



Synthesis, crystal structure, and thermal properties of poly[aqua(μ_5 -2,5-dicarboxybenzene-1,4-dicarboxylato)strontium]

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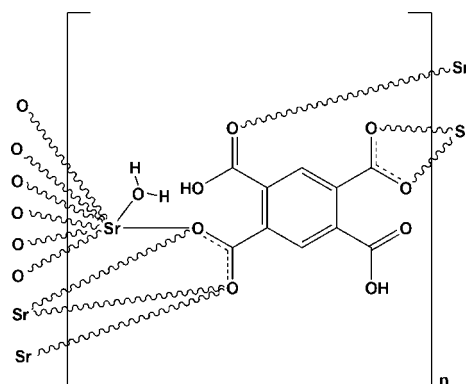
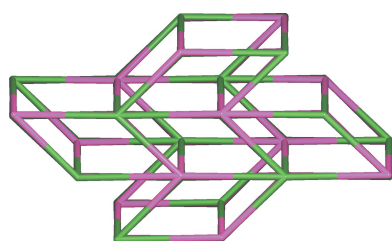
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A coordination polymer formulated as $[\text{Sr}(\text{H}_2\text{BTEC})(\text{H}_2\text{O})]_n$ (H_4BTEC = benzene-1,2,4,5-tetracarboxylic acid, $\text{C}_{10}\text{H}_6\text{O}_8$), was synthesized hydrothermally and characterized by single-crystal and powder X-ray diffraction, scanning electron microscopy and thermal analysis. Its crystal structure is made up of a zigzag inorganic chain formed by edge-sharing of $[\text{SrO}_8]$ polyhedra running along $[001]$. Adjacent chains are connected to each other *via* the carboxylate groups of the ligand, resulting in a double-layered network extending parallel to (100) . $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds of medium-to-weak strength between the layers consolidate the three-dimensional structure. One of the carboxylic OH functions was found to be disordered over two sets of sites with half-occupancy.

1. Chemical context

In recent years, the self-assembly of coordination polymers (CP) and crystal engineering of metal–organic coordination frameworks have attracted great interest because of their varied molecular topologies and the potential applications of these polymers as functional materials (Pan *et al.*, 2004; Jiang *et al.*, 2011; Du *et al.*, 2014). Derivatives of aromatic tetracarboxylic acids such as 1,2,4,5-benzenetetracarboxylic acid (H_4BTEC , commonly known as pyromellitic acid) and their deprotonated forms ($\text{H}_n\text{BTEC}^{(4-n)-}$) belong to an important family of polycarboxylate O-donor ligands, which have been used extensively to prepare CPs (Liu *et al.*, 2009). The variations in the possible binding modes of its four potentially coordinating carboxylic/carboxylate groups, along with the different coordination preferences of the metal ions, gives rise to a great variety of crystal structures.



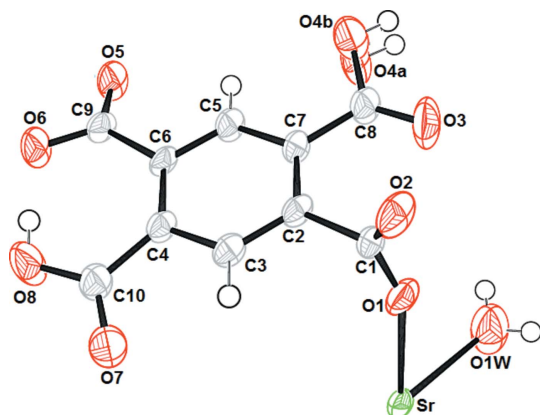


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. (Hydroxy atom O4 is disordered with a 0.5:0.5 ratio.)

In this communication, we report on the synthesis of $[\text{Sr}(\text{H}_2\text{BTEC})(\text{H}_2\text{O})]$, (I), along with its characterization by single-crystal and powder X-ray diffraction, scanning electron microscopy coupled with energy-dispersive X-ray fluorescence, and thermal analysis.

2. Structural commentary

The asymmetric unit of compound (I) comprises one Sr^{II} atom, one doubly deprotonated $(\text{H}_2\text{BTEC})^{2-}$ anion and one coordinating water molecule O1W (Fig. 1). The Sr^{II} atom is bonded to eight oxygen atoms, seven of them coming from five carboxylate or carboxylic groups of five different $(\text{H}_2\text{BTEC})^{2-}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
$\text{O1W---H1W}\cdots\text{O3}^{\text{i}}$	0.83	2.25	3.0666 (3)	170
$\text{O1W---H2W}\cdots\text{O3}^{\text{ii}}$	0.83	2.04	2.864 (4)	171
$\text{O4A---H4A}\cdots\text{O5}^{\text{iii}}$	0.82	1.92	2.68 (2)	152
$\text{O4B---H4B}\cdots\text{O5}^{\text{iii}}$	0.82	1.89	2.696 (16)	166
$\text{O8---H8}\cdots\text{O6}$	0.82	1.59	2.400 (3)	169
$\text{C6---H6}\cdots\text{O4A}^{\text{iii}}$	0.93	2.32	3.240 (18)	169
$\text{C6---H6}\cdots\text{O4B}^{\text{iii}}$	0.93	2.39	3.298 (14)	166

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

ligands, and one oxygen atom from the water molecule. The resulting coordination polyhedron around the alkaline earth cation may be described as a distorted bicapped prism (Fig. 2a). The $\text{Sr}\text{---}\text{O}$ bond lengths span the range 2.4915 (19)–2.8239 (19) \AA for carboxylate/carboxylic acid groups, and the $\text{Sr}\text{---}\text{O}_{(\text{water})}$ bond length is 2.520 (3) \AA . These distances are comparable to those reported in other strontium–carboxylate complexes (He *et al.*, 2014). The $(\text{H}_2\text{BTEC})^{2-}$ anion has a bridging character and connects five Sr^{II} atoms (Fig. 2b) whereby three different coordination modes are realized. The carboxylate group (O1–C1–O2) adopts both a bis-monodentate bridging mode to two Sr^{II} atoms and a bidentate chelating mode to a third Sr^{II} atom; the carboxylic group (O7/C10/O8/H8) is monodentately bound through O7 to a fourth Sr^{II} atom and shows an intramolecular $\text{O8}\text{---}\text{H8}\cdots\text{O6}$ hydrogen bond (Table 1); the carboxylate group (O5/C9/O6) exhibits a bidentate chelating mode to a fifth Sr^{II} atom. The carboxylic group (O3/C8/O4/H4) has a disordered hydroxyl

