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The layer silicate Cs₂Sn^{IV}Si₆O₁₅

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Single crystals of Cs₂SnSi₆O₁₅, dicaesium tin(IV) hexasilicate, were serendipitously obtained from a CsCl/NaCl flux at 923 K, starting from mixtures of CaO, SnO and TeO₂ in a closed silica ampoule. The crystal structure of Cs₂SnSi₆O₁₅ is constructed from {Si₆O₁₅}^{6–} layers extending parallel to (101), and Cs^I cations with a coordination number of eleven as well as isolated [SnO₆] octahedra situated between the silicate layers. Each of the nine different SiO₄ tetrahedra in the silicate layer has a connectedness of Q^3 (three bridging and one terminal O atom), which leads to the formation of five- and eight-membered rings. The same type of silicate layer is found in the crystal structure of the mineral zeravshanite. Comparison with other silicates of the type Cs₂M^{IV}Si₆O₁₅ ($M^{IV} =$ Ti, Zr, Th, U) revealed a *klassengleiche* group–subgroup relationship of index 2 between Cs₂ZrSi₆O₁₅ (Z = 6, space group C2/m) and Cs₂SnSi₆O₁₅ (Z = 12, space group I2/c).

1. Chemical context

Calcium oxotellurate(IV), CaTeO₃, is known to exist in various polymorphic forms that can be obtained either through solid-state reactions (Trömel & Ziethen-Reichenach, 1970; Stöger et al., 2009) or under hydrothermal conditions and subsequent dehydration (Poupon et al., 2015). Some of the CaTeO₃ polymorphs have a non-centrosymmetric crystal structure and show ferroelectric behaviour (Rai et al., 2002) or a second harmonic generation (SHG) effect (Poupon et al., 2015). These features are thought to be related to the presence of the $5s^2$ electron lone pair at the Te^{IV} atom. In a current study it was attempted to incorporate Sn^{II} into CaTeO₃ under formation of solid solutions $(Ca_{1-x}Sn_x)TeO_3$ in order to investigate whether the $5s^2$ electron lone pair at the Sn^{II} atom has any influence on the ferroelectric or SHG characteristics. For that purpose, a flux medium consisting of a eutectic CsCl/NaCl mixture with a melting point of 766 K (Żemcżużny & Rambach, 1909) was chosen as reaction medium in a closed silica ampoule. In comparison with conventional ceramic routes, this allows the lowering of the reaction temperatures by a simultaneous increase of the diffusion pathways. However, neither the intended $(Ca_{1-x}Sn_x)TeO_3$ solid solutions nor other calcium oxotellurates with a partial replacement of $Ca^{\rm II}$ by $Sn^{\rm II}$ could be prepared this way. One of the side products of this reaction was Cs₂Sn^{IV}Si₆O₁₅, which had formed through attack of the silica glass ampoule by the molten salt mixture and concomitant oxidation of Sn^{II} to Sn^{IV}. Its crystal structure along with a structural comparison with other silicates is given here.

М	Ti (single-crystal data) ^a	Ti (powder data) ^b	Zr^{c}	Th $(173 \text{ K data})^d$	Th (293 K data) e	\mathbf{U}^{f}
Space group	C2/c	Сс	C2/m	$Pca2_1$	$Cmc2_1$	$Cmc2_1$
Ż	4	4	6	4	4	4
а	13.386 (5)	12.988 (2)	26.610 (10)	16.2920 (10)	7.2813 (15)	7.2717 (3)
b	7.423 (3)	7.5014 (3)	7.506 (2)	7.2154 (6)	16.420 (3)	16.3061 (7)
с	15.134 (5)	15.156 (3)	11.602 (4)	13.6800 (10)	13.591 (3)	13.4983 (6)
β	107.71 (3)	105.80 (3)	107.43 (2)	90	90	90
V	1432.51	1420.83	2210.92	1608.13	1624.92	1600.53

Table 1Crystal data (Å, °) of $Cs_2M^{IV}Si_6O_{15}$ compounds.

References: (a) Grey et al. (1997); (b) Nyman et al. (2000); (c) Jolicart et al. (1996); (d) Woodward et al. (2005); (e) Mann et al. (2015); (f) Liu & Lii (2011).

2. Structural commentary

The asymmetric unit of $Cs_2SnSi_6O_{15}$ comprises three Cs, two Sn, nine Si and twenty-three O sites. Except for one Sn site (Sn2) and one O site (O23), which are located on Wyckoff positions 4b (site symmetry $\overline{1}$) and 4e (site symmetry 2), respectively, all atoms are on general positions. The crystal structure of $Cs_2SnSi_6O_{15}$ can be described as being built up from silicate layers extending parallel to (101). The silicate layers are linked by caesium cations and isolated [SnO₆] octahedra situated between adjacent silicate layers (Fig. 1).

Each of the three caesium cations exhibits a coordination number of 11, with Cs–O bond lengths ranging from 2.951 (3) to 3.748 (3) Å. The mean Cs–O bond lengths for the three individual [CsO₁₁] polyhedra (Cs1: 3.312 Å; Cs2: 3.355 Å; Cs3: 3.342 Å) are in very good agreement with the overall mean Cs–O bond length of 3.333 (226) Å calculated from 748 bonds for 11-coordinate Cs (Gagné & Hawthorne, 2016). The two Sn^{IV} atoms show slight deviations from a regular octahedral coordination, with Sn–O bond lengths ranging from 2.031 (3) to 2.058 (3) Å. The overall mean Sn^{IV}–O bond length of 2.054 (10) Å calculated from 32 bonds (Gagné & Hawthorne, 2018) is somewhat longer than the mean values for Sn1 (2.037 Å) and Sn2 (2.047 Å).



Figure 1

The crystal structure of Cs₂SnSi₆O₁₅ in a projection along $[0\overline{1}0]$. Cs sites are given in blue, [SnO₆] octahedra in orange and SiO₄ tetrahedra in red. Displacement parameters are drawn at the 74% probability level. For clarity, the disordered Cs3 site with minor occupancy (Cs3*B*) is not shown. [Symmetry code: (i) *x*, *y* + 1, *z* + 1.]

All of the nine SiO₄ tetrahedra in the ${Si_6O_{15}}^{6-}$ layer have one terminal O atom and are linked to three other SiO₄ tetrahedra by common bridging O atoms. Thus, the connectedness of the silicate tetrahedra is Q³ according to the notation of Liebau (1985). The bond lengths distribution in the SiO₄ tetrahedra reflects the different roles of the O atoms in the silicate layer. The Si-O bonds to terminal O atoms are shorter by about 0.03 Å (mean 1.588 Å) than those to bridging O atoms (1.621 Å). The total mean Si - O bond in $Cs_2SnSi_6O_{15}$ has a value of 1.613 Å, which is slightly shorter than the overall mean of 1.625 (24) calculated from 9128 bonds (Gagné & Hawthorne, 2018). The connectedness of the SiO_4 tetrahedra leads to the formation of a ${Si_6O_{15}}^{6-}$ layer comprising five- and eight-membered rings (Fig. 2). The same type of silicate layer is found in the mineral zeravshanite with composition $(Cs_{3.80}Na_{0.18}K_{0.02})Na_2(Zr_{2.73}Ti_{0.19}Sn_{0.04}Fe_{0.04})$ -(Si₁₈O₄₅)(H₂O)₂ (Uvarova et al., 2004).

Crystal-chemical features of silicates comprising the ${Si_6O_{15}}^{6-}$ anion were recently compiled by Wierzbicka-Wieczorek *et al.* (2015). A topological classification of zirconosilicates and their analogues, where the simplest structure units are $[MO_6]$ octahedra and TO_4 tetrahedra united by vertices, was reported some time ago by Ilyushin & Blatov (2002). Since the same structure elements are also present in Cs₂SnSi₆O₁₅ in the form of [SnO₆] octahedra and SiO₄ tetrahedra, a similar analysis can be made. With respect to the concept of the polyhedral microensemble (PME) introduced by Ilyushin & Blatov (2002), Cs₂SnSi₆O₁₅ conforms to the PME type C-1. A comparison of the unit-cell parameters of Cs₂SnSi₆O₁₅ with those of the other reported Cs₂ $M^{IV}Si_6O_{15}$





The ${Si_6O_{15}}^{6-}$ layer in the crystal structure of $Cs_2SnSi_6O_{15}$ shown in a projection along $[\overline{102}]$. Colour code and displacement ellipsoids are as in Fig.1.

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Table 2Experimental details.

Crystal data	
Chemical formula	Cs ₂ SnSi ₆ O ₁₅
M _r	793.05
Crystal system, space group	Monoclinic, I2/c
Temperature (K)	296
a, b, c (Å)	26.3434 (10), 7.4805 (3), 22.9137 (7)
β (°)	107.4020 (7)
$V(Å^3)$	4308.7 (3)
Z	12
Radiation type	Μο Κα
$\mu \text{ (mm}^{-1})$	7.36
Crystal size (mm)	$0.12\times0.03\times0.01$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Krause e. al., 2015).
T_{\min}, T_{\max}	0.539, 0.747
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	51032, 8282, 5013
R _{int}	0.077
$(\sin \theta / \lambda)_{\rm max} ({\rm \AA}^{-1})$	0.772
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.037. 0.082. 1.00
No. of reflections	8282
No. of parameters	331
$\Delta \rho_{\rm max}, \Delta \rho_{\rm min} \ (e \ {\rm \AA}^{-3})$	1.84, -1.48

Computer programs: *APEX3* and *SAINT* (Bruker, 2018), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ATOMS* (Dowty, 2006) and *publCIF* (Westrip, 2010).

 $(M^{IV} = \text{Ti}, \text{Zr}, \text{Th}, \text{U})$ compounds (Table 1) revealed a close relationship between the Sn- and Zr-containing phases. The *a* and *b* axes and the β angle in the two structures are very similar, and the *c* axis of the Sn-containing compound is doubled. Indeed, there is a group–subgroup relationship between the crystal structures of Cs₂ZrSi₆O₁₅ and Cs₂SnSi₆O₁₅. The Sn-containing phase crystallizes in a subgroup (*I*2/*c*; *Z* = 12) of the Zr-containing phase (*C*2/*m*; *Z* = 6), defining a *klassengleiche* relationship of index 2 (Müller, 2013).

