

New mineral names*

ANDREW J. LOCOCK,¹ T. SCOTT ERCIT,^{2,‡} JOHAN KJELLMAN³, AND PAULA C. PIILONEN^{2,†}

¹Department of Earth and Atmospheric Sciences, University of Alberta, Edmonton T6G 2E3, Canada

²Research Division, Canadian Museum of Nature, P.O. Box 3443, Stn. D, Ottawa, ON K1P 6P4, Canada

³Department of Earth Sciences, Uppsala University, SE-752 36 Uppsala, Sweden

ALLANITE-(La)*

P. Orlandi, M. Pasero (2006) Allanite-(La) from Buca della Vena mine, Apuan Alps, Italy, an epidote-group mineral. *Can. Mineral.*, 44, 523–531.

Allanite-(La) is found in close association with calcite and barite in barite veins that cut a dolomitic metamorphosed limestone in the Castello zone of the Buca della Vena mine, near Stazzema, Apuan Alps, Tuscany, Italy. It occurs as prismatic crystals, elongated along [010], up to 2–3 mm in length. The mineral is well crystallized and not metamict, with principal forms {001}, {100}, {101}, {10 $\bar{1}$ }, {210}, and {011}. It is brittle, $H = 6$, transparent to translucent, black with brownish reflections and a brown streak, vitreous, with imperfect cleavage parallel to {001} and conchoidal fracture. Allanite-(La) is biaxial, $n_x = 1.755(5)$, $n_y = 1.760(5)$, $n_z = 1.765(5)$, $2V = 90(2)^\circ$, orientation $Y = b$, has very high dispersion and is strongly pleochroic, with Y greenish to olive green and Z greenish brown. The average of eight electron microprobe analyses gave SiO₂ 32.45, TiO₂ 0.10, ThO₂ 0.31, Al₂O₃ 17.77, Y₂O₃ 0.035, La₂O₃ 8.51, Ce₂O₃ 6.12, Pr₂O₃ 3.16, Nd₂O₃ 3.53, MgO 0.32, CaO 13.01, FeO_{tot} 13.67 (FeO 8.72, Fe₂O₃ 5.50 on the basis of stoichiometry), H₂O (calc) 1.63, sum 100.62 wt% (for FeO_{tot}), 101.17 wt% (for FeO + Fe₂O₃), corresponding (on the basis of 25 negative charges and 8 cations) to: Ca_{1.000}[(La_{0.288}Ce_{0.206}Nd_{0.116}Pr_{0.106}Y_{0.001})_{Σ0.717}Ca_{0.279}Th_{0.006}]_{Σ1.002}(Al_{0.899}Fe_{0.101}³⁺)_{Σ1.000}Al_{1.000}(Fe_{0.669}²⁺Fe_{0.279}³⁺Mg_{0.044}Ti_{0.007})_{Σ0.999}[(Si_{0.978}Al_{0.022})_{Σ1.000}O₄](Si₂O₇)O(OH), which can be simplified as Ca(REE,Ca)Al₂(Fe²⁺,Fe³⁺)(SiO₄)(Si₂O₇)O(OH) with La dominant in the A2 site.

Single-crystal X-ray structure study ($R1 = 0.0328$) confirmed that allanite-(La) is a member of the epidote group: monoclinic, space group $P2_1/m$, $a = 8.914(4)$, $b = 5.726(1)$, $c = 10.132(6)$ Å, $\beta = 114.87(5)^\circ$, $V = 469.1(3)$ Å³. Powder diffraction data were collected with a Gandolfi camera (57.3 mm diameter, CuK α radiation) and yielded refined unit-cell parameters $a = 8.875(6)$, $b = 5.735(2)$, $c = 10.088(7)$ Å, $\beta = 114.88(4)^\circ$, $V = 469.1(3)$ Å³,

* Before publication, minerals marked with an asterisk were approved by the Commission on New Minerals and Mineral Names, International Mineralogical Association.

† E-mail: ppiilonen@mus-nature.ca

‡ English translations of articles are available upon request from T.S.E. (sercit@mus-nature.ca).

and the strongest lines [d in Å (I , hkl): 7.93 (15, $\bar{1}01$), 3.506 (20, $\bar{2}11$), 2.901 (100, $\bar{1}13$), 2.806 (40,020), 2.692 (60,013), 2.611 (50, $\bar{3}11$), 2.283 (15, $\bar{1}14$), 2.174 (25, $\bar{4}01$), 1.632 (20, $\bar{2}33$), 1.432 (15, $\bar{6}13$). $D_{\text{meas}} = 3.93(1)$ g/cm³ by flotation in heavy liquids, $D_{\text{calc}} = 3.94$ g/cm³ for $Z = 2$.

The root name *allanite* honors the Scottish mineralogist Thomas Allan (1777–1833) who first studied the mineral, and the name allanite-(La) reflects its relationship with allanite-(Ce), the Levinson modifier indicating the dominant REE. The authors emphasize that specimens with compositions corresponding to allanite-(La) have been known in the literature for some time, and that although this name has been used previously on an informal basis, the formal description and naming of allanite-(La) fills a gap in the nomenclature of approved epidote-group minerals. The mineral corresponds to IMA mineral no. 2003-065. Type material is deposited in the Centro Interdipartimentale Museo di Storia Naturale e del Territorio of the University of Pisa, under catalog no. 10478. **A.J.L.**

CHISTYAKOVAITE-(Y)*

N.V. Chukanov, G.A. Sidorenko, I.S. Naumova, A.E. Zadov, V.I. Kuz'min (2006) Chistyakovaite, a new mineral Al(VO₂)₂(AsO₄)₂(F,OH)·6.5H₂O. *Dokl. Earth Sci.*, 407, 290–293 (in English); *Dokl. Akad. Nauk*, 406, 816–819 (in Russian).

The new species chistyakovaite occurs in samples collected in the 1950s from the supergene zone of the Bota-Burum deposit, south of Alakol' Lake, southwestern Balkhash area, Zhambyl (Dzhambul) Region, Kazakhstan. This hydrothermal U deposit consists of carbonatized felsite porphyries and tuffaceous breccias of Devonian age that have undergone primary hydrothermal alteration and subsequent supergene alteration. In particular, supergene alteration of hydrothermal arsenopyrite and pitchblende is responsible for liberating the U and As responsible for the new species and many other uranyl-bearing arsenates found at the deposit. The mineral is associated with arsenopyrite, pyrite, galena, scorodite, arseniosiderite, mansfieldite, metazeunerite, trögerite, and sodium uranospinite. It forms imperfect, {100} flattened, yellow crystals to 2 mm across, which are sometimes intergrown. Brittle; Mohs' hardness 2.5; $D_{\text{meas}} 3.62(2)$, $D_{\text{calc}} 3.585$ g/cm³; perfect {100} and imperfect {001} cleavage; stepped fracture. Bright green luminescence in UV light (365 nm). Opti-

cally biaxial (–), colorless, with $\alpha = 1.557(2)$, $\beta = 1.580(1)$, $\gamma = 1.580(1)$, $2V = -10(5)^\circ$, $X = a$, $Z \approx b$, no dispersion. Dissolves in HCl at room temperature with no liberated gas. The infrared spectrum (KBr pellet, 400 to 4000 cm^{-1} range) records vibration and/or flexing bands for H_2O , OH, PO_4 , UO_2 , AsO_4 , and AlO_6 ; a large shoulder at 3130 cm^{-1} implies the existence of some strong hydrogen bonding. Heating in Ar to 850 $^\circ\text{C}$ gives a total weight loss of 12.2%. This, combined with electron microprobe analysis (20 kV, 10 nA, 50 μm , except for F at 15 kV, 70 nA, 50–60 μm beam) gave: Al_2O_3 4.99, UO_2 58.34, As_2O_5 21.40, P_2O_5 1.23, F 1.1, H_2O 12.2, $\text{O}=\text{F} = -0.46$, total 98.80 wt%, yielding the empirical formula (per 2 $\text{AsO}_4 + \text{PO}_4$), $\text{Al}_{0.96}(\text{UO}_2)_{2.00}[(\text{AsO}_4)_{1.83}(\text{PO}_4)_{0.17}][\text{F}_{0.57}(\text{OH})_{0.31}] \cdot 6.50\text{H}_2\text{O}$, or ideally $\text{Al}(\text{UO}_2)_2(\text{AsO}_4)_2(\text{F}, \text{OH}) \cdot 6.50\text{H}_2\text{O}$. Gladstone-Dale compatibility is good. Fracturing and mosaic structure precluded single-crystal study, but powder X-ray diffraction study gave space groups $P2/m$, $P2$ or Pm , $a = 19.99(1)$, $b = 9.79(1)$, $c = 19.62(2)$ \AA , $\beta = 110.7(2)^\circ$, $Z = 8$. The mineral, which would seem to be the arsenate-fluorine analog of threadgoldite, has also possibly been found at the Menzenschwand deposit in the Schwarzwald, Germany. Chistyakovite is named for N.I. Chistyakova, a senior assistant at the All-Russia Research Institute of Mineral Resources (VIMS). Type samples are in the E.V. Kopchenova collection of the Mineralogical Museum at VIMS, (no. 350/59), and in the Fersman Mineralogical Museum, Moscow (no. 3286/1).

Discussion. No mention is made of whether peak shape corrections were applied to the $FK\alpha$ microprobe data. Errors as large as 20% rel. can be incurred without such corrections (Solberg, T.N., 1982, *Microbeam Analysis*, 17, 148–150), an important concern when the (F,OH) site contains only 0.57 F apfu. **T.S.E.**

GABRIELITE*

- S. Graeser, D. Topa, T. Balić-Žunić, E. Makovicky (2006) Gabrielite, $\text{Tl}_2\text{AgCu}_2\text{As}_3\text{S}_7$, a new species of thallium sulfosalt from Lengenbach, Binntal, Switzerland. *Can. Mineral.*, 44, 135–140.
- T. Balić-Žunić, E. Makovicky, L. Karanović, D. Poleti, S. Graeser (2006) The crystal structure of gabrielite, $\text{Tl}_2\text{AgCu}_2\text{As}_3\text{S}_7$, a new species of thallium sulfosalt from Lengenbach, Switzerland. *Can. Mineral.*, 44, 141–158.

