

Hexaaquazinc(II) bis(4-hydroxybenzene-sulfonate) dihydrate

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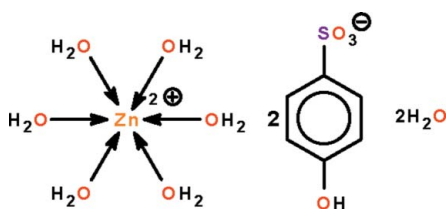
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{O}-\text{C}) = 0.002$ Å; disorder in main residue; R factor = 0.027; wR factor = 0.076; data-to-parameter ratio = 11.9.

In the crystal structure of the title compound, $[\text{Zn}(\text{H}_2\text{O})_6] \cdot (\text{C}_6\text{H}_4\text{SO}_3)_2 \cdot 2\text{H}_2\text{O}$, the Zn^{II} atom lies on a center of inversion. The complex cation interacts with the anion and uncoordinated water molecules by $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, generating a three-dimensional network. The anion is disordered over two equal positions along the hydroxy-sulfonate $\text{C}-\text{C}$ axis.

Related literature

The hexaaquanickel, hexaaquacobalt and hexaaquacopper salts are not isostructural; see: Du *et al.* (2007); Kosnic *et al.* (1992); Liu & Zeng (2007).



Experimental

Crystal data

 $[\text{Zn}(\text{H}_2\text{O})_6] \cdot (\text{C}_6\text{H}_4\text{SO}_3)_2 \cdot 2\text{H}_2\text{O}$
 $M_r = 555.82$

 Triclinic, $P\bar{1}$
 $a = 6.2763$ (5) Å

 $b = 7.0509$ (7) Å

 $c = 13.3151$ (11) Å

 $\alpha = 78.479$ (3)°

 $\beta = 76.832$ (2)°

 $\gamma = 88.051$ (3)°

 $V = 562.15$ (9) Å³
 $Z = 1$

 Mo $K\alpha$ radiation

 $\mu = 1.35$ mm⁻¹
 $T = 293$ K

 $0.23 \times 0.18 \times 0.15$ mm

Data collection

Rigaku R-Axis RAPID IP

diffractometer

Absorption correction: multi-scan

(ABSCOR; Higashi, 1995)

 $T_{\text{min}} = 0.746$, $T_{\text{max}} = 0.823$

5523 measured reflections

2538 independent reflections

 2283 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.076$
 $S = 1.04$

2538 reflections

214 parameters

26 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.47$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1w}-\text{H11} \cdots \text{O1}$	0.82 (1)	2.00 (1)	2.817 (2)	175 (3)
$\text{O1w}-\text{H12} \cdots \text{O3}^{\text{i}}$	0.83 (1)	1.97 (1)	2.801 (2)	176 (2)
$\text{O2w}-\text{H21} \cdots \text{O1}^{\text{ii}}$	0.84 (1)	1.99 (1)	2.818 (2)	168 (2)
$\text{O2w}-\text{H22} \cdots \text{O2}^{\text{iii}}$	0.84 (1)	1.91 (1)	2.730 (2)	165 (2)
$\text{O3w}-\text{H31} \cdots \text{O3}^{\text{iv}}$	0.83 (1)	2.04 (1)	2.845 (2)	166 (3)
$\text{O3w}-\text{H32} \cdots \text{O4}^{\text{v}}$	0.83 (1)	2.02 (1)	2.827 (2)	163 (3)
$\text{O4w}-\text{H41} \cdots \text{O1}$	0.83 (1)	2.02 (1)	2.837 (2)	166 (3)
$\text{O4w}-\text{H42} \cdots \text{O2}^{\text{iii}}$	0.83 (1)	2.05 (1)	2.853 (2)	162 (3)
$\text{O4}-\text{H4} \cdots \text{O4w}^{\text{vi}}$	0.83 (1)	1.79 (1)	2.615 (2)	176 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2624).

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supplementary materials

Acta Cryst. (2009). E65, m1345 [doi:10.1107/S1600536809040604]

Hexaaquazinc(II) bis(4-hydroxybenzenesulfonate) dihydrate

Z.-B. Zhu, S. Gao and S. W. Ng

Experimental

Sodium 3-carboxy-4-hydroxybenzenesulfonate (0.52 g, 2 mmol) was reacted with zinc carbonate (0.25 g, 2 mmol) in water. The mixture was sealed in a 50-ml Teflon-lined stainless-steel bomb and heat at 403 K for three days. The bomb was then allowed to cool naturally to room temperature. Colorless prismatic crystals were obtained. C&H elemental analysis. Calc. for $C_{12}H_{26}O_{16}S_2Zn$: C 25.93, H 4.71%; found: C 25.97, H 4.77%. The carboxyl group of sodium 3-carboxy-4-hydroxybenzenesulfonate was apparently cleaved under the hydrothermal conditions.

