Original paper Stibioústalečite, Cu₆Cu₆(Sb₂Te₂)Se₁₃, the first Te–Se member of tetrahedrite group, from the Ústaleč, Czech Republic

Jiří SEJKORA¹*, Jakub PLÁŠIL², Emil MAKOVICKY³

¹ Department of Mineralogy and Petrology, National Museum, Cirkusová 1740, 193 00 Praha 9 - Horní Počernice, Czech Republic; jiri.sejkora@nm.cz

² Institute of Physics of the CAS, v.v.i., Na Slovance 2, 182 21 Praha 8, Czech Republic

³ Institute for Geoscience and Natural Resources Management, University of Copenhagen, Østervolgade 10, DK-1350,

Copenhagen K, Denmark

* Corresponding author



Stibioústalečite, $Cu_{12}(Sb_2Te_2)Se_{13}$, was approved as a new mineral species from the Ústaleč mine, 15 km west of Horažďovice, SW Bohemia, Czech Republic. It occurs as metallic anhedral grains up to 0.1–0.3 mm in size, dark grey in color, in a calcite gangue. It is directly associated with hakite-(Hg), berzelianite, the not-yet approved phase $Cu_{12}(As_2Te_2)$ Se₁₃ and uraninite. Stibioústalečite is brittle, with an indistinct cleavage and a conchoidal fracture; the calculated density is 5.676 g/cm³. In reflected light, stibioústalečite is isotropic, and grey in color; internal reflections were not observed. Reflectance data for the four COM wavelengths in air are [λ (nm): R (%)]: 470: 33.3; 546: 33.2; 589: 33.1; 650: 33.0. Electron microprobe analysis for holotype material (grain used for single-crystal X-ray study) gave (in wt. % – average of 7 spot analyses): Cu 34.10, Ag 1.22, Fe 0.04, Zn 0.09, Hg 0.33, Sb 9.39, As 0.70, Te 12.41, S 3.76, Se 37.59, total 99.63. On the basis of (As+Sb+Te)=4 atoms per formula unit (*apfu*), the empirical formula of stibioústalečite is ${}^{M(2)}(Cu_{5.75}Ag_{0.25})_{25}{}^{M(1)}(Cu_{5.93}Hg_{0.04}Zn_{0.03}Fe_{0.02})_{26.02}{}^{X(3)}(Te_{2.12}Sb_{1.68}As_{0.20})_{24}(Se_{10.36}S_{2.55})_{212.91}$. The ideal formula is $Cu_6Cu_6(Sb_2Te_2)$ Se₁₃, which requires Cu 33.33, Sb 10.64 Te 11.16 Se 44.87, total 100 wt. %. Stibioústalečite is cubic, *I*43*m*, with unit-cell parameters *a* = 10.828(4) Å, *V* = 1269.6(9) Å³, *Z* = 2. The crystal structure of stibioústalečite was studied by single-crystal X-ray diffraction data and it is isotypic with other members of the tetrahedrite group. The mineral is named after its type locality Ústaleč and its chemical composition, being the (Sb/Te) end-member in the possible ústalečite series.

Keywords: stibioústalečite, new mineral, tetrahedrite group, chemical composition, Ústaleč, Czech Republic Received: 15 February 2022; accepted: 20 September 2022; handling editor: F. Laufek

1. Introduction

Tetrahedrite group minerals are the most common sulfosalts in different kinds of hydrothermal ore deposits. They form a complex isotypic series, with formula ${}^{M(2)}A_{6}{}^{M(1)}(B_{4}C_{2})_{\Sigma 6}{}^{X(3)}D_{4}{}^{S(1)}Y_{12}{}^{S(2)}Z$, characterized by homoand heterovalent substitutions, representing an interesting link between mineralogy and ore geochemistry (Biagioni et al. 2020a). The classification and nomenclature of the tetrahedrite group minerals, in keeping with the current IMA-accepted rules, was recently published by Biagioni et al. (2020a). The general structural formula of minerals belonging to this group can be written as ${}^{M(2)}A_6{}^{M(1)}(B_4C_2)_{\Sigma 6}$ $X^{(3)}D_4^{S(1)}Y_{12}^{S(2)}Z$, where $A = Cu^+$, Ag^+ , \Box (vacancy), and $(Ag_{e})^{4+}$ cluster; B = Cu⁺, and Ag⁺; C = Zn²⁺, Fe²⁺, Hg²⁺, Cd^{2+} , Ni^{2+} , Mn^{2+} , Cu^{2+} , Cu^{+} , and Fe^{3+} ; $D = Sb^{3+}$, As^{3+} , Bi³⁺, and Te⁴⁺; Y = S²⁻, and Se²⁻; and Z = S²⁻, Se²⁻, and \Box (Biagioni et al. 2020a).