Gabrielite occurs as pseudohexagonal prismatic to platy crystals up to 0.4 mm, with aggregates to 1 mm in size. Relative to its pseudohexagonal morphology, the crystals show {001} dominant and are striated parallel to [100]. The tenacity of the mineral is not reported, $\text{VHN}_{10} = 18 \text{ kg/mm}^2$, $H = 1\frac{1}{2}$ –2, opaque, gray to black with a blackish red streak, metallic, with excellent cleavage along (001). In reflected light, gabrielite is white, has common red internal reflections, and shows weak anisotropy; no bireflectance or pleochroism was observed. Reflectance values (in air, WTiC standard) are (R_{max}) 30.53 (470 nm), 29.10 (546 nm), 27.94 (589 nm), and 26.35 (650 nm). The average of eleven electron microprobe analyses gave Tl 37.30, Ag 8.47, Cu 12.60, As 18.90, Sb 1.79, S 20.64, sum 99.70 wt%, corresponding (on the basis of 7 S atoms) to: $\text{Tl}_{1.98}(\text{Ag}_{0.85}\text{Cu}_{2.16})_{\Sigma 3.01}(\text{As}_{2.74}\text{Sb}_{0.16})_{\Sigma 2.90}\text{S}_7$, ideally $\text{Tl}_2\text{AgCu}_2\text{As}_3\text{S}_7$. Single-crystal X-ray structure study ($R1 = 0.0486$) of a sample twinned on (100) showed the mineral to

be triclinic, space group $P\bar{1}$, $a = 12.138(3)$, $b = 12.196(3)$, $c = 15.944(4)$ \AA , $\alpha = 78.537(5)$, $\beta = 84.715(4)$, $\gamma = 60.470(4)^\circ$, $V = 2013(1)$ \AA^3 . The complex crystal structure can be considered to be layered parallel to (001) and to consist of three main slabs of cation-centered polyhedra, two with the idealized trigonal plane-symmetry and one with monoclinic symmetry. One of the pseudotrigonal slabs is the basis of a hypothetical homologous series of cyclically twinned sulfosalt structures. The internal symmetries of the slabs lead to a twin law with (100) as the twin plane, and make possible the existence of several potential OD (order-disorder) polytypes. Metal–metal bonds (Tl–Tl and Tl–Cu) and metal–semimetal (Tl–As) bonds are notable features in the structure and help to explain the low hardness and metallic character of the mineral. Powder diffraction data were collected with a Debye-Scherrer camera (114.6 mm diameter, $\text{FeK}\alpha$ radiation) and yielded refined unit-cell parameters $a = 12.152(7)$, $b = 12.203(7)$, $c = 15.965(5)$ \AA , $\alpha = 78.25(6)$, $\beta = 84.55(6)$, $\gamma = 60.65(7)^\circ$, $V = 2020(2)$ \AA^3 , and the strongest lines [d in \AA (I , hkl): 15.631 (100,001), 5.237 (40,12 $\bar{1}$), 3.944 (40,321), 3.531 (80,300), 3.468 (40,233), 3.263 (50,03 $\bar{1}$), 3.143 (90,21 $\bar{4}$), 2.978 (60,324), 2.911 (70,422), 2.520 (60,2 $\bar{2}$ 3)]. $D_{\text{calc}} = 5.41 \text{ g/cm}^3$ for the ideal formula and $Z = 6$.

The mineral is found in association with numerous other As sulfosalts, including hutchinsonite, hatchite, edenharterite, trechmannite, tennantite, abundant realgar, and rathite, in cavities in a Triassic dolomitic rock at Lengenbach, Binntal, Canton Valais, Switzerland. The name honors Walter Gabriel (b. 1943), of Basel, Switzerland, a well-known mineral photographer and expert on Lengenbach minerals. The mineral corresponds to IMA mineral no. 2002-053. Type material is deposited at the Natural History Museum Basel and the Institute of Mineralogy, University of Basel (X-ray samples) under the catalog number S113.

Discussion. Gabrielite exhibits severe pseudosymmetry; the transformation matrix [010/0 $\bar{1}$ 1/2 $\bar{1}$ 0] gives the pseudohexagonal unit-cell parameters: $a = 12.196$, $b = 18.046$, $c = 21.124$ \AA , $\alpha = 90.03$, $\beta = 90.63$, $\gamma = 120.02^\circ$. **A.J.L.**

IWASHIROITE-(Y)*

- H. Hori, T. Kobayashi, R. Miyawaki, S. Matsubara, K. Yokoyama, M. Shimizu (2005) Iwashiroite-(Y), YTaO_4 , a new mineral from Suishoyama, Kawamata Town, Fukushima Prefecture, Japan. *J. Mineral. Petrol. Sci.*, 101, 170–177.

The new mineral species iwashiroite-(Y) occurs at the Suishoyama mine, Kawamata, Fukushima Prefecture, Japan. The Suishoyama mine worked several NYF-type pegmatites; the mineral was found in the dumps near the no. 1 pit (37 $^\circ$ 40' N, 140 $^\circ$ 37' E). Only one specimen bearing iwashiroite-(Y) was found, an association with quartz, microcline, and annite. Iwashiroite-(Y) is translucent yellow-brown to brown with an adamantine luster and pale brown streak, and is non-fluorescent under UV light (254, 365 nm). Crystals are euhedral {010} plates to 7 mm across, with [101] striae. Cleavage is {010} good, {001} poor; fracture subconchoidal; tenacity brittle. $D_{\text{calc}} = 7.13 \text{ g/cm}^3$; $\text{VHN}_{30} = 766$ –825 kg/cm^2 , corresponding to a Mohs' hardness of 6. Reflectance data for $n_{\text{oil}} = 1.515$ are λ ($^{\text{air}}R_1$, $^{\text{air}}R_2$; $^{\text{oil}}R_1$, $^{\text{oil}}R_2$): 400 (15.3, 14.4; 5.2, 5.2); 470 (14.1, 13.8; 4.4, 4.1); 546 (13.8, 13.6; 4.5, 4.0); 589 (13.9, 13.6; 4.8, 4.2); 650 (14.0, 13.7; 5.0,

4.6); 700 nm (14.3, 14.1; 5.9, 5.8%). An average of 18 spot analyses of non-metamict iwashiroite by electron microprobe gave: Y₂O₃ 29.10, Ce₂O₃ 0.10, Nd₂O₃ 0.10, Sm₂O₃ 0.36, Gd₂O₃ 1.06, Tb₂O₃ 0.25, Dy₂O₃ 2.38, Ho₂O₃ 0.56, Er₂O₃ 2.09, Tm₂O₃ 0.37, Yb₂O₃ 3.33, Lu₂O₃ 0.85, ThO₂ 0.02, UO₂ 0.15, CaO 0.17, Ta₂O₅ 40.64, Nb₂O₅ 16.66, TiO₂ 0.41, total 98.6 wt%, yielding the empirical formula (Y_{0.81}Yb_{0.05}Dy_{0.04}Er_{0.03}Gd_{0.02}Lu_{0.01}Ho_{0.01}Sm_{0.01}Ca_{0.01}Tm_{0.01})_{Σ1.00}(Ta_{0.58}Nb_{0.39}Ti_{0.02})_{Σ0.99}O₄, and thus the ideal formula YTaO₄. The mineral shows zoning in actinide contents, which results in variations in crystallinity: metamict parts of crystals have a significantly higher content of UO₂ + ThO₂ (av. of 2.16 wt%). The powder diffraction pattern (Gandolfi camera, Ni-filtered CuKα radiation, SiO₂ internal standard) gave $a = 5.262(5)$, $b = 5.451(5)$, $c = 5.110(5)$ Å, $\beta = 95.1(1)^\circ$, $Z = 2$, space group $P2_1/a$. The strongest maxima in the pattern are (d Å, $I\%$, hkl): (3.13, 100, $\bar{1}11$), (2.95, 94, 111), (2.73, 26, 020), (2.62, 23, 200), (1.890, 29, 220), (1.862, 29, 022), (1.614, 20, 131). The crystal structure of the mineral was refined to R_1 0.034 using 429 observed [$I > 2\sigma(I)$] single-crystal MoKα X-ray diffraction data. Iwashiroite-(Y) has the M' -fergusonite structure of synthetic YTaO₄. Tantalum is in 4 + 2 distorted octahedral coordination; the TaO₆ octahedra share edges to form zigzag chains along c . Y is 8-coordinated; the YO₈ polyhedra form {100} sheets via edge-sharing. The sheets with YO₈ polyhedra alternate along a with layers consisting only of Ta-bearing octahedral chains. The name is after Iwashiro, the old provincial name for the central part of Fukushima Prefecture. The type sample is deposited with the National Science Museum, Tokyo (no. NSM-M28537).

Discussion. The authors assumed that iwashiroite-(Y) is a polymorph of formanite-(Y) and ytrotantalite-(Y). However, Shih Nicheng and Peng Zhizhong (1981, *Kexue Tongbao*, 26, 548–551) earlier described a non-metamict “formanite-(Y)” from China which seems to be identical to iwashiroite-(Y). Heating of formanite-(Y) from the type locality, in N2 (Lima de Faria, 1964, Identification of metamict minerals by X-ray powder photographs, Junta Invest. Ultramar, Lisbon) resulted in a pattern that can be indexed on the iwashiroite-(Y) cell. Voloshin et al. (2003) did not generate an iwashiroite-like pattern in their heating studies of formanite-(Y) from Russia [see abstract for FORMANITE-(Y), above]. In conclusion, the relationships between formanite-(Y), ytrotantalite-(Y), and iwashiroite-(Y) are muddled, and the possibility exists that formanite-(Y) and iwashiroite-(Y) may be identical. **T.S.E., J.K.**

JOHNSENITE-(CE)*

J.D. Grice, R.A. Gault (2006) Johnsenite-(Ce): a new member of the eudialyte group from Mont Saint-Hilaire, Quebec, Canada. *Can. Mineral.*, 44, 105–115.

