Ba₃[Sn(OH)₆][SeO₄]₂·3H₂O, a hydrated 1:2 double salt of barium hexahydroxidostannate(IV) and barium selenate(VI)

Hans Reuter* and Shouassi Kamaha

Chemistry, Osnabrück University, Barabarstr. 7, 49069 Osnabrück, Germany. *Correspondence e-mail: hreuter@uos.de

Single crystals of tribarium hexahydroxidostannate(IV) bis[selenate(VI)] trihydrate, Ba₃H₂O₁₂Se₂Sn or Ba₃[Sn(OH)₆][SeO₄]₂·3H₂O, prepared from solid BaSnO₃ and aqueous Na₂[SeO₄] solutions have hexagonal (P6₃) symmetry. The structure consists of four different primary building units: a hexahydroxidostannate(IV) ion, two different selenate(VI) ions, all three of point group symmetry C₃, and a mono-capped [BaO₉]-square antiprism of point group symmetry C₁. The secondary building units result from three of the barium coordination polyhedra linked together via common edges. While one of the two tetrahedral voids formed from these trimeric units is filled by one bidentate, chelating μ₂-selenate ion, the other one remains unoccupied as the corresponding second selenate ion only acts as a monodentate, μ₁-ligand. SBUs are completed by hexahydroxidostannate(IV) ions sharing adjacent edges on the uncapped faces of the three, mono-capped square antiprisms. These SBUs are arranged into layers via common edges on the uncapped, square faces of the [BaO₉] coordination polyhedra in a way that the hexahydroxidostannate(IV) ions act as linkage between two neighboring layers.

1. Chemical context

The hexahydroxidostannate(IV) ion, [Sn(OH)₆]²⁻, is a well established tin(IV) anion in chemistry (Scholder, 1981), mineralogy (Strunz & Nickel, 1998) and even archaeology (Basciano et al. 1998), although the number of well defined and structurally described compounds is rather low, especially in case of two-valent cations as these compounds are only slightly soluble. In a former paper (Kamaha & Reuter, 2009), we demonstrated strategies for how to circumvent these difficulties by combining slow anion formation with slow crystallization, mimicking to some extent geochemical crystal formation processes.

Here we present our results on experiments where we offered selenate(VI) anions parallel to the slow formation of hexahydroxidostannate(IV) ions, as possible co-anions during crystallization. In a typical experiment we exposed BaSnO₃ pellets to a Na₂SeO₄ solution, resulting after a long period in the formation of colorless, hexagonal prisms of Ba₃[Sn(OH)₆][SeO₄]₂·3H₂O, a hydrated 1:2 double salt of barium hexahydroxidostannate(IV), Ba[Sn(OH)₆], and barium selenate(VI), Ba[SeO₄]. From both compounds, only the structure of the selenate has been described in the literature (Andara et al., 2005).

2. Structural commentary

The title compound crystallizes in the non-centrosymmetric, hexagonal space group P6₃ and was refined as an inversion
twin, giving a Flack parameter of 0.037 (11). With two formula units in the unit cell, the asymmetric unit consists of 1/3 formula unit: a Ba$^{2+}$ ion and a water molecule, both in general positions, and two crystallographically independent $\left[\text{SeO}_4\right]^{2-}$ ions and one $\left[\text{Sn(OH)}_6\right]^{2-}$ ion, all three having the point group $C_3$. In addition to the $\left[\text{BaO}_9\right]$-coordination polyhedron, these complex anions represent the primary building units, PBUs.