Refinement

The aromatic ring is disordered over two positions in respect of four carbon atoms. 1,2-Related carbon-carbon distances were restrained to 1.39 ± 0.01 Å and the 1,4-related ones to 2.78 ± 0.01 Å. Each component ring was restrained to be nearly flat. As the disorder refined to nearly 1:1, the occupancy of the disordered atoms was set as exactly 0.5.

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to $1.2U(C)$. The water and hydroxy H-atoms were refined with a distance restraint of N—H 0.84 ± 0.01 Å; their temperature factors were refined.

Figures

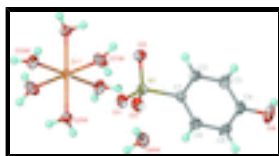


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $[Zn(H_2O)_6] 2[C_6H_5O_4S] 2H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in the aromatic ring is not shown.

Hexaaquazinc(II) bis(4-hydroxybenzenesulfonate) dihydrate

Crystal data

$[Zn(H_2O)_6](C_6H_5O_4S)_2 \cdot 2H_2O$

$M_r = 555.82$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 6.2763$ (5) Å

$b = 7.0509$ (7) Å

$c = 13.3151$ (11) Å

$\alpha = 78.479$ (3)°

$\beta = 76.832$ (2)°

$Z = 1$

$F_{000} = 288$

$D_x = 1.642$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4800 reflections

$\theta = 3.1$ – 27.5 °

$\mu = 1.35$ mm⁻¹

$T = 293$ K

Prism, colorless

supplementary materials

$\gamma = 88.051 (3)^\circ$
 $V = 562.15 (9) \text{ \AA}^3$

$0.23 \times 0.18 \times 0.15 \text{ mm}$

Data collection

Rigaku R-Axis RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
 $T = 293 \text{ K}$
 ω scans
Absorption correction: Multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.746$, $T_{\max} = 0.823$
5523 measured reflections

2538 independent reflections
2283 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\max} = 27.5^\circ$
 $\theta_{\min} = 3.1^\circ$
 $h = -8 \rightarrow 7$
 $k = -9 \rightarrow 9$
 $l = -17 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.076$
 $S = 1.04$
2538 reflections
214 parameters
26 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
 $w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.0371P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.35 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.47 \text{ e \AA}^{-3}$
Extinction correction: none

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Zn1	0.5000	0.5000	0.5000	0.02554 (10)	
S1	0.02762 (6)	0.11701 (5)	0.29910 (3)	0.02660 (11)	
O1	0.0715 (2)	0.28397 (17)	0.34183 (9)	0.0345 (3)	
O2	0.1531 (2)	-0.04947 (19)	0.33502 (10)	0.0451 (3)	
O3	-0.2054 (2)	0.07467 (19)	0.31965 (10)	0.0394 (3)	
O4	0.3707 (3)	0.3376 (3)	-0.15810 (11)	0.0584 (4)	
H4	0.5063 (16)	0.337 (4)	-0.1732 (19)	0.051 (7)*	
O1W	0.4557 (2)	0.2913 (2)	0.41675 (12)	0.0468 (4)	
H11	0.349 (3)	0.290 (4)	0.3908 (19)	0.062 (7)*	
H12	0.556 (3)	0.232 (3)	0.3850 (15)	0.043 (6)*	
O2W	0.2082 (2)	0.62516 (18)	0.47666 (9)	0.0329 (3)	
H21	0.115 (3)	0.637 (3)	0.5314 (12)	0.052 (7)*	
H22	0.207 (4)	0.7338 (19)	0.4375 (14)	0.047 (6)*	