Johnsenite-(Ce) occurs intergrown with zirsilite-(Ce) in a cavity near the margin of a marble xenolith in an igneous breccia along the contact between porphyritic nepheline syenite and sodalite syenite on the level 7 bench of the southeast wall of the Poudrette Quarry, Mont Saint-Hilaire, Quebec, about 40 km east of Montreal. The mineral occurs as deeply etched, skeletal crystals to 4 mm and aggregates of crystals to 1 cm; the partial forms {001} and {101} were observed. It is brittle, $H = 5$ –6, translucent to transparent, pale yellow to bright orange with a

white streak, vitreous, with no discernable cleavage or parting and an uneven fracture. Johnsenite-(Ce) is uniaxial negative, ω 1.648(1), ϵ 1.637(1) for $\lambda = 589$ nm, colorless in transmitted light and non-pleochroic. The average of eight electron microprobe analyses, including three on the grain used for the structure determination, gave Na₂O 10.47, K₂O 0.25, CaO 8.98, SrO 1.60, MnO 5.43, FeO 1.61, Y₂O₃ 0.70, La₂O₃ 1.56, Ce₂O₃ 3.01, Pr₂O₃ 1.14, Nd₂O₃ 0.89, Sm₂O₃ 0.12, Gd₂O₃ 0.33, Dy₂O₃ 0.14, TiO₂ 0.73, ZrO₂ 9.60, HfO₂ 0.04, Nb₂O₅ 0.82, WO₃ 5.23, SiO₂ 43.16, Cl 0.77, CO₂ (calc) 1.27, H₂O (calc) 0.32, O = Cl –0.17, total 98.00 wt%, corresponding [on the basis of one CO₃ group and 29 (Si, Zr, Ti, Hf, Nb, W)] to: Na_{11.74}[(Ce_{0.64}La_{0.33}Dy_{0.03})]_{Σ1.00}Sr_{0.54}Ca_{0.51}Y_{0.22}K_{0.19}Σ_{2.46}(Ca_{5.06}[Pr_{0.24}Nd_{0.18}Gd_{0.06}Sm_{0.02}]]_{Σ0.50}Mn_{0.44})_{Σ6}(Mn_{2.22}Fe_{0.78})_{Σ3}(Zr_{2.71}Ti_{0.32}Hf_{0.01})_{Σ3.04}(W_{0.78}Nb_{0.21})_{0.99}Si_{24.97}O₇₃(CO₃)(OH_{1.25}Cl_{0.75})_{Σ2}, ideally Na₁₂(Ce,La,Sr,Ca)₆Mn₃Zr₃W(Si₂₅O₇₃)(CO₃)(OH,Cl)₂. The results of the structure determination and of infrared spectroscopy support the presence of CO₃ and OH groups in the material. Single-crystal X-ray structure study ($R_1 = 0.040$) of a crystal twinned by merohedry confirmed that johnsenite-(Ce) is a polar member of the eudialyte group: trigonal, space group $R3m$, $a = 14.2675(7)$, $c = 30.0369(14)$ Å, $V = 5295.2(7)$ Å³. Powder diffraction data were collected with a Bruker microdiffractometer (CuKα radiation) and yielded refined unit-cell parameters $a = 14.237(3)$, $c = 30.03(1)$ Å, $V = 5271$ Å³, and the strongest lines [d in Å (I , hkl): 11.299 (95,101), 10.055 (30,003), 9.452 (81,012), 4.291 (34,205), 3.544 (44,220), 3.392 (38,131), 3.164 (75,217), 2.966 (100,315), 2.847 (81,404), 1.7799 (31,440). $D_{\text{meas}} = 3.24(3)$ g/cm³ by flotation in methylene iodide, $D_{\text{calc}} = 3.23$ g/cm³ for $Z = 3$.

Johnsenite-(Ce) occurs in association with: albite, calcite, pectolite, aegirine, fluorapophyllite, zirsilite-(Ce), a burbankite-group mineral, dawsonite, rhodochrosite, epididymite, galena, molybdenite, pyrite, pyrrhotite, quartz, an amphibole-group mineral, sphalerite, stillwellite-(Ce), titanite, cerite-(Ce), tapersuatsiaite, steacyite, catapleiite, zakharovite, natrolite, and microcline. The mineral is the W-analog of zirsilite-(Ce), and is the eighteenth species to be described from the structurally complex eudialyte group. It is also one of eight eudialyte-group species found to date at Mont Saint-Hilaire. The name honors Ole Johnsen (b. 1940), of the Geological Museum, University of Copenhagen, Denmark, and is given in recognition of his extensive research into the eudialyte group and for his scientific and popular contributions to mineralogy. The name is in accord with the recommendations of the Subcommittee on Eudialyte Nomenclature of the CNMMN. The mineral corresponds to IMA mineral no. 2004-026. Holotype material (catalog no. CMNMC 84395) is deposited in the collection of the Canadian Museum of Nature, Ottawa. **A.J.L.**

LEMANSKIITE*

P. Ondruš, F. Veselovský, R. Skála, J. Sejkora, R. Pažout, J. Frýda, A. Gabašová, J. Vajdak (2006) Lemanskiite, NaCaCu₃(AsO₄)₄Cl·5H₂O, a new mineral species from the Abundancia Mine, Chile. *Can. Mineral.*, 44, 523–531.

Lemanskiite occurs intergrown with lammerite in mine dump material from the abandoned Abundancia gold mine, El Guanaco mining district, south of Cerro La Estrella, about 95

km east of Taltal, in Region II, Antofagasta Province, Chile. It occurs as rosette-shaped aggregates (up to 5 mm) of thin lamellar, subparallel, strongly bent intergrowths (0.3 mm × 10 μm) or needle-shaped aggregates of 0.8 mm length and 10 mm in thickness. Individual thin tabular crystals (up to 4 mm in length) are invariably bent. The mineral is brittle, $H = 2\frac{1}{2}$, translucent, dark sky blue with a light blue streak, vitreous, with excellent cleavage parallel to (001). Lemanskiite is uniaxial negative, ω 1.749(2), ϵ 1.647(2), and strongly pleochroic: $O =$ dark green-blue, $E =$ light blue-green (light turquoise). Its chemical composition was determined by an electron microprobe analysis (average of 15 points) and a Perkin Elmer 2400 CHN analyzer to be: Na₂O 3.04(18), CaO 5.33(7), CuO 37.76(44), As₂O₅ 43.53(59), Cl 3.23(7), H₂O 8.50, $O = Cl - 0.73$, sum 100.66 wt%, corresponding (on the basis of 22 anions) to Na_{1.04}Ca_{1.00}Cu_{5.01}(AsO₄)_{4.00}[Cl_{0.96}(OH)_{0.11}]_{Σ1.07}·4.93H₂O, ideally NaCaCu₅(AsO₄)₄Cl·5H₂O. The results of thermogravimetry and infrared spectroscopy support the presence of H₂O in the material. A single-crystal X-ray structure study was not successful as a result of the poor quality of the crystals available. Powder diffraction data were collected with a Philips X'Pert MPD diffractometer (CuK α radiation) and by application of whole-pattern fitting yielded refined unit-cell parameters $a = 9.9758(4)$, $c = 36.714(1)$ Å, $V = 3653.6(2)$ Å³, and the strongest lines [d in Å (I , hkl): 9.600 (9,101), 9.177 (100,004), 4.588 (32,008), 4.167 (10,108), 3.059 (15,0.0.12), 2.924 (5,1.0.12), 2.606 (6,2.0.12), 1.8049 (4,1.0.20), 1.3102 (4,2.2.26), 1.1471 (4,0.0.32)]. Pattern fitting was undertaken assuming tetragonal symmetry and possible space groups $P4_122$ or $P4_322$, based on the data for tetragonal zdenekite. $D_{\text{meas}} = 3.78(1)$ g/cm³ by flotation in Clerici solution, $D_{\text{calc}} = 3.863(5)$ g/cm³ for the empirical formula and $Z = 8$. Lemanskiite is dimorphous with lavendulan and represents the Ca-analog of tetragonal zdenekite.

The mineral occurs as nodules or veinlets in quartz veins and is associated with lammerite, olivenite, mansfieldite, senarmonite, a mineral of the crandallite group, rutile, anatase, and talc. The name honors Chester S. Lemanski, Jr. (b. 1947), a mineral collector who built one of the largest privately held collections in the U.S.A. The mineral corresponds to IMA mineral no. 1999-037. Holotype material labeled P1p14/99 is deposited in the mineralogical collection of the National Museum, Prague, Czech Republic.

Discussion. The authors used powder X-ray diffraction to investigate samples labeled lavendulan from various localities worldwide; most were found to be lemanskiite. The identity of lavendulan from Laurion, Greece, was confirmed, but after several days the powdered material transformed to lemanskiite. Lavendulan from Jáchymov, Czech Republic, was also confirmed, but did not transform to lemanskiite. The apparent ease of transformation from monoclinic lavendulan to tetragonal lemanskiite for some samples may help to explain the two differing results reported for the unit cell and symmetry of the analogous mineral zdenekite, NaPbCu₅(AsO₄)₄Cl·5H₂O: tetragonal, space group $P4_122$ or $P4_322$ (1995, *European Journal of Mineralogy*, 7, 553–557); or monoclinic, space group $P2_1/n$ (2003, *Crystallography Reports*, 48, 939–943). It is noted that the monoclinic structure model described in the latter reference is either incorrect or of poor quality, as its interatomic distances fall well outside of normal ranges. **A.J.L.**

OFTEDALITE*

M.A. Cooper, F.C. Hawthorne, N.A. Ball, P. Černý (2006) Oftedalite, (Sc,Ca,Mn²⁺)₂K(Be,Al)₃Si₁₂O₃₀, a new member of the milarite group from the Heftetjern pegmatite, Tørdal, Norway: description and crystal structure. *Can. Mineral.*, 44, 943–949.

Oftedalite occurs intergrown with Sc-rich milarite in the Heftetjern pegmatite, located at 8° 45' E, 59° 11' N, about 4.3 km NW of Tørdal, Telemark county, southern Norway. As a result of the intimate intergrowth of the two species, properties are reported for the oftedalite–Sc-rich milarite solid solution, which is referred to as oftedalite herein. Oftedalite forms short prismatic hexagonal crystals up to 0.1 mm in diameter with prominent {100} and {001} forms. The mineral is brittle, $H = 6$, grayish white with a colorless streak and vitreous luster. It has poor cleavage parallel to {001} and a conchoidal fracture. Oftedalite is non-pleochroic, uniaxial negative, ω 1.556(2), ϵ 1.553(2) for $\lambda = 590$ nm. Electron microprobe analysis of a small zone of oftedalite in a composite crystal gave SiO₂ 73.32, Al₂O₃ 0.47, Sc₂O₃ 6.77, Y₂O₃ 0.36, FeO 0.26, MnO 1.32, CaO 4.49, K₂O 4.71, BeO (calc) 7.41, sum 99.11 wt%, corresponding to (Sc_{0.96}Ca_{0.79}Mn_{0.18}Fe_{0.04}Y_{0.03}Σ_{2.00}K_{0.98}(Be_{2.91}Al_{0.09}Σ_{3.00}Si_{11.98}O₃₀) on the basis of 30 anions, ideally (Sc,Ca)₂KBe₃Si₁₂O₃₀. Single-crystal X-ray structure study ($R = 0.066$) showed the mineral to be a member of the milarite group: hexagonal, space group $P6/mcc$, $a = 10.097(1)$, $c = 13.991(2)$ Å, $V = 1235.3(6)$ Å³. Powder diffraction data were collected with a Debye-Scherrer camera with a Gandolfi attachment (114.6 mm diameter, CuK α radiation) and yielded refined unit-cell parameters $a = 10.104(2)$, $c = 14.008(3)$ Å, $V = 1238.6(4)$ Å³, and the strongest lines [d in Å (I , hkl): 7.012 (4,002), 5.044 (5,110), 4.097 (7,112), 3.504 (5,004), 3.229 (10,104), 2.880 (8,114), 2.735 (3,204), 1.995 (3,314), 1.836 (4,412), 1.751 (4,008)]. $D_{\text{calc}} = 2.61$ g/cm³ for $Z = 2$.

