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A Contribution to the Stereochemistry of Earth Alkaline Selenites: Synthesis and Crystal Structure of $Ca_2(SeO_3)(Se_2O_5)$, $Ba(SeO_3)$, and $Ba(Se_2O_5)$

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Summary. The compounds $Ca_2(SeO_3)(Se_2O_5)$, $Ba(SeO_3)$, and $Ba(Se_2O_5)$ were obtained at low-hydrothermal conditions from aqueous solutions of SeO_2 by reaction with the respective earth alkaline carbonate. The crystal structures were determined by direct methods from single crystal X-ray diffraction data. $Ca_2(SeO_3)(Se_2O_5)$: space group $P\bar{1}$, $Z=2$, $a=5.517(1)$, $b=8.210(2)$, $c=8.716(2)$ Å, $\alpha=92.47(2)$, $\beta=95.92(2)$, $\gamma=97.15(2)°$, $V=389.0(2)$ Å^3, $R_1=0.017$; $Ba(SeO_3)$: space group $P2_1/m$, $Z=2$, $a=4.677(2)$, $b=5.645(2)$, $c=6.851(3)$ Å, $\beta=107.16(2)°$, $V=172.8(1)$ Å^3, $R_1=0.022$, $Ba(Se_2O_5)$: space group $P2_1/c$, $Z=4$, $a=4.553(1)$, $b=11.724(3)$, $c=9.758(2)$ Å, $\beta=92.66(2)°$, $V=520.3(2)$Å^3, $R_1=0.027$. All three compounds have framework structures; in the case of $Ca_2(SeO_3)(Se_2O_5)$, subunits of edge-sharing CaO_n polyhedra forming sheets parallel to (010) can be emphasized. $Ba(SeO_3)$ belongs to the structure type of $KClO_3$. In $Ba(Se_2O_5)$, chains of face-sharing BaO_9 polyhedra along [100] are present. The calcium atoms are 7- and 8-coordinated with mean Ca–O bond lengths of 2.42 and 2.48 Å, the barium atoms have nine oxygen ligands with mean Ba–O bond lengths of 2.87 Å.

Keywords. $Ca_2(SeO_3)(Se_2O_5)$; $Ba(SeO_3)$; $Ba(Se_2O_5)$, Crystal structure; Crystal chemistry.

Ein Beitrag zur Stereochemie von Erdalkaliseleniten: Synthese und Kristallstruktur von $Ca_2(SeO_3)(Se_2O_5)$, $Ba(SeO_3)$ und $Ba(Se_2O_5)$

Zusammenfassung. Die Verbindungen $Ca_2(SeO_3)(Se_2O_5)$, $Ba(SeO_3)$ und $Ba(Se_2O_5)$ wurden unter niedrig-hydrothermalen Bedingungen aus wäßrigen Lösungen von SeO_2 durch Reaktion mit den jeweiligen Erdalkalikarbonaten erhalten. Die Kristallstrukturen wurden aus Einkristallröntgendaten mittels direkter Methoden bestimmt. $Ca_2(SeO_3)(Se_2O_5)$: Raumgruppe $P\bar{1}$, $Z=2$, $a=5.517(1)$, $b=8.210(2)$, $c=8.716(2)$ Å, $\alpha=92.47(2)$, $\beta=95.92(2)$, $\gamma=97.15(2)°$, $V=389.0(2)$ Å^3, $R_1=0.017$; $Ba(SeO_3)$: Raumgruppe $P2_1/m$, $Z=2$, $a=4.677(2)$, $b=5.645(2)$, $c=6.851(3)$ Å, $\beta=107.16(2)°$, $V=172.8(1)$ Å^3, $R_1=0.022$; $Ba(Se_2O_5)$: Raumgruppe $P2_1/c$, $Z = 4$, $a = 4.553(1)$, $b=11.724(3)$, $c=9.758(2)$ Å, $\beta=92.66(2)°$, $V=520.3(2)$ Å^3, $R_1=0.027$. Alle drei Verbindungen besitzen Gerüststrukturen; im Fall des $Ca_2(SeO_3)(Se_2O_5)$ können Einheiten von kantenverknüpften CaO_n Polyedern hervorgehoben werden, die Schichten parallel zu (010) bilden. $Ba(SeO_3)$ gehört

