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# Hexaaquazinc(II) bis(4-hydroxybenzenesulfonate) dihydrate

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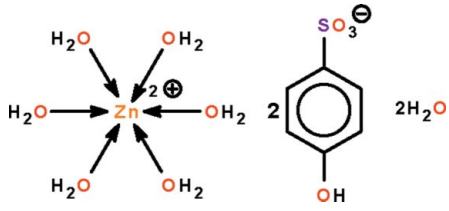
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(O–C) = 0.002 Å; disorder in main residue; $R$ factor = 0.027; $wR$ factor = 0.076; data-to-parameter ratio = 11.9.

In the crystal structure of the title compound, $[Zn(H_2O)_6](C_6H_5O_4S)_2\cdot 2H_2O$, the $Zn^{II}$ atom lies on a center of inversion. The complex cation interacts with the anion and uncoordinated water molecules by O—H···O hydrogen bonds, generating a three-dimensional network. The anion is disordered over two equal positions along the hydroxy–sulfonate C—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

$[Zn(H_2O)_6](C_6H_5O_4S)_2\cdot 2H_2O$
$M_r$ = 555.82
Triclinic, $P\overline{1}$
$a$ = 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) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 1.35 mm$^{-1}$
$T$ = 293 K
0.23 × 0.18 × 0.15 mm

### Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.746, $T_{max}$ = 0.823
5523 measured reflections
2538 independent reflections
2283 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1w—H11···O1 | 0.82 (1) | 2.00 (1) | 2.817 (2) | 175 (3) |
| O1w—H12···O3$^{i}$ | 0.83 (1) | 1.97 (1) | 2.801 (2) | 176 (2) |
| O2w—H21···O1$^{ii}$ | 0.84 (1) | 1.99 (1) | 2.818 (2) | 168 (2) |
| O2w—H22···O2$^{iii}$ | 0.84 (1) | 1.91 (1) | 2.730 (2) | 165 (2) |
| O3w—H31···O3$^{iv}$ | 0.83 (1) | 2.04 (1) | 2.845 (2) | 166 (3) |
| O3w—H32···O4$^{v}$ | 0.83 (1) | 2.02 (1) | 2.827 (2) | 163 (3) |
| O4w—H41···O1 | 0.83 (1) | 2.02 (1) | 2.837 (2) | 166 (3) |
| O4w—H42···O2$^{iii}$ | 0.83 (1) | 2.05 (1) | 2.853 (2) | 162 (3) |
| O4—H4···O4w$^{vi}$ | 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/MSC, 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: *publCIF* (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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# supporting information

*Acta Cryst.* (2009). E**65**, m1345 [https://doi.org/10.1107/S1600536809040604]

## Hexaaquazinc(II) bis(4-hydroxybenzenesulfonate) dihydrate

**Zhi-Biao Zhu, Shan Gao and Seik Weng Ng**

### S1. 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.

### S2. 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 1.2*U*(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.

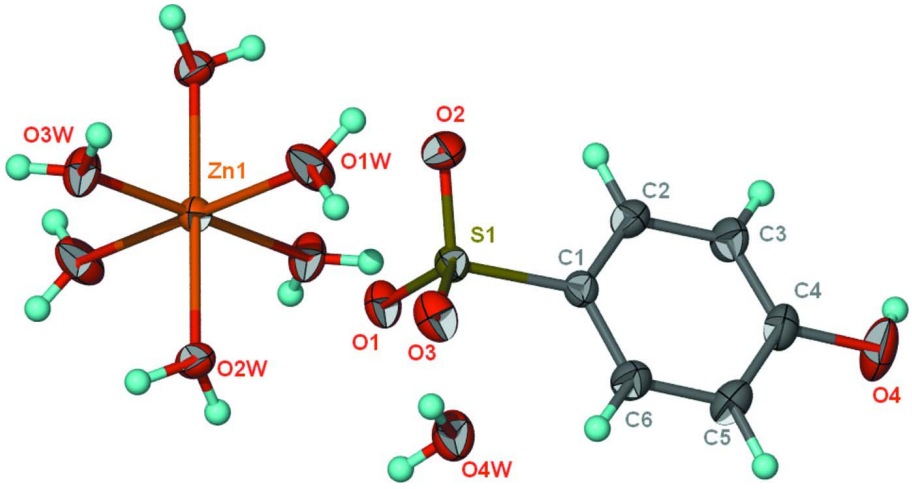


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $[Zn(H_2O)_6]$ $2[C_6H_5O_4S]\cdot 2H_2O$ 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, $P\overline{1}$
Hall symbol: -P 1
$a = 6.2763\ (5)$ Å
$b = 7.0509\ (7)$ Å
$c = 13.3151\ (11)$ Å
$\alpha = 78.479\ (3)°$
$\beta = 76.832\ (2)°$
$\gamma = 88.051\ (3)°$
$V = 562.15\ (9)$ Å$^3$
$Z = 1$
$F(000) = 288$
$D_x = 1.642$ 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
0.23 × 0.18 × 0.15 mm

*Data collection*

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ 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 $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -8\rightarrow7$
$k = -9\rightarrow9$
$l = -17\rightarrow16$

*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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å$^{-3}$
$\Delta\rho_{min} = -0.47$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| 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 code: (i) −*x*+1, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1w—H11···O1 | 0.82 (1) | 2.00 (1) | 2.817 (2) | 175 (3) |
| O1w—H12···O3$^{ii}$ | 0.83 (1) | 1.97 (1) | 2.801 (2) | 176 (2) |
| O2w—H21···O1$^{iii}$ | 0.84 (1) | 1.99 (1) | 2.818 (2) | 168 (2) |
| O2w—H22···O2$^{iv}$ | 0.84 (1) | 1.91 (1) | 2.730 (2) | 165 (2) |

| | | | | |
|---|---|---|---|---|
| O3w—H31···O3$^{v}$ | 0.83 (1) | 2.04 (1) | 2.845 (2) | 166 (3) |
| O3w—H32···O4$^{vi}$ | 0.83 (1) | 2.02 (1) | 2.827 (2) | 163 (3) |
| 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) $-x+1, -y+1, -z$.