

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

A ramsayite-type oxide, $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$ Hisanori Yamane,^{a*} Shunsuke Abe,^a Rong Tu^b and Takashi Goto^b

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Received 28 August 2010; accepted 12 September 2010

Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{Al}-\text{O}) = 0.002\text{ \AA}$; R factor = 0.018; wR factor = 0.043; data-to-parameter ratio = 12.2.

The title compound, dicalcium nonaoxidodistannate(IV)-dialuminate, is the second example which crystallizes in the isotypic structure of a pyroxene silicate, $\text{Na}_2\text{Ti}_2\text{Si}_2\text{O}_9$ (ramsayite). $\infty^1[\text{Sn}_2\text{O}_8]$ chains and pyroxene-type $\infty^1[\text{Al}_2\text{O}_6]$ chains are formed along the b axis by sharing O atoms. The Ca atoms are situated in the resulting channels and exhibit a coordination number of 7.

Related literature

For the structure of ramsayite, $\text{Na}_2\text{Ti}_2\text{Si}_2\text{O}_9$, see: Sundberg *et al.* (1987). For the synthesis of $\text{Ca}_8\text{Sn}_7\text{Al}_{10}\text{O}_{37}$, see: Barbanyagre & Kotlyarov (2001). For the structure of a related stannate silicate, $\text{Ca}_2\text{SnSi}_2\text{O}_9$, see: Blasse *et al.* (1995). For bond-valence parameters, see: Brese & O'Keeffe (1991). For the $\text{CaO}-\text{Al}_2\text{O}_3$ system, see: Jerebtsov & Mikhailov (2001). For the Inorganic Crystal Structure Database, see: ICSD (2009).

Experimental

Crystal data

$\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$	$V = 735.18 (18)\text{ \AA}^3$
$M_r = 515.50$	$Z = 4$
Orthorhombic, $Pbcn$	Mo $K\alpha$ radiation
$a = 8.9866 (6)\text{ \AA}$	$\mu = 8.46\text{ mm}^{-1}$
$b = 5.4894 (11)\text{ \AA}$	$T = 293\text{ K}$
$c = 14.9030 (18)\text{ \AA}$	$0.17 \times 0.15 \times 0.07\text{ mm}$

Data collection

Rigaku R-AXIS RAPID diffractometer	Absorption correction: numerical (NUMABS; Higashi, 1999)
	$T_{\min} = 0.427$, $T_{\max} = 0.717$
	6534 measured reflections

845 independent reflections
788 reflections with $I > 2\sigma(I)$

 $R_{\text{int}} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.018$
 $wR(F^2) = 0.043$
 $S = 1.08$
845 reflections

69 parameters
 $\Delta\rho_{\text{max}} = 0.72\text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.72\text{ e \AA}^{-3}$

Table 1

Selected bond lengths (\AA).

Ca1—O3 ⁱ	2.303 (2)	Al1—O2	1.763 (2)
Ca1—O2	2.391 (2)	Al1—O1 ^{iv}	1.777 (3)
Ca1—O1 ⁱⁱ	2.404 (2)	Sn1—O4 ^v	2.002 (2)
Ca1—O4 ⁱ	2.412 (2)	Sn1—O3	2.032 (2)
Ca1—O2 ⁱ	2.463 (2)	Sn1—O3 ⁱ	2.053 (2)
Ca1—O5	2.486 (2)	Sn1—O5 ^{vi}	2.0682 (13)
Ca1—O3 ⁱⁱⁱ	2.624 (2)	Sn1—O1 ⁱ	2.106 (2)
Al1—O2 ⁱ	1.735 (2)	Sn1—O1	2.207 (2)
Al1—O4	1.745 (2)		

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

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

This work was supported in part by a Grant-in-Aid for Scientific Research (B) (No. 21350113, 2009) from the Ministry of Education, Culture, Sports and Technology (MEXT), Japan, and performed under the auspices of the Inter-university Cooperative Research Program of the Institute for Materials Research, Tohoku University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2147).