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dem $KClO_3$-Strukturtyp an. In $Ba(Se_2O_5)$ treten Ketten von flächenverknüpften BaO_9 Polyedern entlang [100] auf. Die Calciumatome sind 7- und 8-koordiniert mit mittleren Ca–O Bindungslängen von 2.42 und 2.48 Å: die beiden Bariumatome weisen neun Sauerstoffliganden mit mittleren Ba–O Bindungslängen von 2.87 Å auf.

Introduction

In selenium oxysalts, the electronic configuration of the Se(IV) ion leads to a trigonal pyramidal coordination to three oxygen ligands. The non-bonding lone-pair electrons *E* of the *s*-orbital, however, complete a rather rigid pseudotetrahedron $([E]SeO_3)^{2-}$ with typical Se–O bond distances and O–Se–O bond angles of 1.70 Å and 100°, respectively. Many synthetic selenite compounds have been reported in the literature; for a detailed survey cf. Ref. [1] and references cited therein. Up to now, 14 selenites are known to occur also as minerals [2]. The crystal structures of some of them have been studied at our laboratory [3–5], and hence the synthesis of selenites, the general principles of their interpolyhedral connections, and the role of the lone-pair electrons became a main field of our interest.

One of the authors (*G. G.*) especially studied Fe(III) selenites in complex systems including also mono- and/or divalent cations [6]. The three earth alkaline compounds presented in the current paper resulted therefrom and encouraged a more detailed investigation of selenites containing exclusively the elements Ca, Sr and Ba. Among them, the crystal structures of $Ca(SeO_3)\cdot H_2O$ [7], $Ca(Se_2O_5)$ [8], $Ca(HSeO_3)_2\cdot H_2O$ and $Ca_2(HSeO_3)_2(Se_2O_5)$ [9], and $Sr(Se_2O_5)$ [10] have been reported up to now. Data on synthesis and solubility, thermal analysis, X-ray powder diffraction, and IR spectroscopy have been given for two modifications of $Ca(SeO_3)$ [11], for $Ca(SeO_3)\cdot H_2O$ [11, 12], $Ca(HSeO_3)_2\cdot H_2O$ [11, 12], $Ca(Se_2O_5)$ and $Ca_2(Se_3O_8)$ [11], and for $Sr(SeO_3)$, $Sr(SeO_3)\cdot H_2O$, $Sr(SeO_3)\cdot 2H_2O$, $Sr(HSeO_3)_2$, $Sr(Se_2O_5)\cdot H_2O$, $Ba(SeO_3)$, $Ba(HSeO_3)_2$, and $Ba(Se_2O_5)$ [12]. From the strongest powder pattern lines, $Ca_2(Se_3O_8)$ [11] is identified to be $Ca_2(SeO_3)(Se_2O_5)$ which is described in the present work.

Results and Discussion

Structure of $Ca_2(SeO_3)(Se_2O_5)$

The complex framework structure of $Ca_2(SeO_3)(Se_2O_5)$ consists of CaO_7 and CaO_8 polyhedra, linked by SeO_3 and Se_2O_5 groups. All atoms occupy general sites. Sheets (Fig. 1a) can be described within (010): the $Ca(1)O_7$ polyhedra share one edge each and *vice versa* with two neighbouring Ca(1) and with three neighbouring Ca(2) polyhedra. Further, each CaO_n group is linked within the sheet to three $Se(1)O_3$ pyramids *via* one common edge and two common corners. This atomic arrangement is also reflected in the morphology of the crystals which form platelets flattened parallel to (010). These sheets are combined to a framework by the diselenite groups as illustrated in Fig. 1b: the diselenite Se(2)O(4,5)-O6-Se(3)O(7,8) is bound *via* the edge O7–O8 and the corner O5 to one sheet and by the corner O4 to the next one. Interstitials are occupied by the lone-pair electrons

