

## Telluronevskite, $\text{Bi}_3\text{TeSe}_2$ , a new mineral

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**Abstract:** The new mineral telluronevskite, ideally  $\text{Bi}_3\text{TeSe}_2$ , has been found as irregular grains disseminated in quartzite from the volcanic Vihorlat Mts near Košice in eastern Slovakia, Slovak Republic. The mineral forms massive aggregates up to 2 mm in diameter and/or individual disseminated tabular crystals flattened along (0001). Telluronevskite is megascopically steel grey in colour, with a metallic lustre and black streak. In reflected light, it is white with a yellow tint, very weak pleochroism and moderate anisotropy. Maximum and minimum values of reflectance measured in air for 470, 546, 589 and 650 nm are ( $R_{\text{max}}/R_{\text{min}}$  in %): 48.5/46.6; 51.1/48.5; 51.9/49.5; 52.8/50.5. Vickers micro-hardness ( $\text{VHN}_{10}$  in  $\text{kp.mm}^{-2}$ ) varied in the range 63–137 with mean value of 100. Microprobe analyses yield the empirical formula  $(\text{Bi}_{2.92}\text{Pb}_{0.02})\text{Te}_{1.01}(\text{Se}_{1.73}\text{S}_{0.32})$ . It is trigonal with space group  $P\bar{3}m1$ . The unit-cell dimensions refined from X-ray powder microdiffraction data are  $a = 4.264(6)$  Å and  $c = 23.25(3)$  Å with  $c : a = 5.453 : 1$ . For  $Z = 2$  the calculated density is  $D_x = 8.08(2)$   $\text{g.cm}^{-3}$ ; measured density  $D_m = 8.1(2)$   $\text{g.cm}^{-3}$ . The five strongest lines in the diffraction pattern are ( $d$  (Å),  $hkl$ ): 4.66, 19, 005; 3.12, 100, 104; 2.28, 33, 108; 2.13, 36, 110, 109; 1.355, 18, 1.0.16, 214. Constrained structure refinement from combined powder and precession data revealed ordering of Te and Se atoms within the telluronevskite crystal structure. Telluronevskite belongs to the tsumoite subgroup of the tetradymite group.

**Key-words:** telluronevskite, new mineral, tsumoite subgroup, tetradymite group, crystal structure, bismuth selenide telluride, Vihorlat Mts, Slovakia.

### Introduction

Bismuth selenides-tellurides were discovered during a regional geological prospecting programme in the volcanic Vihorlat Mountains, approximately 8 km SSE of Snina and 20 km of Humenné in the eastern part of Slovakia. Later detailed mineralogical study revealed that one of these phases is a new mineral, telluronevskite. The new mineral and its name have been approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Associ-

ation (CNMMN IMA No. 93-027a). The mineral name reflects its chemical similarity to nevskite with one atom of selenium substituted by tellurium within the formula unit. The type material is deposited at the mineralogical collection of the Museum of Bohemian Paradise in Turnov, Czech Republic, under No. 593/99, and at the mineralogical collections of the Museum of Eastern Slovakia in Košice, Slovak Republic, under No. G 10772.

Telluronevskite, ideally  $\text{Bi}_3\text{TeSe}_2$ , belongs to the tsumoite subgroup of the tetradymite group as

defined by Bayliss (1991). Other Bi-members of this subgroup are tsumoite (Shimazaki & Ozawa, 1978), nevskite (Nechelyustov *et al.*, 1984) and sulphotsumoite (Zavalyov & Begizov, 1982). Bayliss (1991) also lists ingodite (Zavalyov & Begizov, 1981) as a member of this subgroup though it very probably does not belong there and forms an individual subgroup. Ideal chemistry of all these minerals is shown in Fig. 1.