3. Synthesis and crystallization

1.2 mmol of CaO (0.067 g), 0.13 mmol SnO (0.018 g) and 1.3 mmol of TeO₂ (0.207 g) were intimately mixed with 1 g of an NaCl (35 mol%):CsCl (65 mol%) mixture and filled in a silica ampoule that was subsequently evacuated and torchsealed. The ampoule was then heated at 923 K for 2 d before the power of the furnace was switched off. The silica ampoule showed a severe attack from the halide flux but was still intact. After washing the recrystallized flux with several portions of warm water and drying the remaining solid in air, a few lathshaped crystals of the title compound could be isolated under a polarizing microscope. Single-crystal diffraction of other selected crystals revealed α -CaTeO₃ (Stöger *et al.*, 2009), CaTe₂O₅ (Weil & Stöger, 2008) and Ca₄Te₅O₁₄ (Weil, 2004) as products. Powder X-ray diffraction of the bulk showed the reflections of these phases together with those of SnO₂ and also some reflections of non-assignable phase(s).

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. For better comparison of Cs₂SnSi₆O₁₅ with the crystal structure of Cs₂ZrSi₆O₁₅, the unconventional setting *I*2/*c* of space group type *C*2/*c* (No. 15) was chosen, so that unit-cell parameters *a*, *b*, *c* and β of the Sncontaining phase correspond to *a*, *b*, 2*c* and β of the Zrcontaining phase (Jolicart *et al.*, 1996; Table 1). The Cs3 atom in Cs₂SnSi₆O₁₅ was found to be disordered over two sites in a 0.934 (5):0.066 ratio and was refined with common displacement parameters for the two sites (*A* and *B*).

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Computing details

Data collection: *APEX3* (Bruker, 2018); cell refinement: *SAINT* (Bruker, 2018); data reduction: *SAINT* (Bruker, 2018); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ATOMS* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Dicaesium tin(IV) hexasilicate

Crystal data

Cs₂SnSi₆O₁₅ $M_r = 793.05$ Monoclinic, I2/c a = 26.3434 (10) Å b = 7.4805 (3) Å c = 22.9137 (7) Å $\beta = 107.4020$ (7)° V = 4308.7 (3) Å³ Z = 12

Data collection

Bruker APEXII CCD diffractometer ω - and φ -scans Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015). $T_{\min} = 0.539$, $T_{\max} = 0.747$ 51032 measured reflections

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.037$ $wR(F^2) = 0.082$ S = 1.008282 reflections 331 parameters F(000) = 4368 $D_x = 3.668 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 4399 reflections $\theta = 2.8-32.4^{\circ}$ $\mu = 7.36 \text{ mm}^{-1}$ T = 296 KLath, colourless $0.12 \times 0.03 \times 0.01 \text{ mm}$

8282 independent reflections 5013 reflections with $I > 2\sigma(I)$ $R_{int} = 0.077$ $\theta_{max} = 33.3^\circ$, $\theta_{min} = 2.8^\circ$ $h = -40 \rightarrow 40$ $k = -11 \rightarrow 11$ $l = -35 \rightarrow 35$

0 restraints $w = 1/[\sigma^2(F_o^2) + (0.0259P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.002$ $\Delta\rho_{max} = 1.84 \text{ e} \text{ Å}^{-3}$ $\Delta\rho_{min} = -1.48 \text{ e} \text{ Å}^{-3}$

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.

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	Occ. (<1)
Cs1	0.39755 (2)	-0.01953 (4)	0.18693 (2)	0.01982 (7)	
Cs2	0.57484 (2)	-0.51580 (4)	0.00767 (2)	0.02128 (7)	
Cs3A	0.74609 (2)	-0.98408 (7)	0.32160 (8)	0.02213 (18)	0.934 (5)
Cs3B	0.7514 (3)	-0.9776 (11)	0.3439 (8)	0.02213 (18)	0.066 (5)
Sn1	0.67822 (2)	-0.49735 (4)	-0.17784 (2)	0.00700 (6)	
Sn2	0.500000	0.000000	0.000000	0.00681 (7)	
Si1	0.62500 (5)	-0.70216 (15)	0.18853 (6)	0.0075 (2)	
Si2	0.63425 (5)	-0.30679 (15)	0.18719 (6)	0.0091 (2)	
Si3	0.69676 (5)	-0.70648 (15)	-0.04744 (6)	0.0077 (2)	
Si4	0.63589 (4)	-0.99872 (15)	-0.00070 (5)	0.0067 (2)	
Si5	0.81053 (5)	-0.81223 (15)	0.04445 (6)	0.0086 (2)	
Si6	0.68624 (4)	-0.99635 (15)	0.13636 (5)	0.0078 (2)	
Si7	0.50782 (5)	-0.80838 (15)	0.13301 (6)	0.0080 (2)	
Si8	0.51736 (5)	-0.20099 (15)	0.13222 (6)	0.0081 (2)	
Si9	0.45804 (4)	-0.50114 (15)	0.18261 (5)	0.0066 (2)	
01	0.65897 (13)	-0.7024 (4)	0.25901 (15)	0.0129 (7)	
O2	0.56382 (13)	-0.7463 (4)	0.18108 (15)	0.0167 (7)	
O3	0.64737 (13)	-0.8469 (4)	0.15066 (16)	0.0199 (8)	
O4	0.62794 (13)	-0.5077 (4)	0.15681 (13)	0.0140 (6)	
O5	0.66980 (12)	-0.3096 (4)	0.25683 (15)	0.0115 (6)	
O6	0.66307 (13)	-0.1918 (4)	0.14653 (15)	0.0162 (7)	
O7	0.57564 (13)	-0.2302 (4)	0.18125 (15)	0.0170 (7)	
08	0.70020 (13)	-0.6982 (4)	-0.11572 (15)	0.0119 (7)	
O9	0.75309 (13)	-0.7544 (5)	0.00067 (17)	0.0187 (7)	
O10	0.65155 (12)	-0.8509 (4)	-0.04422 (15)	0.0134 (7)	
O11	0.67790 (13)	-0.5157 (4)	-0.02671 (14)	0.0144 (6)	
O12	0.57747 (12)	-0.9680 (4)	0.00220 (15)	0.0144 (7)	
O13	0.68113 (12)	-0.9797 (4)	0.06475 (13)	0.0123 (6)	
O14	0.85664 (13)	-0.6934 (4)	0.02893 (16)	0.0147 (7)	
O15	0.81334 (13)	-0.7987 (4)	0.11477 (14)	0.0125 (7)	
O16	0.74525 (12)	-0.9636 (4)	0.17887 (14)	0.0136 (7)	
O17	0.50824 (13)	-0.7996 (4)	0.06370 (15)	0.0127 (7)	
O18	0.46185 (12)	-0.6903 (4)	0.14849 (15)	0.0129 (7)	
O19	0.49642 (12)	-0.0117 (4)	0.15154 (14)	0.0119 (6)	
O20	0.51978 (13)	-0.1991 (4)	0.06375 (15)	0.0121 (7)	
O21	0.47656 (13)	-0.3514 (4)	0.14152 (16)	0.0171 (7)	
O22	0.39930 (12)	-0.4614 (4)	0.18260 (15)	0.0149 (7)	
O23	0.500000	-0.5021 (6)	0.250000	0.0193 (10)	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (A^2)

supporting information

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.01741 (15)	0.02075 (15)	0.02457 (17)	-0.00118 (12)	0.01126 (13)	-0.00080 (13)
Cs2	0.01832 (15)	0.02304 (15)	0.02465 (17)	-0.00150 (14)	0.00974 (13)	-0.00107 (14)
Cs3A	0.01454 (17)	0.02048 (16)	0.0320 (5)	0.00139 (14)	0.0080(2)	0.0013 (2)
Cs3B	0.01454 (17)	0.02048 (16)	0.0320 (5)	0.00139 (14)	0.0080(2)	0.0013 (2)
Sn1	0.00705 (12)	0.00726 (12)	0.00620 (13)	0.00027 (11)	0.00124 (10)	0.00007 (12)
Sn2	0.00707 (17)	0.00700 (17)	0.00653 (18)	0.00038 (16)	0.00229 (14)	0.00016 (17)
Si1	0.0074 (6)	0.0074 (5)	0.0069 (6)	-0.0006 (4)	0.0011 (5)	-0.0018 (4)
Si2	0.0098 (6)	0.0086 (5)	0.0082 (7)	-0.0011 (4)	0.0013 (5)	0.0012 (4)
Si3	0.0086 (6)	0.0076 (5)	0.0064 (7)	0.0007 (4)	0.0016 (5)	0.0012 (4)
Si4	0.0063 (5)	0.0065 (5)	0.0079 (5)	-0.0005 (4)	0.0031 (4)	0.0001 (5)
Si5	0.0093 (6)	0.0071 (5)	0.0091 (7)	0.0004 (4)	0.0021 (5)	0.0010 (4)
Si6	0.0077 (5)	0.0091 (5)	0.0065 (5)	0.0003 (5)	0.0020 (4)	-0.0002 (5)
Si7	0.0086 (6)	0.0063 (5)	0.0091 (7)	-0.0002 (4)	0.0025 (5)	-0.0012 (4)
Si8	0.0089 (6)	0.0072 (5)	0.0086 (7)	0.0011 (4)	0.0031 (5)	0.0020 (4)
Si9	0.0068 (5)	0.0064 (5)	0.0071 (5)	-0.0012 (5)	0.0029 (4)	-0.0004 (5)
01	0.0160 (17)	0.0111 (15)	0.0096 (18)	0.0011 (12)	0.0008 (14)	-0.0006 (12)
O2	0.0086 (16)	0.0259 (18)	0.0147 (19)	-0.0032 (13)	0.0020 (14)	-0.0048 (14)
03	0.0168 (18)	0.0198 (17)	0.022 (2)	0.0065 (14)	0.0036 (16)	-0.0121 (14)
O4	0.0229 (17)	0.0077 (13)	0.0097 (15)	-0.0037 (13)	0.0026 (13)	-0.0007 (12)
05	0.0119 (16)	0.0099 (14)	0.0110 (18)	-0.0009 (12)	0.0011 (14)	0.0037 (12)
06	0.0219 (19)	0.0129 (15)	0.0154 (19)	-0.0034 (13)	0.0079 (16)	0.0028 (13)
O7	0.0102 (17)	0.0242 (18)	0.0131 (19)	0.0048 (13)	-0.0019 (14)	0.0041 (14)
08	0.0164 (17)	0.0092 (14)	0.0105 (18)	0.0016 (12)	0.0049 (14)	0.0024 (12)
09	0.0121 (16)	0.0264 (17)	0.0146 (17)	0.0030 (13)	-0.0005 (13)	0.0072 (13)
O10	0.0129 (17)	0.0145 (15)	0.0105 (17)	-0.0063 (12)	0.0001 (14)	0.0045 (12)
011	0.0209 (17)	0.0096 (14)	0.0175 (17)	-0.0002 (13)	0.0131 (14)	-0.0014 (13)
O12	0.0071 (15)	0.0177 (15)	0.0203 (18)	-0.0010 (12)	0.0068 (13)	-0.0010 (13)
013	0.0134 (15)	0.0193 (16)	0.0030 (14)	-0.0020 (13)	0.0006 (12)	0.0005 (12)
O14	0.0124 (17)	0.0131 (15)	0.018 (2)	-0.0025 (12)	0.0042 (15)	0.0036 (13)
015	0.0196 (18)	0.0097 (14)	0.0070 (17)	0.0016 (12)	0.0022 (14)	0.0007 (12)
016	0.0083 (15)	0.0237 (17)	0.0081 (16)	-0.0012 (12)	0.0013 (12)	-0.0024 (13)
O17	0.0195 (18)	0.0111 (14)	0.0072 (18)	-0.0012 (13)	0.0036 (14)	-0.0039 (12)
O18	0.0117 (16)	0.0096 (14)	0.0178 (19)	0.0030 (12)	0.0052 (14)	-0.0048 (12)
019	0.0146 (15)	0.0106 (14)	0.0132 (15)	0.0011 (13)	0.0084 (13)	0.0002 (13)
O20	0.0162 (17)	0.0106 (14)	0.0107 (18)	0.0033 (12)	0.0060 (14)	0.0009 (12)
O21	0.0201 (19)	0.0143 (16)	0.017 (2)	-0.0077 (13)	0.0064 (16)	0.0061 (13)
O22	0.0081 (15)	0.0155 (15)	0.0211 (18)	0.0013 (12)	0.0042 (14)	-0.0025 (13)
O23	0.020 (2)	0.025 (2)	0.011 (2)	0.000	0.0024 (19)	0.000

