

# Poly[[tetraqua( $\mu_3$ -naphthalene-1,6-disulfonato- $\kappa^4 O^1:O^6, O^6':O^6''$ )-strontium(II)] monohydrate]

Shan Gao<sup>a</sup> and Seik Weng Ng<sup>b,c,\*</sup>

<sup>a</sup>Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, Heilongjiang University, Harbin 150080, People's Republic of China, <sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and <sup>c</sup>Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia

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

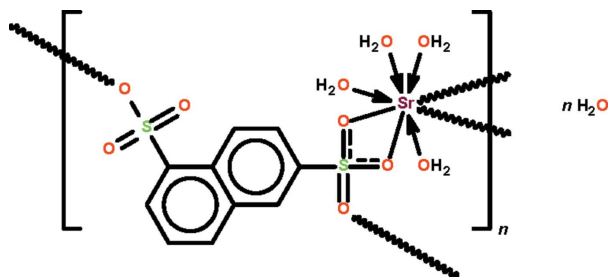
Received 4 November 2011; accepted 9 November 2011

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å; disorder in main residue;  $R$  factor = 0.024;  $wR$  factor = 0.057; data-to-parameter ratio = 17.2.

In the crystal structure of the polymeric title compound,  $\{[\text{Sr}(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)(\text{H}_2\text{O})_4]\cdot\text{H}_2\text{O}\}_n$ , the naphthalene-1,6-disulfonate dianion uses one  $-\text{SO}_3$  unit to  $O, O'$ -chelate to an  $\text{Sr}^{\text{II}}$  cation and its third O atom to bind to another  $\text{Sr}^{\text{II}}$  cation. The other  $-\text{SO}_3$  unit binds to yet another  $\text{Sr}^{\text{II}}$  atom. The four coordinated water molecules are monodentate but one is disordered over two positions in a 1:1 ratio. The  $\mu_3$ -bonding mode of the dianion generates a polymeric three-dimensional network; the network is consolidated by  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds. The  $\text{Sr}^{\text{II}}$  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

$[\text{Sr}(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)(\text{H}_2\text{O})_4]\cdot\text{H}_2\text{O}$   
 $M_r = 463.97$

Orthorhombic,  $P2_12_12_1$   
 $a = 7.1067$  (16) Å

$b = 14.080$  (4) Å  
 $c = 16.745$  (6) Å  
 $V = 1675.6$  (9) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 3.52$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.22 \times 0.17 \times 0.15$  mm

### Data collection

Rigaku R-Axis RAPID IP diffractometer  
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\text{min}} = 0.511$ ,  $T_{\text{max}} = 0.620$

16056 measured reflections  
3786 independent reflections  
3497 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.057$   
 $S = 1.02$   
3786 reflections  
220 parameters  
15 restraints

H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.36$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.29$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983),  
1584 Friedel pairs  
Flack parameter:  $-0.017$  (4)

**Table 1**

Selected bond lengths (Å).

Sr1—O1	2.737 (2)	Sr1—O1W	2.641 (2)
Sr1—O2	2.721 (2)	Sr1—O2W	2.562 (2)
Sr1—O3 <sup>i</sup>	2.583 (2)	Sr1—O3W	2.500 (2)
Sr1—O4 <sup>ii</sup>	2.5352 (19)	Sr1—O4W	2.585 (14)

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1w—H12 $\cdots$ O2 <sup>iii</sup>	0.84	2.25	2.809 (3)	124
O2w—H21 $\cdots$ O5 <sup>iv</sup>	0.84	2.03	2.793 (3)	151
O2w—H22 $\cdots$ O5w <sup>v</sup>	0.84	1.95	2.763 (3)	164
O3w—H31 $\cdots$ O6 <sup>vi</sup>	0.84	2.09	2.829 (3)	147
O3w—H32 $\cdots$ O5w <sup>v</sup>	0.84	1.99	2.754 (3)	151
O5w—H51 $\cdots$ O6 <sup>ii</sup>	0.84	2.06	2.874 (3)	163
O5w—H52 $\cdots$ O1w	0.84	2.02	2.831 (3)	160

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

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).

This work was supported by the Key Project of the Natural Science Foundation of Heilongjiang Province (No. ZD200903), the Key Project of the Education Bureau of Heilongjiang Province (No. 12511z023) and the University of Malaya.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5382).