This compositional diversity is reflected in the relatively large number of mineral species belonging to this group that has been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA-CNMNC). In addition to the eleven mineral species redefined in Biagioni et al. (2020a), thirteen new mineral species have been described in two years, emphasizing the chemical variability of this isotypic group.

The Te-rich members of tetrahedrite group have been known for a long time. The first descriptions of goldfieldite were given by Sharwood (1907) and Ransome (1909), Thompson (1946) proved it to show isotypic relations with tetrahedrite. Kato and Sakurai (1970) and Kalbskopf (1974) found that Te does not substitute for S but behaves similarly as Sb and As in the crystal structure of tetrahedrite or tennantite. Several authors have debated the actual definition of goldfieldite (e.g., Trudu and Knittel 1998) and it was finally solved in the nomenclature of the tetrahedrite group by Biagioni et al. (2020a). Increased Se-contents in Te-rich members have so far been known only in samples from the epithermal Au deposits at Kamchatka, Russia (Spiridonov and Okrugin 1985; Pohl et al. 1996; Spiridonov et al. 2014), and from the Wild Dog epithermal Au system on Bougainville Island, Papua New Guinea (Noviello 1989), and they do not exceed 3.0 apfu Se.



Fig. 1 Stibioústalečite (U) as anhedral grains up to 0.3 mm in length in calcite gangue in association with hakite-(Hg) (H) and berzelianite (B); \mathbf{a} – reflected light microscopy (partly crossed polars); \mathbf{b} – BSE photo.

Actually, new chemical data available for samples from locality Ústaleč (western Bohemia, Czech Republic) show Se-dominant composition with (As+Sb)/Te atomic ratios close to 1, with Sb>As, i.e., close to the end-member formula Cu₁₂(Sb₂Te₂)Se₁₃. It allowed the submission of a proposal to the IMA-CNMNC to give a definition of the Se-analogue of stibiogoldfieldite. The mineral and its name have been approved (IMA 2021-071). Stibioústalečite ("stibio-oostaletchite") is named after its type locality Ústaleč and its chemical composition, being the (Sb/Te) end-member in the possible ústalečite series. The name is in analogy with the proposal of Biagioni et al. (2020a) for the goldfieldite series. Holotype material of stibioústalečite (polished section) is deposited in the collections of the Department of Mineralogy and Petrology, National Museum in Prague, Cirkusová 1740, 19300 Praha 9, Czech Republic, under the catalog number P1P 7/2021.

2. Occurrence

Stibioústalečite was found at the small Ústaleč uranium deposit, mined by (now abandoned) Ústaleč mine located 500 m northeast of the village Ústaleč, 15 km west of Horažďovice, western Bohemia, Czech Republic (GPS coordinates: 49°19'15.04"N, 13°30'21.40"E). The small Ústaleč uranium deposit belongs to the Horažďovice uranium district, similarly to several analogous deposits and occurrences, including Újezd u Kasejovic, Nalžovské Hory, Těchonice and others. The hydrothermal uranium mineralization exhibits structural control by the regional Horažďovice fault zone trending WNW-ESE. The deposit is located in metamorphic rocks of the Varied Group of the Moldanubian complex at contact with the Chanovice apophysis of the Central Bohemian Plutonic Complex (Litochleb et al. 1999). Three main fault systems are important in the tectonic structure

veins. The vein zones 1–15 m thick are represented by zones of crushed rocks carrying numerous carbonate and quartz veins and veinlets showing an en-echelon pattern. The uranium mineralization in vein zones attains 5 to 80 cm thickness. The predominating contrasting veins are up to 1 m thick, with vein filling of tectonic clay, carbonates, quartz and uranium minerals with accompanying sulfides and selenides. The third group includes vein structures of complicated course, usually 50 cm to 1 m thick. Crushed rocks, carbonates, quartz, fluorite and local uranium mineralization, usually of uneconomic character, fill the latter type of veins (Litochleb et al. 1999). Selenide mineralization of this deposit is tied to white or yellowish, post-ore calcite (younger than uranium mineralization). Selenides penetrate uraninite along grain interfaces and they overgrow or replace spheroidal uraninite aggregates at places. Litochleb et al. (1999) described berzelianite, bukovite, clausthalite, eskebornite, eucairite, ferroselite, hakite, giraudite, chaméanite and

of the deposit. The first set is represented by mylonite

zones practically free of mineralization, trending E-W

to WNW-ESE, dipping 65-80° to SE. The second group

contains northeast-trending structures dipping 45-80°

SE, accompanied by two morphological types of uranium

mineralization - vein-zones and so-called contrasting

3. Physical and optical properties

umangite there.

