

## Strontium diibuprofenate dihydrate, strontium malonate sesquihydrate, strontium diascorbate dihydrate and strontium 2-oxidobenzoate hydrate at 120 K

Kenny Stahl,<sup>a\*</sup> Jens E. T. Andersen<sup>a</sup> and Stephan Christgau<sup>b</sup>

<sup>a</sup>Department of Chemistry, Technical University of Denmark, DK-2800 Lyngby, Denmark, and <sup>b</sup>Osteologix A/S, Symbion Science Park, Fruebjergvej 3, DK-2100 Copenhagen Ø, Denmark

Correspondence e-mail: kenny@kemi.dtu.dk

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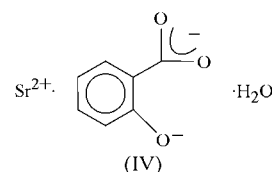
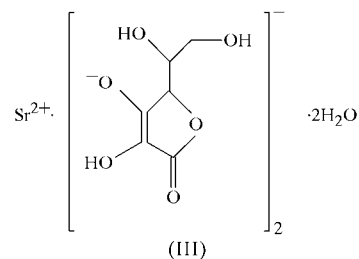
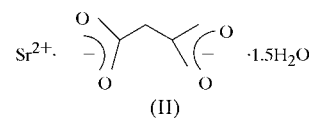
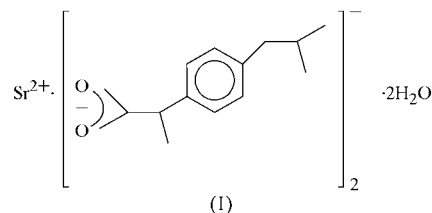
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Four strontium(II) salts with organic acids have been studied. Poly[di aquadi- $\mu$ -ibuprofenato-strontium(II)] or poly[di aquabis[ $\mu$ -2-(4-isobutylphenyl)propionato]strontium(II)], [Sr(C<sub>13</sub>H<sub>17</sub>O<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub>, crystallizes with eight-coordinated Sr atoms. The coordination polyhedra are interconnected by edge-sharing to form chains. The Sr coordination chains are packed into layers, which are stacked by van der Waals interactions. Poly[ $\mu$ -aqua-diaquadi- $\mu$ -malonato-distrontium(II)], [Sr<sub>2</sub>(C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>3</sub>]<sub>n</sub>, crystallizes with nine-coordinated Sr atoms three-dimensionally interconnected into a framework structure. One of the two crystallographically independent water molecules is located on a twofold axial site. *catena*-Poly[[diaqua(ascorbato)strontium(II)]- $\mu$ -ascorbato], [Sr(C<sub>6</sub>H<sub>7</sub>O<sub>6</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub>, crystallizes with isolated eight-coordinated Sr polyhedra. One of the ascorbate ligands bridges two Sr atoms, forming zigzag polyhedral ascorbate chains. These chains are tied together by a three-dimensional hydrogen-bonding network. Poly[aqua- $\mu$ -2-oxidobenzoato-strontium(II)], [Sr(C<sub>7</sub>H<sub>4</sub>O<sub>3</sub>)(H<sub>2</sub>O)]<sub>n</sub>, crystallizes with eight-coordinated Sr atoms. The polyhedra are interconnected by face- and edge-sharing into layers. These layers are stacked by van der Waals forces between the protruding 2-oxidobenzoate ligands.

