

## New Mineral Names\*

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### CALVERTITE\*

J.L. Jambor, A.C. Roberts, L.A. Groat, C.J. Stanley, A.J. Criddle, and M.N. Feinglos (2007) Calvertite, Cu<sub>5</sub>Ge<sub>0.5</sub>S<sub>4</sub>, a new mineral species from Tsumeb, Namibia. Can. Mineral., 45, 1519–1523.

Calvertite was discovered during the examination of another new mineral (gallobeaudanite) from the Tsumeb mine. The un-oxidized portions of the sample in which calvertite was found consist mainly of calvertite and reinerite with minor tennantite and gallite inclusions. Calvertite occurs in a granular texture formed by a network of chalcocite veins. The calvertite grains are anhedral, elongate to elliptical with the largest grains up to 100 µm across. The calvertite postdates the reinerite as evidenced by veins of calvertite cutting reinerite. Other associated minerals in the sample are goethite, hematite, quartz, Hg-rich native silver, stolzite, otjisumerite, and various members of the alunite supergroup.

Calvertite has a metallic luster, irregular to conchoidal fracture, brittle tenacity, and no cleavage or parting. It is macroscopically black. The VHN is 283 kg/mm<sup>2</sup> (Mohs hardness 4 to 5). It is opaque and pale bluish-gray in reflected light. No birefringence, pleochroism, or internal reflections were observed. Reflectance percentages in air are 26.3 (470 nm), 23.1 (546), 22.2 (589), and 21.5% (650).

Chemical composition was measured using an electron microprobe. Weight percent results (and ranges in parentheses) are as follows: Cu 63.10 (62.55–63.70), Fe 1.66 (1.49–1.84), Zn 0.55 (0.22–0.92), Ge 5.76 (5.58–5.98), As 1.50 (1.35–1.56), Ga 0.36 (0.31–0.39), V 0.05 (0.04–0.05), S 26.63 (26.4–26.78), corresponding to an empirical formula (based of four S atoms per formula unit) of (Cu<sub>4.782</sub>Fe<sub>0.143</sub>Zn<sub>0.041</sub>Ga<sub>0.025</sub>V<sub>0.005</sub>)<sub>Σ4.996</sub>(Ge<sub>0.382</sub>As<sub>0.096</sub>)<sub>Σ0.478</sub>S<sub>4</sub>, Z = 1,  $D_{\text{calc}}$  = 5.239 g/cm<sup>3</sup>.

The powder diffraction pattern for calvertite consists of only four lines: [ $d$  in Å ( $I\%$ ,  $hkl$ )]: 3.053(100, 111), 2.639(10, 200), 1.869(90, 220), and 1.595(30, 311). These lines do not definitively identify the mineral. The X-ray pattern of synthetic Cu<sub>5</sub>GeS<sub>4</sub> also consists only of four lines, all of which moderately match those of calvertite. The strongest lines of reinerite, germanocolusite, and germanite also agree well with those of calvertite.

Single-crystal X-ray studies of a grain removed from a polished section indicate the mineral is cubic, with  $a$  = 5.337(1) with allowable space groups of *Fm3m*, *F432*, and *F43m*. A re-analysis a year later of the same single crystal produced no reflections, but the original powder sample showed no change after 11 years.

The authors suggest that the small unit cell and the unstable character of calvertite indicate that it is a metastable, highly disordered mineral whose ordered equivalent would be Cu<sub>10</sub>GeS<sub>8</sub> with  $a$  = 2 × 5.337 Å. It is named for Lauriston (Larry) Derwent Calvert (1924–1993) of the National Research Council, Ottawa, Canada. Cotype polished sections of calvertite are in the Canadian Museum of Nature, Ottawa (CMNMC 85731), and the Natural History Museum, London, U.K. (BM 2004, 78). G.P.

