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Poly[tetraqua(μ_8 -butane-1,2,3,4-tetra-carboxylato)distrontium]Pei-Chi Cheng,^a Jun-Xiang Zhan,^b Cheng-You Wu^b and Chia-Her Lin^{b*}^aDepartment of Chemistry, R&D Center for Membrane Technology, Center for Nanotechnology, Chung-Yuan Christian University, Chung-Li 320, Taiwan, and^bDepartment of Chemistry, Chung-Yuan Christian University, Chung-Li 320, Taiwan

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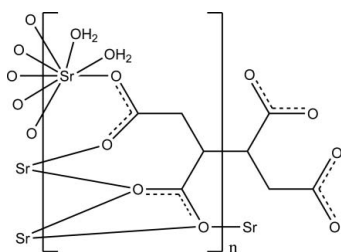
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.028; wR factor = 0.061; data-to-parameter ratio = 17.5.

In the title compound, $[\text{Sr}_2(\text{C}_8\text{H}_6\text{O}_8)(\text{H}_2\text{O})_4]_n$, the Sr^{II} ion is coordinated by six O atoms of four symmetry-related ligands and two water molecules in a distorted bicapped trigonal-prismatic environment. The butane-1,2,3,4-tetracarboxylate ligands lie on inversion centers and bridge Sr^{II} ions, forming a three-dimensional network. Within the three-dimensional structure, there are $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds involving the water molecules and carboxylate O atoms.

Related literature

For general background to coordination polymers, see: Jiang & Xu (2011); Kam *et al.* (2007); Kitagawa *et al.* (2004); Liu *et al.* (2009). For related structures, see: Ma & Yan (2009); Wu (2009).



Experimental

Crystal data

 $[\text{Sr}_2(\text{C}_8\text{H}_6\text{O}_8)(\text{H}_2\text{O})_4]$ $M_r = 477.44$ Monoclinic, $P2_1/n$ $a = 8.7085$ (4) Å $b = 7.9671$ (4) Å $c = 10.0697$ (4) Å $\beta = 95.409$ (2)°
 $V = 695.54$ (5) Å³
 $Z = 2$
Mo $K\alpha$ radiation $\mu = 7.73$ mm⁻¹
 $T = 296$ K
 $0.25 \times 0.15 \times 0.13$ mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2010)
 $T_{\text{min}} = 0.248$, $T_{\text{max}} = 0.433$ 7782 measured reflections
1746 independent reflections
1443 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.072$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.061$
 $S = 0.97$
1746 reflections100 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.58$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.46$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1W}-\text{H1WA}\cdots\text{O3}^{\text{i}}$	0.85	1.90	2.729 (3)	164.5
$\text{O1W}-\text{H1WB}\cdots\text{O4}^{\text{ii}}$	0.85	2.14	2.944 (3)	159.1
$\text{O2W}-\text{H2WA}\cdots\text{O4}$	0.85	2.06	2.841 (3)	153.1
$\text{O2W}-\text{H2WB}\cdots\text{O1W}^{\text{iii}}$	0.88	1.99	2.864 (3)	170.1

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

Data collection: APEX2 (Bruker, 2010); cell refinement: SAINT (Bruker, 2010); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2010); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5368).

References

- Brandenburg, K. (2010). DIAMOND. Crystal Impact GbR, Bonn, Germany.
Bruker (2010). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
Jiang, H.-L. & Xu, Q. (2011). Chem. Commun. **47**, 3351–3370.
Kam, K. C., Young, K. L. M. & Cheetham, A. K. (2007). Cryst. Growth Des. **7**, 1522–1532.
Kitagawa, S., Kitaura, R. & Noro, S. (2004). Angew. Chem. Int. Ed. **43**, 2334–2375.
Liu, H. K., Tsao, T. H., Zhang, Y. T. & Lin, C. H. (2009). CrystEngComm, **11**, 1462–1468.
Ma, C.-H. & Yan, Y.-S. (2009). Acta Cryst. E **65**, m1555.
Sheldrick, G. M. (2008). Acta Cryst. A **64**, 112–122.
Wu, L. (2009). Acta Cryst. E **65**, m1425.