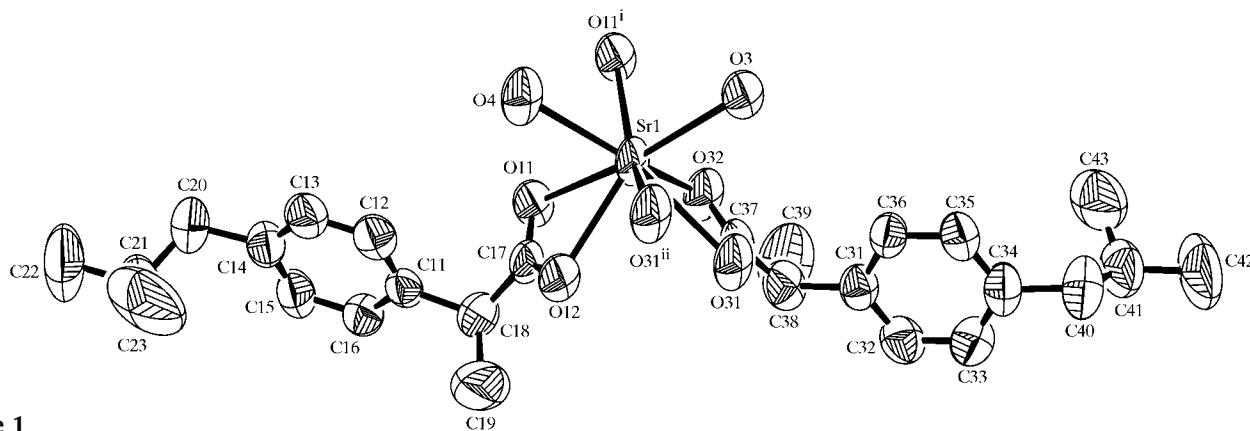
### Comment

In recent years, it has been found that strontium has a positive effect on the development and growth of bone, and the effect of dose on bone structure has been investigated in great detail (Schrooten *et al.*, 2003). 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). The present paper presents

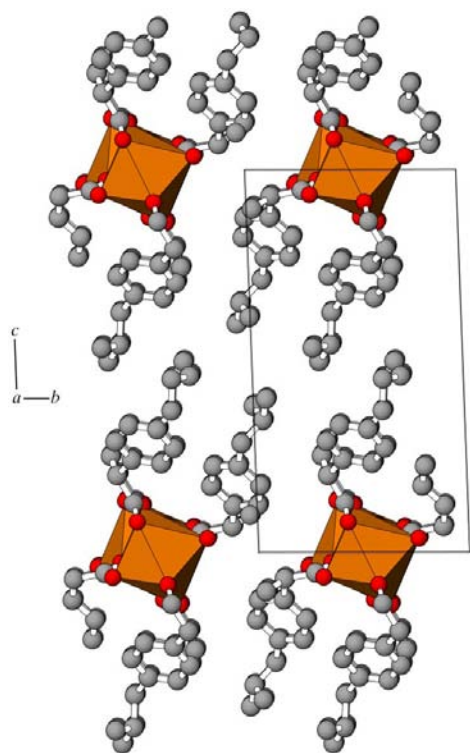
a structural investigation of four such new strontium(II) salts with organic acids.



In strontium diibuprofenate dihydrate, (I), the Sr atom is eight-coordinated in a distorted square antiprism by six O atoms from the asymmetric unit and two additional carboxylate O atoms from neighbouring ibuprofenate ligands (O11<sup>i</sup> and O31<sup>ii</sup> in Fig. 1). The ibuprofenate pair in the asymmetric unit (shown in Fig. 1) have the same absolute configuration. The strontium polyhedra share edges to form chains in the *a* direction (Fig. 2). The chains are stacked in layers in the *ab* plane, with the ibuprofenate ligands protruding in the *c* direction. These layers are in turn stacked in the *c* direction, in both cases by van der Waals interactions only. Viewed in the *a* direction (Fig. 2), the strontium ibuprofenate complexes appear slightly tilted. This causes a difference in the packing of the two independent ibuprofenate ligands. One ibuprofenate ligand, (IA), extends further towards the next layer than the other, (IB), which is more confined to the space between the chains. This difference in packing may explain the observation of larger disorder of the terminal methyl groups of the (IA) ibuprofenate ligand. The torsion angles of the isobutyl and propionate ends are very similar for the two ibuprofenate ligands (Table 3). Compared with the torsion angles of ibuprofen (Hansen *et al.*, 2003), the differences in the isobutyl ends are minor, 6–8°, while the propionate ends show differences of 26–47° (Table 3). The ibuprofen conformations minimize the benzene–propionate interactions, while in (I), the coordination and packing requirements cause more strained conformations. Hydrogen bonding plays a minor role in the packing. Only one H atom of

**Figure 1**

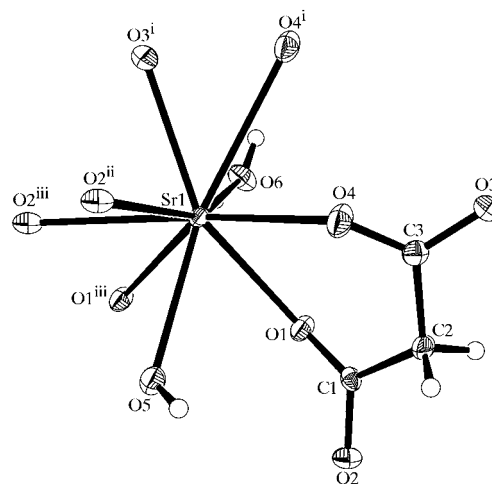
The asymmetric unit of (I), showing 75% probability displacement ellipsoids and the atomic numbering. H atoms have been omitted for clarity. The symmetry positions are as indicated in Table 1.

