Decaaquabis[μ_2-(5-carboxylato-*m*-phenylenedioxy)diacetato]trizinc(II) dihydrate

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In the crystal structure of the title compound, $[Zn_3(C_{11}H_7O_8)_2(H_2O)_{10}]\cdot 2H_2O$, the trianionic carboxylate unit uses one oxyacetate $-OCH_2CO_2^-$ arm to chelate a Zn atom through the ether and carboxylate O atoms. The other oxyacetate arm is free; the $-CO_2^-$ end has a formal negative charge. The central Zn atom lies on a special position of site symmetry $\bar{1}$. The uncoordinated water molecules form a three-dimensional hydrogen-bonded network. One solvent water molecule is disordered over two positions in a 2:1 ratio.

Related literature

The reaction of zinc cations and (5-carboxylato-*m*-phenylenedioxy)diacetate trianions in water gives crystalline hexaaquazinc bis[[(5-carboxylato-*m*-phenylenedioxy)diacetato]-triaquazincate] heptahydrate, whose anion exists as a carboxylate-bridged chain (Wen & Ng, 2007).
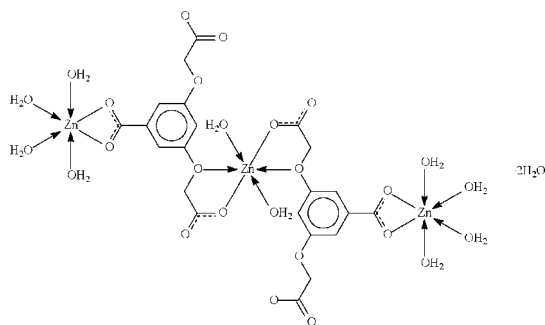
Experimental

Crystal data

$[Zn_3(C_{11}H_7O_8)_2(H_2O)_{10}]\cdot 2H_2O$
$M_r = 946.63$
Triclinic, $P\bar{1}$
$a = 7.3125\ (1)$ Å
$b = 9.0935\ (1)$ Å
$c = 13.4543\ (2)$ Å
$\alpha = 79.271\ (1)°$
$\beta = 82.6340\ (1)°$
$\gamma = 74.064\ (1)°$
$V = 842.42\ (2)$ Å^3
$Z = 1$
Mo $K\alpha$ radiation
$\mu = 2.23$ mm^{-1}
$T = 295\ (2)$ K
$0.32 \times 0.16 \times 0.06$ mm

Data collection

Bruker APEX2 area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.742$, $T_{max} = 0.878$
14462 measured reflections
3858 independent reflections
3176 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.067$
$S = 1.04$
3858 reflections
299 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1w—H1w1$\cdots$O5^i	0.85 (1)	1.95 (1)	2.786 (2)	170 (3)
O1w—H1w2$\cdots$O7^{ii}	0.85 (1)	2.10 (2)	2.836 (2)	145 (3)
O2w—H2w1$\cdots$O7^{iii}	0.84 (1)	1.82 (1)	2.657 (2)	172 (3)
O2w—H2w2$\cdots$O6w	0.84 (1)	2.09 (2)	2.843 (4)	150 (3)
O3w—H3w1$\cdots$O8^i	0.84 (1)	1.93 (1)	2.761 (2)	167 (2)
O3w—H3w2$\cdots$O2^{iv}	0.85 (1)	1.93 (1)	2.772 (2)	172 (3)
O4w—H4w1$\cdots$O4^v	0.86 (3)	1.91 (1)	2.758 (3)	173 (3)
O4w—H4w2$\cdots$O8^{vi}	0.85 (1)	1.81 (1)	2.655 (2)	180 (3)
O5w—H5w1$\cdots$O2^{vii}	0.85 (1)	1.84 (1)	2.685 (2)	170 (2)
O5w—H5w2$\cdots$O6w^{viii}	0.85 (1)	1.97 (2)	2.708 (3)	144 (3)
O5w—H5w2$\cdots$O6w'^{viii}	0.85 (1)	1.90 (1)	2.732 (6)	168 (3)
O6w—H6w1$\cdots$O8^{vi}	0.85 (1)	1.94 (2)	2.747 (3)	158 (4)
O6w—H6w2$\cdots$O5w^{ix}	0.86 (1)	1.98 (2)	2.791 (3)	156 (4)