supporting information

Acta Cryst. (2011). E67, m1700 [https://doi.org/10.1107/S1600536811046265]

Poly[tetraqua(μ_8 -butane-1,2,3,4-tetracarboxylato)distrontium]**Pei-Chi Cheng, Jun-Xiang Zhan, Cheng-You Wu and Chia-Her Lin****S1. Comment**

Multicarboxylate ligands, are widely used to construct coordination polymers with interesting properties (Kam, *et al.*, 2007; Liu, *et al.*, 2009, Kitagawa *et al.*, 2004; Jiang & Xu, 2011). The butane-1,2,3,4-tetracarboxylato ligand has already been reported in crystal structures (Ma & Yan, 2009; Wu, 2009). In our continuing investigations on metal coordination polymers we report here the structure of a new Sr coordination polymer based on butane-1,2,3,4-tetracarboxylic acid.

The asymmetric unit of the title compound consists of one strontium, one half carboxylate ligand and two coordinated water molecules (Fig. 1). The strontium is eight coordinated by six O atoms of four symmetry related ligands and two water molecules. The Sr—O distances range from 2.5491 (18) to 2.688 (2) Å. The ligands bridge the neighboring Sr^{II} centers forming a three-dimensional framework structure (Fig. 2). The hydrogen bonds involving the water molecules and the carboxylate O atoms further stabilize the three dimensional structure.

S2. Experimental

Solvothermal reactions were carried out at 363 K for 2 d in a Teflon-lined acid digestion bomb with an internal volume of 23 ml followed by slow cooling at 6 K/h to room temperature. A single-phase product consisting of colorless crystals of was obtained from a mixture of butane-1,2,3,4-tetracarboxylic acid (C₈H₁₀O₈, 0.0468 g, 0.2 mmol), Sr(NO₃)₂ (0.0847 g, 0.4 mmol), and ethanol (5.0 ml) and H₂O (1.0 ml).

S3. Refinement

H atoms were constrained to ideal geometries, with C—H = 0.96–0.98 Å, O—H = 0.85–0.88 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}); U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