**Figure 2**

The crystal packing of (I), viewed down the *a* axis. The Sr eight-coordination is shown as polyhedra. H atoms have been omitted for clarity.

each water molecule is employed in hydrogen bonding (Table 2), and hydrogen bonding is, because of the bulkiness of the ibuprofenate ligands, restricted to carboxyl O atoms in neighbouring strontium polyhedra within a polyhedral chain.

In strontium malonate sesquihydrate, (II) (Fig. 3), the Sr atom is nine-coordinated by all available malonate and water O atoms. The irregular polyhedra are connected by edge- and face-sharing into a three-dimensional framework structure. Atoms O3 and O6 are still unshared between polyhedra. The channel system thus created is occupied by the malonate carbon backbone (Fig. 4). All water H atoms are involved in

**Figure 3**

The asymmetric unit of (II), showing 75% probability displacement ellipsoids and the atomic numbering. The symmetry positions are as indicated in Table 4.

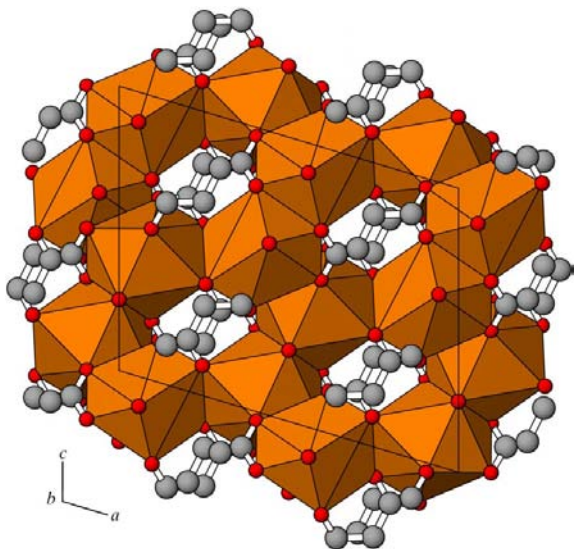
hydrogen bonding to carboxyl O atoms (Table 5). Strontium malonate anhydride (Briggman & Oskarsson, 1977) forms a similar three-dimensional polyhedral network, but all O atoms are shared between Sr polyhedra. This configuration results in a relatively dense packing [ $D_x = 2.78 \text{ Mg m}^{-3}$ , compared with  $2.48 \text{ Mg m}^{-3}$  in (II)]. The higher degree of interconnection and denser packing is the most probable cause of the irreversible dehydration of (II) (see *Experimental*).

In strontium diascorbate dihydrate, (III) (Fig. 5), the Sr atom is eight-coordinated by ascorbate and water O atoms, forming isolated irregular polyhedra. The two independent ascorbate ligands are coordinated differently. One ascorbate ligand, (IIIA), uses atoms O11, O13, O15 and O16 to coordinate two Sr atoms, thus linking the Sr polyhedra into zigzag chains in the *b* direction, while the other ligand, (IIIB), has a one-sided coordination through atoms O25 and O26 (Fig. 6). The ascorbate polyhedral chains are further connected by a three-dimensional hydrogen-bonding network. The conformations of the independent ascorbate ions are different; the O14–C17–C18–C19 [in (IIIA)] and O24–C27–C28–C29