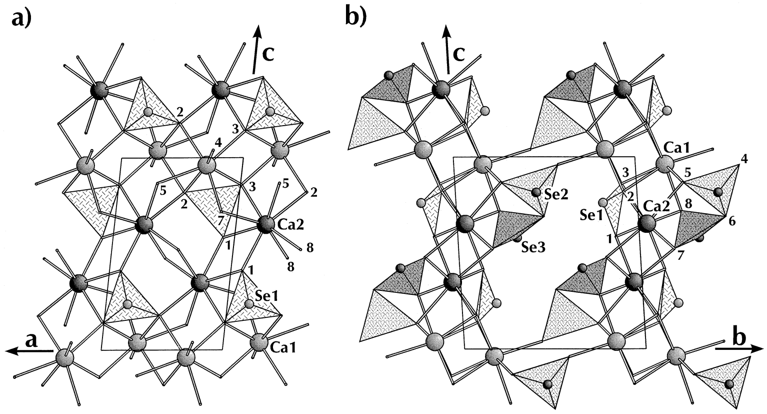

Fig. 1. Crystal structure of $Ca_2(SeO_3)(Se_2O_5)$ in projections parallel to a) [010] and b) [100]; the (Se_2O_5) groups are omitted in Fig. 1a, the oxygen atoms are labelled by number; the drawings have been performed with the program ATOMS [13]

of the selenium atoms. Except O6, bridging Se(2) and Se(3), all oxygen atoms are coordinated to one selenium atom and in addition to one (O4), two (O1, O5, O7, O8), or three (O2, O3) calcium atoms.

Related structures

To the authors' best knowledge, no compounds which are isotypic with $Ca_2(SeO_3)(Se_2O_5)$ have been reported in the literature. A compilation of selected structural details for various calcium selenites is given in Table 1. The geometry of coordination polyhedra of the title compound complies well with these data.

Structure of $Ba(SeO_3)$

The structure of $Ba(SeO_3)$ is built up from BaO_9 polyhedra and trigonal pyramidal SeO_3 groups (both polyhedra have symmetry m) which are combined by common edges and corners to a three-dimensional framework (Fig. 2). The Ba atoms are 7+2 coordinated to oxygen atoms, sharing a common edge each with eight neighbouring BaO_9 polyhedra. The selenite group is linked to six BaO_9 polyhedra *via* three common edges and three corners, respectively. Both oxygen atoms are coordinated to one Se and three Ba atoms in a distorted tetrahedral coordination.

Related structures

$Ba(SeO_3)$ is isotypic with the minerals molybdomenite ($Pb(SeO_3)$, [3, 14]) and scotlandite ($Pb(SO_3)$, [15]) and further with $Ba(TeO_3)$-I [16] and $K(ClO_3)$ [17, 18]. A close relationship exists to the high-temperature form of $La(BO_3)$ [19]. Differences are caused by the specific requirements of the respective polyhedra. Except the planar BO_3 groups in $La(BO_3)$, the anion groups are trigonal pyramids which are completed by the lone-pair electrons to form tetrahedra. The nine-coordinated cations are 7+2 coordinated in $Ba(TeO_3)$-I (with a more pronounced

Table 1. Structural details for Ca-selenites; * bridging oxygen atom, # protonated oxygen atom