O3W	0.3176 (2)	0.32548 (19)	0.63807 (9)	0.0377 (3)	
H31	0.292 (4)	0.2107 (17)	0.639 (2)	0.061 (7)*	
H32	0.313 (4)	0.346 (4)	0.6979 (11)	0.060 (7)*	
O4W	0.2020 (3)	0.6528 (2)	0.21483 (10)	0.0459 (3)	
H41	0.142 (4)	0.551 (3)	0.2522 (18)	0.073 (9)*	
H42	0.159 (4)	0.729 (3)	0.2548 (18)	0.064 (8)*	
C1	0.1270 (3)	0.1789 (2)	0.16170 (12)	0.0269 (3)	
C4	0.2937 (3)	0.2822 (3)	-0.05256 (13)	0.0371 (4)	
C2	0.3442 (7)	0.1495 (7)	0.1195 (3)	0.0359 (9)	0.50
H2	0.4364	0.0899	0.1639	0.043*	0.50
C3	0.4286 (7)	0.2065 (7)	0.0124 (3)	0.0376 (11)	0.50
H3	0.5803	0.1929	-0.0160	0.045*	0.50
C5	0.0730 (6)	0.3207 (7)	-0.0106 (3)	0.0390 (8)	0.50
H5	-0.0173	0.3845	-0.0550	0.047*	0.50
C6	-0.0097 (6)	0.2634 (7)	0.0973 (3)	0.0349 (8)	0.50
H6	-0.1598	0.2821	0.1267	0.042*	0.50
C2'	0.3409 (6)	0.2436 (7)	0.1239 (3)	0.0324 (9)	0.50
H2'	0.4300	0.2539	0.1715	0.039*	0.50
C3'	0.4255 (8)	0.2935 (7)	0.0161 (3)	0.0374 (11)	0.50
H3'	0.5736	0.3353	-0.0103	0.045*	0.50
C5'	0.0822 (6)	0.2055 (7)	-0.0137 (3)	0.0416 (9)	0.50
H5'	-0.0043	0.1873	-0.0611	0.050*	0.50
C6'	-0.0028 (6)	0.1555 (7)	0.0946 (3)	0.0335 (7)	0.50
H6'	-0.1480	0.1061	0.1214	0.040*	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02646 (15)	0.02624 (15)	0.02455 (15)	0.00073 (9)	-0.00629 (10)	-0.00595 (9)
S1	0.0311 (2)	0.0229 (2)	0.02348 (19)	-0.00025 (15)	-0.00199 (16)	-0.00367 (13)
O1	0.0408 (7)	0.0331 (6)	0.0298 (6)	-0.0060 (5)	-0.0032 (5)	-0.0110 (4)
O2	0.0593 (9)	0.0357 (7)	0.0329 (6)	0.0145 (6)	-0.0056 (6)	0.0030 (5)
O3	0.0338 (6)	0.0404 (7)	0.0410 (7)	-0.0092 (5)	0.0023 (5)	-0.0117 (5)
O4	0.0538 (10)	0.0940 (13)	0.0232 (6)	-0.0074 (9)	-0.0055 (7)	-0.0044 (7)
O1W	0.0357 (7)	0.0558 (9)	0.0648 (9)	0.0112 (6)	-0.0203 (7)	-0.0403 (7)
O2W	0.0306 (6)	0.0357 (7)	0.0282 (6)	0.0056 (5)	-0.0048 (5)	0.0005 (5)
O3W	0.0504 (8)	0.0336 (7)	0.0254 (6)	-0.0108 (6)	-0.0037 (5)	-0.0009 (5)
O4W	0.0596 (9)	0.0382 (8)	0.0342 (7)	-0.0030 (6)	-0.0011 (6)	-0.0044 (6)
C1	0.0320 (8)	0.0238 (7)	0.0236 (7)	0.0008 (6)	-0.0041 (6)	-0.0044 (5)
C4	0.0449 (10)	0.0421 (10)	0.0240 (8)	-0.0014 (8)	-0.0075 (7)	-0.0061 (7)
C2	0.039 (2)	0.038 (2)	0.0278 (18)	0.007 (2)	-0.0079 (15)	-0.0010 (18)
C3	0.033 (2)	0.047 (3)	0.0263 (19)	0.002 (2)	0.0006 (15)	-0.002 (2)
C5	0.044 (2)	0.043 (2)	0.0318 (19)	-0.0016 (18)	-0.0157 (16)	-0.0018 (16)
C6	0.0322 (19)	0.040 (2)	0.0327 (18)	0.0040 (17)	-0.0096 (14)	-0.0059 (16)
C2'	0.0311 (18)	0.045 (2)	0.0228 (16)	-0.0036 (19)	-0.0072 (13)	-0.0081 (18)
C3'	0.034 (2)	0.043 (3)	0.032 (2)	-0.003 (2)	0.0011 (15)	-0.008 (2)
C5'	0.046 (2)	0.055 (3)	0.0289 (18)	0.001 (2)	-0.0176 (16)	-0.0102 (18)
C6'	0.0317 (18)	0.039 (2)	0.0320 (18)	-0.0016 (16)	-0.0082 (14)	-0.0093 (16)

supplementary materials

Geometric parameters (\AA , $^\circ$)

