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catena-Poly[[tetraaquazinc(II)]-μ-5-sulfo-salicylato-κ^2O:O']

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Key indicators

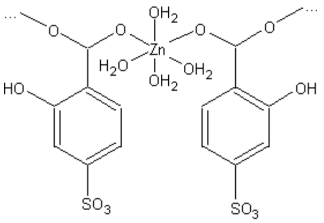
Single-crystal X-ray study
T = 213 K
Mean σ(C–C) = 0.005 Å
R factor = 0.030
wR factor = 0.086
Data-to-parameter ratio = 12.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title coordination polymer, $[Zn(C_7H_4O_6S)(H_2O)_4]_n$, comprises octahedral Zn atoms bonded to two carboxylate O atoms of the acid ligands and four water molecules. The zinc(II) ions are bridged by carboxylate moieties, creating a one-dimensional chain structure. The Zn—O bond distances lie in the range 2.074 (3)–2.118 (3) Å. The water molecules are involved in hydrogen bonds.

Comment

Coordination polymers have attracted considerable attention, due not only to their fascinating structural diversity but also to their potential applications. 5-Sulfosalicylic acid, which is known as a flexible multidentate ligand with versatile binding ability, is widely used as a chelating ligand for the analysis of different metal ions in solution. The structures of several divalent metal complexes with carboxylic acid ligands have been reported (*e.g.* van Albada *et al.*, 2004; Gao *et al.*, 2004; Yang *et al.*, 2003).



(I)

In the title compound, (I) (Fig. 1), the Zn atom adopts an octahedral geometry, formed by two O atoms of the bridging carboxylate ligand [Zn—O = 2.118 (3) and 2.076 (3) Å] and four O atoms of coordinated water molecules [Zn—O = 2.061 (3)–2.140 (3) Å] (Table 1). As a result of the bridging effect of the carboxylate groups, one-dimensional polymeric chains are formed, which may be considered as the main structural feature of (I). The crystal packing of (I) is stabilized by intricate intermolecular hydrogen bonding between the water molecules and the O atoms of the SO_3 moieties, with O$\cdots$O distances in the range 2.714 (3)–3.078 (3) Å (Table 2 and Fig. 2).

Experimental

The title compound, (I), was prepared by a procedure analogous to that of Gao *et al.* (2004) by reaction of equimolar amounts (10 mmol) of zinc acetate dihydrate with 5-sulfosalicylic acid in acetone to yield a colourless precipitate. The resulting solid was collected and dried *in vacuo*. Suitable crystals were obtained by evaporation of a water solution. Analysis calculated for $C_7H_{12}O_{10}SZn$: C 23.80, H 3.39, Zn 18.41%; found: C 24.01, H 3.56, Zn 18.28%.

Crystal data

$[Zn(C_7H_4O_6S)(H_2O)_4]$
$M_r = 353.60$
Monoclinic, *Cc*
$a = 10.454$ (6) Å
$b = 16.192$ (6) Å
$c = 7.0777$ (14) Å
$\beta = 94.47$ (5)°
$V = 1194.4$ (9) Å^3
$Z = 4$

$D_x = 1.966$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2444 reflections
$\theta = 2$–28°
$\mu = 2.28$ mm^{-1}
$T = 213$ (2) K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.445$, $T_{max} = 0.634$
3595 measured reflections

2444 independent reflections
2424 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 28.3°$
$h = -13 \rightarrow 13$
$k = -21 \rightarrow 18$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.086$
$S = 1.09$
2444 reflections
201 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.064P)^2 + 1.0831P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.039$
$\Delta\rho_{max} = 0.90$ e Å^{-3}
$\Delta\rho_{min} = -0.72$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0101 (9)
Absolute structure: Flack (1983), 982 Friedel pairs
Flack parameter = 0.068 (11)