Stibioústalečite occurs as anhedral grains up to 0.1-0.3 mm in size (Figs 1 and 2), dark grey in color with a grey streak. It is opaque and luster is metallic. The Mohs hardness may be close to $3\frac{1}{2}-4$, in agreement with other members of the tetrahedrite group. Stibioústalečite is brittle, with an indistinct cleavage and a conchoidal fracture. Density was not measured, owing to the small amount of available material; based on the empirical



Fig. 2 Stibioústalečite (U) as anhedral grains up to 0.2 mm in length in calcite gangue in association with berzelianite (B) and uraninite (white in BSE); the area of the extracted fragment for the single-crystal study is outlined by red color; \mathbf{a} – reflected light microscopy (partly crossed polars); \mathbf{b} – BSE photo.

Tab. 1 Reflectance data of stibioústalečite from Ústaleč

λ (nm)	R (%)	λ (nm)	R (%)
400	32.8	560	33.1
420	33.1	580	33.1
440	33.1	589	33.1
460	33.2	600	33.1
470	33.3	620	33.0
480	33.3	640	33.0
500	33.3	650	33.0
520	33.2	660	32.9
540	33.1	680	33.9
546	33.2	700	32.9

formula and the single-crystal unit-cell parameters, the calculated density is 5.676 g/cm³. In reflected light, stibioústalečite is isotropic. It is grey; internal reflections were not observed. Reflectance values, measured in the air using a spectrophotometer MSP400 Tidas at

Leica microscope and standard WTiC (Zeiss 370), with a 100× objective, are given in Tab. 1 and shown in Fig. 3. Stibioústalečite was identified in samples of calcite gangue. It is directly associated with hakite-(Hg), berzelianite, the not-yet approved "arsenoústalečite" and uraninite. Other associated minerals

Fig. 3 Reflectance curve for stibioústalečite from Ústaleč. For the sake of comparison, the curves for stibiogoldfieldite (1) from Mohawk mine (Biagioni et al. 2022), stibiogoldfieldite (2) from Goldfield (Criddle and Stanley 1993, p. 208, described as *goldfieldite*) and *arsenogoldfieldite* (3) from Tramway mine (Criddle and Stanley 1993, p. 209, described as *goldfieldite*) are shown.



4. Chemical composition

Chemical analyses were performed using a Cameca SX100 electron microprobe (National Museum, Prague) operating in wavelength-dispersive mode (25 kV, 20 nA and 1 μ m wide beam). The following standards and X-ray lines were used to minimize line overlap: Ag (AgL_a), Au (AuM_a), Bi (BiM_β), CdTe (CdL_a), Co (CoK_a), chalcopyrite (CuK_a), pyrite (FeK_a, SK_a), HgTe (HgM_a), NiAs (NiK_a, AsL_β), PbS (PbM_a), PbSe (SeL_a), PbTe (TeL_a), Sb₂S₃ (SbL_a), Tl(BrI) (TlL_a) and ZnS (ZnK_a). Peak counting times were 20 s for all elements and one-half of the peak



Tab. 2 Chemical data for stibioústalečite (grain used for SCXRD)

constituent	mean	range	(σ)
Cu	34.10	31.62-35.55	1.37
Ag	1.22	0.16-3.70	1.34
Fe	0.04	0.00-0.14	0.05
Zn	0.09	0.00-0.14	0.05
Hg	0.33	0.00-0.92	0.36
Sb	9.39	9.09-9.64	0.22
As	0.70	0.56-0.97	0.13
Te	12.41	11.73-13.12	0.46
S	3.76	3.04-4.44	0.55
Se	37.59	36.44-38.29	0.63
total	99.63		

 (σ) - estimated standard deviation

time for each background. Other elements, such as Au, Bi, Co, Ni and Pb were found to be below the detection limits (0.02–0.05 wt. %). Raw intensities were converted to the concentrations of elements using the automatic "PAP" (Pouchou and Pichoir 1985) matrix-correction software. There are several different approaches for calculating the chemical formula of the tetrahedrite group



minerals; due to possible vacancies at $^{M(2)}A$ -site in the Te-rich members, the best approach is (Biagioni et al. 2020a, 2022) normalization on the basis of (As + Sb + Te) = 4 *apfu*, taking into account that previous studies (e.g., Johnson et al. 1986) revealed that negligible variations concerning the ideal number of X(3) atoms occur.