Geometric parameters (Å, °)

Cs1—O19	2.951 (3)	Sn1—O22 ⁱⁱⁱ	2.036 (3)
Cs1—O1 ⁱ	3.237 (3)	Sn1—O1 ^x	2.036 (3)
Cs1—O18 ⁱⁱ	3.256 (3)	Sn1—O15 ^{vi}	2.038 (3)
Cs1—O10 ⁱⁱⁱ	3.282 (3)	Sn1—O16 ^{vi}	2.039 (3)

supporting information

Cs1—O7 ^{iv}	3.291 (3)	Sn1—O5 ^x	2.044 (3)
Cs1—O5 ^{iv}	3.299 (3)	Sn2—O12 ⁱⁱⁱ	2.040 (3)
Cs1—O22	3.308 (3)	Sn2—O12 ⁱⁱ	2.040 (3)
Cs1—O15 ^v	3.336 (3)	Sn2—O20	2.042 (3)
Cs1—O8 ⁱⁱⁱ	3.352 (3)	Sn2—O20 ^{xi}	2.042 (3)
Cs1—O2 ⁱ	3.538 (3)	Sn2—O17 ⁱⁱⁱ	2.058 (3)
Cs1—O21	3.588 (3)	Sn2—O17 ⁱⁱ	2.058 (3)
Cs1—Cs3A ⁱ	3.7396 (5)	Si1—O1	1.595 (4)
Cs2—011	3.045 (3)	Si1—O2	1.604 (3)
Cs2—O20	3.238 (3)	Si1-03	1.606 (3)
Cs2—017	3.253 (3)	Si1-04	1.638 (3)
$Cs2 = O14^{vi}$	3.268 (3)	Si2-05	1.590 (3)
Cs2 = 04	3 283 (3)	Si2-07	1 614 (3)
$Cs2 = O17^{iii}$	3 300 (3)	Si2-06	1.615(3)
$C_{s2} = O_{1}^{s2}$	3316(3)	Si2-04	1.612(3)
$C_{82} = 0.20$	3 387 (3)	Si2-01 Si308	1 595 (3)
$C_{s2} = O_{12}^{s2}$	3 426 (4)	Si3	1.692(4)
$C_{s2} = 0.21$	3 636 (3)	Si3-010	1.602(4)
$C_{s2} = 0.10^{10}$	3.748(3)	Si3-010	1.020(3) 1.628(3)
$C_{s2} = C_{s2}^{iii}$	3 8508 (6)	Si4_012	1.020(3)
$C_{32} - C_{32}$	3 120 (3)	Si4 012	1.577(3)
$C_{\rm s3A} = 01$	3.129(3)	Si4 010	1.013(3) 1.623(3)
$C_{3}A = O_{4}$	3 206 (3)	Si4 = O10	1.025(3) 1.629(3)
$C_{s3A} = O_{7}^{ix}$	3.200(3)	Si5 015	1.029(3) 1 504(3)
$C_{s3A} = 0.5$	3.223(3)	Si5_00	1.394(3)
$C_{3}A = 015$	3.227(3)	$S_{15} = 0.9$	1.003(4) 1.628(3)
$C_{3}A = O_{10}$	3.208(3)	Si5_014	1.028(3)
$C_{s3A} = 00^{\circ}$	3.331(3)	SIS-014 Si6 016	1.028(3) 1.587(3)
$C_{s3A} = O10$	5.557(5)	Si6_012	1.387(3)
C_{s3A} S_{s3A}	3.5765(15)	Si6_02	1.011(3) 1.615(3)
$C_{s3A} = O_{3}^{m}$	3.392(3)	S10-03	1.013(3)
$C_{s3A} = 0.15$	3.033(3)	Si0-00**	1.028(3)
	3.007(10)	SI/01/	1.593(3)
$C_{\rm S3B} = 08^{\rm m}$	3.050 (9)	517018	1.622(3)
$C_{s3B} = O4^{viii}$	3.186 (8)	S1/-02	1.623 (4)
$C_{s3B} = O_{b}^{sm}$	3.308 (8)	S1/019 ¹	1.631 (3)
Cs3B—OI	3.334(12)	S18-020	1.589 (3)
$C_{s3B} = O_{16}^{im}$	3.347 (9)	S18-021	1.614 (3)
	3.494 (13)	S18-07	1.623 (4)
$C_{33}B = O_{3}^{10}$	3.580 (8)	518-019	1.629 (3)
C_{s3B} $-S_{12}$ $-S_{$	3.6/0 (8)	S19-022	1.576(3)
Cs3B—O16	3.738 (18)	S19—O23	1.6078 (12)
Cs3B— $S11$ Viii	3.796 (8)	S19—021	1.629 (3)
Sn1—O8	2.031 (3)	S19—018	1.634 (3)
019—Cs1—O1 ⁱ	129.44 (8)	O1—Si1—Cs3A ^{viii}	79.54 (12)
O19—Cs1—O18 ⁱⁱ	48.50 (7)	O2—Si1—Cs3A ^{viii}	166.44 (14)
O1 ⁱ —Cs1—O18 ⁱⁱ	83.41 (7)	O3—Si1—Cs3A ^{viii}	74.38 (13)
O19—Cs1—O10 ⁱⁱⁱ	81.34 (8)	O4—Si1—Cs3Aviii	58.51 (12)

O1 ⁱ —Cs1—O10 ⁱⁱⁱ	120.55 (8)	O1—Si1—Cs3B ^{viiii}	86.8 (3)
O18 ⁱⁱ —Cs1—O10 ⁱⁱⁱ	92.05 (8)	O2—Si1—Cs3B ^{viii}	161.0 (3)
O19—Cs1—O7 ^{iv}	107.28 (8)	O3—Si1—Cs3B ^{viii}	70.0 (2)
$O1^{i}$ — $Cs1$ — $O7^{iv}$	89.80 (8)	O4—Si1—Cs3B ^{viii}	56.05 (18)
$O18^{ii}$ — $Cs1$ — $O7^{iv}$	128.63 (8)	Cs3A ^{viii} —Si1—Cs3B ^{viii}	7.4 (2)
$O10^{iii}$ — $Cs1$ — $O7^{iv}$	133.27 (8)	O1—Si1—Cs1 ^{xiii}	54.50 (11)
O19—Cs1—O5 ^{iv}	137.94 (8)	O2—Si1—Cs1 ^{xiii}	65.38 (13)
$O1^{i}$ — $Cs1$ — $O5^{iv}$	88.26 (7)	O3—Si1—Cs1 ^{xiii}	98.41 (13)
$O18^{ii}$ — $Cs1$ — $O5^{iv}$	170.79 (7)	O4—Si1—Cs1 ^{xiii}	154.79 (12)
$O10^{iii}$ — $Cs1$ — $O5^{iv}$	95.58 (7)	Cs3A ^{viii} —Si1—Cs1 ^{xiii}	127.81 (4)
$O7^{iv}$ —Cs1—O5 ^{iv}	47.11 (8)	Cs3B ^{viii} —Si1—Cs1 ^{xiii}	133.4 (2)
O19—Cs1—O22	89.45 (8)	O1—Si1—Cs2	156.41 (12)
O1 ⁱ —Cs1—O22	139.09 (7)	O2—Si1—Cs2	87.35 (13)
O18 ⁱⁱ —Cs1—O22	137.29 (7)	O3—Si1—Cs2	75.41 (14)
O10 ⁱⁱⁱ —Cs1—O22	71.33 (8)	O4—Si1—Cs2	46.31 (11)
O7 ^{iv} —Cs1—O22	63.12 (8)	Cs3A ^{viii} —Si1—Cs2	80.71 (3)
O5 ^{iv} —Cs1—O22	50.83 (7)	Cs3B ^{viii} —Si1—Cs2	74.0 (3)
O19—Cs1—O15 ^v	111.12 (8)	Cs1 ^{xiii} —Si1—Cs2	148.79 (3)
$O1^{i}$ —Cs1—O15 ^v	49.69 (8)	O1—Si1—Cs3A	36.91 (11)
$O18^{ii}$ — $Cs1$ — $O15^{v}$	69.44 (7)	O2—Si1—Cs3A	119.24 (13)
$O10^{iii}$ — $Cs1$ — $O15^{v}$	73.23 (8)	O3—Si1—Cs3A	74.66 (14)
$O7^{iv}$ —Cs1—O15 ^v	136.47 (7)	O4—Si1—Cs3A	129.29 (12)
$O5^{iv}$ — $Cs1$ — $O15^{v}$	107.90 (7)	Cs3A ^{viii} —Si1—Cs3A	74.28 (3)
O22—Cs1—O15 ^v	135.35 (8)	Cs3B ^{viii} —Si1—Cs3A	79.2 (2)
O19—Cs1—O8 ⁱⁱⁱ	119.44 (8)	Cs1 ^{xiii} —Si1—Cs3A	54.428 (19)
$O1^{i}$ — $Cs1$ — $O8^{iii}$	105.87 (7)	Cs2—Si1—Cs3A	145.09 (3)
O18 ⁱⁱ —Cs1—O8 ⁱⁱⁱ	136.95 (8)	O5—Si2—O7	110.53 (17)
O10 ⁱⁱⁱ —Cs1—O8 ⁱⁱⁱ	46.58 (7)	O5—Si2—O6	110.39 (18)
O7 ^{iv} —Cs1—O8 ⁱⁱⁱ	93.90 (8)	O7—Si2—O6	111.42 (18)
O5 ^{iv} —Cs1—O8 ⁱⁱⁱ	49.56 (8)	O5—Si2—O4	111.56 (16)
O22—Cs1—O8 ⁱⁱⁱ	51.07 (7)	O7—Si2—O4	108.41 (18)
O15 ^v —Cs1—O8 ⁱⁱⁱ	84.72 (7)	O6—Si2—O4	104.37 (16)
O19—Cs1—O2 ⁱ	99.87 (8)	O5—Si2—Cs3A ^{viii}	77.67 (12)
$O1^{i}$ — $Cs1$ — $O2^{i}$	45.36 (8)	O7—Si2—Cs3A ^{viii}	170.77 (14)
$O18^{ii}$ — $Cs1$ — $O2^{i}$	75.78 (8)	O6—Si2—Cs3A ^{viii}	68.05 (12)
$O10^{iii}$ — $Cs1$ — $O2^{i}$	161.62 (7)	O4—Si2—Cs3A ^{viii}	63.62 (12)
$O7^{iv}$ —Cs1—O2 ⁱ	64.15 (7)	O5—Si2—Cs3B ^{viii}	85.3 (3)
$O5^{iv}$ — $Cs1$ — $O2^{i}$	95.55 (7)	O7—Si2—Cs3B ^{viii}	163.7 (3)
$O22$ — $Cs1$ — $O2^i$	126.86 (8)	O6—Si2—Cs3B ^{viii}	64.3 (2)
$O15^{v}$ — $Cs1$ — $O2^{i}$	89.43 (7)	O4—Si2—Cs3B ^{viii}	60.1 (2)
O8 ⁱⁱⁱ —Cs1—O2 ⁱ	139.69 (7)	Cs3A ^{viii} —Si2—Cs3B ^{viii}	7.6 (3)
O19—Cs1—O21	45.41 (7)	O5—Si2—Cs1 ^{iv}	56.99 (11)
O1 ⁱ —Cs1—O21	172.30 (8)	O7—Si2—Cs1 ^{iv}	56.83 (13)
O18 ⁱⁱ —Cs1—O21	92.93 (7)	O6—Si2—Cs1 ^{iv}	112.15 (12)
O10 ⁱⁱⁱ —Cs1—O21	66.22 (8)	O4—Si2—Cs1 ^{iv}	143.45 (12)
$O7^{iv}$ —Cs1—O21	87.19 (8)	Cs3A ^{viii} —Si2—Cs1 ^{iv}	132.30 (5)
$O5^{iv}$ —Cs1—O21	94.85 (7)	Cs3B ^{viii} —Si2—Cs1 ^{iv}	139.4 (3)
O22—Cs1—O21	44.39 (7)	O5—Si2—Cs2	154.76 (12)