The two crystallographically different Sn–O distances within the hexahydroxidostannate(IV) anion (Fig. 1, Table 1) are identical within standard deviations $[d(\text{Sn1–O1}) = 2.052 (2) \text{ Å}]$ and $d(\text{Sn1–O2}) = 2.054 (2) \text{ Å}$. The mean value of 2.053 (2) Å is somewhat shorter than the mean value of 2.060 (10) Å observed in other hexahydroxidostannates (Kamaha & Reuter, 2009), but lies in the observed range of 2.039–2.075 Å. Deviations from the geometry of a regular octahedron are better expressed in terms of the bond angles, which show bond angles of 178.7 (1)$^\circ$. All oxygen atoms of the $\left[\text{Sn(OH)}_6\right]^{2-}$ ion coordinate to three barium ions. On the other hand, the three basal oxygen atoms act as acceptor of one hydrogen bond and also perform coordinative bonds, each to a different barium ion, in the first selenate ion while those of the second selenate ion accept two hydrogen bonds. Besides bond-length differences, deviations from the geometry of a regular tetrahedron result in both selenate ions having bond angles of slightly flattened trigonal pyramids rather than strict tetrahedra (Fig. 2).

The coordination sphere of the barium ion consists of nine oxygen atoms: two from water molecules, four from two $\left[\text{Sn(OH)}_6\right]^{2-}$ ions, one from the first selenate ion and two,
respectively, from the second selenate ion (Fig. 3). In summary, this \( \text{Ba}\left(\mu_2-\text{OH}\right)_4(\text{H}_2\text{O})_2(\mu_2-\text{OSe}_2)\text{Se}_1\) coordination sphere has the shape of a mono-capped square antiprism. The uncapped face of this coordination polyhedron only is built up from the oxygen atoms of two hexahydroxidostannate ions. Its shape is almost square [maximal angle deviations from rectangular: \(\pm 0.6\) (1)°, maximal deviation from planarity: \(\pm 0.0132\) Å, side lengths: 2.7705 (2)–3.1720 (2) Å]. In contrast, the capped face of the square antiprism consists of oxygen atoms from two water molecules and from \(\text{basal}\) oxygen atoms of the two different selenate ions. Its shape [maximal deviation from planarity: \(\pm 0.0022\) (2) Å] is much better described as an acute trapezoid with a longer/shorter base of 4.4606 (2)/3.7164 (2) Å, legs of 3.4108 (2)/3.2331 (2) Å and angles between 103.01 (1) and 78.42 (1)°. The dihedral angle between these planes is 5.64 (1)°. These deviations from a regular square antiprism are mainly caused by coordination to the selenate ions, as the \(\text{apical}\) oxygen atom of the second one constitutes the cap of the \(\text{[BaO}_9\) coordination polyhedron, giving rise to a bidentate-chelating coordination mode of this selenate ion while the first selenate ion only acts as monodentate ligand. \(\text{Ba—O}\) bond lengths (Table 3) range from 2.715 (2) to 3.106 (3) Å, mean value 2.837 Å. Bonds between the barium ion and the oxygen atoms of the hexahydroxidostannate ions are of comparable lengths \([d(\text{Ba—O}_1/\text{O}_2) = 2.737 (2)–2.782 (2) \text{ Å}]\) as are those between the barium ion and the water molecules \([2.880 (2)/2.931 (2) \text{ Å}]\). The longest bond \([d(\text{Ba—O}_7) = 3.106 (3) \text{ Å}]\) is between the barium ion and the \(\text{basal}\) oxygen atom of the second selenate ion, while the shortest one \([d(\text{Ba—O}_3) = 2.715 (2) \text{ Å}]\) leads to the \(\text{basal}\) atom of the first selenate ion.

3. Supramolecular features

The interaction of the four different PBUs is visualized in Fig. 4. The most prominent part of the resulting secondary building units, SBUs, consists of three \(\text{[BaO}_9\) coordination polyhedra related to each other via the threefold rotation axes.
in Wyckoff position $b$. These three PBUs are linked together via common edges, each of them composed of the coordinated water molecule and the apical oxygen atom of the second selenate ion. In addition, this selenate ion shares its remaining three, basal oxygen atoms with the three surrounding barium ions, thus filling the tetrahedral void between the three [BaO$_9$] coordination polyhedra. On the other hand, the opposite void of the trimeric [BaO$_9$] unit is empty, as the first selenate ion only shares its three basal oxygen atoms with the three [BaO$_9$] coordination polyhedra but not the apical one. Each SBU is completed by a hexahydroxidostannate(IV) ion sharing one edge with the uncapped face of the mono-capped [BaO$_9$] antiprisms.

