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# Poly[bis($\mu_3$-dodecyl sulfato)calcium]

**Genta Sakane,* Masahiro Tomohara, Yasuhiro Katayama and Koya Hayashi**

Department of Chemistry, Okayama University of Science, Ridai-cho, Okayama 700-0005, Japan
Correspondence e-mail: gsakane@chem.ous.ac.jp

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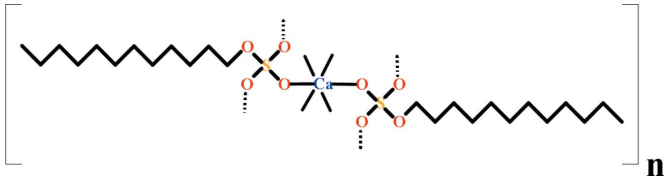
Key indicators: single-crystal X-ray study; $T$ = 93 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.031; $wR$ factor = 0.088; data-to-parameter ratio = 10.6.

In the title compound $[Ca(C_{12}H_{25}O_4S)_2]_n$, 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

$[Ca(C_{12}H_{25}O_4S)_2]$ $M_r$ = 570.84
Triclinic, $P\overline{1}$
$a$ = 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) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.39 mm$^{-1}$
$T$ = 93 K
0.50 × 0.10 × 0.10 mm

### Data collection

Rigaku R-AXIS IV diffractometer
4361 measured reflections
2500 independent reflections
2396 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.39 e Å$^{-3}$
$\Delta\rho_{min}$ = −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*.

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

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# supporting information

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## Poly[bis($\mu_3$-dodecyl sulfato)calcium]

**Genta Sakane, Masahiro Tomohara, Yasuhiro Katayama and Koya Hayashi**

### 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.

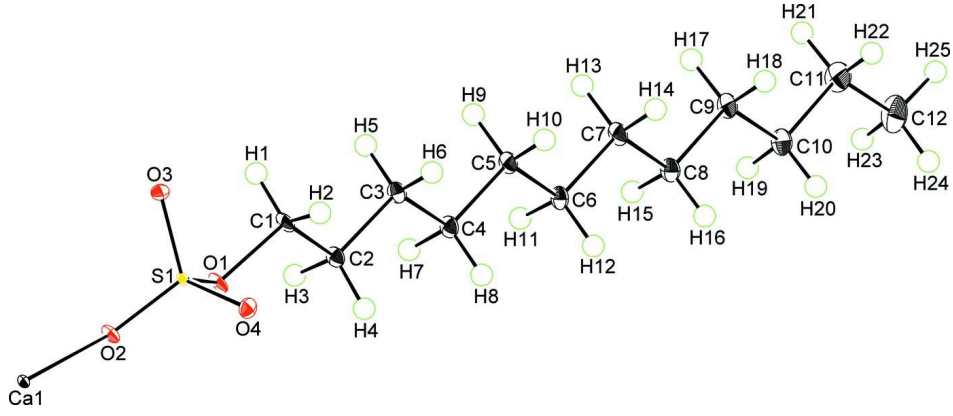


**Figure 1**

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

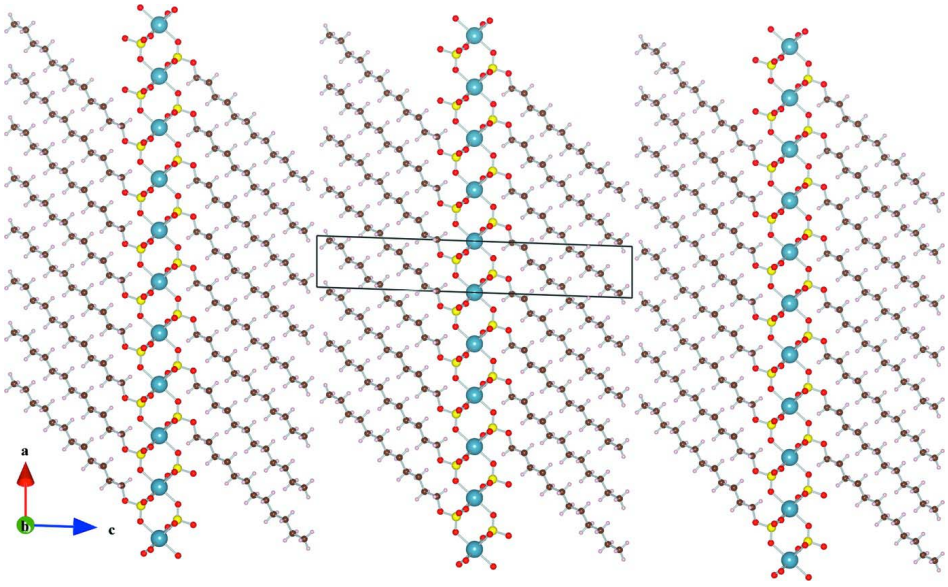


**Figure 2**

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

**Poly[bis($\mu_3$-dodecyl sulfato)calcium]**

*Crystal data*

$[Ca(C_{12}H_{25}O_4S)_2]$
$M_r = 570.84$
Triclinic, $P\overline{1}$
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) Å$^3$
$Z = 1$
$F(000) = 310$
$D_x = 1.275$ 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 × 0.10 × 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$^{-1}$
$\omega$ scans
4361 measured reflections
2500 independent reflections
2396 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.4°$
$h = -5 \rightarrow 5$
$k = -6 \rightarrow 6$
$l = -35 \rightarrow 35$

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

$\Delta\rho_{max} = 0.39$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ e Å$^{-3}$

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |

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| 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) |

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| 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) $x+1, y, z$.