	$Ca(SeO_3)\cdot H_2O$	$Ca(HSeO_3)_2\cdot H_2O$	$Ca_2(HSeO_3)_2(Se_2O_5)$	$Ca(Se_2O_5)$	$Ca_2(SeO_3)Se_2O_5$
Space group	$P2_1/c$	$P\bar{1}$	C2/m	Pbca	$P\bar{1}$
Coordination of Ca	7	8	7	7	7, 8
Ca site symm.	1	1	1	1	1
Range Ca-O (Å)	2.327–2.511	2.393–2.615	2.368–2.566	2.341–2.487	2.300–2.550, 2.400–2.604
⟨Ca-O⟩ (Å)	2.424	2.468	2.434	2.431	2.419, 2.479
Ca-Ca linkage	sheet by edges + corners	chain by edges	sheet by edges + corners	sheet by edges	sheet by edges
Se-O (Å)	1.668, 1.704, 1.714	1.653, 1.663, 1.784#	1.671, 1.686, 1.773#	1.663, 1.664, 1.800*	1.682, 1.705, 1.707
		1.668, 1.724, 1.749#	1.636, 1.649, 1.744*	1.642, 1.685, 1.856*	1.633, 1.668, 1.849*
					1.670, 1.671, 1.795*
Se-O-Se(°)			131.3	124.1	127.1
Structure	sheet, conn. by H-bonds	framework	framework	framework	framework
References	[7]	[9]	[9]	[8]	this work

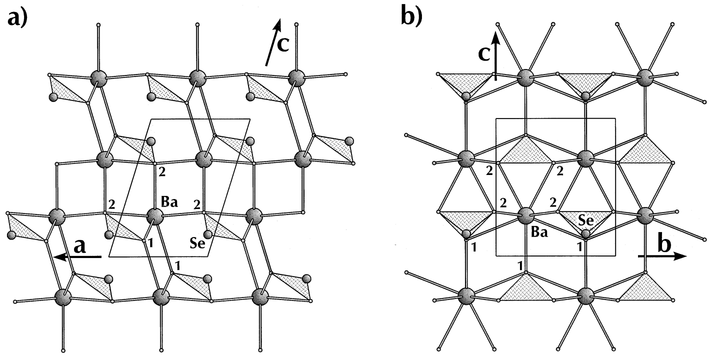

Fig. 2. Crystal structure of $Ba(SeO_3)$ in projections parallel to a) [010] and b) [100]

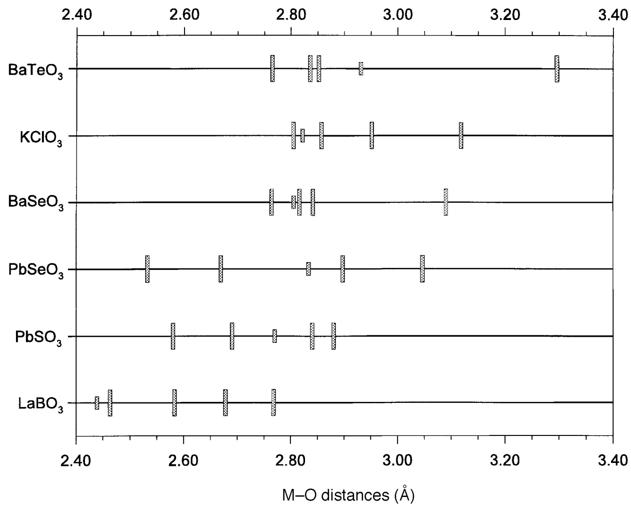

Fig. 3. Individual M–O distances in $Ba(TeO_3)$-I [16], $K(ClO_3)$ [18], $Ba(SeO_3)$, $Pb(SeO_3)$ [14], $Pb(SO_3)$ [15], and $La(BO_3)$ [19] in the order of mean M–O distances for 9-coordination; the larger bars indicate two equivalent values each

separation) and in $K(ClO_3)$, whereas in case of Pb and La the spread of M–O distances is more continuous (Fig. 3).

Structure of $Ba(Se_2O_5)$

The framework structure of $Ba(Se_2O_5)$ is composed by BaO_9 polyhedra and Se_2O_5 groups as illustrated in Figs. 4a,b. The BaO_9 polyhedra share common faces to form infinite chains along [100]; each polyhedron is further linked to two neighbouring chains by a corner and to one close chain by two common edges. The Ba ion bridges to seven diselenite groups *via* seven corners and one common edge. The nine oxygen ligands of Ba are in the range of 2.731–2.946 Å, one further oxygen atom is 3.375 Å apart. Except the bridging O3 atom, all oxygens are coordinated to one selenium atom and to two (O1, O2, O4) or three (O5) barium atoms.