O15 ^v —Cs1—O21	135.03 (8)	O7—Si2—Cs2	89.01 (13)
O8 ⁱⁱⁱ —Cs1—O21	81.42 (7)	O6—Si2—Cs2	74.77 (13)
O2 ⁱ —Cs1—O21	127.16 (8)	O4—Si2—Cs2	44.80 (11)
O19—Cs1—Cs3A ⁱ	161.21 (7)	Cs3A ^{viii} —Si2—Cs2	81.95 (4)
O1 ⁱ —Cs1—Cs3A ⁱ	52.70 (6)	Cs3B ^{viii} —Si2—Cs2	74.7 (3)
O18 ⁱⁱ —Cs1—Cs3A ⁱ	122.16 (5)	Cs1 ^{iv} —Si2—Cs2	145.67 (4)
O10 ⁱⁱⁱ —Cs1—Cs3A ⁱ	82.98 (6)	O5—Si2—Cs3A ⁱⁱ	38.62 (11)
O7 ^{iv} —Cs1—Cs3A ⁱ	91.03 (6)	O7—Si2—Cs3A ⁱⁱ	107.08 (13)
O5 ^{iv} —Cs1—Cs3A ⁱ	54.06 (6)	O6—Si2—Cs3A ⁱⁱ	77.00 (13)
O22—Cs1—Cs3A ⁱ	95.29 (5)	O4—Si2—Cs3A ⁱⁱ	140.89 (12)
O15 ^v —Cs1—Cs3A ⁱ	53.91 (5)	Cs3A ^{viii} —Si2—Cs3A ⁱⁱ	81.93 (4)
O8 ⁱⁱⁱ —Cs1—Cs3A ⁱ	53.22 (5)	Cs3B ^{viiii} —Si2—Cs3A ⁱⁱ	87.7 (2)
O2 ⁱ —Cs1—Cs3A ⁱ	91.81 (5)	Cs1 ^{iv} —Si2—Cs3A ⁱⁱ	54.01 (2)
O21—Cs1—Cs3A ⁱ	134.39 (5)	Cs2—Si2—Cs3A ⁱⁱ	151.10 (3)
O11—Cs2—O20	129.98 (8)	O8—Si3—O9	111.77 (18)
O11—Cs2—O17	136.90 (8)	O8—Si3—O10	109.12 (18)
O20—Cs2—O17	87.84 (7)	O9—Si3—O10	111.11 (18)
O11—Cs2—O14 ^{vi}	47.93 (7)	O8—Si3—O11	111.35 (16)
O20—Cs2—O14 ^{vi}	84.79 (7)	O9—Si3—O11	107.22 (19)
O17—Cs2—O14 ^{vi}	170.85 (8)	O10—Si3—O11	106.12 (16)
O11—Cs2—O4	97.70 (8)	O8—Si3—Cs1 ⁱⁱⁱ	55.75 (12)
O20—Cs2—O4	71.06 (8)	O9—Si3—Cs1 ⁱⁱⁱ	131.64 (14)
O17—Cs2—O4	73.34 (8)	O10—Si3—Cs1 ⁱⁱⁱ	53.45 (12)
O14 ^{vi} —Cs2—O4	99.06 (8)	O11—Si3—Cs1 ⁱⁱⁱ	120.94 (13)
O11—Cs2—O17 ⁱⁱⁱ	112.47 (8)	O8—Si3—Cs3B ^{xiv}	43.6 (2)
O20—Cs2—O17 ⁱⁱⁱ	50.51 (7)	O9—Si3—Cs3B ^{xiv}	82.2 (2)
O17—Cs2—O17 ⁱⁱⁱ	107.82 (6)	O10—Si3—Cs3B ^{xiv}	92.32 (16)
O14 ^{vi} —Cs2—O17 ⁱⁱⁱ	71.38 (8)	O11—Si3—Cs3B ^{xiv}	153.9 (2)
O4—Cs2—O17 ⁱⁱⁱ	121.04 (7)	Cs1 ⁱⁱⁱ —Si3—Cs3B ^{xiv}	56.65 (16)
O11—Cs2—O20 ⁱⁱⁱ	117.98 (7)	O8—Si3—Cs2	125.15 (13)
O20-Cs2-O20 ⁱⁱⁱ	107.85 (6)	O9—Si3—Cs2	121.49 (14)
O17—Cs2—O20 ⁱⁱⁱ	50.25 (7)	O10—Si3—Cs2	63.86 (12)
O14 ^{vi} —Cs2—O20 ⁱⁱⁱ	137.65 (8)	O11—Si3—Cs2	42.26 (11)
O4—Cs2—O20 ⁱⁱⁱ	123.29 (7)	Cs1 ⁱⁱⁱ —Si3—Cs2	93.96 (3)
O17 ⁱⁱⁱ —Cs2—O20 ⁱⁱⁱ	85.76 (7)	Cs3B ^{xiv} —Si3—Cs2	150.41 (15)
O11—Cs2—O12	87.76 (7)	O8—Si3—Cs3A ^{xiv}	38.41 (11)
O20—Cs2—O12	139.65 (7)	O9—Si3—Cs3A ^{xiv}	87.05 (14)
O17—Cs2—O12	51.84 (7)	O10—Si3—Cs3A ^{xiv}	93.01 (12)
O14 ^{vi} —Cs2—O12	135.12 (7)	O11—Si3—Cs3A ^{xiv}	149.35 (12)
O4—Cs2—O12	92.86 (8)	Cs1 ⁱⁱⁱ —Si3—Cs3A ^{xiv}	53.629 (19)
O17 ⁱⁱⁱ —Cs2—O12	135.53 (8)	Cs3B ^{xiv} —Si3—Cs3A ^{xiv}	5.5 (2)
O20 ⁱⁱⁱ —Cs2—O12	50.21 (7)	Cs2—Si3—Cs3A ^{xiv}	147.54 (4)
O11—Cs2—O21 ⁱⁱⁱ	81.88 (8)	O12—Si4—O13	113.92 (17)
O20—Cs2—O21 ⁱⁱⁱ	121.19 (8)	O12—Si4—O10	110.94 (17)
O17—Cs2—O21 ⁱⁱⁱ	96.07 (7)	O13—Si4—O10	104.91 (17)
O14 ^{vi} —Cs2—O21 ⁱⁱⁱ	92.39 (8)	O12-Si4-O14 ^{xii}	112.47 (17)
O4—Cs2—O21 ⁱⁱⁱ	164.18 (7)	O13—Si4—O14 ^{xii}	107.67 (17)
O17 ⁱⁱⁱ —Cs2—O21 ⁱⁱⁱ	72.97 (8)	O10—Si4—O14 ^{xii}	106.39 (17)
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O20 ⁱⁱⁱ —Cs2—O21 ⁱⁱⁱ	46.12 (7)	O12—Si4—Cs2	56.81 (11)
O12—Cs2—O21 ⁱⁱⁱ	71.33 (8)	O13—Si4—Cs2	94.11 (11)
O11—Cs2—O10	44.74 (7)	O10—Si4—Cs2	65.92 (11)
O20—Cs2—O10	173.27 (8)	O14 ^{xii} —Si4—Cs2	158.21 (14)
O17—Cs2—O10	95.59 (7)	O12—Si4—Cs1 ⁱⁱⁱ	97.51 (13)
O14 ^{vi} —Cs2—O10	91.21 (7)	O13—Si4—Cs1 ⁱⁱⁱ	146.31 (11)
O4—Cs2—O10	104.34 (7)	O10—Si4—Cs1 ⁱⁱⁱ	49.59 (12)
O17 ⁱⁱⁱ —Cs2—O10	133.00 (7)	O14 ^{xii} —Si4—Cs1 ⁱⁱⁱ	68.28 (12)
O20 ⁱⁱⁱ —Cs2—O10	78.73 (7)	Cs2—Si4—Cs1 ⁱⁱⁱ	93.20 (2)
O12—Cs2—O10	43.92 (6)	O12—Si4—Cs2 ^{ix}	75.01 (11)
O21 ⁱⁱⁱ —Cs2—O10	64.29 (8)	O13—Si4—Cs2 ^{ix}	102.93 (11)
O11—Cs2—O18 ⁱⁱⁱ	75.42 (8)	O10—Si4—Cs2 ^{ix}	145.47 (12)
O20—Cs2—O18 ⁱⁱⁱ	93.42 (7)	O14 ^{xii} —Si4—Cs2 ^{ix}	44.83 (11)
O17—Cs2—O18 ⁱⁱⁱ	129.03 (8)	Cs2—Si4—Cs2 ^{ix}	131.69 (3)
O14 ^{vi} —Cs2—O18 ⁱⁱⁱ	57.05 (8)	Cs1 ⁱⁱⁱ —Si4—Cs2 ^{ix}	96.43 (2)
O4—Cs2—O18 ⁱⁱⁱ	153.40 (7)	O15—Si5—O9	111.40 (18)
O17 ⁱⁱⁱ —Cs2—O18 ⁱⁱⁱ	44.71 (7)	O15—Si5—O11 ^{xii}	110.88 (16)
O20 ⁱⁱⁱ —Cs2—O18 ⁱⁱⁱ	81.50 (7)	O9—Si5—O11 ^{xii}	107.93 (19)
O12—Cs2—O18 ⁱⁱⁱ	112.20 (7)	O15—Si5—O14	111.96 (18)
O21 ⁱⁱⁱ —Cs2—O18 ⁱⁱⁱ	41.79 (7)	O9—Si5—O14	110.00 (18)
O10-Cs2-O18 ⁱⁱⁱ	88.92 (6)	O11 ^{xii} —Si5—O14	104.38 (16)
O11—Cs2—Cs2 ⁱⁱⁱ	160.41 (6)	O15—Si5—Cs2 ^{xii}	122.11 (13)
O20—Cs2—Cs2 ⁱⁱⁱ	54.87 (6)	O9—Si5—Cs2 ^{xii}	126.10 (14)
O17—Cs2—Cs2 ⁱⁱⁱ	54.48 (6)	O11 ^{xii} —Si5—Cs2 ^{xii}	48.26 (11)
O14 ^{vi} —Cs2—Cs2 ⁱⁱⁱ	123.98 (6)	O14—Si5—Cs2 ^{xii}	56.37 (11)
O4—Cs2—Cs2 ⁱⁱⁱ	101.49 (5)	O15—Si5—Cs3B ^{viii}	39.9 (2)
O17 ⁱⁱⁱ —Cs2—Cs2 ⁱⁱⁱ	53.35 (5)	O9—Si5—Cs3B ^{viii}	76.6 (2)
O20 ⁱⁱⁱ —Cs2—Cs2 ⁱⁱⁱ	52.98 (5)	O11 ^{xii} —Si5—Cs3B ^{viii}	143.06 (18)
O12—Cs2—Cs2 ⁱⁱⁱ	95.13 (5)	O14—Si5—Cs3B ^{viii}	108.28 (16)
O21 ⁱⁱⁱ —Cs2—Cs2 ⁱⁱⁱ	80.72 (5)	Cs2 ^{xii} —Si5—Cs3B ^{viii}	154.58 (17)
O10—Cs2—Cs2 ⁱⁱⁱ	131.69 (5)	O15—Si5—Cs1 ^{xv}	47.65 (11)
O18 ⁱⁱⁱ —Cs2—Cs2 ⁱⁱⁱ	85.59 (5)	O9—Si5—Cs1 ^{xv}	121.39 (14)
O1—Cs3A—O8 ^{vii}	112.49 (8)	O11 ^{xii} —Si5—Cs1 ^{xv}	130.40 (13)
O1—Cs3A—O4 ^{viii}	131.83 (8)	O14—Si5—Cs1 ^{xv}	64.99 (13)
O8 ^{vii} —Cs3A—O4 ^{viii}	115.45 (8)	Cs2 ^{xii} —Si5—Cs1 ^{xv}	100.22 (3)
O1—Cs3A—O5 ^{ix}	91.53 (8)	Cs3B ^{viii} —Si5—Cs1 ^{xv}	54.65 (16)
O8 ^{vii} —Cs3A—O5 ^{ix}	51.50 (8)	O16—Si6—O13	112.41 (16)
O4 ^{viii} —Cs3A—O5 ^{ix}	122.05 (8)	O16—Si6—O3	109.44 (18)
O1—Cs3A—O15 ^{viii}	51.50 (8)	O13—Si6—O3	106.76 (18)
O8 ^{vii} —Cs3A—O15 ^{viii}	89.11 (8)	O16—Si6—O6 ^{ix}	113.01 (18)
O4 ^{viii} —Cs3A—O15 ^{viii}	124.22 (9)	O13—Si6—O6 ^{ix}	107.14 (17)
O5 ^{ix} —Cs3A—O15 ^{viii}	112.54 (8)	O3—Si6—O6 ^{ix}	107.78 (18)
O1—Cs3A—O16	74.06 (8)	O16—Si6—Cs3B ^{viii}	59.0 (2)
O8 ^{vii} —Cs3A—O16	126.48 (9)	O13—Si6—Cs3B ^{viii}	87.2 (3)
O4 ^{viii} —Cs3A—O16	81.50 (8)	O3—Si6—Cs3B ^{viiii}	67.37 (17)
O5 ^{ix} —Cs3A—O16	75.98 (8)	O6 ^{ix} —Si6—Cs3B ^{viii}	165.6 (3)
O15 ^{viii} —Cs3A—O16	124.23 (8)	O16—Si6—Cs3A ^{viii}	55.21 (12)
O1—Cs3A—O6 ^{viii}	166.14 (10)	O13—Si6—Cs3A ^{viii}	94.08 (11)