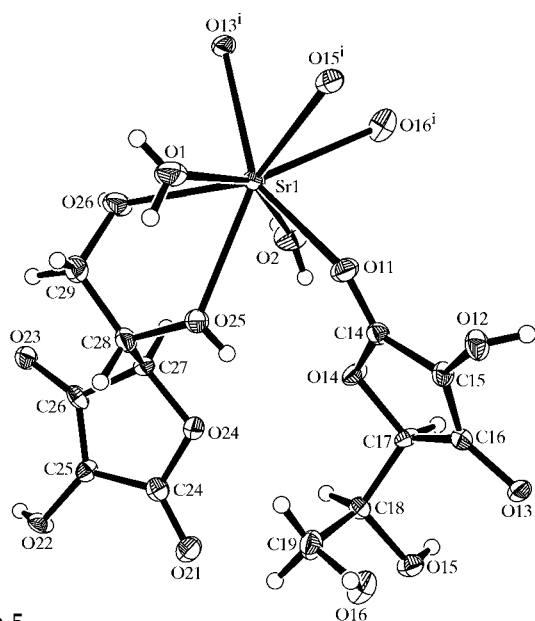
[in (IIIB)] torsion angles are  $-69.9(2)$  and  $176.4(2)^\circ$ , respectively. The O14—C17—C18—C19 [in (IIIA)] torsion angle is similar to the corresponding torsion angles in ascorbic acid, with values of  $-68.3(3)$  and  $-55.5(3)^\circ$  for its two independent molecules (Hvoslef, 1968). The O15—C18—C18—O16 [in (IIIA)] and O25—C28—C29—O26 [in (IIIB)] torsion angles are  $48.8(2)$  and  $50.4(2)^\circ$ , respectively, bringing them into almost eclipsed conformations and allowing for simultaneous Sr coordination of the O-atom pairs. In ascorbic

acid, the corresponding O—C—C—O torsion angles are  $171.2(3)$  and  $171.4(3)^\circ$ , *i.e.* close to staggered conformations (Hvoslef, 1968). All H-atom donors are involved in hydrogen bonding, forming a three-dimensional network. It is interesting to note that the shortest hydrogen bonds ( $H \cdots A < 2 \text{ \AA}$ ) all involve uncoordinated O atoms from (IIIB) (Table 7), which may be explained by a higher packing/conformational flexibility of the one-sided Sr coordination of (IIIB).

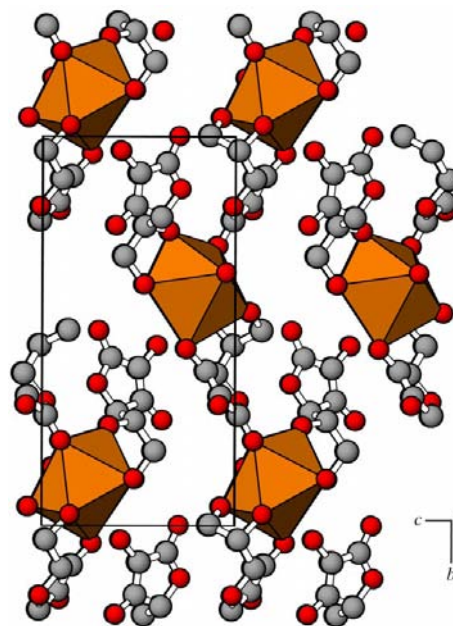
In strontium 2-oxidobenzoate hydrate, (IV) (Fig. 7), the Sr atom is eight-coordinated in an approximately square antiprismatic configuration. The antiprisms are pairwise connected through face-sharing, and these pairs are further connected by edge-sharing into layers in the *ac* plane (Fig. 8). The 2-oxidobenzoate ligands protrude from the layers and



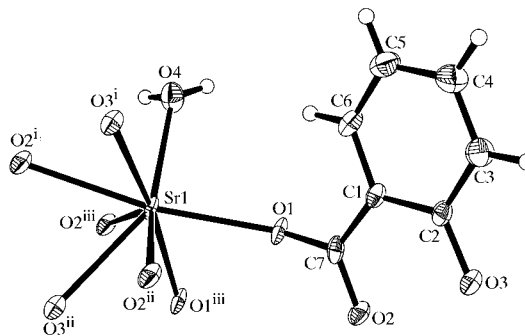
**Figure 4**  
The crystal packing of (II), viewed down the *b* axis. The Sr nine-coordination is shown as polyhedra. H atoms have been omitted for clarity.



**Figure 5**  
The asymmetric unit of (III), showing 75% probability displacement ellipsoids and the atomic numbering. The symmetry positions are as indicated in Table 6.