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

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2561).

metal-organic compounds

References

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supplementary materials

Decaaquabis[*μ*$_2$-(5-carboxylato-*m*-phenylenedioxy)diacetato]trizinc(II) dihydrate

Y.-H. Wen, X. Feng and S. W. Ng

Comment

(type here to add)

Experimental

(5-Carboxy-*m*-phenylenedioxy)diacetic acid (0.282 g, 1 mol) and zinc nitrate hexahydrate (0.298 g, 1 mmol)) were mixed in 20 ml e thanol-water (1:1, *v/v*) solution. The pH value was adjusted to 7 by sodium carbonate solution. The filtered solution was set aside for the growth of crystals which appeared after a week.

In an earlier attempt, the filtered solution was set aside for a week for the growth of hexaaquazinc bis[(5-carboxylato-*m*-phenylenedioxy)diacetatotriaquazincate] heptahydrate (Wen & Ng, 2007). In the present study, the solution was kept at 278 K for two months to yield a compound of a different composition.

Refinement

The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.85 (1) Å and H···H 1.39 (1) Å; their temperature factors were freely refined. For the disordered lattce water molecule, hydrogen atoms were placed on the major component only. The carbon-bound H-atoms were generated geometrically (C–H 0.93 to 0.97 Å); they were included in the refinement in the riding model approximation, with U(H) set to $1.2U_{eq}$(C).

Figures
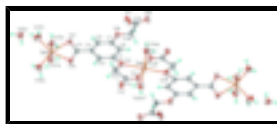
Fig. 1. **Figure 1**. Thermal ellipsoid plot depicting the coordination geometries of the two zinc atoms; displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius. The minor disorder component of the lattice water molecule is not shown. [Symmery code (i) $2 - x$, $-y$, $1 - z$.]

Decaaquabis[μ$_2$-(5-carboxylato-*m*-phenylenedioxy)diacetato]trizinc(II) dihydrate

Crystal data

[Zn$_3$(C$_{11}$H$_7$O$_8$)$_2$(H$_2$O)$_{10}$]·2H$_2$O	$Z = 1$
$M_r = 946.63$	$F_{000} = 484$
Triclinic, $P\bar{1}$	$D_x = 1.866$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.3125$ (1) Å	Cell parameters from 5082 reflections
$b = 9.0935$ (1) Å	$\theta = 2.6–27.2°$

