

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

 Poly[bis(μ_3 -dodecyl sulfato)calcium]

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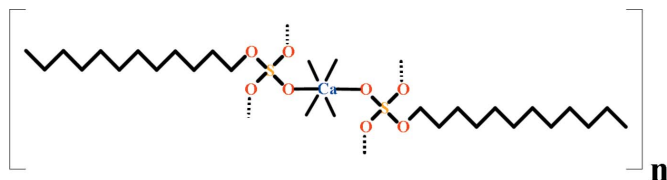
Received 20 May 2010; accepted 31 May 2010

 Key indicators: single-crystal X-ray study; $T = 93$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.031; wR factor = 0.088; data-to-parameter ratio = 10.6.

In the title compound $[\text{Ca}(\text{C}_{12}\text{H}_{25}\text{O}_4\text{S})_2]_n$, the unique Ca^{II} ion lies on an inversion center and is coordinated in a slightly distorted octahedral environment by six O atoms from dodecyl sulfate anions. The crystal structure is based on hydrocarbon (dodecyl sulfate) layers which sandwich the Ca^{II} ions. Within the layers, the hydrocarbon zigzag chains are parallel to one another and interact *via* van der Waals forces.

Related literature

For studies of the title compound using atomic force microscopy, see: Rodriguez *et al.* (2002). For the Krafft point of the title compound, see: Hato & Shinoda (1973).



Experimental

Crystal data

 $[\text{Ca}(\text{C}_{12}\text{H}_{25}\text{O}_4\text{S})_2]$
 $M_r = 570.84$

 Triclinic, $P\bar{1}$
 $a = 5.3888$ (3) Å
 $b = 5.3834$ (3) Å
 $c = 29.1922$ (16) Å
 $\alpha = 93.4321$ (19)°
 $\beta = 90.099$ (4)°
 $\gamma = 118.393$ (5)°

 $V = 743.22$ (7) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.39$ mm⁻¹
 $T = 93$ K
 $0.50 \times 0.10 \times 0.10$ mm

Data collection

 Rigaku R-Axis IV diffractometer
 4361 measured reflections
 2500 independent reflections

 2396 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.088$
 $S = 1.08$
 2500 reflections

 235 parameters
 All H-atom parameters refined
 $\Delta\rho_{\text{max}} = 0.39$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.43$ e Å⁻³

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *Yadokari-XG 2009* (Kabuto *et al.*, 2009); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Yadokari-XG 2009* and *VESTA* (Momma *et al.*, 2008); software used to prepare material for publication: *Yadokari-XG 2009*.

This work was supported by matching fund subsidy for private universities from MEXT (Ministry of Education, Culture, Sports, Science and Technology, Japan).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5055).

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supporting information

Acta Cryst. (2010). E66, m749 [doi:10.1107/S1600536810020659]

Poly[bis(μ_3 -dodecyl sulfato)calcium]

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S1. Comment

The crystal of the title compound, (I) (Fig. 1), is mechanically flexible because (I) is a two-dimensional layered compound which is characterized by strong covalent bonds and coordination bonds within the layers and weak van der Waals forces between the layers (Fig. 2).

S2. Experimental

The title compound was prepared by the addition of CaCl_2 to sodium dodecyl sulfate (SDS) in a water-ethanol mixed solvent. A crystal suitable for single-crystal X-ray diffraction was selected directly from the prepared sample.

S3. Refinement

All H atoms were located in a difference map as peaks of density and refined with isotropic thermal parameters; the range of C—H bond lengths is 0.94 (2)–1.03 (3) Å.

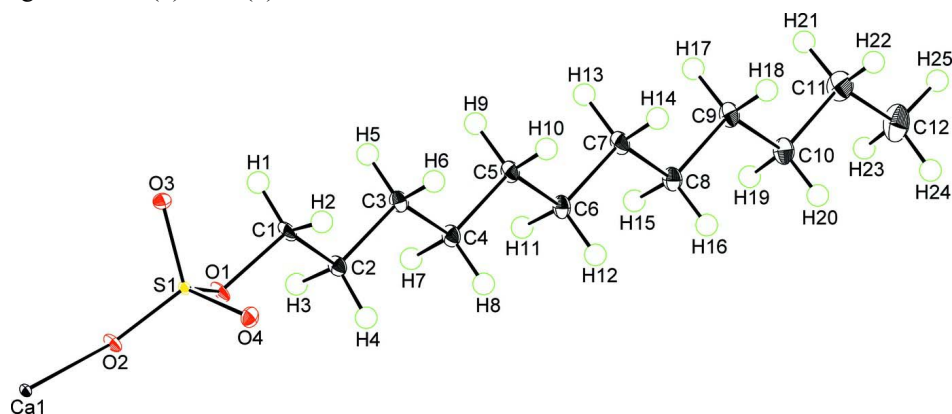


Figure 1

The asymmetric unit of (I) with atom labels and 50% probability displacement ellipsoids for non-H atoms. H atoms are shown as spheres of arbitrary radius.

