Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquazinc(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

Xi-Shi Tai,[a]* Jie Yin[b] and Ming-Yang Hao[c]

[a]Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, [b]Department of Chemistry and Chemical Engineering, Ningxia University, Yinchuan 750021, People's Republic of China, and [c]Clinical College of Weifang Medical University, Weifang 261042, People's Republic of China
Correspondence e-mail: taixishi@lzu.edu.cn

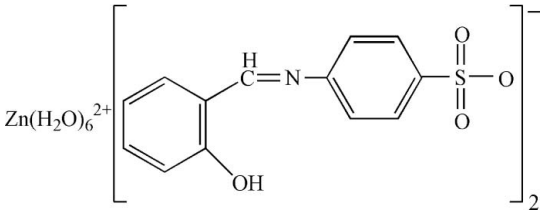
Received 7 May 2007; accepted 21 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.068; wR factor = 0.168; data-to-parameter ratio = 13.2.

In the title compound, $[Zn(H_2O)_6](C_{13}H_{10}NO_4S)_2$, a distorted ZnO_6 octahedron results from the coordination by the six water molecules. Only three of the water molecules are crystallographically unique, as the Zn atom lies on an inversion center. The Zn—O bond lengths are in the range 2.054 (4)–2.073 (4) Å. A network of hydrogen bonds helps to establish the crystal packing.

Related literature

For related literature, see: Tai *et al.* (2005).



Experimental

Crystal data

$[Zn(H_2O)_6](C_{13}H_{10}NO_4S)_2$
M_r = 726.03
Monoclinic, $P2_1/n$
a = 6.3255 (10) Å
b = 35.312 (3) Å
c = 6.9832 (10) Å
β = 90.391 (2)°
V = 1559.8 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 298 (2) K
0.35 × 0.33 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.723, T_{max} = 0.826
6994 measured reflections
2708 independent reflections
2170 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.168
S = 1.08
2708 reflections
205 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7B···O3^{i}	0.85	1.93	2.760 (6)	166
O7—H7A···O1	0.85	1.93	2.779 (5)	177
O6—H6B···O1^{ii}	0.85	1.92	2.773 (6)	176
O6—H6A···O2^{iii}	0.85	1.92	2.770 (6)	175
O5—H5B···O3	0.85	1.90	2.745 (6)	171
O5—H5A···O2^{ii}	0.85	1.91	2.742 (6)	167
O4—H4···N1	0.82	1.93	2.602 (7)	139

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China (20671073), NingXia Natural Gas Transferring Key Laboratory (2004007), the Science and Technology Foundation of Weifang and Weifang University for research grants.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PR2013).

References

Bruker (1997). *SMART* (Version 5.044), *SAINT* (Version 5.01), *SADABS* (Version 2.0) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tai, X. S., Liu, W. Y., Liu, Y. Z. & Li, Y. Z. (2005). *Acta Cryst.* E**61**, o389–o390.

supporting information

Acta Cryst. (2008). E**64**, m273 [doi:10.1107/S1600536807061703]

Hexaaquazinc(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

Xi-Shi Tai, Jie Yin and Ming-Yang Hao

S1. Comment

As part of our onging studies of metal coordination complexes with Shiff base ligands (Tai *et al.*, 2005), the synthesis and structure of the title compound, (I), is reported. Six water molecules are attached to the zinc atom, resulting in a distorted ZnO_6 octahedron (Fig. 1). The C7=N1 bond length [1.280 (9) Å] implies double bond character, while C4—O9 [1.332 (9) Å] is well regarded as a single bond. The dihedral angle between the two benzene ring mean planes (C1—C6 and C8—C13) is 32.2 (3)°. A network of hydrogen bonds helps to establish the crystal packing.