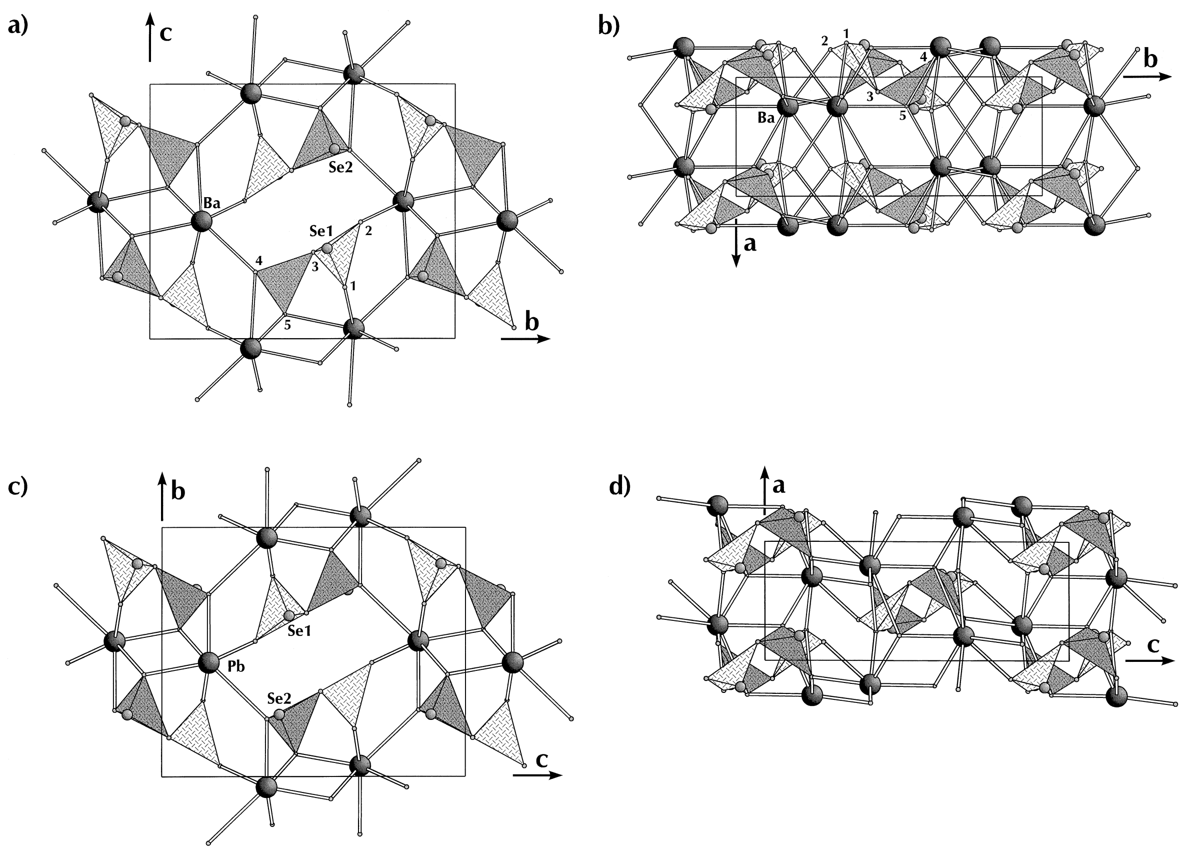

Fig. 4. Comparison of the crystal structures of a,b) $Ba(Se_2O_5)$ and c,d) $Pb(Se_2O_5)$

Related structures

As illustrated in Figs. 4c,d the atomic assemblage of $Pb(Se_2O_5)$ [20], space group $P2_1/n$, $a = 4.515$, $b = 9.503$, $c = 11.618$ Å, $\beta = 90.33°$, is in part related to that of $Ba(Se_2O_5)$. Relevant differences are found in the orientation of the diselenite group; the structures of both compounds are arranged in a different way with respect to the symmetry elements. This might be caused by the lone pair electrons of the Pb^{2+} ion, favouring a more distorted, one-sided coordination polyhedron around Pb: the Pb atom is six-coordinated with Pb–O bonds in the range of 2.48–2.88 Å, further Pb–O distances are 3.10, 3.14, 3.29, and 3.48 Å.