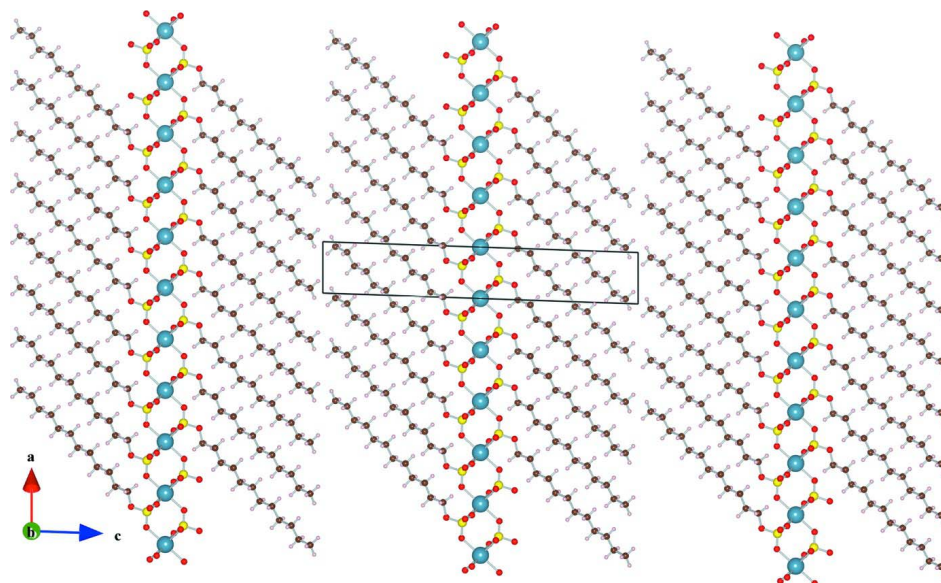


Figure 2

The packing of (I), viewed along the b axis, showing hydrocarbon (dodecyl sulfate) layers which sandwich Ca atoms.

Poly[bis(μ_3 -dodecyl sulfato)calcium]

Crystal data

$[\text{Ca}(\text{C}_{12}\text{H}_{25}\text{O}_4\text{S})_2]$

$M_r = 570.84$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 5.3888$ (3) Å

$b = 5.3834$ (3) Å

$c = 29.1922$ (16) Å

$\alpha = 93.4321$ (19)°

$\beta = 90.099$ (4)°

$\gamma = 118.393$ (5)°

$V = 743.22$ (7) Å³

$Z = 1$

$F(000) = 310$

$D_x = 1.275$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 3581 reflections

$\theta = 1.4$ – 25.5 °

$\mu = 0.39$ mm⁻¹

$T = 93$ K

Needle, colourless

$0.50 \times 0.10 \times 0.10$ mm

Data collection

Rigaku R-AXIS IV

diffractometer

Radiation source: rotating-anode X-ray

Graphite Monochromator monochromator

Detector resolution: 10.0 pixels mm⁻¹

ω scans

4361 measured reflections

2500 independent reflections

2396 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\text{max}} = 25.5$ °, $\theta_{\text{min}} = 1.4$ °

$h = -5 \rightarrow 5$

$k = -6 \rightarrow 6$

$l = -35 \rightarrow 35$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.088$

$S = 1.08$

2500 reflections

235 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

All H-atom parameters refined

$$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.4436P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.43 \text{ e } \text{\AA}^{-3}$$