### Geological setting

The Vihorlatské vrchy Mts, which are composed of the Humenské vrchy Mts, the Vihorlat Mts and the Popriečny Mts subunits, have a complex geological structure, consisting of Mesozoic rocks of the Humenské vrchy Mts subunit and the Klippen Belt unit, Paleogene sequences of the Magura unit, the Klippen Belt and the Inner Carpathian unit, molasse sediments and volcanics of Neogene age, and Quaternary sediments (Kaličiak *et al.*, 1995; Žec, 1997). Neogene calc-alkaline volcanics (Lexa *et al.*, 1993) cover an essential part of the region and are of two distinct types (Mahel', 1978; Slávik *et al.*, 1986). The first is a broadly scattered type of rhyodacite and dacite volcanism. The second type corresponds to a basaltic-andesitic volcanism of volcanic-arc type, characterized by a large number of stratovolcanoes, related to two major fault systems. The volcanic Vihorlat Mts are situated over the intersection of NE-SW running faults of the Vrbica fault system and the Pieniny Klippen Belt (Fusán *et al.*, 1971, 1979; Burian *et al.*, 1985). The volcanic activity was affected by the Alpine tectonics. A total of five volcanic stages are recognized in the area (Orlický *et al.*, 1970) ranging from Upper Badenian to Pannonian age.

Metallogenetic processes operated in the volcanic zone near the Morské oko Lake, Porubský potok Creek and Sokolský potok Creek valleys. The intrusive complex, consisting of hydrothermally altered rocks, comprises a surface area of 3.5 km<sup>2</sup>. The area shows significant geochemical anomalies of Mo, Sn and Bi related to an intrusive body of diorite porphyrite, carbonatic rocks and secondary quartzite. A strong wallrock alteration hosts the geochemical anomalies of Pb, Zn, Cu, Hg and Ag (Bacsó & Ďud'a, 1988). The polymetallic mineralization discovered in borehole VH-4 near the Čremošná Creek consists of pyrite, pyrrothite, sphalerite, chalcopyrite and stannite (Bacsó, 1979). The entire mineralization occurs in an area

composed of alumo-metasomatites of hydrothermal origin with corundum, andalusite, topaz, tourmaline, sericite and micas. No exploitable deposits of ores occur in the region of the Vihorlat Mts.

The mineralization of Bi-selenides and tellurides, located in the central part of the Vihorlat Mountains (48°58'69" N, 22°08'28" E) bound to bodies of secondary quartzites, was found in the central area of the Central Volcanic Vihorlat Zone near Morské oko Lake, Porubský and Sokolský potok Valleys.

### Occurrence and paragenesis

The mineral studied was originally described as tetradymite and wehrlite (Sopková, 1977) and was taken from the body of secondary quartzite, which covered an area of 120 × 160 m about 1.5 km E-SE of the secondary quartzites of the Porubský potok Creek located about 2 km southwestwards Morské oko Lake. This is not far from Remetský Hámer, which is about 11 km north of Sobrance near Michalovce. The grains and/or aggregates of telluronevskite are found in opal-quartz veinlets or they are disseminated directly in quartzite. Telluronevskite occurs either in massive aggregates of platy lamellar crystals from 0.05 mm up to 1 mm across in size, which are flattened along (0001), or individual disseminated platy grains up to 1.5 or 2 mm in diameter, resembling tetradymite or tellurobismuthite.

The bodies of secondary quartzites are found at the contact between the superposed lava flows and underlying pyroclastic rocks in the central part of the Vihorlat Mts between the Morské oko Lake and Skalný potok Creek (Bacsó, 1971). The origin of the secondary quartzites relates either to the contact effect of a magmatic body, which had intruded the andesites and andesite tuffs in depth, or with a hydrothermal alteration of the primary rocks (Derco *et al.*, 1977). The secondary quartzites were formed together with epigenetic mineralization during the Upper Sarmatian (Bacsó, 1979).

The largest body of the secondary quartzites constitutes a 100-200 m thick semi-circular zone with an area of 350 × 200 m (Bacsó, 1979; Derco *et al.*, 1977), which is located at the contact of diorite porphyrite and quartz diorite dikes and stocks, piercing a dome-shaped body consisting of pyroxene andesite north of Kapka Valley. Smaller outcrops of the secondary quartzites are known in the vicinity of Morské oko Lake and in the valleys of Skalný, Porubský and Čremošná creeks. The various types of secondary

quartzites (Bacsó, 1971; Derco *et al.*, 1977) typically have high fluorine content (1-19 wt%). They consist of the following three rock types:

- I. Compact green-grey rocks consisting of ammonium hydromica, boehmite, diaspore, topaz, andalusite, mullite and corundum (Kováč *et al.*, 1977);
- II. Massive grey-pink to brown-red rocks containing predominantly topaz, andalusite, biotite, kaolinite and fluorite;
- III. Compact grey to greenish, partly kaolinized rocks with quartz, topaz and kaolinite (Derco *et al.*, 1977).

