

Poly[μ_2 -aqua-aqua- μ_5 -naphthalene-2,7-disulfonato-strontium]

Shan Gao^a and Seik Weng Ng^{b,c,*}

^aKey Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, Heilongjiang University, Harbin 150080, People's Republic of China, ^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and ^cChemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia

Correspondence e-mail: seikweng@um.edu.my

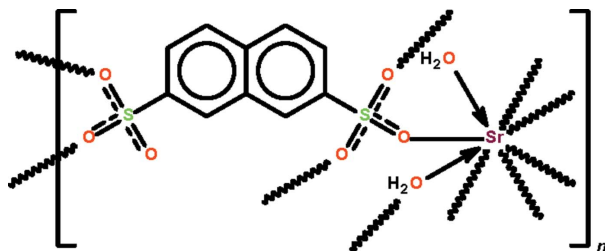
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.028; wR factor = 0.071; data-to-parameter ratio = 15.6.

In the crystal structure of the polymeric title compound, $[\text{Sr}(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)(\text{H}_2\text{O})_2]_n$, the naphthalene-2,7-disulfonate dianion uses one $-\text{SO}_3^-$ unit to bind to two Sr^{II} cations and the other $-\text{SO}_3^-$ unit to bind to three Sr^{II} cations; of the two coordinated water molecules, one is monodentate to one Sr^{II} cation, whereas the other bridges two Sr^{II} cations. The μ_5 -bridging mode of the dianion and the μ_2 -bridging mode of the water molecule generate a polymeric three-dimensional network which is consolidated by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds. The Sr^{II} cation exists in an undefined eight-coordinate environment.

Related literature

For a review of metal arenesulfonates, see: Cai (2004). For a related strontium naphthalenedisulfonate, see: Cai *et al.* (2001).



Experimental

Crystal data

$[\text{Sr}(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)(\text{H}_2\text{O})_2]$
 $M_r = 409.92$
 Orthorhombic, $Pna2_1$
 $a = 13.064$ (6) Å
 $b = 19.324$ (9) Å
 $c = 5.1989$ (17) Å

$V = 1312.5$ (9) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 4.46$ mm⁻¹
 $T = 293$ K
 $0.18 \times 0.12 \times 0.12$ mm

Data collection

Rigaku R-Axis RAPID IP
 diffractometer
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.501$, $T_{\text{max}} = 0.616$

11845 measured reflections
 2962 independent reflections
 2646 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.071$
 $S = 1.04$
 2962 reflections
 190 parameters
 1 restraint

H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.60$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.51$ e Å⁻³
 Absolute structure: Flack (1983),
 1584 Friedel pairs
 Flack parameter: -0.011 (6)

Table 1

Selected bond lengths (Å).

Sr1—O1	2.612 (2)	Sr1—O6 ^{iv}	2.540 (2)
Sr1—O2 ⁱ	2.494 (2)	Sr1—O1 ^w	2.614 (2)
Sr1—O3 ⁱⁱ	2.595 (2)	Sr1—O2 ^w	2.756 (3)
Sr1—O5 ⁱⁱⁱ	2.549 (2)	Sr1—O2 ^w ^v	2.974 (3)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1 ^w —H1 ^w 1 \cdots O4 ^{vi}	0.84	2.29	3.066 (4)	154
O1 ^w —H1 ^w 2 \cdots O4 ^{vii}	0.84	2.27	2.904 (4)	132
O2 ^w —H2 ^w 2 \cdots O4 ^{vii}	0.84	2.03	2.856 (3)	167

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5381).