The general structural formula of the tetrahedrite group minerals can be best defined as ${}^{M(2)}A_6{}^{M(1)}(B_4C_2)$ ${}^{X(3)}D_4{}^{S(1)}Y_{12}{}^{S(2)}Z$ (Biagioni et al. 2020a). Analytical data for the grain from holotype sample used for the single-crystal study (7 analyses) are given in Tab. 2 and give the following formula: $(Cu_{11.68}Ag_{0.25}Hg_{0.04}Zn_{0.03}Fe_{0.02})_{\Sigma12.02}$ (Sb_{1.68}As_{0.20}Te_{2.12})_{$\Sigma4$}(Se_{10.36}S_{2.55})_{$\Sigma12.91$}. On the basis of the crystal structure of goldfieldites (Biagioni et al. 2020a, 2022), the crystal-chemical formula of stibioústalečite can be written as ${}^{M(2)}(Cu_{5.75}Ag_{0.25})_{\Sigma6}{}^{M(1)}(Cu_{5.93}Hg_{0.04}Zn_{0.03}Fe_{0.02})_{\Sigma6.02}{}^{X(3)}(Te_{2.12}Sb_{1.68}As_{0.20})_{\Sigma4}(Se_{10.36}S_{2.55})_{\Sigma12.91}$. The simplified formula is $(Cu,Ag)_6(Cu^+,Hg,Zn,Fe)_6[(Sb,As,Te)_2Te_2]_{\Sigma4}$ (Se,S)₁₃ and end-member formula is $Cu_6Cu_6(Sb_2Te_2)Se_{13}$, corresponding to (in wt. %) Cu 33.33, Sb 10.64 Te 11.16 Se 44.87, total 100.

The chemical composition for other grains and samples of stibioústalečite from Ústaleč is given in Tab. 3 and presented in Figs 4 and 5. Besides prevailing stibioústalečite, some grains with As > Sb contents (Tab. 3) corresponding to the not-yet approved end-member "arsenoústalečite" were also observed in the material studied (Fig. 4); it has the chemical formula (mean of 11 analyses) $^{M(2)}(Cu_{5.73}Ag_{0.27})_{\Sigma 6}$ $^{M(1)}(Cu_{6.17}Fe_{0.03}Hg_{0.02}Zn_{0.01})_{\Sigma 6.53}$ $x^{(3)}(\text{Te}_{1.73}^{1.31}\text{As}_{1.31}^{1.31}\text{Sb}_{0.96}^{0.02})_{\Sigma4}(\text{Se}_{10.81}^{1.203}\text{S}_{1.79})_{\Sigma12.60}$. The minor Ag contents for all studied grains of ústalečite series are found in the range 0.03-0.77 apfu and do not correlate with Sb, Te or S contents. The determined Me²⁺ (Hg+Fe+Zn+Cd) contents in the minerals of ústalečite series do not exceed 0.35 apfu (Fig. 5a) which are fully in line with substitution $M^{(1)}Me^{2+} + X^{(3)}(Sb/$ $(As)^{3+} = M(1)Cu^{+} + X(3)Te^{4+}, pub$ lished for Te-members of tetrahedrite group with Te contents

Fig. 4 Ternary Te–Sb–As graph (at. unit) for Te-bearing tetrahedrite-group minerals from Ústaleč.

				stib	ioústaleči	te					"arse	noústaleči	ite"	
Ag	0.89	0.20	1.87	2.14	0.67	2.33	0.28	0.28	0.30	0.93	1.54	0.56	0.24	0.31
Fe	0.00	0.48	0.00	0.00	0.09	0.00	0.08	0.30	0.00	0.00	0.00	0.09	0.23	0.40
Tl	0.00	0.00	0.45	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00
Zn	0.19	0.48	0.20	0.14	0.12	0.15	0.15	0.07	0.00	0.07	0.00	0.08	0.11	0.00
Hg	2.03	0.09	2.03	0.90	0.33	0.81	0.08	0.00	0.00	0.51	0.22	0.12	0.00	0.00
Cu	34.34	37.05	34.71	33.81	34.91	33.91	34.37	35.30	34.18	34.51	36.46	36.28	35.45	34.73
Sb	9.36	11.03	10.87	10.29	6.30	10.06	5.86	5.77	8.94	5.56	4.81	4.71	5.72	5.26
As	4.14	2.19	1.35	1.08	3.50	0.85	3.36	3.53	0.50	4.99	4.78	5.44	3.71	3.77
Se	39.62	32.32	38.33	38.94	41.33	37.91	41.33	40.05	38.35	41.22	37.92	38.19	39.60	40.34
Te	6.71	8.89	8.54	10.32	10.63	10.80	10.96	11.65	12.71	10.16	10.42	10.44	11.65	11.66
S	2.85	5.93	2.36	2.39	1.87	2.38	1.76	2.88	3.31	3.59	3.54	4.04	3.27	2.61
total	100.13	98.66	100.70	100.01	99.75	99.20	98.22	99.83	98.29	101.59	99.69	99.95	99.98	99.08
Ag	0.179	0.039	0.398	0.441	0.138	0.484	0.058	0.056	0.062	0.180	0.309	0.108	0.047	0.062
Cu ^A	5.821	5.961	5.602	5.559	5.862	5.516	5.942	5.944	5.938	5.820	5.691	5.892	5.953	5.938
ΣA	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Cu ^{B+C}	5.880	6.342	6.940	6.277	6.228	6.434	6.156	6.014	6.034	5.500	6.716	5.933	5.929	5.885
Fe	0.000	0.181	0.000	0.000	0.034	0.000	0.033	0.116	0.000	0.000	0.000	0.033	0.088	0.155
T1	0.000	0.000	0.051	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.000	0.000	0.000	0.000
Zn	0.063	0.156	0.069	0.048	0.039	0.051	0.050	0.023	0.000	0.022	0.000	0.025	0.036	0.000
Hg	0.219	0.010	0.233	0.100	0.037	0.090	0.009	0.000	0.000	0.053	0.024	0.012	0.000	0.000
$\Sigma B + C$	6.163	6.687	7.292	6.425	6.339	6.576	6.248	6.153	6.034	5.580	6.740	6.004	6.053	6.040
Sb	1.665	1.912	2.050	1.880	1.139	1.850	1.077	1.020	1.634	0.952	0.854	0.801	1.001	0.935
As	1.197	0.618	0.414	0.321	1.028	0.254	1.003	1.014	0.149	1.388	1.380	1.504	1.055	1.089
Te	1.139	1.470	1.536	1.799	1.833	1.895	1.921	1.965	2.217	1.660	1.766	1.695	1.945	1.977
ΣX	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000
Se	10.865	8.637	11.146	10.971	11.518	10.752	11.708	10.919	10.810	10.882	10.385	10.018	10.682	11.052
S	1.925	3.902	1.686	1.658	1.282	1.662	1.227	1.934	2.298	2.334	2.388	2.610	2.172	1.761
$\Sigma S+Se$	12.790	12.539	12.833	12.629	12.800	12.414	12.935	12.853	13.108	13.216	12.773	12.628	12.854	12.813