Mineral assemblages in the secondary quartzites show a zonal structure. The central parts of the bodies are enriched with corundum. Andalusite with topaz or tourmaline was found in argillitized quartzites in two surrounding zones, the latter one passing into propylitized andesites with pyrrhotite impregnations which rims the bodies (Bacsó, 1971; Slavkay, 1975).

Table 1. Chemical analyses of telluronevskite, their arithmetic mean (in wt%) and empirical formula based on 6 atoms per formula unit.

Chemical analyses				
No.	1	2	3	4
Bi	68.75	68.94	68.95	68.73
Pb	0.59	0.20	0.29	0.58
Se	15.49	15.23	15.37	15.54
Te	14.64	14.92	14.66	14.11
S	1.01	1.05	1.25	1.26
Total	100.48	100.34	100.52	100.22
wt%				
	Mean	e.s.d.	Min	Max
Bi	68.84	0.06	68.73	68.95
Pb	0.42	0.10	0.20	0.59
Se	15.41	0.07	15.23	15.54
Te	14.58	0.17	14.11	14.92
S	1.14	0.07	1.01	1.26
Total	100.39			
Empirical formula				
	Mean	e.s.d.		
Bi	2.92	0.01		
Pb	0.02	0.00		
Se	1.73	0.01		
Te	1.01	0.01		
S	0.32	0.02		

JEOL JXA-50A electron microprobe; standards: metallic Bi, PbSe, PbTe, ZnS, PbS and tetradymite; X-ray lines used for quantifying: BiM, PbM, SeL, TeL, SK

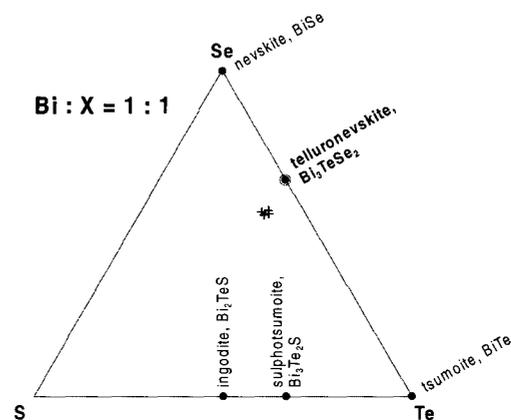


Fig. 1. Ternary diagram Se-Te-S showing the end-member composition of members of the tsumoite subgroup of the tetradymite group as defined by Bayliss (1991). The ideal composition of telluronevskite is indicated by a circled dot; crosses represent the measured composition of natural telluronevskite.

## Chemical composition

Several grains of telluronevskite were analysed using a JEOL JXA-50A wavelength-dispersive electron microprobe. The operating conditions were 20 kV and 25 nA. The following X-ray lines were used: AgL $\alpha$ , AsL $\alpha$ , CuK $\alpha$ , BiM $\alpha$ , PbM $\alpha$ , SeL $\alpha$ , TeL $\alpha$ , SK $\alpha$  and ZnK $\alpha$ . Pure metallic Ag and Bi, synthetic PbSe and PbTe (for Se and Te), ZnS (for S) and PbS (for Pb) as well as the mineral tetradymite (for Te) were utilized as the microprobe standards. No elements other than Bi, Pb, Se, Te and S were detected. The analytical corrections of ZAF type applied were those provided by the microprobe manufacturer.

Four typical analyses of telluronevskite selected from a total of 15, their mean, and the corresponding empirical formula calculated on the basis of 6 atoms per formula unit are summarized in Table 1. The mineral seems to be homogeneous, with little intra- and inter-grain compositional variation. Sulphur and lead represent only minor substituents and, if they are neglected, the ideal chemical formula of telluronevskite is Bi<sub>3</sub>TeSe<sub>2</sub>. Real composition, however, indicates minor Bi  $\leftrightarrow$  Te substitution and a more pronounced Se  $\leftrightarrow$  S one resulting in the simplified formula (Bi,Te)<sub>3</sub>Te(Se,S)<sub>2</sub>. The assignment of tellurium to a special position has been confirmed by crystal structure refinement – see below.