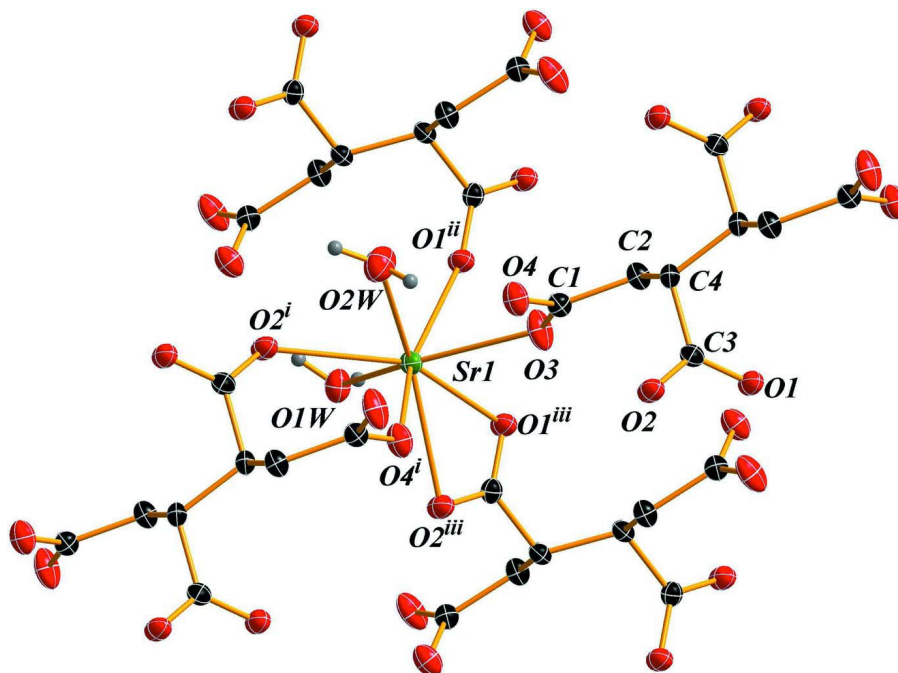


Figure 1

A view of part of the title structure, showing 50% probability displacement ellipsoids. [symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $-x + 1/2, y + 1/2, -z + 1/2$; (iii) $x - 1/2, -y - 1/2, z + 1/2$].

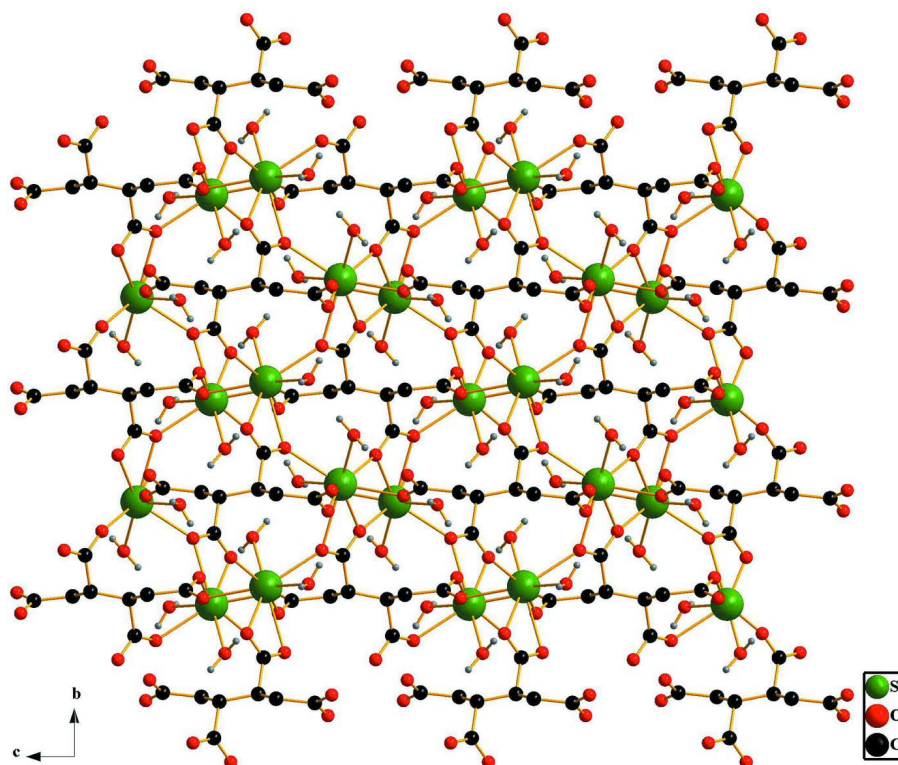


Figure 2

Part of the crystal structure of the title compound viewed along the *a* axis.

Poly[tetraaqua(μ_8 -butane-1,2,3,4-tetracarboxylato)distrontium]

Crystal data

[Sr₂(C₈H₆O₈)(H₂O)₄]

$M_r = 477.44$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.7085$ (4) Å

$b = 7.9671$ (4) Å

$c = 10.0697$ (4) Å

$\beta = 95.409$ (2)°

$V = 695.54$ (5) Å³

$Z = 2$

$F(000) = 468$

$D_x = 2.280$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4783 reflections

$\theta = 3.0$ – 28.5 °

$\mu = 7.73$ mm⁻¹

$T = 296$ K

Tabular, colourless

$0.25 \times 0.15 \times 0.13$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.3333 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2010)