Oftedalite occurs as compositionally heterogeneous crystals (intergrown with Sc-rich milarite) found in late stage assemblages in vugs and fractures of the Heftetjern pegmatite. Minerals directly associated with oftedalite–Sc-rich milarite include green tourmaline, yttrian milarite, bazzite, thortveitite, kristiansenite, and bertrandite. The name honors Ivar Oftedal (1894–1976), former Professor of Mineralogy at the Institute of Geology, University of Oslo, who contributed extensively to the geochemistry of Sc, and who wrote the first papers on the mineralogy of the Tørdal pegmatites. Oftedalite is only the tenth mineral described to require essential scandium. The mineral corresponds to IMA mineral no. 2003-045a. Type material labeled H04/98 is deposited in the Canadian Museum of Nature, Ottawa, and a small fragment is also stored at the Steiermärkisches Landesmuseum, Graz, Austria. **A.J.L.**

PAKHOMOVSKYITE*

V.N. Yakovenchuk, G.Yu. Ivanyuk, Yu.A. Mikhailova, E.A. Selivanova, S.V. Krivovichev (2006) Pakhomovskiyte, Co₃(PO₄)₂·8H₂O, a new mineral species from Kovdor, Kola Peninsula, Russia. *Can. Mineral.*, 44, 117–123.

Pakhomovskiyte is found in leached fissures within dykes of dolomite carbonatite in the “Anomalous” ore of the Iron-Ore

complex, Kovdor massif (67°33' N, 30°31' E), Kola Peninsula, Russia. The mineral occurs as groups (up to 3 × 2 cm) of small spherulites (up to 0.5 mm diameter) and rosettes of well-formed crystals (up to 0.05 mm diameter). The mineral is flexible in thin flakes, $H \sim 2$, translucent to transparent, bright pink with a pink streak, with a dull (in aggregates) to pearly (in separate flakes) luster, and perfect cleavage parallel to {010}. Pakhomovskiyite is biaxial positive, $n_x = 1.581(2)$, $n_y = 1.600(2)$, $n_z = 1.631(2)$ for $\lambda = 590$ nm, $2V_{\text{meas}} = 75\text{--}80^\circ$, $2V_{\text{calc}} = 77^\circ$, with orientation $X = b$ and $Y \wedge c$ 22–23° in the obtuse β angle, weak dispersion ($r < v$), and is pleochroic, with Y pale pink and Z pinkish gray. It is easily soluble in dilute cold $\text{HCl}_{(\text{aq})}$. The chemical composition from the average of electron microprobe analyses from 14 specimens (each 6–10 points) and a Penfield determination of H_2O is: CoO 34.88(40), MgO 2.97(10), MnO 2.41(5), FeO 0.40(2), NiO 0.53(2), P_2O_5 27.95(50), H_2O 29.50(50), sum 98.64 wt%, corresponding (on the basis of 5 non-H cations) to: $(\text{Co}_{2.38}\text{Mg}_{0.38}\text{Mn}_{0.17}\text{Ni}_{0.04}\text{Fe}_{0.03}^{2+})_{\Sigma 2.99}(\text{PO}_4)_{2.01} \cdot 8.35\text{H}_2\text{O}$, ideally $\text{Co}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$. Single-crystal X-ray study with a precession camera showed the mineral to be monoclinic, space group $C2/m$, $a = 10.034(4)$, $b = 13.341(3)$, $c = 4.670(3)$ Å, $\beta = 105.02(2)^\circ$, $V = 603.8$ Å³. Powder diffraction data were collected with a camera (type unspecified, 114.6 mm diameter, $\text{FeK}\alpha$ radiation) and yielded the strongest lines [d in Å (I , hkl): 7.84 (3,110), 6.67 (10,020), 4.85 (4,200), 3.84 (4,20 $\bar{1}$), 3.195 (6,13 $\bar{1}$), 2.948 (7,31 $\bar{1}$), 2.691 (7,221), 2.521 (6,24 $\bar{1}$), 2.408 (6,40 $\bar{1}$), 2.206 (3,241)]. $D_{\text{meas}} = 2.71(2)$ g/cm³ by flotation in dilute-Clerici solution, $D_{\text{calc}} = 2.71$ g/cm³ for $Z = 2$. Pakhomovskiyite is a new member of the isotypic vivianite group, and is the Co-analog of vivianite, and the P-analog of erythrite.

Pakhomovskiyite occurs in association with bakhchisaraitsevite, bobierite, magnetite, kovdorskite, rimkorolite, juonniite, nosethite, chalcopyrite, phlogopite, pyrrhotite, and pyrite. It is the last low-temperature hydrothermal mineral to form, and results from the dissolution of primary ore minerals by alkaline phosphate-bearing solutions. The mineral is named in honor of Yakov A. Pakhomovsky (b. 1948), a mineralogist of the Geological Institute of the Kola Science Center, Russian Academy of Sciences, who has made significant contributions to the mineralogy of the alkaline massifs of the Kola Peninsula. The mineral corresponds to IMA mineral no. 2004-021. Type material has been deposited in the Mineralogical Museum of St. Petersburg State University, Russia, and in the Geological and Mineralogical Museum of the Geological Institute of the Kola Science Center of the Russian Academy of Sciences, Apatity, Russia. **A.J.L.**

PERHAMITE

S. Mills, G. Mumme, I. Grey, P. Bordet (2006) The crystal structure of perhamite. *Mineral. Mag.*, 70, 201–209.

Perhamite was encountered at the Moculta quarry, Mount Lofty Ranges, South Australia, where it occurs as crandallite-like bladed rosettes on a matrix of apatite and quartz. Crystal quality precluded single-crystal structure analysis; however, crystals of perhamite from the Emmons pegmatite, Greenwood, Maine were sufficient for structure analysis. Four electron microprobe analyses of perhamite samples from the Emmons quarry gave

an average of P_2O_5 21.24, CaO 11.66, SiO_2 13.47, Al_2O_3 29.33, H_2O (by diff.) 24.2 wt%, very similar to the analysis of the type sample from the Bell pit, Newry, Maine. Upper-level precession photographs about c^* show trigonal symmetry. Single-crystal X-ray intensity data collection involving a CCD area detector (295 K; $\text{MoK}\alpha$; 847 total unique reflections, 618 unique observed [$F > 4\sigma(F)$] reflections; $R_1 = 0.070$, $R_{1\text{obs}} = 0.044$, $wR_2 = 0.157$) gave $a = 7.021(1)$, $c = 20.218$ Å, average space group $P\bar{3}m1$, $D_{\text{calc}} = 2.49$ g/cm³. The crystal structure consists of ordered blocks of a well-defined crandallite-type structure separated by ill-defined, disordered regions. The crandallite-type region shows six-coordinated Al and four-coordinated P; the disordered region shows TO_4 tetrahedra predominantly occupied by Si, and is cross-linked to the crandallite region by tetrahedra predominantly occupied by Al. Corner linking of the AlO_4 and SiO_4 tetrahedra results in 4-member rings that are interconnected in (001) planes to form chains. Framework connectivity between the crandallite and disordered regions results in zeolitic cavities occupied by Ca and H_2O . The average structure combined with the chemical analysis indicates that the formula of perhamite is $(\text{Ca},\text{Sr})_{3.7}\text{Al}_{7.7}\text{Si}_3\text{P}_4\text{O}_{23.5}(\text{OH})_{14.1} \cdot 8\text{H}_2\text{O}$. The authors discuss two possibilities for local ordering in the disordered region of the structure. One of these involves a non-centrosymmetric arrangement of AlO_4 and SiO_4 tetrahedra; the other involves five-coordinated Si. At the present it is not possible to state which model is more likely. **T.S.E.**

NEW DATA

ALLOCHALCOSELITE*

S.V. Krivovichev, S.K. Filatov, P.C. Burns, L.P. Vergasova (2006) The crystal structure of allochalcoseelite, $\text{Cu}^+\text{Cu}^{2+}_3\text{PbO}_2(\text{SeO}_3)_2\text{Cl}_5$. *Can. Mineral.*, 44, 507–514.

Single-crystal X-ray study of allochalcoseelite ($R1 = 0.047$), $\text{Cu}^+\text{Cu}^{2+}_3\text{PbO}_2(\text{SeO}_3)_2\text{Cl}_5$, indicated that it is monoclinic, space group $C2/m$, $a = 18.468(2)$, $b = 6.1475(8)$, $c = 15.314(2)$ Å, $\beta = 119.284(2)^\circ$, $V = 1516.5(3)$ Å³, $Z = 4$, $D_{\text{calc}} = 4.61$ g/cm³. Allochalcoseelite is only the second mineral known to contain both Cu^+ and Cu^{2+} positions (paramelaconite, Cu_4O_3 , is the other). The structure contains one Pb site coordinated by three O and four Cl atoms. There are two Se sites, which form SeO_3 trigonal pyramids. There are six Cu sites, four of which are occupied by Cu^{2+} and two [Cu5 and Cu6] by Cu^+ cations. The Cu1–Cu3 sites are in distorted octahedral coordination by O and Cl atoms. The Cu4 site occurs as a trigonal bipyramid, CuO_3Cl_2 . The Cu^+ cations are both coordinated by two Cl[−] anions to form linear anions $[\text{Cu}^+\text{Cl}_2]^-$, with Cl–Cu–Cl angles of 180°. The structure can be described in terms of arrangements of the strong $M\text{--O}$ bonds ($M = \text{Se}^{4+}$, Cu^{2+} and Pb^{2+}) in layers parallel to (100), with some of the Cl[−] anions sandwiched between them. The $[\text{SeO}_3]^{2-}$ pyramids are attached to oxocentered tetrahedra in “face-to-face” positions to form complex $([\text{O}_2\text{Cu}_5\text{Pb}][\text{SeO}_3]_2)^{4+}$ chains that are linked together to form a metal–oxygen layer parallel to (100). The layer has large pores that are occupied by the $[\text{Cu}^+\text{Cl}_2]^-$ anions, which are held in the structure via weak $\text{Cu}^{2+}\text{--Cl}^-$ bonds. Allochalcoseelite can be therefore considered as a host–guest system with $[\text{Cu}^+\text{Cl}_2]^-$ anions included into the Cu^{2+} oxoselenite chloride matrix. According to the authors, the relatively isolated and

weakly bonded positions of the $[\text{Cu}^+\text{Cl}_2]^-$ anions in the structure may indicate the stability of such complexes and their possible role in the transport of Cu by volcanic gases. **A.J.L.**

BERRYITE*

D. Topa, E. Makovicky, H. Putz, W.G. Mumme (2006) The crystal structure of berryite, $\text{Cu}_3\text{Ag}_2\text{Pb}_3\text{Bi}_7\text{S}_{16}$. *Can. Mineral.*, 44, 465–480.

