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catena-Poly[[[tetraaqua(3-carboxy-4-hydroxybenzenesulfonato)strontium(II)]-μ_3-3-carboxy-4-hydroxybenzenesulfonato] dihydrate]

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The title complex, $\{[Sr(C_7H_5O_6S)_2(H_2O)_4]\cdot 2H_2O\}_n$, exists as a ladder chain of Sr^{II} ions connected by 3-carboxy-4-hydroxybenzenesulfonate anions through μ_2-sulfonate and carboxyl groups, and solvent water molecules, forming a three-dimensional hydrogen-bonded framework. The Sr^{II} ion exhibits a distorted square antiprismatic coordination geometry defined by three O atoms of two sulfonate groups, one carboxyl O and four water molecules. The 3-carboxy-4-hydroxybenzenesulfonate anions show two types of coordination to strontium, *viz.* μ_2-sulfonate + monodentate-carboxyl bridging and monodentate sulfonate–O coordination.

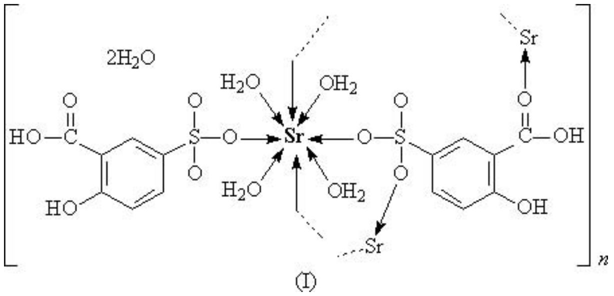
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.062
Data-to-parameter ratio = 13.6

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

Comment

In recent years, the assembly of multifunctional ligands with metal ions has received growing attention due to their use in constructing higher dimensional polymers with interesting structures and properties [for a recent review, see Çoté & Shimizu (2003)]. 3-Carboxy-4-hydroxybenzenesulfonic acid (H_2L) is such a ligand and has three different potential coordinating groups and therefore varied coordination modes. The structure of the hydrate of the ligand has been reported (Attig, 1975). Some crystal structures of metal coordination complexes with this ligand are also documented (Aliev *et al.*, 1994; Sharutin *et al.*, 1997; Sun *et al.*, 1995), in particular, two recent Ag^I complexes, *viz.* $[Ag_2L(H_2O)]_n$ and $\{[Ag_2(HL)_2(H_2O)_3]\cdot H_2O\}_n$ (Ma *et al.*, 2005), which exhibit three- and two-dimensional extended structures, respectively. In such complexes, the ligand adopts various coordination modes. We report here a one-dimensional chain Sr^{II} complex, (I), which was obtained by the reaction of $Sr(CO_3)_2$ and H_2L in water.



(I)

The structure of (I) consists of $[Sr(HL)_2(H_2O)_4]$ neutral ladder chains and solvent water molecules. The coordination environment around the Sr^{II} ion and the linkage modes of ligands together with the atom-numbering scheme of (I) are shown in Fig. 1 and selected geometrical parameters are listed in Table 1. The eight-coordinate Sr^{II} ion is bound by three O atoms of two sulfonate groups, one carboxyl O atom and four

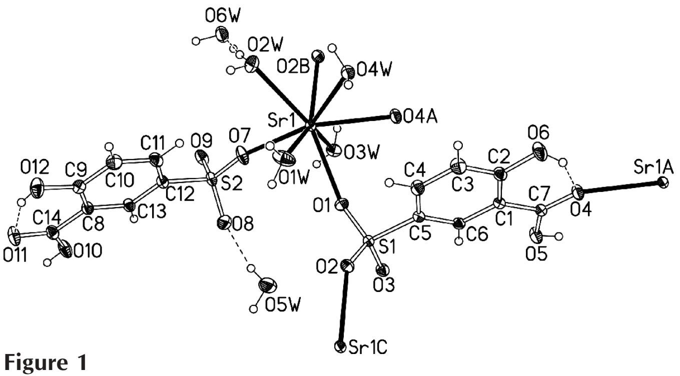


Figure 1
The local coordination environments of the sulfonate ligand and the Sr^{II} center in (I). The dashed lines denote hydrogen bonds and displacement ellipsoids are shown at the 50% probability level. The atom-numbering scheme of the asymmetric unit is shown, together with symmetry-equivalent atoms [symmetry codes: (*A*) $1 - x, 1 - y, 1 - z$; (*B*) $x, y - 1, z$; (*C*) $x, y + 1, z$].