These secondary building units are linked together with three others, each via a common edge of the uncapped square of the [BaO$_9$] coordination polyhedra. In this way, each [BaO$_9$] coordination polyhedron shares two opposite edges of its square faces with two neighboring barium coordination polyhedra, resulting in a trigonal–prismatic void between the three interconnected PBUs. All corners of these voids consist of hydroxyl groups from [Sn(OH)$_6$]$_2$ ions with the tin atoms of these PBUs situated on threefold rotation axes in Wyckoff position $a$.

In summary, the PBUs are arranged in layers perpendicular to the $c$ axis direction (Fig. 5). The pores within these layers are occupied by selenate ions (Se2) of adjacent layers. These selenate ions are connected with the layer via hydrogen bonds (Table 2) to the water molecules and hydroxyl groups of the [Sn(OH)$_6$]$_2$ ions, while the latter cross-link adjacent layers. Adjacent layers are rotated through 120° against each other, resulting in a compact crystal packing without any accessible holes, channels or pores (Fig. 6). To some extent, the complex composition of the title compound expressed by the formula $M^+$[X$^{IV}$(OH)$_6$]Y$^{IV}$O$_{12}$·3H$_2$O has similarities to those of the mineral thauamsite, Ca$_3$[Si(OH)$_6$][SO$_4$][CO$_3$]·3H$_2$O (Edge & Taylor, 1971; Effenberger et al., 1983), also crystallizing in space group $P6_3$. In contrast to the title compound, the coordination polyhedron of the earth metal in this mineral is reduced from nine to eight and may be described as a one-face distorted square antiprism. While the hexahydroxidosilicate adopt a similar position as the hexahydroxidostannate ion, the two other complex anions of thaumasite are only linked via hydrogen bonds to the trimeric units of [CaO$_9$] polyhedra as these secondary building units are not cross-linked into layers.

Figure 5
Polyhedral model showing the aufbau principle of the layers (top view above, side view below) as result of the interconnection of the PBUs. Polyhedral colors according to Fig. 1 to 3. Isolated selenate ions (Se2) in the three-sided pores belong to adjacent layers. The corresponding hydrogen bonds are omitted for clarity.

Figure 6
Polyhedral model showing the packing of two layers.
4. Synthesis and crystallization

Single crystals of the title compound were obtained in a long-duration experiment exposing a BaSnO$_3$ (Celest) pellet prepared by heating equimolar amounts of SnO$_2$ and BaO for 40 h at 1688 K to 10 ml of a solution of Na$_2$SeO$_4$ (Fluka) in a rolled rim glass vessel closed with a snap-on lid. Colorless, hexagonal prisms occurred after several months in the sludge of the mouldered BaSnO$_3$ pellet.

5. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 4. All H atoms were clearly identified in difference Fourier syntheses. Their positions were modeled with respect to a common O—H distance of 0.96 Å and a bond angle of 104.9° in case of the water molecule before they were fixed and allowed to ride on the corresponding oxygen atoms. Refinement of two common isotropic temperature factors, one for the hydrogen atoms of the hydroxyl groups and one for the hydrogen atoms of the water molecule, allowed us to check the reliability of their positions.

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Ba₃[Sn(OH)₆][SeO₄]₂·3H₂O, a hydrated 1:2 double salt of barium hexahydroxidostannate(IV) and barium selenate(VI)

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Computing details
Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT (Bruker, 2009); program(s) used to solve structure: SHELXS97 (Sheldrick 2008); program(s) used to refine structure: SHELXL2014/7 (Sheldrick, 2015); molecular graphics: DIAMOND (Brandenburg, 2006), Mercury (Macrae et al. 2020); software used to prepare material for publication: publCIF (Westrip, 2010).