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supporting information

Acta Cryst. (2010). E66, i72 [doi:10.1107/S1600536810036445]

A ramsayite-type oxide, $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$

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S1. Comment

Barbanyagre and Kotlyarov (2001) reported a quaternary oxide $\text{Ca}_8\text{Al}_{10}\text{Sn}_7\text{O}_{37}$ with a powder X-ray diffraction (PXRD) pattern, but they did not clarify the crystal structure. We have prepared single crystals of $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$ by slow cooling of a Ca—Al—Sn—O melt. The PXRD pattern of $\text{Ca}_8\text{Al}_{10}\text{Sn}_7\text{O}_{37}$ was similar to that calculated with the crystal structure parameters of $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$ analyzed by the present study.

$\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$ is isostructural with ramsayite (lorenzenite) $\text{Na}_2\text{Ti}_2\text{Si}_2\text{O}_9$ ($a = 8.7128$ (10), $b = 5.2327$ (5), $c = 14.487$ (2) Å) (Sundberg, *et al.*, 1987). Other compounds crystallizing in the isotopic structure were not found in the Inorganic Crystal Structure Database (ICSD, 2009).

The selected bond distances in $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$ are summarized in Table 1. The coordination environments of Ca, Sn and Al are drawn with displacement ellipsoids in Fig. 1. The Sn site is in a distorted oxygen octahedron with the Sn—O distances varying from 2.002 (2) to 2.207 (2) Å, (average 2.08 (8) Å). The bond valence sum (BVS) calculated for Sn atoms with the bond valence parameter of $R(\text{Sn—O}) = 1.905$ Å (Brese & O'Keeffe, 1991) was 3.815, a little smaller than the IV valence of Sn. These Sn—O bond lengths and the BVS are consistent with those reported for $\text{Ca}_3\text{SnSi}_2\text{O}_9$ (2.007–2.134 Å, avg. 2.08 (4) Å, BVS 3.803) (Blasse *et al.*, 1995).

Each SnO_6 octahedron shares O1—O3 edges with both adjacent sides of SnO_6 octahedra and a one-dimensional chain $\infty^1[\text{Sn}_2\text{O}_8]$ is formed along the b axis. Al atoms are tetrahedrally coordinated by O atoms and the AlO_4 tetrahedra form pyroxene-type $\infty^1[\text{Al}_2\text{O}_6]$ chains along the b axis by sharing O2. The Al—O bond lengths are from 1.735 to 1.777 (3) Å (avg. 1.755 (19) Å) and the BVS of 3.02 is consistent with trivalent of Al(III). The chains of $\infty^1[\text{Al}_2\text{O}_6]$ and $\infty^1[\text{Sn}_2\text{O}_8]$ are bridged by sharing O4, and the $\infty^1[\text{Sn}_2\text{O}_8]$ chains are linked each other by sharing O5 on a two-fold axis, forming rectangular channels along the b axis (Fig. 2). Ca sites are situated in the channels and surrounded by 7 oxygen atoms with the distances from 2.303 (2) to 2.624 (2) Å. The BVS of Ca atoms is 2.01 and well agrees with the valence number of Ca(II).

A permittivity of 48 and a $\tan\delta$ of 0.02 were measured at room temperature with an impedance analyzer (Solartron 1260 and 1296) for the polycrystalline sample which was mainly composed of $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$ with a small amount of CaSnO_3 which crystallized at the initial stage of solid state reaction.

S2. Experimental

The starting materials used were CaCO_3 (Rare Metallic, 99.99% purity), SnO_2 (Rare Metallic, 99.99% purity) and Al_2O_3 (Rare Metallic, 99.99% purity). The powders were weighed, mixed in an agate mortar with a pestle, and pressed into pellets, which were placed on a platinum plate and heated in an electric furnace in air. Single crystals of $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$ were prepared from a starting mixture with an atomic ratio Ca: Sn: Al = 5:1:4. The pellet of the mixture was heated to 1823 K at a heating rate of 200 K/h, and then cooled to 1773 K at a cooling rate of 5 K/h. The single crystals were probably grown in a flux with a composition close to a $\text{Ca}_3\text{Al}_2\text{O}_6$ — CaAl_2O_4 mixture which has the eutectic point of 1644

K (Jerebtsov & Mikhailov, 2001). The samples were then cooled in the furnace by shutting off the electric power. The obtained sample was crushed into fragments and colorless transparent single crystals of about 0.06–0.14 mm were picked up under an optical microscope. A polycrystalline sample was prepared by heating the pellets of the starting mixtures with stoichiometric metal ratios Ca:Sn:Al = 1:1:1 at around 1600 K for 24 h.