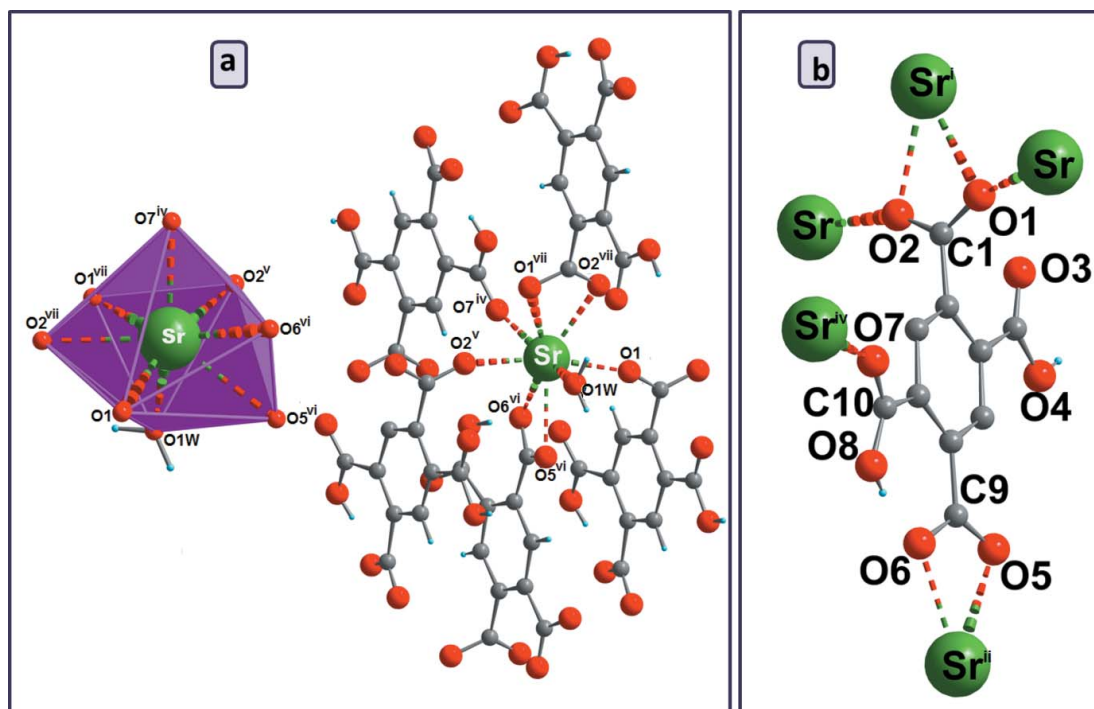


Figure 2
(a) Perspective view of the coordination environment of Sr^{II} and (b) coordination modes of the $(\text{H}_2\text{BTEC})^{2-}$ anion in (I). [Symmetry codes: (i) $x, -y + 2, z - \frac{1}{2}$; (ii) $x, -y + 1, z - \frac{3}{2}$; (iv) $-x + \frac{3}{2}, -y + \frac{3}{2}, -z + 2$; (v) $x, y, z + 1$; (vi) $x, -y + 1, z + \frac{1}{2}$; (vii) $x, -y + 2, z + \frac{1}{2}$]

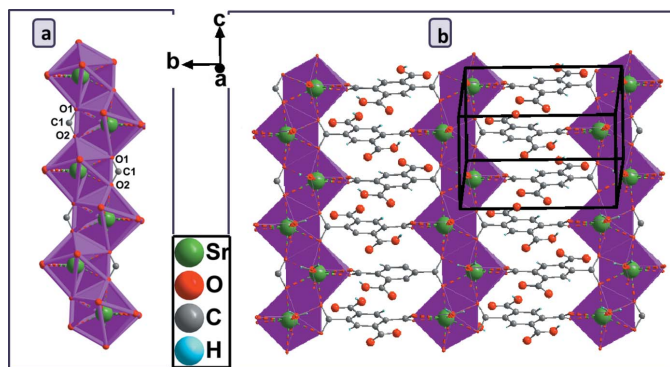


Figure 3
(a) View of the inorganic chain and (b) the two-dimensional layer structure in the crystal structure of (I).

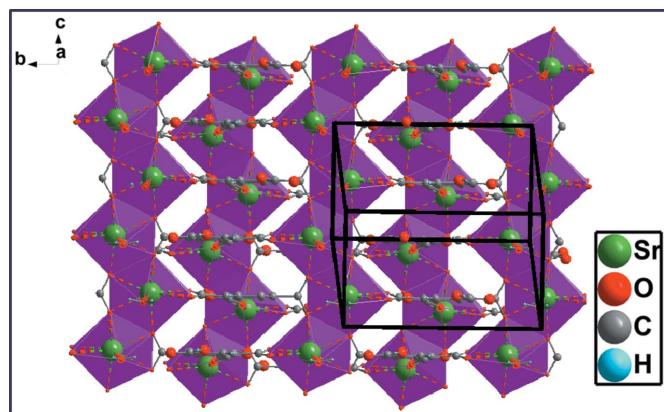


Figure 6
View of the double-layered network along the *a* axis.