## References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
- Cai, J. (2004). *Coord. Chem. Rev.* **248**, 1061–1083.
- Cai, J., Chen, C.-H., Liao, C.-Z., Feng, X.-L. & Chen, X.-M. (2001). *Acta Cryst.* **B57**, 520–530.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MSO (2002). *CrystalClear*. Rigaku/MSO Inc., The Woodlands, Texas, USA.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

**supplementary materials**

*Acta Cryst.* (2011). E67, m1767-m1768 [ doi:10.1107/S1600536811047593 ]

**Poly[[tetraaqua( $\mu_3$ -naphthalene-1,6-disulfonato- $\kappa^4 O^1:O^6, O^6':O^6''$ )strontium(II)] monohydrate]**

**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  $\text{Sr}(\text{H}_2\text{O})_4(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)\cdot\text{H}_2\text{O}$ , the  $\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2^{2-}$  dianion uses one  $-\text{SO}_3$  unit to  $O, O'$ -chelate to an  $\text{Sr}^{\text{II}}$  atom and its third O atom to bind to another  $\text{Sr}^{\text{II}}$  atom. The other  $-\text{SO}_3$  unit binds to yet another  $\text{Sr}^{\text{II}}$  atom (Scheme I, Fig. 1). The four coordinated water molecules are monodentate but one is disordered over two positions in a 1:1 ratio. The  $\mu_3$  bonding mode of the dianion 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-1,6-disulfonate (1 mmol) were dissolved in water (10 ml). The solution was filtered and set aside; yellow crystals were isolated from the filtrate after several days.

**Refinement**

Carbon-bound H-atoms were generated geometrically and were included in the riding model approximation [C—H 0.93 Å,  $U$ , 1.2 $U_{\text{eq}}(\text{C})$ ]. The water H-atoms were placed in calculated positions [O—H 0.84 Å,  $U$  1.5 $U_{\text{eq}}(\text{O})$ ] on the basis of hydrogen bonding interactions; however, only some are involved and others are not.

One of the water molecules is disordered over two positions in a 1:1 ratio.

**Figures**

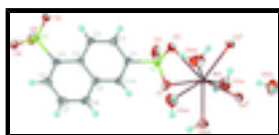


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of a fragment of polymeric  $\text{Sr}(\text{H}_2\text{O})_4(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)\cdot\text{H}_2\text{O}$  at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

**Poly[[tetraaqua( $\mu_3$ -naphthalene-1,6-disulfonato-  $\kappa^4 O^1:O^6, O^6':O^6''$ )strontium] monohydrate]**

*Crystal data*

$[\text{Sr}(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)(\text{H}_2\text{O})_4]\cdot\text{H}_2\text{O}$

$F(000) = 936$

$M_r = 463.97$

$D_x = 1.839 \text{ Mg m}^{-3}$

# supplementary materials

Orthorhombic,  $P2_12_12_1$   
Hall symbol: P 2ac 2ab  
 $a = 7.1067$  (16) Å  
 $b = 14.080$  (4) Å  
 $c = 16.745$  (6) Å  
 $V = 1675.6$  (9) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
Cell parameters from 14836 reflections  
 $\theta = 3.1$ – $27.1^\circ$   
 $\mu = 3.52$  mm<sup>-1</sup>  
 $T = 293$  K  
Prism, yellow  
 $0.22 \times 0.17 \times 0.15$  mm

## Data collection

Rigaku R-Axis RAPID IP  
diffractometer  
Radiation source: fine-focus sealed tube  
graphite  
 $\omega$  scan  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.511$ ,  $T_{\max} = 0.620$   
16056 measured reflections

3786 independent reflections  
3497 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$   
 $\theta_{\max} = 27.1^\circ$ ,  $\theta_{\min} = 3.1^\circ$   
 $h = -8 \rightarrow 9$   
 $k = -16 \rightarrow 18$   
 $l = -21 \rightarrow 21$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.057$   
 $S = 1.02$   
3786 reflections  
220 parameters  
15 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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.36$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.29$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983), 1584 Friedel pairs  
Flack parameter:  $-0.017$  (4)

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sr1	0.17295 (3)	0.709854 (16)	0.858456 (15)	0.02516 (7)	
S1	-0.05018 (9)	0.60924 (5)	1.00949 (4)	0.03027 (15)	
S2	0.03060 (8)	0.15903 (4)	1.19980 (4)	0.02706 (14)	
O1	-0.1183 (2)	0.61336 (14)	0.92809 (12)	0.0384 (5)	
O2	0.1341 (3)	0.65457 (14)	1.01330 (13)	0.0419 (5)	
O3	-0.1813 (3)	0.64691 (14)	1.06765 (13)	0.0512 (6)	
O4	0.1872 (3)	0.20770 (14)	1.23766 (11)	0.0367 (4)	
O5	-0.1493 (3)	0.18114 (15)	1.23623 (12)	0.0435 (5)	
O6	0.0641 (3)	0.05717 (13)	1.19636 (13)	0.0355 (4)	
O1W	-0.0894 (3)	0.84232 (15)	0.86687 (16)	0.0516 (6)	