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supplementary materials

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Poly[μ_2 -aqua-aqua- μ_5 -naphthalene-2,7-disulfonato-strontium]

S. Gao and S. W. Ng

Comment

A review of metal arenesulfonates that are synthesized in aqueous medium explains the reasons for the ability of the ions to form stable metal-organic frameworks owing to multiple coordination modes of the sulfonate $-\text{SO}_3$ groups (Cai, 2004). Among the divalent metal derivatives, the strontium system has been less studied (Cai *et al.*, 2001). In the crystal structure of $\text{Sr}(\text{H}_2\text{O})_2(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)$, the $\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2^{2-}$ dianion uses one $-\text{SO}_3$ unit to bind to two Sr^{II} atoms and the other $-\text{SO}_3$ unit to bind to three Sr^{II} atoms; of the two water molecules, one is monodentate to one Sr atom whereas the other bridge two Sr atoms (Scheme I, Fig. 1). The μ_5 -bridging mode of the dianion and the μ_2 -bridging mode of the water molecule generates a polymeric three-dimensional network; the network is consolidated by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1). The Sr atom exists in an undefined eight-coordinate environment.

Experimental

Strontium nitrate (1 mmol) and sodium naphthalene-2,7-disulfonate (1 mmol) were dissolved in water (10 ml). The solution was filtered and set aside; colorless crystals were isolated from the filtrate after several days.

Refinement

Hydrogen atoms were generated geometrically and were included in the riding model approximation [C—H 0.93 Å and O—H 0.84 Å, U 1.2 to $1.5U_{\text{eq}}(\text{C},\text{O})$]. The 3 7 2 reflection was omitted owing to bad agreement.

Figures

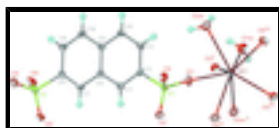


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of a fragment of polymeric $\text{Sr}(\text{H}_2\text{O})_2(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Poly[μ_2 -aqua-aqua- μ_5 -naphthalene-2,7-disulfonato-strontium]

Crystal data

[$\text{Sr}(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)(\text{H}_2\text{O})_2$]

$M_r = 409.92$

Orthorhombic, $Pna2_1$

Hall symbol: P 2c -2n

$a = 13.064(6)$ Å

$F(000) = 816$

$D_x = 2.075$ Mg m^{-3}

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

Cell parameters from 10271 reflections

$\theta = 3.1\text{--}27.5^\circ$

supplementary materials

$b = 19.324 (9) \text{ \AA}$
 $c = 5.1989 (17) \text{ \AA}$
 $V = 1312.5 (9) \text{ \AA}^3$
 $Z = 4$

$\mu = 4.46 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
Prism, colorless
 $0.18 \times 0.12 \times 0.12 \text{ mm}$

Data collection

Rigaku R-Axis RAPID IP
diffractometer
Radiation source: fine-focus sealed tube
graphite
 ω scan
Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.501$, $T_{\max} = 0.616$
11845 measured reflections

2962 independent reflections
2646 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.1^\circ$
 $h = -16 \rightarrow 16$
 $k = -24 \rightarrow 25$
 $l = -6 \rightarrow 6$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.071$
 $S = 1.04$
2962 reflections
190 parameters
1 restraint
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
 $w = 1/[\sigma^2(F_o^2) + (0.0383P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.60 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.51 \text{ e \AA}^{-3}$
Absolute structure: Flack (1983), 1584 Friedel pairs
Flack parameter: $-0.011 (6)$

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	-0.008465 (18)	0.635847 (12)	0.49937 (9)	0.02043 (9)
S1	0.14037 (4)	0.47764 (3)	0.49983 (18)	0.01857 (14)
S2	0.64351 (5)	0.24848 (3)	0.49376 (18)	0.01863 (14)
O1	0.14590 (15)	0.55148 (11)	0.5589 (4)	0.0294 (6)
O2	0.12497 (16)	0.43544 (11)	0.7268 (4)	0.0256 (5)
O3	0.06622 (16)	0.46443 (12)	0.2980 (4)	0.0285 (5)
O4	0.74894 (15)	0.27350 (11)	0.5219 (6)	0.0310 (5)
O5	0.63559 (18)	0.19599 (11)	0.2968 (4)	0.0294 (5)
O6	0.59963 (17)	0.22808 (12)	0.7371 (4)	0.0288 (5)
O1w	0.13881 (15)	0.72744 (11)	0.5039 (7)	0.0376 (5)
H1w1	0.1543	0.7369	0.6567	0.056*
H1w2	0.1903	0.7113	0.4278	0.056*
O2w	0.08346 (17)	0.63163 (10)	0.0225 (6)	0.0315 (5)