Tribarium hexahydroxidostannate(IV) bis[selenate(VI)] trihydrate

Crystal data
Ba₃[Sn(OH)₆][SeO₄]₂·3H₂O
Mr = 972.73
Hexagonal, P6₃
a = 9.2550 (6) Å
C = 11.4441 (8) Å
V = 848.92 (13) Å³
Z = 2
F(000) = 868

Data collection
Bruker APEXII CCD
diffraetor
c and o scans
Absorption correction: multi-scan
(SADABS; Krause et al., 2015)

Tmin = 0.314, T max = 0.741
112431 measured reflections

Refinement
Refinement on F²
Least-squares matrix: full
R[F² > 2σ(F²)] = 0.008
wR(F²) = 0.018
S = 1.13
1659 reflections
74 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
H-atom parameters constrained

w = 1/[σ²(F²) + (0.0035P)² + 1.0003P]
where P = (F² + 2Fc²)/3
(Δ/σ) max = 0.001
Δρ max = 0.54 e Å⁻³
Δρ min = −0.37 e Å⁻³
Extinction correction: SHELXL-2014/7
(Sheldrick 2015,
Fc*=kFc[1+0.001xFc²λ²/sin(2θ)]⁻¹/4
Extinction coefficient: 0.00210 (7)
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.037 (11)
supporting information

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. Refined as a 2-component inversion twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

| Atom | x         | y         | z         | Uiso* / Ueq |
|------|-----------|-----------|-----------|-------------|
| Ba1  | 0.85513 (2) | 0.67674 (2) | 0.76533 (2) | 0.00444 (4) |
| Sn1  | 1.0000    | 1.0000    | 0.51521 (5) | 0.00320 (5) |
| O1   | 0.9097 (3) | 0.7983 (3) | 0.4052 (2)  | 0.0057 (4)  |
| H1   | 0.8736    | 0.6914    | 0.4403     | 0.030 (7)*  |
| O2   | 1.1069 (3) | 0.9077 (3) | 0.6279 (2)  | 0.0056 (4)  |
| H2   | 1.1548    | 0.8586    | 0.5787     | 0.030 (7)*  |
| Se1  | 0.6667    | 0.3333    | 0.50722 (5) | 0.00388 (9) |
| Se2  | 0.6667    | 0.3333    | 0.96470 (5) | 0.00512 (9) |
| O6   | 0.6667    | 0.3333    | 0.8207 (3)  | 0.0072 (7)  |
| O4   | 0.6667    | 0.3333    | 0.3627 (4)  | 0.0076 (6)  |
| O3   | 0.7824 (3) | 0.5248 (3) | 0.55332 (19)| 0.0108 (4)  |
| O7   | 0.6848 (3) | 0.1745 (3) | 1.0066 (2)  | 0.0106 (4)  |
| O8   | 0.9600 (3) | 0.4949 (2) | 0.23440 (18)| 0.0095 (4)  |
| H8A  | 0.8628    | 0.4361    | 0.2827     | 0.054 (11)* |
| H8B  | 0.9175    | 0.4875    | 0.1568     | 0.054 (11)* |

Atomic displacement parameters (Å²)

|       | U¹¹  | U¹²  | U¹³  | U²²  | U²³  | U³³  |
|-------|------|------|------|------|------|------|
| Ba1   | 0.00500 (6) | 0.00347 (6) | 0.00436 (6) | 0.00175 (5) | -0.00001 (8) | -0.00006 (8) |
| Sn1   | 0.00351 (7) | 0.00351 (7) | 0.00258 (10) | 0.00175 (3) | 0.000 | 0.000 |
| O1    | 0.0070 (11) | 0.0036 (11) | 0.0054 (10) | 0.0018 (9) | 0.0002 (8) | -0.0001 (8) |
| O2    | 0.0062 (11) | 0.0066 (11) | 0.0057 (10) | 0.0044 (10) | 0.0001 (8) | 0.0009 (8) |
| Se1   | 0.00407 (14) | 0.00407 (14) | 0.0035 (2) | 0.00204 (7) | 0.000 | 0.000 |
| Se2   | 0.00486 (14) | 0.00486 (14) | 0.0057 (2) | 0.00243 (7) | 0.000 | 0.000 |
| O6    | 0.0085 (10) | 0.0085 (10) | 0.0046 (17) | 0.0043 (5) | 0.000 | 0.000 |
| O4    | 0.0103 (10) | 0.0103 (10) | 0.0023 (13) | 0.0051 (5) | 0.000 | 0.000 |
| O3    | 0.0137 (11) | 0.0049 (10) | 0.0087 (9) | 0.0008 (8) | -0.0013 (8) | -0.0022 (8) |
| O7    | 0.0133 (11) | 0.0089 (10) | 0.0125 (9) | 0.0077 (9) | -0.0017 (9) | 0.0024 (8) |
| O8    | 0.0071 (8) | 0.0113 (9) | 0.0096 (10) | 0.0041 (7) | 0.0001 (7) | 0.0006 (7) |

