Poly[[tetraaquatris(monomethyl fumarato)-distrontium(II)] monomethyl fumarate] at 120 K

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The title compound, $\{[Sr_2(C_5H_5O_4)_3(H_2O)_4](C_5H_5O_4)\}_n$, crystallizes with three methyl fumarate ions and four water molecules coordinating the two independent strontium(II) ions. The coordination polyhedra are interconnected by edge-sharing to form chains, which are connected by hydrogen bonds into layers. The layers, in turn, are stacked with the fourth methyl fumarate anion intercalated.

Comment

Recent preclinical and clinical investigations have revealed that strontium(II) reduces bone resorption while at the same time it provides stimulation for new bone formation (Marie *et al.*, 2001). These investigations have led to a growing interest in strontium(II) salts, their crystal structures and synthetic methods that may provide products of high yield and purity (Christgau *et al.*, 2005; Stahl *et al.*, 2006). The present paper presents the structural investigation of such a new strontium(II) salt, (I).

(I)
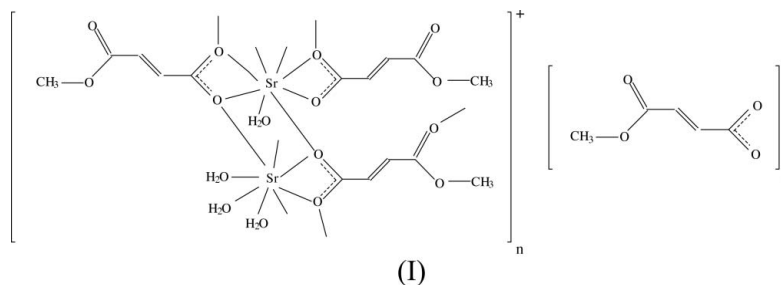
The two independent strontium(II) ions are both eight-coordinated by three methyl fumarate ions and four water molecules (Table 1 and Fig. 1). The coordination polyhedra are interconnected by edge-sharing to form chains in the *a*-axis direction (Fig. 2). Hydrogen bonds (Table 2) between water molecules and to the second, Sr-coordinated, methyl fumarate anion connect the chains into layers in the *ab* plane. Additional hydrogen bonds bind the uncoordinated methyl fumarate to these layers. The layers, in turn, are connected by electrostatic and van der Waals interactions between the layers including the fourth methyl fumarate anion. Three of the methyl fumarate ions are approximately planar, while in the fourth methyl fumarate ion the carboxylate group is twisted by approximately 60° (Table 3) to allow for its Sr coordination and packing.

Experimental

The title compound was synthesized by sprinkling powdered strontium carbonate into a saturated solution of methyl fumarate in a

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molar ratio of 1:2 at 313 K. More methyl fumarate was added after cessation of the initial effervescence, followed by addition of strontium carbonate in a molar ratio of 1:2. The procedure was continued in this stepwise manner until a permanent precipitate was observed. Cooling to 293 K and filtration gave the title compound in high yield and purity.

Crystal data

$[Sr_2(C_5H_5O_4)_3(H_2O)_4](C_5H_5O_4)$
$M_r = 763.66$
Triclinic, $P\bar{1}$
$a = 7.1336\ (6)$ Å
$b = 10.7203\ (8)$ Å
$c = 20.9384\ (17)$ Å
$\alpha = 100.676\ (2)°$
$\beta = 96.322\ (2)°$
$\gamma = 107.096\ (2)°$

$V = 1480.7\ (2)$ Å^3
$Z = 2$
$D_x = 1.713$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.69$ mm^{-1}
$T = 120\ (2)$ K
Needle, colorless
$0.23 \times 0.05 \times 0.03$ mm

Data collection

Bruker SMART APEX
   diffractometer
ω scans
Absorption correction: multi-scan
   (SADABS; Sheldrick, 2002)
   $T_{min} = 0.484$, $T_{max} = 0.897$

19750 measured reflections
8421 independent reflections
5753 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 30.8°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.095$
$S = 0.87$
8421 reflections
407 parameters

H atoms treated by a mixture of
   independent and constrained
   refinement
$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.48$ e Å^{-3}
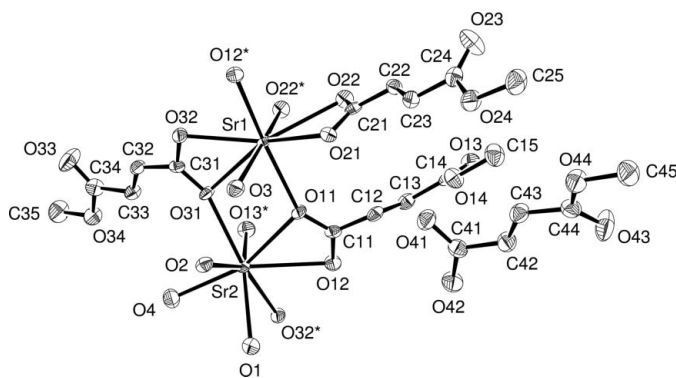$\Delta\rho_{min} = -0.71$ e Å^{-3}

