

Aqua{2-[(*E*)-3,5-dibromo-2-oxidobenzylidene-
amino]ethanesulfonato}(1,10-phenanthroline)-
zinc(II) ethanol solvateShu-Hua Zhang,^{a*} Yi-Min Jiang^b
and Kai-Bei Yu^c^aDepartment of Materials and Chemistry Engineering, Guilin University of Technology, Guilin, Guangxi 541004, People's Republic of China, ^bCollege of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin, Guangxi 541004, People's Republic of China, and ^cAnalysis and Test Center, Chinese Academy of Sciences, Chengdu, Sichuan 610041, People's Republic of China

Correspondence e-mail: zsh720108@21cn.com

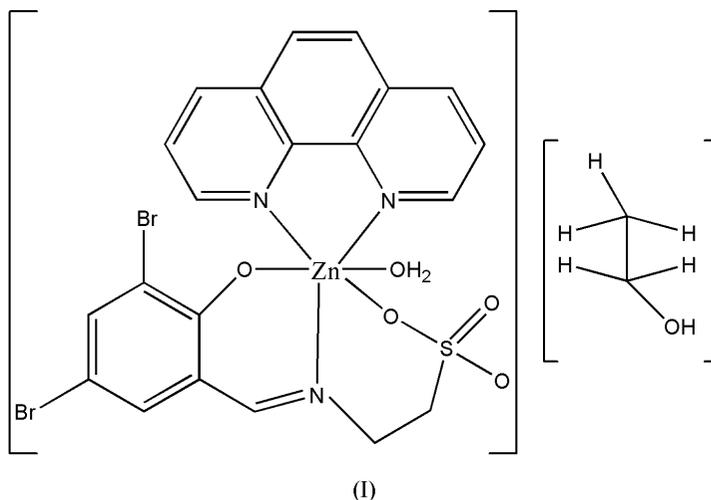
Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.034
 wR factor = 0.062
Data-to-parameter ratio = 14.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $[\text{Zn}(\text{C}_9\text{H}_9\text{Br}_2\text{NO}_4\text{S})(\text{C}_8\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot \text{C}_2\text{H}_5\text{OH}$, was synthesized in a water–ethanol solution. In the structure, one Zn atom is six-coordinated by three ligands to form the neutral complex, in which the Zn atom has a distorted octahedral coordination geometry. Molecules form dimers through $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds.

Comment

Schiff base complexes containing sulfur and Schiff bases complexes containing amino acids have been studied for many years (Casella & Gullotti, 1981; Wang *et al.*, 1994; Casella & Gullotti, 1986; Jiang, Zhang, Xu & Xiao, 2003; Jiang, Zhang, Zhou & Zhong, 2003; Zhang *et al.*, 2003) and have aroused increasing interest because of their antiviral, anticancer and antibacterial activities. Taurine, an amino acid containing sulfur, is indispensable to human beings and has important physiological functions. Recently, Schiff base complexes derived from taurine have been reported (Zhang & Jiang, 2002, 2003; Jiang *et al.*, 2004; Xu *et al.*, 2004). We report here the synthesis and crystal structure of a new zinc(II) complex, (I), prepared by the reaction of $\text{Zn}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$, and the sodium salt of the Schiff base ligand 2-[(*E*)-3,5-dibromo-2-oxidobenzylideneamino]ethanesulfonic acid, which was derived in turn by the reaction of taurine, 3,5-dibromosalicylaldehyde and 1,10-phenanthroline (phen).



As shown in Fig. 1, the molecule of (I) is mononuclear. The Zn atom is coordinated by one N and two O atoms of the tridentate ligand (*L*), two N atoms of the bidentate ligand (phen) and one O atom of the coordinated water molecule, forming a slightly distorted octahedral geometry with O atoms

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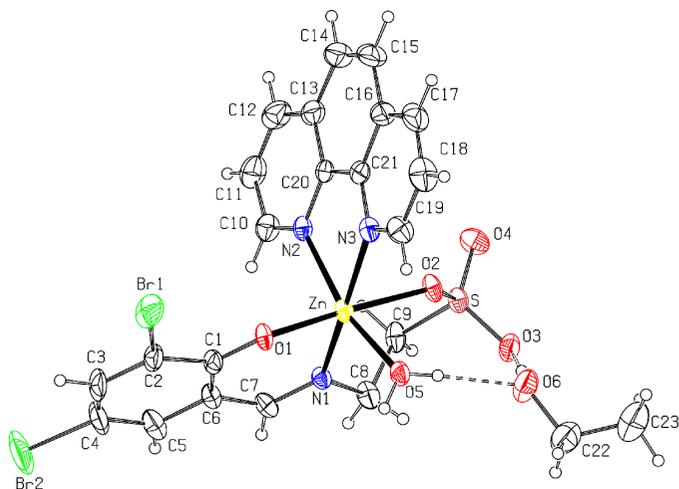


Figure 1
View of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates a hydrogen bond.