S2. Experimental

One mmol of zinc acetate was added to a solution of salicylaldehyde-4-aminobenzene sulfonic acid (1 mmol) in 20 ml of 95% CH_3CH_2OH. The mixture was continuously stirred for 2 h at refluxing temperature, evaporating some methanol, then, upon cooling, the solid product was collected by filtration and dried *in vacuo* (yield 76%). Clear blocks of (I) were obtained by evaporation from a methanol solution after a week.

S3. Refinement

The water H atoms were located in a difference map and refined as riding in their as-found relative positions with U_{iso}(H) = 1.2U_{eq}(O)". Other H atoms were placed geometrically (C—H = 0.93–0.97 Å, O—H = 0.82 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(O).

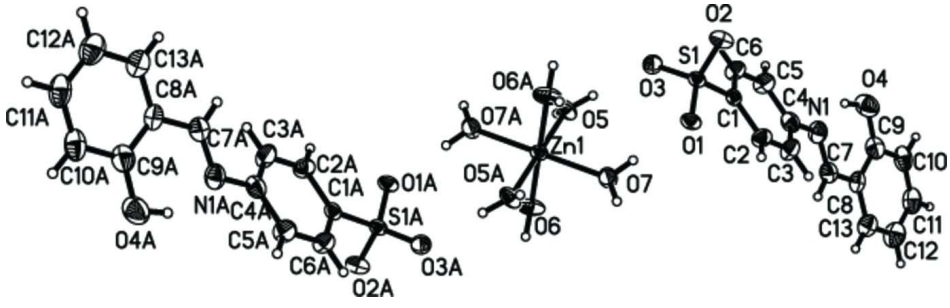


Figure 1

The complex molecule in (I) with 50% probabiility ellipsoids (arbitrary spheres for the H atoms).

Hexaaquazinc(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

Crystal data

$[Zn(H_2O)_6](C_{13}H_{10}NO4S)_2$
M_r = 726.03
Monoclinic, $P2_1/n$
a = 6.3255 (10) Å
b = 35.312 (3) Å
c = 6.9832 (10) Å
β = 90.391 (2)°
V = 1559.8 (4) Å^3

$Z = 2$
$F(000) = 752$
$D_x = 1.546$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2287 reflections

$\theta = 2.3$–$23.1°$
$\mu = 0.99$ mm^{-1}
$T = 298$ K
Block, colourless
0.35 × 0.33 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.723$, $T_{max} = 0.826$

6994 measured reflections
2708 independent reflections
2170 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -7 \rightarrow 5$
$k = -42 \rightarrow 32$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.168$
$S = 1.08$
2708 reflections
205 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 5.0428P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ e Å^{-3}

Special details

Experimental. '*SADABS* v2.0 (Bruker, 1997)'

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}
Zn1	1.0000	0.0000	0.0000	0.0366 (3)
N1	0.4209 (9)	0.23101 (16)	0.5074 (8)	0.0590 (15)
O1	0.8397 (6)	0.06182 (11)	0.5063 (6)	0.0432 (10)
O2	0.5147 (6)	0.05114 (12)	0.6744 (6)	0.0517 (11)
O3	0.5147 (6)	0.05133 (12)	0.3282 (6)	0.0508 (11)
O4	0.1459 (9)	0.28426 (15)	0.5713 (9)	0.0841 (17)
H4	0.1765	0.2635	0.5271	0.126*
O5	0.7091 (6)	0.02586 (12)	0.0024 (6)	0.0508 (11)
H5A	0.6633	0.0365	−0.0989	0.061*
H5B	0.6403	0.0352	0.0953	0.061*