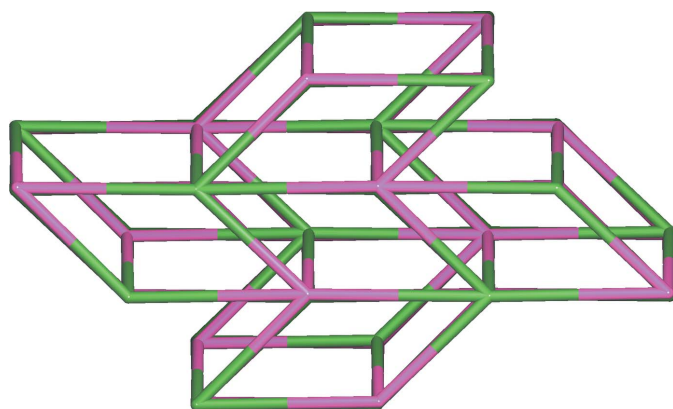


Figure 4
The uninodal five-connected net for (I).

group and does not bind to a cation. The $[\text{SrO}_8]$ polyhedra share edges through (O1–O2), thus forming an infinite zigzag chain running parallel to [001] (Fig. 3*a*). These chains are further connected through the carboxylate groups (O1/C1/O2 and O5/C9/O6) into double layers parallel to (100) that are stacked along [100] (Fig. 3*b*). A topological analysis (Blatov *et al.*, 2014) revealed that the overall structure of the coordination polymer (I) can be defined as a uninodal five-connected net with the Schläfli symbol $\{4^8.6^2\}$, and the vertex symbols of Sr^{II} and $(\text{H}_2\text{BTEC})^{2-}$ node is $[4.4.4.4.4.4.4.6(3).6(3)]$ (Fig. 4).

3. Supramolecular features

In the crystal structure of (I), neighbouring layers are linked to each other along the stacking direction by intermolecular O–H...O hydrogen bonds of medium-to-weak strength involving the coordinating water molecule with the carbonyl O atom (O3) of the non-coordinating carboxylic acid group as acceptor, as well as the disordered O4–H4 function of this carboxylic acid group and carboxylate O atom O4 as an acceptor group (Table 1). The hydrogen-bonding scheme is completed by two weak intermolecular C–H...O interactions involving aromatic H atoms (Table 1). Based on the connectivity of these hydrogen bonds, four different motifs (Etter *et al.*, 1990) can be distinguished, *viz.* $R_2^2(8)$, $R_2^2(10)$, $R_2^2(13)$ and $R_2^2(15)$ (Fig. 5), leading to a three-dimensional supramolecular structure (Figs. 6, 7).

4. Crystal morphology and characterization

SEM images show the appearance of the microcrystalline powder, while EDX measurements provided qualitative confirmation about the presence of all non-hydrogen atoms (Fig. 8). The FT-IR spectrum of complex (I) (Fig. S1 in the supporting information) shows broad absorption bands near 3440 cm^{-1} , which are assigned to O–H stretching vibrations of the –COOH groups and water molecules, respectively. The

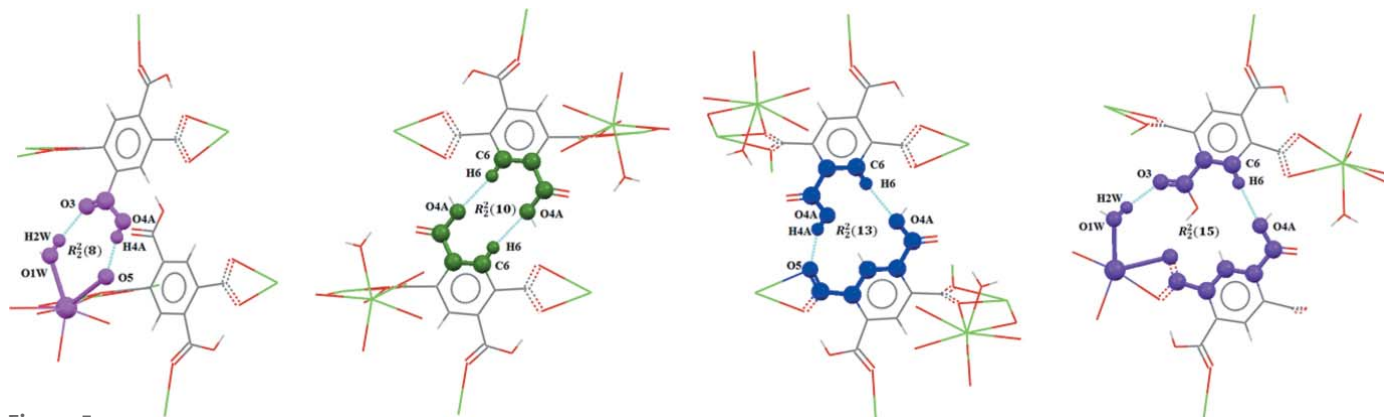


Figure 5
The hydrogen-bonded-ring patterns found in (I).

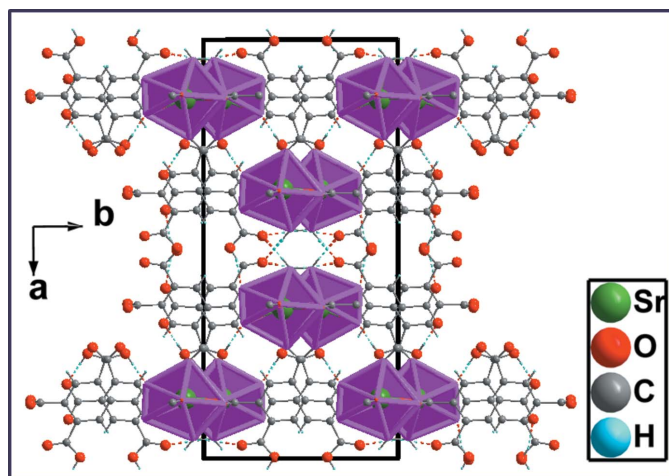


Figure 7
Projection of the three-dimensional structure along [001] axis with hydrogen-bonding interactions shown as dashed lines.

bands located at 3164 cm^{-1} can be attributed to aromatic C–H stretching vibration. In addition, the symmetric [$\nu_s(\text{OCO}) =$

