zn1—O7—Zn3 | −106.6 (3) | Zn3$^{viii}$—O6—C9—O5 | −27.8 (9) |
| O2—Zn1—O7—Zn3 | 130.78 (17) | Zn3$^{viii}$—O6—C9—C3 | 149.8 (4) |
| O2$^{iii}$—Zn1—O7—Zn3 | −49.22 (17) | C4—C3—C9—O5 | 151.0 (6) |
| C6—C1—C2—C3 | −1.3 (8) | C2—C3—C9—O5 | −24.6 (8) |
| C7—C1—C2—C3 | 177.3 (5) | C4—C3—C9—O6 | −26.8 (8) |
| C6—C1—C2—C8 | −174.3 (5) | C2—C3—C9—O6 | 157.6 (5) |

Symmetry codes: (i) −*y*+3/4, *x*−1/4, −*z*+3/4; (ii) *y*+1/4, −*x*+1/4, *z*+1/4; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*+1, −*y*−1/2, *z*; (v) −*y*+3/4, *x*−3/4, *z*+1/4; (vi) *y*+3/4, −*x*+3/4, *z*−1/4; (vii) −*y*+1/4, *x*−1/4, *z*−1/4; (viii) *y*+1/4, −*x*+3/4, −*z*+3/4.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*WA*···O2*W* | 0.86 (2) | 2.37 (4) | 3.121 (7) | 146 (6) |
| O1*W*—H1*WB*···O2$^{v}$ | 0.86 (2) | 2.28 (5) | 2.981 (6) | 139 (6) |
| O1*W*—H1*WB*···O5$^{iii}$ | 0.86 (2) | 2.40 (4) | 3.084 (6) | 137 (5) |
| O7—H7*O*···O3$^{ii}$ | 0.79 (2) | 2.38 (2) | 3.174 (5) | 179 (5) |
| O2*W*—H2*WA*···O3*W*$^{i}$ | 0.64 | 2.30 | 2.776 (18) | 134 |
| O3*W*—H3*WA*···O2*W*$^{viii}$ | 0.86 | 1.94 | 2.776 (18) | 164 |
| O3*W*—H3*WB*···O4$^{ix}$ | 0.90 | 2.24 | 2.811 (15) | 121 |

Symmetry codes: (i) −*y*+3/4, *x*−1/4, −*z*+3/4; (ii) *y*+1/4, −*x*+1/4, *z*+1/4; (iii) −*x*+1, −*y*, −*z*+1; (v) −*y*+3/4, *x*−3/4, *z*+1/4; (viii) *y*+1/4, −*x*+3/4, −*z*+3/4; (ix) −*x*+1/2, −*y*−1/2, −*z*+1/2.