Table 2. Reflectance data of telluronevskite.

$\lambda$ [nm]	$R_{\max}$ [%]	$R_{\min}$ [%]
420	45.5	42.5
440	46.7	44.7
460	47.8	45.9
470	COM	46.6
480	49.2	46.9
500	50.4	48.1
520	50.5	48.5
540	51.0	48.4
546	COM	48.5
560	51.6	49.4
580	51.8	49.4
589	COM	49.5
600	52.0	49.7
620	52.6	50.2
640	52.7	50.4
650	COM	50.5
660	52.9	50.5
680	53.1	50.6
700	53.2	50.8

Measurement conditions: plane polarized light, normal incidence, monochromator, photomultiplier with the cathode S<sub>20</sub>, standard SiC, objective 16, half field prism illuminator, obliquity corrected through  $(R_{\perp} + R_{\parallel}) / 2$

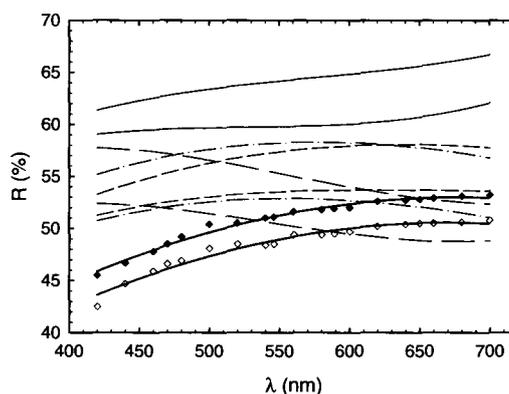


Fig. 2. Reflectance data for telluronevskite measured in air. Filled diamonds correspond to  $R_{\max}$  whereas open ones represent  $R_{\min}$  values. The reflectance curves of telluronevskite are compared to other members of the tsumoite subgroup and ingodite. The line styles used: heavy solid line = telluronevskite; solid line = tsumoite; long-dashed line = nevskite; short-dashed line = sulphotsumoite; dash-dotted line = ingodite.

Table 3. Comparison of individual Bi-members of the tsumoite subgroup of the tetradymite group.

Mineral name	telluronevskite	tsumoite	sulphotsumoite	nevskite	ingodite
Formula	Bi <sub>3</sub> TeSe <sub>2</sub>	BiTe <sup>(a)</sup> Bi <sub>2</sub> Te <sub>2</sub> <sup>(b)</sup>	Bi(Te,S) <sup>(a)</sup> Bi <sub>3</sub> Te <sub>2</sub> S <sup>(b)</sup>	BiSe <sup>(a)</sup> Bi <sub>2</sub> (Se,S) <sub>2</sub> <sup>(b)</sup>	Bi(S,Te) <sup>(a)</sup> Bi <sub>2</sub> TeS <sup>(b)</sup>
Crystal system			Trigonal		
Space group			<i>P3m1</i>		
Unit cell		(c)	(c)	(c)	(g)
<i>a</i> (Å)	4.264	4.422	4.316	4.197	4.247
<i>c</i> (Å)	23.25	24.05	23.43	22.8	69.9
Powder data		(d)	(e)	(f)	(g)
	<i>d</i> <i>I</i>	<i>d</i> <i>I</i>	<i>d</i> <i>I</i>	<i>d</i> <i>I</i>	<i>d</i> <i>I</i>
	4.66    19	4.81    6	4.67    30	22.8    16	4.66    30
	3.32    13		3.69    20	4.56    12	3.66    20
	3.12    100	3.23    100	3.16    100	3.58    16	3.11    100
			2.70    20	3.06    100	
	2.28    33	2.37    35	2.32    60	2.24    35	2.28    60
	2.13    36	2.31    31	2.16    50	2.09    30	2.12    50
	1.94    16	2.00    8	1.96    50	1.90    12	1.94    40
$F_N$	$F_{28}=2(0.164,83)$	$F_{26}=2(0.093,154)^{(h)}$	$F_{30}=2(0.149,104)^{(i)}$	$F_{23}=1(0.165,116)^{(j)}$	$F_{27}=2(0.111,83)^{(k)}$
$D_x$	8.08	8.23 <sup>(c)</sup>	8.13 <sup>(c)</sup>	7.85 <sup>(c)</sup>	7.88 <sup>(c)</sup>
$D_m$	8.10	8.16 <sup>(c)</sup>	n.d. <sup>(c)</sup>	n.d. <sup>(c)</sup>	n.d. <sup>(c)</sup>
VHN	63 – 137	51 – 90 <sup>(c)</sup>	63.9 – 66.2 <sup>(c)</sup>	60 – 114 <sup>(c)</sup>	60.9 – 64.6 <sup>(c)</sup>