Experimental

Synthesis and characterization

Crystals of $Ca_2(SeO_3)(Se_2O_5)$ were prepared as follows: SeO_2 was added in small portions to a suspension of 0.5 g $CaCO_3$ in 25 ml H_2O until the release of CO_2 was completed. Subsequently, this mixture was enclosed in a Teflon vessel of 50 ml capacity and heated in a steel autoclave for several days at a temperature of 220°C, followed by a 12 h period of cooling to room temperature. A single-phase white reaction product consisting of clear platelets exhibiting the crystallographic forms {100}, {010} and [001} was separated by filtering, washing with diluted acetone, and drying at 50 °C.

Analogous experiments using $SrCO_3$ and $BaSO_3$ as starting reagents, respectively, led to large crystals of $Sr(Se_2O_5)$ [10] and to strongly elongated, commonly intergrown crystals of $Ba(Se_2O_5)$. A TG investigation of 25.8 mg $Ba(Se_2O_5)$ (Mettler M3 microbalance, TA 4000 Thermo Analysis System, nitrogen atmosphere, heating rate $5°C \cdot min^{-1}$, temperature range 30 to 800°C) yielded a weight loss of 29.5%, which is in best agreement with the thermal decomposition [12] to $Ba(SeO_3)$ and $SeO_2\uparrow$. The IR powder spectrum (Perkin-Elmer FTIR spectrometer 1760X, TGS detector, KBr microdisks) of the original substance resembles that reported for of $Ba(Se_2O_5)$ [12]. Samples of $Ba(SeO_3)$ were synthesized from the starting materials $FeC_2O_4 \cdot 2H_2O$, $BaCO_3$, and SeO_2, and treated hydrothermally similar to the procedure described above. The major reaction product was identified as $BaFe_2(SeO_3)_4$ [21], easily distinguishable from the associated colourless crystals of $Ba(SeO_3)$ by its yellow colour.

Table 2. Crystal data and details of the intensity measurements and structure refinements for $Ca_2(SeO_3)(Se_2O_5)$, $Ba(SeO_3)$, and $Ba(Se_2O_5)$

	$Ca_2(SeO_3)(Se_2O_5)$	$Ba(SeO_3)$	$Ba(Se_2O_5)$
Space group	$P\bar{1}$	$P2_1/m$	$P2_1/c$
a (Å)	5.517(1)	4.677(2)	4.553(1)
b (Å)	8.210(2)	5.645(2)	11.724(3)
c (Å)	8.716(2)	6.851(3)	9.758(2)
α (°)	92.47(2)	90	90
β (°)	95.92(2)	107.16(2)	92.66(2)
γ (°)	97.15(2)	90	90
V (°)	389.0(2)	172.8(1)	520.3(2)
Z	2	2	4
Formula weight	445.0	264.3	375.3
$\rho_{calc}(g \cdot cm^{-3})$	3.799	5.079	4.790
$\mu(MoK\alpha)(cm^{-1})$	155	218	216
$2\theta_{max}(°)$	60	80	60
Measured reflections	4395	4294	6087
Unique data set	2244	1156	1519
Data with $F_o > 4\sigma(F_o)$	2037	1015	1343
Variables	119	29	74
Extinction coefficient	0.0106(6)	0.006(1)	0.0027
R_1 (for $F_o > 4\sigma(F_o)$)*	0.017	0.022	0.027
wR_2 (for all F_o^2)*	0.041	0.046	0.066
a, b*	0.02/0	0.02/0	0.034/1.0
$\Delta\rho_{min}$ and $_{max}(e \cdot Å^{-3})$	−0.6/0.8	−1.7/2.2	−0.9/2.4