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.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ca1	-1.0000	-0.5000	0.5000	0.00470 (14)
S1	-0.37678 (7)	-0.17886 (7)	0.442177 (11)	0.00452 (13)
O1	-0.2874 (2)	-0.2127 (2)	0.39188 (3)	0.0088 (3)
O2	-0.6786 (2)	-0.3652 (2)	0.44018 (3)	0.0082 (2)
O3	-0.3024 (2)	0.1177 (2)	0.45120 (3)	0.0086 (2)
O4	-0.2238 (2)	-0.2644 (2)	0.47274 (3)	0.0106 (3)
C1	0.0057 (3)	-0.0139 (3)	0.38163 (5)	0.0099 (3)
C2	0.0898 (3)	-0.1473 (3)	0.34179 (5)	0.0098 (3)
C3	0.3718 (4)	0.0621 (3)	0.32332 (5)	0.0106 (3)
C4	0.4633 (4)	-0.0705 (3)	0.28353 (5)	0.0110 (3)
C5	0.7364 (4)	0.1365 (3)	0.26211 (5)	0.0108 (3)
C6	0.8242 (4)	0.0010 (3)	0.22225 (5)	0.0113 (3)
C7	1.0951 (4)	0.2073 (3)	0.20023 (5)	0.0121 (3)
C8	1.1836 (4)	0.0689 (3)	0.16093 (5)	0.0121 (3)
C9	1.4510 (4)	0.2760 (4)	0.13817 (5)	0.0135 (4)
C10	1.5462 (4)	0.1376 (4)	0.09979 (5)	0.0141 (4)
C11	1.8122 (4)	0.3468 (4)	0.07713 (6)	0.0202 (4)
C12	1.9121 (5)	0.2066 (5)	0.03986 (6)	0.0248 (4)
H1	-0.004 (5)	0.149 (5)	0.3738 (8)	0.030*
H2	0.129 (5)	0.029 (5)	0.4080 (8)	0.030*
H3	-0.066 (5)	-0.220 (5)	0.3174 (8)	0.030*
H4	0.095 (5)	-0.318 (5)	0.3516 (8)	0.030*
H5	0.352 (5)	0.218 (5)	0.3138 (8)	0.030*
H6	0.512 (5)	0.139 (5)	0.3479 (8)	0.030*
H7	0.302 (5)	-0.159 (5)	0.2590 (8)	0.030*
H8	0.484 (5)	-0.230 (5)	0.2944 (8)	0.030*
H9	0.708 (5)	0.296 (5)	0.2513 (7)	0.030*
H10	0.886 (5)	0.224 (5)	0.2861 (8)	0.030*
H11	0.670 (5)	-0.078 (5)	0.1986 (8)	0.030*
H12	0.850 (5)	-0.157 (5)	0.2328 (8)	0.030*
H13	1.065 (5)	0.367 (5)	0.1885 (8)	0.030*
H14	1.251 (5)	0.302 (5)	0.2243 (8)	0.030*

H15	1.032 (5)	-0.013 (5)	0.1384 (8)	0.030*
H16	1.216 (5)	-0.082 (5)	0.1722 (8)	0.030*