O8 ^{vii} —Cs3A—O6 ^{viii}	72.76 (8)	O3—Si6—Cs3A ^{viii}	65.97 (13)
O4viii—Cs3A—O6viii	46.33 (7)	O6 ^{ix} —Si6—Cs3A ^{viii}	158.73 (13)
O5 ^{ix} —Cs3A—O6 ^{viii}	81.91 (8)	Cs3B ^{viii} —Si6—Cs3A ^{viii}	6.9 (2)
O15 ^{viii} —Cs3A—O6 ^{viii}	142.36 (10)	O16—Si6—Cs3A	49.66 (11)
O16—Cs3A—O6 ^{viii}	92.45 (8)	O13—Si6—Cs3A	161.93 (12)
O1—Cs3A—O16 ^{viii}	50.82 (8)	O3—Si6—Cs3A	81.01 (14)
O8 ^{vii} —Cs3A—O16 ^{viii}	141.13 (8)	O6 ^{ix} —Si6—Cs3A	85.16 (13)
O4 ^{viii} —Cs3A—O16 ^{viii}	87.21 (7)	Cs3B ^{viii} —Si6—Cs3A	80.7 (3)
O5 ^{ix} —Cs3A—O16 ^{viii}	141.80 (8)	Cs3A ^{viii} —Si6—Cs3A	73.88 (3)
O15 ^{viii} —Cs3A—O16 ^{viii}	52.43 (7)	O16—Si6—Cs3B ^{xvi}	78.5 (2)
O16—Cs3A—O16 ^{viii}	86.00 (8)	O13—Si6—Cs3B ^{xvi}	95.3 (3)
O6 ^{viii} —Cs3A—O16 ^{viii}	132.99 (8)	O3—Si6—Cs3B ^{xvi}	150.6 (2)
O1—Cs3A—Si2 ^{viii}	143.72 (7)	O6 ^{ix} —Si6—Cs3B ^{xvi}	45.60 (15)
O8 ^{vii} —Cs3A—Si2 ^{viii}	99.10 (6)	Cs3B ^{viii} —Si6—Cs3B ^{xvi}	134.4 (2)
O4 ^{viii} —Cs3A—Si2 ^{viii}	27.34 (5)	Cs3A ^{viii} —Si6—Cs3B ^{xvi}	132.72 (14)
05^{ix} Cs3A Si2 ^{viii}	94.72 (6)	Cs3A—Si6—Cs3B ^{xvi}	83.8 (2)
015^{viii} Cs3A Si2 ^{viii}	150.05 (8)	016—Si6—Cs3A ^{xvi}	74 65 (12)
016 C_{33} S_{12}	72 93 (6)	013—Si6—Cs3A ^{xvi}	101.69(12)
$O6^{\text{viii}}$ $Cs3A$ $Si2^{\text{viii}}$	72.93(0) 26.72(5)	O3—Si6—Cs3A ^{xvi}	146 41 (14)
016^{viii} $C_{\text{s}34}$ $S_{\text{i}2}^{\text{viii}}$	$111 \ 97 \ (5)$	$O6^{ix}$ Si6 Cs3A ^{xvi}	45 44 (12)
$01 - C_{33} - 05^{viii}$	111.57 (5)	$C_{s3}B^{viii}$ Si6 $C_{s3}A^{xvi}$	132 32 (15)
08^{vii} Cs3A 05^{viii}	106.15(7)	$C_{s3}\Delta^{vii}$ Si6 $C_{s3}\Delta^{xvi}$	129 68 (4)
04^{viii} C_{33} A O_{5}^{viii}	45 90 (7)	$C_{3}A = Si6 = C_{3}A^{xvi}$	77 24 (3)
$O_{4}^{ix} = C_{3}^{ix} = O_{5}^{ix}$	43.90 (7) 80.67 (8)	$C_{s3}B_{xvi}$ Si6 $C_{s3}A_{xvi}$	66(2)
$015^{\text{viii}} C_{\text{S}} 3 05^{\text{viii}}$	164.32(7)	$017 \ 57 \ 018$	0.0(2)
015 - Cs3A - 05	104.32 (7)	017 = 517 = 018	113.08(18) 112.00(17)
$O_{10} C_{33} A O_{5}^{\text{viii}}$	43.09(3)	017 - 517 - 02	112.90(17) 106.40(17)
$00 - c_{33A} - 05$	111 00 (7)	$017 \text{ Si7} 010^{\text{ix}}$	100.40(17) 110.79(16)
$C_{10} = C_{33} = C_{33}$	111.39(7)	018 Si7 019	110.79(10) 104.08(15)
SIZ = CSSA = OS	23.03(0)	018 - 517 - 019	104.08(13) 106.01(18)
$O_1 = C_{SSA} = O_2$	92.49(0)	02-31/-019	100.91(10)
$O_{4}^{\text{viii}} = C_{3}^{2} A = O_{3}^{2}^{\text{viii}}$	143.14(10) 12.06(7)	O18 Si7 Calix	124.89 (13)
$O_{4} = C_{3} = O_{4} = O_{4}$	43.90(7)	$O_{18} = S_{17} = C_{81}$	37.03(11)
$03^{}$ $03^{}$ $03^{}$	138.91 (8)	$O_2 = S_1 = C_S_1 = C_S_1$	121.33(13)
O15 - Cs3A - O3 - O3	83.90 (7)	017 Si7 Cs2iii	40.64 (10)
$O_{10} = C_{33} = O_{3}$	85.25 (8)	$017 - 517 - C_{2}2^{11}$	49.62 (12)
$00^{}$ CS3A $03^{}$	89.48 (7)	018 - 517 - 0.52	00.05(12)
C_{22}	43.55 (7)	02-51/-0.02	121.72(13)
$S12^{m} - CS3A - O3^{m}$	70.25 (5)	$O19^{$	131.32(13)
03^{m} 03^{m}	/9./1 (/)	$Cs1^{m}$ $S1/$ $Cs2^{m}$	102.84 (3)
$OI - Cs3A - Cs1^{xiii}$	55.38 (6)	020-518-021	111.19 (18)
$O8^{vn}$ —Cs3A—Cs1 ^{xin}	57.17(6)	020-518-07	112.06 (18)
$O4^{\text{vm}}$ —Cs3A—Cs1 ^{xm}	172.38 (6)	021—S18—07	110.13 (18)
$O5^{1n}$ — $Cs3A$ — $Cs1^{xm}$	55.98 (5)	020—S18—019	112.18 (16)
$O15^{vm}$ — $Cs3A$ — $Cs1^{xm}$	56.64 (6)	021—S18—019	106.10 (17)
O16—Cs3A—Cs1 ^{xiii}	104.31 (6)	O7—Si8—O19	104.83 (18)
O6 ^{viii} —Cs3A—Cs1 ^{xiii}	127.54 (5)	O20—Si8—Cs1	125.41 (13)
$O16^{vin}$ —Cs3A—Cs1 ^{xin}	98.01 (5)	O21—Si8—Cs1	64.70 (12)
Si2 ^{viii} —Cs3A—Cs1 ^{xiii}	149.39 (3)	O7—Si8—Cs1	120.29 (13)

