

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Diaquabis[3-(2-sulfanylphenyl)prop-2-enoato]zinc(II) dihydrate

Qiang Wang, Jian Hou, Li-Jun Wang and Qing-Fu Zeng*

 Engineering Research Center for Clean Production of Textile Dyeing and Printing, Ministry of Education, Wuhan 430073, People's Republic of China
 Correspondence e-mail: qfzeng@wuse.edu.cn

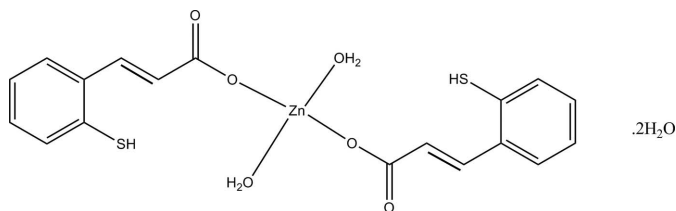
Received 27 August 2009; accepted 28 August 2009

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.067; wR factor = 0.185; data-to-parameter ratio = 12.4.

In the title compound, $[\text{Zn}(\text{C}_9\text{H}_7\text{O}_2\text{S})_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$, the Zn^{II} atom (site symmetry $\bar{1}$) is four-coordinated by two O atoms from 3-(2-sulfanylphenyl)prop-2-enoate anions and two aqua O atoms in a slightly distorted ZnO_4 square-planar arrangement. In the crystal, $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds help to establish the packing.

Related literature

For background to coordination networks, see: Cheng *et al.*, (2006). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $[\text{Zn}(\text{C}_9\text{H}_7\text{O}_2\text{S})_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$
 $M_r = 495.85$

 Monoclinic, $P2_1/c$
 $a = 18.4398$ (5) Å

 $b = 7.7188$ (3) Å

 $c = 7.3258$ (2) Å

 $\beta = 98.578$ (2)°

 $V = 1031.04$ (6) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 1.44$ mm⁻¹
 $T = 298$ K

 $0.30 \times 0.20 \times 0.14$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer

 Absorption correction: ψ scan (North *et al.*, 1968)

 $T_{\text{min}} = 0.673$, $T_{\text{max}} = 0.824$

6272 measured reflections

 1811 independent reflections
 1441 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.092$

200 standard reflections

 every 3 reflections
 intensity decay: 1%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.185$
 $S = 1.06$

1811 reflections

146 parameters

6 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.93$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.88$ e Å⁻³
Table 1

Selected bond lengths (Å).

Zn1—O1	1.969 (4)	Zn1—O3	1.953 (4)
--------	-----------	--------	-----------

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O}3-\text{H}3\text{A} \cdots \text{O}4^{\text{i}}$	0.82 (4)	2.56 (5)	3.033 (7)	118 (5)
$\text{O}3-\text{H}3\text{B} \cdots \text{O}1^{\text{ii}}$	0.82 (4)	2.44 (5)	3.221 (6)	159 (4)
$\text{O}4-\text{H}4\text{A} \cdots \text{O}2$	0.83 (3)	1.95 (4)	2.716 (7)	155 (5)
$\text{O}4-\text{H}4\text{B} \cdots \text{O}2^{\text{iii}}$	0.83 (4)	2.30 (6)	2.951 (7)	136 (4)

 Symmetry codes: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The project was supported by the Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry, Educational Commission of Hubei Province (D20091703) and the Natural Science Foundation of Hubei Province (2008CDB038).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5073).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Cheng, K., Zhu, H.-L. & Li, Y.-G. (2006). *Z. Anorg. Allg. Chem.* **632**, 2326–2330.
- Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
- Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2009). E65, m1183 [doi:10.1107/S1600536809034473]

Diaquabis[3-(2-sulfanylphenyl)prop-2-enoato]zinc(II) dihydrate

Q. Wang, J. Hou, L.-J. Wang and Q.-F. Zeng

Comment

There has been much research interest in acid metal complexes due to their molecular architectures and biological activities (e.g. Cheng *et al.*, 2006). In this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The Zn^{II} atom is four-coordinated by two O atoms from the 3-(2-sulfanylphenyl)propanoate and two O atoms from the water molecules, forming a slightly distorted square-planar coordination.

Experimental

A mixture of 3-(2-sulfanylphenyl)propanoic acid (364 mg, 2 mmol) and ZnCl₂ (1 mmol, 134 mg) in methanol (10 ml) was stirred for 3 h. After keeping the filtrate in air for 7 d, colourless blocks of (I) were formed.

Refinement

The water H atoms were located in a difference map and their positions were refined with restraints of O—H = 0.82 (1) Å. The other H atoms were positioned geometrically (C—H = 0.93 Å, S—H = 1.20 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Figures

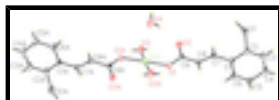


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids. Atoms with the suffix A are generated by the symmetry operation (2-x, 1-y, 1-z).