S3. Refinement

The highest peak in the difference electron density map is 0.94 Å from Sn1 while the deepest hole is 1.08 Å from the same atom.

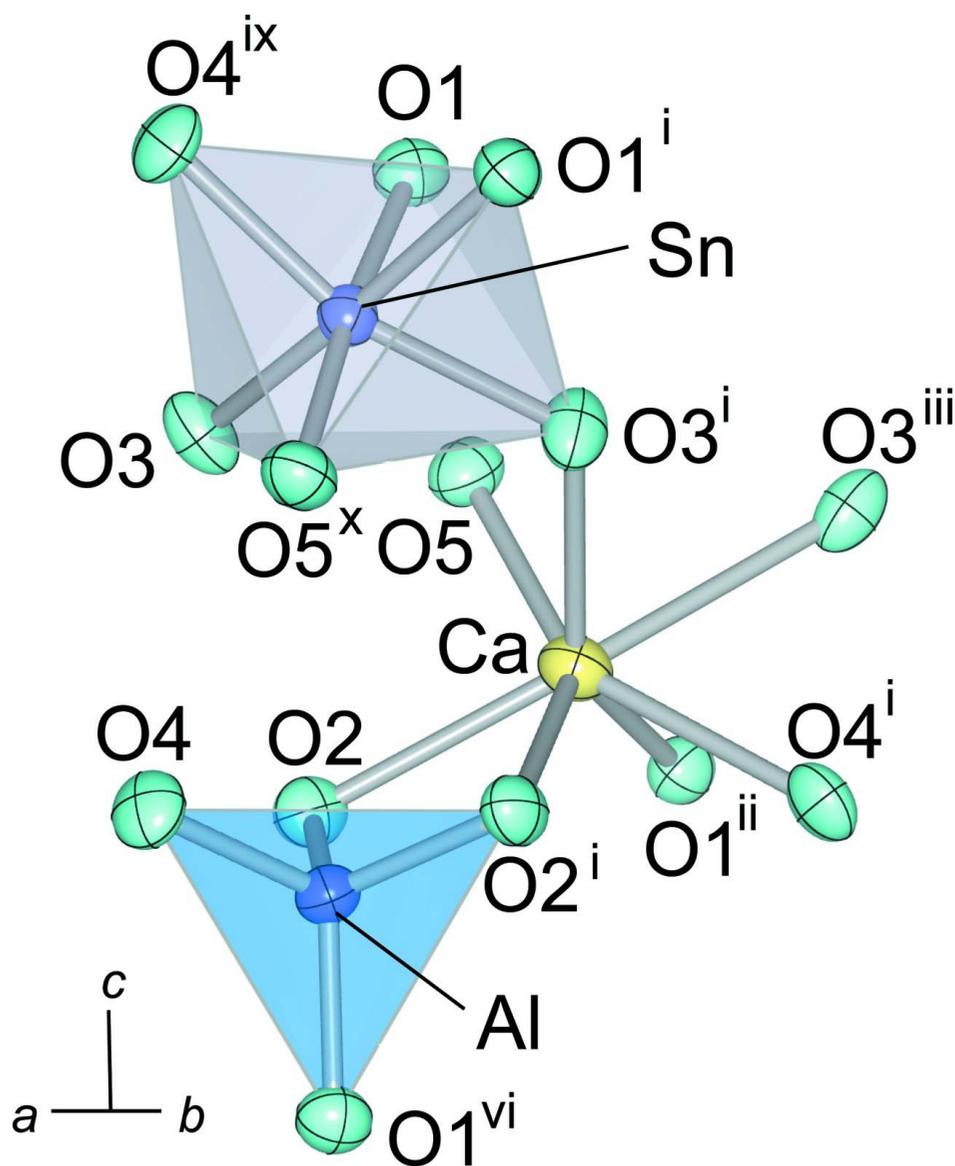
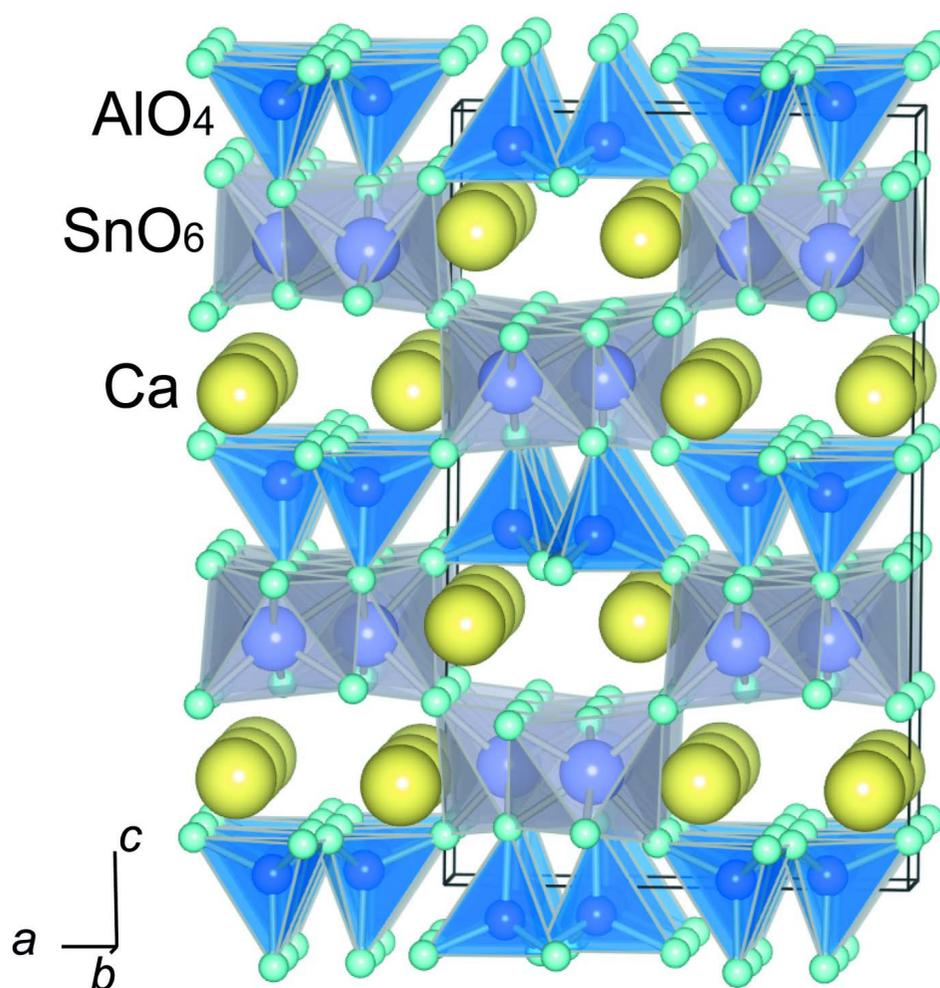