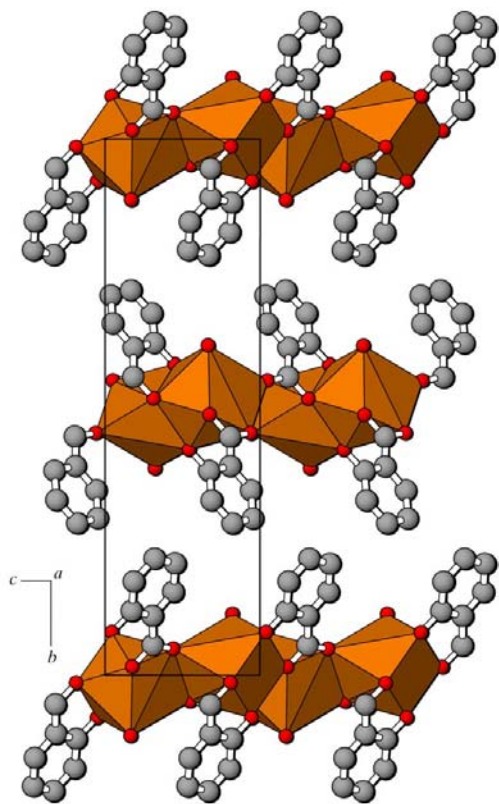
**Figure 6**  
The crystal packing of (III), viewed down the *a* axis. The Sr eight-coordination is shown as polyhedra. H atoms have been omitted for clarity.



**Figure 7**  
The asymmetric unit of (IV), showing 75% probability displacement ellipsoids and the atomic numbering. The symmetry positions are as indicated in Table 8.

connect them through van der Waals forces in the *b* direction. In contrast, strontium disalicylate dihydrate (Debuyst *et al.* 1979) forms polyhedral chains, where the hydroxy group takes part in a three-dimensional hydrogen-bonding network connecting these chains. In (IV), only one of the water H-atom donors, H4B, participates in a conventional hydrogen bond (Table 9). However, atom H4A points towards the centre of a neighbouring benzene ring with a distance of 2.83 (3) Å to the ring centre (*A*) and an O4—H4A...*A* angle of 154 (3)°.

Strontium(II) salts of organic acids are generally octa- to decacoordinated by O atoms, with coordination distances in the range 2.4–3.0 Å. The Sr polyhedra show various degrees of condensation depending on the number of available carboxylic acid and water O atoms, and the size of the organic group. The resulting structures are thus observed with isolated Sr polyhedra as in (III), or with polyhedra connected into chains as in (I), layers as in (IV) or three-dimensional networks as in (II). The average Sr—O distance is primarily determined by the coordination number, *viz.* 2.6803 (4) Å for nine-coordinate (II), and 2.5940 (9), 2.5927 (6) and 2.6034 (7) Å for the eight-coordinated (I), (III) and (IV), respectively. An increasing degree of condensation causes a minor increase in the average Sr—O distances when comparing the eight-coordinated complexes [2.5927 (6) Å for (III) (isolated), 2.5940 (9) Å for (I) (chains) and 2.6034 (7) Å for (IV) (layers)].



**Figure 8**  
The crystal packing of (IV), viewed down the *a* axis. The Sr eight-coordination is shown as polyhedra. H atoms have been omitted for clarity.

## Experimental

For the preparation of (I), solid strontium carbonate was added to a saturated solution of racemic ibuprofen at 317 K in a molar ratio of 1:2. The product was obtained in high yield and purity after cooling to room temperature and filtration. For the preparation of (II), an equimolar amount of solid strontium carbonate was added to a saturated aqueous solution of malonic acid at 303–317 K. The product precipitated upon cooling to room temperature. Consecutive cycles of evaporation of the solvent below 343 K followed by filtration at room temperature resulted in yields of between 90 and 100%. Heating of the product above 343 K resulted in complete dehydration and irreversible transformation to anhydrous strontium malonate. For the preparation of (III), strontium chloride hexahydrate was added to a solution of sodium ascorbate in a molar ratio of 1:2. More strontium chloride hexahydrate, approximately 100 g in total, and sodium ascorbate, approximately 77 g in total, were added to the solution at 317 K until a transparent yellow syrup was obtained. The syrup was suction filtered for 12 h and the product was obtained by drying the syrup in a desiccator. The final product was a white powder with a yellow tarnish, while the selected single crystals appeared colourless. The product was also obtained by pouring an aqueous solution of ascorbic acid and powdered strontium carbonate into a large volume of acetone according to the procedure of Ruskin & Merrill (1947). For the preparation of (IV), powdered strontium carbonate was added to an equimolar amount of a saturated solution of salicylic acid at 313 K. Strontium 2-oxidobenzoate hydrate was obtained in high yield and purity as a precipitate on cooling to 293 K.