supplementary materials

$c = 13.4543\ (2)$ Å

$\alpha = 79.271\ (1)°$

$\beta = 82.6340\ (1)°$

$\gamma = 74.064\ (1)°$

$V = 842.42\ (2)$ Å^3

$\mu = 2.23$ mm^{-1}

$T = 295\ (2)$ K

Prism, colorless

$0.32 \times 0.16 \times 0.06$ mm

Data collection

Bruker APEX-II area-detector diffractometer	3858 independent reflections
Radiation source: fine-focus sealed tube	3176 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
$T = 295(2)$ K	$\theta_{max} = 27.5°$
φ and ω scans	$\theta_{min} = 1.6°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{min} = 0.742$, $T_{max} = 0.878$	$k = -11 \rightarrow 11$
14462 measured reflections	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.027$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.2695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
3858 reflections	$\Delta\rho_{max} = 0.42$ e Å^{-3}
299 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
18 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
Zn1	1.0000	0.0000	0.5000	0.02497 (9)	
Zn2	0.25698 (3)	0.73433 (3)	0.898344 (17)	0.02466 (8)	
O1	0.9264 (2)	−0.15104 (16)	0.61275 (10)	0.0281 (3)	
O2	0.7610 (2)	−0.19883 (17)	0.75921 (11)	0.0298 (3)	
O3	0.7885 (2)	0.15379 (15)	0.60092 (10)	0.0262 (3)	
O4	0.4623 (2)	0.54817 (17)	0.84086 (10)	0.0281 (3)	
O5	0.3464 (2)	0.75350 (16)	0.73226 (11)	0.0281 (3)	
O6	0.7776 (2)	0.65455 (16)	0.41363 (10)	0.0270 (3)	
O7	0.8774 (3)	0.83786 (18)	0.25159 (12)	0.0449 (5)	
O8	0.9369 (2)	0.65423 (17)	0.15490 (11)	0.0310 (4)	

O1w	0.7706 (2)	−0.00283 (19)	0.42077 (12)	0.0326 (4)	
H1w1	0.741 (4)	0.0793 (17)	0.3784 (17)	0.069 (10)*	
H1w2	0.794 (5)	−0.0807 (19)	0.3909 (19)	0.080 (12)*	
O2w	0.0493 (2)	0.94000 (19)	0.89410 (14)	0.0400 (4)	
H2w1	0.066 (4)	1.016 (2)	0.8510 (17)	0.062 (9)*	
H2w2	−0.061 (2)	0.957 (3)	0.922 (2)	0.083 (12)*	
O3w	0.0360 (2)	0.63529 (19)	0.89035 (13)	0.0331 (4)	
H3w1	0.059 (3)	0.5422 (12)	0.8821 (18)	0.044 (8)*	
H3w2	−0.042 (4)	0.693 (2)	0.8485 (19)	0.070 (10)*	
O4w	0.2654 (3)	0.6729 (2)	1.05019 (12)	0.0404 (4)	
H4w1	0.355 (3)	0.603 (3)	1.079 (2)	0.073 (10)*	
H4w2	0.1602 (19)	0.667 (3)	1.0834 (18)	0.054 (9)*	
O5w	0.4649 (2)	0.8552 (2)	0.89952 (12)	0.0313 (4)	
H5w1	0.550 (3)	0.847 (3)	0.8501 (12)	0.047 (8)*	
H5w2	0.520 (4)	0.837 (4)	0.9540 (11)	0.090 (13)*	
O6w	−0.2748 (4)	0.8784 (3)	1.0180 (2)	0.0378 (10)	0.671 (6)
H6w1	−0.223 (6)	0.793 (3)	1.054 (3)	0.126 (17)*	
H6w2	−0.338 (7)	0.941 (4)	1.058 (3)	0.17 (2)*	
O6w'	−0.4015 (10)	0.8303 (8)	1.0841 (6)	0.062 (3)	0.329 (6)
C1	0.8089 (3)	−0.1096 (2)	0.68481 (15)	0.0223 (4)	
C2	0.7164 (3)	0.0612 (2)	0.68664 (16)	0.0297 (5)	
H2A	0.5793	0.0811	0.6859	0.036*	
H2B	0.7422	0.0892	0.7486	0.036*	
C3	0.7317 (3)	0.3135 (2)	0.59859 (14)	0.0204 (4)	
C4	0.6293 (3)	0.3834 (2)	0.67841 (15)	0.0220 (4)	
H4	0.5972	0.3243	0.7389	0.026*	
C5	0.5750 (3)	0.5446 (2)	0.66633 (15)	0.0205 (4)	
C6	0.6244 (3)	0.6330 (2)	0.57711 (14)	0.0215 (4)	
H6	0.5864	0.7405	0.5693	0.026*	
C7	0.7317 (3)	0.5591 (2)	0.49913 (14)	0.0210 (4)	
C8	0.7852 (3)	0.3998 (2)	0.50908 (15)	0.0219 (4)	
H8	0.8562	0.3510	0.4564	0.026*	
C9	0.4563 (3)	0.6204 (2)	0.75028 (14)	0.0207 (4)	
C10	0.8699 (3)	0.5819 (2)	0.32888 (15)	0.0229 (4)	
H10A	0.7941	0.5190	0.3120	0.027*	
H10B	0.9937	0.5147	0.3458	0.027*	
C11	0.8944 (3)	0.7035 (2)	0.23948 (15)	0.0252 (4)	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0323 (2)	0.01893 (18)	0.02016 (18)	−0.00585 (14)	0.00617 (14)	−0.00096 (13)
Zn2	0.02595 (14)	0.02400 (14)	0.02075 (13)	−0.00288 (10)	0.00454 (10)	−0.00511 (10)
O1	0.0366 (9)	0.0184 (7)	0.0240 (8)	−0.0050 (6)	0.0098 (6)	−0.0014 (6)
O2	0.0328 (9)	0.0246 (8)	0.0268 (8)	−0.0082 (7)	0.0064 (6)	0.0040 (6)
O3	0.0374 (9)	0.0147 (7)	0.0220 (7)	−0.0049 (6)	0.0101 (6)	−0.0030 (6)
O4	0.0319 (8)	0.0261 (8)	0.0195 (7)	0.0005 (6)	0.0040 (6)	−0.0029 (6)
O5	0.0313 (8)	0.0226 (8)	0.0239 (8)	0.0038 (6)	0.0003 (6)	−0.0055 (6)