H2w1	0.1187	0.5953	0.0242	0.038*
H2w2	0.1257	0.6644	0.0242	0.038*
C1	0.3192 (2)	0.40460 (13)	0.4846 (8)	0.0208 (5)
H1	0.2958	0.3826	0.6325	0.025*
C2	0.2615 (2)	0.45518 (15)	0.3713 (5)	0.0187 (6)
C3	0.2939 (2)	0.48863 (15)	0.1474 (6)	0.0240 (7)
H3	0.2526	0.5222	0.0717	0.029*
C4	0.3857 (2)	0.47221 (15)	0.0399 (6)	0.0230 (7)
H4	0.4072	0.4949	-0.1083	0.028*
C5	0.4485 (2)	0.42073 (15)	0.1525 (6)	0.0195 (6)
C6	0.4143 (2)	0.38578 (15)	0.3764 (6)	0.0196 (6)
C7	0.4773 (2)	0.33370 (14)	0.4836 (9)	0.0205 (6)
H7	0.4555	0.3097	0.6287	0.025*
C8	0.5694 (2)	0.31837 (15)	0.3767 (5)	0.0196 (6)
C9	0.6062 (3)	0.35484 (15)	0.1587 (6)	0.0247 (7)
H9	0.6707	0.3451	0.0920	0.030*
C10	0.5462 (2)	0.40419 (15)	0.0481 (6)	0.0241 (7)
H10	0.5694	0.4274	-0.0974	0.029*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.02020 (14)	0.02060 (13)	0.02050 (13)	-0.00055 (9)	-0.00006 (17)	0.00153 (17)
S1	0.0168 (3)	0.0174 (3)	0.0215 (3)	0.0006 (2)	0.0002 (4)	-0.0011 (4)
S2	0.0182 (3)	0.0182 (3)	0.0195 (3)	-0.0003 (2)	-0.0002 (4)	0.0013 (4)
O1	0.0256 (12)	0.0186 (10)	0.0439 (18)	0.0013 (8)	0.0031 (10)	-0.0054 (9)
O2	0.0238 (12)	0.0276 (12)	0.0252 (11)	-0.0004 (9)	0.0028 (9)	0.0027 (9)
O3	0.0219 (12)	0.0363 (13)	0.0273 (11)	0.0012 (10)	-0.0039 (10)	-0.0047 (10)
O4	0.0206 (10)	0.0311 (11)	0.0414 (13)	-0.0040 (8)	-0.0073 (12)	0.0085 (14)
O5	0.0360 (14)	0.0235 (12)	0.0287 (12)	0.0056 (9)	-0.0051 (11)	-0.0047 (10)
O6	0.0355 (14)	0.0249 (11)	0.0260 (12)	0.0005 (10)	0.0050 (10)	0.0045 (10)
O1w	0.0341 (12)	0.0421 (13)	0.0366 (12)	-0.0059 (9)	-0.0008 (16)	-0.0050 (16)
O2w	0.0313 (11)	0.0307 (11)	0.0324 (13)	-0.0031 (9)	0.0037 (14)	-0.0060 (11)
C1	0.0234 (13)	0.0192 (12)	0.0197 (12)	-0.0033 (10)	-0.0004 (17)	-0.0003 (15)
C2	0.0143 (14)	0.0210 (14)	0.0210 (14)	-0.0008 (11)	-0.0003 (11)	-0.0046 (12)
C3	0.0243 (17)	0.0208 (14)	0.0270 (15)	0.0016 (12)	-0.0040 (14)	0.0028 (13)
C4	0.0253 (15)	0.0245 (14)	0.0193 (19)	-0.0021 (11)	-0.0002 (13)	0.0025 (12)
C5	0.0208 (16)	0.0184 (14)	0.0192 (15)	-0.0036 (12)	-0.0012 (12)	-0.0001 (12)
C6	0.0210 (16)	0.0159 (14)	0.0219 (14)	-0.0016 (12)	-0.0027 (12)	-0.0023 (12)
C7	0.0221 (13)	0.0210 (13)	0.0185 (14)	-0.0015 (10)	-0.0001 (16)	0.0049 (18)
C8	0.0224 (16)	0.0162 (14)	0.0202 (13)	0.0005 (12)	-0.0027 (12)	-0.0015 (11)
C9	0.0236 (17)	0.0257 (16)	0.0248 (16)	-0.0001 (12)	0.0064 (14)	0.0002 (13)
C10	0.0271 (16)	0.0243 (15)	0.021 (2)	0.0001 (12)	0.0041 (12)	0.0032 (12)

