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Hexaaquazinc(II) 3-carboxy-4-hydroxybenzenesulfonate tetrahydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.088
Data-to-parameter ratio = 12.5

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

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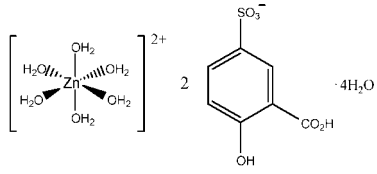
In the title compound, $[Zn(H_2O)_6]L_2\cdot 4H_2O$, where H$L$ = 3-carboxy-4-hydroxybenzenesulfonic acid ($C_7H_6O_6S$), each Zn^{II} cation lies on an inversion center and is octahedrally coordinated by six water molecules. The L^- anions do not coordinate to zinc, but act as counter-anions. The crystal structure is composed of alternating layers of $[Zn(H_2O)_6]^{2+}$ cations and sulfonate anions. The $[Zn(H_2O)_6]^{2+}$ cations, water molecules and L^- anions are connected through a complex pattern of hydrogen-bonding interactions.

Comment

The crystal structures of five transition metal (Mn, Co, Ni, Cu and Zn) 3-carboxy-4-hydroxybenzenesulfonates have been determined. The structures of the manganese (Ma *et al.*, 2003*a*), cobalt (Ma *et al.*, 2003*b*), nickel (Ma *et al.*, 2003*c*) and copper compound (Ma *et al.*, 2003*d*) have been reported in the preceding papers. The crystal structure of the zinc compound, (I), is presented here.



(I)

The Zn^{II} atom is located on an inversion center, and all other atoms are in general positions. Selected bond lengths and angles are given in Table 1. Fig. 1 shows the asymmetric unit, together with the complete coordination environment of the Zn^{II} cation. Compound (I) is isostructural with the cobalt compound (Ma *et al.*, 2003*b*) and nickel compound (Ma *et al.*, 2003*c*). The Zn—O distances range from 2.059 (2) to 2.099 (2) Å. The average Zn—O distance of 2.082 Å is slightly shorter than the values in other zinc compounds (Li *et al.*, 2002).

The alternating layers of $[Zn(H_2O)_6]^{2+}$ cations and sulfonate anions in (I) are shown in Fig. 2. Selected hydrogen-bond parameters are listed in Table 2.

Experimental

A mixture of 3-carboxy-4-hydroxybenzenesulfonic acid (0.44 g, 2 mmol) and ZnO (0.081 g, 1 mmol) in water (10 ml) was stirred at room temperature for 30 min. Colorless crystals of compound (I) were obtained after leaving the solution to stand at room temperature for several days. Analysis calculated for $C_{14}H_{30}CoO_{22}S_2$: C 24.73, H 4.45%; found: C 24.59, H 4.39%.

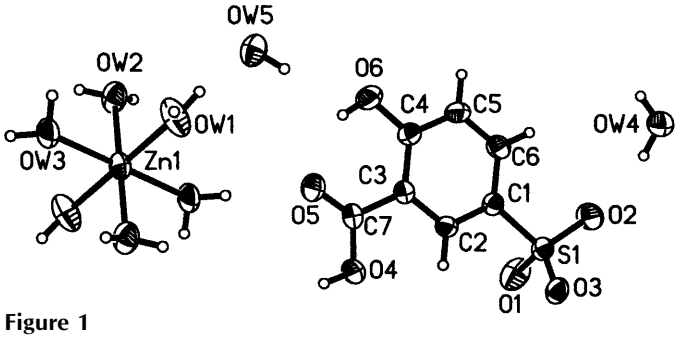


Figure 1
View of the asymmetric unit, expanded to show the complete coordination, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

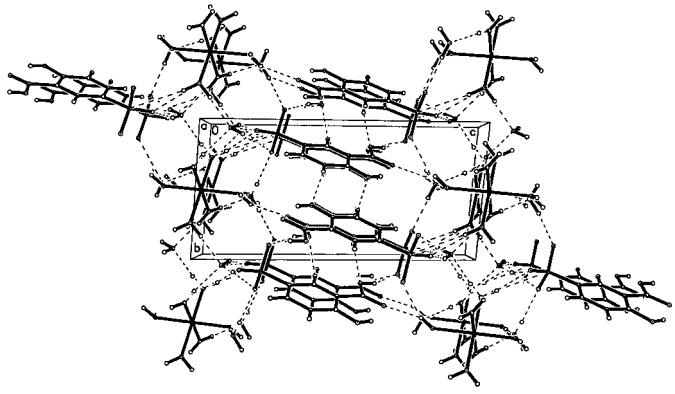


Figure 2
View of the alternating layers of cations and anions, along the *a* axis.