## Compound (I)

### Crystal data

[Sr(C<sub>13</sub>H<sub>17</sub>O<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]  
*M<sub>r</sub>* = 534.18  
 Triclinic, *P*1̄  
*a* = 7.9116 (7) Å  
*b* = 10.4870 (10) Å  
*c* = 18.2493 (17) Å  
 $\alpha$  = 86.088 (2)°  
 $\beta$  = 79.784 (2)°  
 $\gamma$  = 70.605 (2)°  
*V* = 1405.5 (2) Å<sup>3</sup>

*Z* = 2  
*D<sub>x</sub>* = 1.262 Mg m<sup>-3</sup>  
 Mo K $\alpha$  radiation  
 Cell parameters from 3382 reflections  
 $\theta$  = 2.3–27.6°  
 $\mu$  = 1.95 mm<sup>-1</sup>  
*T* = 120 (2) K  
 Plate, colourless  
 0.35 × 0.06 × 0.03 mm

### Data collection

Bruker SMART APEX  
 diffractometer  
 $\omega$  scan  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 2002)  
*T<sub>min</sub>* = 0.548, *T<sub>max</sub>* = 0.944  
 19139 measured reflections

8160 independent reflections  
 5038 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.051  
 $\theta_{max}$  = 31.0°  
*h* = -11 → 11  
*k* = -15 → 14  
*l* = -26 → 26

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.058  
*wR*(*F*<sup>2</sup>) = 0.145  
*S* = 0.98  
 8160 reflections  
 310 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0724P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.79 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.44 \text{ e \AA}^{-3}$

**Table 1**

Selected bond lengths (Å) for (I).

Sr1—O11 <sup>i</sup>	2.476 (2)	Sr1—O12	2.595 (2)
Sr1—O31 <sup>ii</sup>	2.486 (2)	Sr1—O32	2.599 (3)
Sr1—O3	2.563 (3)	Sr1—O31	2.728 (2)
Sr1—O4	2.563 (3)	Sr1—O11	2.742 (2)

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

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O3—H31...O12 <sup>ii</sup>	0.804 (18)	1.92 (2)	2.706 (3)	165 (4)
O4—H41...O32 <sup>i</sup>	0.798 (19)	1.91 (2)	2.704 (3)	171 (5)

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

**Table 3**  
Selected torsion angles in (I) (°).

	(I)	Ibuprofen <sup>a</sup>
C14—C20—C21—C22	−174.1 (5)	−168.3 (5)
C34—C40—C41—C42	−176.9 (4)	168.7 (5)
C12—C11—C18—C19	104.8 (5)	144.4 (4)
C36—C31—C38—C39	101.9 (4)	151.2 (4)
C11—C18—C17—O11	−59.6 (5)	−95.9 (4)
C31—C38—C37—O31	−58.0 (4)	−83.6 (4)

Note: (a) Hansen *et al.* (2003).

**Compound (II)**

*Crystal data*

[Sr<sub>2</sub>(C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>3</sub>]  
*M<sub>r</sub>* = 433.38  
 Monoclinic, *C*2/*c*  
*a* = 14.3345 (9) Å  
*b* = 7.3458 (5) Å  
*c* = 11.5075 (7) Å  
 $\beta$  = 106.710 (1)°  
*V* = 1160.55 (13) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 2.480 Mg m<sup>−3</sup>

*Data collection*

Bruker SMART APEX diffractometer  
 $\omega$  scan  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)  
*T<sub>min</sub>* = 0.06, *T<sub>max</sub>* = 0.48  
 7363 measured reflections  
 1708 independent reflections

*Refinement*

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.016  
*wR* (*F*<sup>2</sup>) = 0.041  
*S* = 1.08  
 1708 reflections  
 97 parameters  
 H atoms treated by a mixture of independent and constrained refinement

Mo *K*α radiation  
 Cell parameters from 5770 reflections  
 $\theta$  = 3.0–30.9°  
 $\mu$  = 9.25 mm<sup>−1</sup>  
*T* = 120 (2) K  
 Irregular, colourless  
 0.33 × 0.30 × 0.08 mm

