Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[tetraaqua(μ_3-naphthalene-1,6-disulfonato-$\kappa^4O^1:O^6,O^{6'}:O^{6''}$)-strontium(II)] monohydrate]

Shan Gao[a] and Seik Weng Ng[b,c]*

[a]Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, Heilongjiang University, Harbin 150080, People's Republic of China, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

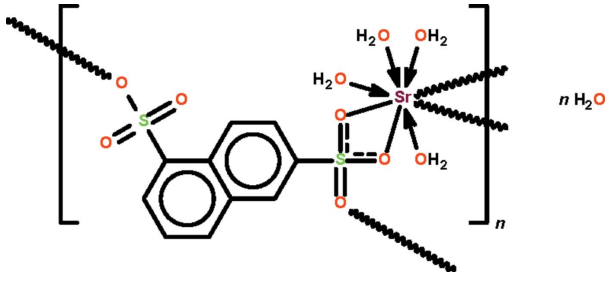
Received 4 November 2011; accepted 9 November 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–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, $\{[Sr(C_{10}H_6O_6S_2)(H_2O)_4]\cdot H_2O\}_n$, the naphthalene-1,6-disulfonate dianion uses one $-SO_3$ unit to O,O'-chelate to an Sr^{II} cation and its third O atom to bind to another Sr^{II} cation. The other $-SO_3$ unit binds to yet another Sr^{II} atom. The four coordinated water molecules are monodentate but one is disordered over two positions in a 1:1 ratio. The μ_3-bonding mode of the dianion generates a polymeric three-dimensional network; the network is consolidated by O—H···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

$[Sr(C_{10}H_6O_6S_2)(H_2O)_4]\cdot H_2O$
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^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.52 mm^{-1}
T = 293 K
0.22 × 0.17 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
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_{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
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Absolute structure: Flack (1983), 1584 Friedel pairs
Flack parameter: −0.017 (4)

Table 1
Selected bond lengths (Å).

Sr1—O1	2.737 (2)	Sr1—O1*W*	2.641 (2)
Sr1—O2	2.721 (2)	Sr1—O2*W*	2.562 (2)
Sr1—O3^{i}	2.583 (2)	Sr1—O3*W*	2.500 (2)
Sr1—O4^{ii}	2.5352 (19)	Sr1—O4*W*	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—H···A	D—H	H···A	D···A	D—H···A
O1w—H12···O2^{iii}	0.84	2.25	2.809 (3)	124
O2w—H21···O5^{iv}	0.84	2.03	2.793 (3)	151
O2w—H22···O5w^{v}	0.84	1.95	2.763 (3)	164
O3w—H31···O6^{vi}	0.84	2.09	2.829 (3)	147
O3w—H32···O5w^{v}	0.84	1.99	2.754 (3)	151
O5w—H51···O6^{ii}	0.84	2.06	2.874 (3)	163
O5w—H52···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/MSC, 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: *publCIF* (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.* B**57**, 520–530.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, m1767–m1768 [https://doi.org/10.1107/S1600536811047593]

Poly[[tetraaqua(μ_3-naphthalene-1,6-disulfonato-κ^4O^1:O^6,$O^{6'}$:$O^{6''}$)strontium(II)] monohydrate]

Shan Gao and Seik Weng Ng

S1. 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 $-SO_3$ groups (Cai, 2004). Among the divalent metal derivatives, the strontium system has been less studied (Cai *et al.*, 2001). In the crystal structure of $Sr(H_2O)_4(C_{10}H_6O_6S_2)\cdot H_2O$, the $C_{10}H_6O_6S_2^{2-}$ dianion uses one $-SO_3$ unit to *O*,*O*′-chelate to an Sr^{II} atom and its third O atom to bind to another Sr^{II} atom. The other $-SO_3$ unit binds to yet another Sr^{II} atom (Scheme I, Fig. 1). T; the four coordinated water molecules are monodentate but one is disordered over two positions in a 1:1 ratio. The μ_3 bonding mode of the dianon generates a polymeric three-dimensional network; the network is consolidated by O–H···O hydrogen bonds (Table 1). The Sr atom exists in an undefined eight-coordinate environment.

S2. 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.

S3. Refinement

Carbon-bound H-atoms were generated geometrically and were included in the riding model approximation [C—H 0.93 Å, *U*, 1.2U_{eq}(C)]. The water H-atoms were placed in calculated positions [O—H 0.84 Å, *U* 1.5U_{eq}(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.