Tab. 3 Representative chemical analyses for members of ústalečite series from Ústaleč

Coefficients of empirical formula calculated on the basis 4 apfu = Sb + Bi + Te

up to 2 *apfu* (Biagioni et al. 2020a, 2022). Associated hakite-(Hg) shows Me²⁺ contents in the range 1.22–1.56 *apfu* (Fig. 5a); members with Te < 1 and Me²⁺ in the range 0.37–1.01 *apfu* (Fig. 5a) probably correspond to the notyet approved end-member "*hakite-(Cu)*" with variable ratios Cu⁺/Cu²⁺.

The determined Sb/(Sb+As) ratios do not correlate with Te contents (Fig. 5b). Both Sb- (prevailing) and As-dominant members have been observed in the material studied. The range of SeS₋₁ substitution is limited to $3.90 \ apfu$ S (Fig. 5c).

5. X-ray crystallography

Powder X-ray diffraction data could not be collected due to the paucity of available material. Consequently, powder X-ray diffraction data, given in Tab. 4, were calculated through the software *PowderCell* 2.3 (Kraus and Nolze 1996) on the basis of the crystal structure model (our stoichiometry and unit-cell parameter, atom coordinates from stibiogoldfieldite, Biagioni et al. 2022).

A short prismatic fragment of stibioústalečite, $30 \times 24 \times 12$ µm in size, extracted from the polished section

and analyzed using an electron microprobe (Fig. 2), was mounted on glass fiber and examined with an Rigaku SuperNova single-crystal diffractometer equipped with an Atlas S2 CCD detector and a microfocus MoK_{a} source. Data reduction was performed using CrysAlisPro Version 1.171.39.46 (Rigaku 2019). The cubic [space group: $I\overline{4}3m$ (#217)] unit-cell parameter determined from single-crystal data is a = 10.828(4) Å, V = 1269.6(9) Å³ and Z = 2. The single-crystal X-ray diffraction data were corrected for Lorentz factor, polarization effect (Rigaku 2019) and for absorption (Gaussian type in Jana2006). The attempts to refine the structure of stibioústalečite (using the Jana2006 program, Petříček et al. 2014) from these data resulted only in a very problematic refinement due to extremely poor diffraction intensities, $R_{int} =$ 21.4 %. During the refinement, severe correlations, the impossibility to let the occupancies be refined freely, large atomic displacement parameters, and several additional issues (significantly large errors on a few variables, such as on inversion twin fractions) appeared. Therefore we do not present the results of refinement here and the collected single crystal diffraction data were used for the space group assignment and refinement of the unit-cell parameter of stibioústalečite.



6. Discussion and conclusions

An unambiguous determination of stibioústalečite as a member of the tetrahedrite group is based on its chemical composition (stoichiometry), symmetry and unit-cell parameter refined from single-crystal X-ray diffraction data. The increase of unit-cell parameter (due to the SeS, substitution) for stibiogoldfieldite (Biagioni et al. 2022)/ stibioústalečite (this paper), 0.48 Å, is comparable with the value of 0.41 Å, observed in the case of tetrahedrite-(Hg) (Rožňava, Biagioni et al. 2020b)/hakite-(Hg) (Škácha et al. 2016).