H11	-0.0628	0.8806	0.9036	0.077*	
H12	-0.1939	0.8169	0.8764	0.077*	
O2W	-0.0715 (3)	0.68007 (15)	0.74884 (13)	0.0430 (5)	
H21	-0.1701	0.7106	0.7592	0.065*	
H22	-0.0964	0.6218	0.7467	0.065*	
O3W	0.2189 (3)	0.54239 (15)	0.81275 (15)	0.0550 (6)	
H31	0.3323	0.5340	0.8004	0.082*	
H32	0.1506	0.5320	0.7728	0.082*	
O4W	0.518 (2)	0.6538 (11)	0.8714 (6)	0.069 (2)	0.50
H41	0.5845	0.6977	0.8902	0.103*	0.50
H42	0.5236	0.6071	0.9026	0.103*	0.50
O4W'	0.506 (2)	0.6686 (11)	0.9022 (6)	0.069 (2)	0.50
H43	0.5283	0.6115	0.8912	0.103*	0.50
H44	0.5160	0.6770	0.9517	0.103*	0.50
O5W	0.0879 (3)	0.98623 (17)	0.77588 (17)	0.0621 (7)	
H51	0.1881	0.9625	0.7577	0.093*	
H52	0.0479	0.9502	0.8123	0.093*	
C1	-0.0216 (3)	0.48828 (18)	1.03469 (16)	0.0273 (6)	
C2	-0.0014 (4)	0.4641 (2)	1.11612 (16)	0.0311 (6)	
H2	0.0027	0.5116	1.1547	0.037*	
C3	0.0120 (3)	0.37121 (17)	1.13822 (17)	0.0307 (5)	
H3	0.0240	0.3561	1.1921	0.037*	
C4	0.0081 (3)	0.29677 (19)	1.08087 (14)	0.0242 (5)	
C5	0.0181 (3)	0.19898 (19)	1.09993 (15)	0.0257 (5)	
C6	0.0120 (3)	0.1312 (2)	1.04032 (17)	0.0328 (6)	
H6	0.0171	0.0671	1.0536	0.039*	
C7	-0.0016 (4)	0.1581 (2)	0.96025 (18)	0.0371 (7)	
H7	-0.0033	0.1118	0.9206	0.045*	
C8	-0.0124 (4)	0.2518 (2)	0.93974 (17)	0.0346 (6)	
H8	-0.0236	0.2688	0.8863	0.042*	
C9	-0.0066 (3)	0.32300 (18)	0.99881 (15)	0.0260 (5)	
C10	-0.0232 (3)	0.42029 (19)	0.97758 (16)	0.0290 (6)	
H10	-0.0353	0.4374	0.9242	0.035*	

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sr1	0.02683 (11)	0.02339 (11)	0.02527 (12)	-0.00045 (10)	-0.00087 (10)	0.00222 (10)
S1	0.0361 (3)	0.0258 (3)	0.0289 (4)	0.0041 (3)	0.0054 (3)	0.0052 (3)
S2	0.0299 (3)	0.0254 (3)	0.0259 (3)	-0.0017 (3)	0.0003 (3)	0.0027 (3)
O1	0.0372 (10)	0.0418 (11)	0.0361 (12)	0.0039 (8)	-0.0012 (8)	0.0105 (10)
O2	0.0464 (12)	0.0381 (11)	0.0412 (13)	-0.0101 (9)	-0.0084 (9)	0.0077 (10)
O3	0.0737 (13)	0.0331 (11)	0.0468 (14)	0.0164 (11)	0.0289 (13)	0.0041 (10)
O4	0.0434 (9)	0.0365 (10)	0.0302 (10)	-0.0086 (11)	-0.0086 (8)	0.0029 (9)
O5	0.0395 (11)	0.0529 (13)	0.0381 (12)	0.0061 (9)	0.0154 (9)	0.0089 (10)
O6	0.0417 (10)	0.0255 (10)	0.0392 (12)	0.0007 (8)	-0.0055 (9)	0.0042 (9)
O1W	0.0457 (11)	0.0422 (12)	0.0667 (16)	0.0074 (9)	0.0137 (11)	-0.0032 (12)
O2W	0.0438 (10)	0.0432 (13)	0.0420 (13)	0.0003 (9)	-0.0116 (9)	0.0002 (10)