O5 ^{viii} —Cs3A—Cs1 ^{xiii}	135.18 (6)	O19—Si8—Cs1	41.45 (10)
O3 ^{viii} —Cs3A—Cs1 ^{xiii}	140.35 (5)	O20—Si8—Cs2 ⁱⁱⁱ	53.68 (12)
O15 ^{viii} —Cs3B—O8 ^{vii}	96.1 (3)	O21—Si8—Cs2 ⁱⁱⁱ	57.85 (13)
O15 ^{viii} —Cs3B—O4 ^{viii}	133.3 (4)	O7—Si8—Cs2 ⁱⁱⁱ	134.84 (13)
O8 ^{vii} —Cs3B—O4 ^{viii}	120.4 (3)	O19—Si8—Cs2 ⁱⁱⁱ	120.30 (13)
O15 ^{viii} —Cs3B—O6 ^{viii}	158.8 (6)	Cs1—Si8—Cs2 ⁱⁱⁱ	94.85 (3)
O8 ^{vii} —Cs3B—O6 ^{viii}	74.9 (2)	O20—Si8—Cs1 ^{iv}	141.77 (13)
O4 ^{viii} —Cs3B—O6 ^{viii}	46.66 (13)	O21—Si8—Cs1 ^{iv}	105.59 (14)
O15 ^{viii} —Cs3B—O1	51.35 (16)	O7—Si8—Cs1 ^{iv}	42.51 (12)
O8 ^{vii} —Cs3B—O1	110.8 (3)	O19—Si8—Cs1 ^{iv}	65.46 (12)
O4 ^{viii} —Cs3B—O1	125.0 (4)	Cs1—Si8—Cs1 ^{iv}	79.75 (2)
O6 ^{viii} —Cs3B—O1	149.8 (6)	Cs2 ⁱⁱⁱ —Si8—Cs1 ^{iv}	162.95 (3)
O15 ^{viii} —Cs3B—O16 ^{viii}	54.21 (15)	O20—Si8—Cs2	39.22 (11)
O8 ^{vii} —Cs3B—O16 ^{viii}	150.0 (3)	O21—Si8—Cs2	94.95 (13)
O4 ^{viii} —Cs3B—O16 ^{viii}	87.7 (2)	Q7—Si8—Cs2	86.44 (12)
$O6^{\text{viii}}$ —Cs3B—O16 ^{viii}	134.3 (3)	O19—Si8—Cs2	150.46 (11)
01 —Cs3B— 016^{viii}	49.38 (16)	Cs1— $Si8$ — $Cs2$	150.06 (4)
015^{viii} Cs3B 05^{ix}	111.0(2)	Cs^{2iii} —Si8—Cs2	55 205 (18)
$O8^{\text{vii}}$ —Cs3B—O5 ^{ix}	49.88 (16)	$Cs2^{iv}$ —Si8—Cs2	12874(3)
$O4^{\text{viii}}$ $Cs3B$ $O5^{\text{ix}}$	114 6 (4)	022 = 8i9 = 023	113 21 (14)
$O6^{\text{viii}}$ $C83B$ $O5^{\text{ix}}$	78 3 (2)	022 - Si9 - 023	109 52 (18)
$01 - C_{3}B - O_{5}^{ix}$	83.6 (3)	022 - 519 - 021	109.62(10) 108.63(19)
$O16^{\text{viii}}$ $Cs3B$ $O5^{\text{ix}}$	1307(5)	022 - Si9 - 018	111 34 (17)
015^{viii} Cs3B 03^{viii}	90.6 (2)	022 = 519 = 010 023 = 519 = 018	1094(2)
$O8^{\text{vii}}$ $C83B$ $O3^{\text{viii}}$	157 1 (5)	025 - 519 - 018	109.1(2) 104 29 (17)
$O4^{\text{viii}}$ $Cs3B$ $O3^{\text{viii}}$	44 73 (12)	022 - Si9 - Cs1	54 89 (11)
$O6^{\text{viii}}$ $Cs3B$ $O3^{\text{viii}}$	91.09(19)	022 Sig 03	98 43 (16)
$01 - C_{33B} - 03^{viii}$	90 5 (2)	025 Si9 031	65 20 (12)
016^{viii} Cs3B 03^{viii}	44 18 (12)	018—Si9—Cs1	152 14 (13)
$O_{5ix} = C_{53B} = O_{3viii}$	145.7(5)	$022 - Si9 - Cs^{2iii}$	95 56 (13)
015^{viii} Cs3B Si2 ^{viii}	1599(3)	$023 - Si9 - Cs2^{iii}$	150 37 (5)
$O_{\text{S}}^{\text{vii}}$ C_{S}^{S} $B_{\text{S}}^{\text{viii}}$	999(2)	025 - 519 - 032 $021 - 519 - 032^{iii}$	51 79 (13)
$O4^{\text{viii}}$ C_{s3B} $Si2^{\text{viii}}$	26 56 (9)	$018 - 5i9 - Cs^{2iii}$	63 31 (12)
Of^{viii} C_{s3B} S_{i2}^{viii}	26.10 (8)	C_{s1} Si9 C_{s2}	92.24(2)
$01 - C_{33B} - S_{12}^{viii}$	1310(5)	$022 - Si9 - Cs1^{ix}$	78 16 (11)
016^{viii} Cs3B Si2 ^{viii}	1100(2)	$022 \text{Si}9 \text{Cs}1^{\text{ix}}$	97.46 (16)
$O_{10} = C_{33} = S_{12}$	88 7 (3)	$025 - 519 - Cs1^{ix}$	145 97 (13)
$O_{3}^{\text{viii}} = C_{3}^{3}B = S_{12}^{3}$	70.04(14)	$018 - Si9 - Cs1^{ix}$	44 82 (11)
015^{viii} C $3B$ 016	1162(4)	C_{s1} Sig C_{s1}	132.96 (3)
$O_{\rm S}^{\rm vii}$ C $_{\rm S}^{\rm 3B}$ O16	116.2(4)	$C_{s}2^{iii}$ SiQ $C_{s}1^{ix}$	152.90(3)
$O_{4}^{\text{viii}} = C_{3}^{2} P_{4} O_{1}^{16}$	74.8(3)	$C_{52} = -S_{15} = C_{51}$	93.20(2)
$O4 = C_{33} = O10$	74.8(3) 84.9(3)	$S_{11} = O_1 = S_{11}$	131.37(17) 125.27(15)
$01 C_{3}^{3}P = 016$	65 8 (3)	$Sn1_{xvii}$ $O1_{xvii}$ $O1_{xvii}$	123.27(13) 100.12(12)
$O1 = C_{33} = O10$ $O16^{\text{viii}} = C_{3} = O16$	70.0(3)	$SiII \longrightarrow C_{1} C_{2}I^{xiii}$	100.12(12) 101.85(14)
$O_{10} = C_{30} = O_{10}$	(7.0(3))	$S_{11} = O_{11} = O_{11}$	101.03(14) 108(12(12))
$O_3 = C_{33} = O_{10}$	70 8 (3)	$C_{s}^{3} = O_{s}^{1} = O_{s}^{1} = O_{s}^{1}$	71 01 (6)
S_{12} V_{111} C_{12} C_{12} C_{10}	668(2)	$C_{3}A_{-}U_{1} - C_{3}P_{-}$	(1.71(0))
512 - C55D - C10 $C15$ $C_{2}2D - C_{2}1$ x^{iii}	57.45(14)	$S_{11} = 01 = 0.000$	133.0(3)
U13US3BUS1	37.43 (14)	SII1—OI—CS3B	93.2 (3)