The role of tellurium in the crystal structure of tetrahedrite group minerals was recently reviewed by Biagioni et al. (2020a; 2022). Kato and Sakurai (1970) and Kalbskopf (1974) realized that Te does not substitute for S (as believed earlier, e.g., Nowacki 1969) but behaves like As and Sb in the tennantite-tetrahedrite series, as proposed by Lévy (1967). In addition, Kalbskopf (1974) observed the appearance of vacancies at the trigonally coordinated M(2) site. Similar results were later found by Dmitrieva et al. (1987) and Pohl et al. (1996).

Later, several authors (e.g., Novgorodova et al. 1978; Kase 1986; Knittel 1989) proposed that the accommodation of Te^{4+} (up to 2 Te *apfu*) in the crystal structure of a tetrahedrite group mineral is possible through an increase of Cu⁺

Fig. 5 Compositional variation of Tebearing tetrahedrite-group minerals from Ústaleč. **a** – The (Zn+Fe+Zn+Cd) vs. Te (*apfu*) graph for Te-bearing tetrahedrite-group minerals. **b** – The Sb/(Sb+As) vs. Te (*apfu*) graph for minerals of ústalečite series. **c** – The Se vs. S (*apfu*) graph for minerals of ústalečite series.

Tab. 4 Calculated X-ray powder diffraction data for stibioústalečite

I _{cale}	d _{calc}	h	k	l
0.9	5.4140	2	0	0
4.9	4.4205	2	1	1
9.6	3.8283	2	2	0
6.3	3.4241	3	1	0
100.0	3.1258	2	2	2
10.9	2.8939	3	2	1
6.7	2.7070	4	0	0
2.3	2.5522	3	3	0
9.3	2.5522	4	1	1
1.3	2.4212	4	2	0
1.5	2.3085	3	3	2
2.8	2.2103	4	2	2
4.2	2.1236	5	1	0
3.4	2.1236	4	3	1
11.1	1.9769	5	2	1
71.1	1.9141	4	4	0
2.4	1.8570	4	3	3
7.9	1.7565	6	1	1
1.3	1.7565	5	3	2
2.9	1.7121	6	2	0
33.4	1.6324	6	2	2
1.1	1.5629	4	4	4
1.6	1.5313	5	5	0
2.8	1.5313	5	4	3
1.0	1.5313	7	1	0
1.3	1.4735	6	3	3
9.1	1.3535	8	0	0
1.4	1.3328	5	5	4
1.4	1.3328	7	4	1
5.7	1.2942	6	5	3

Intensity and $d_{\rm hkl}$ were calculated using the software *PowderCell2.4* (Kraus and Nolze 1996) on the basis of the crystal structure model (our stoichiometry and unit-cell parameter, atom coordinates of stibiogold-fieldite, Biagioni et al. 2022). Only reflections with $I_{\rm cale} > 1$ are listed. The eight strongest reflections are given in bold.

content (and minor Ag⁺) from 10 to 12 *apfu*, according to the substitution $^{M(1)}Me^{2+} + ^{X(3)}(Sb/As)^{3+} = ^{M(1)}Cu^+ + ^{X(3)}Te^{4+}$, where Me = Fe, Zn, Hg and others. For Te contents between 2 and 4 *apfu*, the charge balance is maintained through the creation of vacancies at the M(2) site, according to the substitution mechanism $^{M(2)}Cu^+ + ^{X(3)}(Sb/As)^{3+} = ^{M(2)}\Box + ^{X(3)}Te^{4+}$. A discussion of the crystal chemistry of the substitutional series between tetrahedrite/tennantite series and goldfieldite is reported in Trudu and Knittel (1998). Makovicky and Karup-Møller (2017) performed syntheses of the complete tetrahedrite–goldfieldite and tennantite–goldfieldite sections and reviewed recently published chemical analyses.

Increased Se-contents with a maximum of 3.0 *apfu* are known in Te-rich members of tetrahedrite group only from samples from the epithermal Au deposits at Kam-chatka, Russia (Spiridonov and Okrugin 1985; Pohl et al. 1996; Spiridonov et al. 2014), and from the Wild Dog

Tab. 5 Crystal and experimental data for stibioústalečite

Crystal data				
Crystal size (mm ³)	$0.030 \times 0.024 \times 0.012$			
Cell setting, space group	Cubic, <i>I</i> 43 <i>m</i>			
a (Å)	10.828(4)			
$V(Å^3)$	1269.6(9)			
Z	2			
Data collection				
Radiation, wavelength (Å)	MoK_a , $\lambda = 0.71073$			
Temperature (K)	297.29(18)			
$\theta_{\max}(^{\circ})$	29.3			
Measured reflections	3776			
Unique reflections	3761			
Reflections with $F_0 > 3\sigma(F_0)$	632			
R _{int}	0.214			
R_{σ}	0.335			
	$13 \le h \le 13,$			
Range of h, k, l	$-13 \le k \le 10,$			
	$-9 \le l \le 14$			

epithermal Au system on Bougainville Island, Papua New Guinea (Noviello 1989). The experiments at 340 °C by de Medicis and Giasson (1971) on the system Cu–Te–Se failed to produce the Se-bearing analogs of goldfieldite, Trudu and Knittel (1998) could not assess whether complete Se-for-S substitution exists in goldfieldite.

