metal-organic papers

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Key indicators

Poly[diaqua-μ_3-hydrogenglutarato-μ_2-hydrogen-glutarato-strontium(II)]

The title compound, $[Sr(C_5H_7O_4)_2(H_2O)_2]_n$, crystallizes with an infinite polymeric network. The layered structure is built up from cross-linked infinite chains of one edge-sharing $SrO_7(H_2O)_2$ polyhedra. One of the two crystallographically distinct ligands acts by its deprotonated group in bis-bridging-chelating mode and the second involves its two ends in bidentate and monodentate modes, respectively. The inorganic layers are pillared by methylene spacers and form empty channels. Interlayer hydrogen bonds involve mainly the protonated ends of the ligands as donors.

Comment

Polymeric inorganic–organic compounds are controlled self-assembly frameworks which can be considered as advanced materials having the advantages of combining the properties of their inorganic and organic parts and consequently are good precursors for the synthesis of materials with various applications (Rao *et al.*, 2004; Rosi *et al.*, 2002; James, 2003). In order to develop an available rational design in mild synthesis conditions of such compounds based on alkaline-earth metals (Djeghri, 1999), we have obtained crystals of the title compound, $[Sr(C_5H_7O_4)_2(H_2O)_2]$, (I).

(I)

Complex (I) is a layered structure formed by cross-linked infinite chains of one-edge-sharing polyhedra running along
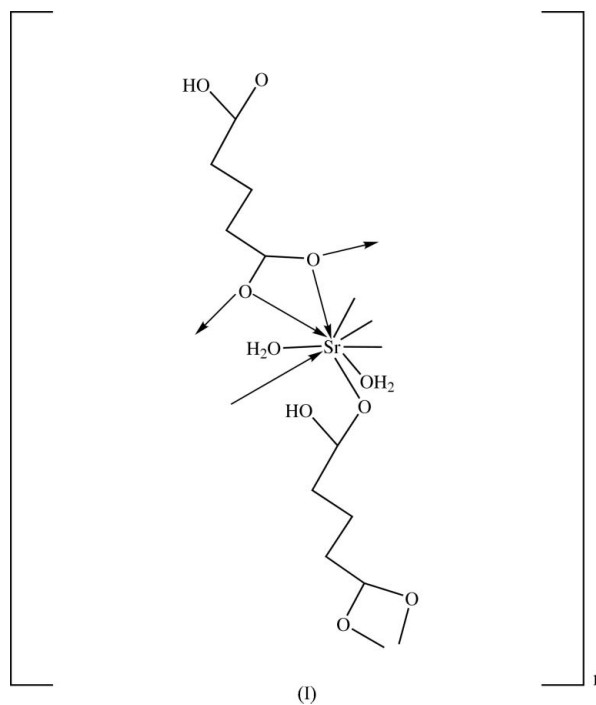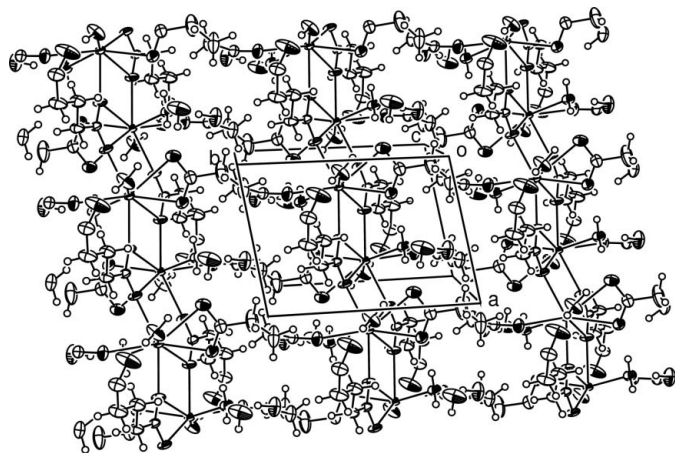
Figure 1
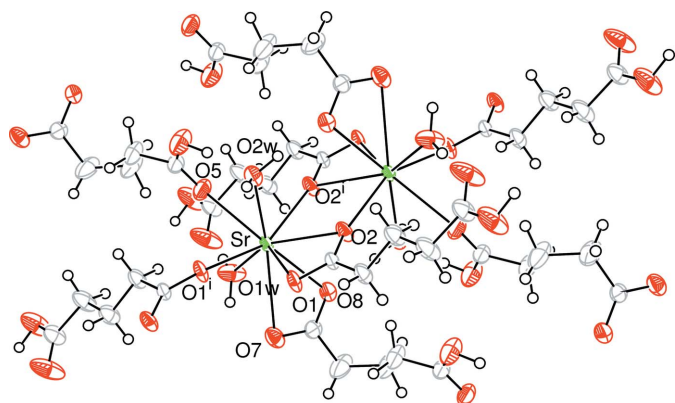Perspective view of the packing seen along the *c* axis

Figure 2
View of the linkage between two Sr atoms, including the labelling scheme, with 50% probability displacement ellipsoids. See Table 1 for symmetry code.

the *a* axis and exhibiting channels. The carbon backbones of the ligands form organic pillars completing these channels by surrounding them with their methylene groups (Fig. 1). In the inorganic layers each Sr^{II} ion is linked to two others *via* two triply coordinated O atoms (O2 and O1), with an Sr$\cdots$Sr distance of 4.2727 (1) Å, and *via* doubly coordinated O atoms (O7 and O8) with a distance of 5.0378 (1) Å. Sr^{II} is nine-coordinate and links to four O atoms from the bis-bridging-chelating ligand, and three from the ligand involving its two end functional groups in bidentate and monodentate mode, respectively (Fig. 2). The corresponding coordination polyhedron is distorted, and its geometry is intermediate between a monocapped dodecahedron and a tricapped trigonal prism.