### CASSAGNAITE\*

R. Basso, C. Carbone, and A. Palenzona (2008) Cassagnaite, a new, V-bearing silicate mineral from the Cassagna mine, northern Apennines, Italy. Eur. J. Mineral., 20, 95–100.

Cassagnaite is a new mineral found in the Val Graveglia manganese district (Northern Apennines, Liguria, Italy) at the Cassagna mine. Cassagnaite was found in fractures in braunit + quartz layered mineralization, together with piemontite. Hydrothermal fluid circulation, along later extensional fractures under decreasing *P-T* metamorphic conditions, induced the concentration of commonly dispersed elements that were involved into the genesis of As-, Ba-, Cu-, Sr-, and V-rich mineral assemblages. Vanadium minerals have been previously discovered at the two other mines in the area (Gambatesa and Molinello mines) such as cavoite, medaite, palenzonite, repaiata, saneroite, tiragalloite, vanadiocarpholite, and vanadomalayaite, this is the first time a newly described vanadium mineral was discovered at this mine. Cassagnaite appears as very rare isolated prismatic to tabular {001} crystals, usually elongated along [100], and as entangled aggregates of a few crystals. The crystals are generally very small, with a maximum size of 0.06 mm.

Cassagnaite is transparent with vitreous luster, golden brown in color, and the streak is nearly white. The morphology of the crystals is generally dominated by the prism {011} and the pinacoids {001} and {100}. It is brittle and exhibits {001} cleavage (or parting). Due to the unusual scarcity of available material and to the reduced size of the crystals, the determinations of physical and optical properties are not complete. The calculated density is 3.22 g/cm<sup>3</sup>. The mineral does not fluoresce under short and long-

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

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wave ultraviolet light. Optically, cassagnaite is biaxial and some optical measurements were performed on the largest face, likely parallel to the {001} cleavage, of a prismatic crystal elongated along [100]. The refractive index values are  $N$  (parallel to  $a$ ): 1.810 ( $\pm 0.005$ ) and  $n$ : 1.800 ( $\pm 0.005$ ), measured by Cargille's liquids at 25 °C ( $\lambda = 589$  nm). The pleochroism is very weak:  $N$  = golden yellow-brown and  $n$  = pale golden yellow-brown.

The crystal structure, refined in the space group  $Cmcm$  with unit-cell parameters  $a = 6.066(1)$  Å,  $b = 8.908(1)$  Å,  $c = 18.995(2)$  Å, and  $Z = 2$ , may be described as a layer stacking along [001] of a fundamental building block of composition  $[M1_2(OH)_2(SiO_4)]^{4-}$  that alternates with intersheets, randomly occurring in a ratio ideally 1:1, of type 1  $[(Ca, Mn^{2+})_2SiO_2]^{4-}$  and of type 2  $(Ca, Mn^{2+})_2M_2(OH)_2O_2]^{4-}$ , where  $Fe^{3+}$  and  $Mn^{3+}$  populate 3/4 of the M1 site and Al the remaining 1/4, while  $V^{3+}$ , Mg, and Al occupy in nearly equal proportions the M2 site. All the checked crystals exhibit very poor reflection quality, almost all exhibited a large quantity of streaked reflections, likely related to a high degree of structural disorder, and generally weak reflections likely due to the small size. The proposed structure of cassagnaite represents at present an averaged model of a high disordered structure and attempts will be made to improve it.

Quantitative analyses (seven points on two crystals) were performed by means of an electron microprobe (PHILIPS SEM 515 electron microscope equipped with EDAXPV9100 spectrometer) in energy-dispersion mode, with an accelerating voltage of 15 kV and a beam current of about 2 nA.  $H_2O$  content could not be directly determined because of the lack of material but a micro-Raman analysis has been carried out with a Renishaw 2000 Ramascope equipment using a laser operating at 633 nm; the large band in the range 3500–3000 cm<sup>-1</sup> of the Raman shift shows the presence of  $(OH)^-$  ions in the structure of cassagnaite. The empirical formula, based on 26 oxygen atoms pfu taking into account crystal-chemical considerations and the indications of the structure refinement, is  $Ca_{3.3}Mn_{0.7}^{2+}Fe_{1.6}^{3+}Mn_{1.4}^{3+}Al_{1.5}V_{0.7}^{3+}Mg_{0.6}Si_{5.2}O_{26}H_{6.5}$ .