1630 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.023  
 $\theta_{\max}$  = 30.7°  
*h* = −19 → 19  
*k* = −10 → 10  
*l* = −16 → 15

$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 0.6829P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.003$   
 $\Delta\rho_{\max} = 0.55 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.49 \text{ e \AA}^{-3}$   
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.0044 (2)

**Table 4**  
Selected bond lengths (Å) for (II).

Sr1—O4	2.5386 (10)	Sr1—O1 <sup>iii</sup>	2.6850 (10)
Sr1—O1	2.5801 (9)	Sr1—O5	2.6956 (9)
Sr1—O6	2.5839 (10)	Sr1—O2 <sup>iii</sup>	2.8423 (10)
Sr1—O3 <sup>i</sup>	2.5942 (9)	Sr1—O4 <sup>i</sup>	2.9836 (11)
Sr1—O2 <sup>ii</sup>	2.6201 (10)		

Symmetry codes: (i)  $-x + \frac{3}{2}, -y + \frac{1}{2}, -z + 1$ ; (ii)  $x, -y, z + \frac{1}{2}$ ; (iii)  $-x + 1, y, -z + \frac{1}{2}$ .

**Table 5**  
Hydrogen-bond geometry (Å, °) for (II).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5...O3 <sup>iv</sup>	0.824 (14)	1.902 (14)	2.7165 (12)	169.7 (19)
O6—H6A...O3 <sup>v</sup>	0.797 (15)	2.179 (17)	2.8662 (14)	144.6 (19)
O6—H6B...O2 <sup>vi</sup>	0.805 (15)	2.150 (16)	2.9328 (14)	164.2 (19)

Symmetry codes: (iv)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (v)  $x - \frac{1}{2}, y + \frac{1}{2}, z$ ; (vi)  $x, -y + 1, z + \frac{1}{2}$ .

**Compound (III)**

*Crystal data*

[Sr(C<sub>6</sub>H<sub>7</sub>O<sub>6</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]  
*M<sub>r</sub>* = 473.88  
 Monoclinic, *P*2<sub>1</sub>  
*a* = 6.4358 (5) Å  
*b* = 16.1040 (13) Å  
*c* = 8.3646 (7) Å  
 $\beta$  = 107.696 (1)°  
*V* = 825.90 (12) Å<sup>3</sup>  
*Z* = 2  
*D<sub>x</sub>* = 1.906 Mg m<sup>−3</sup>

Mo *K*α radiation  
 Cell parameters from 6673 reflections  
 $\theta$  = 2.5–30.7°  
 $\mu$  = 3.34 mm<sup>−1</sup>  
*T* = 120 (2) K  
 Irregular, colourless  
 0.28 × 0.05 × 0.04 mm

*Data collection*

Bruker SMART APEX diffractometer  
 $\omega$  scan  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)  
*T<sub>min</sub>* = 0.455, *T<sub>max</sub>* = 0.878  
 10978 measured reflections  
 4728 independent reflections

4507 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.023  
 $\theta_{\max}$  = 30.9°  
*h* = −9 → 9  
*k* = −22 → 23  
*l* = −12 → 11

*Refinement*

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.025  
*wR* (*F*<sup>2</sup>) = 0.057  
*S* = 1.04  
 4728 reflections  
 274 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.73 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.28 \text{ e \AA}^{-3}$   
 Absolute structure: Flack (1983)  
 Flack parameter: −0.017 (4)

**Table 6**  
Selected bond lengths (Å) for (III).

Sr1—O11	2.5446 (16)	Sr1—O2	2.5790 (17)
Sr1—O13 <sup>i</sup>	2.5688 (15)	Sr1—O1	2.6016 (16)
Sr1—O16 <sup>i</sup>	2.5699 (16)		