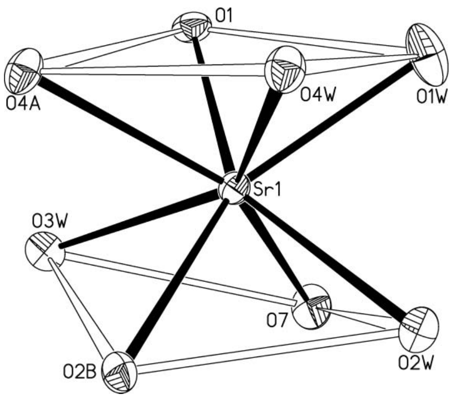


Figure 2
The geometry around the Sr^{II} ion in (I).

water molecules to give a distorted square antiprism (Fig. 2). In contrast to other reported metal complexes mentioned above, in (I) the 3-carboxy-4-hydroxybenzenesulfonate ligands show two types of coordination modes, *viz.* μ_2-sulfonate + monodentate-carboxyl bridging and monodentate sulfonate-O coordination. For the former, a sulfonate group adopting a μ_2-bridging coordination mode uses its two O atoms to link two adjacent Sr^{II} ions to form an Sr—OSO— single chain, in which the Sr1···Sr1*B* [symmetry code: (*B*) $x, 1 + y, z$] separation is 7.078 (1) Å (Fig. 3). Two such single chains are linked by the ligand skeleton through carboxyl atom O4 coordinated to Sr^{II} ions to give a ladder-like double chain structure containing dinuclear grid units. In the dinuclear unit, the Sr1···Sr1*A* [symmetry code: (*A*) $1 - x, 1 - y, 1 - z$] distance is 10.660 (3) Å. The other sulfonate O-monodentate ligands are located on the periphery of the double chain to complete the coordination of the Sr^{II} ions. In the one-dimensional chain, the phenyl ring planes (such as C1–C6, C8–C13 and C1*A*–C6*A*) are almost parallel with each other, the dihedral angle between the ring planes C1–C6 and C8–C13 being 15.4 (1)°. In addition, both intra- and intermolecular hydrogen bonds (Fig. 1 and Table 2) are observed. The latter assemble one-dimensional chains with solvent water molecules to form a three-dimensional framework.

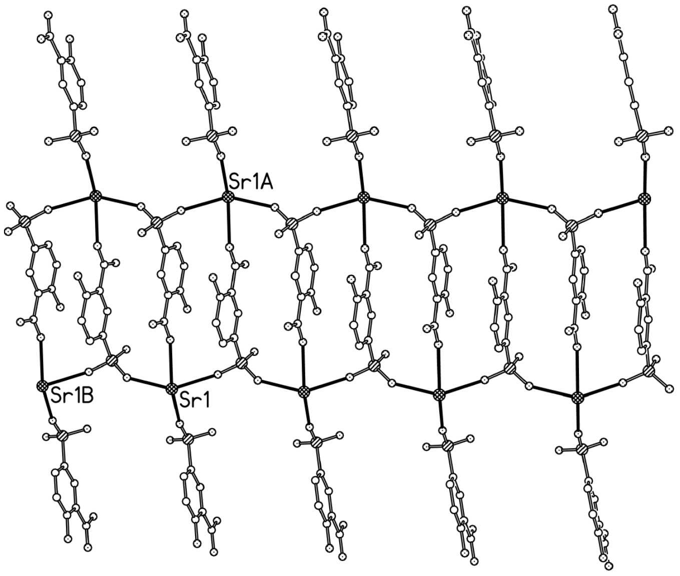


Figure 3
A perspective view of the one-dimensional chain structure of (I). H atoms and water molecules have been omitted.

Experimental

The title complex, (I), was synthesized by the addition of $Sr(CO_3)_2$ (410 mg, 2 mmol) to an aqueous solution (50 ml) of 3-carboxy-4-hydroxybenzenesulfonic acid (660 mg, 3 mmol). The resulting solution was stirred for 2 h at room temperature and then filtered. The filtrate was allowed to evaporate slowly. After about 10 d, colorless crystals of (I) were isolated (yield: 21%, based on Sr). Analysis calculated (%) for $C_{14}H_{22}O_{18}S_2Sr$: C 26.69, H 3.52; found: C 26.10, H 3.82.