Zn1—O2W ⁱ	2.0660 (11)	C1—C6'	1.375 (4)
Zn1—O2W	2.0660 (11)	C1—C2	1.377 (4)
Zn1—O1W	2.0713 (13)	C1—C2'	1.380 (4)
Zn1—O1W ⁱ	2.0713 (13)	C1—C6	1.387 (4)
Zn1—O3W	2.1066 (12)	C4—C3	1.367 (4)
Zn1—O3W ⁱ	2.1066 (12)	C4—C3'	1.380 (5)
S1—O2	1.4530 (12)	C4—C5'	1.395 (4)
S1—O3	1.4552 (13)	C4—C5	1.409 (4)
S1—O1	1.4651 (12)	C2—C3	1.384 (5)
S1—C1	1.7624 (15)	C2—H2	0.9500
O4—C4	1.358 (2)	C3—H3	0.9500
O4—H4	0.83 (1)	C5—C6	1.392 (5)
O1W—H11	0.82 (1)	C5—H5	0.9500
O1W—H12	0.83 (1)	C6—H6	0.9500
O2W—H21	0.84 (1)	C2'—C3'	1.389 (5)
O2W—H22	0.84 (1)	C2'—H2'	0.9500
O3W—H31	0.83 (1)	C3'—H3'	0.9500
O3W—H32	0.83 (1)	C5'—C6'	1.395 (5)
O4W—H41	0.83 (1)	C5'—H5'	0.9500
O4W—H42	0.83 (1)	C6'—H6'	0.9500
O2W ⁱ —Zn1—O2W	180.000 (1)	C6'—C1—S1	120.64 (18)
O2W ⁱ —Zn1—O1W	90.22 (5)	C2—C1—S1	119.18 (18)
O2W—Zn1—O1W	89.78 (5)	C2'—C1—S1	118.08 (17)
O2W ⁱ —Zn1—O1W ⁱ	89.78 (5)	C6—C1—S1	120.43 (18)
O2W—Zn1—O1W ⁱ	90.22 (5)	O4—C4—C3	121.5 (2)
O1W—Zn1—O1W ⁱ	180.0	O4—C4—C3'	120.7 (2)
O2W ⁱ —Zn1—O3W	92.58 (5)	O4—C4—C5'	119.52 (19)
O2W—Zn1—O3W	87.42 (5)	C3—C4—C5'	111.2 (3)
O1W—Zn1—O3W	89.15 (6)	C3'—C4—C5'	119.8 (3)
O1W ⁱ —Zn1—O3W	90.85 (6)	O4—C4—C5	117.71 (19)
O2W ⁱ —Zn1—O3W ⁱ	87.42 (5)	C3—C4—C5	120.6 (3)
O2W—Zn1—O3W ⁱ	92.58 (5)	C3'—C4—C5	112.2 (3)
O1W—Zn1—O3W ⁱ	90.85 (6)	C1—C2—C3	120.2 (3)
O1W ⁱ —Zn1—O3W ⁱ	89.15 (6)	C1—C2—H2	119.9
O3W—Zn1—O3W ⁱ	180.0	C3—C2—H2	119.9
O2—S1—O3	112.90 (9)	C4—C3—C2	120.0 (4)
O2—S1—O1	110.94 (8)	C4—C3—H3	120.0
O3—S1—O1	112.10 (7)	C2—C3—H3	120.0
O2—S1—C1	105.84 (7)	C6—C5—C4	118.6 (3)
O3—S1—C1	107.93 (8)	C6—C5—H5	120.7
O1—S1—C1	106.68 (7)	C4—C5—H5	120.7
C4—O4—H4	110.5 (17)	C1—C6—C5	120.0 (3)
Zn1—O1W—H11	122.4 (17)	C1—C6—H6	120.0