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

Sr1—O1	2.612 (2)	O1w—H1w2	0.8400
Sr1—O2 ⁱ	2.494 (2)	O2w—Sr1 ^{viii}	2.974 (3)

supplementary materials

Sr1—O3 ⁱⁱ	2.595 (2)	O2w—H2w1	0.8400
Sr1—O5 ⁱⁱⁱ	2.549 (2)	O2w—H2w2	0.8400
Sr1—O6 ^{iv}	2.540 (2)	C1—C2	1.367 (4)
Sr1—O1w	2.614 (2)	C1—C6	1.412 (4)
Sr1—O2w	2.756 (3)	C1—H1	0.9300
Sr1—O2w ^v	2.974 (3)	C2—C3	1.397 (4)
S1—O2	1.448 (2)	C3—C4	1.360 (4)
S1—O3	1.451 (2)	C3—H3	0.9300
S1—O1	1.461 (2)	C4—C5	1.417 (4)
S1—C2	1.772 (3)	C4—H4	0.9300
S2—O6	1.444 (2)	C5—C6	1.418 (4)
S2—O5	1.445 (2)	C5—C10	1.423 (4)
S2—O4	1.467 (2)	C6—C7	1.414 (4)
S2—C8	1.769 (3)	C7—C8	1.358 (4)
O2—Sr1 ⁱⁱ	2.494 (2)	C7—H7	0.9300
O3—Sr1 ⁱ	2.595 (2)	C8—C9	1.418 (4)
O5—Sr1 ^{vi}	2.549 (2)	C9—C10	1.362 (4)
O6—Sr1 ^{vii}	2.540 (2)	C9—H9	0.9300
O1w—H1w1	0.8400	C10—H10	0.9300
O2 ⁱ —Sr1—O6 ^{iv}	78.25 (8)	S1—O3—Sr1 ⁱ	139.31 (13)
O2 ⁱ —Sr1—O5 ⁱⁱⁱ	101.47 (8)	S2—O5—Sr1 ^{vi}	142.79 (14)
O6 ^{iv} —Sr1—O5 ⁱⁱⁱ	72.56 (8)	S2—O6—Sr1 ^{vii}	147.99 (15)
O2 ⁱ —Sr1—O3 ⁱⁱ	75.53 (8)	Sr1—O1w—H1w1	109.5
O6 ^{iv} —Sr1—O3 ⁱⁱ	135.12 (7)	Sr1—O1w—H1w2	109.5
O5 ⁱⁱⁱ —Sr1—O3 ⁱⁱ	77.77 (8)	H1w1—O1w—H1w2	109.5
O2 ⁱ —Sr1—O1	101.17 (7)	Sr1—O2w—Sr1 ^{viii}	130.23 (8)
O6 ^{iv} —Sr1—O1	149.72 (7)	Sr1—O2w—H2w1	104.7
O5 ⁱⁱⁱ —Sr1—O1	135.70 (8)	Sr1 ^{viii} —O2w—H2w1	104.7
O3 ⁱⁱ —Sr1—O1	71.79 (7)	Sr1—O2w—H2w2	104.7
O2 ⁱ —Sr1—O1w	145.90 (10)	Sr1 ^{viii} —O2w—H2w2	104.7
O6 ^{iv} —Sr1—O1w	82.82 (8)	H2w1—O2w—H2w2	105.7
O5 ⁱⁱⁱ —Sr1—O1w	99.51 (9)	C2—C1—C6	119.8 (3)
O3 ⁱⁱ —Sr1—O1w	135.57 (9)	C2—C1—H1	120.1
O1—Sr1—O1w	81.56 (8)	C6—C1—H1	120.1
O2 ⁱ —Sr1—O2w	74.84 (7)	C1—C2—C3	121.5 (3)
O6 ^{iv} —Sr1—O2w	75.06 (7)	C1—C2—S1	120.3 (2)
O5 ⁱⁱⁱ —Sr1—O2w	147.45 (7)	C3—C2—S1	118.1 (2)
O3 ⁱⁱ —Sr1—O2w	130.00 (7)	C4—C3—C2	120.1 (3)
O1—Sr1—O2w	75.62 (7)	C4—C3—H3	120.0
O1w—Sr1—O2w	72.99 (10)	C2—C3—H3	120.0
O2 ⁱ —Sr1—O2w ^v	138.66 (7)	C3—C4—C5	120.3 (3)
O6 ^{iv} —Sr1—O2w ^v	134.37 (7)	C3—C4—H4	119.8
O5 ⁱⁱⁱ —Sr1—O2w ^v	73.79 (7)	C5—C4—H4	119.8