Single-crystal X-ray study of berryite ($R1 = 0.064$), $\text{Cu}_3\text{Ag}_2\text{Pb}_3\text{Bi}_7\text{S}_{16}$, indicated that it is monoclinic, space group $P2_1/m$, $a = 12.703(2)$, $b = 4.0305(7)$, $c = 28.925(5)$ Å, $\beta = 102.484(2)^\circ$, $V = 1445.9(4)$ Å³, $Z = 2$, $D_{\text{calc}} = 6.90$ g/cm³. The average of ten electron microprobe analyses gave Cu 6.18(6), Ag 6.888(14), Pb 20.90(13), Bi 49.04(15), S 17.08(9), sum 100.08(26) wt%, corresponding to $\text{Cu}_{2.93}\text{Ag}_{1.92}\text{Pb}_{3.04}\text{Bi}_{7.07}\text{S}_{16.04}$ on the basis of 31 atoms. The structure of berryite shows modular affinities with the non-commensurate structure of cannizzarite, and with the pavonite homologous series, and is analogous to the modular structures of the synthetic compounds $\text{Ca}_2\text{Sb}_2\text{S}_5$ and $\text{La}_4\text{In}_5\text{S}_{13}$. There are three Pb sites, seven Bi sites, two Ag sites, 3 Cu sites and sixteen S sites in the asymmetric unit. The Pb sites and two Bi sites are located on the surfaces of PbS-like slabs four layers thick; four Bi sites and the Ag sites are located in the interior of the slabs. Copper atoms in triangular coordination lie in a single S layer, with pseudohexagonal geometry. The remaining Bi site straddles the pseudo-tetragonal PbS-like slab and the S–Cu layer. Three primitive pseudotetragonal subcells of the PbS-like slab match with two hexagonal subcells of the Cu–S layer; this semicomensurate lock-in structure is made possible by the extension of the a parameter of the PbS-like slab by insertion of wide AgS_{2+4} octahedra (linear S–Ag–S coordinations). Model structures of orthorhombic berryite (a polytypic variant) and of watkinsonite, $\text{Cu}_2\text{PbBi}_4(\text{Se},\text{S})_8$ are derived from that of monoclinic berryite. **A.J.L.**

BLIXITE*

S.V. Krivovichev, P.C. Burns, (2006) The crystal structure of $\text{Pb}_8\text{O}_5(\text{OH})_2\text{Cl}_4$, a synthetic analogue of blixite? *Can. Mineral.*, 44, 515–522.

Single-crystal X-ray study of hydrothermally synthesized $\text{Pb}_8\text{O}_5(\text{OH})_2\text{Cl}_4$ ($R1 = 0.047$), indicated that it is monoclinic, space group $C2/c$, $a = 26.069(5)$, $b = 5.8354(11)$, $c = 22.736(4)$ Å, $\beta = 102.612(6)^\circ$, $V = 3375.3(11)$ Å³, $Z = 8$, $D_{\text{calc}} = 7.53$ g/cm³. The crystal studied was twinned on (100). The compound $\text{Pb}_8\text{O}_5(\text{OH})_2\text{Cl}_4$ is considered very likely to be identical to the mineral blixite, empirical formula $(\text{Pb}_{1.95}\text{Ca}_{0.02})_{\Sigma 1.97}[\text{O}_{1.27}(\text{OH})_{0.41}\Sigma 1.68]\text{Cl}_{1.02}$, on the basis of similarity of chemical composition and the correspondence of the powder diffraction pattern calculated from the structure of $\text{Pb}_8\text{O}_5(\text{OH})_2\text{Cl}_4$ with the data measured for blixite. The unit-cell volume determined for $\text{Pb}_8\text{O}_5(\text{OH})_2\text{Cl}_4$ is exactly four times larger than that reported for blixite, and the authors suggest that the previous orthorhombic unit cell of blixite corresponds to a subcell. The structure is based (OPb₄) oxocentered tetrahedra that share edges to form $[\text{O}_5\text{Pb}_8]$ sheets parallel to (100). Hydroxyl groups form two short (OH)–Pb bonds that result in (OH)Pb₂ dimers attached to the $[\text{O}_5\text{Pb}_8]$ sheets. Chlorine

atoms link the $\{[\text{O}_5\text{Pb}_8](\text{OH})_2\}$ sheets in the third dimension. The structure is closely related to other structures based on PbO-type defect sheets. **A.J.L.**

EMILITE*

D. Topa, W.H. Paar, T. Balić-Žunić (2006) Emilite, $\text{Cu}_{10.72}\text{Pb}_{10.72}\text{Bi}_{21.28}\text{S}_{48}$, the last missing link of the bismuthinite-aikinite series? *Can. Mineral.*, 44, 459–464.

The structure and composition of the new mineral emilite were published before its complete description as a new mineral (2002, *Canadian Mineralogist*, 40, 239–245 and 982), and an abstract of that research was presented in *American Mineralogist*, 89, 1826. Complementary data are abstracted here.

Emilite is found in an assemblage of sulfides and sulfosalts in the quartz veins of the Felbertal scheelite deposit, located in the Hohe Tauern massif, about 10 km south of the town of Mittersill, Salzburg Province, Austria. The mineral occurs as small elongate crystals, not exceeding 0.3 mm in length and 0.1 mm in diameter, and is brittle, $\text{VHN}_{50-100} = 242-287$ kg/mm², $H = 3\frac{1}{2}-4$, opaque, tin-white, with a grayish black streak and metallic luster. It has uneven fracture and imperfect $\{0kl\}$ cleavage. In reflected light, emilite is creamy white, without internal reflections and with very weak bireflectance in air and in oil, whitish to yellowish tints. Anisotropy is moderate in air and in oil with greenish to grayish rotation tints under crossed polarizers. Reflectance values of emilite (in air, WTiC standard) are (R_1 – R_2) 39.40–46.95 (470 nm), 39.21–48.25 (546 nm), 38.98–48.35 (589 nm), and 38.30–44.69 (650 nm). Electron microprobe analysis of the two crystals used for structure determination gave Cu 7.50, 7.68; Pb 25.12, 25.42; Bi 50.07, 49.91; S 17.44, 17.60; sum 100.13, 100.61 wt%; corresponding (on the basis of $\text{Bi} + [(\text{Pb} + \text{Cu})/2] = 8$) to: $\text{Cu}_{2.63-2.68}\text{Pb}_{2.70-2.72}\text{Bi}_{5.34-5.30}\text{S}_{12.10-12.18}$, ideally $\text{Cu}_{2.68}\text{Pb}_{2.68}\text{Bi}_{5.32}\text{S}_{12}$. Single-crystal X-ray structure study ($R1 = 0.076$, 0.066) showed the mineral to be the Cu-rich 45 Å derivative in the bismuthinite-aikinite series: orthorhombic, space group $Pmc2_1$, $a = 4.0285(8)$, $b = 44.986(9)$, $c = 11.599(2)$ Å, $V = 2102.1(7)$ Å³. Powder diffraction data were calculated from the structure using Powder Cell 2.3 ($\lambda = \text{CuK}\alpha$), strongest lines [d in Å (l, hkl)] are 4.04 (49,082), 3.793 (21,140), 3.656 (100,043), 3.605 (49,141), 3.567 (81,0,12,1), 3.174 (71,142), 3.152 (78,181), 2.852 (95,182), 2.671 (46,1,12,1), 2.577 (49,084). $D_{\text{calc}} = 7.02$ g/cm³ for the ideal formula and $Z = 4$.

Emilite is the Cu-rich member of the bismuthinite-aikinite series with a periodicity of order equal to a fourfold multiple of the bismuthinite substructure motif. For comparison, the entire series follows with their chemical formulas recast to a basis of $\text{Bi} + [(\text{Pb} + \text{Cu})/2] = 8$ and $\text{S} = 12$ atoms, and their cell multiplicity listed relative to bismuthinite: bismuthinite, Bi_8S_{12} , onefold; pekoite, $\text{Cu}_{0.67}\text{Pb}_{0.67}\text{Bi}_{7.33}(\text{S},\text{Se})_{12}$, threefold; gladite, $\text{Cu}_{1.33}\text{Pb}_{1.33}\text{Bi}_{6.67}\text{S}_{12}$, threefold; salzburgite, $\text{Cu}_{1.6}\text{Pb}_{1.6}\text{Bi}_{6.4}\text{S}_{12}$, fourfold; paarite, $\text{Cu}_{1.7}\text{Pb}_{1.7}\text{Bi}_{6.3}\text{S}_{12}$, fivefold; krupkaite, $\text{Cu}_2\text{Pb}_2\text{Bi}_6\text{S}_{12}$, onefold; lindströmite, $\text{Cu}_{2.4}\text{Pb}_{2.4}\text{Bi}_{5.6}\text{S}_{12}$, fivefold; emilite, $\text{Cu}_{2.68}\text{Pb}_{2.68}\text{Bi}_{5.32}\text{S}_{12}$, fourfold; hammarite, $\text{Cu}_{2.67}\text{Pb}_{2.67}\text{Bi}_{5.33}\text{S}_{12}$, threefold; friedrichite, $\text{Cu}_{3.33}\text{Pb}_{3.33}\text{Bi}_{4.67}\text{S}_{12}$, threefold; aikinite, $\text{Cu}_4\text{Pb}_4\text{Bi}_4\text{S}_{12}$, onefold.