Diaquabis[3-(2-sulfanylphenyl)prop-2-enoato]zinc(II) dihydrate

Crystal data

[Zn(C₉H₇O₂S)₂(H₂O)₂].2H₂O

$M_r = 495.85$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 18.4398$ (5) Å

$b = 7.7188$ (3) Å

$c = 7.3258$ (2) Å

$\beta = 98.578$ (2)°

$V = 1031.04$ (6) Å³

$F_{000} = 512$

$D_x = 1.597$ Mg m⁻³

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

Cell parameters from 25 reflections

$\theta = 9\text{--}12^\circ$

$\mu = 1.44$ mm⁻¹

$T = 298$ K

Block, colourless

0.30 × 0.20 × 0.14 mm

supplementary materials

$Z = 2$

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{\text{int}} = 0.092$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 25.0^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 2.2^\circ$
$T = 298$ K	$h = -21 \rightarrow 18$
$\omega/2\theta$ scans	$k = -9 \rightarrow 8$
Absorption correction: ψ scan (North <i>et al.</i> , 1968)	$l = -8 \rightarrow 8$
$T_{\text{min}} = 0.673$, $T_{\text{max}} = 0.824$	200 standard reflections
6272 measured reflections	every 3 reflections
1811 independent reflections	intensity decay: 1%
1441 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.185$	$w = 1/[\sigma^2(F_o^2) + (0.1071P)^2 + 0.9875P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
1811 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
146 parameters	$\Delta\rho_{\text{max}} = 0.93 \text{ e } \text{\AA}^{-3}$
6 restraints	$\Delta\rho_{\text{min}} = -0.88 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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 (\AA^2)

x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
-----	-----	-----	----------------------------------

C1	0.6975 (3)	0.9228 (8)	0.6126 (7)	0.0401 (13)
C2	0.6254 (3)	0.8922 (8)	0.6435 (8)	0.0442 (14)
C3	0.5803 (4)	1.0275 (10)	0.6681 (10)	0.0590 (19)
H3	0.5327	1.0042	0.6892	0.071*
C4	0.6020 (4)	1.1926 (10)	0.6630 (11)	0.070 (2)
H4	0.5700	1.2818	0.6811	0.084*
C5	0.6739 (4)	1.2307 (10)	0.6300 (10)	0.066 (2)
H5	0.6898	1.3446	0.6253	0.079*
C6	0.7196 (3)	1.0945 (8)	0.6051 (9)	0.0500 (16)
H6	0.7669	1.1183	0.5825	0.060*
C7	0.7479 (3)	0.7796 (7)	0.5892 (7)	0.0374 (12)
H7	0.7326	0.6685	0.6150	0.045*
C8	0.8132 (3)	0.7942 (7)	0.5345 (7)	0.0361 (12)
H8	0.8281	0.9030	0.5003	0.043*
C9	0.8630 (3)	0.6463 (7)	0.5254 (7)	0.0354 (12)
H3A	1.0261 (19)	0.464 (7)	0.180 (6)	0.043*
H4A	0.866 (2)	0.294 (4)	0.419 (8)	0.043*
H3B	0.964 (2)	0.558 (6)	0.165 (6)	0.043*
H4B	0.861 (2)	0.133 (5)	0.346 (8)	0.043*
O1	0.92576 (19)	0.6850 (5)	0.4821 (5)	0.0401 (9)
O2	0.8441 (3)	0.4964 (5)	0.5594 (7)	0.0530 (12)
O3	0.9908 (3)	0.4908 (6)	0.2311 (6)	0.0499 (11)
O4	0.8892 (3)	0.2064 (6)	0.3989 (8)	0.0666 (13)
S1	0.59232 (9)	0.6819 (2)	0.6468 (3)	0.0601 (6)
H1	0.5970	0.6126	0.5024	0.090*
Zn1	1.0000	0.5000	0.5000	0.0327 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.038 (3)	0.044 (3)	0.039 (3)	0.008 (3)	0.008 (2)	-0.006 (3)
C2	0.040 (3)	0.050 (4)	0.045 (3)	0.005 (3)	0.013 (3)	0.001 (3)
C3	0.040 (4)	0.071 (5)	0.069 (5)	0.018 (3)	0.018 (3)	0.003 (4)
C4	0.063 (5)	0.062 (5)	0.088 (5)	0.033 (4)	0.020 (4)	-0.004 (4)
C5	0.078 (5)	0.042 (4)	0.079 (5)	0.013 (4)	0.021 (4)	-0.012 (3)
C6	0.040 (3)	0.041 (4)	0.072 (4)	0.005 (3)	0.017 (3)	-0.004 (3)
C7	0.034 (3)	0.034 (3)	0.045 (3)	0.005 (2)	0.008 (2)	0.002 (2)
C8	0.037 (3)	0.032 (3)	0.040 (3)	0.005 (2)	0.011 (2)	0.003 (2)
C9	0.037 (3)	0.038 (3)	0.032 (3)	0.007 (2)	0.009 (2)	-0.002 (2)
O1	0.032 (2)	0.045 (2)	0.045 (2)	0.0091 (16)	0.0099 (17)	0.0037 (17)
O2	0.052 (3)	0.035 (3)	0.075 (3)	0.0035 (19)	0.019 (2)	0.000 (2)
O3	0.062 (3)	0.052 (3)	0.040 (2)	0.017 (2)	0.021 (2)	0.0060 (18)
O4	0.074 (3)	0.049 (3)	0.082 (4)	0.014 (2)	0.030 (3)	-0.004 (3)
S1	0.0465 (9)	0.0555 (11)	0.0842 (13)	-0.0072 (8)	0.0287 (9)	0.0035 (9)
Zn1	0.0348 (6)	0.0360 (6)	0.0300 (5)	0.0075 (4)	0.0139 (4)	0.0046 (3)