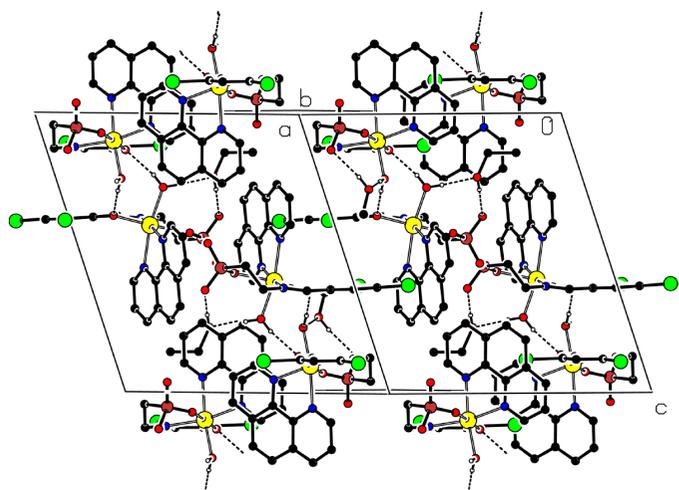


Figure 2
Packing diagram (Spek, 2003) of the title complex, showing the hydrogen bonding as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

(O1 and O2) of the ligand (*L*) in axial positions. The sum of the equatorial coordination angles (see Table 1) is close to 360° (359.28°), and the bond angles involving the Zn atom are similar to values observed in zinc complexes of a salicylaldehyde Schiff base and are in good agreement with those in other taurine-containing complexes. The Zn1—O1 bond length is shorter than Zn1—N1, indicating that the hydroxyl O atom has stronger coordinating ability than the imine N atom, while sulfonate atom O2 has a stronger coordinating ability than water atom O5, indicating that the coordinating ability of the sulfonate has been reinforced by chemical modification (Cai *et al.*, 2001).

Molecules, related by twofold axes, form dimers through O—H...O hydrogen bonding (see Table 2 and Fig. 2). These dimers are, in turn, connected by weaker C—H...O interactions (which are not discussed in detail here) into a three-dimensional network.

Experimental

The sodium salt of the Schiff base ligand 2-[(*E*)-3,5-dibromo-2-oxidobenzylideneamino]ethanesulfonic acid was synthesized as reported previously (Xu *et al.*, 2004). The ligand (2.0 mmol) was dissolved in aqueous ethanol (25 ml). To this solution, Zn(OAc)₂·4H₂O (2.0 mmol) was added and the mixture was stirred and refluxed at 343 K for 8 h. Phen (2.0 mmol) was then added and the reaction was continued for another 4 h. After cooling to room temperature and filtration, the filtrate was left to stand at room temperature and suitable for X-ray diffraction were obtained in a yield of 52%. Analysis found (%): C 37.69, H 3.35, N 6.08, S 4.59, Zn 9.44; C₂₃H₂₃ZnN₃O₆S requires (%): C 37.76, H 3.33, N 6.05, S 4.62, Zn 9.41; IR (KBr, ν cm⁻¹): 1033.1, 1038.1, 1148.6, 1185.0 (—SO₃), 1627.3 (ν C=N), 1603.3, 1521.2 (ν C=N +C=C), 3419.5 (ν O—H).

Crystal data

[Zn(C₉H₉Br₂NO₄S)(C₈H₈N₂)·(H₂O)]·C₂H₆O
M_r = 694.69
 Monoclinic, *C*2/*c*
a = 18.700 (3) Å
b = 19.717 (4) Å
c = 15.728 (3) Å
 β = 114.45 (1)°
V = 5278.6 (16) Å³
Z = 8

D_x = 1.748 Mg m⁻³
 Mo Kα radiation
 Cell parameters from 34 reflections
 θ = 2.8–15.2°
 μ = 4.08 mm⁻¹
T = 296 (2) K
 Prism, red
 0.58 × 0.40 × 0.30 mm

Data collection

Siemens P4 diffractometer
 ω scans
 Absorption correction: empirical (SADABS; Sheldrick, 1996)
T_{min} = 0.160, *T_{max}* = 0.290
 5343 measured reflections
 4793 independent reflections
 2528 reflections with *I* > 2σ(*I*)

R_{int} = 0.016
 θ_{max} = 25.3°
h = 0 → 22
k = 0 → 23
l = -18 → 17
 3 standard reflections every 97 reflections
 intensity decay: 5.1%

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.034
wR (*F*²) = 0.062
S = 0.83
 4793 reflections
 340 parameters
 H atoms treated by a mixture of independent and constrained refinement

w = 1/[σ²(*F_o*²) + (0.0244*P*)²]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δσ)_{max} = 0.001
 Δρ_{max} = 0.44 e Å⁻³
 Δρ_{min} = -0.59 e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.00063 (3)

Table 1

Selected geometric parameters (Å, °).

Zn—O1	2.013 (2)	Zn—N3	2.147 (3)
Zn—O5	2.094 (3)	Zn—O2	2.160 (2)
Zn—N1	2.117 (3)	Zn—N2	2.207 (3)
O1—Zn—O5	91.53 (11)	N1—Zn—O2	89.87 (10)
O1—Zn—N1	89.74 (11)	N3—Zn—O2	83.01 (10)
O5—Zn—N1	96.68 (12)	O1—Zn—N2	97.25 (10)
O1—Zn—N3	97.89 (11)	O5—Zn—N2	166.35 (12)
O5—Zn—N3	92.09 (13)	N1—Zn—N2	93.81 (11)
N1—Zn—N3	168.22 (12)	N3—Zn—N2	76.40 (12)
O1—Zn—O2	176.73 (10)	O2—Zn—N2	86.01 (10)
O5—Zn—O2	85.30 (11)		

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5A \cdots O6	0.820 (10)	1.926 (11)	2.745 (4)	176 (4)
O5—H5B \cdots O1 ¹	0.817 (10)	1.960 (13)	2.765 (4)	168 (4)
O6—H6O \cdots O3	0.824 (10)	1.995 (13)	2.812 (5)	171 (5)

Symmetry code: (i) $1-x, y, \frac{3}{2}-z$.

The H atoms of O5 and O6 were located in a difference Fourier map and their positions and isotropic displacement parameters were refined. All other H atoms were positioned geometrically and were refined as riding, with C—H distances of 0.93–0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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