The mineral is associated with bismuthinite-derivative sulfosalts in the range krupkaite-hammarite, cannizzarite, cosalite,

galenobismutite, makovickyite, pavonite, and members of the gustavite-lillianite series, native Bi, chalcopyrite, and pyrite in the quartz veins, stringers and laminae of the metamorphosed scheelite deposit of Felbertal, Austria. The mineral is named in honor of Prof. Emil Makovicky (b. 1940), of the University of Copenhagen, in acknowledgement of his contributions to the crystal chemistry and modular description of diverse sulfosalts families, including those from the Felbertal deposit. The mineral corresponds to IMA mineral no. 2001-015. Type material is deposited under catalog number 14954 in the Mineral Reference Collection of the Division of Mineralogy, University of Salzburg, and at the Geological Institute and Museum of the University of Copenhagen. **A.J.L.**

FORMANITE-(Y)*

A.V. Voloshin, L.M. Lyalina, Ye.E. Savchenko, A.N. Bogdanova (2003) Formanite-(Y) from the amazonite randpegmatites of Western Keivy (Kola Peninsula). Zap. Vser. Mineral. Obshch., 132(1), 82–94 (in Russian).

Formanite-(Y) has been found to occur in the amazonite-bearing granitic “randpegmatites” (= marginal or stockscheider pegmatites) of Ploskaya Mt., Western Keivy area, Kola Peninsula, Russia. It forms faintly greenish to colorless, flattened prismatic crystals along the margins of plumbomicrocline crystals, but is more commonly found as narrow (0.2–0.3 mm thick) fracture fillings and veinlets within plumbomicrocline. It is metamict; heating between 600 and 850 °C induces the fergusonite (a.k.a. *T*-fergusonite) structure, whereas heating from 900 to 1100 °C induces the beta-fergusonite (a.k.a. *M*-fergusonite) structure. Electron microprobe analysis gives the compositional range $(Y_{0.60-0.81}Yb_{0.16-0.30}REE_{0.29-0.49})_{1.05-1.19}(Ta_{0.61-0.67}Nb_{0.23-0.30}Ti_{0.01-0.02})_{0.91-0.98}O_4$. In terms of the Nb/Ta ratio, there is a distinct composition gap between (earlier) fergusonite-(Y) and formanite-(Y) at Ploskaya Mt. The formanite-(Y) is riddled with inclusions of galena, native bismuth, löllingite and an unknown U–Pb oxide mineral.

Discussion. There are indexing errors in the monoclinic pattern (8 indices violate *I*-centering); nonetheless, the structural interpretations are valid. The question still remains as to whether the formanite-(Y) was tetragonal or monoclinic in its pre-metamict state. **T.S.E., J.K.**

GALENOBISMUTITE* (CL-BEARING)

D. Pinto, T. Balić-Žunić, E. Bonaccorsi, Y.S. Borodaev, A. Garavelli, C. Garbarino, E. Makovicky, N.N. Mosgova, F. Vurro (2006) Rare sulfosalts from Vulcano, Aeolian Islands, Italy. VII. Cl-bearing galenobismutite. Can. Mineral., 44, 443–457.

Galenobismutite, nominally $PbBi_2S_4$, collected from a high-temperature fumarole incrustation in the La Fossa crater of Vulcano, Italy, is shown to be enriched in chlorine. The Cl-bearing galenobismutite (with Cl ranging from 0.12–1.45 wt%) is commonly associated with bismuthinite, cannizzarite, galena, heyrovskýite, and lillianite, and rarely with kirkiite, vurroite, and other less well-characterized Pb–Bi sulfochlorides. The range of compositions determined from 28 electron microprobe analyses of several crystal fragments (in wt%) is: Pb 28.15–34.94 (mean 31.37, σ 1.67), Bi 47.36–55.34 (mean 50.56, σ 1.95), S 14.72–

16.60 (mean 15.98, σ 0.35), Se 0.40–1.03 (mean 0.86, σ 0.14), Cl 0.12–1.45 (mean 0.85, σ 0.33), As 0–0.23 (mean 0.07, σ 0.09), Ag 0–0.23 (mean 0.03, σ 0.05), Zn 0–0.22 (mean 0.02, σ 0.05), Cu 0–0.10 (mean 0.01, σ 0.02). Single-crystal X-ray structure study of two samples ($R1 = 0.0310$, conventional X-ray source; 0.0149, synchrotron X-ray source) showed the structure of Cl-bearing galenobismutite to be topologically identical to that of Cl-free galenobismutite. The composition (from electron microprobe analysis) of the refined crystal with $R1 = 0.0310$ is $(Pb_{1.14}Bi_{1.85})_{\Sigma 2.99}(S_{3.75}Se_{0.09}Cl_{0.17})_{\Sigma 4.01}$, with unit-cell parameters in space group *Pnam*: $a = 11.832(1)$, $b = 14.640(2)$, $c = 4.0817(4)$ Å, $V = 707.0(1)$ Å³. $D_{calc} = 7.10$ g/cm³ for the empirical formula and $Z = 4$. The principal mechanism of Cl substitution into galenobismutite is the coupled exchange mechanism $Pb^{2+} + Cl^- \leftrightarrow Bi^{3+} + S^{2-}$, and the proportion of this coupled exchange is approximately linearly correlated with increases in the *a* and *b* cell dimensions. Evidence of a preferential distribution of Cl among the anion positions was not observed. The general empirical formula for Cl-bearing galenobismutite may be expressed as $Pb_{1+x}Bi_{2-x}(S_{4-x}Cl_xSe_y)$ with $0 < x < 0.3$ and $0 < y < 0.2$. **A.J.L.**

GORCEIXITE*

T.J. Dzikowski, L.A. Groat, J.L. Jambor (2006) The symmetry and crystal structure of gorceixite, $BaAl_3[(PO_3(O,OH))_2(OH)]_6$, a member of the alunite supergroup. Can. Mineral., 44, 951–958.

Re-investigation of the structure of gorceixite, $BaAl_3[(PO_3(O,OH))_2(OH)]_6$, by single-crystal X-ray methods ($R1 = 0.023$) indicated that it is rhombohedral, space group $R\bar{3}m$, with cell parameters $a = 7.0538(3)$, $c = 17.2746(6)$ Å, $V = 744.36(5)$ Å³, $Z = 3$, $D_{calc} = 3.42$ g/cm³. The results of electron microprobe analysis are consistent with full occupancy of the Ba site, but in the crystal structure analysis the site refines to 88% occupancy. The reason for this discrepancy is not clear. Although $R\bar{3}m$ is the most appropriate space group for the crystal studied, the authors do not insist that all gorceixite samples adopt this space group. Rather, it is suggested that different conditions of formation and compositions may be responsible for the lower symmetry (space group *Cm*) previously reported for the species, although the mechanism causing the adoption of lower symmetry is not determined. **A.J.L.**

HOLFERTITE*

D. I. Belakovskiy, L.A. Pautov, E. Sokolova, F.C. Hawthorne, A.V. Mokhov (2006) Holfertite, a new hydroxyl-hydrated uranium titanate from Starvation Canyon, Thomas Range, Utah. Mineral. Record, 37, 311–317.

The structure and composition of the new mineral holfertite were published before its complete description as a new mineral (2005, *Canadian Mineralogist*, 43, 1545–1552), and an abstract of that research was presented in *American Mineralogist*, 91, 1204. Complementary data are abstracted here.

Holfertite, ideally $U_{1.75}^{6+}Ti^{4+}Ca_{0.25}O_{7.5}(H_2O)_3$ or $U_{1.75}^{6+}Ti^{4+}Ca_{0.25}O_{7.17}(OH)_{0.67}(H_2O)_3$, occurs as a pneumatolytic phase with hematite, bixbyite, fluorite, topaz, and red beryl in cavities and fractures in rhyolite from Starvation (formerly Searle) Canyon, Thomas Range, Utah, U.S.A. The crystals are often hollow and

form elongated hexagonal prisms up to 1×5 mm. The mineral is brittle, $H = 4$, translucent to transparent, canary-yellow to orange-yellow with a pale yellow streak and adamantine luster. It has perfect cleavage on $\{110\}$ and an uneven to conchoidal fracture. Holfertite is non-pleochroic, colorless, uniaxial positive, ω 1.815(8), ε 1.910(8) for $\lambda = 590$ nm. Powder diffraction data were collected with a Debye-Scherrer camera (57.3 mm diameter, FeK α radiation) and yielded the strongest lines [d in Å (I): 4.60 (10), 3.05 (2), 2.90 (8), 1.87 (3), 1.747 (3), 1.531 (2), 1.211 (3). $D_{\text{calc}} = 4.22$ for the empirical formula $\text{U}_{1.74}^{6+}\text{Ti}_{0.97}^{4+}\text{Ca}_{0.27}\text{Fe}_{0.04}^{3+}\text{K}_{0.04}\text{O}_{7.5}(\text{H}_2\text{O})_3$, 4.26 g/cm³ for the empirical formula $\text{U}_{1.74}^{6+}\text{Ti}_{0.97}^{4+}\text{Ca}_{0.27}\text{Fe}_{0.04}^{3+}\text{K}_{0.04}\text{O}_{7.17}(\text{OH})_{0.67}(\text{H}_2\text{O})_3$, and $Z = 3$. The mineral corresponds to IMA mineral no. 2003-009.

The color, habit, X-ray diffraction pattern, crystal class, and cell dimensions of holfertite resemble those of an unnamed Ca-U-Ti-HREE oxide mineral described in 1995 by Foord et al. from the same locality (*Mineralogical Record*, 26, 122–128). However, the authors point out that the reports of the two phases differ considerably in chemical composition, optical properties, and density, and suggest that the previous investigation may have mistakenly conflated two separate materials. **A.J.L.**

HORSFORDITE

M.N. Feinglos, B.B. Cannon V, F.H. Cocks (2006) The true nature of "horsfordite". *Can. Mineral.*, 44, 409–413.

Horsfordite was described in 1888 as a mineral species with composition Cu_5Sb from the area of Mytilene (formerly Lesbos, now Lesvos, Mytilini or Mitilini). Both copper-, and antimony-mineralization occur in the region, but neither recent data nor recent samples of horsfordite are known. A specimen labeled horsfordite, from the Ferrier Collection at the Redpath Museum, McGill University, the acquisition of which dates to the time of the original description of the species, was investigated with an electron microprobe. The specimen consists of a mixture of antimony-bearing copper, a phase of nominal composition Cu_4Sb , and a phase of nominal composition Cu_3Sb . The bulk composition of this three-phase mixture corresponds to that reported originally for horsfordite. The dendritic texture of the intergrown phases and the presence of vacuoles are consistent with the mixture being a metallurgical product; evidence of its existence in Nature is lacking.

Discussion. Horsfordite appears to be discredited as a mineral species by these findings. In the literature, it has long been considered an inadequately described species, for which no original type material is available. Formal approval by the IMA Commission on New Minerals and Mineral Names of the discreditation of horsfordite (cf. *American Mineralogist*, 75, 928–930) does not appear to have been obtained. **A.J.L.**

JAGUÉITE*, CHRISSTANLEYITE*

D. Topa, E. Makovicky, T. Balić-Žunić (2006) The crystal structures of jaguéite, $\text{Cu}_2\text{Pd}_3\text{Se}_4$, and chrisstanleyite, $\text{Ag}_2\text{Pd}_3\text{Se}_4$. *Can. Mineral.*, 44, 497–505.