The holotype sample is deposited in the collection of the Dipartimento per lo Studio del Territorio e delle sue Risorse (Dip.Te.Ris), Università di Genova, Italy. **K.T.T.**

### CHUKANOVITE\*

I.V. Pekovi, N. Perchiazzi, S. Merlino, V.N. Kalachev, M. Merlini, and A.E. Zadov (2007) Chukanovite,  $Fe_2(CO_3)(OH)_2$ , a new mineral from the weathered iron meteorite Dronino. *Eur. J. Mineral.*, 19, 891–898.

Chukanovite is the product of terrestrial alteration, found in cavities in the Dronino meteorite. The Dronino meteorite is an ataxite iron meteorite mainly consisting of kamacite and containing minor amounts of taenite and chromite. Sporadically it is extremely enriched in troilite and poorly studied Fe-Ni sulfides (Russell et al. 2004; Grokhovsky et al. 2005). The Dronino meteorite shower fell approximately 5000–8000 years ago, after the last glaciation period. Numerous fragments of the meteorite have been found in glacial and post-glacial deposits, mainly at a depth of 0.5–1 m under the surface. The sample used in this study was found in 2000 near the Dronino village in Kasimov

district, Ryazan' Oblast, 350 km east-south of Moscow, Russia (54°44.8' N; 41°25.3' E).

Chukanovite is monoclinic  $P2_1/a$ , with  $a = 12.396(1)$  Å,  $b = 9.407(1)$  Å,  $c = 3.2152(3)$  Å,  $\beta = 97.78^\circ$  and closely related to the minerals of the malachite-rosasite group. The strongest lines of the X-ray powder pattern [ $d$  in Å  $(I^0, hkl)$ ] are: 6.14(40,200), 5.15(60,231), 3.73(80,310), 2.645(100,230), 2.361(40,510), 2.171(40,520). The structure of chukanovite was refined on synchrotron data by the Rietveld method up to  $R_p = 3.43\%$ ,  $wR_p = 4.51\%$ , and  $R_{Bragg} = 2.48\%$ .

Unaltered chukanovite is transparent, pale-green, or colorless. The surface of aggregates is brownish-green. Streak is white, luster is vitreous, cleavage is perfect, probably on {021}, and the fracture is uneven. The mineral is brittle, the Mohs hardness is 3.5–4, and the calculated density is 3.60 g/cm<sup>3</sup>. It is optically biaxial (–) with  $\alpha = 1.673(3)$ ,  $\beta = 1.770(5)$ ,  $\gamma = 1.780(5)$ ,  $2V_{meas} = 10(5)^\circ$ . Chukanovite occurs as acicular to fibrous individuals, elongated along [001], up to 0.5 mm long and up to 2–3 µm thick usually combined in spherulites up to 0.3 mm (rarely up to 1 mm) in diameter. Botryoidal spherulitic clusters and parallel- or radial-columnar aggregates forming crusts up to 1 mm thick are typical. Aggregates are usually porous; the core of some spherulites contains grains of kamacite, taenite, sulfides, or iron hydroxides.

The infrared spectrum of the new mineral is close to the spectra of pokrovskite (the most similar), malachite, and members of the rosasite group. Absorption bands in the IR spectrum of chukanovite (in cm<sup>-1</sup>; frequencies of the most intensive bands are italic, sh = shoulder) are: 3475, 3325, 1755, 1521, 1400sh, 1364, 1069, 1055sh, 955, 861, 837, 781, 710sh, 695, 655, 504, 452.