Crystal data

$[Zn(H_2O)_6](C_7H_5O_6S)_2\cdot4H_2O$
$M_r = 679.87$
Triclinic, $P\overline{1}$
$a = 6.5367\ (14)$ Å
$b = 7.2555\ (18)$ Å
$c = 14.616\ (4)$ Å
$\alpha = 92.83\ (2)^\circ$
$\beta = 96.321\ (19)^\circ$
$\gamma = 102.839\ (17)^\circ$
$V = 669.8\ (3)$ Å^3
$Z = 1$
$D_x = 1.685$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 22 reflections
$\theta = 4.8$–8.7°
$\mu = 1.17$ mm^{-1}
$T = 293\ (2)$ K
Block, colorless
0.52 × 0.36 × 0.32 mm

Data collection

Siemens *P*4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.517$, $T_{max} = 0.688$
3445 measured reflections
2615 independent reflections
2101 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 26.0^\circ$
$h = -1 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -17 \rightarrow 17$
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.088$
$S = 1.03$
2615 reflections
209 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.083 (4)

Table 1
Selected geometric parameters (Å, °).

C4—O6	1.349 (3)	O3—S1	1.4582 (18)
C7—O5	1.227 (3)	*OW*1—Zn1	2.059 (2)
C7—O4	1.311 (3)	*OW*2—Zn1	2.088 (2)
O1—S1	1.463 (2)	*OW*3—Zn1	2.099 (2)
O2—S1	1.440 (2)		
O5—C7—O4	123.6 (2)	*OW*1—Zn1—*OW*2	89.56 (10)
O2—S1—O3	112.10 (12)	*OW*1—Zn1—*OW*3	88.60 (9)
O2—S1—O1	113.37 (14)	*OW*2—Zn1—*OW*3	89.95 (9)
O3—S1—O1	109.74 (13)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
*OW*1—H1*A*···*OW*4^{i}	0.891 (18)	1.964 (19)	2.827 (3)	162 (3)
*OW*1—H1*B*···*OW*5	0.868 (18)	1.950 (19)	2.797 (3)	165 (3)
*OW*2—H2*A*···*OW*4^{ii}	0.889 (18)	1.891 (18)	2.775 (3)	173 (3)
*OW*2—H2*B*···O2^{iii}	0.870 (18)	2.035 (19)	2.889 (3)	167 (3)
*OW*3—H3*A*···*OW*5^{iv}	0.887 (18)	1.868 (19)	2.754 (3)	178 (3)
*OW*3—H3*B*···O5^{v}	0.878 (18)	2.111 (19)	2.938 (3)	157 (3)
*OW*4—H4*A*···O2	0.901 (18)	1.971 (19)	2.845 (3)	163 (3)
*OW*4—H4*B*···O1^{vi}	0.890 (18)	1.981 (19)	2.866 (3)	173 (3)
*OW*5—H5*A*···O3^{vii}	0.859 (18)	1.934 (19)	2.738 (3)	155 (3)
*OW*5—H5*B*···O1^{iii}	0.846 (18)	1.964 (19)	2.796 (3)	167 (3)
O4—H4···O3^{viii}	0.82	1.88	2.653 (3)	156
O6—H6···O5	0.82	1.92	2.637 (3)	146

Symmetry codes: (i) $x, y, 1+z$; (ii) $x, 1+y, 1+z$; (iii) $1-x, 1-y, 1-z$; (iv) $2-x, 1-y, 2-z$; (v) $1-x, 1-y, 2-z$; (vi) $1+x, y, z$; (vii) $1-x, -y, 1-z$; (viii) $-x, -y, 1-z$.

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the carboxyl group and hydroxyl group were also positioned geometrically and refined as riding atoms, with O—H = 0.82 Å and $U_{iso}(H) = 1.5U_{eq}(O)$. The water H atoms were located in a difference Fourier map and refined with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL*97.

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