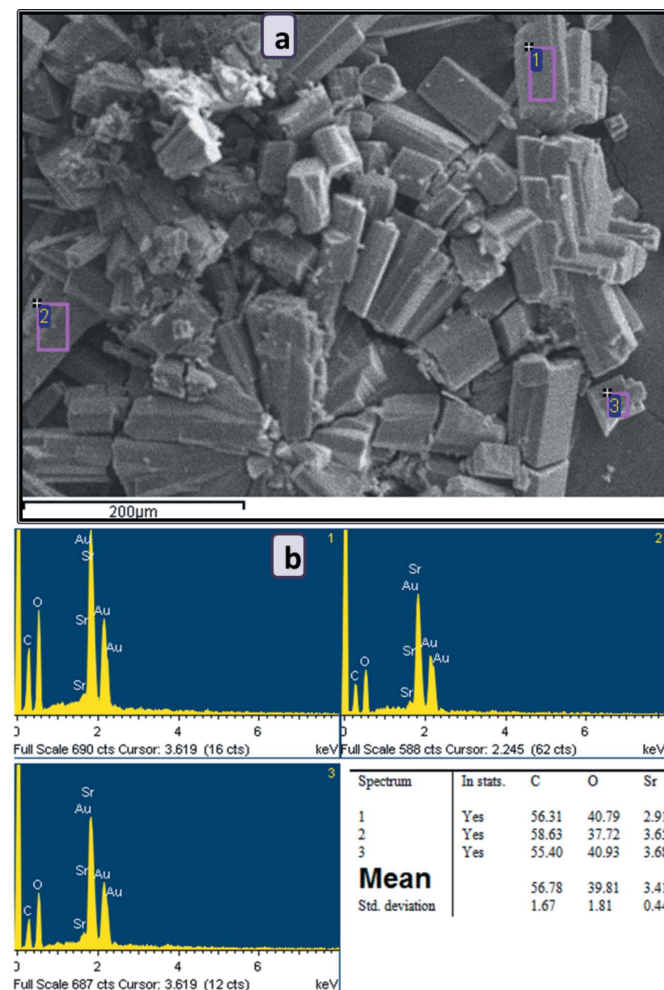


Figure 8
(a) SEM images and (b) a typical EDX spectrum with a table of the quantitative analysis results for Sr, O and C (in at%).

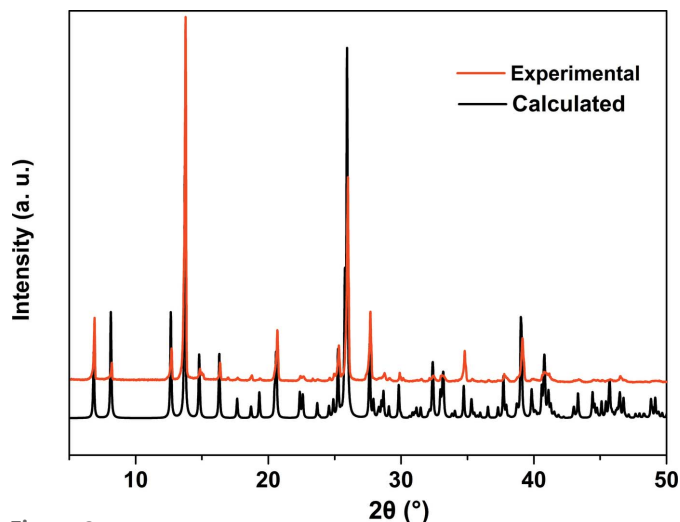


Figure 9
Powder XRD patterns of (I) compared with the calculated one.

1414 and 1346 cm^{-1}] and asymmetric [$\nu_{as}(\text{OCO}) = 1626$ and 1533 cm^{-1}] stretching vibrations in (I) can be attributed to the split of the absorption bands of the carboxylate groups. The $\Delta(\nu_{as}-\nu_s)$ values of $187\text{--}212\text{ cm}^{-1}$ indicate that some of the carboxylate groups are monodentate and bridging to the Sr^{II} atoms. A strong absorption at 1731 cm^{-1} confirms the presence of the carboxylic acid function. All these results are in agreement with the crystallographic data.

Plots of the experimental and simulated powder X-ray diffraction (PXRD) patterns of the title compound are shown in Fig. 9, revealing a good match and thus phase purity and repeatable synthesis. TG/DTG, SDTA curves and the mass spectrometry analysis are depicted in Fig. 10a. TG/DTG curves of (I) reveal a total mass loss of *ca* 60.5% (calc. 58.1%) from room temperature up to 1273 K, with SrO as the final product. The mass loss of (I), under a dry N_2 atmosphere, proceeds in four steps. The first one, between 298 and 550 K with a mass loss of *ca* 5.2% (cal. 5.0%), is associated with an endothermic reaction (491 K in the SDTA curve) and corresponds to the loss of the coordinating water molecule. The second step, between 557 and 719 K with a mass loss of *ca* 22.1% (calc. 25.7%) and an endothermic reaction (peak at 609 K), is attributed to the beginning of the decomposition of the $(\text{H}_2\text{BTEC})^{2-}$ ligand. The third step, between 706 and 908 K with a mass loss of about 15.3% is exothermic (peak at 882 K), and may be attributed to the complete decomposition of the organic anion. The fourth step, between 908 and 1147 K with a mass loss of 17.9% is also exothermic (peak at 1121 K), and may be due to another evaporation of trapped organic moieties. The associated mass spectrometry m/z 18 (H_2O), 44 (CO_2), and 76 (C_6H_4) curves (Fig. 10b) are in agreement with the TG/DTG data. The m/z 18 curve has four maxima, the first and second maxima at 565 and 639 K correspond to the loss of the coordinating water molecules. The third maximum at 682 K coincides with the m/z 44 and 76 curves, which is attributed to the first decomposition step of the organic anion, and the last maximum at 806 K coincides with the second maximum of m/z 44 and 76.