Average chemical composition (wt%; electron probe,  $H_2O$  by modified Penfield method,  $CO_2$  by selective sorption) is  $MgO$  0.1,  $FeO$  68.8,  $NiO$  0.6,  $CO_2$  19.8,  $H_2O$  10.9, total 100.2 wt%. The empirical formula calculated on the basis of two metal atoms is  $(Fe_{1.97}^{2+}Ni_{0.02}Mg_{0.01})_{\Sigma 2.00}(CO_3)_{0.93}(OH)_{2.14} \cdot 0.18 H_2O$ , ideally  $Fe_2(CO_3)(OH)_2$ .

The mineral was named in honor of Nikita V. Chukanov (b. 1953), Russian physicist and mineralogist. The holotype specimen is deposited in the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow. **K.T.T.**

### FERROSKUTTERUDITE\*

E.M. Spiridonov, Yu.D. Gritsenko, and I.M. Kulikova (2007) Ferroskutterudite  $(Fe, Co)As_3$ : A new mineral species from the dolomite-calcite veins of the Noril'sk Ore Field. *Doklady Earth Sciences*, 417, 1278–1280.

Ferroskutterudite,  $(Fe, Co)As_3$ , was discovered in antimonide-arsenide mineralization among the Ni-Cu ores of the Noril'sk ore field, Russia. Antimonide-arsenide mineralization (164–122 Ma) post-dates the Ni-Cu mineralization of the main ore field (~250 Ma). The antimonide-arsenide mineralization occurs in hydrothermally derived carbonate and apophyllite-anhydrite-carbonate veins precipitated from  $NaCl-MgCl_2$  solutions at low salinity (0.2–1.4 wt% NaCl equiv.) at  $P = 0.1$ –0.9 kbar and  $T = 127$ –216 °C. The mineral occurs in dolomite-calcite veins, which contain triarsenides that cross-cut calcite veins containing both arsenides and diarsenides. It is associated with wurtzite, sphalerite, galena,

chalcopyrite, pyrrhotite, cubanite, and chalcocite. Ferroskutterudite is a rare mineral, occurring where aggregates of Co and Co-Ni skutterudite are replaced by granular intergrowths of low-Co nickelskutterudite, Fe-skutterudite, and ferroskutterudite. Ferroskutterudite occurs as 30–100 µm grains, has a tin white color, and metallic luster. It is indistinguishable from skutterudite, characterized by high-relief, and has a microindentation hardness of  $VHN_{50} = 700\text{--}1050 \text{ kg/mm}^2$ . Ferroskutterudite has a high reflectance (54–58%), is white and isotropic. The reflectance in air (based on certified standard WTiC) is 57.2 (400 nm), 57.6 (420 nm), 58.0 (440 nm), 58.2 (460 nm), 58.2 (470 nm), 58.2 (480 nm), 58.0 (500 nm), 57.6 (520 nm), 57.3 (540 nm), 57.2 (546 nm), 56.9 (560 nm), 56.4 (580 nm), 56.2 (589 nm), 56.0 (600 nm) 55.5 (620 nm) 55.2 (640 nm), 54.9 (650 nm), 54.7 (660 nm), 54.3 (680 nm), and 53.8% (700 nm).

The average chemical composition of ferroskutterudite (electron microprobe, 4 analyses) gave Ni 0.05, Co 8.38, Fe 12.09, As 78.01, S 1.34, total 99.87 wt%, corresponding to  $(\text{Fe}_{0.600}\text{Co}_{0.394}\text{Ni}_{0.002})_{20.996}(\text{As}_{2.888}\text{S}_{0.116})_{\Sigma 3.004}$  (based on 4 atoms), or, simplified,  $(\text{Fe},\text{Co})(\text{As},\text{S})_3$ . Ferroskutterudite is cubic,  $Im\bar{3}m$ ,  $a = 8.17(1)$  Å,  $V = 545.34(3)$  Å<sup>3</sup>,  $Z = 8$ . The strongest lines on the powder X-ray diffraction pattern (57.3 mm Debye-Scherer camera,  $\text{CuK}\alpha$  radiation, indexed by analogy with skutterudite) include [ $d$  in Å (1%,  $hkl$ )]: 2.858(100, 310), 2.182(90, 321), 1.829(70, 420), 1.667(50, 422), 1.602(70, 510), 1.402(60, 530).