O8 ^{vii} —Cs3B—Cs1 ^{xiii}	57.53 (14)	Cs3A—O1—Cs3B	7.9 (2)
O4viii—Cs3B—Cs1xiii	167.5 (5)	Cs1 ^{xiii} —O1—Cs3B	70.34 (15)
O6 ^{viii} —Cs3B—Cs1 ^{xiii}	126.7 (3)	Si1—O1—Cs3A ^{viii}	76.02 (12)
O1—Cs3B—Cs1 ^{xiii}	53.63 (14)	Sn1 ^{xvii} —O1—Cs3A ^{viii}	90.90 (10)
O16 ^{viii} —Cs3B—Cs1 ^{xiii}	97.3 (2)	Cs3A—O1—Cs3A ^{viii}	88.33 (8)
O5 ^{ix} —Cs3B—Cs1 ^{xiii}	53.71 (15)	Cs1 ^{xiii} —O1—Cs3A ^{viii}	154.40 (9)
O3 ^{viii} —Cs3B—Cs1 ^{xiii}	141.5 (3)	Cs3B—O1—Cs3A ^{viii}	92.2 (2)
Si2 ^{viii} —Cs3B—Cs1 ^{xiii}	142.4 (4)	Si1—O2—Si7	144.3 (2)
O16—Cs3B—Cs1xiii	94.8 (4)	Si1—O2—Cs1 ^{xiii}	90.29 (14)
O15 ^{viii} —Cs3B—Si1 ^{viii}	114.8 (2)	Si7—O2—Cs1 ^{xiii}	112.69 (15)
O8 ^{vii} —Cs3B—Si1 ^{viii}	145.5 (3)	Si1—O3—Si6	159.1 (3)
O4 ^{viii} —Cs3B—Si1 ^{viii}	25.25 (8)	Si1—O3—Cs3B ^{viii}	85.1 (2)
O6 ^{viii} —Cs3B—Si1 ^{viii}	70.77 (15)	Si6—O3—Cs3B ^{viii}	88.02 (19)
O1—Cs3B—Si1 ^{viii}	100.8 (3)	Si1—O3—Cs3A ^{viii}	80.57 (13)
O16 ^{viii} —Cs3B—Si1 ^{viii}	63.64 (15)	Si6—O3—Cs3Aviii	90.22 (14)
O5 ^{ix} —Cs3B—Si1 ^{viii}	123.9 (4)	Cs3B ^{viii} —O3—Cs3A ^{viii}	7.7 (3)
O3 ^{viii} —Cs3B—Si1 ^{viii}	24.92 (7)	Si1—O4—Si2	129.51 (19)
Si2 ^{viii} —Cs3B—Si1 ^{viii}	46.82 (10)	Si1—O4—Cs3B ^{viii}	98.7 (2)
O16—Cs3B—Si1 ^{viii}	64.7 (2)	Si2—O4—Cs3B ^{viii}	93.4 (2)
Cs1 ^{xiii} —Cs3B—Si1 ^{viii}	153.4 (4)	Si1—O4—Cs3A ^{viii}	95.66 (14)
O8—Sn1—O22 ⁱⁱⁱ	89.80 (12)	Si2—O4—Cs3A ^{viii}	89.04 (13)
$O8$ — $Sn1$ — $O1^x$	177.68 (12)	Cs3B ^{viii} —O4—Cs3A ^{viii}	8.8 (3)
$O22^{iii}$ —Sn1—O1 ^x	92.32 (13)	Si1—O4—Cs2	112.55 (14)
O8—Sn1—O15 ^{vi}	95.43 (12)	Si2—O4—Cs2	114.54 (14)
O22 ⁱⁱⁱ —Sn1—O15 ^{vi}	92.48 (12)	Cs3B ^{viii} —O4—Cs2	96.3 (3)
O1 ^x —Sn1—O15 ^{vi}	85.41 (12)	Cs3A ^{viii} —O4—Cs2	105.03 (9)
O8—Sn1—O16 ^{vi}	91.37 (12)	Si2—O5—Sn1 ^{xvii}	130.27 (17)
O22 ⁱⁱⁱ —Sn1—O16 ^{vi}	176.09 (13)	Si2—O5—Cs3A ⁱⁱ	123.44 (14)
O1 ^x —Sn1—O16 ^{vi}	86.45 (12)	Sn1 ^{xvii} —O5—Cs3A ⁱⁱ	106.29 (13)
O15 ^{vi} —Sn1—O16 ^{vi}	91.12 (12)	Si2—O5—Cs1 ^{iv}	99.16 (13)
$O8$ — $Sn1$ — $O5^x$	86.35 (12)	Sn1 ^{xvii} —O5—Cs1 ^{iv}	97.58 (10)
$O22^{iii}$ —Sn1—O5 ^x	88.07 (12)	Cs3A ⁱⁱ —O5—Cs1 ^{iv}	69.96 (6)
$O1^{x}$ — $Sn1$ — $O5^{x}$	92.80 (12)	Si2—O5—Cs3B ⁱⁱ	129.9 (3)
$O15^{vi}$ — $Sn1$ — $O5^{x}$	178.14 (12)	Sn1 ^{xvii} —O5—Cs3B ⁱⁱ	99.8 (3)
$O16^{vi}$ — $Sn1$ — $O5^{x}$	88.28 (12)	Cs3A ⁱⁱ —O5—Cs3B ⁱⁱ	7.0 (2)
O8—Sn1—Cs3B ^x	122.9 (3)	Cs1 ^{iv} —O5—Cs3B ⁱⁱ	67.68 (14)
O22 ⁱⁱⁱ —Sn1—Cs3B ^x	125.41 (13)	Si2—O5—Cs3A ^{viii}	76.70 (12)
O1 ^x —Sn1—Cs3B ^x	56.3 (3)	Sn1 ^{xvii} —O5—Cs3A ^{viii}	96.58 (10)
O15 ^{vi} —Sn1—Cs3B ^x	47.0 (2)	Cs3A ⁱⁱ —O5—Cs3A ^{viii}	99.33 (8)
O16 ^{vi} —Sn1—Cs3B ^x	56.66 (14)	Cs1 ^{iv} —O5—Cs3A ^{viii}	164.22 (9)
O5 ^x —Sn1—Cs3B ^x	131.4 (2)	Cs3B ⁱⁱ —O5—Cs3A ^{viii}	103.00 (19)
O8—Sn1—Cs3A ^x	129.10 (9)	Si2—O6—Si6 ⁱⁱ	145.3 (2)
O22 ⁱⁱⁱ —Sn1—Cs3A ^x	125.11 (8)	Si2—O6—Cs3B ^{viii}	89.6 (2)
O1 ^x —Sn1—Cs3A ^x	49.99 (9)	Si6 ⁱⁱ —O6—Cs3B ^{viii}	113.8 (2)
O15 ^{vi} —Sn1—Cs3A ^x	52.78 (8)	Si2—O6—Cs3A ^{viii}	85.23 (13)
O16 ^{vi} —Sn1—Cs3A ^x	56.45 (9)	Si6 ⁱⁱ —O6—Cs3A ^{viii}	114.18 (15)
O5 ^x —Sn1—Cs3A ^x	125.54 (8)	Cs3B ^{viii} —O6—Cs3A ^{viii}	8.5 (3)
Cs3B ^x —Sn1—Cs3A ^x	7.0 (2)	Si2—07—Si8	142.1 (2)

O8—Sn1—Cs1 ⁱⁱⁱ	54.30 (9)	Si2—O7—Cs1 ^{iv}	98.93 (15)
O22 ⁱⁱⁱ —Sn1—Cs1 ⁱⁱⁱ	53.05 (8)	Si8—O7—Cs1 ^{iv}	118.02 (15)
O1 ^x —Sn1—Cs1 ⁱⁱⁱ	126.61 (9)	Si3—O8—Sn1	128.90 (17)
O15 ^{vi} —Sn1—Cs1 ⁱⁱⁱ	128.78 (8)	Si3—O8—Cs3B ^{xiv}	115.3 (3)
$O16^{vi}$ — $Sn1$ — $Cs1^{iii}$	125.17 (9)	Sn1—O8—Cs3B ^{xiv}	115.8 (3)
O5 ^x —Sn1—Cs1 ⁱⁱⁱ	52.84 (8)	Si3—O8—Cs3A ^{xiv}	123.52 (15)
Cs3B ^x —Sn1—Cs1 ⁱⁱⁱ	175.7 (2)	Sn1—O8—Cs3A ^{xiv}	107.58 (12)
Cs3A ^x —Sn1—Cs1 ⁱⁱⁱ	176.60 (2)	Cs3B ^{xiv} —O8—Cs3A ^{xiv}	8.6 (3)
O8—Sn1—Cs3A ^{xiv}	45.47 (8)	Si3—O8—Cs1 ⁱⁱⁱ	101.09 (13)
O22 ⁱⁱⁱ —Sn1—Cs3A ^{xiv}	106.03 (8)	Sn1—O8—Cs1 ⁱⁱⁱ	96.22 (12)
O1 ^x —Sn1—Cs3A ^{xiv}	132.83 (9)	Cs3B ^{xiv} —O8—Cs1 ⁱⁱⁱ	72.34 (19)
O15 ^{vi} —Sn1—Cs3A ^{xiv}	135.00 (9)	Cs3A ^{xiv} —O8—Cs1 ⁱⁱⁱ	69.61 (6)
O16 ^{vi} —Sn1—Cs3A ^{xiv}	72.31 (9)	Si3—O9—Si5	175.2 (3)
O5 ^x —Sn1—Cs3A ^{xiv}	46.38 (9)	Si4—O10—Si3	143.6 (2)
Cs3B ^x —Sn1—Cs3A ^{xiv}	128.32 (11)	Si4—O10—Cs1 ⁱⁱⁱ	108.30 (14)
Cs3A ^x —Sn1—Cs3A ^{xiv}	128.760 (13)	Si3—O10—Cs1 ⁱⁱⁱ	103.11 (14)
Cs1 ⁱⁱⁱ —Sn1—Cs3A ^{xiv}	52.982 (8)	Si4—O10—Cs2	90.03 (13)
O8—Sn1—Cs1 ^{xi}	136.49 (8)	Si3—O10—Cs2	92.47 (13)
$O22^{iii}$ —Sn1—Cs1 ^{xi}	72.06 (8)	Cs1 ⁱⁱⁱ —O10—Cs2	115.94 (9)
$O1^x$ — $Sn1$ — $Cs1^{xi}$	45.31 (8)	Si5 ^{vi} —O11—Si3	130.59 (18)
$O15^{vi}$ — $Sn1$ — $Cs1^{xi}$	48.21 (9)	Si5 ^{vi} —O11—Cs2	108.23 (14)
O16 ^{vi} —Sn1—Cs1 ^{xi}	109.41 (9)	Si3—O11—Cs2	116.67 (14)
$O5^{x}$ — $Sn1$ — $Cs1^{xi}$	130.44 (9)	Si4—O12—Sn2 ^{ix}	164.45 (19)
Cs3B ^x —Sn1—Cs1 ^{xi}	53.90 (11)	Si4—O12—Cs2	100.26 (13)
Cs3A ^x —Sn1—Cs1 ^{xi}	53.058 (9)	Sn2 ^{ix} —O12—Cs2	94.97 (10)
$Cs1^{iii}$ — $Sn1$ — $Cs1^{xi}$	125.031 (10)	Si6—O13—Si4	138.7 (2)
Cs3A ^{xiv} —Sn1—Cs1 ^{xi}	176.69 (2)	Si5—O14—Si4 ^{vi}	139.6 (2)
O8—Sn1—Cs3A ^{vi}	116.76 (8)	Si5—O14—Cs2 ^{xii}	99.13 (13)
O22 ⁱⁱⁱ —Sn1—Cs3A ^{vi}	130.18 (9)	Si4 ^{vi} —O14—Cs2 ^{xii}	114.59 (14)
O1 ^x —Sn1—Cs3A ^{vi}	61.07 (9)	Si5—O14—Cs1 ^{xv}	92.19 (14)
O15 ^{vi} —Sn1—Cs3A ^{vi}	123.03 (8)	Si4 ^{vi} —O14—Cs1 ^{xv}	88.28 (13)
O16 ^{vi} —Sn1—Cs3A ^{vi}	46.12 (9)	$Cs2^{xii}$ —O14—Cs1 ^{xv}	122.15 (10)
O5 ^x —Sn1—Cs3A ^{vi}	55.46 (8)	Si5—O15—Sn1 ^{xii}	129.25 (17)
Cs3B ^x —Sn1—Cs3A ^{vi}	76.1 (2)	Si5—O15—Cs3B ^{viii}	120.2 (4)
Cs3A ^x —Sn1—Cs3A ^{vi}	70.79 (2)	Sn1 ^{xii} —O15—Cs3B ^{viii}	103.3 (3)
Cs1 ⁱⁱⁱ —Sn1—Cs3A ^{vi}	108.007 (10)	Si5—O15—Cs3A ^{viii}	128.03 (16)
Cs3A ^{xiv} —Sn1—Cs3A ^{vi}	74.36 (3)	Sn1 ^{xii} —O15—Cs3A ^{viii}	97.02 (10)
Cs1 ^{xi} —Sn1—Cs3A ^{vi}	104.687 (12)	Cs3B ^{viii} —O15—Cs3A ^{viii}	8.1 (3)
O12 ⁱⁱⁱ —Sn2—O12 ⁱⁱ	180.00 (18)	Si5—O15—Cs1 ^{xv}	111.68 (14)
O12 ⁱⁱⁱ —Sn2—O20	88.36 (12)	Sn1 ^{xii} —O15—Cs1 ^{xv}	104.69 (12)
O12 ⁱⁱ —Sn2—O20	91.64 (12)	Cs3B ^{viii} —O15—Cs1 ^{xv}	73.1 (2)
$O12^{iii}$ — $Sn2$ — $O20^{xi}$	91.64 (12)	Cs3A ^{viii} —O15—Cs1 ^{xv}	69.45 (6)
$O12^{ii}$ — $Sn2$ — $O20^{xi}$	88.36 (12)	Si6—O16—Sn1 ^{xii}	139.84 (18)
O20—Sn2—O20 ^{xi}	180.0	Si6—O16—Cs3A	108.61 (13)
O12 ⁱⁱⁱ —Sn2—O17 ⁱⁱⁱ	90.26 (12)	Sn1 ^{xii} —O16—Cs3A	107.16 (12)
O12 ⁱⁱ —Sn2—O17 ⁱⁱⁱ	89.74 (12)	Si6—O16—Cs3Bviii	97.1 (3)
O20—Sn2—O17 ⁱⁱⁱ	85.77 (12)	Sn1 ^{xii} —O16—Cs3B ^{viii}	92.74 (16)
O20 ^{xi} —Sn2—O17 ⁱⁱⁱ	94.23 (12)	Cs3A—O16—Cs3B ^{viii}	102.1 (3)

