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Poly[bis(μ_3-dodecyl sulfato)calcium]

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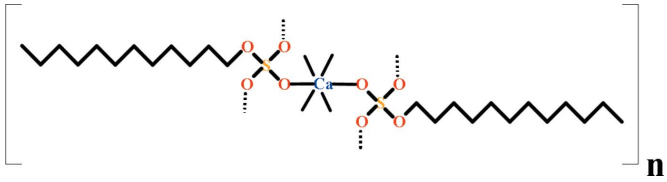
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.088; data-to-parameter ratio = 10.6.

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
α = 93.4321 (19)°
β = 90.099 (4)°
γ = 118.393 (5)°
V = 743.22 (7) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 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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supplementary materials

Acta Cryst. (2010). E**66**, m749 [**doi:10.1107/S1600536810020659**]

Poly[bis(μ_3-dodecyl sulfato)calcium]

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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).

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.

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.

Figures

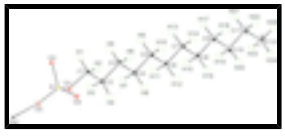


Fig. 1. The asymmetric unit of (I) with atom labels and 50% probability displacement ellipsoids for non-H atoms. H atoms are shown as spheres of arbitary radius.

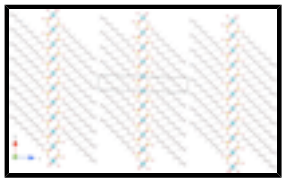


Fig. 2. The packing of (I), viewed along the *b* axis, showing hydrocarbon (dodecyl sulfate) layers which sandwich Ca atoms.

Poly[bis(μ$_3$-dodecyl sulfato)calcium]

Crystal data

$[Ca(C_{12}H_{25}O_4S)_2]$	$Z = 1$
$M_r = 570.84$	$F(000) = 310$
Triclinic, $P\overline{1}$	$D_x = 1.275$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
$a = 5.3888$ (3) Å	Cell parameters from 3581 reflections
$b = 5.3834$ (3) Å	$\theta = 1.4$–$25.5°$
$c = 29.1922$ (16) Å	$\mu = 0.39$ mm^{-1}

α = 93.4321 (19)°	T = 93 K
β = 90.099 (4)°	Needle, colourless
γ = 118.393 (5)°	0.50 × 0.10 × 0.10 mm
V = 743.22 (7) Å^3	

Data collection

Rigaku R-AXIS IV diffractometer	2396 reflections with $I > 2\sigma(I)$
Radiation source: rotating-anode X-ray	R_{int} = 0.031
Graphite Monochromator	θ_{max} = 25.5°, θ_{min} = 1.4°
Detector resolution: 10.0 pixels mm^{-1}	h = −5→5
ω scans	k = −6→6
4361 measured reflections	l = −35→35
2500 independent reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.031	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.088	All H-atom parameters refined
S = 1.08	$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.4436P]$ where $P = (F_o^2 + 2F_c^2)/3$
2500 reflections	$(\Delta/\sigma)_{max}$ = 0.001
235 parameters	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −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 (Å^2)

	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, °)

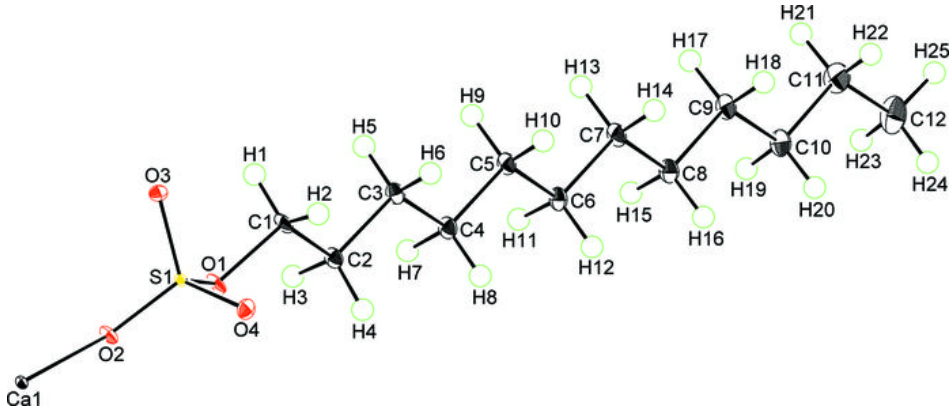
Ca1—O4^{i}	2.2955 (11)	C4—H8	0.99 (2)
Ca1—O4^{ii}	2.2956 (11)	C5—C6	1.529 (2)
Ca1—O3^{iii}	2.3177 (10)	C5—H9	1.01 (2)
Ca1—O3^{iv}	2.3178 (11)	C5—H10	0.98 (2)
Ca1—O2	2.3544 (10)	C6—C7	1.524 (2)
Ca1—O2^{v}	2.3544 (10)	C6—H11	0.99 (2)
Ca1—S1^{v}	3.4589 (4)	C6—H12	0.99 (2)
Ca1—S1	3.4589 (4)	C7—C8	1.528 (2)
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*.

Fig. 1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C10
H1
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H15
C1
H20
C4
H11
H16
S1
O1
C2
H12
H7
H3
H8
O4
H4
O2
Ca1

Fig. 2