## supplementary materials

O3W	0.0486 (12)	0.0399 (12)	0.0765 (19)	0.0157 (10)	0.0014 (11)	-0.0116 (12)
O4W	0.036 (2)	0.094 (4)	0.075 (6)	0.011 (2)	-0.010 (5)	-0.009 (5)
O4W'	0.036 (2)	0.094 (4)	0.075 (6)	0.011 (2)	-0.010 (5)	-0.009 (5)
O5W	0.0504 (12)	0.0479 (14)	0.088 (2)	0.0178 (11)	0.0124 (12)	0.0176 (14)
C1	0.0272 (12)	0.0259 (13)	0.0287 (15)	0.0009 (10)	0.0038 (10)	0.0067 (11)
C2	0.0434 (15)	0.0261 (13)	0.0237 (15)	0.0025 (11)	-0.0002 (11)	-0.0010 (10)
C3	0.0439 (14)	0.0294 (13)	0.0187 (13)	-0.0003 (11)	-0.0009 (12)	0.0045 (12)
C4	0.0233 (10)	0.0288 (13)	0.0207 (12)	-0.0010 (10)	0.0003 (9)	-0.0016 (12)
C5	0.0251 (11)	0.0284 (13)	0.0238 (13)	0.0010 (11)	0.0001 (9)	0.0009 (11)
C6	0.0339 (14)	0.0284 (14)	0.0361 (17)	-0.0007 (11)	-0.0043 (12)	-0.0028 (12)
C7	0.0439 (16)	0.0365 (17)	0.0309 (16)	0.0010 (14)	-0.0008 (13)	-0.0134 (13)
C8	0.0399 (14)	0.0418 (16)	0.0222 (15)	0.0024 (12)	-0.0030 (11)	-0.0032 (12)
C9	0.0228 (11)	0.0304 (14)	0.0248 (14)	0.0027 (10)	0.0019 (10)	-0.0005 (11)
C10	0.0335 (13)	0.0333 (14)	0.0202 (14)	0.0016 (11)	0.0016 (10)	0.0036 (11)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Sr1—O1	2.737 (2)	O3W—H32	0.8400
Sr1—O2	2.721 (2)	O4W—H41	0.8400
Sr1—O3 <sup>i</sup>	2.583 (2)	O4W—H42	0.8400
Sr1—O4 <sup>ii</sup>	2.5352 (19)	O4W'—H43	0.8400
Sr1—O1W	2.641 (2)	O4W'—H44	0.8401
Sr1—O2W	2.562 (2)	O5W—H51	0.8430
Sr1—O3W	2.500 (2)	O5W—H52	0.8433
Sr1—O4W	2.585 (14)	C1—C10	1.353 (4)
Sr1—O4W'	2.542 (15)	C1—C2	1.413 (4)
S1—O1	1.448 (2)	C2—C3	1.363 (4)
S1—O3	1.448 (2)	C2—H2	0.9300
S1—O2	1.458 (2)	C3—C4	1.422 (4)
S1—C1	1.766 (3)	C3—H3	0.9300
S2—O5	1.450 (2)	C4—C5	1.415 (4)
S2—O4	1.4526 (19)	C4—C9	1.427 (3)
S2—O6	1.4550 (19)	C5—C6	1.382 (4)
S2—C5	1.767 (3)	C6—C7	1.397 (4)
O3—Sr1 <sup>iii</sup>	2.583 (2)	C6—H6	0.9300
O4—Sr1 <sup>iv</sup>	2.5352 (19)	C7—C8	1.366 (4)
O1W—H11	0.8401	C7—H7	0.9300
O1W—H12	0.8399	C8—C9	1.409 (4)
O2W—H21	0.8399	C8—H8	0.9300
O2W—H22	0.8399	C9—C10	1.420 (4)
O3W—H31	0.8401	C10—H10	0.9300
O3W—Sr1—O4 <sup>ii</sup>	97.84 (7)	S1—O3—Sr1 <sup>iii</sup>	150.00 (13)
O3W—Sr1—O4W'	75.6 (3)	S2—O4—Sr1 <sup>iv</sup>	149.83 (12)
O4 <sup>ii</sup> —Sr1—O4W'	88.3 (3)	Sr1—O1W—H11	109.5
O3W—Sr1—O2W	73.44 (7)	Sr1—O1W—H12	109.5
O4 <sup>ii</sup> —Sr1—O2W	76.65 (7)	H11—O1W—H12	109.5
O4W'—Sr1—O2W	143.1 (2)	Sr1—O2W—H21	109.5