H17	1.415 (5)	0.426 (5)	0.1260 (8)	0.030*
H18	1.606 (5)	0.369 (5)	0.1619 (8)	0.030*
H19	1.399 (5)	0.041 (5)	0.0767 (8)	0.030*
H20	1.580 (5)	-0.007 (5)	0.1123 (8)	0.030*
H21	1.773 (5)	0.488 (5)	0.0641 (8)	0.030*
H22	1.955 (5)	0.437 (5)	0.1011 (8)	0.030*
H23	1.771 (6)	0.110 (5)	0.0152 (9)	0.037*
H24	1.940 (6)	0.050 (5)	0.0518 (8)	0.037*
H25	2.097 (6)	0.344 (5)	0.0273 (8)	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0033 (2)	0.0043 (2)	0.0060 (2)	0.00128 (17)	0.00087 (15)	0.00124 (15)
S1	0.0037 (2)	0.0044 (2)	0.00495 (19)	0.00141 (16)	0.00119 (13)	0.00066 (13)
O1	0.0050 (6)	0.0096 (6)	0.0069 (5)	-0.0003 (4)	0.0035 (4)	-0.0005 (4)
O2	0.0053 (6)	0.0081 (5)	0.0079 (5)	0.0005 (4)	0.0019 (4)	0.0005 (4)
O3	0.0090 (6)	0.0064 (5)	0.0099 (5)	0.0034 (4)	0.0004 (4)	-0.0006 (4)
O4	0.0099 (6)	0.0116 (5)	0.0120 (5)	0.0061 (5)	-0.0008 (4)	0.0036 (4)
C1	0.0061 (8)	0.0096 (8)	0.0106 (7)	0.0008 (6)	0.0044 (6)	0.0015 (6)
C2	0.0083 (8)	0.0110 (8)	0.0091 (7)	0.0039 (6)	0.0033 (6)	0.0005 (6)
C3	0.0091 (9)	0.0122 (8)	0.0099 (7)	0.0045 (6)	0.0036 (6)	0.0023 (6)
C4	0.0096 (8)	0.0130 (8)	0.0107 (7)	0.0057 (6)	0.0037 (6)	0.0015 (6)
C5	0.0094 (9)	0.0127 (8)	0.0103 (7)	0.0051 (7)	0.0043 (6)	0.0026 (6)
C6	0.0096 (9)	0.0149 (8)	0.0106 (7)	0.0066 (7)	0.0033 (6)	0.0019 (6)
C7	0.0094 (8)	0.0145 (8)	0.0116 (7)	0.0050 (7)	0.0050 (6)	0.0016 (6)
C8	0.0110 (9)	0.0150 (8)	0.0110 (7)	0.0066 (7)	0.0038 (6)	0.0019 (6)
C9	0.0117 (9)	0.0168 (9)	0.0128 (7)	0.0075 (7)	0.0064 (6)	0.0024 (6)
C10	0.0130 (9)	0.0187 (9)	0.0119 (7)	0.0087 (7)	0.0042 (6)	0.0009 (6)
C11	0.0215 (10)	0.0244 (10)	0.0181 (8)	0.0131 (8)	0.0113 (7)	0.0060 (7)
C12	0.0256 (11)	0.0392 (12)	0.0179 (9)	0.0216 (9)	0.0116 (7)	0.0067 (8)