The classification of Te-bearing minerals of the tetrahedrite group has been debated for a long time and different nomenclatural approaches have been proposed. When establishing the nomenclature of tetrahedrite group, Biagioni et al. (2020a) recognized this inconsistency and based their revision on three end-member formulas for Te-bearing tetrahedrite-group minerals, i.e., $Cu_6Cu_6(Sb_2Te_2)S_{13}$, $Cu_6Cu_6(As_2Te_2)S_{13}$, and $(Cu_4\Box_2)$ $Cu_6Te_4S_{13}$. In order to avoid further confusion, they proposed to use the name goldfieldite to indicate the end-member composition $(Cu_4\Box_2)Cu_6Te_4S_{13} = Cu_{10}Te_4S_{13}$, in agreement with Moëlo et al. (2008). New names are to be proposed for the other two end-member (sensu Hawthorne 2002) compositions. In the tetrahedrite/tennantite-goldfieldite series, the following boundaries were proposed by Biagioni et al. (2020a):

- (1) tetrahedrite/tennantite, with 0 < Te (apfu) < 1;
- (2) new names, for the compositions with 1<Te (*apfu*)<3. Two different names (e.g., stibiogoldfieldite; *arseno-goldfieldite*) should be applied, taking into account the dominant trivalent constituent;
- (3) goldfieldite, with 3 < Te(apfu) < 4.

The proposed new mineral stibioústalečite, $Cu_6Cu_6(Sb_2Te_2)Se_{13}$, is evidently a Se-analog of stibiogoldfieldite (Biagioni et al. 2022), and therefore, following the classification of Biagioni et al. (2020a), we propose the same type of scheme for possible members of the ústalečite series:

(1) hakite/giraudite, with 0 < Te (apfu) < 1;

- (2) new names, with 1 < Te (*apfu*) < 3. Two different names stibioústalečite, which is described here, and a potential *"arsenoústalečite"* should be applied, taking into account the dominant trivalent constituent;
- (3) possible "ústalečite", with 3 < Te (apfu) < 4.

Acknowledgments. The study was financially supported by the Ministry of Culture of the Czech Republic (long-term project DKRVO 2019-2023/1.II.d; National Museum, 00023272). We acknowledge CzechNano-Lab Research Infrastructure supported by MEYS CR (LM2018110) for financial support for the collection of diffraction data. The referee, Pavel Škácha, and the handling editor, František Laufek, are highly acknowledged for comments and suggestions that helped to improve the manuscript.

References

- BIAGIONI C, GEORGE LG, COOK NJ, MAKOVICKY E, MOËLO
 Y, PASERO M, SEJKORA J, STANLEY CJ, WELCH MD, BOSI
 F (2020a) The tetrahedrite group: Nomenclature and classification. Amer Miner 105: 109–122
- BIAGIONI C, SEJKORA J, MUSETTI S, VELEBIL D, PASERO M (2020b) Tetrahedrite-(Hg), a new 'old'member of the tetrahedrite group. Mineral Mag 84(4): 584–592
- BIAGIONI C, SEJKORA J, MUSETTI S, MAKOVICKY E, PAGANO R, PASERO M, DOLNÍČEK Z (2022) Stibiogoldfieldite, $Cu_{12}(Sb_2Te_2)S_{13}$, a new tetrahedrite group mineral. Mineral Mag 86(1): 168–175.
- CRIDDLE AJ, STANLEY CJ (1993) Quantitative data file for ore minerals, third edition. Chapman & Hall, London pp 1–666
- DE MEDICIS R, GIASSON G (1971) Le système Cu–Se–Te. C R Acad Sci, Ser D 272: 513–515
- DMITRIEVA MT, YEFREMOV VA, KOVALENKER VA (1987) Crystal structure of As-goldfieldite. Dokl Akad Nauk SSSR, Earth Sci Sec 297: 141–144
- HAWTHORNE FC (2002) The use of end-member chargearrangements in defining new mineral species and heterovalent substitutions in complex minerals. Can Mineral 40: 699–710
- JOHNSON NE, CRAIG JR, RIMSTIDT JD (1986) Compositional trends in tetrahedrite. Canad Mineral 24: 385–397
- KALBSKOPF R (1974) Synthese und Kristallstruktur von Cu_{12-x}Te₄S₁₃, dem Tellur-Endglied der Fahlerze. Tschermaks Mineral Petrogr Mitt 21: 1–10
- KASE K (1986) Tellurian tennantite from the Besshi-type deposits in Sambagawa metamorphic belt, Japan. Canad Mineral 24: 399–404
- KATO A, SAKURAI K (1970) Re-definition of goldfieldite Cu₁₂(Te,As,Sb)₄S₁₃. J Mineral Soc Jap 10: 122 (in Japanese)