O6	0.0405 (9)	0.0179 (7)	0.0188 (7)	−0.0066 (6)	0.0097 (6)	−0.0032 (6)
O7	0.0838 (14)	0.0222 (8)	0.0266 (8)	−0.0166 (9)	0.0076 (9)	−0.0024 (7)
O8	0.0445 (10)	0.0279 (8)	0.0183 (7)	−0.0088 (7)	0.0053 (7)	−0.0042 (6)
O1w	0.0403 (10)	0.0250 (9)	0.0313 (9)	−0.0059 (7)	−0.0043 (7)	−0.0042 (7)
O2w	0.0313 (10)	0.0245 (9)	0.0532 (11)	−0.0030 (7)	0.0090 (8)	0.0067 (8)
O3w	0.0348 (9)	0.0224 (8)	0.0419 (10)	−0.0070 (7)	−0.0044 (8)	−0.0042 (7)
O4w	0.0290 (9)	0.0576 (12)	0.0245 (8)	−0.0037 (9)	0.0030 (7)	0.0043 (8)
O5w	0.0289 (9)	0.0415 (10)	0.0262 (8)	−0.0127 (7)	0.0045 (7)	−0.0112 (7)
O6w	0.0391 (17)	0.0333 (16)	0.0384 (17)	0.0018 (12)	−0.0112 (13)	−0.0101 (13)
O6w'	0.065 (5)	0.049 (4)	0.074 (5)	0.001 (3)	−0.031 (4)	−0.018 (4)
C1	0.0242 (11)	0.0210 (10)	0.0212 (10)	−0.0068 (8)	−0.0014 (8)	−0.0011 (8)
C2	0.0355 (13)	0.0222 (11)	0.0262 (11)	−0.0072 (9)	0.0113 (9)	−0.0011 (9)
C3	0.0224 (10)	0.0157 (9)	0.0213 (10)	−0.0019 (8)	0.0000 (8)	−0.0042 (8)
C4	0.0246 (10)	0.0206 (10)	0.0181 (10)	−0.0049 (8)	0.0030 (8)	−0.0010 (8)
C5	0.0207 (10)	0.0199 (10)	0.0199 (10)	−0.0024 (8)	−0.0008 (8)	−0.0059 (8)
C6	0.0246 (10)	0.0168 (10)	0.0217 (10)	−0.0027 (8)	−0.0005 (8)	−0.0042 (8)
C7	0.0237 (10)	0.0205 (10)	0.0178 (10)	−0.0061 (8)	0.0013 (8)	−0.0019 (8)
C8	0.0248 (10)	0.0209 (10)	0.0180 (10)	−0.0038 (8)	0.0039 (8)	−0.0048 (8)
C9	0.0219 (10)	0.0208 (10)	0.0205 (10)	−0.0062 (8)	0.0016 (8)	−0.0068 (8)
C10	0.0278 (11)	0.0208 (10)	0.0196 (10)	−0.0061 (8)	0.0034 (8)	−0.0059 (8)
C11	0.0296 (11)	0.0220 (11)	0.0223 (11)	−0.0062 (9)	0.0012 (9)	−0.0019 (8)