O3 ⁱⁱ —Sr1—O2w ^v	63.25 (7)	C4—C5—C6	119.4 (3)
O1—Sr1—O2w ^v	64.07 (7)	C4—C5—C10	121.3 (3)
O1w—Sr1—O2w ^v	73.33 (9)	C6—C5—C10	119.2 (3)
O2w—Sr1—O2w ^v	130.23 (8)	C1—C6—C7	122.6 (3)
O2—S1—O3	113.41 (13)	C1—C6—C5	118.8 (3)
O2—S1—O1	112.68 (14)	C7—C6—C5	118.6 (3)
O3—S1—O1	110.90 (13)	C8—C7—C6	120.6 (3)
O2—S1—C2	107.06 (13)	C8—C7—H7	119.7
O3—S1—C2	106.29 (14)	C6—C7—H7	119.7
O1—S1—C2	105.92 (13)	C7—C8—C9	121.2 (3)
O6—S2—O5	113.63 (13)	C7—C8—S2	120.7 (2)
O6—S2—O4	112.04 (16)	C9—C8—S2	118.0 (2)
O5—S2—O4	111.67 (15)	C10—C9—C8	119.4 (3)
O6—S2—C8	107.02 (14)	C10—C9—H9	120.3
O5—S2—C8	104.65 (14)	C8—C9—H9	120.3
O4—S2—C8	107.23 (14)	C9—C10—C5	120.8 (3)
S1—O1—Sr1	123.13 (12)	C9—C10—H10	119.6
S1—O2—Sr1 ⁱⁱ	149.15 (13)	C5—C10—H10	119.6
O2—S1—O1—Sr1	-99.69 (16)	O2—S1—C2—C1	1.7 (3)
O3—S1—O1—Sr1	28.67 (19)	O3—S1—C2—C1	-119.8 (3)
C2—S1—O1—Sr1	143.58 (13)	O1—S1—C2—C1	122.2 (3)
O2 ⁱ —Sr1—O1—S1	-14.73 (16)	Sr1—S1—C2—C1	151.7 (2)
O6 ^{iv} —Sr1—O1—S1	-100.53 (18)	O2—S1—C2—C3	179.3 (2)
O5 ⁱⁱⁱ —Sr1—O1—S1	104.78 (16)	O3—S1—C2—C3	57.8 (2)
O3 ⁱⁱ —Sr1—O1—S1	55.81 (15)	O1—S1—C2—C3	-60.2 (3)
O1w—Sr1—O1—S1	-160.21 (17)	Sr1—S1—C2—C3	-30.7 (3)
O2w—Sr1—O1—S1	-85.71 (15)	C1—C2—C3—C4	-1.4 (4)
O2w ^v —Sr1—O1—S1	124.29 (16)	S1—C2—C3—C4	-179.0 (2)
O3—S1—O2—Sr1 ⁱⁱ	-22.5 (3)	C2—C3—C4—C5	0.6 (4)
O1—S1—O2—Sr1 ⁱⁱ	104.6 (3)	C3—C4—C5—C6	0.9 (4)
C2—S1—O2—Sr1 ⁱⁱ	-139.4 (2)	C3—C4—C5—C10	-178.0 (3)
Sr1—S1—O2—Sr1 ⁱⁱ	64.1 (3)	C2—C1—C6—C7	-179.7 (3)
O2—S1—O3—Sr1 ⁱ	-62.7 (2)	C2—C1—C6—C5	0.7 (4)
O1—S1—O3—Sr1 ⁱ	169.39 (18)	C4—C5—C6—C1	-1.5 (4)
C2—S1—O3—Sr1 ⁱ	54.7 (2)	C10—C5—C6—C1	177.4 (3)
Sr1—S1—O3—Sr1 ⁱ	-173.4 (2)	C4—C5—C6—C7	178.9 (3)
O6—S2—O5—Sr1 ^{vi}	72.0 (3)	C10—C5—C6—C7	-2.2 (4)
O4—S2—O5—Sr1 ^{vi}	-160.0 (2)	C1—C6—C7—C8	-178.4 (3)
C8—S2—O5—Sr1 ^{vi}	-44.4 (3)	C5—C6—C7—C8	1.1 (5)
O5—S2—O6—Sr1 ^{vii}	0.2 (3)	C6—C7—C8—C9	1.4 (5)
O4—S2—O6—Sr1 ^{vii}	-127.6 (2)	C6—C7—C8—S2	-174.7 (2)
C8—S2—O6—Sr1 ^{vii}	115.2 (3)	O6—S2—C8—C7	-13.3 (3)
O2 ⁱ —Sr1—O2w—Sr1 ^{viii}	37.85 (9)	O5—S2—C8—C7	107.5 (3)