Type material of ferroskutterudite (IMA no. 2006-0210) has been deposited at the Fersman Mineralogical Museum, Russian Academy of Sciences, Moscow, Russia (no. 3440/1). **P.C.P.**

### HINGGANITE-(Ce)\*, HINGANNITE-(Y)\*

R. Miyawaki, S. Matsubara, K. Yokoyama, and A. Okamoto (2007) Hingannite-(Ce) and hingannite-(Y) from Tahara, Hirukawa-mura, Gifu Prefecture, Japan: The description on a new mineral species of the Ce-analogue of hingannite-(Y) with a refinement of the crystal structure of hingannite-(Y). *J. Mineral. Petrol. Sciences*, 102, 1–7.

Hingannite-(Ce) was unofficially described in 1987 by Miyawaki et al. (*J. Mineral. Soc. Japan*, 18, 17–30). This recent paper represents the formal, approved description of hingannite-(Ce) from a pegmatite at Tahara, Hirukawa-mura, Gifu Prefecture, Japan, along with a crystal-structure refinement of hingannite-(Y) from the same locality. Hingannite-(Ce) occurs as rims on euhedral, prismatic crystals of hingannite-(Y) from 1 to 5 mm in length. It is associated with quartz, potassium feldspar, albite, zinnwaldite, cassiterite, stokesite, fluorite, chlorite, titanite, and an undetermined Ca-rich mineral related to hingannite-(Y). Hingannite-(Ce) is transparent, pale tan, has a vitreous luster, a white streak, and a Mohs hardness of 5–6. It does not fluoresce in either short or long wave UV light. Cleavage was not observed, and the density could not be determined due to the small crystal size ( $D_{\text{calc}} = 4.28 \text{ g/cm}^3$ ). Hingannite-(Ce) is biaxial (+),  $2V > 75^\circ$ ,  $\alpha = 1.745(5)$ ,  $\gamma = 1.770(5)$ .

Chemical analyses of hingannite-(Ce) and hingannite-(Y) were performed by electron microprobe, with Be and B contents confirmed by SIMS. The average composition of hingannite-(Ce) is  $\text{La}_2\text{O}_3$  11.11,  $\text{Ce}_2\text{O}_3$  28.32,  $\text{Pr}_2\text{O}_3$  2.11,  $\text{Nd}_2\text{O}_3$  4.70,  $\text{Sm}_2\text{O}_3$  0.39,