Geometric parameters (Å, °)

Ca1—O4 ⁱ	2.2955 (11)	C4—H8	0.99 (2)
Ca1—O4 ⁱⁱ	2.2956 (11)	C5—C6	1.529 (2)
Ca1—O3 ⁱⁱⁱ	2.3177 (10)	C5—H9	1.01 (2)
Ca1—O3 ^{iv}	2.3178 (11)	C5—H10	0.98 (2)
Ca1—O2	2.3544 (10)	C6—C7	1.524 (2)
Ca1—O2 ^v	2.3544 (10)	C6—H11	0.99 (2)
Ca1—S1 ^v	3.4589 (4)	C6—H12	0.99 (2)
Ca1—S1	3.4589 (4)	C7—C8	1.528 (2)
S1—O4	1.4474 (11)	C7—H13	1.03 (2)
S1—O2	1.4476 (11)	C7—H14	1.00 (2)
S1—O3	1.4558 (11)	C8—C9	1.525 (2)
S1—O1	1.5732 (10)	C8—H15	0.96 (2)

O1—C1	1.4703 (18)	C8—H16	0.98 (2)
O3—Ca1 ^{vi}	2.3177 (10)	C9—C10	1.530 (2)
O4—Ca1 ^{vii}	2.2956 (11)	C9—H17	1.00 (2)
C1—C2	1.512 (2)	C9—H18	0.99 (2)
C1—H1	0.94 (2)	C10—C11	1.522 (2)
C1—H2	0.96 (2)	C10—H19	0.96 (2)
C2—C3	1.522 (2)	C10—H20	0.97 (2)
C2—H3	1.01 (2)	C11—C12	1.528 (2)
C2—H4	0.99 (2)	C11—H21	0.98 (2)
C3—C4	1.529 (2)	C11—H22	0.96 (2)
C3—H5	0.95 (2)	C12—H23	0.97 (3)
C3—H6	0.96 (2)	C12—H24	1.00 (3)
C4—C5	1.525 (2)	C12—H25	1.00 (3)
C4—H7	1.03 (2)		
O4 ⁱ —Ca1—O4 ⁱⁱ	179.997 (1)	C2—C3—H6	109.6 (14)
O4 ⁱ —Ca1—O3 ⁱⁱⁱ	86.81 (4)	C4—C3—H6	111.4 (15)
O4 ⁱⁱ —Ca1—O3 ⁱⁱⁱ	93.19 (4)	H5—C3—H6	105.4 (19)
O4 ⁱ —Ca1—O3 ^{iv}	93.19 (4)	C5—C4—C3	114.00 (13)
O4 ⁱⁱ —Ca1—O3 ^{iv}	86.81 (4)	C5—C4—H7	110.0 (13)
O3 ⁱⁱⁱ —Ca1—O3 ^{iv}	179.997 (1)	C3—C4—H7	108.4 (14)
O4 ⁱ —Ca1—O2	92.58 (4)	C5—C4—H8	109.4 (14)
O4 ⁱⁱ —Ca1—O2	87.43 (4)	C3—C4—H8	109.1 (13)
O3 ⁱⁱⁱ —Ca1—O2	87.11 (4)	H7—C4—H8	105.6 (19)
O3 ^{iv} —Ca1—O2	92.90 (4)	C4—C5—C6	113.36 (13)
O4 ⁱ —Ca1—O2 ^v	87.43 (4)	C4—C5—H9	107.5 (14)
O4 ⁱⁱ —Ca1—O2 ^v	92.57 (4)	C6—C5—H9	110.2 (13)
O3 ⁱⁱⁱ —Ca1—O2 ^v	92.89 (4)	C4—C5—H10	109.0 (14)
O3 ^{iv} —Ca1—O2 ^v	87.10 (4)	C6—C5—H10	111.1 (15)
O2—Ca1—O2 ^v	179.998 (2)	H9—C5—H10	105.3 (19)
O4 ⁱ —Ca1—S1 ^v	80.30 (3)	C7—C6—C5	113.72 (13)
O4 ⁱⁱ —Ca1—S1 ^v	99.70 (3)	C7—C6—H11	108.4 (13)
O3 ⁱⁱⁱ —Ca1—S1 ^v	75.13 (3)	C5—C6—H11	107.9 (14)
O3 ^{iv} —Ca1—S1 ^v	104.86 (3)	C7—C6—H12	108.5 (14)
O2—Ca1—S1 ^v	161.13 (3)	C5—C6—H12	110.0 (13)
O2 ^v —Ca1—S1 ^v	18.87 (3)	H11—C6—H12	108.1 (19)
O4 ⁱ —Ca1—S1	99.70 (3)	C6—C7—C8	113.32 (13)
O4 ⁱⁱ —Ca1—S1	80.30 (3)	C6—C7—H13	108.1 (14)
O3 ⁱⁱⁱ —Ca1—S1	104.86 (3)	C8—C7—H13	109.9 (13)
O3 ^{iv} —Ca1—S1	75.14 (3)	C6—C7—H14	109.6 (13)
O2—Ca1—S1	18.87 (3)	C8—C7—H14	110.4 (14)
O2 ^v —Ca1—S1	161.13 (3)	H13—C7—H14	105.1 (18)
S1 ^v —Ca1—S1	180.0	C9—C8—C7	113.44 (13)
O4—S1—O2	113.59 (6)	C9—C8—H15	108.9 (14)
O4—S1—O3	111.92 (6)	C7—C8—H15	107.6 (15)
O2—S1—O3	112.94 (6)	C9—C8—H16	108.1 (15)
O4—S1—O1	107.44 (6)	C7—C8—H16	110.0 (13)
O2—S1—O1	103.17 (6)	H15—C8—H16	108.7 (19)