O6	1.1063 (6)	0.03918 (14)	−0.1984 (7)	0.0634 (13)
H6A	1.2325	0.0438	−0.2321	0.076*
H6B	1.0273	0.0452	−0.2926	0.076*
O7	1.1046 (6)	0.03394 (15)	0.2234 (6)	0.0659 (14)
H7A	1.0205	0.0428	0.3067	0.079*
H7B	1.2285	0.0364	0.2696	0.079*
S1	0.6114 (2)	0.06635 (4)	0.5026 (2)	0.0358 (4)
C1	0.5612 (8)	0.11535 (16)	0.4999 (7)	0.0352 (12)
C2	0.7196 (10)	0.14097 (18)	0.5569 (9)	0.0504 (16)
H2	0.8529	0.1323	0.5932	0.060*
C3	0.6734 (12)	0.17949 (19)	0.5582 (10)	0.0616 (19)
H3	0.7770	0.1968	0.5946	0.074*
C4	0.4756 (11)	0.19220 (18)	0.5058 (10)	0.0534 (16)
C5	0.3215 (11)	0.16672 (18)	0.4537 (10)	0.0577 (18)
H5	0.1871	0.1755	0.4217	0.069*
C6	0.3630 (9)	0.12829 (17)	0.4482 (9)	0.0486 (15)
H6	0.2584	0.1113	0.4100	0.058*
C7	0.5591 (11)	0.25692 (19)	0.4805 (9)	0.0551 (17)
H7	0.6977	0.2500	0.4540	0.066*
C8	0.5058 (12)	0.29691 (18)	0.4902 (10)	0.0567 (17)
C9	0.3022 (13)	0.3086 (2)	0.5377 (11)	0.067 (2)
C10	0.2618 (15)	0.3473 (2)	0.5562 (11)	0.072 (2)
H10	0.1281	0.3554	0.5926	0.086*
C11	0.4158 (15)	0.3734 (2)	0.5214 (11)	0.073 (2)
H11	0.3849	0.3991	0.5311	0.087*
C12	0.6194 (16)	0.3620 (2)	0.4714 (12)	0.082 (2)
H12	0.7243	0.3798	0.4477	0.098*
C13	0.6621 (13)	0.3239 (2)	0.4578 (11)	0.067 (2)
H13	0.7978	0.3160	0.4264	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0234 (4)	0.0495 (6)	0.0370 (5)	−0.0006 (4)	−0.0002 (3)	−0.0018 (4)
N1	0.064 (4)	0.047 (3)	0.066 (4)	0.013 (3)	−0.002 (3)	−0.007 (3)
O1	0.0223 (18)	0.062 (3)	0.046 (2)	0.0040 (17)	0.0003 (16)	0.003 (2)
O2	0.037 (2)	0.066 (3)	0.052 (3)	0.003 (2)	0.0060 (19)	0.018 (2)
O3	0.032 (2)	0.064 (3)	0.057 (3)	0.0026 (19)	−0.0060 (19)	−0.011 (2)
O4	0.085 (4)	0.068 (3)	0.100 (5)	0.013 (3)	0.027 (3)	0.005 (3)
O5	0.035 (2)	0.079 (3)	0.038 (2)	0.016 (2)	0.0023 (18)	0.002 (2)
O6	0.031 (2)	0.099 (4)	0.060 (3)	−0.005 (2)	−0.003 (2)	0.030 (3)
O7	0.029 (2)	0.109 (4)	0.060 (3)	−0.002 (2)	−0.004 (2)	−0.038 (3)
S1	0.0239 (7)	0.0472 (8)	0.0362 (7)	0.0032 (6)	0.0008 (5)	−0.0001 (6)
C1	0.028 (3)	0.047 (3)	0.031 (3)	0.005 (2)	−0.001 (2)	−0.005 (2)
C2	0.039 (3)	0.060 (4)	0.053 (4)	−0.005 (3)	−0.010 (3)	0.000 (3)
C3	0.066 (5)	0.049 (4)	0.069 (5)	−0.007 (3)	−0.007 (4)	−0.012 (3)
C4	0.053 (4)	0.051 (4)	0.056 (4)	0.012 (3)	0.010 (3)	−0.002 (3)
C5	0.046 (4)	0.048 (4)	0.079 (5)	0.007 (3)	−0.007 (3)	0.000 (3)