(a) Bayliss, 1991; (b) Chvileva *et al.*, 1988; (c) Anthony *et al.*, 1990; (d) JCPDS 31-200; (e) Zavyalov & Begizov, 1982; (f) JCPDS 29-249; (g) Zavyalov & Begizov, 1981; (h) JCPDS 31-201; (i) JCPDS 38-442; (j) JCPDS 37-442; (k) JCPDS 41-1408.

Fig. 1 displays the Bi end-members of the tsumoite subgroup of the tetradymite group as defined by Bayliss (1991) – *i.e.* including ingodite – plotted on the ternary diagram using atomic percentages of selenium, tellurium and sulphur. The ideal and measured composition of telluronevskite are shown, with up to 11 at.% sulphur substitution in this mineral compared to the ideal formula.

### Physical and optical properties

Aggregates of telluronevskite are megascopically steel grey with a metallic lustre and black streak. When altered, telluronevskite becomes greyish black with dull lustre and a reddish brown rimming of grains. Telluronevskite has a variable habit ranging from irregular grains to poorly shaped laths or prisms. Quite often, the grains occur as polycrystals, each characterized by a number of small crystal domains. Crystals flattened along (0001) exhibit perfect cleavage parallel to (0001) and are usually strongly deformed and display deformation lamellae. Thin platy crystals of telluronevskite are also flexible.

In polished section, telluronevskite grains vary from lath-shaped to nearly equant to irregular. Many grains range from 0.1 mm to 1 mm in size. The colour is white with a yellow tint; birefractance is weak, noticeable in oil (yellowish white to grey), but not perceptible in air. The anisotropy is moderate without any strong chromatic effects. The polarization colours vary from grey to bluish grey. No internal reflections were observed. Reflectance data were measured in air and are listed in Table 2 and plotted in Fig. 2.

Vickers microhardness VHN (30 indentations, 10 g load) is 100 kp.mm<sup>-2</sup> (a range 62.9–137.0 kp.mm<sup>-2</sup>). A microhardness anisotropy was observed. Sections approximately perpendicular to [0001] have VHN<sub>10</sub> = 62.9 kp.mm<sup>-2</sup> whereas sections approximately parallel to [0001] VHN<sub>10</sub> = 137.0 kp.mm<sup>-2</sup>. Table 3 shows that telluronevskite is harder than tsumoite, sulphotsumoite and ingodite while its microhardness is very close to that of nevskite.

The average of five density measurements in a pycnometer is 8.1 (2) g.cm<sup>-3</sup>.

### X-ray diffraction and crystal structure

The powder X-ray microdiffraction study was carried out using a 76.4 mm diameter Debye-Scherrer camera with Bradley-Jay arrangement. CuK Ni-fil-

tered radiation was employed for powder diffraction study. Intensities were calculated as the arithmetic mean of three measurements by an analogue optical two-beam photo-densitometer. Powder data are listed in Table 4. The figures-of-merit were calculated for the above-mentioned powder pattern and their values are  $M_{20} = 3.09$  (de Wolff, 1968) and  $F_{28} = 2$  (0.164, 83) (Smith & Snyder, 1979). These low values of figures-of-merit are

Table 4. Powder X-ray diffraction data for telluronevskite.