Crystal data

$[Sr(C_7H_5O_6S)_2(H_2O)_4]\cdot 2H_2O$
$M_r = 630.06$
Triclinic, $P\overline{1}$
$a = 6.893$ (1) Å
$b = 7.078$ (1) Å
$c = 24.754$ (5) Å
$\alpha = 96.41$ (3)°
$\beta = 90.83$ (3)°
$\gamma = 108.49$ (3)°
$V = 1136.5$ (4) Å^3
$Z = 2$
$D_x = 1.841$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6098 reflections
$\theta = 3.1$–27.4°
$\mu = 2.64$ mm^{-1}
$T = 293$ (2) K
Block, colorless
0.26 × 0.26 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.509$, $T_{max} = 0.530$
11 145 measured reflections
5160 independent reflections
4497 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 8$
$l = -32 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.062$
$S = 1.03$
5160 reflections
380 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0319P)^2 + 0.4193P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sr1—O1	2.566 (2)	Sr1—O4*W*	2.728 (2)
Sr1—O2$^{\rm i}$	2.546 (2)	Sr1—O3*W*	2.732 (2)
Sr1—O1*W*	2.534 (2)	Sr1—O4$^{\rm ii}$	2.620 (2)
Sr1—O2*W*	2.660 (2)	Sr1—O7	2.533 (2)
O1—Sr1—O2*W*	148.03 (6)	O2$^{\rm i}$—Sr1—O4*W*	83.02 (6)
O1—Sr1—O3*W*	72.46 (6)	O2*W*—Sr1—O3*W*	132.48 (6)
O1—Sr1—O4$^{\rm ii}$	75.35 (6)	O2*W*—Sr1—O4*W*	68.85 (6)
O1—Sr1—O4*W*	108.70 (6)	O4$^{\rm ii}$—Sr1—O2*W*	127.40 (6)
O1*W*—Sr1—O1	72.64 (6)	O4$^{\rm ii}$—Sr1—O3*W*	70.43 (6)
O1*W*—Sr1—O2$^{\rm i}$	143.54 (6)	O4$^{\rm ii}$—Sr1—O4*W*	68.07 (5)
O1*W*—Sr1—O2*W*	76.67 (7)	O4*W*—Sr1—O3*W*	136.37 (5)
O1*W*—Sr1—O3*W*	141.31 (6)	O7—Sr1—O1	89.84 (6)
O1*W*—Sr1—O4$^{\rm ii}$	115.51 (7)	O7—Sr1—O1*W*	88.72 (7)
O1*W*—Sr1—O4*W*	71.63 (6)	O7—Sr1—O2$^{\rm i}$	99.44 (6)
O2$^{\rm i}$—Sr1—O1	142.11 (5)	O7—Sr1—O2*W*	80.67 (6)
O2$^{\rm i}$—Sr1—O2*W*	69.84 (6)	O7—Sr1—O3*W*	75.03 (6)
O2$^{\rm i}$—Sr1—O3*W*	74.67 (6)	O7—Sr1—O4$^{\rm ii}$	145.10 (5)
O2$^{\rm i}$—Sr1—O4$^{\rm ii}$	76.32 (6)	O7—Sr1—O4*W*	146.59 (6)

Symmetry codes: (i) $x, y-1, z$; (ii) $1-x, 1-y, 1-z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H15*A*···O5*W*$^{\rm iii}$	0.85 (1)	2.02 (1)	2.839 (3)	163 (3)
O1*W*—H15*B*···O6W$^{\rm iv}$	0.85 (1)	1.89 (1)	2.740 (3)	176 (3)
O2*W*—H16*A*···O6W	0.85 (1)	1.86 (1)	2.703 (3)	173 (3)
O2*W*—H16*B*···O8$^{\rm iv}$	0.84 (1)	2.08 (1)	2.894 (3)	162 (3)
O3*W*—H17*B*···O2*W*$^{\rm v}$	0.84 (1)	2.14 (2)	2.926 (3)	155 (3)
O3*W*—H17*A*···O3$^{\rm i}$	0.85 (1)	2.04 (2)	2.852 (2)	159 (4)
O4*W*—H18*B*···O3$^{\rm iii}$	0.84 (1)	1.96 (1)	2.797 (2)	176 (3)
O4*W*—H18*A*···O3*W*$^{\rm iii}$	0.84 (1)	2.11 (1)	2.951 (2)	176 (3)
O5—H22···O4*W*$^{\rm ii}$	0.81 (3)	1.87 (3)	2.667 (2)	169 (3)
O5*W*—H19*B*···O8	0.84 (1)	1.95 (1)	2.775 (3)	168 (3)
O5*W*—H19*A*···O9$^{\rm iv}$	0.84 (1)	1.98 (1)	2.815 (3)	174 (4)
O6—H21···O4	0.90 (4)	1.76 (4)	2.576 (2)	149 (3)
O6W—H20*A*···O5*W*$^{\rm i}$	0.85 (1)	2.01 (1)	2.838 (3)	166 (3)
O6W—H20*B*···O11$^{\rm vi}$	0.85 (1)	1.92 (1)	2.756 (2)	170 (3)
O10—H24···O9$^{\rm vii}$	0.82 (3)	1.94 (3)	2.739 (2)	163 (3)
O12—H23···O11	0.80 (3)	1.89 (4)	2.627 (3)	152 (3)

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

The H atoms of the water molecules, carboxyl and hydroxyl groups were located in Fourier difference maps. The water molecule O—H distances were restrained to 0.85 (1) Å. The aromatic H atoms were placed in calculated positions and treated as riding in the refinement [C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)]

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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