Figure 1
The asymmetric unit of (I), showing 75% probability displacement ellipsoids and the atomic numbering. H atoms have been omitted for clarity. O12*, O22*, O13* and O32* are added to complete the Sr coordination, with symmetry codes (cf Table 1) i, ii, iv and iii, respectively.
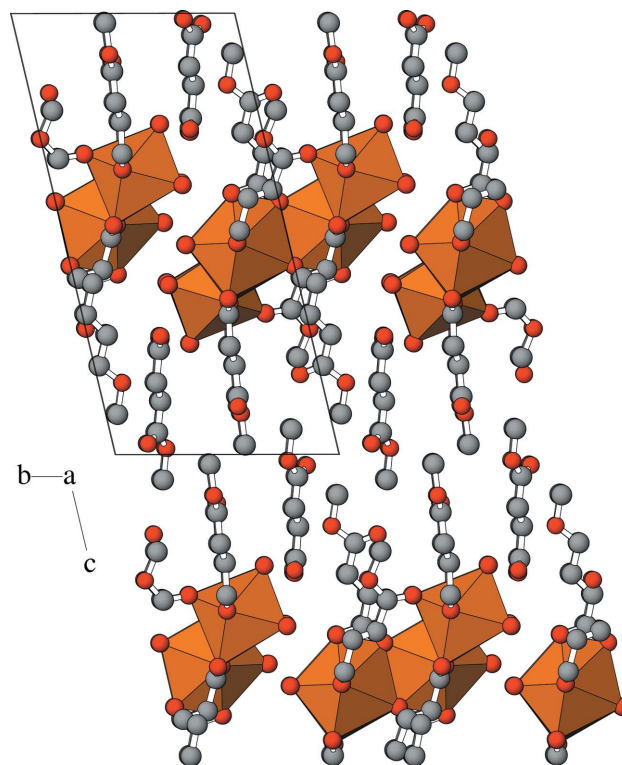
Table 1
Selected bond lengths (Å).

Sr1—O11	2.499 (2)	Sr2—O4	2.569 (3)
Sr1—O12^i	2.509 (2)	Sr2—O32^{iii}	2.571 (2)
Sr1—O22^{ii}	2.537 (2)	Sr2—O31	2.597 (2)
Sr1—O3	2.598 (3)	Sr2—O13^{iv}	2.600 (2)
Sr1—O32	2.601 (2)	Sr2—O2	2.621 (2)
Sr1—O21	2.617 (2)	Sr2—O11	2.664 (2)
Sr1—O31	2.775 (2)	Sr2—O1	2.671 (2)
Sr1—O22	2.807 (2)	Sr2—O12	2.812 (2)

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

Figure 2
The crystal packing of (I), viewed down the a axis. The eight-coordinate Sr atoms are shown as polyhedra. H atoms have been omitted for clarity.

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O1—H1A$\cdots$O42^v	0.834 (18)	1.850 (19)	2.681 (3)	174 (4)
O1—H1B$\cdots$O21^{vi}	0.818 (18)	2.02 (2)	2.813 (3)	163 (4)
O2—H2A$\cdots$O21^{vi}	0.809 (18)	2.017 (19)	2.822 (3)	174 (4)
O2—H2B$\cdots$O41^{vi}	0.837 (18)	1.835 (19)	2.667 (3)	173 (4)
O3—H3A$\cdots$O1^i	0.810 (18)	1.98 (2)	2.775 (4)	169 (4)
O3—H3B$\cdots$O2	0.792 (18)	2.03 (2)	2.819 (4)	171 (4)
O4—H4A$\cdots$O41^{vi}	0.821 (18)	2.05 (3)	2.788 (4)	149 (4)
O4—H4B$\cdots$O42^v	0.807 (18)	2.07 (2)	2.835 (4)	159 (4)

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

Table 3
Selected methyl fumarate torsion angles (°).

O11—C11—C12—C13	−122.1 (4)	O31—C31—C32—C33	−5.7 (5)
O13—C14—C13—C12	−167.8 (3)	O33—C34—C33—C32	7.1 (6)
C15—O14—C14—C13	−179.7 (3)	C35—O34—C34—C33	−177.5 (3)
O21—C21—C22—C23	10.8 (5)	O41—C41—C42—C43	12.5 (5)
O23—C24—C23—C22	10.8 (6)	O43—C44—C43—C42	9.2 (6)
C25—O24—C24—C23	177.6 (3)	C45—O44—C44—C43	−178.8 (3)

All H parameters were initially refined freely. In the final cycles the H atoms of the CH groups were placed in calculated positions with C—H = 0.93 Å and refined as riding atoms. The CH$_3$ groups were placed in calculated positions and the torsion angle allowed to refine

(C—H = 0.96 Å). For the water molecules, the O—H distances were restrained to 0.82 (2) Å. The displacement parameters were set to 1.2 (CH and CH$_3$) or 1.5 (OH) times U_{eq} of the corresponding C or O atoms. The highest peak is located 0.83 Å from atom Sr1.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus* and *SADABS* (Sheldrick, 2002); 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 *ATOMS* (Dowty, 2000); software used to prepare material for publication: *SHELXL97*.

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