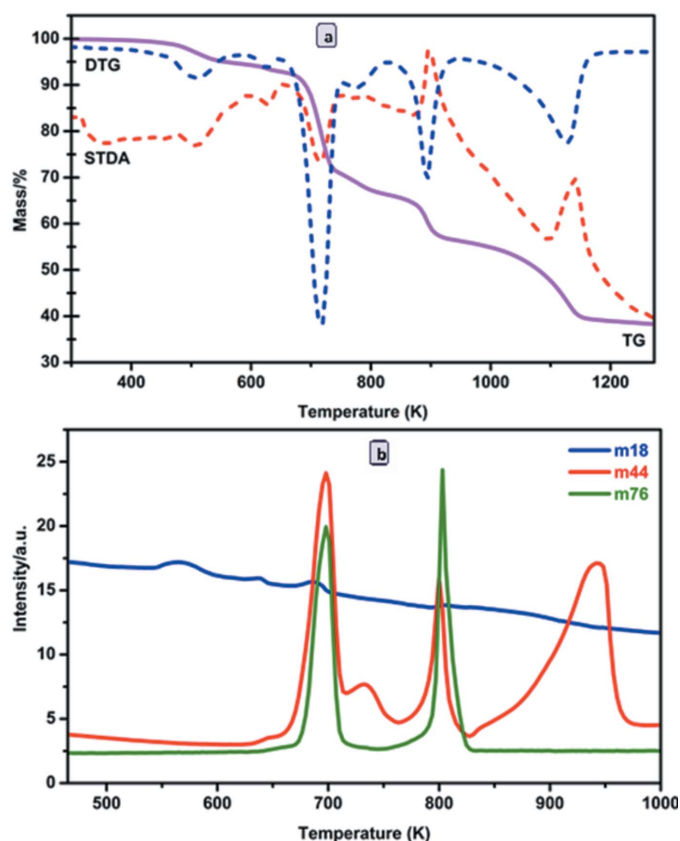


Figure 10 (a) TG–DTG–SDTA curves and (b) m/z 18 (H_2O), m/z 44 (CO_2) and m/z 76 (C_6H_4) MS signals for (I).

5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, update November 2018; Groom *et al.*, 2016) resulted in 196 hits for the $(\text{H}_4\text{BTEC})^{2-}$ dianion. To the best of our knowledge, there are only two alkaline earth coordination polymers made up from the $(\text{H}_2\text{BTEC})^{2-}$ dianion, *viz.* $\text{Ba}(\text{H}_2\text{BTEC})(\text{H}_2\text{O})_5)_n$ (Dale *et al.*, 2003) and $[\text{Sr}_2(\text{H}_2\text{BTEC})_2(\text{H}_2\text{O})_2]_n$ (Balegroune *et al.*, 2011). In the Ba compound, the alkaline earth cation displays a monocapped square-antiprismatic coordination environment, and the coordination mode of the $(\text{H}_2\text{BTEC})^{2-}$ ligand is monodentate to four cations at a time. The Sr compound is based on $[\text{SrO}_8]$ and $[\text{SrO}_6]$ polyhedra sharing edges, with the two independent $(\text{H}_2\text{BTEC})^{2-}$ ligands coordinating to five- and six-metal cations, respectively. Compound (I) with its layered structure has a different set-up and is not comparable with these two previously reported structures.

6. Synthesis and crystallization

6.1. Synthesis

Chemicals were purchased from commercial sources and used without any further purification. Compound (I) was synthesized under hydrothermal conditions. 0.26 g (1 mmol) of $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$, 0.25 g (1 mmol) of pyromellitic acid (H_4BTEC)

Table 2

Experimental details.

Crystal data	
Chemical formula	$[\text{Sr}(\text{C}_{10}\text{H}_4\text{O}_8)(\text{H}_2\text{O})]$
M_r	357.77
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	295
a, b, c (Å)	25.8191 (7), 11.9726 (3), 7.1467 (2)
β (°)	90.662 (2)
V (Å ³)	2209.05 (10)
Z	8
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	4.93
Crystal size (mm)	0.23 × 0.14 × 0.10
Data collection	
Diffractometer	Oxford Diffraction Xcalibur, Ruby, Gemini
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2015)
T_{\min} , T_{\max}	0.833, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16106, 3417, 2700
R_{int}	0.045
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.734
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.086, 1.08
No. of reflections	3417
No. of parameters	199
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.70, -0.41

Computer programs: *CrysAlis CCD* (Oxford Diffraction, 2015), *CrysAlis RED* (Oxford Diffraction, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Berndt, 2001).

and 0.04 g (1 mmol) of NaOH were dissolved in water (13 ml). The reaction mixture was stirred at room temperature to homogeneity and then placed in a Teflon-lined stainless vessel (40 ml) and heated to 433 K for 3 d under autogenous pressure, and afterwards cooled to room temperature. The resulting product of plate-like single crystals and microcrystalline powder was filtered off, washed thoroughly with distilled water, and finally air-dried at room temperature.

6.2. Experimental details

Powder X-ray diffraction patterns were recorded on a Philips X'pert diffractometer with Cu $K\alpha$ radiation. The samples were gently ground in an agate mortar in order to minimize the preferred orientation. All data were collected at room temperature over the 2θ angular range of 4–60° with a step of 0.01° and a counting time of 1.5 s per step. IR spectra were recorded with a JASCO FTIR-6300 spectrometer in the region 4000–600 cm⁻¹. SEM micrographs and X-ray microanalysis (SEM/EDX) were recorded by using a JEOL-6610LV scanning electron microscope operating at 30 kV coupled with an Oxford X-Max microanalysis system (EDX). A Mettler-Toledo TGA/SDTA851e was used for the thermal analysis in a nitrogen dynamic atmosphere (50 ml min⁻¹) at a heating rate of 10 K min⁻¹. In this case, *ca* 10 mg of a powder sample were thermally treated, and blank runs were performed with the empty crucible.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound hydrogen atoms were placed in idealized positions and refined with $C-H = 0.93 \text{ \AA}$ and $U_{\text{iso}} = 1.2U_{\text{eq}}(C)$. The hydrogen atoms of the water molecule and of the carboxylic groups were located in a difference-Fourier map and were refined with $O-H = 0.93$ and 0.92 \AA , respectively, and with $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(O)$. One of the carboxylic OH functions (O4–H4) was found to be disordered over two sets of sites of equal occupancy.