Figure 1

O-atom coordination around Ca, Al, and Sn atoms in the structure of $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$. Displacement ellipsoids are drawn at 99% probability level. [Symmetry codes as in Table 1.]

**Figure 2**

Crystal structure of $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$, illustrated with distorted Sn-centered oxygen octahedra and Al-centered oxygen tetrahedra.

dicalcium nonaoxydistanate(IV) dialuminate

Crystal data

$\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$

$M_r = 515.50$

Orthorhombic, *Pbcn*

Hall symbol: $-P\ 2n\ 2ab$

$a = 8.9866\ (6)\ \text{\AA}$

$b = 5.4894\ (11)\ \text{\AA}$

$c = 14.9030\ (18)\ \text{\AA}$

$V = 735.18\ (18)\ \text{\AA}^3$

$Z = 4$

$F(000) = 952$

$D_x = 4.657\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71075\ \text{\AA}$

Cell parameters from 5414 reflections

$\theta = 3.6\text{--}27.8^\circ$

$\mu = 8.46\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Platelet, colourless

$0.17 \times 0.15 \times 0.07\ \text{mm}$

Data collection

Rigaku R-AXIS RAPID
diffractometer

Radiation source: fine-focus sealed tube
Graphite monochromator

Detector resolution: $10.00\ \text{pixels mm}^{-1}$
 ω scans

Absorption correction: numerical
(*NUMABS*; Higashi, 1999)

$T_{\min} = 0.427$, $T_{\max} = 0.717$
 6534 measured reflections
 845 independent reflections
 788 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.6^\circ$
 $h = -11 \rightarrow 11$
 $k = -7 \rightarrow 7$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.018$
 $wR(F^2) = 0.043$
 $S = 1.08$
 845 reflections
 69 parameters
 0 restraints

Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map
 $w = 1/[\sigma^2(F_o^2) + (0.002P)^2 + 2.2176P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.72 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.72 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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	0.06714 (7)	0.36160 (11)	0.14603 (5)	0.00676 (14)
Al1	0.34369 (10)	0.31037 (18)	0.02817 (7)	0.0055 (2)
Sn1	0.34459 (2)	0.36611 (4)	0.333981 (15)	0.00525 (9)
O1	0.1618 (2)	0.1912 (4)	0.40897 (16)	0.0070 (5)
O2	0.2277 (2)	0.0795 (4)	0.07144 (15)	0.0071 (4)
O3	0.3314 (2)	0.0365 (4)	0.27250 (16)	0.0079 (5)
O4	0.5156 (2)	0.2310 (4)	0.07402 (16)	0.0078 (4)
O5	0.0000	0.0250 (6)	0.2500	0.0077 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0069 (3)	0.0071 (3)	0.0062 (3)	-0.0007 (2)	0.0006 (2)	-0.0003 (2)
Al1	0.0057 (5)	0.0058 (5)	0.0050 (5)	-0.0001 (3)	-0.0004 (3)	0.0001 (4)
Sn1	0.00529 (13)	0.00501 (14)	0.00544 (14)	0.00004 (7)	-0.00022 (7)	-0.00022 (8)
O1	0.0080 (11)	0.0067 (11)	0.0064 (12)	-0.0008 (8)	-0.0004 (8)	-0.0002 (9)
O2	0.0089 (11)	0.0054 (10)	0.0070 (11)	-0.0007 (8)	-0.0005 (9)	-0.0003 (9)
O3	0.0077 (11)	0.0064 (11)	0.0096 (13)	-0.0008 (8)	0.0026 (9)	-0.0019 (9)
O4	0.0059 (10)	0.0088 (11)	0.0087 (11)	-0.0003 (8)	-0.0024 (9)	-0.0011 (9)
O5	0.0086 (15)	0.0078 (15)	0.0066 (16)	0.000	-0.0014 (13)	0.000

Geometric parameters (Å, °)