$l_{obs}$	$d_{obs}$	$d_{calc}$	$h$	$k$	$l$
19	4.66	4.65	0	0	5
9	3.65	3.65	1	0	1
13	3.32	{ 3.33 3.32	1 0	0	3 7
100	3.12	3.12	1	0	4
6	2.68	2.67	1	0	6
33	2.28	2.28	1	0	8
36	2.13	{ 2.13 2.12	1 1	1 0	0 9
16	1.935	{ 1.938 1.938	1 0	1 0	5 12
8	1.843	{ 1.841 1.836	2 1	0 0	1 11
7	1.797	{ 1.797 1.795	2 1	0 1	3 7
9	1.758	1.760	2	0	4
2	1.669	1.661	0	0	14
2	1.613	1.610	1	0	13
12	1.559	{ 1.559 1.550	2 0	0 0	8 15
10	1.434	{ 1.446 1.434 1.429	2 1 1	0 1 0	10 12 15
18	1.355	{ 1.358 1.353	2 1	1 0	4 16
7	1.307	{ 1.314 1.310	1 1	2 1	6 14
7	1.261	{ 1.258 1.254	1 1	2 1	8 15
11	1.231	{ 1.231 1.229	3 2	0 1	0 9
2	1.215	{ 1.224 1.219	0 1	0 0	19 18

76.4 mm diameter Debye-Scherrer camera with Bradley-Jay film arrangement, Ni-filtered CuK radiation.

Table 5. Unit-cell dimensions for telluronevskite.

Parameter		Value
	Powder data	
$a$ [Å]		4.264(6)
$c$ [Å]		23.25(3)
$V$ [Å <sup>3</sup> ]		366(1)
	Precession data	
$a$ [Å]		4.28(1)
$c$ [Å]		23.26(8)
$V$ [Å <sup>3</sup> ]		369(3)
	Cone-axis photograph	
$a$ [Å]		4.25(8)
$c$ [Å]		23.4(1)
$V$ [Å <sup>3</sup> ]		366(2)

common for all natural phases within the tsumoite subgroup (Table 3). There are generally two reasons for such low values. One is the use of non-focusing diffraction techniques with lower resolution for the description of all these minerals. The other is the crystal structure of these phases, which leads to strong substructure reflections and rather weak superstructure ones. The latter are not usually recorded in powder data, which consequently lowers the figures-of-merit.

Thin platelets of mineral were picked from an aggregate of tabular crystals in quartzite rock to be as smooth as possible to produce sharp, undeformed reflections. However, even very small grains that seemed to fulfil these requirements under a binocular lens with magnification of 20 to 40 times gave either multiple sets of reflections corresponding to misoriented domains, or streaked reflections showing mechanical effects like crystal bending. Eventually, several platy crystals roughly  $0.4 \times 0.3$  mm in cross-section and up to several tens of micrometres in thickness were selected to carry out a single-crystal study of telluronevskite. A precession camera was used employing mostly MoK Zr-filtered radiation. The precession angle  $\mu$  was set to  $10^\circ$  for orientational photographs and to  $28^\circ$  for zero-level photographs of adjusted reciprocal lattices. To check the correctness of unit-cell dimensions, cone-axis photographs were also taken using Zr-filtered Mo-radiation.

Oriental photographs taken along  $c$  with unfiltered radiation and without layer-line screen showed trigonal symmetry due to superimposed spots and white-radiation streaks from upper levels although the plane symmetry of the  $hk0$  reciprocal plane is  $p6mm$ . This trigonal symmetry was veri-

fied by cone-axis photograph as well. Plane symmetries of the  $h0l$  and  $hhl$  reciprocal planes are  $p2$  and  $p2mm$ , respectively, and plane symmetry of cone-axis  $c$  photograph is  $p3m1$ , revealing Laue group symmetry  $\bar{3}m$ . No systematic absences were observed. The corresponding space groups are  $P\bar{3}m1$ ,  $P3m1$ ,  $P321$ . By analogy to other extensively studied members of the tsumoite subgroup of tetradymite group and their synthetic analogues, the space group of telluronevskite is  $P\bar{3}m1$ .

Unit-cell parameters from powder data in Table 5 were refined using the program of Burnham (1962) with a correction term for sample displacement. Unit-cell dimensions from precession data were measured on uncalibrated reciprocal photographs taken with MoK $\alpha$  radiation. The size of parameter  $a$  was determined from photographs of  $h0l$  and  $hk0$  reciprocal lattices. For the parameter  $c$  both  $h0l$  and  $hhl$  photographs were examined. The procedure of Rieder (1973) was used to evaluate individual measurements. Final parameters were computed as grand means of extrapolated values, arithmetic means and weighed means given by the program by Rieder (1973). Photograph taken along  $c$  using cone-axis technique provided additional information on the direct lattice translation along  $c$  from -1, +1, +2, +3 and +4 levels. The parameter  $c$  calculated from cone-axis photograph was extrapolated employing the procedure of Quarashi & Barnes (1953). Unit-cell dimensions of telluronevskite are listed in Table 5. Calculated density for  $Z = 2$  is  $D_x = 8.08$  (2) g.cm<sup>-3</sup> which is in fair agreement with the measured value.

