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

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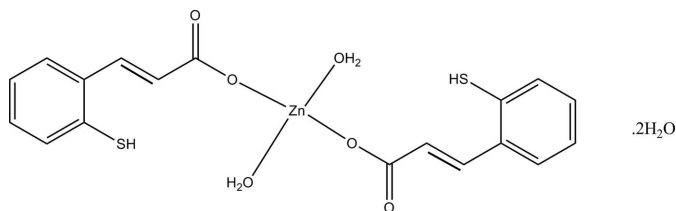
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.067; wR factor = 0.185; data-to-parameter ratio = 12.4.

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)
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Table 2

Hydrogen-bond geometry (Å, °).

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

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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.

supporting information

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

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

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

S1. 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.

S2. 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.

S3. 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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

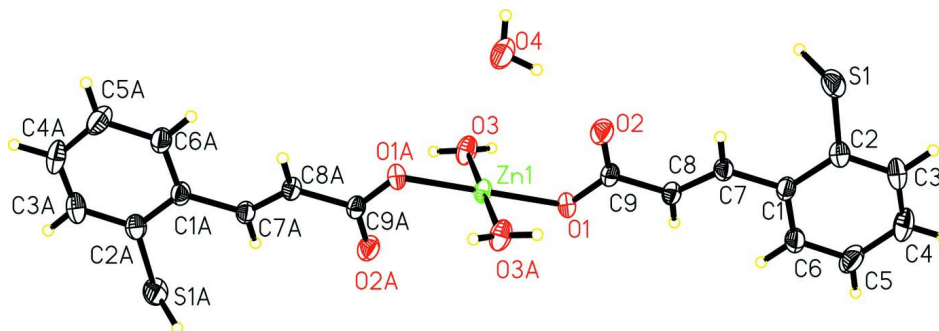


Figure 1

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

$Z = 2$

$F(000) = 512$
 $D_x = 1.597 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 25 reflections
 $\theta = 9\text{--}12^\circ$

$\mu = 1.44 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Block, colourless
 $0.30 \times 0.20 \times 0.14 \text{ mm}$

Data collection

Enraf–Nonius CAD-4
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 $\omega/2\theta$ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.673$, $T_{\max} = 0.824$
 6272 measured reflections

1811 independent reflections
 1441 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.092$
 $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.2^\circ$
 $h = -21 \rightarrow 18$
 $k = -9 \rightarrow 8$
 $l = -8 \rightarrow 8$
 200 standard reflections every 3 reflections
 intensity decay: 1%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.185$
 $S = 1.06$
 1811 reflections
 146 parameters
 6 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
 $w = 1/[\sigma^2(F_o^2) + (0.1071P)^2 + 0.9875P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.93 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.88 \text{ e \AA}^{-3}$

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (Å²)

	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 (Å, °)

C1—C6	1.390 (10)	C8—C9	1.473 (7)
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 code: (i) $-x+2, -y+1, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
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) $x, -y+1/2, z-1/2$.