

catena-Poly[[diaquazinc(II)]- μ -4,4'-sulfonyldibenzoato- κ^2 O:O']

Peng-Bin Pan,^{a,b} Lei Zhang,^a Zhao-Ji Li,^a Xin-Yi Cao^a and Yuan-Gen Yao^{a*}

^aState Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China, and ^bGraduate School, Chinese Academy of Sciences, Beijing 100039, People's Republic of China
Correspondence e-mail: yyg@fjirsm.ac.cn

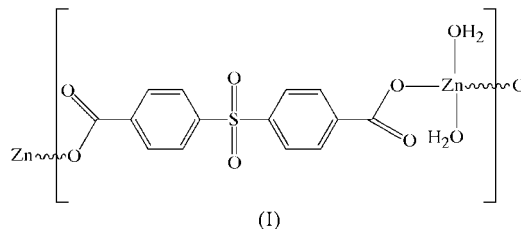
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The title compound, $[Zn(C_{14}H_8O_6S)(H_2O)_2]_n$, is the first reported metal complex of the 4,4'-sulfonyldibenzoate anion. The structure comprises zigzag chains of alternating $[Zn(H_2O)_2]^{2+}$ and sulfonyldibenzoate units, the central Zn and S atoms of which lie on crystallographic twofold axes. The Zn^{II} centre occupies a strongly distorted tetrahedral environment $[O-Zn-O = 83.30(7)-136.19(8)^\circ]$, coordinated by the two water O atoms $[Zn-O = 1.986(2) \text{ \AA}]$ and one O atom from each of two carboxylate groups $[Zn-O = 1.9942(19) \text{ \AA}]$, with much longer contacts to the other O atoms of these carboxylates $[Zn-O = 2.528(2) \text{ \AA}]$. Hydrogen bonds between carboxylate O atoms and coordinated water molecules in adjacent chains lead to the formation of a three-dimensional network structure.

Comment

In recent years, much attention has been focused on the design and synthesis of supramolecular complexes because of their novel structural architectures and potential applications in catalysis, magnetism, ion exchange and nonlinear optics (Atwood *et al.*, 1996; Barton *et al.*, 1999; Lo *et al.*, 2000). The basic strategy for the synthesis of such compounds involves connecting metal-containing building blocks with various multidentate ligands. As an important family of these multidentate ligands, organic aromatic polycarboxylate ligands such as benzene-1,2-dicarboxylate, benzene-1,3,5-tricarboxylate, 4,4'-carbonylbis(benzene-1,2-dicarboxylate) and benzene-1,2,4,5-tetracarboxylate have been extensively employed in the preparation of such metal-organic complexes. These products exhibit both high dimensionality in their structures and interesting properties (Chui *et al.*, 1999; Li *et al.*, 1999; Zhang *et al.*, 2004). Similarly, the 4,4'-sulfonyldibenzoate anion (hereinafter DSDC) can act as a versatile ligand for the construction of novel metal-organic hybrid compounds, due to the presence of two carboxylate functions and its structural flexibility. However, to the best of our knowledge, no metal

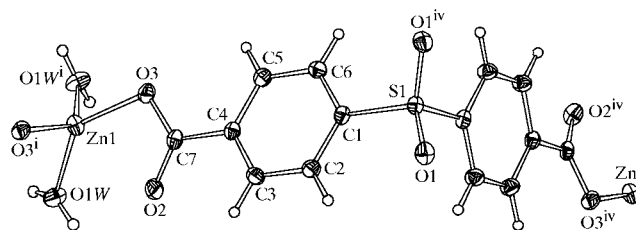
complexes with DSDC have been reported to date. Therefore, with the aim of exploring the coordination chemistry of DSDC, the title complex, (I), was obtained from the hydrothermal reaction of dimethyl 4,4'-sulfonyldibenzoate with zinc acetate and sodium hydroxide.