Geometric parameters (Å, °)

| Bond          | Length (Å) | Angle (°) |
|---------------|------------|-----------|
| Ba1—O3        | 2.715 (2)  |           |
| Ba1—O2        | 2.737 (2)  |           |
| Ba1—Se1       | 2.777 (2)  |           |
| Ba1—Se2       | 2.779 (2)  |           |
| Ba1—O1        | 2.779 (2)  |           |
| Ba1—O4        | 2.782 (2)  |           |

Acta Cryst. (2022). E78, 809-813
| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|-----------------------|--------------|-----------------------|--------------|
| Ba1—O6                | 2.829 (1)    | Se1—O3                | 1.634 (2)    |
| Ba1—O8^iv             | 2.880 (2)    | Se1—O3                | 1.634 (2)    |
| Ba1—O8^i              | 2.931 (2)    | Se1—O3                | 1.634 (2)    |
| Ba1—O7^v              | 3.106 (3)    | Se2—O7^iv             | 1.633 (2)    |
| Ba1—Se2               | 3.5786 (4)   | Se2—O7^v              | 1.633 (2)    |
| Ba1—Sn1               | 3.8639 (5)   | Se2—O7                | 1.633 (2)    |
| Sn1—O1^iii            | 2.052 (2)    | Se2—Ba1^v             | 3.5786 (4)   |
| Sn1—O1                | 2.052 (2)    | Se2—Ba1^v             | 3.5786 (4)   |
| Sn1—O2                | 2.054 (2)    | O6—Ba1^v              | 2.8288 (8)   |
| Sn1—O2^v              | 2.054 (2)    | O6—Ba1^v              | 2.8288 (8)   |
| O3—Ba1—O2             | 77.58 (7)    | Ba1^vii—Sn1—Ba1^ix    | 71.188 (11)  |
| O3—Ba1—O1^i           | 142.66 (7)   | O1^iii—Sn1—Ba1^x      | 43.93 (7)    |
| O2—Ba1—O1^i           | 99.65 (6)    | O1—Sn1—Ba1^x          | 94.36 (7)    |
| O3—Ba1—O1^ii          | 144.19 (7)   | O1^v—Sn1—Ba1^x        | 43.93 (7)    |
| O2—Ba1—O1^ii          | 70.22 (5)    | O2—Sn1—Ba1^x          | 137.27 (7)   |
| O1^i—Ba1—O1^i         | 60.66 (10)   | O2^v—Sn1—Ba1^x        | 86.69 (7)    |
| O3—Ba1—O2^iii         | 77.32 (7)    | O2^v—Sn1—Ba1^x        | 135.94 (6)   |
| O2—Ba1—O2^iii         | 60.20 (10)   | Ba1^vii—Sn1—Ba1^x     | 71.188 (11)  |
| O1^i—Ba1—O2^iii       | 69.60 (5)    | Ba1^vii—Sn1—Ba1^x     | 71.188 (11)  |
| O1^ii—Ba1—O2^iii      | 99.11 (6)    | O1^iii—Sn1—Ba1        | 136.01 (7)   |
| O3—Ba1—O6             | 76.38 (9)    | O1—Sn1—Ba1            | 85.66 (7)    |
| O2—Ba1—O6             | 144.30 (7)   | O1^v—Sn1—Ba1          | 136.07 (7)   |