$T_{\min} = 0.248$, $T_{\max} = 0.433$

7782 measured reflections

1746 independent reflections

1443 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.072$

$\theta_{\max} = 28.7$ °, $\theta_{\min} = 3.0$ °

$h = -11 \rightarrow 11$

$k = -8 \rightarrow 10$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.061$

$S = 0.97$

1746 reflections

100 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.58$ e Å⁻³

$\Delta\rho_{\min} = -0.46$ e Å⁻³

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.22086 (2)	0.04306 (3)	0.60530 (2)	0.01806 (9)

O3	0.2772 (2)	-0.0137 (3)	0.36082 (19)	0.0333 (5)
O1W	0.0092 (2)	0.0561 (3)	0.7699 (2)	0.0285 (5)
H1WA	-0.0857	0.0434	0.7437	0.043*
H1WB	0.0108	0.1483	0.8122	0.043*
O2W	0.4040 (2)	0.2833 (3)	0.5536 (2)	0.0405 (6)
H2WA	0.4624	0.2227	0.5104	0.061*
H2WB	0.4420	0.3623	0.6089	0.061*
O1	0.5067 (2)	-0.3138 (2)	0.03110 (18)	0.0249 (4)
O2	0.69087 (19)	-0.2208 (3)	0.17764 (18)	0.0249 (4)
O4	0.5123 (2)	0.0870 (3)	0.34605 (19)	0.0281 (5)
C1	0.3872 (3)	0.0252 (4)	0.2949 (2)	0.0194 (5)
C2	0.3645 (3)	0.0043 (4)	0.1447 (2)	0.0202 (6)
H2A	0.3107	0.1013	0.1075	0.024*
H2B	0.3001	-0.0920	0.1243	0.024*
C3	0.5739 (3)	-0.1966 (4)	0.0963 (2)	0.0183 (5)
C4	0.5134 (3)	-0.0185 (4)	0.0755 (2)	0.0174 (5)
H4A	0.5914	0.0597	0.1156	0.021*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01577 (12)	0.01900 (17)	0.01883 (12)	-0.00105 (10)	-0.00146 (8)	-0.00014 (10)
O3	0.0215 (9)	0.0593 (17)	0.0201 (9)	-0.0077 (9)	0.0072 (8)	-0.0053 (9)
O1W	0.0222 (9)	0.0352 (14)	0.0281 (10)	0.0005 (8)	0.0025 (8)	-0.0077 (9)
O2W	0.0443 (12)	0.0363 (15)	0.0418 (12)	-0.0080 (11)	0.0088 (10)	-0.0065 (11)
O1	0.0272 (9)	0.0188 (12)	0.0268 (9)	-0.0009 (8)	-0.0074 (8)	-0.0012 (8)
O2	0.0249 (9)	0.0185 (11)	0.0295 (10)	0.0031 (8)	-0.0080 (8)	-0.0007 (8)
O4	0.0196 (9)	0.0405 (15)	0.0237 (9)	-0.0016 (8)	-0.0004 (7)	-0.0038 (9)
C1	0.0171 (11)	0.0219 (16)	0.0193 (12)	0.0025 (11)	0.0027 (9)	0.0002 (11)
C2	0.0157 (11)	0.0272 (17)	0.0177 (11)	-0.0007 (10)	0.0016 (9)	0.0003 (11)
C3	0.0181 (11)	0.0195 (16)	0.0176 (11)	-0.0007 (10)	0.0029 (9)	0.0026 (10)
C4	0.0182 (11)	0.0195 (16)	0.0144 (11)	-0.0016 (10)	0.0016 (9)	-0.0024 (10)

Geometric parameters (\AA , $^\circ$)