Funding information

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supporting information

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Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2015); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2015); data reduction: *CrysAlis RED* (Oxford Diffraction, 2015); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Poly[aqua(μ_5 -2,5-dicarboxybenzene-1,4-dicarboxylato)strontium]

Crystal data

[Sr(C₁₀H₄O₈)(H₂O)]
 $M_r = 357.77$
 Monoclinic, *C2/c*
 Hall symbol: -C 2yc
 $a = 25.8191$ (7) Å
 $b = 11.9726$ (3) Å
 $c = 7.1467$ (2) Å
 $\beta = 90.662$ (2)°
 $V = 2209.05$ (10) Å³
 $Z = 8$

$F(000) = 1408$
 $D_x = 2.151$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 5087 reflections
 $\theta = 2.9$ – 30.9 °
 $\mu = 4.93$ mm⁻¹
 $T = 295$ K
 Prism, colorless
 $0.23 \times 0.14 \times 0.10$ mm

Data collection

Oxford Diffraction Xcalibur, Ruby, Gemini diffractometer
 Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
 Graphite monochromator
 Detector resolution: 10.2673 pixels mm⁻¹
 CCD rotation images, thick slices scans
 Absorption correction: multi-scan (*CrysAlis Pro*; Oxford Diffraction, 2015)

$T_{\min} = 0.833$, $T_{\max} = 1.000$
 16106 measured reflections
 3417 independent reflections
 2700 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$
 $\theta_{\max} = 31.5$ °, $\theta_{\min} = 2.9$ °
 $h = -36$ → 37
 $k = -17$ → 16
 $l = -9$ → 10

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.086$
 $S = 1.08$

3417 reflections
 199 parameters
 2 restraints
 0 constraints
 Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0329P)^2 + 3.281P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.007$
 $\Delta\rho_{\max} = 0.70 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.41 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.86646 (10)	0.8405 (2)	0.6041 (4)	0.0220 (5)	
C2	0.86705 (10)	0.7142 (2)	0.6075 (3)	0.0212 (5)	
C3	0.82120 (11)	0.6600 (2)	0.6499 (4)	0.0245 (6)	
H3	0.7921	0.703	0.6754	0.029*	
C4	0.81681 (10)	0.5436 (2)	0.6561 (4)	0.0222 (5)	
C5	0.86102 (10)	0.4787 (2)	0.6146 (3)	0.0206 (5)	
C6	0.90708 (11)	0.5344 (2)	0.5760 (4)	0.0252 (6)	
H6	0.9366	0.4923	0.5527	0.03*	
C7	0.91076 (11)	0.6508 (2)	0.5708 (4)	0.0240 (6)	
C8	0.96109 (11)	0.7054 (2)	0.5286 (4)	0.0310 (6)	
C9	0.86422 (11)	0.3525 (2)	0.6049 (4)	0.0253 (6)	
C10	0.76333 (11)	0.5051 (2)	0.7169 (4)	0.0290 (6)	
O1	0.86950 (8)	0.89053 (15)	0.7574 (3)	0.0306 (5)	
O2	0.86043 (9)	0.88916 (15)	0.4518 (3)	0.0346 (5)	
O1W	0.95292 (11)	0.9470 (2)	1.1096 (5)	0.0641 (8)	
H2W	0.9779 (14)	0.908 (4)	1.077 (7)	0.096*	
H1W	0.959 (2)	1.012 (2)	1.076 (7)	0.096*	
O3	0.96836 (9)	0.80320 (18)	0.5342 (5)	0.0607 (8)	
O4A	1.0004 (6)	0.6356 (8)	0.533 (7)	0.049 (6)	0.50 (7)
H4A	1.0275	0.6705	0.5217	0.073*	0.50 (7)
O4B	0.9931 (6)	0.6371 (9)	0.438 (6)	0.044 (4)	0.50 (7)
H4B	1.022	0.6653	0.4338	0.066*	0.50 (7)
O5	0.90652 (8)	0.30446 (16)	0.5932 (3)	0.0361 (5)	
O6	0.82258 (8)	0.29547 (16)	0.6041 (3)	0.0393 (5)	
O7	0.73445 (9)	0.57112 (19)	0.7873 (4)	0.0531 (7)	
O8	0.74913 (10)	0.40310 (19)	0.7001 (5)	0.0699 (10)	
H8	0.7727	0.3666	0.6541	0.105*	
Sr	0.85719 (2)	0.90596 (2)	1.10167 (3)	0.02469 (9)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0257 (14)	0.0109 (11)	0.0295 (13)	0.0010 (9)	0.0059 (11)	0.0014 (10)
C2	0.0295 (14)	0.0118 (11)	0.0222 (12)	0.0040 (10)	-0.0010 (11)	0.0013 (10)
C3	0.0274 (14)	0.0143 (12)	0.0318 (14)	0.0049 (10)	0.0014 (11)	0.0000 (11)