Crystal structure refinement was performed on a combined intensity data set comprising inte-

Table 6. Atomic and displacement parameters in the crystal structure of telluronevskite. Standard deviations are given in parentheses.

Site	Atom	SOF	$x$	$y$	$z$	$B_{iso}$ (Å <sup>2</sup> )
Bi1	Bi	0.98(6)	0	0	0.1265(7)	0.54(9)
	Te	0.02				
Bi2	Bi	0.98(6)	1/3	2/3	0.2942(6)	0.54(9)
	Te	0.02				
Bi3	Bi	0.98(6)	2/3	1/3	0.4589(7)	0.54(9)
	Te	0.02				
Te1	Te	0.95(10)	1/3	2/3	0.0566(8)	1.38(10)
	Se	0.05				
Se1	Se	0.84(9)	2/3	1/3	0.2157(8)	1.38(10)
	S	0.16				
Se2	Se	0.84(9)	0	0	0.3686(7)	1.38(10)
	S	0.16				

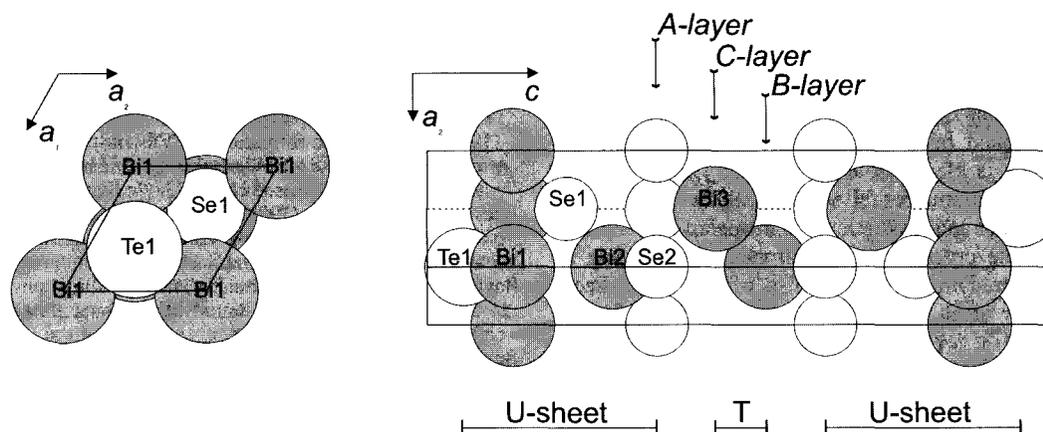


Fig. 3. Crystal structure of telluronevskite. Projections onto the  $a_1$ - $a_2$  and  $a_2$ - $c$  planes.

Table 7. Interatomic distances in the telluronevskite crystal structure.

	$d$ (Å)	$\sigma$
$d(\text{Te1}-\text{Te1})$	3.604	0.020
$d(\text{Bi1}-\text{Te1})$	2.950	0.014
$d(\text{Bi1}-\text{Se1})$	3.219	0.016
$d(\text{Bi2}-\text{Se1})$	3.065	0.014
$d(\text{Bi2}-\text{Se2})$	3.009	0.013
$d(\text{Bi3}-\text{Se2})$	3.236	0.015
$d(\text{Bi3}-\text{Bi3})$	3.117	0.014

grated intensities from the powder diffractogram and data from the precession films. The refinement was carried out using the program FullProf.98 (Rodríguez-Carvajal, 1998). The refinement was soft-constrained based on the knowledge of interatomic distances found in  $\text{Bi}_2\text{Se}_2$  (Stasova, 1967),  $\text{Bi}_{1.007}\text{Se}_{0.993}$  (Gaudin *et al.*, 1995),  $\text{BiTe}$  (Yamana *et al.*, 1979) and tsumoite (Shimazaki & Ozawa, 1978). Isotropic displacement parameters were not refined for all sites separately but instead for sites of the Bi and (Se,Te) type only. Site occupancies were constrained based on the chemical formula  $\text{Bi}_{2.94}\text{Te}_{1.01}\text{Se}_{1.73}\text{S}_{0.32}$ . Structure refinement eventually converged to  $RF^2 = 15.4\%$  and  $wRF^2 = 17.2\%$ . These excessively high agreement factors are mainly because we were not able to employ an absorption correction for combined powder and precession data. Resulting atomic and isotropic displacement parameters are summarized in Table 6. The crystal structure is presented in projections down  $c$  and perpendicular to the  $a_2$ - $c$  plane in Fig. 3. Selected interatomic distances are listed in Table 7.