Sr1—O4 ⁱ	2.5491 (18)	O1—Sr1 ^{iv}	2.5689 (17)
Sr1—O1 ⁱⁱ	2.5690 (17)	O1—Sr1 ^v	2.6666 (18)
Sr1—O2W	2.576 (2)	O2—C3	1.260 (3)
Sr1—O1W	2.5946 (19)	O2—Sr1 ⁱ	2.6565 (18)
Sr1—O3	2.5948 (19)	O2—Sr1 ^v	2.688 (2)
Sr1—O2 ⁱ	2.6565 (18)	O4—C1	1.260 (3)
Sr1—O1 ⁱⁱⁱ	2.6666 (18)	O4—Sr1 ⁱ	2.5492 (18)
Sr1—O2 ⁱⁱⁱ	2.688 (2)	C1—C2	1.516 (3)
Sr1—C3 ⁱⁱⁱ	3.040 (3)	C2—C4	1.540 (3)
Sr1—H2WA	2.7869	C2—H2A	0.9615
O3—C1	1.254 (3)	C2—H2B	0.9614
O1W—H1WA	0.8501	C3—C4	1.521 (4)
O1W—H1WB	0.8483	C3—Sr1 ^v	3.040 (3)

O2W—H2WA	0.8499	C4—C4 ^{vi}	1.544 (5)
O2W—H2WB	0.8836	C4—H4A	0.9800
O1—C3	1.254 (3)		
O4 ⁱ —Sr1—O1 ⁱⁱ	157.86 (6)	O4 ⁱ —Sr1—H2WA	64.6
O4 ⁱ —Sr1—O2W	76.72 (7)	O1 ⁱⁱ —Sr1—H2WA	99.1
O1 ⁱⁱ —Sr1—O2W	91.33 (6)	O2W—Sr1—H2WA	17.7
O4 ⁱ —Sr1—O1W	125.67 (6)	O1W—Sr1—H2WA	143.4
O1 ⁱⁱ —Sr1—O1W	76.42 (6)	O3—Sr1—H2WA	63.1
O2W—Sr1—O1W	126.16 (7)	O2 ⁱ —Sr1—H2WA	80.7
O4 ⁱ —Sr1—O3	82.01 (6)	O1 ⁱⁱⁱ —Sr1—H2WA	141.8
O1 ⁱⁱ —Sr1—O3	77.02 (6)	O2 ⁱⁱⁱ —Sr1—H2WA	132.8
O2W—Sr1—O3	76.20 (7)	C3 ⁱⁱⁱ —Sr1—H2WA	141.7
O1W—Sr1—O3	145.32 (6)	Sr1 ^{vii} —Sr1—H2WA	125.9
O4 ⁱ —Sr1—O2 ⁱ	82.57 (6)	C1—O3—Sr1	132.92 (17)
O1 ⁱⁱ —Sr1—O2 ⁱ	110.61 (6)	Sr1—O1W—H1WA	121.7
O2W—Sr1—O2 ⁱ	68.51 (6)	Sr1—O1W—H1WB	112.2
O1W—Sr1—O2 ⁱ	67.72 (6)	H1WA—O1W—H1WB	103.2
O3—Sr1—O2 ⁱ	143.85 (6)	Sr1—O2W—H2WA	95.3
O4 ⁱ —Sr1—O1 ⁱⁱⁱ	112.11 (6)	Sr1—O2W—H2WB	127.1
O1 ⁱⁱ —Sr1—O1 ⁱⁱⁱ	70.75 (7)	H2WA—O2W—H2WB	121.4
O2W—Sr1—O1 ⁱⁱⁱ	151.93 (6)	C3—O1—Sr1 ^{iv}	155.35 (16)
O1W—Sr1—O1 ⁱⁱⁱ	71.71 (6)	C3—O1—Sr1 ^v	94.78 (14)
O3—Sr1—O1 ⁱⁱⁱ	78.74 (6)	Sr1 ^{iv} —O1—Sr1 ^v	109.25 (7)
O2 ⁱ —Sr1—O1 ⁱⁱⁱ	137.41 (6)	C3—O2—Sr1 ⁱ	127.36 (17)