C4	0.0276 (14)	0.0143 (12)	0.0247 (13)	0.0012 (10)	0.0004 (11)	0.0000 (10)
C5	0.0283 (13)	0.0089 (10)	0.0247 (12)	0.0030 (10)	0.0017 (10)	-0.0009 (10)
C6	0.0272 (14)	0.0132 (12)	0.0352 (15)	0.0028 (10)	0.0025 (11)	0.0009 (11)
C7	0.0288 (14)	0.0114 (12)	0.0321 (14)	0.0007 (10)	0.0050 (11)	0.0014 (10)
C8	0.0293 (15)	0.0159 (13)	0.0479 (18)	0.0019 (11)	0.0065 (13)	0.0005 (12)
C9	0.0360 (16)	0.0126 (12)	0.0276 (13)	0.0001 (11)	0.0051 (12)	0.0004 (11)
C10	0.0270 (14)	0.0197 (13)	0.0405 (16)	0.0008 (11)	0.0028 (12)	-0.0007 (12)
O1	0.0493 (13)	0.0143 (9)	0.0283 (10)	-0.0005 (8)	0.0061 (9)	-0.0026 (8)
O2	0.0604 (15)	0.0153 (9)	0.0281 (10)	0.0013 (9)	-0.0010 (10)	0.0045 (8)
O1W	0.0398 (15)	0.0346 (14)	0.118 (3)	0.0015 (12)	0.0062 (16)	-0.0016 (17)
O3	0.0397 (13)	0.0185 (11)	0.124 (3)	-0.0074 (10)	0.0248 (14)	-0.0081 (13)
O4A	0.028 (3)	0.016 (2)	0.103 (18)	0.005 (2)	0.017 (6)	0.011 (5)
O4B	0.030 (4)	0.024 (3)	0.079 (12)	0.004 (2)	0.017 (5)	0.004 (4)
O5	0.0336 (11)	0.0132 (9)	0.0617 (14)	0.0025 (8)	0.0069 (10)	-0.0006 (9)
O6	0.0342 (11)	0.0135 (9)	0.0704 (15)	-0.0028 (8)	0.0131 (10)	-0.0022 (10)
O7	0.0299 (12)	0.0283 (12)	0.102 (2)	0.0011 (10)	0.0166 (13)	-0.0157 (13)
O8	0.0455 (15)	0.0218 (12)	0.143 (3)	-0.0086 (10)	0.0482 (17)	-0.0161 (14)
Sr	0.03497 (15)	0.01095 (12)	0.02837 (14)	-0.00125 (10)	0.01032 (10)	-0.00039 (10)

Geometric parameters (Å, °)

C1—O2	1.243 (3)	C10—O7	1.201 (3)
C1—O1	1.251 (3)	C10—O8	1.280 (3)
C1—C2	1.512 (3)	O1—Sr	2.4915 (19)
C1—Sr ⁱ	3.045 (3)	O1—Sr ⁱ	2.6959 (19)
C2—C3	1.386 (4)	O2—Sr ⁱⁱⁱ	2.510 (2)
C2—C7	1.388 (4)	O2—Sr ⁱ	2.6785 (19)
C3—C4	1.400 (4)	O1W—Sr	2.520 (3)
C3—H3	0.93	O1W—H2W	0.830 (19)
C4—C5	1.415 (3)	O1W—H1W	0.826 (19)
C4—C10	1.524 (4)	O4A—H4A	0.82
C5—C6	1.394 (4)	O4B—H4B	0.82
C5—C9	1.516 (4)	O5—Sr ⁱⁱ	2.8238 (19)
C6—C7	1.397 (3)	O6—Sr ⁱⁱ	2.572 (2)
C6—H6	0.93	O7—Sr ^{iv}	2.519 (2)
C7—C8	1.488 (4)	O8—H8	0.82
C8—O3	1.187 (3)	Sr—O2 ^v	2.510 (2)
C8—O4A	1.314 (12)	Sr—O7 ^{iv}	2.519 (2)
C8—O4B	1.337 (12)	Sr—O6 ^{vi}	2.572 (2)
C9—O5	1.238 (3)	Sr—O2 ^{vii}	2.6785 (19)
C9—O6	1.273 (3)	Sr—O1 ^{vii}	2.6959 (19)
C9—Sr ⁱⁱ	3.099 (3)	Sr—O5 ^{vi}	2.8239 (19)
O2—C1—O1	123.3 (2)	C1—O2—Sr ⁱⁱⁱ	155.89 (18)
O2—C1—C2	119.0 (2)	C1—O2—Sr ⁱ	94.78 (16)
O1—C1—C2	117.7 (2)	Sr ⁱⁱⁱ —O2—Sr ⁱ	108.93 (7)
O2—C1—Sr ⁱ	61.23 (14)	Sr—O1W—H2W	131 (4)
O1—C1—Sr ⁱ	62.05 (13)	Sr—O1W—H1W	112 (4)