Geometric parameters (Å, °)

Zn1—O1	1.9744 (14)	O2w—H2w2	0.84 (1)
Zn1—O1^i	1.9744 (14)	O3w—H3w1	0.84 (1)
Zn1—O1w	2.1078 (16)	O3w—H3w2	0.85 (3)
Zn1—O1w^i	2.1078 (16)	O4w—H4w1	0.86 (3)
Zn1—O3^i	2.2742 (14)	O4w—H4w2	0.85 (1)
Zn1—O3	2.2742 (14)	O5w—H5w1	0.85 (1)
Zn2—O4w	2.0194 (16)	O5w—H5w2	0.85 (1)
Zn2—O2w	2.0566 (16)	O6w—H6w1	0.85 (1)
Zn2—O3w	2.0771 (16)	O6w—H6w2	0.86 (1)
Zn2—O5w	2.1091 (16)	C1—C2	1.518 (3)
Zn2—O4	2.1242 (15)	C2—H2A	0.9700
Zn2—O5	2.2347 (14)	C2—H2B	0.9700
O1—C1	1.251 (2)	C3—C4	1.380 (3)
O2—C1	1.244 (2)	C3—C8	1.384 (3)
O3—C3	1.392 (2)	C4—C5	1.393 (3)
O3—C2	1.429 (2)	C4—H4	0.9300
O4—C9	1.272 (2)	C5—C6	1.381 (3)
O5—C9	1.255 (2)	C5—C9	1.488 (3)
O6—C7	1.371 (2)	C6—C7	1.389 (3)
O6—C10	1.425 (2)	C6—H6	0.9300
O7—C11	1.233 (3)	C7—C8	1.378 (3)
O8—C11	1.271 (2)	C8—H8	0.9300
O1w—H1w1	0.85 (1)	C10—C11	1.503 (3)
O1w—H1w2	0.85 (1)	C10—H10A	0.9700