Single-crystal X-ray structure study of jaguéite, ideally $\text{Cu}_2\text{Pd}_3\text{Se}_4$, and of chrisstanleyite, ideally $\text{Ag}_2\text{Pd}_3\text{Se}_4$, has confirmed that the two species are isostructural. The minerals are

monoclinic, space group $P2_1/c$. Jaguéite ($R1 = 0.0552$) has cell parameters $a = 5.672(5)$, $b = 9.909(9)$, $c = 6.264(6)$ Å, $\beta = 115.40(2)^\circ$, $V = 318.0(5)$, $Z = 2$, $D_{\text{calc}} = 7.96$ g/cm³ for the ideal formula. Chrisstanleyite ($R1 = 0.083$) has cell parameters $a = 5.676(2)$, $b = 10.342(4)$, $c = 6.341(2)$ Å, $\beta = 114.996(4)^\circ$, $V = 337.3(2)$, $Z = 2$, $D_{\text{calc}} = 8.38$ g/cm³ for the ideal formula, $D_{\text{calc}} = 8.20$ g/cm³ for the empirical formula. The crystal of chrisstanleyite investigated was twinned, twin law matrix $[100/0\bar{1}0/\bar{1}0\bar{1}]$ with (001) as the twin plane. Electron microprobe analysis for jaguéite and chrisstanleyite gave Cu 15.70, 3.09; Ag 1.59, 20.55; Pd 42.04, 38.64; Se 40.15, 37.54; sum 99.48, 99.82 wt%, respectively, corresponding (on the basis of 9 atoms) to: $\text{Cu}_{1.91}\text{Ag}_{0.11}\text{Pd}_{3.05}\text{Se}_{3.93}$ for jaguéite, and $\text{Cu}_{0.41}\text{Ag}_{1.59}\text{Pd}_{3.03}\text{Se}_{3.97}$ for chrisstanleyite. The structure contains two Pd sites, one Cu (or Ag) site and two Se sites. The Pd sites are in square planar coordination by Se, to form PdSe_4 squares, whereas the d^{10} cation site (Cu or Ag) is coordinated by Se to form an elongated tetrahedron. Atom Pd1 forms isolated square arrangements PdSe_4 , whereas the adjacent arrangements involving Pd2 are paired via a common edge. The (Cu,Ag) coordination tetrahedra form (100) layers which, together with the Pd2–Cu(Ag)–Pd1–Cu(Ag)–Pd2 system of metal–metal bonds, help to stabilize the framework structure composed of PdSe_4 squares. In contrast to jaguéite, the d^{10} cation site in chrisstanleyite is modeled as a split position with Ag (80% occupancy) separated from Cu (20% occupancy) by 0.37 Å. Jaguéite and chrisstanleyite are members of a new structure-type, for which a sulfide analog is lacking.

Discussion. The calculated density reported for chrisstanleyite is erroneous; corrected values are given above. **A.J.L.**

KIRKIITE*

E. Makovicky, T. Balić-Žunić, L. Karanović, D. Poleti (2006) The crystal structure of kirkiite, $\text{Pb}_{10}\text{Bi}_3\text{As}_3\text{S}_{19}$. *Can. Mineral.*, 44, 177–188.

Single-crystal X-ray structure study of kirkiite, $\text{Pb}_{10}\text{Bi}_3\text{As}_3\text{S}_{19}$, ($R1 = 0.069$), indicated that it is monoclinic, space group $P2_1/m$, with cell parameters $a = 8.621(4)$, $b = 26.03(1)$, $c = 8.810(4)$ Å, $\beta = 119.21(1)^\circ$, $V = 1726(1)$ Å³, $Z = 2$, $D_{\text{calc}} = 6.80$ g/cm³ (for the ideal formula). The mineral is strongly pseudo-hexagonal and commonly twinned with (20 $\bar{1}$) as the twin plane and [100] as the twin axis. The distortion of the pseudo-hexagonal lattice is in accordance with the alignment of lone-electron-pair micelles in rows parallel to (001). The structure can be described as composed of slabs based on a transitional PbS–SnS archetype, with tightly bonded layers parallel to (083) of kirkiite; the slabs are unit-cell-twinned on (010) reflection planes. Kirkiite and jordanite, $\text{Pb}_{28}\text{As}_{12}\text{S}_{46}$, are two members of a homologous series whose general formula is $\text{Pb}_{8N-4}\text{Me}_{12}^3\text{S}_{8N+14}$. The data resolve previous uncertainties about the symmetry and space group of kirkiite, which had been suggested to be either orthorhombic or monoclinic, and because of its pseudosymmetry, to have apparent space group $P6_322$ (cf. abstract in *American Mineralogist*, 71, 1278–1279). **A.J.L.**

LENAITE*

L. Bindi, P.G. Spry, G. Pratesi (2006) Lenaite from the Gies gold–silver telluride deposit, Judith Mountains, Montana,

USA: occurrence, composition, and crystal structure. *Can. Mineral.*, 44, 177–188.

Lenaite, AgFeS_2 , is described from its fourth locality worldwide, and its structure determined. A sample of the mineral in the mineralogical collection of the Natural History Museum of Florence is from the Gies gold–silver telluride deposit, Judith Mountains, Montana. It occurs as anhedral grains up to 0.2 mm across, $\text{VHN}_{10} = 285 \text{ kg/mm}^2$, $H = 4\text{--}4\frac{1}{2}$, steel-gray with a black streak and no cleavage. In reflected light, lenaite is grayish white, non-pleochroic, moderately anisotropic in yellowish tints, and shows no birefractance. Reflectance values of the mineral (in air, SiC standard) are (R_1 – R_2): 28.2–30.6 (471.1 nm), 31.8–35.8 (548.3 nm), 32.8–36.5 (586.6 nm), and 30.9–35.0 (652.3 nm). The average of six electron microprobe analyses on the same crystal gave Ag 45.86(40), Fe 24.97(30), S 28.53 (30), sum 99.36 wt%, corresponding (on the basis of 4 atoms) to: $\text{Ag}_{0.96}\text{Fe}_{1.01}\text{S}_{2.02}$. Single-crystal X-ray structure study of lenaite ($R1 = 0.0363$), indicated that it is isostructural with chalcopyrite: tetragonal, space group $I\bar{4}2d$, with cell parameters $a = 5.4371(2)$, $c = 10.8479(9)$ Å, $V = 320.69(3)$ Å³, $Z = 4$, $D_{\text{calc}} = 4.72 \text{ g/cm}^3$ (for the ideal formula). The space group determined differs from that originally proposed on the basis of powder diffraction data, $P4_2mc$, (cf. *American Mineralogist*, 81, 1283); the present authors question the purity of the type material.

Discussion. The reflectance values listed above are given at wavelengths within 3 nm of the four standard wavelengths recommended by the IMA Commission on Ore Mineralogy: 470, 546, 589, and 650 nm. **A.J.L.**

MISERITE*

I.V. Rozhdstvenskaya, M.D. Evdokimov (2006) Refinement of the miserite crystal structure ($\text{K}_{1.29}\text{□}_{0.21}$)[$\text{Ca}_{5.51}\text{M}_{0.49}^{2+}$]($\text{Si}_6(\text{O},\text{OH})_{15}$)(Si_2O_7)(F,OH)₂·0.25H₂O (M = Y, REE, Fe, Ti, Mn, Mg, Na) from the Dara-i-Pioz occurrence, Pamirs, Tajikistan. *Dokl. Earth Sci.*, 406, 74–78 (in English); *Dokl. Akad. Nauk*, 406, 236–240 (in Russian).

The crystal structure of miserite from the Dara-i-Pioz deposit has been refined from single-crystal X-ray $\text{MoK}\alpha$ diffraction data (2589 independent reflections, sample shape corrections by DIFABS) giving $a = 10.120(3)$, $b = 16.079(3)$, $c = 7.378(3)$ Å, $\alpha = 96.62(2)$, $\beta = 111.15(2)$, $\gamma = 76.33(2)^\circ$, space group $P\bar{1}$, $Z = 2$, $R = R_w = 0.043$, $\text{GoF} = 1.04$. Electron microprobe analysis and L.O.I. gave the empirical formula $\text{K}_{1.33}(\text{Ca}_{5.52}\text{Y}_{0.18}\text{REE}_{0.18}\text{Fe}_{0.04}\text{Mn}_{0.03}\text{Mg}_{0.02}\text{Na}_{0.02}\text{Ti}_{0.01})(\text{Si}_{7.99}\text{Al}_{0.01})(\text{O},\text{OH})_{22}(\text{OH}_{1.45}\text{F}_{0.55})$. The refinement confirms the basic structural features of Scott (1976, *Can. Mineral.*, 14, 515–528). Newly recognized features from the current refinement include: (1) Only Ca1 is completely occupied by Ca. Instead of ordered into one site, REE and Y are dispersed over the other 6 Ca sites, with Ca6 showing the strongest preference. (2) The Z site of Scott (1976) is shown to be fractionally occupied by K, not dominantly occupied by Ca. (3) There is considerable occupancy of the F site by OH. (4) The ideal formula is $\text{K}_{1.5-x}(\text{Ca}, \text{Y}, \text{REE})_{25}[\text{Si}_6\text{O}_{15}][\text{Si}_2\text{O}_7](\text{OH}, \text{F})_2\cdot\text{yH}_2\text{O}$. **T.S.E.**

PADĚRAITE*

D. Topa, E. Makovicky (2006) The crystal structure of padĚraite, $\text{Cu}_7(\text{X}_{0.33}\text{Pb}_{1.33}\text{Bi}_{11.33})_{\Sigma 13}\text{S}_{22}$, with X = Cu or Ag: new data and interpretation. *Can. Mineral.*, 44, 481–495.