O4 ⁱ —Sr1—O2 ⁱⁱⁱ	70.72 (6)	C3—O2—Sr1 ^v	93.61 (16)
O1 ⁱⁱ —Sr1—O2 ⁱⁱⁱ	118.62 (5)	Sr1 ⁱ —O2—Sr1 ^v	134.76 (7)
O2W—Sr1—O2 ⁱⁱⁱ	147.38 (6)	C1—O4—Sr1 ⁱ	131.09 (19)
O1W—Sr1—O2 ⁱⁱⁱ	76.83 (6)	O3—C1—O4	123.7 (2)
O3—Sr1—O2 ⁱⁱⁱ	97.05 (7)	O3—C1—C2	117.8 (2)
O2 ⁱ —Sr1—O2 ⁱⁱⁱ	108.31 (3)	O4—C1—C2	118.5 (2)
O1 ⁱⁱⁱ —Sr1—O2 ⁱⁱⁱ	48.59 (5)	C1—C2—C4	115.4 (2)
O4 ⁱ —Sr1—C3 ⁱⁱⁱ	90.58 (7)	C1—C2—H2A	108.3
O1 ⁱⁱ —Sr1—C3 ⁱⁱⁱ	94.92 (6)	C4—C2—H2A	108.6
O2W—Sr1—C3 ⁱⁱⁱ	159.30 (7)	C1—C2—H2B	108.6
O1W—Sr1—C3 ⁱⁱⁱ	74.52 (6)	C4—C2—H2B	108.0
O3—Sr1—C3 ⁱⁱⁱ	86.00 (7)	H2A—C2—H2B	107.8
O2 ⁱ —Sr1—C3 ⁱⁱⁱ	126.65 (6)	O1—C3—O2	122.4 (2)
O1 ⁱⁱⁱ —Sr1—C3 ⁱⁱⁱ	24.28 (6)	O1—C3—C4	118.9 (2)
O2 ⁱⁱⁱ —Sr1—C3 ⁱⁱⁱ	24.44 (6)	O2—C3—C4	118.7 (2)
O4 ⁱ —Sr1—Sr1 ^{vii}	142.42 (5)	O1—C3—Sr1 ^v	60.94 (13)
O1 ⁱⁱ —Sr1—Sr1 ^{vii}	36.13 (4)	O2—C3—Sr1 ^v	61.95 (14)
O2W—Sr1—Sr1 ^{vii}	124.41 (5)	C4—C3—Sr1 ^v	172.02 (16)
O1W—Sr1—Sr1 ^{vii}	70.29 (4)	C3—C4—C2	110.1 (2)
O3—Sr1—Sr1 ^{vii}	75.10 (4)	C3—C4—C4 ^{vi}	109.4 (3)
O2 ⁱ —Sr1—Sr1 ^{vii}	132.19 (4)	C2—C4—C4 ^{vi}	111.5 (2)
O1 ⁱⁱⁱ —Sr1—Sr1 ^{vii}	34.62 (4)	C3—C4—H4A	108.6

O2 ⁱⁱⁱ —Sr1—Sr1 ^{vii}	82.83 (3)	C2—C4—H4A	108.6
C3 ⁱⁱⁱ —Sr1—Sr1 ^{vii}	58.82 (5)	C4 ^{vi} —C4—H4A	108.6

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1 <i>W</i> —H1 <i>WA</i> \cdots O3 ^{vii}	0.85	1.90	2.729 (3)	164.5
O1 <i>W</i> —H1 <i>WB</i> \cdots O4 ^{viii}	0.85	2.14	2.944 (3)	159.1
O2 <i>W</i> —H2 <i>WA</i> \cdots O4	0.85	2.06	2.841 (3)	153.1
O2 <i>W</i> —H2 <i>WB</i> \cdots O1 <i>W</i> ^{ix}	0.88	1.99	2.864 (3)	170.1

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