O2w—H2w1	0.84 (1)	C10—H10B	0.9700
O1—Zn1—O1^i	180.0	Zn2—O4w—H4w2	115.9 (18)
O1—Zn1—O1w	90.41 (6)	H4w1—O4w—H4w2	108.3 (15)
O1^i—Zn1—O1w	89.59 (6)	Zn2—O5w—H5w1	114.5 (17)
O1—Zn1—O1w^i	89.59 (6)	Zn2—O5w—H5w2	116 (2)
O1^i—Zn1—O1w^i	90.41 (6)	H5w1—O5w—H5w2	108.2 (15)
O1w—Zn1—O1w^i	180.00 (7)	H6w1—O6w—H6w2	107.9 (17)
O1—Zn1—O3^i	102.88 (5)	H6w1—O6w'—H6w2	67.6 (17)
O1^i—Zn1—O3^i	77.12 (5)	O2—C1—O1	124.92 (19)
O1w—Zn1—O3^i	91.35 (6)	O2—C1—C2	115.08 (18)
O1w^i—Zn1—O3^i	88.65 (6)	O1—C1—C2	119.98 (17)
O1—Zn1—O3	77.12 (5)	O3—C2—C1	110.61 (17)
O1^i—Zn1—O3	102.88 (5)	O3—C2—H2A	109.5
O1w—Zn1—O3	88.65 (6)	C1—C2—H2A	109.5
O1w^i—Zn1—O3	91.35 (6)	O3—C2—H2B	109.5
O3^i—Zn1—O3	180.00 (5)	C1—C2—H2B	109.5
O4w—Zn2—O2w	99.31 (8)	H2A—C2—H2B	108.1
O4w—Zn2—O3w	94.63 (7)	C4—C3—C8	121.46 (18)
O2w—Zn2—O3w	85.62 (7)	C4—C3—O3	123.55 (18)
O4w—Zn2—O5w	88.50 (7)	C8—C3—O3	114.99 (17)
O2w—Zn2—O5w	89.36 (7)	C3—C4—C5	118.54 (18)
O3w—Zn2—O5w	174.46 (6)	C3—C4—H4	120.7
O4w—Zn2—O4	103.16 (7)	C5—C4—H4	120.7
O2w—Zn2—O4	157.52 (7)	C6—C5—C4	120.94 (18)
O3w—Zn2—O4	91.76 (6)	C6—C5—C9	120.35 (18)
O5w—Zn2—O4	91.97 (6)	C4—C5—C9	118.68 (18)
O4w—Zn2—O5	161.01 (6)	C5—C6—C7	119.11 (18)
O2w—Zn2—O5	97.82 (6)	C5—C6—H6	120.4
O3w—Zn2—O5	94.79 (6)	C7—C6—H6	120.4
O5w—Zn2—O5	83.55 (6)	O6—C7—C8	123.42 (17)
O4—Zn2—O5	60.09 (5)	O6—C7—C6	115.68 (17)
C1—O1—Zn1	121.99 (13)	C8—C7—C6	120.90 (18)
C3—O3—C2	116.78 (15)	C7—C8—C3	119.02 (18)
C3—O3—Zn1	132.71 (12)	C7—C8—H8	120.5
C2—O3—Zn1	110.27 (11)	C3—C8—H8	120.5
C9—O4—Zn2	92.45 (11)	O5—C9—O4	119.59 (18)
C9—O5—Zn2	87.87 (12)	O5—C9—C5	120.62 (17)
C7—O6—C10	116.56 (15)	O4—C9—C5	119.76 (17)
Zn1—O1w—H1w1	110 (2)	O6—C10—C11	109.57 (17)
Zn1—O1w—H1w2	113 (2)	O6—C10—H10A	109.8
H1w1—O1w—H1w2	109.8 (16)	C11—C10—H10A	109.8
Zn2—O2w—H2w1	118.4 (18)	O6—C10—H10B	109.8
Zn2—O2w—H2w2	128.7 (19)	C11—C10—H10B	109.8
H2w1—O2w—H2w2	111.9 (16)	H10A—C10—H10B	108.2
Zn2—O3w—H3w1	120.8 (17)	O7—C11—O8	125.04 (19)
Zn2—O3w—H3w2	111.1 (19)	O7—C11—C10	120.39 (19)