Zn1—O1W—H12	124.5 (16)	C5—C6—H6	120.0
H11—O1W—H12	109 (2)	C1—C2'—C3'	119.9 (3)
Zn1—O2W—H21	115.9 (16)	C1—C2'—H2'	120.1
Zn1—O2W—H22	120.5 (16)	C3'—C2'—H2'	120.1
H21—O2W—H22	103 (2)	C4—C3'—C2'	119.7 (4)
Zn1—O3W—H31	119.8 (18)	C4—C3'—H3'	120.1
Zn1—O3W—H32	122.9 (19)	C2'—C3'—H3'	120.1
H31—O3W—H32	112 (2)	C4—C5'—C6'	120.3 (3)
H41—O4W—H42	100 (3)	C4—C5'—H5'	119.9
C6'—C1—C2	111.5 (2)	C6'—C5'—H5'	119.9
C6'—C1—C2'	121.2 (2)	C1—C6'—C5'	118.9 (3)
C2—C1—C6	120.3 (2)	C1—C6'—H6'	120.6
C2'—C1—C6	112.6 (2)	C5'—C6'—H6'	120.6
O2—S1—C1—C6'	112.2 (3)	C5'—C4—C5—C6	76.9 (5)
O3—S1—C1—C6'	-8.9 (3)	C6'—C1—C6—C5	-83.1 (5)
O1—S1—C1—C6'	-129.6 (2)	C2—C1—C6—C5	-0.7 (6)
O2—S1—C1—C2	-32.7 (3)	C2'—C1—C6—C5	30.0 (5)
O3—S1—C1—C2	-153.8 (3)	S1—C1—C6—C5	176.7 (3)
O1—S1—C1—C2	85.5 (3)	C4—C5—C6—C1	3.1 (6)
O2—S1—C1—C2'	-65.2 (3)	C6'—C1—C2'—C3'	2.6 (6)
O3—S1—C1—C2'	173.7 (2)	C2—C1—C2'—C3'	79.8 (6)
O1—S1—C1—C2'	53.1 (3)	C6—C1—C2'—C3'	-32.5 (5)
O2—S1—C1—C6	149.9 (2)	S1—C1—C2'—C3'	179.9 (4)
O3—S1—C1—C6	28.7 (3)	O4—C4—C3'—C2'	177.4 (4)
O1—S1—C1—C6	-91.9 (3)	C3—C4—C3'—C2'	-82.7 (8)
C6'—C1—C2—C3	35.6 (5)	C5'—C4—C3'—C2'	-5.3 (6)
C2'—C1—C2—C3	-80.8 (6)	C5—C4—C3'—C2'	31.8 (5)
C6—C1—C2—C3	0.9 (6)	C1—C2'—C3'—C4	1.4 (7)
S1—C1—C2—C3	-176.6 (4)	O4—C4—C5'—C6'	-177.3 (4)
O4—C4—C3—C2	-179.3 (4)	C3—C4—C5'—C6'	33.0 (5)
C3'—C4—C3—C2	84.4 (8)	C3'—C4—C5'—C6'	5.4 (6)
C5'—C4—C3—C2	-30.3 (6)	C5—C4—C5'—C6'	-80.6 (5)
C5—C4—C3—C2	6.3 (6)	C2—C1—C6'—C5'	-32.4 (5)
C1—C2—C3—C4	-3.7 (7)	C2'—C1—C6'—C5'	-2.5 (6)
O4—C4—C5—C6	179.4 (4)	C6—C1—C6'—C5'	80.8 (5)
C3—C4—C5—C6	-6.0 (6)	S1—C1—C6'—C5'	-179.8 (3)
C3'—C4—C5—C6	-33.9 (5)	C4—C5'—C6'—C1	-1.5 (6)

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

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>
O1w—H11 \cdots O1	0.82 (1)	2.00 (1)	2.817 (2)	175 (3)
O1w—H12 \cdots O3 ⁱⁱ	0.83 (1)	1.97 (1)	2.801 (2)	176 (2)
O2w—H21 \cdots O1 ⁱⁱⁱ	0.84 (1)	1.99 (1)	2.818 (2)	168 (2)
O2w—H22 \cdots O2 ^{iv}	0.84 (1)	1.91 (1)	2.730 (2)	165 (2)
O3w—H31 \cdots O3 ^v	0.83 (1)	2.04 (1)	2.845 (2)	166 (3)
O3w—H32 \cdots O4 ^{vi}	0.83 (1)	2.02 (1)	2.827 (2)	163 (3)

supplementary materials

O4w—H41…O1	0.83 (1)	2.02 (1)	2.837 (2)	166 (3)
O4w—H42…O2 ^{iv}	0.83 (1)	2.05 (1)	2.853 (2)	162 (3)
O4—H4…O4w ^{vii}	0.83 (1)	1.79 (1)	2.615 (2)	176 (3)

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

Fig. 1