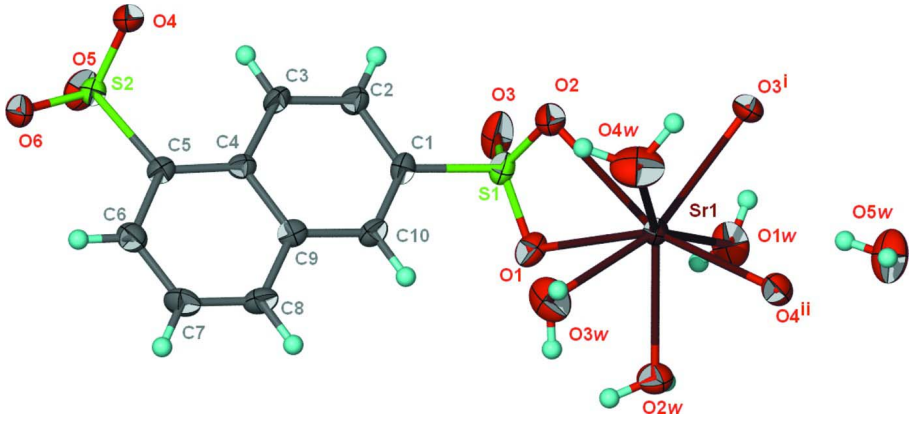


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of a fragment of polymeric $Sr(H_2O)_4(C_{10}H_6O_6S_2)\cdot H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Poly[[tetraaqua(μ_3-naphthalene-1,6-disulfonato-κ^4O^1:O^6,$O^{6'}$:$O^{6''}$)strontium] monohydrate]

Crystal data

$[Sr(C_{10}H_6O_6S_2)(H_2O)_4]\cdot H_2O$
$M_r = 463.97$
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^3
$Z = 4$
$F(000) = 936$
$D_x = 1.839$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14836 reflections
$\theta = 3.1$–$27.1°$
$\mu = 3.52$ mm^{-1}
$T = 293$ K
Prism, yellow
0.22 × 0.17 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω 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 $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.1°$, $\theta_{min} = 3.1°$
$h = -8\rightarrow9$
$k = -16\rightarrow18$
$l = -21\rightarrow21$

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^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Absolute structure: Flack (1983), 1584 Friedel pairs
Absolute structure parameter: −0.017 (4)

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

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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)
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 (Å, º)

Sr1—O1	2.737 (2)	O3W—H32	0.8400
Sr1—O2	2.721 (2)	O4W—H41	0.8400
Sr1—O3^{i}	2.583 (2)	O4W—H42	0.8400
Sr1—O4^{ii}	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^{iii}	2.583 (2)	C6—H6	0.9300
O4—Sr1^{iv}	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^{ii}	97.84 (7)	S1—O3—Sr1^{iii}	150.00 (13)
O3W—Sr1—O4W′	75.6 (3)	S2—O4—Sr1^{iv}	149.83 (12)
O4^{ii}—Sr1—O4W′	88.3 (3)	Sr1—O1W—H11	109.5
O3W—Sr1—O2W	73.44 (7)	Sr1—O1W—H12	109.5
O4^{ii}—Sr1—O2W	76.65 (7)	H11—O1W—H12	109.5
O4W′—Sr1—O2W	143.1 (2)	Sr1—O2W—H21	109.5
O3W—Sr1—O3^{i}	146.15 (7)	Sr1—O2W—H22	109.5
O4^{ii}—Sr1—O3^{i}	82.38 (7)	H21—O2W—H22	109.5
O4W′—Sr1—O3^{i}	70.6 (3)	Sr1—O3W—H31	109.5
O2W—Sr1—O3^{i}	137.99 (7)	Sr1—O3W—H32	109.5
O3W—Sr1—O4W	67.3 (3)	H31—O3W—H32	109.5
O4^{ii}—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^{i}—Sr1—O4W	79.5 (3)	Sr1—O4W—H43	114.0
O3W—Sr1—O1W	140.76 (7)	Sr1—O4W′—H43	109.6
O4^{ii}—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^{i}—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^{ii}—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^{i}—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^{ii}—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^{i}—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)
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^{ii}—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^{i}—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^{ii}—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^{i}—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^{iii}	−82.0 (3)	C7—C8—C9—C4	−0.8 (4)
O2—S1—O3—Sr1^{iii}	42.7 (3)	C5—C4—C9—C8	0.5 (4)
C1—S1—O3—Sr1^{iii}	160.3 (3)	C3—C4—C9—C8	−179.6 (2)
O5—S2—O4—Sr1^{iv}	23.0 (3)	C5—C4—C9—C10	177.9 (2)
O6—S2—O4—Sr1^{iv}	−103.6 (2)	C3—C4—C9—C10	−2.2 (3)
C5—S2—O4—Sr1^{iv}	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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H12···O2^{iii}	0.84	2.25	2.809 (3)	124
O2w—H21···O5^{v}	0.84	2.03	2.793 (3)	151
O2w—H22···O5w^{vi}	0.84	1.95	2.763 (3)	164
O3w—H31···O6^{vii}	0.84	2.09	2.829 (3)	147
O3w—H32···O5w^{vi}	0.84	1.99	2.754 (3)	151
O5w—H51···O6^{ii}	0.84	2.06	2.874 (3)	163
O5w—H52···O1w	0.84	2.02	2.831 (3)	160

Symmetry codes: (ii) −*x*+1/2, −*y*+1, *z*−1/2; (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.