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

C1—C6	1.390 (10)	C8—C9	1.473 (7)
-------	------------	-------	-----------

supplementary materials

C1—C2	1.402 (8)	C8—H8	0.9300
C1—C7	1.470 (8)	C9—O2	1.245 (6)
C2—C3	1.364 (9)	C9—O1	1.280 (6)
C2—S1	1.735 (7)	Zn1—O1	1.969 (4)
C3—C4	1.338 (10)	Zn1—O3	1.953 (4)
C3—H3	0.9300	O3—H3A	0.824 (10)
C4—C5	1.413 (11)	O3—H3B	0.823 (10)
C4—H4	0.9300	O4—H4A	0.821 (10)
C5—C6	1.376 (9)	O4—H4B	0.819 (10)
C5—H5	0.9300	S1—H1	1.2000
C6—H6	0.9300	Zn1—O3 ⁱ	1.953 (4)
C7—C8	1.330 (7)	Zn1—O1 ⁱ	1.969 (4)
C7—H7	0.9300		
C6—C1—C2	117.2 (5)	C1—C7—H7	117.0
C6—C1—C7	121.3 (5)	C7—C8—C9	123.2 (5)
C2—C1—C7	121.5 (6)	C7—C8—H8	118.4
C3—C2—C1	120.3 (6)	C9—C8—H8	118.4
C3—C2—S1	119.4 (5)	O2—C9—O1	123.9 (5)
C1—C2—S1	120.3 (5)	O2—C9—C8	121.0 (5)
C4—C3—C2	122.3 (7)	O1—C9—C8	115.0 (5)
C4—C3—H3	118.9	C9—O1—Zn1	117.3 (4)
C2—C3—H3	118.9	Zn1—O3—H3A	121 (4)
C3—C4—C5	119.7 (6)	Zn1—O3—H3B	121 (4)
C3—C4—H4	120.1	H3A—O3—H3B	110.2 (18)
C5—C4—H4	120.1	H4A—O4—H4B	110.3 (18)
C6—C5—C4	118.2 (7)	C2—S1—H1	109.5
C6—C5—H5	120.9	O3 ⁱ —Zn1—O3	180.0
C4—C5—H5	120.9	O3 ⁱ —Zn1—O1 ⁱ	90.25 (17)
C5—C6—C1	122.3 (6)	O3—Zn1—O1 ⁱ	89.75 (17)
C5—C6—H6	118.8	O3 ⁱ —Zn1—O1	89.75 (17)
C1—C6—H6	118.8	O3—Zn1—O1	90.25 (17)
C8—C7—C1	126.0 (5)	O1 ⁱ —Zn1—O1	180.0
C8—C7—H7	117.0		
C6—C1—C2—C3	-1.1 (9)	C7—C1—C6—C5	-178.8 (6)
C7—C1—C2—C3	178.8 (6)	C6—C1—C7—C8	-10.0 (9)
C6—C1—C2—S1	177.7 (4)	C2—C1—C7—C8	170.1 (6)
C7—C1—C2—S1	-2.4 (8)	C1—C7—C8—C9	175.9 (5)
C1—C2—C3—C4	0.4 (11)	C7—C8—C9—O2	4.1 (8)
S1—C2—C3—C4	-178.5 (6)	C7—C8—C9—O1	-175.4 (5)
C2—C3—C4—C5	0.4 (12)	O2—C9—O1—Zn1	-7.6 (7)
C3—C4—C5—C6	-0.4 (11)	C8—C9—O1—Zn1	171.9 (3)
C4—C5—C6—C1	-0.4 (10)	C9—O1—Zn1—O3 ⁱ	-70.7 (4)
C2—C1—C6—C5	1.2 (9)	C9—O1—Zn1—O3	109.3 (4)

Symmetry codes: (i) $-x+2, -y+1, -z+1$.

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3A \cdots O4 ⁱⁱ	0.82 (4)	2.56 (5)	3.033 (7)	118 (5)
O3—H3B \cdots O1 ⁱⁱⁱ	0.82 (4)	2.44 (5)	3.221 (6)	159 (4)
O4—H4A \cdots O2	0.83 (3)	1.95 (4)	2.716 (7)	155 (5)
O4—H4B \cdots O2 ^{iv}	0.83 (4)	2.30 (6)	2.951 (7)	136 (4)

Symmetry codes: (ii) $-x+2, y+1/2, -z+1/2$; (iii) $x, -y+3/2, z-1/2$; (iv) $x, -y+1/2, z-1/2$.

Fig. 1