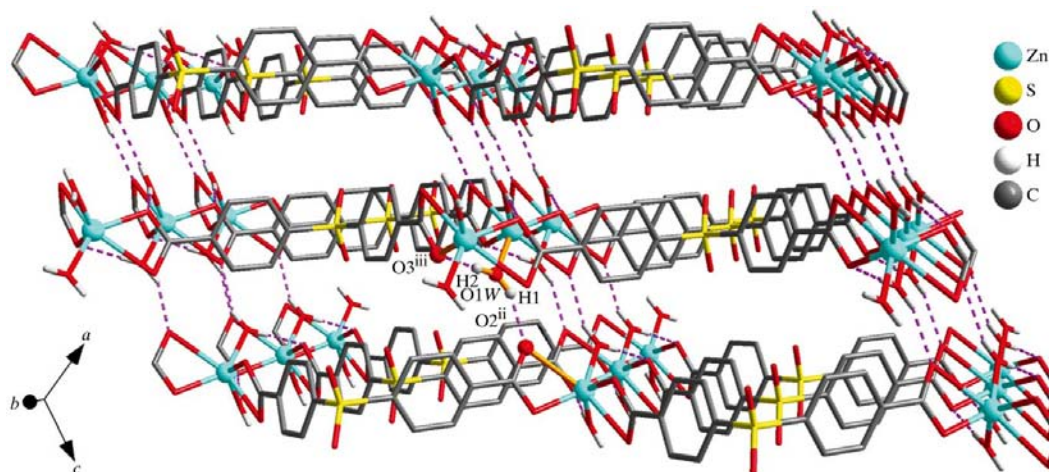


As shown in Fig. 1, the Zn centres in (I) are four-coordinate in a highly distorted tetrahedral environment involving two O-atom donors of two DSDC ligands and two coordinated water molecules. The Zn^{II} centre occupies a strongly distorted tetrahedral environment $[O-Zn-O = 83.30(7)-136.19(8)^\circ]$, coordinated by the two water O atoms $[Zn-O = 1.986(2) \text{ \AA}]$ and one O atom from each of two carboxylate groups $[Zn-O = 1.9942(19) \text{ \AA}]$, with much longer contacts to the other O atoms of these carboxylates $[Zn-O = 2.528(2) \text{ \AA}]$. The bonded distances are in agreement with values reported in other zinc-carboxylate complexes (Monge *et al.*, 2005; Wang *et al.*, 2006; He *et al.*, 2006). The DSDC group acts as a bidentate ligand in this structure, with both carboxylate groups coordinating in an essentially monodentate manner to the Zn^{II} centres.

The structure of (I) comprises zigzag chains of alternating $[Zn(H_2O)_2]^{2+}$ and sulfonyldibenzoate units, with their respective Zn and S atoms lying on crystallographic twofold axes. The zigzag nature of the chains, which run along the $[101]$ direction (Fig. 2), can be traced to the $O3-Zn1-O3$ and $C1-S1-S1$ angles of $99.67(12)$ and $104.04(17)^\circ$, respectively. The two benzene ring planes in the each DSDC ligand are almost perpendicular, with a dihedral angle of $80.99(7)^\circ$, imparting a slight twist to the chains. The carboxylate group is not coplanar with the aromatic ring to which it is attached but is twisted from the mean plane through the aromatic ring by $17.61(6)^\circ$.

As illustrated in Fig. 2, a major structural feature of (I) is the connection of adjacent zigzag chains *via* $O-H \cdots O$ hydrogen bonds. The water H atoms participate in hydrogen



**Figure 2**

A view of (I), showing the three-dimensional framework constructed via O—H \cdots O hydrogen bonds. Hydrogen bonds are depicted as dashed lines. [Symmetry codes: (ii) $-x + 1, -y, -z + 1$; (iii) $-x + 1, y - 1, -z + \frac{1}{2}$.]

bonds with different carboxylate O atoms as acceptors, *viz.* O1W—H1 \cdots O2 and O1W—H2 \cdots O3, to form a three-dimensional framework.

Experimental

Zn(CH₃CO₂)₂·2H₂O (0.111 g, 0.5 mmol), dimethyl 4,4'-sulfonyldibenzoate (0.168 g, 0.5 mmol) and NaOH (0.039 g, 1 mmol) in a 1:1:2 molar ratio, with water (15 ml), were placed in a 25 ml Teflon-lined stainless steel reactor and heated to 453 K for 76 h. When the reactor was cooled to room temperature over a period of 3 d, colourless prismatic single crystals of (I) suitable for X-ray diffraction were obtained.

Crystal data

[Zn(C ₁₄ H ₈ O ₆ S)(H ₂ O) ₂]	$V = 727.95 (17) \text{ \AA}^3$
$M_r = 405.70$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 13.307 (2) \text{ \AA}$	$\mu = 1.87 \text{ mm}^{-1}$
$b = 5.0336 (5) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 12.1142 (18) \text{ \AA}$	$0.30 \times 0.10 \times 0.03 \text{ mm}$
$\beta = 116.218 (5)^\circ$	

Data collection

Siemens P4 diffractometer	5356 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1668 independent reflections
$T_{\min} = 0.799, T_{\max} = 0.945$	1454 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	110 parameters
$wR(F^2) = 0.090$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
1668 reflections	$\Delta\rho_{\text{min}} = -0.43 \text{ e \AA}^{-3}$

All H atoms, except water atoms H1 and H2, were positioned geometrically and refined using a riding model [C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. Atoms H1 and H2 were located from a difference map and refined isotropically, with the O—H distances fixed at 0.82 Å, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1994); data reduction: SAINT and SHELXTL (Siemens, 1995); program(s) used to solve structure: SHELXTL; program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

Table 1

Selected geometric parameters (Å, °).

Zn1—O1W	1.986 (2)	Zn1—O3	1.9942 (19)
Zn1—O2	2.528 (2)		
O1W ⁱ —Zn1—O1W	91.73 (12)	O1W—Zn1—O2	83.30 (7)
O1W ⁱ —Zn1—O3	100.18 (9)	O2—Zn1—O3	56.45 (7)
O1W—Zn1—O3	136.19 (8)	O2—Zn1—O3 ⁱ	94.65 (7)
O3—Zn1—O3 ⁱ	99.67 (12)	O2—Zn1—O2 ⁱ	137.11 (9)
O1W ⁱ —Zn1—O2	128.74 (8)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1 \cdots O2 ⁱⁱ	0.82	1.97	2.709 (3)	149
O1W—H2 \cdots O3 ⁱⁱⁱ	0.90	1.89	2.790 (3)	178

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BM3026). Services for accessing these data are described at the back of the journal.

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