H3w1—O3w—H3w2	109.7 (15)	O8—C11—C10	114.55 (18)
Zn2—O4w—H4w1	124 (2)		
O1w—Zn1—O1—C1	−88.19 (16)	Zn1—O3—C3—C4	−166.41 (14)
O1w^i—Zn1—O1—C1	91.81 (16)	C2—O3—C3—C8	−172.49 (17)
O3^i—Zn1—O1—C1	−179.67 (15)	Zn1—O3—C3—C8	13.7 (3)
O3—Zn1—O1—C1	0.33 (15)	C8—C3—C4—C5	1.8 (3)
O1—Zn1—O3—C3	172.76 (18)	O3—C3—C4—C5	−177.99 (18)
O1^i—Zn1—O3—C3	−7.24 (18)	C3—C4—C5—C6	−0.9 (3)
O1w—Zn1—O3—C3	−96.51 (17)	C3—C4—C5—C9	177.00 (17)
O1w^i—Zn1—O3—C3	83.49 (17)	C4—C5—C6—C7	−0.7 (3)
O1—Zn1—O3—C2	−1.31 (13)	C9—C5—C6—C7	−178.56 (18)
O1^i—Zn1—O3—C2	178.69 (13)	C10—O6—C7—C8	6.0 (3)
O1w—Zn1—O3—C2	89.42 (14)	C10—O6—C7—C6	−173.57 (17)
O1w^i—Zn1—O3—C2	−90.58 (14)	C5—C6—C7—O6	−179.03 (17)
O4w—Zn2—O4—C9	−169.99 (12)	C5—C6—C7—C8	1.4 (3)
O2w—Zn2—O4—C9	12.0 (2)	O6—C7—C8—C3	180.00 (17)
O3w—Zn2—O4—C9	94.84 (12)	C6—C7—C8—C3	−0.5 (3)
O5w—Zn2—O4—C9	−81.07 (12)	C4—C3—C8—C7	−1.2 (3)
O5—Zn2—O4—C9	0.33 (11)	O3—C3—C8—C7	178.66 (18)
O4w—Zn2—O5—C9	29.9 (3)	Zn2—O5—C9—O4	0.56 (18)
O2w—Zn2—O5—C9	−175.84 (12)	Zn2—O5—C9—C5	178.66 (17)
O3w—Zn2—O5—C9	−89.61 (12)	Zn2—O4—C9—O5	−0.58 (19)
O5w—Zn2—O5—C9	95.70 (12)	Zn2—O4—C9—C5	−178.70 (16)
O4—Zn2—O5—C9	−0.33 (11)	C6—C5—C9—O5	24.9 (3)
Zn1—O1—C1—O2	−177.86 (15)	C4—C5—C9—O5	−152.95 (19)
Zn1—O1—C1—C2	0.7 (3)	C6—C5—C9—O4	−156.98 (18)
C3—O3—C2—C1	−173.21 (17)	C4—C5—C9—O4	25.1 (3)
Zn1—O3—C2—C1	1.9 (2)	C7—O6—C10—C11	175.12 (16)
O2—C1—C2—O3	176.85 (17)	O6—C10—C11—O7	16.0 (3)
O1—C1—C2—O3	−1.9 (3)	O6—C10—C11—O8	−165.57 (17)
C2—O3—C3—C4	7.4 (3)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O5^{ii}	0.85 (1)	1.95 (1)	2.786 (2)	170 (3)
O1w—H1w2···O7^{iii}	0.85 (1)	2.10 (2)	2.836 (2)	145 (3)
O2w—H2w1···O7^{iv}	0.84 (1)	1.82 (1)	2.657 (2)	172 (3)
O2w—H2w2···O6w	0.84 (1)	2.09 (2)	2.843 (4)	150 (3)
O3w—H3w1···O8^{ii}	0.84 (1)	1.93 (1)	2.761 (2)	167 (2)
O3w—H3w2···O2^{v}	0.85 (3)	1.93 (1)	2.772 (2)	172 (3)
O4w—H4w1···O4^{vi}	0.86 (3)	1.91 (1)	2.758 (2)	173 (3)
O4w—H4w2···O8^{vii}	0.85 (1)	1.81 (1)	2.655 (2)	180 (3)
O5w—H5w1···O2^{viii}	0.85 (1)	1.84 (1)	2.685 (2)	170 (2)
O5w—H5w2···O6w^{ix}	0.85 (1)	1.97 (2)	2.708 (3)	144 (3)

O5w—H5w2···O6w$^{\text{ix}}$	0.85 (1)	1.90 (1)	2.732 (6)	168 (3)
O6w—H6w1···O8$^{\text{vii}}$	0.85 (1)	1.94 (2)	2.747 (3)	158 (4)
O6w—H6w2···O5w$^{\text{x}}$	0.86 (1)	1.98 (2)	2.791 (3)	156 (4)

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

Fig. 1