C6	0.037 (3)	0.047 (4)	0.062 (4)	0.005 (3)	−0.014 (3)	0.001 (3)
C7	0.058 (4)	0.055 (4)	0.053 (4)	0.008 (3)	0.001 (3)	−0.005 (3)
C8	0.068 (4)	0.048 (4)	0.053 (4)	0.003 (4)	−0.002 (3)	−0.014 (3)
C9	0.081 (6)	0.061 (5)	0.058 (5)	0.006 (4)	0.006 (4)	−0.001 (4)
C10	0.104 (7)	0.052 (4)	0.059 (5)	0.019 (4)	0.005 (4)	−0.003 (3)
C11	0.108 (7)	0.047 (4)	0.062 (5)	0.019 (4)	−0.006 (4)	−0.002 (4)
C12	0.109 (8)	0.052 (5)	0.084 (6)	0.002 (5)	−0.007 (5)	0.003 (4)
C13	0.073 (5)	0.059 (5)	0.071 (5)	0.002 (4)	−0.008 (4)	−0.007 (4)

Geometric parameters (Å, º)

Zn1—O5^{i}	2.054 (4)	C1—C2	1.406 (8)
Zn1—O5	2.054 (4)	C2—C3	1.391 (9)
Zn1—O7^{i}	2.072 (4)	C2—H2	0.9300
Zn1—O7	2.072 (4)	C3—C4	1.376 (9)
Zn1—O6	2.073 (4)	C3—H3	0.9300
Zn1—O6^{i}	2.073 (4)	C4—C5	1.374 (9)
N1—C7	1.280 (9)	C5—C6	1.383 (9)
N1—C4	1.413 (8)	C5—H5	0.9300
O1—S1	1.453 (4)	C6—H6	0.9300
O2—S1	1.453 (4)	C7—C8	1.454 (9)
O3—S1	1.459 (4)	C7—H7	0.9300
O4—C9	1.332 (9)	C8—C13	1.394 (10)
O4—H4	0.8200	C8—C9	1.394 (10)
O5—H5A	0.8500	C9—C10	1.397 (10)
O5—H5B	0.8499	C10—C11	1.365 (11)
O6—H6A	0.8500	C10—H10	0.9300
O6—H6B	0.8500	C11—C12	1.396 (12)
O7—H7A	0.8500	C11—H11	0.9300
O7—H7B	0.8500	C12—C13	1.375 (10)
S1—C1	1.759 (6)	C12—H12	0.9300
C1—C6	1.380 (8)	C13—H13	0.9300
O5^{i}—Zn1—O5	180.0 (2)	C3—C2—H2	120.6
O5^{i}—Zn1—O7^{i}	91.04 (17)	C1—C2—H2	120.6
O5—Zn1—O7^{i}	88.96 (17)	C4—C3—C2	120.5 (6)
O5^{i}—Zn1—O7	88.96 (17)	C4—C3—H3	119.7
O5—Zn1—O7	91.04 (17)	C2—C3—H3	119.7
O7^{i}—Zn1—O7	180.0 (3)	C5—C4—C3	119.9 (6)
O5^{i}—Zn1—O6	89.80 (17)	C5—C4—N1	117.6 (6)
O5—Zn1—O6	90.20 (17)	C3—C4—N1	122.4 (6)
O7^{i}—Zn1—O6	89.2 (2)	C4—C5—C6	121.0 (6)
O7—Zn1—O6	90.8 (2)	C4—C5—H5	119.5
O5^{i}—Zn1—O6^{i}	90.20 (17)	C6—C5—H5	119.5
O5—Zn1—O6^{i}	89.80 (17)	C1—C6—C5	119.4 (6)
O7^{i}—Zn1—O6^{i}	90.8 (2)	C1—C6—H6	120.3
O7—Zn1—O6^{i}	89.2 (2)	C5—C6—H6	120.3
O6—Zn1—O6^{i}	180.0 (3)	N1—C7—C8	121.9 (7)