| O1^i—Ba1—O6           | 115.84 (7)   | O2—Sn1—Ba1            | 42.73 (7)    |
| O1^ii—Ba1—O6          | 123.39 (8)   | O2^v—Sn1—Ba1          | 93.29 (7)    |
| O2^iv—Ba1—O6          | 134.70 (7)   | O2^v—Sn1—Ba1          | 44.06 (6)    |
| O3—Ba1—O8^iv          | 70.52 (6)    | Ba1^vii—Sn1—Ba1       | 108.832 (5)  |
| O2—Ba1—O8^iv          | 81.46 (7)    | Ba1^vii—Sn1—Ba1       | 108.833 (5)  |
| O1^i—Ba1—O8^iv        | 146.58 (6)   | Ba1^vii—Sn1—Ba1       | 179.974 (12) |
| O1^ii—Ba1—O8^iv       | 89.23 (6)    | O1^iii—Sn1—Ba1^vii    | 136.08 (7)   |
| O2^iv—Ba1—O8^iv       | 134.31 (6)   | O1—Sn1—Ba1^vii        | 136.01 (7)   |
| O6—Ba1—O8^iv          | 67.08 (4)    | O1^v—Sn1—Ba1^vii      | 85.66 (7)    |
| O3—Ba1—O8^i           | 74.22 (6)    | O2—Sn1—Ba1^vii        | 44.06 (6)    |
| O2—Ba1—O8^i           | 127.90 (6)   | O2^v—Sn1—Ba1^vii      | 42.73 (7)    |
| O1^i—Ba1—O8^i         | 79.11 (7)    | O2^v—Sn1—Ba1^vii      | 93.29 (7)    |
| O1^ii—Ba1—O8^i        | 139.10 (6)   | Ba1^vii—Sn1—Ba1^vii   | 179.974 (12) |
| O2^ii—Ba1—O8^i        | 71.31 (7)    | Ba1^vii—Sn1—Ba1^vii   | 108.832 (5)  |
| O6—Ba1—O8^i           | 66.39 (4)    | Ba1^vii—Sn1—Ba1^vii   | 108.832 (5)  |
| O8^iii—Ba1—O8^i       | 126.49 (7)   | Ba1—Sn1—Ba1^vii       | 71.147 (11)  |
| O3—Ba1—O7^v           | 126.88 (6)   | O1^iii—Sn1—Ba1^ii     | 85.66 (7)    |
| Bond                  | Angle (°) (σ) |
|----------------------|--------------|
| O2—Ba1—O7"          | 136.68 (7)   |
| O1i—Ba1—O7"         | 80.61 (7)    |
| O1ii—Ba1—O7"        | 72.68 (6)    |
| O2ii—Ba1—O7"        | 148.89 (7)   |
| O6—Ba1—O7"          | 52.54 (8)    |
| O8vi—Ba1—O7"        | 76.42 (6)    |
| O8vii—Ba1—O7"       | 94.97 (6)    |
| O3—Ba1—Se2          | 103.02 (5)   |
| O2—Ba1—Se2          | 155.03 (5)   |
| O1i—Ba1—Se2         | 94.54 (5)    |
| O1ii—Ba1—Se2        | 99.78 (5)    |
| O2iii—Ba1—Se2       | 144.71 (5)   |
| O6—Ba1—Se2          | 26.66 (7)    |
| O8vi—Ba1—Se2        | 75.44 (4)    |
| O8vii—Ba1—Se2       | 74.87 (4)    |
| O7vii—Ba1—Se2       | 78.11 (4)    |
| O3—Ba1—Sn1vi        | 164.39 (5)   |
| O2—Ba1—Sn1vi        | 89.44 (5)    |
| O1i—Ba1—Sn1vi       | 30.84 (5)    |
| O1ii—Ba1—Sn1vi      | 30.85 (5)    |
| O2iii—Ba1—Sn1vi     | 88.77 (5)    |
