Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquazinc(II) bis(4-hydroxybenzenesulfonate) dihydrate

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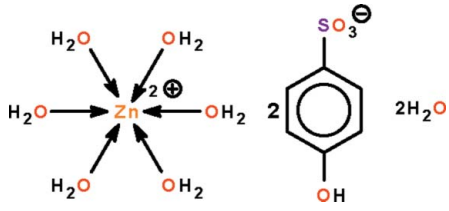
Received 28 September 2009; accepted 5 October 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(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
α = 78.479 (3)°
β = 76.832 (2)°
γ = 88.051 (3)°
V = 562.15 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 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).

We thank the Natural Science Foundation of Heilongjiang Province (No. B200501), Heilongjiang University, China, and the University of Malaya for supporting this study.

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). E**65**, 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 1.2*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.

Figures

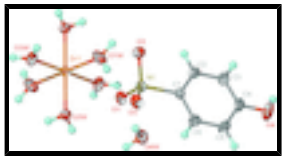

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $[Zn(H_2O)_6]$ $2[C_6H_5O_4S]\cdot 2H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in the aromatic ring is not shown.

Hexaaquazinc(II) bis(4-hydroxybenzenesulfonate) dihydrate

Crystal data

$[Zn(H_2O)_6](C_6H_5O_4S)_2\cdot 2H_2O$	$Z = 1$
$M_r = 555.82$	$F_{000} = 288$
Triclinic, $P\overline{1}$	$D_x = 1.642$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.2763$ (5) Å	Cell parameters from 4800 reflections
$b = 7.0509$ (7) Å	$\theta = 3.1$–27.5°
$c = 13.3151$ (11) Å	$\mu = 1.35$ mm^{-1}
$\alpha = 78.479$ (3)°	$T = 293$ K
$\beta = 76.832$ (2)°	Prism, colorless

γ = 88.051 (3)°	0.23 × 0.18 × 0.15 mm
V = 562.15 (9) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	2538 independent reflections
Radiation source: fine-focus sealed tube	2283 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 293 K	θ_{max} = 27.5°
ω scans	θ_{min} = 3.1°
Absorption correction: Multi-scan (ABSCOR; Higashi, 1995)	h = −8→7
T_{min} = 0.746, T_{max} = 0.823	k = −9→9
5523 measured reflections	l = −17→16

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
$wR(F^2)$ = 0.076	$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.0371P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
2538 reflections	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
214 parameters	$\Delta\rho_{min}$ = −0.47 e Å^{-3}
26 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	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 (Å^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)

Geometric parameters (Å, °)

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 (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^{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*.

Fig. 1