O3—S1—O1	107.04 (6)	C8—C9—C10	113.78 (14)
O4—S1—Ca1	94.37 (5)	C8—C9—H17	107.8 (14)
O2—S1—Ca1	31.74 (4)	C10—C9—H17	110.3 (13)
O3—S1—Ca1	100.49 (5)	C8—C9—H18	108.8 (13)
O1—S1—Ca1	134.58 (4)	C10—C9—H18	108.4 (14)
C1—O1—S1	115.39 (9)	H17—C9—H18	107.7 (18)
S1—O2—Ca1	129.39 (6)	C11—C10—C9	113.27 (14)
S1—O3—Ca1 ^{vi}	138.18 (7)	C11—C10—H19	108.9 (14)
S1—O4—Ca1 ^{vii}	160.70 (7)	C9—C10—H19	110.8 (15)
O1—C1—C2	107.53 (12)	C11—C10—H20	109.1 (15)
O1—C1—H1	103.4 (15)	C9—C10—H20	108.9 (14)
C2—C1—H1	112.3 (14)	H19—C10—H20	105.6 (19)
O1—C1—H2	111.0 (14)	C10—C11—C12	113.14 (16)
C2—C1—H2	111.6 (15)	C10—C11—H21	107.9 (15)
H1—C1—H2	111 (2)	C12—C11—H21	110.1 (13)
C1—C2—C3	111.44 (13)	C10—C11—H22	106.5 (14)
C1—C2—H3	107.7 (14)	C12—C11—H22	109.9 (15)
C3—C2—H3	111.5 (13)	H21—C11—H22	109.1 (19)
C1—C2—H4	109.4 (13)	C11—C12—H23	112.2 (16)
C3—C2—H4	111.2 (14)	C11—C12—H24	111.7 (14)
H3—C2—H4	105.3 (19)	H23—C12—H24	103 (2)
C2—C3—C4	112.23 (13)	C11—C12—H25	112.3 (14)
C2—C3—H5	107.4 (15)	H23—C12—H25	111 (2)
C4—C3—H5	110.6 (14)	H24—C12—H25	107 (2)
O4 ⁱ —Ca1—S1—O4	161.30 (7)	Ca1—S1—O1—C1	176.64 (8)
O4 ⁱⁱ —Ca1—S1—O4	-18.69 (7)	O4—S1—O2—Ca1	56.79 (10)
O3 ⁱⁱⁱ —Ca1—S1—O4	-109.44 (5)	O3—S1—O2—Ca1	-72.04 (9)
O3 ^{iv} —Ca1—S1—O4	70.56 (5)	O1—S1—O2—Ca1	172.76 (7)
O2—Ca1—S1—O4	-129.73 (10)	O4 ⁱ —Ca1—O2—S1	112.94 (8)
O2 ^v —Ca1—S1—O4	50.26 (10)	O4 ⁱⁱ —Ca1—O2—S1	-67.06 (8)
S1 ^v —Ca1—S1—O4	-136 (16)	O3 ⁱⁱⁱ —Ca1—O2—S1	-160.39 (9)
O4 ⁱ —Ca1—S1—O2	-68.96 (9)	O3 ^{iv} —Ca1—O2—S1	19.61 (9)
O4 ⁱⁱ —Ca1—S1—O2	111.04 (9)	O2 ^v —Ca1—O2—S1	-17 (11)
O3 ⁱⁱⁱ —Ca1—S1—O2	20.30 (9)	S1 ^v —Ca1—O2—S1	180.0
O3 ^{iv} —Ca1—S1—O2	-159.71 (9)	O4—S1—O3—Ca1 ^{vi}	1.53 (12)
O2 ^v —Ca1—S1—O2	179.998 (2)	O2—S1—O3—Ca1 ^{vi}	131.22 (9)
S1 ^v —Ca1—S1—O2	-6 (16)	O1—S1—O3—Ca1 ^{vi}	-115.93 (9)
O4 ⁱ —Ca1—S1—O3	48.05 (5)	Ca1—S1—O3—Ca1 ^{vi}	100.63 (9)
O4 ⁱⁱ —Ca1—S1—O3	-131.95 (5)	O2—S1—O4—Ca1 ^{vii}	80.8 (2)
O3 ⁱⁱⁱ —Ca1—S1—O3	137.31 (7)	O3—S1—O4—Ca1 ^{vii}	-149.8 (2)
O3 ^{iv} —Ca1—S1—O3	-42.70 (7)	O1—S1—O4—Ca1 ^{vii}	-32.6 (2)
O2—Ca1—S1—O3	117.01 (9)	Ca1—S1—O4—Ca1 ^{vii}	107.0 (2)
O2 ^v —Ca1—S1—O3	-62.99 (9)	S1—O1—C1—C2	156.54 (11)
S1 ^v —Ca1—S1—O3	111 (16)	O1—C1—C2—C3	170.34 (13)
O4 ⁱ —Ca1—S1—O1	-78.87 (7)	C1—C2—C3—C4	178.97 (14)
O4 ⁱⁱ —Ca1—S1—O1	101.13 (7)	C2—C3—C4—C5	176.61 (13)
O3 ⁱⁱⁱ —Ca1—S1—O1	10.38 (7)	C3—C4—C5—C6	-179.75 (13)

O3 ^{iv} —Ca1—S1—O1	-169.62 (7)	C4—C5—C6—C7	179.24 (13)
O2—Ca1—S1—O1	-9.91 (10)	C5—C6—C7—C8	179.09 (13)
O2 ^v —Ca1—S1—O1	170.08 (10)	C6—C7—C8—C9	178.78 (14)
S1 ^v —Ca1—S1—O1	-16 (16)	C7—C8—C9—C10	178.20 (14)
O4—S1—O1—C1	-68.41 (11)	C8—C9—C10—C11	179.60 (15)
O2—S1—O1—C1	171.31 (11)	C9—C10—C11—C12	178.15 (15)
O3—S1—O1—C1	51.95 (12)		

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