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.061 (3)	Zn1—O6	2.076 (3)
Zn1—O2	2.140 (3)	S1—O8	1.461 (2)
Zn1—O3	2.074 (3)	S1—O9	1.460 (3)
Zn1—O4	2.098 (3)	S1—O10	1.461 (2)
Zn1—O5^{i}	2.118 (3)	Zn1—O5^{ii}	2.118 (3)
O1—Zn1—O3	91.22 (11)	O6—Zn1—O5^{ii}	96.61 (9)
O1—Zn1—O6	84.06 (11)	O4—Zn1—O5^{ii}	88.51 (10)
O3—Zn1—O6	175.22 (10)	O1—Zn1—O2	95.74 (11)
O1—Zn1—O4	178.75 (12)	O3—Zn1—O2	93.61 (10)
O3—Zn1—O4	90.03 (10)	O6—Zn1—O2	86.19 (10)
O6—Zn1—O4	94.69 (10)	O4—Zn1—O2	84.21 (10)
O1—Zn1—O5^{ii}	91.59 (11)	O5^{ii}—Zn1—O2	172.39 (9)
O3—Zn1—O5^{ii}	84.19 (10)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7···O6	0.83	1.88	2.600 (4)	145
O4—H4*B*···O5	0.84 (3)	2.09 (4)	2.820 (4)	145 (3)

The O2–O4 water H atoms were initially located in a difference Fourier map, but were included in the refinement with O—H distances restrained to 0.85 (2) Å and H···H distances restrained to 1.37 (2) Å. The H atoms of O1 were located in a difference Fourier map and freely refined. The H atom on O7 was placed in its geometrically idealized position. All aromatic H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.94 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

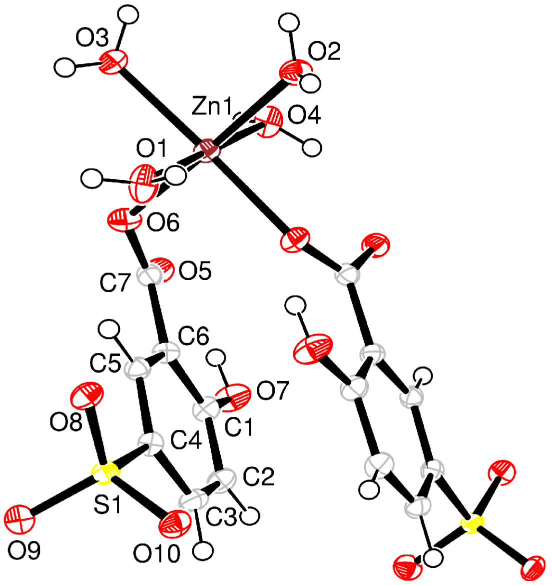


Figure 1
View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

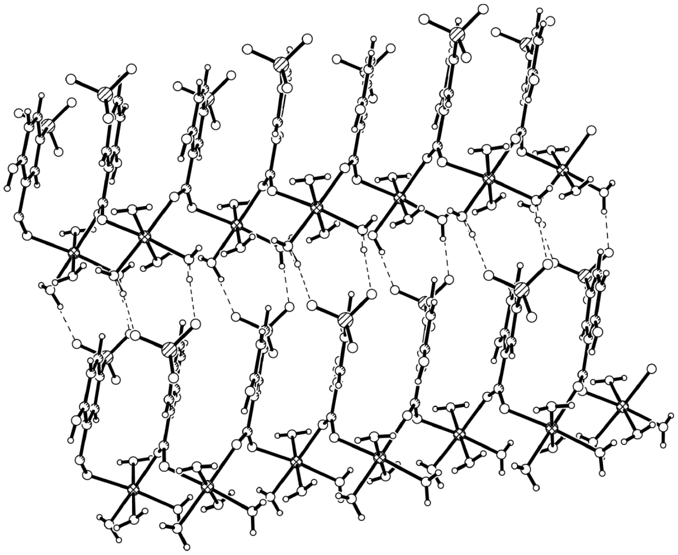


Figure 2
The molecular packing of (I), viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2001).

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