| O6—Ba1—Sn1vi        | 118.99 (7)   |
| O8v—Ba1—Sn1vi       | 116.51 (4)   |
| O8—Ba1—Sn1vi        | 108.24 (4)   |
| O7vii—Ba1—Sn1vi     | 68.67 (4)    |
| Se2—Ba1—Sn1vi       | 92.415 (12)  |
| O3—Ba1—Sn1          | 68.85 (5)    |
| O2—Ba1—Sn1          | 30.61 (5)    |
| O1i—Ba1—Sn1         | 89.73 (5)    |
| O1ii—Ba1—Sn1        | 89.69 (5)    |
| O2iii—Ba1—Sn1       | 30.89 (5)    |
| O6—Ba1—Sn1          | 144.71 (7)   |
| O8—Ba1—Sn1          | 105.32 (4)   |
| O8vii—Ba1—Sn1       | 97.70 (4)    |
| O7vi—Ba1—Sn1        | 62.33 (4)    |
| Se2—Ba1—Sn1         | 170.516 (10) |
| Sn1vi—Ba1—Sn1       | 95.571 (6)   |
| O1i—Sn1—O1          | 86.27 (10)   |
| O1i—Sn1—O1vii       | 86.27 (10)   |
| O1—Sn1—O1vii        | 86.27 (10)   |
| O1ii—Sn1—O2         | 178.66 (12)  |
| O1—Sn1—O2           | 178.66 (12)  |
| O1—Sn1—O2v          | 93.93 (9)    |
| O1i—Sn1—O2v         | 95.06 (9)    |
| O1—Sn1—O2vii        | 95.07 (9)    |
| O1ii—Sn1—O2vii      | 178.66 (12)  |
| O1—Sn1—O2viii       | 93.93 (9)    |
| O1i—Sn1—O2viii      | 95.06 (9)    |
| O1—Sn1—O2vii        | 95.07 (9)    |
O1—Sn1—O2̂ 95.06 (9)  Ba1v—Se2—Ba1  83.696 (12)
O1v—Sn1—O2̂ 178.66 (12)  Se2—O6—Ba1i  102.95 (7)
O2—Sn1—O2̂  84.73 (10)  Se2—O6—Ba1v  102.95 (7)
O2v—Sn1—O2̂  84.73 (10)  Ba1v—O6—Ba1  115.13 (5)
O2̂i—Sn1—Ba1viii  44.00 (7)  Ba1v—O6—Ba1  115.13 (5)
O2̂ii—Sn1—Ba1viii  94.36 (7)  Ba1v—O6—Ba1  115.13 (5)
O2̂—Sn1—Ba1viii  135.94 (6)  Se1—O3—Ba1  135.14 (12)
O2̂—Sn1—Ba1viii  137.27 (7)  Se2—O7—Ba1xi  92.78 (11)
O2̂—Sn1—Ba1viii  137.27 (7)  Se2—O7—Ba1xi  92.78 (11)
O1i—Sn1—Ba1viii  86.69 (7)  Ba1vii—O8—H8A  105.3
O1—Sn1—Ba1viii  43.93 (7)  Ba1vii—O8—H8A  119.5
O1i—Sn1—Ba1viii  43.93 (7)  Ba1vii—O8—H8B  114.2
O2—Sn1—Ba1viii  86.69 (7)  Ba1vii—O8—H8B  102.6
O2i—Sn1—Ba1viii  135.94 (6)  H8A—O8—H8B  105.0
O2ii—Sn1—Ba1viii  137.27 (7)  H8A—O8—H8B  105.0

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

**Hydrogen-bond geometry (Å, °)**

| D—H···A | D—H | H···A | D···A | D—H···A |
|----------|-----|-------|-------|---------|
| O1—H1···O3 | 0.96 | 1.86  | 2.772 (3) | 158 |
| O2—H2···O7viii | 0.96 | 1.85  | 2.773 (3) | 160 |
| O8—H8A···O4 | 0.96 | 1.82  | 2.775 (3) | 173 |
| O8—H8B···O7viii | 0.96 | 1.98  | 2.923 (3) | 169 |

Symmetry codes: (viii) −x+2, −y+1, z−1/2; (xiii) −y+1, x−y, z−1.