O12 ⁱⁱⁱ —Sn2—O17 ⁱⁱ	89.74 (12)	Si6-016-Cs3Aviii	101.94 (14)
O12 ⁱⁱ —Sn2—O17 ⁱⁱ	90.26 (12)	Sn1 ^{xii} —O16—Cs3A ^{viii}	93.15 (10)
O20—Sn2—O17 ⁱⁱ	94.23 (12)	Cs3A—O16—Cs3A ^{viii}	94.00 (8)
$O20^{xi}$ — $Sn2$ — $O17^{ii}$	85.77 (12)	Cs3B ^{viii} —O16—Cs3A ^{viii}	8.4 (3)
O17 ⁱⁱⁱ —Sn2—O17 ⁱⁱ	180.00 (18)	Si6—O16—Cs3B	110.77 (18)
O12 ⁱⁱⁱ —Sn2—Cs2 ⁱⁱⁱ	55.33 (8)	Sn1 ^{xii} —O16—Cs3B	105.33 (17)
O12 ⁱⁱ —Sn2—Cs2 ⁱⁱⁱ	124.67 (8)	Cs3A—O16—Cs3B	2.28 (13)
O20—Sn2—Cs2 ⁱⁱⁱ	53.35 (9)	Cs3B ^{viii} —O16—Cs3B	101.0 (3)
$O20^{xi}$ — $Sn2$ — $Cs2^{iii}$	126.65 (9)	Cs3A ^{viii} —O16—Cs3B	92.79 (14)
O17 ⁱⁱⁱ —Sn2—Cs2 ⁱⁱⁱ	51.61 (8)	Si7—O17—Sn2 ^{ix}	130.26 (17)
O17 ⁱⁱ —Sn2—Cs2 ⁱⁱⁱ	128.39 (8)	Si7—O17—Cs2	125.86 (15)
O12 ⁱⁱⁱ —Sn2—Cs2 ⁱⁱ	124.67 (8)	Sn2 ^{ix} —O17—Cs2	98.65 (10)
O12 ⁱⁱ —Sn2—Cs2 ⁱⁱ	55.33 (8)	Si7—O17—Cs2 ⁱⁱⁱ	108.81 (14)
O20—Sn2—Cs2 ⁱⁱ	126.65 (9)	Sn2 ^{ix} —O17—Cs2 ⁱⁱⁱ	104.82 (12)
$O20^{xi}$ — $Sn2$ — $Cs2^{ii}$	53.35 (9)	Cs2—O17—Cs2 ⁱⁱⁱ	72.17 (6)
O17 ⁱⁱⁱ —Sn2—Cs2 ⁱⁱ	128.39 (8)	Si7—O18—Si9	137.1 (2)
O17 ⁱⁱ —Sn2—Cs2 ⁱⁱ	51.61 (8)	Si7—O18—Cs1 ^{ix}	97.47 (13)
Cs2 ⁱⁱⁱ —Sn2—Cs2 ⁱⁱ	180.0	Si9—O18—Cs1 ^{ix}	114.47 (14)
O12 ⁱⁱⁱ —Sn2—Cs2	109.74 (8)	Si7—O18—Cs2 ⁱⁱⁱ	90.66 (13)
O12 ⁱⁱ —Sn2—Cs2	70.26 (8)	Si9—O18—Cs2 ⁱⁱⁱ	93.76 (13)
O20—Sn2—Cs2	45.77 (8)	Cs1 ^{ix} —O18—Cs2 ⁱⁱⁱ	124.26 (10)
O20 ^{xi} —Sn2—Cs2	134.23 (8)	Si8—O19—Si7 ⁱⁱ	129.52 (18)
O17 ⁱⁱⁱ —Sn2—Cs2	47.71 (9)	Si8—O19—Cs1	117.12 (14)
O17 ⁱⁱ —Sn2—Cs2	132.29 (9)	Si7 ⁱⁱ —O19—Cs1	109.67 (13)
Cs2 ⁱⁱⁱ —Sn2—Cs2	54.535 (8)	Si8—O20—Sn2	129.48 (17)
Cs2 ⁱⁱ —Sn2—Cs2	125.465 (8)	Si8—O20—Cs2	122.70 (15)
$O12^{iii}$ — $Sn2$ — $Cs2^{xi}$	70.26 (8)	Sn2—O20—Cs2	107.37 (11)
O12 ⁱⁱ —Sn2—Cs2 ^{xi}	109.74 (8)	Si8—O20—Cs2 ⁱⁱⁱ	103.61 (14)
O20—Sn2—Cs2 ^{xi}	134.23 (8)	Sn2—O20—Cs2 ⁱⁱⁱ	97.05 (12)
$O20^{xi}$ — $Sn2$ — $Cs2^{xi}$	45.77 (8)	Cs2—O20—Cs2 ⁱⁱⁱ	72.15 (6)
$O17^{iii}$ — $Sn2$ — $Cs2^{xi}$	132.29 (9)	Si8—O21—Si9	151.9 (3)
O17 ⁱⁱ —Sn2—Cs2 ^{xi}	47.71 (9)	Si8—O21—Cs2 ⁱⁱⁱ	98.65 (14)
$Cs2^{iii}$ — $Sn2$ — $Cs2^{xi}$	125.466 (8)	Si9—O21—Cs2 ⁱⁱⁱ	106.27 (15)
Cs2 ⁱⁱ —Sn2—Cs2 ^{xi}	54.534 (8)	Si8—O21—Cs1	91.31 (13)
Cs2—Sn2—Cs2 ^{xi}	180.0	Si9—O21—Cs1	90.47 (13)
O1—Si1—O2	110.44 (18)	Cs2 ⁱⁱⁱ —O21—Cs1	113.55 (10)
O1—Si1—O3	111.15 (18)	Si9—O22—Sn1 ⁱⁱⁱ	160.20 (19)
O2—Si1—O3	108.86 (18)	Si9—O22—Cs1	102.17 (14)
O1—Si1—O4	111.33 (16)	Sn1 ⁱⁱⁱ —O22—Cs1	97.49 (10)
O2—Si1—O4	108.37 (18)	Si9 ^{iv} —O23—Si9	179.5 (3)
O3—Si1—O4	106.57 (18)		

Symmetry codes: (i) -x+1, y+1, -z+1/2; (ii) x, y+1, z; (iii) -x+1, -y-1, -z; (iv) -x+1, y, -z+1/2; (v) x-1/2, -y-1/2, z; (vi) -x+3/2, y+1/2, -z; (vii) x, -y-2, z+1/2; (viii) -x+3/2, -y-3/2, -z+1/2; (ix) x, y-1, z; (x) x, -y-1, z-1/2; (xi) -x+3/2, y-1/2, -z; (xiii) -x+3/2, y+1/2, -z; (vii) x, -y-2, z+1/2; (viii) -x+3/2, -y-3/2, -z+1/2; (ix) x, y-1, z-1/2; (xi) -x+1, -y, -z; (xii) -x+3/2, y-1/2, -z; (xiii) -x+1, y-1, -z+1/2; (xiv) x, -y-2, z-1/2; (xv) x+1/2, -y-1/2, z; (xvi) -x+3/2, -y-5/2, -z+1/2; (xvii) x, -y-1, z+1/2.