C7—N1—C4	121.6 (6)	N1—C7—H7	119.1
C9—O4—H4	109.5	C8—C7—H7	119.1
Zn1—O5—H5A	119.3	C13—C8—C9	119.6 (7)
Zn1—O5—H5B	129.9	C13—C8—C7	119.5 (7)
H5A—O5—H5B	106.9	C9—C8—C7	120.9 (7)
Zn1—O6—H6A	128.5	O4—C9—C8	122.6 (7)
Zn1—O6—H6B	119.5	O4—C9—C10	118.6 (8)
H6A—O6—H6B	106.6	C8—C9—C10	118.8 (8)
Zn1—O7—H7A	122.0	C11—C10—C9	120.9 (8)
Zn1—O7—H7B	129.4	C11—C10—H10	119.5
H7A—O7—H7B	106.4	C9—C10—H10	119.5
O1—S1—O2	111.6 (2)	C10—C11—C12	120.6 (7)
O1—S1—O3	112.7 (2)	C10—C11—H11	119.7
O2—S1—O3	112.2 (3)	C12—C11—H11	119.7
O1—S1—C1	106.7 (2)	C13—C12—C11	118.8 (8)
O2—S1—C1	107.2 (3)	C13—C12—H12	120.6
O3—S1—C1	105.9 (2)	C11—C12—H12	120.6
C6—C1—C2	120.4 (5)	C12—C13—C8	121.2 (8)
C6—C1—S1	119.5 (4)	C12—C13—H13	119.4
C2—C1—S1	120.1 (4)	C8—C13—H13	119.4
C3—C2—C1	118.8 (6)		

O1—S1—C1—C6	163.8 (5)	S1—C1—C6—C5	177.4 (5)
O2—S1—C1—C6	−76.5 (5)	C4—C5—C6—C1	1.4 (10)
O3—S1—C1—C6	43.5 (5)	C4—N1—C7—C8	−177.3 (6)
O1—S1—C1—C2	−18.6 (5)	N1—C7—C8—C13	−179.4 (7)
O2—S1—C1—C2	101.1 (5)	N1—C7—C8—C9	2.8 (11)
O3—S1—C1—C2	−138.9 (5)	C13—C8—C9—O4	−179.7 (7)
C6—C1—C2—C3	−0.7 (9)	C7—C8—C9—O4	−1.9 (11)
S1—C1—C2—C3	−178.3 (5)	C13—C8—C9—C10	−1.5 (11)
C1—C2—C3—C4	0.5 (10)	C7—C8—C9—C10	176.3 (7)
C2—C3—C4—C5	0.7 (11)	O4—C9—C10—C11	−179.3 (7)
C2—C3—C4—N1	179.1 (6)	C8—C9—C10—C11	2.5 (12)
C7—N1—C4—C5	−152.7 (7)	C9—C10—C11—C12	−1.7 (12)
C7—N1—C4—C3	28.8 (10)	C10—C11—C12—C13	0.0 (12)
C3—C4—C5—C6	−1.7 (11)	C11—C12—C13—C8	0.9 (12)
N1—C4—C5—C6	179.8 (6)	C9—C8—C13—C12	−0.1 (11)
C2—C1—C6—C5	−0.2 (9)	C7—C8—C13—C12	−178.0 (7)

Symmetry code: (i) $-x+2, -y, -z$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*B*···O3^{ii}	0.85	1.93	2.760 (6)	166
O7—H7*A*···O1	0.85	1.93	2.779 (5)	177
O6—H6*B*···O1^{iii}	0.85	1.92	2.773 (6)	176
O6—H6*A*···O2^{iv}	0.85	1.92	2.770 (6)	175

O5—H5*B*···O3	0.85	1.90	2.745 (6)	171
O5—H5*A*···O2^{iii}	0.85	1.91	2.742 (6)	167
O4—H4···N1	0.82	1.93	2.602 (7)	139

Symmetry codes: (ii) *x*+1, *y*, *z*; (iii) *x*, *y*, *z*−1; (iv) *x*+1, *y*, *z*−1.