O3W—Sr1—O3 <sup>i</sup>	146.15 (7)	Sr1—O2W—H22	109.5
O4 <sup>ii</sup> —Sr1—O3 <sup>i</sup>	82.38 (7)	H21—O2W—H22	109.5
O4W'—Sr1—O3 <sup>i</sup>	70.6 (3)	Sr1—O3W—H31	109.5
O2W—Sr1—O3 <sup>i</sup>	137.99 (7)	Sr1—O3W—H32	109.5
O3W—Sr1—O4W	67.3 (3)	H31—O3W—H32	109.5
O4 <sup>ii</sup> —Sr1—O4W	80.5 (3)	Sr1—O4W—H41	109.9
O4W'—Sr1—O4W	12.6 (3)	Sr1—O4W—H42	109.6
O2W—Sr1—O4W	130.8 (2)	H41—O4W—H42	108.4
O3 <sup>i</sup> —Sr1—O4W	79.5 (3)	Sr1—O4W—H43	114.0
O3W—Sr1—O1W	140.76 (7)	Sr1—O4W'—H43	109.6
O4 <sup>ii</sup> —Sr1—O1W	89.77 (7)	H41—O4W'—H43	109.5
O4W'—Sr1—O1W	143.4 (3)	Sr1—O4W'—H44	109.5
O2W—Sr1—O1W	71.03 (7)	H43—O4W'—H44	109.5
O3 <sup>i</sup> —Sr1—O1W	72.92 (8)	H51—O5W—H52	107.9
O4W—Sr1—O1W	151.7 (3)	C10—C1—C2	120.8 (2)
O3W—Sr1—O2	92.01 (8)	C10—C1—S1	120.8 (2)
O4 <sup>ii</sup> —Sr1—O2	158.59 (6)	C2—C1—S1	118.3 (2)
O4W'—Sr1—O2	75.8 (3)	C3—C2—C1	120.0 (3)
O2W—Sr1—O2	124.55 (7)	C3—C2—H2	120.0
O3 <sup>i</sup> —Sr1—O2	78.91 (7)	C1—C2—H2	120.0
O4W—Sr1—O2	85.9 (3)	C2—C3—C4	121.5 (3)
O1W—Sr1—O2	94.57 (7)	C2—C3—H3	119.2
O3W—Sr1—O1	76.18 (7)	C4—C3—H3	119.2
O4 <sup>ii</sup> —Sr1—O1	149.74 (6)	C5—C4—C3	124.3 (2)
O4W'—Sr1—O1	117.8 (4)	C5—C4—C9	118.2 (2)
O2W—Sr1—O1	73.20 (7)	C3—C4—C9	117.5 (2)
O3 <sup>i</sup> —Sr1—O1	119.14 (8)	C6—C5—C4	120.5 (2)
O4W—Sr1—O1	122.0 (4)	C6—C5—S2	117.7 (2)
O1W—Sr1—O1	78.10 (6)	C4—C5—S2	121.72 (19)
O2—Sr1—O1	51.35 (6)	C5—C6—C7	120.6 (3)
O1—S1—O3	113.78 (13)	C5—C6—H6	119.7
O1—S1—O2	108.91 (12)	C7—C6—H6	119.7
O3—S1—O2	112.83 (14)	C8—C7—C6	120.5 (3)
O1—S1—C1	107.58 (13)	C8—C7—H7	119.8
O3—S1—C1	105.46 (12)	C6—C7—H7	119.8
O2—S1—C1	107.94 (12)	C7—C8—C9	120.6 (3)
O5—S2—O4	112.99 (12)	C7—C8—H8	119.7
O5—S2—O6	111.86 (12)	C9—C8—H8	119.7
O4—S2—O6	110.92 (11)	C8—C9—C10	120.5 (3)
O5—S2—C5	106.59 (12)	C8—C9—C4	119.6 (2)
O4—S2—C5	107.54 (11)	C10—C9—C4	119.8 (2)
O6—S2—C5	106.53 (13)	C1—C10—C9	120.3 (2)
S1—O1—Sr1	99.67 (9)	C1—C10—H10	119.8
S1—O2—Sr1	100.05 (10)	C9—C10—H10	119.8
O3—S1—O1—Sr1	125.47 (11)	O3—S1—C1—C2	-42.8 (2)
O2—S1—O1—Sr1	-1.34 (13)	O2—S1—C1—C2	78.0 (2)