MoKα-radiation, 2θ-ω-scans; 40/45/40 steps per reflection, increased for α_1-α_2 splitting, 2×5 steps for background correction; 0.03° step width, 0.5–2 sec per seep; three standard reflections every 120 min, lattice parameters refined from 50/46/46 reflections in the 2θ-ranges 25°–37°/29°–39°/28°–40°; $^*R_1 = \Sigma\|F_o| - |F_c\|/\Sigma|F_o$, $wR_2 = (\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^4)^{1/2}$, $w = 1/(\sigma^2(F_o^2) + (a \times P)^2 + b \times P)$, $P = ((\max \text{ of } (0 \text{ or } F_o^2)) + 2F_c^2)/3$

Table 3. Atomic coordinates and displacement parameters U_{eq} with e.s.d. s in parentheses for $Ca_2(SeO_3)(Se_2O_5)$, $Ba(SeO_3)$, and $Ba(Se_2O_5)$; an extended Table with anisotropic displacement parameters can be obtained from the authors upon request

	x	*y*	*z*	U_{eq}
Ca1	0.29175(6)	0.16220(5)	0.96155(4)	0.01013(8)
Ca2	0.24211(6)	0.95587(5)	0.34827(4)	0.01060(8)
Se1	0.17758(3)	0.80866(2)	0.76168(2)	0.00937(6)
Se2	0.22937(3)	0.55578(2)	0.18454(2)	0.01392(6)
Se3	0.27558(3)	0.32582(3)	0.57942(2)	0.01117(6)
O1	0.0909(2)	0.8705(2)	0.58523(16)	0.0145(3)
O2	0.4516(2)	0.92545(18)	0.82102(16)	0.0118(3)
O3	−0.0082(2)	0.91657(19)	0.86009(16)	0.0126(3)
O4	0.2526(3)	0.4280(2)	0.0396(2)	0.0236(3)
O5	0.3174(2)	0.74511(19)	0.13201(17)	0.0149(3)
O6	0.5062(3)	0.5211(2)	0.31114(19)	0.0206(3)
O7	0.1319(2)	0.23660(19)	0.71953(16)	0.0128(3)
O8	0.4504(2)	0.1876(2)	0.52199(17)	0.0142(3)
Ba	0.65676(4)	0.25	0.29275(2)	0.01229(5)
Se	0.06726(6)	0.75	0.16147(4)	0.01141(6)
O1	0.6922(5)	0.75	0.1179(4)	0.0201(4)
O2	0.1762(4)	0.5174(3)	0.3224(2)	0.0165(3)
Ba	0.24479(6)	0.16946(2)	0.46238(3)	0.01299(10)
Se1	0.73077(9)	0.08114(4)	0.14525(5)	0.01219(12)
Se2	0.81676(9)	0.10451(4)	0.75716(5)	0.01242(12)
O1	0.7097(8)	0.1395(3)	0.2990(4)	0.0216(7)
O2	0.7641(8)	0.1914(3)	0.0396(4)	0.0214(7)
O3	0.1142(7)	0.0366(3)	0.1588(4)	0.0191(7)
O4	0.1577(7)	0.1551(3)	0.7591(4)	0.0178(7)
O5	0.7589(8)	0.0586(3)	0.5967(4)	0.0178(7)

X-Ray crystallography and structure determination

Selected single crystals were chosen for X-ray data collection at room temperature on a Stoe AED2 four-circle diffractometer equipped with a graphite monochromator. A summary of crystal data and details of the structure refinements are given in Table 2. The measured intensities were corrected for *Lorentz* and polarization effects and for absorption by evaluation of ψ-scans ($Ba(SeO_3)$ and $Ba(Se_2O_5)$) or by numerical correction ($Ca_2(SeO_3)(Se_2O_5)$). The crystal structures were determined by direct methods [22] and subsequent *Fourier* and difference *Fourier* syntheses. Final structure parameters of the title compounds, obtained by full-matrix least-squares techniques on F^2 [23] are summarized in Table 3, selected interatomic distances and angles in Table 4.