Re-investigation of the structure of padĚraite by single-crystal X-ray methods, using both Ag-bearing and Ag-free materials, has confirmed that it is monoclinic, space group $P2_1/m$. For the Ag-bearing material, $R1 = 0.0772$, $a = 17.585(4)$, $b = 3.9386(9)$, $c = 28.453(7)$ Å, $\beta = 105.41(1)^\circ$, $V = 1899.8(8)$ Å³, $Z = 2$, $D_{\text{calc}} = 6.69 \text{ g/cm}^3$. For the Ag-free material, $R1 = 0.0504$, $a = 17.573(2)$, $b = 3.9426(4)$, $c = 28.423(3)$ Å, $\beta = 105.525(2)^\circ$, $V = 1897.3(6)$ Å³, $Z = 2$, $D_{\text{calc}} = 6.69 \text{ g/cm}^3$. Electron microprobe analysis of the two crystals used for structure determination (average of 4 and 6 points, respectively) gave Cu 11.83(2), 12.08(6); Ag 0.51(1), 0; Pb 7.44(5), 7.24(6); Bi 61.88(11), 61.71(24); Sb 0.10(1), 0.09(1), Te 0.23(1), 0; S 18.49(2), 18.33(4); sum 100.48(11), 99.45(24) wt%; corresponding (on the basis of 42 atoms) to: $\text{Cu}_{7.09}\text{Ag}_{0.18}\text{Pb}_{1.37}\text{Bi}_{11.28}\text{Sb}_{0.03}\text{S}_{21.98}\text{Te}_{0.07}$ and $\text{Cu}_{7.30}\text{Pb}_{1.34}\text{Bi}_{11.35}\text{Sb}_{0.03}\text{S}_{21.97}$, respectively. The structural results are similar to those of W.G. Mumme (1986, *Canadian Mineralogist*, 24, 513–521), but with superior resolution of the site occupancies, and the resultant structure is re-interpreted in a modular description as an intergrowth of “Q slabs,” which on their own make up a structure related to nordströmite or kobellite, with kupĚkite-like “K slabs”. A homologous series based on KQ^n derivatives of padĚraite is discussed along with regular intergrowths of padĚraite and the cuprobismutite homologous series. **A.J.L.**

PEARCEITE*

L. Bindi, M. Evain, S. Menchetti (2006) Temperature dependence of the silver distribution in the crystal structure of natural pearceite, $(\text{Ag},\text{Cu})_{16}(\text{As},\text{Sb})_2\text{S}_{11}$. *Acta Cryst.*, B62, 212–219.

Single-crystal X-ray structure study of pearceite, $(\text{Ag},\text{Cu})_{16}(\text{As},\text{Sb})_2\text{S}_{11}$, at 300, 120, and 15 K ($R1 = 0.046$ for the refinement at 300 K), indicated that it is trigonal, space group $P\bar{3}m1$, with cell parameters (at 300 K) $a = 7.3876(4)$, $c = 11.8882(11)$ Å, $V = 561.89(5)$ Å³, $Z = 1$, $D_{\text{calc}} = 6.31 \text{ g/cm}^3$ (for the composition determined by structure refinement). The average of seven electron microprobe analyses yielded the chemical formula $(\text{Ag}_{12.15}\text{Cu}_{3.84})_{\Sigma 15.99}(\text{As}_{1.18}\text{Sb}_{0.83})_{\Sigma 2.01}\text{S}_{11.00}$, in agreement with that derived from the structural analysis at 300 K, $(\text{Ag}_{13.03}\text{Cu}_{2.97})_{\Sigma 16}(\text{As}_{1.18}\text{Sb}_{0.82})_{\Sigma 2}\text{S}_{11}$. The crystal structure can be described as a regular alternation of two kinds of layers along stacked along the c axis: the first layer, ~6.15 Å thick, has general composition $[(\text{Ag},\text{Cu})_6(\text{As},\text{Sb})_2\text{S}_7]^{2-}$, and the second layer, ~5.75 Å thick, has general composition $[\text{Ag}_9\text{Cu}_4\text{S}_4]^{2+}$. The (As,Sb) atoms form isolated (As,Sb)S₃ pyramids, as typically occur in sulfosalts, and copper atoms link two S atoms in linear coordination, whereas the silver atoms are highly disordered and are distributed along well-defined diffusion-like paths joining low-coordination sites. The diffusion-like paths for silver have been determined by means of a combination of a Gram–Charlier description of the anisotropic displacement parameters and a split-atom model.

According to the authors, as the temperature decreases the silver positions (electron densities) condense into better defined modes but, contrary to what is commonly observed for classical ionic conductors such as argyrodite, the joint probability density function still exhibits a strong overlapping of neighboring sites and the disorder is not resolved. **A.J.L.**

POLYBASITE*

M. Evain, L. Bindi, S. Menchetti (2006) Structural complexity in minerals: twinning, polytypism and disorder in the crystal structure of polybasite, $(\text{Ag,Cu})_{16}(\text{Sb,As})_2\text{S}_{11}$. *Acta Cryst.*, B62, 447–456.

Single-crystal X-ray structure study of two twinned samples of polybasite, $(\text{Ag,Cu})_{16}(\text{Sb,As})_2\text{S}_{11}$, at 120 and 100 K, respectively, have shown that at least two polytypes exist, 221-polybasite, and 222-polybasite. The average of eight electron microprobe analyses yielded the chemical formula (on the basis of 29 atoms): $(\text{Ag}_{14.27}\text{Cu}_{1.69(8)}\text{Zn}_{0.03}\text{Bi}_{0.01})_{\Sigma 16}(\text{Sb}_{1.99}\text{As}_{0.08})_{\Sigma 2.07}(\text{S}_{10.77}\text{Se}_{0.16(2)})_{\Sigma 10.93}$ for 221-polybasite, and $(\text{Ag}_{14.48}\text{Cu}_{1.29}\text{Pb}_{0.01}\text{Bi}_{0.01})_{\Sigma 15.79}(\text{Sb}_{1.98}\text{As}_{0.09})_{\Sigma 2.07}\text{S}_{11.14}$ for 222-polybasite, in agreement with the formulas derived from the structure refinements: $\text{Ag}_{14.52}\text{Cu}_{1.48}\text{Sb}_2\text{S}_{11}$ and $\text{Ag}_{14.814}\text{Cu}_{1.186}\text{Sb}_2\text{S}_{11}$, respectively. Refinement of the 221-polybasite structure at 120 K ($R1 = 0.036$) indicated that it is trigonal, space group $P321$, $a = 15.0954(12)$, $c = 11.8825(8)$ Å, $V = 2344.9(3)$ Å³, $Z = 4$, $D_{\text{calc}} = 6.39$ g/cm³. Refinement of the 222-polybasite structure at 100 K ($R1 = 0.050$) indicated that it is monoclinic (pseudo-orthorhombic), space group $C2/c$, $a = 26.188(3)$, $b = 15.1199(18)$, $c = 23.784(3)$ Å, $\beta = 90^\circ$, $Z = 16$, $D_{\text{calc}} = 6.40$ g/cm³; no experimental uncertainty is given for the angle β . These structures are closely related to that of pearceite (*Acta Crystallographica*, B62, 212–219), and consist of the stacking of $[(\text{Ag,Cu})_6\text{Sb}_2\text{S}_7]^{2-}$, and $[\text{Ag}_9\text{CuS}_4]^{2+}$ module layers along the c axis. The Sb atoms form isolated SbS_3 pyramids, as typically occur in sulfosalts, and copper atoms link two S atoms in linear coordination, and silver occupies sites with coordination ranging from quasi-linear to almost tetrahedral. In contrast to pearceite, the metal atoms in both types of polybasite do not exhibit positional disorder. The stacking sequences of the layers in 221-polybasite and 222-polybasite differ, and the nature of the structure adopted appears to be a function of the Cu content. With low substitution of Cu for Ag, the symmetry is monoclinic (222-polybasite), and with increasing Cu the average symmetry becomes trigonal (221-polybasite). A further increase gives rise to a folding of the cell along the a and b dimensions as found in

the pearceite structure.

Discussion. These structures are closely related to that of pearceite, and the prefixes 221- and 222- refer to the size of the unit cell (in a trigonal or pseudo-trigonal setting) as multiples of a common pearceite-like subcell of approximate dimensions $a = 7.4$, $c = 11.9$ Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 120^\circ$. Thus, for trigonal 221-polybasite with cell dimensions $a = 15.095$ and $c = 11.883$ Å, the transformation matrix from the small trigonal subcell to the true cell is $[200/020/001]$, giving rise to the 221-prefix. For 222-polybasite, the C -centered pseudo-orthorhombic cell $a = 26.188$, $b = 15.120$, $c = 23.784$ Å, $\beta = 90^\circ$, can be transformed by the matrix $[\frac{1}{2}\frac{1}{2}0/\frac{1}{2}\frac{1}{2}0/001]$ to a pseudotrigonal cell $a = 15.120$, $c = 23.784$ Å. The transformation matrix from the small trigonal subcell to this larger pseudotrigonal cell is $[200/020/002]$, giving rise to the 222-prefix. The use of such prefixes is not in accord with the previous schemes of nomenclature used for minerals of the polybasite group, and does not appear to have been approved by the IMA-CNMMN. In addition, as there appears to be a compositional control on the nature of the structures in the polybasite group (e.g., Cu content), these structures should likely be considered polytypoids, rather than a family of polytypes. **A.J.L.**

STRONALSITE*, BANALSITE*

R.P. Liferovich, A.J. Locock, R.H. Mitchell, A.K. Shpachenko (2006) The crystal structure of stronalsite and a redetermination of the structure of banalsite. *Can. Mineral.*, 44, 533–546.

Single-crystal X-ray structure study of stronalsite, $\text{SrNa}_2\text{Al}_4\text{Si}_4\text{O}_{16}$, ($R1 = 0.043$), and of two crystals of banalsite, $\text{BaNa}_2\text{Al}_4\text{Si}_4\text{O}_{16}$, ($R1 = 0.031, 0.027$), has confirmed that the two minerals are isostructural, and crystallize in the orthorhombic non-centrosymmetric space group $Iba2$, rather than the centrosymmetric space group $Ibam$ previously assigned to banalsite. The structural models are similar, but the lower symmetry results from the ordering of Al and Si onto separate tetrahedral sites. Unit-cell parameters for stronalsite are: $a = 8.4080(9)$, $b = 9.8699(11)$, $c = 16.7083(18)$ Å, $V = 1386.6(3)$ Å³, $Z = 4$, $D_{\text{calc}} = 2.92$ g/cm³; for banalsite from Wales: $a = 8.5400(7)$, $b = 10.0127(9)$, $c = 16.7897(14)$ Å, $V = 1435.7(2)$ Å³, $D_{\text{calc}} = 3.05$ g/cm³; for banalsite from Sweden: $a = 8.5068(16)$, $b = 9.9811(18)$, $c = 16.7485(31)$ Å, $V = 1422.1(5)$ Å³, $D_{\text{calc}} = 3.08$ g/cm³. The data resolve previous uncertainties about the symmetry and space group of stronalsite and banalsite. **A.J.L.**