## Discussion

Telluronevskite is a member of the tsumoite subgroup of the tetradymite group as defined by Bayliss (1991). The Bi-members of the tsumoite subgroup are characterized by space group  $P\bar{3}m1$ , unit-cell dimensions  $a \sim 4.2 - 4.4$  Å and  $c \sim 22.8 - 24.1$  Å and formula  $\text{Bi}(\text{Te},\text{Se},\text{S})$  with  $Z = 6$ . Telluronevskite is compared to other Bi-minerals within the tsumoite subgroup in Fig. 2 and Table 3.

Fig. 2 compares the reflectance data of telluronevskite with other Bi-members of the tsumoite subgroup and ingodite. Apparently, telluronevskite reflectance curves resemble those for tsumoite, sulphotsumoite and ingodite, whereas curves for nevskite have just opposite slope. Reflectance values of telluronevskite lie below those for other minerals within the tsumoite subgroup as well as ingodite except nevskite; nevskite reflectance is higher than that for telluronevskite in low wavelengths, in higher wavelengths, however, reflectance curves for telluronevskite and nevskite (Nechelyustov *et al.*, 1984) intersect each other. The negative slope for reflectance curves of nevskite seems to be a common feature for all Se-rich members of the tetradymite group – *cf.* Fig. 39 and 121 in Chvileva *et al.* (1988). Similarly, the reflectance seems to depend on tellurium content among Te-rich minerals of the tsumoite group – the higher the Te content, the higher the reflectance (again *cf.* Fig. 39 in Chvileva *et al.*, 1988).

The size of unit-cell parameters for Bi-members of the tsumoite subgroup appears also to be a function of tellurium content. The higher the content of tellurium, the larger the unit-cell dimensions

(Table 3). Data for telluronevskite are relatively well consistent with observed chemical composition. They are only slightly off the tie-line between BiSe and BiTe end members but this fact can be explained by the observed Se ↔ S substitution – this is clearly true for data of sulphotsumoite whose parameters fall significantly below those for tsumoite and synthetic BiTe, respectively.

The crystal structure of phases belonging to the tetradymite group consists of individual sheets which are  $A$  ( $0; 0; z_A$ ),  $B$  ( $1/3; 2/3; z_B$ ), and  $C$  ( $2/3; 1/3; z_C$ ) (Abrikosov & Stasova, 1985; Stasova, 1967). Particular sheets are arranged to form two-sheet layers Bi-Bi ( $T$ ) and five-sheet layers X-Bi-X-Bi-X ( $U$ ) where X stands for chalcogenide (Te, Se, S) atom or atoms. The overall sheet stacking sequence observed in tsumoite-like phases is  $ACB$  and the structure is built up by the layer sequence ... $UTU$ ... (Abrikosov & Stasova, 1985; Stasova, 1967; Stasova & Karpinskii, 1967). The total number of sheets in the unit cell is thus  $N = 12$ . On the contrary, ingodite is characterized by the number of structural sheets  $N = 36$ . Bayliss (1991) retained parameter  $c$  quoted by abstractors in *Amer. Mineral.* 1982, Vol. 67, p. 855. However, Zavyalov & Begizov (1981) in their original description of ingodite pointed out that there are several superstructure reflections, which cannot be indexed satisfactorily using  $c = 23.2$  Å; they instead proposed a cell with  $c = 69.6$  Å and calculated  $Z = 9$  correspondingly ( $Z$  is then correctly cited in the abstract but it does not correspond to the cell with  $c = 23.3$  Å). Obviously, ingodite does not belong to the tsumoite subgroup of the tetradymite group but it forms an individual subgroup, which is characterized by the number of structural sheets  $N = 36$  per unit cell.

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