Table 4. Selected interatomic distances (Å) and angles (°) in $Ca_2(SeO_3)(Se_2O_5)$, $Ba(SeO_3)$, and $Ba(Se_2O_5)$

Cal-O4	1×	2.300(2)		**Ba(SeO₃)**	
Ca1-O7	1×	2.337(2)	Ba-O2	2×	2.764(2)
Ca1-O3	1×	2.371(1)	Ba-O1	1×	2.805(3)
Ca1-O5	1×	2.429(1)	Ba-O2	2×	2.816(2)
Ca1-O2	1×	2.436(2)	Ba-O2	2×	2.841(2)
Ca1-O3	1×	2.510(2)	Ba-O1	2×	3.090(1)
Ca1-O2	1×	2.550(2)	⟨Ba-O⟩		2.870
⟨Ca1-O⟩		2.419			
			Se-O1	1×	1.690(3)
Ca2-O8	1×	2.400(2)	Se-O2	2×	1.693(2)
Ca2-O1	1×	2.406(2)	⟨Se-O⟩		1.692
Ca2-O7	1×	2.441(2)			
Ca2-O3	1×	2.465(2)	O1-Se-O2	2×	102.3(1)
Ca2-O8	1×	2.466(2)	O2-Se-O2	1×	101.7(1)
Ca2-O2	1×	2.492(2)	⟨O-Se-O⟩		102.1
Ca2-O1	1×	2.558(2)			
Ca2-O5	1×	2.604(2)			
⟨Ca2-O⟩		2.479		**Ba(Se₂O₅)**	
			Ba-O1	1×	2.731(4)
Sel-O1	1×	1.682(2)	Ba-O5	1×	2.735(4)
Se1-O2	1×	1.705(1)	Ba-O2	1×	2.858(4)
Se1-O3	1×	1.707(1)	Ba-O1	1×	2.870(4)
⟨Se1-O⟩		1.698	Ba-O4	1×	2.872(4)
			Ba-O5	1×	2.927(4)
O1-Se1-O2	1×	105.2(1)	Ba-O5	1×	2.933(4)
O1-Se1-O3	1×	96.9(1)	Ba-O2	1×	2.941(4)
O2-Se1-O3	1×	98.6(1)	Ba-O4	1×	2.946(4)
⟨O-Se1-O⟩		100.2	⟨Ba-O⟩	1×	2.868
Se2-O4	1×	1.633(2)	Se1-O1	1×	1.656(4)
Se2-O5	1×	1.668(2)	Se1-O2	1×	1.665(4)
Se2-O6	1×	1.849(2)	Se1-O3	1×	1.821(3)
⟨Se2-O⟩		1.717	⟨Se1-O⟩		1.714
O4-Se2-O5	1×	107.5(1)	O1-Se1-O2	1×	104.6(2)
O4-Se2-O6	1×	99.1(1)	O1-Se1-O3	1×	98.5(2)
O5-Se2-O6	1×	100.2(1)	O2-Se1-O3	1×	98.8(2)
⟨O-Se2-O⟩		102.3	⟨O-Se1-O⟩		100.6
Se3-O7	1×	1.670(1)	Se2-O4	1×	1.661(3)
Se3-O8	1×	1.671(2)	Se2-O5	1×	1.665(4)
Se3-O6	1×	1.795(2)	Se2-O3	1×	1.867(4)
⟨Se3-O⟩		1.712	⟨Se2-O⟩		1.731
O7-Se3-O8	1×	104.3(1)	O4-Se2-O5	1×	103.5(2)
O7-Se3-O6	1×	101.3(1)	O4-Se2-O3	1×	100.0(2)
O8-Se3-O6	1×	103.1(1)	O5-Se2-O3	1×	98.2(2)
⟨O-Se3-O⟩		102.9	⟨O-Se2-O⟩		100.6
Se3-O6-Se2	1×	127.1(1)	Se1-O3-Se2	1×	115.3(2)

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