supplementary materials

O6 ^{iv} —Sr1—O2w—Sr1 ^{viii}	-43.75 (10)	O4—S2—C8—C7	-133.7 (3)
O5 ⁱⁱⁱ —Sr1—O2w—Sr1 ^{viii}	-49.76 (17)	O6—S2—C8—C9	170.5 (2)
O3 ⁱⁱ —Sr1—O2w—Sr1 ^{viii}	93.43 (12)	O5—S2—C8—C9	-68.6 (3)
O1—Sr1—O2w—Sr1 ^{viii}	143.91 (11)	O4—S2—C8—C9	50.1 (3)
O1w—Sr1—O2w—Sr1 ^{viii}	-130.67 (11)	C7—C8—C9—C10	-2.7 (5)
O2w ^v —Sr1—O2w—Sr1 ^{viii}	180.0	S2—C8—C9—C10	173.4 (2)
S1—Sr1—O2w—Sr1 ^{viii}	123.51 (9)	C8—C9—C10—C5	1.6 (5)
C6—C1—C2—C3	0.7 (4)	C4—C5—C10—C9	179.7 (3)
C6—C1—C2—S1	178.3 (2)	C6—C5—C10—C9	0.8 (4)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1w—H1w1 \cdots O4 ^{ix}	0.84	2.29	3.066 (4)	154
O1w—H1w2 \cdots O4 ^x	0.84	2.27	2.904 (4)	132
O2w—H2w2 \cdots O4 ^x	0.84	2.03	2.856 (3)	167

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

Fig. 1