The average Sr—O(carboxylate ligands) distance, consistent with usual distances for nine-coordinated Sr^{II} ions (Stein & Ruschewitz, 2005), is slightly longer than the average length of Sr—O(aqua ligands) (Table 1). Within the ligands, other geometric parameters (C—O, C—C distances and O—C—O, O—C—C angles) all lie in the expected ranges, as found for other hydrogenoglutarate or glutarate compounds (Benmerad

et al., 2000, 2004; Rahahlia *et al.*, 2006). The bis-bridging-chelating ligand is in an *anti-anti* conformation illustrated by the C2—C3—C4—C5 [174.8 (3)°] and C1—C2—C3—C4 [179.5 (2)°] torsion angles, while the ligand involving its two functional ends is in an intermediate conformation (Kim *et al.*, 2004), exhibiting C6—C7—C8—C9 [161.1 (3)°] and C10—C9—C8—C7 [48.6 (5)°] torsion angles far from the ideal values of the *syn--anti* conformation (60 and 180°).

The protonated ends are involved in hydrogen bonding as donors (Table 2). Additional hydrogen bonds are observed between aqua ligands (O1w and O2w) as donors, and the O atoms of the carboxylate (O3^v, O3^{ii}) and carboxylic ends (O7^{vi}, O8^{vii}) as acceptors (symmetry codes as in Table 2). The main structural features in the resulting hydrogen-bonding scheme are the great linearity of the bond angles, and the coexistence around water molecules of two-centred and three-centred hydrogen bonds. In this study, no assembly cage is constructed around the metal, and hence the typical *M*—O—*M* subfeature distinguishing alkaline earth and rare earth dicarboxylates is present.

Experimental

Crystal data

[Sr(C$_5$H$_7$O$_4$)$_2$(H$_2$O)$_2$]	V = 777.4 (3) Å^3
M_r = 385.86	Z = 2
Triclinic, $P\bar{1}$	D_x = 1.648 Mg m^{-3}
a = 7.019 (1) Å	Mo $K\alpha$ radiation
b = 10.225 (1) Å	μ = 3.51 mm^{-1}
c = 11.600 (1) Å	T = 298 (2) K
α = 104.25 (5)°	Prism, colourless
β = 101.92 (5)°	0.3 × 0.2 × 0.2 mm
γ = 96.60 (5)°	

Data collection

Nonius KappaCCD diffractometer	44196 measured reflections
ω scans	5660 independent reflections
Absorption correction: multi-scan	4752 reflections with $I > 2\sigma(I)$
(*DENZO–SMN*; Otwinowski &	R_{int} = 0.049
Minor, 1997)	θ_{max} = 32.6°
T_{min} = 0.332, T_{max} = 0.494	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0014P)^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$+ 1.0612P]$
$wR(F^2)$ = 0.070	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max}$ = 0.001
5660 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
208 parameters	$\Delta\rho_{min}$ = -0.48 e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

metal-organic papers

Table 1
Selected geometric parameters (Å, °).

Sr1—O1[i]	2.5137 (16)	Sr1—O7[iii]	2.920 (3)
Sr1—O1	2.6645 (18)	Sr1—O8[iii]	2.592 (2)
Sr1—O2[ii]	2.4827 (15)	Sr1—O1W	2.578 (2)
Sr1—O2	2.836 (2)	Sr1—O2W	2.692 (3)
Sr1—O5	2.7269 (17)		
Sr1[i]—O1—Sr1	111.17 (6)	Sr1[ii]—O2—Sr1	107.10 (7)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O3W—H5W$\cdots$O7[iv]	0.97 (3)	1.66 (3)	2.623 (3)	175
O4W—H6W$\cdots$O2W	0.95 (3)	1.68 (3)	2.619 (3)	174 (4)
O1W—H1W$\cdots$O3[v]	0.93 (3)	1.96 (3)	2.862 (3)	164
O1W—H2W$\cdots$O3[ii]	0.94 (3)	1.89 (3)	2.831 (3)	173
O2W—H3W$\cdots$O7[vi]	0.92 (3)	1.90 (3)	2.798 (2)	166
O2W—H4W$\cdots$O8[vii]	0.93 (3)	1.82 (2)	2.718 (3)	164

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

All H atoms belonging to the coordinated water molecules were located in a difference Fourier map and refined with restrained O—H distances of 0.97 Å, and with U_{iso}(H) = 1.5U_{eq}(O). Methylene H atoms were placed in geometrically idealized positions with fixed C—H distances (0.97 Å) and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *KappaCCD Software* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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