- KNITTEL U (1989) Composition and association of arsenian goldfieldite from the Marian Gold Deposit, Northern Luzon, Philippines. Mineral Petrol 40: 145–154
- KRAUS W, NOLZE G (1996) POWDER CELL a program for the representation and manipulation of crystal structures and calculation of the resulting X-ray powder patterns. J Appl Crystallogr 29: 301–303
- Lévy C (1967) Contribution a la minéralogie des sulfures de cuivre du type Cu_3XS_4 . Mém Bur Rech Géol Min 54: 1–178
- LITOCHLEB J, ŠREIN V, NOVICKÁ Z, ŠREINOVÁ B (1999) Selenides from the uranium deposit Ústaleč (SW Bohemia). Bull mineral-petrolog odd Nár muz (Praha) 7: 98–108 (in Czech)
- MAKOVICKY E, KARUP-MØLLER S (2017) Exploratory studies of substitutions in the tetrahedrite/tennantitegoldfieldite solid solution. Canad Mineral 55: 233–244
- MOËLO Y, MAKOVICKY E, MOZGOVA NN, JAMBOR JL, COOK N, PRING A, PAAR WH, NICKEL EH, GRAESER S, KARUP-MØLLER S, BALIĆ-ŽUNIĆ T, MUMME WG, VURRO F, TOPA D, BINDI L, BENTE K, SHIMIZU M (2008) Sulfosalt systematics: a review. Report of the sulfosalt sub-committee of the IMA Commission on Ore Mineralogy. Eur J Mineral 20: 7–46
- NOVGORODOVA MI, TSEPIN AI, DMITRIYEVA MT (1978) The new isomorphous series in grey ore group. Zap Vsesojuz Mineral Obsch 107: 100–110 (in Russian)
- NOVIELLO SP (1989) Paragenesis, fluid inclusion study, microprobe analysis and geochemistry of the gold–telluride mineralizing fluids at the Wild Dog Prospect, PNG. B.Sc. (Hon.) thesis, Monash Univ., Clayton, Victoria. Australia
- NOWACKI W (1969) Zur Klassifikation und Kristallchemie der Sulfosalze. Schweiz mineral petrogr Mitt 49: 109–156
- PETŘÍČEK V, DUŠEK M, PALATINUS L (2014) Crystallographic computing system Jana2006: general features. Z Kristallogr 229: 345–352
- POHL D, LIESSMANN W, OKRUGIN VM (1996) Rietveld analysis of selenium-bearing goldfieldites. Neu Jb Mineral, Mh 1996: 1–8
- POUCHOU JL, PICHOIR F (1985) "PAP" (jρZ) procedure for improved quantitative microanalysis. *In*: ARMSTRONG JT (ed) Microbeam Analysis. San Francisco Press, San Francisco, pp 104–106
- RANSOME FL (1909) Geology and ore deposits of Goldfield, Nevada. U.S. Geological Survey, Professional Papers 66
- RIGAKU (2019) CrysAlis CCD and CrysAlis RED. Rigaku-Oxford Diffraction Ltd, Yarnton, Oxfordshire, UK
- SHARWOOD WJ (1907) Gold tellurides. Mining and Scientific Press 94: 731–732
- ŠKÁCHA P, SEJKORA J, PALATINUS L, MAKOVICKY E, PLÁŠIL J, MACEK I, GOLIÁŠ V (2016) Hakite from Příbram, Czech Republic: compositional variability, crystal structure and the role in Se mineralization. Mineral Mag 80(6): 1115–1128

- SPIRIDONOV EM, OKRUGIN VM (1985) Selenium goldfieldite, a new fahlore variety. Dokl Akad Nauk SSSR 280: 474–478
- SPIRIDONOV EM, IVANOVA YUN, YAPASKURT VO (2014) Selenium-bearing goldfieldite and fischesserite AuAg₃ Se₂-petzite AuAg₃Te₂ solid solutions in ores from the Ozernovskoe volcanogenic deposit (Kamchatka). Dokl Earth Sci 458: 1139–1142
- THOMPSON RM (1946) Goldfieldite = tellurian tetrahedrite. Univ Tor Stud, Geol Ser 50: 77–78
- TRUDU A, KNITTEL U (1998) Crystallography, mineral chemistry, and chemical nomenclature of goldfieldite, the tellurian member of the tetrahedrite solid-solution series. Canad Mineral 36: 1115–1137