Ca1—O3 ⁱ	2.303 (2)	Sn1—O1 ⁱ	2.106 (2)
Ca1—O2	2.391 (2)	Sn1—O1	2.207 (2)
Ca1—O1 ⁱⁱ	2.404 (2)	O1—Al1 ^{vii}	1.777 (3)
Ca1—O4 ⁱ	2.412 (2)	O1—Sn1 ^{viii}	2.106 (2)
Ca1—O2 ⁱ	2.463 (2)	O1—Ca1 ⁱⁱ	2.404 (2)
Ca1—O5	2.486 (2)	O2—Al1 ^{viii}	1.735 (2)
Ca1—O3 ⁱⁱⁱ	2.624 (2)	O2—Ca1 ^{viii}	2.463 (2)
Al1—O2 ⁱ	1.735 (2)	O3—Sn1 ^{viii}	2.053 (2)
Al1—O4	1.745 (2)	O3—Ca1 ^{viii}	2.303 (2)
Al1—O2	1.763 (2)	O3—Ca1 ^{ix}	2.624 (2)
Al1—O1 ^{iv}	1.777 (3)	O4—Sn1 ^v	2.002 (2)
Sn1—O4 ^v	2.002 (2)	O4—Ca1 ^{viii}	2.412 (2)
Sn1—O3	2.032 (2)	O5—Sn1 ^x	2.0682 (13)
Sn1—O3 ⁱ	2.053 (2)	O5—Sn1 ^{viii}	2.0682 (13)
Sn1—O5 ^{vi}	2.0682 (13)	O5—Ca1 ⁱⁱ	2.486 (2)
O3 ⁱ —Ca1—O2	114.30 (8)	O3 ⁱ —Sn1—O1 ⁱ	80.21 (9)
O3 ⁱ —Ca1—O1 ⁱⁱ	141.26 (8)	O5 ^{vi} —Sn1—O1 ⁱ	88.98 (9)
O2—Ca1—O1 ⁱⁱ	96.08 (8)	O4 ^v —Sn1—O1	87.66 (9)
O3 ⁱ —Ca1—O4 ⁱ	97.80 (8)	O3—Sn1—O1	78.32 (9)
O2—Ca1—O4 ⁱ	121.59 (8)	O3 ⁱ —Sn1—O1	81.41 (9)
O1 ⁱⁱ —Ca1—O4 ⁱ	84.93 (8)	O5 ^{vi} —Sn1—O1	173.05 (6)
O3 ⁱ —Ca1—O2 ⁱ	82.57 (8)	O1 ⁱ —Sn1—O1	94.57 (9)
O2—Ca1—O2 ⁱ	69.69 (4)	Al1 ^{vii} —O1—Sn1 ^{viii}	121.70 (13)
O1 ⁱⁱ —Ca1—O2 ⁱ	132.50 (8)	Al1 ^{vii} —O1—Sn1	121.93 (11)
O4 ⁱ —Ca1—O2 ⁱ	67.76 (7)	Sn1 ^{viii} —O1—Sn1	96.90 (9)
O3 ⁱ —Ca1—O5	84.02 (7)	Al1 ^{vii} —O1—Ca1 ⁱⁱ	108.61 (10)
O2—Ca1—O5	87.41 (7)	Sn1 ^{viii} —O1—Ca1 ⁱⁱ	97.21 (9)
O1 ⁱⁱ —Ca1—O5	73.48 (6)	Sn1—O1—Ca1 ⁱⁱ	107.17 (10)
O4 ⁱ —Ca1—O5	145.85 (7)	Al1 ^{viii} —O2—Al1	134.02 (15)
O2 ⁱ —Ca1—O5	145.50 (6)	Al1 ^{viii} —O2—Ca1	120.07 (11)
O3 ⁱ —Ca1—O3 ⁱⁱⁱ	77.78 (9)	Al1—O2—Ca1	93.51 (9)
O2—Ca1—O3 ⁱⁱⁱ	159.97 (8)	Al1 ^{viii} —O2—Ca1 ^{viii}	91.78 (9)
O1 ⁱⁱ —Ca1—O3 ⁱⁱⁱ	67.00 (8)	Al1—O2—Ca1 ^{viii}	94.11 (10)
O4 ⁱ —Ca1—O3 ⁱⁱⁱ	69.47 (7)	Ca1—O2—Ca1 ^{viii}	123.82 (10)
O2 ⁱ —Ca1—O3 ⁱⁱⁱ	129.46 (7)	Sn1—O3—Sn1 ^{viii}	104.43 (10)
O5—Ca1—O3 ⁱⁱⁱ	77.73 (6)	Sn1—O3—Ca1 ^{viii}	135.82 (11)
O2 ⁱ —Al1—O4	113.24 (12)	Sn1 ^{viii} —O3—Ca1 ^{viii}	118.71 (10)
O2 ⁱ —Al1—O2	104.92 (9)	Sn1—O3—Ca1 ^{ix}	94.02 (9)
O4—Al1—O2	101.59 (11)	Sn1 ^{viii} —O3—Ca1 ^{ix}	104.41 (10)
O2 ⁱ —Al1—O1 ^{iv}	111.43 (12)	Ca1 ^{viii} —O3—Ca1 ^{ix}	84.64 (7)
O4—Al1—O1 ^{iv}	114.50 (11)	Al1—O4—Sn1 ^v	137.01 (13)
O2—Al1—O1 ^{iv}	110.23 (11)	Al1—O4—Ca1 ^{viii}	96.38 (10)
O4 ^v —Sn1—O3	90.89 (9)	Sn1 ^v —O4—Ca1 ^{viii}	101.55 (9)
O4 ^v —Sn1—O3 ⁱ	163.28 (9)	Sn1 ^x —O5—Sn1 ^{viii}	130.13 (15)
O3—Sn1—O3 ⁱ	99.18 (9)	Sn1 ^x —O5—Ca1 ⁱⁱ	121.78 (5)

O4 ^v —Sn1—O5 ^{vi}	98.44 (7)	Sn1 ^{viii} —O5—Ca1 ⁱⁱ	95.75 (4)
O3—Sn1—O5 ^{vi}	98.16 (9)	Sn1 ^x —O5—Ca1	95.75 (4)
O3 ⁱ —Sn1—O5 ^{vi}	93.33 (8)	Sn1 ^{viii} —O5—Ca1	121.78 (5)
O4 ^v —Sn1—O1 ⁱ	88.14 (9)	Ca1 ⁱⁱ —O5—Ca1	83.96 (10)
O3—Sn1—O1 ⁱ	172.86 (9)		

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