C2—C1—Sr ⁱ	176.01 (17)	H2W—O1W—H1W	107 (5)
C3—C2—C7	118.9 (2)	C8—O4A—H4A	109.5
C3—C2—C1	117.6 (2)	C8—O4B—H4B	109.5
C7—C2—C1	123.5 (2)	C9—O5—Sr ⁱⁱ	90.82 (16)
C2—C3—C4	122.9 (2)	C9—O6—Sr ⁱⁱ	102.06 (16)
C2—C3—H3	118.6	C10—O7—Sr ^{iv}	142.5 (2)
C4—C3—H3	118.6	C10—O8—H8	109.5
C3—C4—C5	118.3 (2)	O1—Sr—O2 ^v	167.19 (7)
C3—C4—C10	112.6 (2)	O1—Sr—O7 ^{iv}	116.75 (9)
C5—C4—C10	129.0 (2)	O2 ^v —Sr—O7 ^{iv}	73.47 (9)
C6—C5—C4	118.1 (2)	O1—Sr—O1W	84.28 (10)
C6—C5—C9	114.9 (2)	O2 ^v —Sr—O1W	88.39 (10)
C4—C5—C9	127.0 (2)	O7 ^{iv} —Sr—O1W	153.66 (10)
C5—C6—C7	122.7 (2)	O1—Sr—O6 ^{vi}	89.16 (7)
C5—C6—H6	118.6	O2 ^v —Sr—O6 ^{vi}	85.74 (7)
C7—C6—H6	118.6	O7 ^{iv} —Sr—O6 ^{vi}	76.84 (7)
C2—C7—C6	119.0 (2)	O1W—Sr—O6 ^{vi}	121.57 (8)
C2—C7—C8	120.8 (2)	O1—Sr—O2 ^{vii}	70.61 (6)
C6—C7—C8	120.2 (2)	O2 ^v —Sr—O2 ^{vii}	118.11 (5)
O3—C8—O4A	120.3 (7)	O7 ^{iv} —Sr—O2 ^{vii}	93.44 (8)
O3—C8—O4B	121.4 (6)	O1W—Sr—O2 ^{vii}	78.18 (9)
O3—C8—C7	124.4 (3)	O6 ^{vi} —Sr—O2 ^{vii}	150.91 (7)
O4A—C8—C7	113.1 (5)	O1—Sr—O1 ^{vii}	117.32 (5)
O4B—C8—C7	112.1 (5)	O2 ^v —Sr—O1 ^{vii}	70.04 (6)
O5—C9—O6	119.8 (2)	O7 ^{iv} —Sr—O1 ^{vii}	83.01 (7)
O5—C9—C5	121.0 (2)	O1W—Sr—O1 ^{vii}	72.76 (8)
O6—C9—C5	119.2 (2)	O6 ^{vi} —Sr—O1 ^{vii}	152.13 (7)
O5—C9—Sr ⁱⁱ	65.65 (14)	O2 ^{vii} —Sr—O1 ^{vii}	48.19 (6)
O6—C9—Sr ⁱⁱ	54.25 (13)	O1—Sr—O5 ^{vi}	81.37 (6)
C5—C9—Sr ⁱⁱ	173.12 (18)	O2 ^v —Sr—O5 ^{vi}	86.56 (7)
O7—C10—O8	119.3 (3)	O7 ^{iv} —Sr—O5 ^{vi}	121.96 (7)
O7—C10—C4	119.3 (3)	O1W—Sr—O5 ^{vi}	74.46 (8)
O8—C10—C4	121.4 (2)	O6 ^{vi} —Sr—O5 ^{vi}	47.19 (6)
C1—O1—Sr	153.31 (17)	O2 ^{vii} —Sr—O5 ^{vi}	142.39 (6)
C1—O1—Sr ⁱ	93.76 (15)	O1 ^{vii} —Sr—O5 ^{vi}	139.83 (6)
Sr—O1—Sr ⁱ	108.96 (7)		
O2—C1—C2—C3	-96.5 (3)	C6—C7—C8—O4B	22 (2)
O1—C1—C2—C3	79.9 (3)	C6—C5—C9—O5	10.9 (4)
O2—C1—C2—C7	83.5 (3)	C4—C5—C9—O5	-169.8 (3)
O1—C1—C2—C7	-100.0 (3)	C6—C5—C9—O6	-167.3 (2)
C7—C2—C3—C4	-0.5 (4)	C4—C5—C9—O6	12.0 (4)
C1—C2—C3—C4	179.5 (2)	C3—C4—C10—O7	-14.4 (4)
C2—C3—C4—C5	-0.9 (4)	C5—C4—C10—O7	162.8 (3)
C2—C3—C4—C10	176.7 (2)	C3—C4—C10—O8	167.8 (3)
C3—C4—C5—C6	2.1 (4)	C5—C4—C10—O8	-15.0 (5)
C10—C4—C5—C6	-175.0 (3)	O2—C1—O1—Sr	149.6 (3)
C3—C4—C5—C9	-177.2 (2)	C2—C1—O1—Sr	-26.7 (5)

C10—C4—C5—C9	5.8 (5)	Sr ⁱ —C1—O1—Sr	148.8 (4)
C4—C5—C6—C7	-2.1 (4)	O2—C1—O1—Sr ⁱ	0.8 (3)
C9—C5—C6—C7	177.3 (3)	C2—C1—O1—Sr ⁱ	-175.5 (2)
C3—C2—C7—C6	0.6 (4)	O1—C1—O2—Sr ⁱⁱⁱ	168.9 (3)
C1—C2—C7—C6	-179.5 (3)	C2—C1—O2—Sr ⁱⁱⁱ	-14.9 (6)
C3—C2—C7—C8	-178.7 (3)	Sr ⁱ —C1—O2—Sr ⁱⁱⁱ	169.7 (5)
C1—C2—C7—C8	1.3 (4)	O1—C1—O2—Sr ⁱ	-0.8 (3)
C5—C6—C7—C2	0.7 (4)	C2—C1—O2—Sr ⁱ	175.5 (2)
C5—C6—C7—C8	-180.0 (3)	O6—C9—O5—Sr ⁱⁱ	-3.8 (3)
C2—C7—C8—O3	4.7 (5)	C5—C9—O5—Sr ⁱⁱ	178.0 (2)
C6—C7—C8—O3	-174.6 (3)	O5—C9—O6—Sr ⁱⁱ	4.3 (3)
C2—C7—C8—O4A	168 (2)	C5—C9—O6—Sr ⁱⁱ	-177.48 (19)
C6—C7—C8—O4A	-12 (2)	O8—C10—O7—Sr ^{iv}	-9.8 (6)
C2—C7—C8—O4B	-159.0 (19)	C4—C10—O7—Sr ^{iv}	172.4 (3)

Symmetry codes: (i) $x, -y+2, z-1/2$; (ii) $x, -y+1, z-1/2$; (iii) $x, y, z-1$; (iv) $-x+3/2, -y+3/2, -z+2$; (v) $x, y, z+1$; (vi) $x, -y+1, z+1/2$; (vii) $x, -y+2, z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O3 ^{vii}	0.83	2.25	3.0666 (3)	170
O1W—H2W \cdots O3 ^{viii}	0.83	2.04	2.864 (4)	171
O4A—H4A \cdots O5 ^{ix}	0.82	1.92	2.68 (2)	152
O4B—H4B \cdots O5 ^{ix}	0.82	1.89	2.696 (16)	166
O8—H8 \cdots O6	0.82	1.59	2.400 (3)	169
C6—H6 \cdots O4A ^{ix}	0.93	2.32	3.240 (18)	169
C6—H6 \cdots O4B ^{ix}	0.93	2.39	3.298 (14)	166

Symmetry codes: (vii) $x, -y+2, z+1/2$; (viii) $-x+2, y, -z+3/2$; (ix) $-x+2, -y+1, -z+1$.