## supplementary materials

C1—S1—O1—Sr1	-118.10 (10)	C10—C1—C2—C3	-1.6 (4)
O3W—Sr1—O1—S1	104.94 (11)	S1—C1—C2—C3	176.90 (19)
O4 <sup>ii</sup> —Sr1—O1—S1	-173.28 (9)	C1—C2—C3—C4	0.6 (4)
O4W'—Sr1—O1—S1	39.8 (3)	C2—C3—C4—C5	-178.8 (2)
O2W—Sr1—O1—S1	-178.50 (12)	C2—C3—C4—C9	1.2 (4)
O3 <sup>i</sup> —Sr1—O1—S1	-42.42 (12)	C3—C4—C5—C6	179.6 (2)
O4W—Sr1—O1—S1	53.5 (3)	C9—C4—C5—C6	-0.5 (3)
O1W—Sr1—O1—S1	-104.96 (11)	C3—C4—C5—S2	1.7 (3)
O2—Sr1—O1—S1	0.87 (8)	C9—C4—C5—S2	-178.37 (17)
O1—S1—O2—Sr1	1.35 (13)	O5—S2—C5—C6	-110.1 (2)
O3—S1—O2—Sr1	-126.00 (12)	O4—S2—C5—C6	128.4 (2)
C1—S1—O2—Sr1	117.88 (11)	O6—S2—C5—C6	9.5 (2)
O3W—Sr1—O2—S1	-71.35 (11)	O5—S2—C5—C4	67.8 (2)
O4 <sup>ii</sup> —Sr1—O2—S1	171.05 (13)	O4—S2—C5—C4	-53.7 (2)
O4W'—Sr1—O2—S1	-145.9 (3)	O6—S2—C5—C4	-172.64 (19)
O2W—Sr1—O2—S1	-0.13 (14)	C4—C5—C6—C7	0.8 (4)
O3 <sup>i</sup> —Sr1—O2—S1	141.52 (12)	S2—C5—C6—C7	178.7 (2)
O4W—Sr1—O2—S1	-138.4 (3)	C5—C6—C7—C8	-1.1 (4)
O1W—Sr1—O2—S1	69.94 (11)	C6—C7—C8—C9	1.1 (4)
O1—Sr1—O2—S1	-0.87 (8)	C7—C8—C9—C10	-178.2 (2)
O1—S1—O3—Sr1 <sup>iii</sup>	-82.0 (3)	C7—C8—C9—C4	-0.8 (4)
O2—S1—O3—Sr1 <sup>iii</sup>	42.7 (3)	C5—C4—C9—C8	0.5 (4)
C1—S1—O3—Sr1 <sup>iii</sup>	160.3 (3)	C3—C4—C9—C8	-179.6 (2)
O5—S2—O4—Sr1 <sup>iv</sup>	23.0 (3)	C5—C4—C9—C10	177.9 (2)
O6—S2—O4—Sr1 <sup>iv</sup>	-103.6 (2)	C3—C4—C9—C10	-2.2 (3)
C5—S2—O4—Sr1 <sup>iv</sup>	140.3 (2)	C2—C1—C10—C9	0.6 (4)
O1—S1—C1—C10	13.9 (2)	S1—C1—C10—C9	-177.81 (19)
O3—S1—C1—C10	135.7 (2)	C8—C9—C10—C1	178.6 (2)
O2—S1—C1—C10	-103.5 (2)	C4—C9—C10—C1	1.3 (4)
O1—S1—C1—C2	-164.6 (2)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1w—H12 $\cdots$ O2 <sup>iii</sup>	0.84	2.25	2.809 (3)	124
O2w—H21 $\cdots$ O5 <sup>v</sup>	0.84	2.03	2.793 (3)	151
O2w—H22 $\cdots$ O5w <sup>vi</sup>	0.84	1.95	2.763 (3)	164
O3w—H31 $\cdots$ O6 <sup>vii</sup>	0.84	2.09	2.829 (3)	147
O3w—H32 $\cdots$ O5w <sup>vi</sup>	0.84	1.99	2.754 (3)	151
O5w—H51 $\cdots$ O6 <sup>ii</sup>	0.84	2.06	2.874 (3)	163
O5w—H52 $\cdots$ O1w	0.84	2.02	2.831 (3)	160

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

Fig. 1