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

**Table 7**  
Hydrogen-bond geometry (Å, °) for (III).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1A...O23 <sup>ii</sup>	0.829 (18)	1.879 (18)	2.708 (2)	177 (3)
O1—H1B...O21 <sup>iii</sup>	0.797 (17)	1.963 (19)	2.736 (2)	163 (3)
O2—H2A...O12 <sup>iv</sup>	0.820 (17)	2.104 (18)	2.920 (2)	175 (3)
O2—H2B...O15 <sup>v</sup>	0.804 (17)	2.25 (2)	2.971 (2)	150 (3)
O12—H12...O23 <sup>vi</sup>	0.821 (17)	1.756 (18)	2.571 (2)	172 (3)
O15—H15...O22 <sup>vii</sup>	0.791 (17)	1.978 (17)	2.768 (2)	177 (3)
O16—H16...O21 <sup>ii</sup>	0.802 (18)	1.997 (19)	2.783 (2)	167 (3)
O22—H22...O13 <sup>viii</sup>	0.782 (17)	1.86 (2)	2.579 (2)	154 (3)
O25—H25...O14	0.783 (17)	2.25 (2)	2.893 (2)	140 (3)
O26—H26...O14 <sup>v</sup>	0.785 (17)	2.348 (19)	3.100 (2)	161 (4)

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



## Compound (IV)

## Crystal data

[Sr(C<sub>7</sub>H<sub>4</sub>O<sub>3</sub>)(H<sub>2</sub>O)]  
*M<sub>r</sub>* = 241.74  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 5.0993 (4) Å  
*b* = 22.808 (2) Å  
*c* = 6.9811 (6) Å  
 $\beta$  = 109.755 (2)°  
*V* = 764.15 (11) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 2.101 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 4077 reflections  
 $\theta$  = 3.2–30.4°  
 $\mu$  = 7.02 mm<sup>-1</sup>  
*T* = 120 (2) K  
 Irregular, colourless  
 0.14 × 0.10 × 0.02 mm

## Data collection

Bruker SMART APEX diffractometer  
 $\omega$  scan, frame data integration  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)  
*T<sub>min</sub>* = 0.440, *T<sub>max</sub>* = 0.872  
 10002 measured reflections

2251 independent reflections  
 1917 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.040  
 $\theta_{\text{max}}$  = 30.9°  
*h* = -7 → 7  
*k* = -32 → 32  
*l* = -9 → 10

## Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.038  
*wR*(*F*<sup>2</sup>) = 0.092  
*S* = 1.08  
 2251 reflections  
 115 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.1094P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 1.87 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -1.00 \text{ e } \text{Å}^{-3}$

Table 8

Selected bond lengths (Å) for (IV).

Sr1—O1	2.469 (2)	Sr1—O3 <sup>ii</sup>	2.605 (2)
Sr1—O4	2.502 (2)	Sr1—O2 <sup>iii</sup>	2.666 (2)
Sr1—O3 <sup>i</sup>	2.579 (2)	Sr1—O1 <sup>iii</sup>	2.677 (2)
Sr1—O2 <sup>i</sup>	2.591 (2)	Sr1—O2 <sup>ii</sup>	2.738 (2)

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

Table 9

Hydrogen-bond geometry (Å, °) for (IV).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O4—H4B...O3 <sup>iv</sup>	0.823 (18)	1.90 (2)	2.718 (3)	170 (4)

Symmetry code: (iv) *x* - 1, *y*, *z* + 1.

In all refinements, all H-atom sites were initially located in difference Fourier maps and refined freely. In the final cycles, H atoms of the CH, CH<sub>2</sub> and CH<sub>3</sub> groups were placed in calculated positions, with C—H distances of 0.93 (aromatic CH), 0.98 (aliphatic

CH), 0.97 (CH<sub>2</sub>) and 0.96 Å (CH<sub>3</sub>), and refined as riding atoms. In water molecules and OH groups, the O—H distances were restrained to 0.82 (2) Å. The displacement parameters were set at 1.2 (CH, CH<sub>2</sub> and CH<sub>3</sub>) or 1.5 (OH) times *U<sub>eq</sub>* of the corresponding C or O atoms. In (I), several of the terminal methyl groups showed signs of disorder. Several models with split positions for atoms C19, C22 and C23 were tried, with up to ten different positions. Using 353 parameters with mixed anisotropic and isotropic displacement parameters for the different split sites, but not including the corresponding H-atom positions, resulted in a *wR2* value of 0.154, while the unsplit model, including H-atom positions with 310 parameters, resulted in a *wR2* value of 0.145. The unsplit model was therefore judged as appropriate at the present level of experimental resolution. The absolute structure determination of (III) is based on 2226 Bijvoet pairs.

For all compounds, 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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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1898). Services for accessing these data are described at the back of the journal.

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