$\text{Gd}_2\text{O}_3$  0.08,  $\text{Tb}_2\text{O}_3$  trace,  $\text{Dy}_2\text{O}_3$  0.05,  $\text{Ho}_2\text{O}_3$  trace,  $\text{Er}_2\text{O}_3$  trace,  $\text{Tm}_2\text{O}_3$  trace,  $\text{Yb}_2\text{O}_3$  trace,  $\text{Lu}_2\text{O}_3$  trace,  $\text{Y}_2\text{O}_3$  0.72,  $\text{CaO}$  7.07,  $\text{FeO}$  3.61,  $\text{SiO}_2$  25.47,  $\text{BeO}_{\text{calc}}$  10.60,  $\text{H}_2\text{O}_{\text{calc}}$  2.88, total 97.10 wt%, corresponding to  $(\text{Ce}_{0.82}\text{La}_{0.32}\text{Nd}_{0.13}\text{Pr}_{0.06}\text{Y}_{0.03}\text{Sm}_{0.01}\text{Gd}_{0.002}\text{Dy}_{0.001}\text{Ca}_{0.60})_{\Sigma 1.97}\text{Fe}_{0.24}\text{Be}_{2.02}\text{Si}_{2.02}\text{O}_{8.20}(\text{OH})_{1.52}$ , based on 4( $\text{REE} + \text{Ca} + \text{Si}$ ). The simplified formula of hingannite-(Ce) is  $(\text{Ce},\text{Ca})_2(\square,\text{Fe})\text{Be}_2\text{Si}_2\text{O}_8[(\text{OH}),\text{O}]_2$ , and the ideal formula is  $\text{Ce}_2\square\text{Be}_2\text{Si}_2\text{O}_8(\text{OH})_2$  or  $\text{CeBeSiO}_4(\text{OH})$ , which requires  $\text{Ce}_2\text{O}_3$  63.56,  $\text{SiO}_2$  23.27,  $\text{BeO}$  9.69,  $\text{H}_2\text{O}$  3.49, total 100 wt%. The average composition of hingannite-(Y) (grain used for single-crystal X-ray refinement) is  $\text{La}_2\text{O}_3$  0.28,  $\text{Ce}_2\text{O}_3$  1.58,  $\text{Pr}_2\text{O}_3$  0.50,  $\text{Nd}_2\text{O}_3$  2.48,  $\text{Sm}_2\text{O}_3$  1.26,  $\text{Gd}_2\text{O}_3$  2.56,  $\text{Tb}_2\text{O}_3$  0.36,  $\text{Dy}_2\text{O}_3$  2.51,  $\text{Ho}_2\text{O}_3$  1.30,  $\text{Er}_2\text{O}_3$  1.85,  $\text{Tm}_2\text{O}_3$  0.41,  $\text{Yb}_2\text{O}_3$  2.20,  $\text{Lu}_2\text{O}_3$  0.95,  $\text{Y}_2\text{O}_3$  31.11,  $\text{CaO}$  3.57,  $\text{FeO}$  3.70,  $\text{SiO}_2$  28.27,  $\text{BeO}_{\text{calc}}$  11.77,  $\text{H}_2\text{O}_{\text{calc}}$  3.17, total 99.83 wt%, corresponding to  $(\text{Y}_{1.21}\text{Ca}_{0.29}\text{Nd}_{0.06}\text{Gd}_{0.06}\text{Dy}_{0.06}\text{Yb}_{0.05}\text{Er}_{0.04}\text{Ce}_{0.04}\text{Sm}_{0.03}\text{Ho}_{0.03}\text{Lu}_{0.02}\text{Pr}_{0.01}\text{Tm}_{0.01}\text{ Tb}_{0.01}\text{La}_{0.01})_{\Sigma 1.92}\text{Fe}_{0.23}\text{Be}_{2.07}\text{Si}_{2.07}\text{O}_{8.19}(\text{OH})_{1.55}$ , based on 4( $\text{REE} + \text{Ca} + \text{Si}$ ).

A single-crystal X-ray refinement of hingannite-(Ce) was not possible due to the small size of the crystals. Powder X-ray diffraction data were obtained (114.6 mm Gandolfi camera and imaging plate,  $\text{CuK}\alpha$  radiation) and unit-cell parameters determined using the Rietveld method with positional and isotropic displacement parameters fixed to those of hingannite-(Y). Hingannite-(Ce) is isostructural with hingannite-(Y), monoclinic,  $P2_1/a$ ,  $Z = 2$ ,  $a = 9.8973(1)$ ,  $b = 7.6282(8)$ ,  $c = 4.7505(6)$  Å,  $\beta = 90.416(8)^\circ$ ,  $V = 358.64(7)$  Å<sup>3</sup>. The strongest lines on the powder X-ray diffraction pattern include [ $d$  in Å (1%,  $hkl$ )]: 6.06(42, 110), 3.74(37,  $\bar{1}11$ ), 3.56(28, 120), 3.44(34,  $\bar{2}01$ ), 3.13(86,  $\bar{2}11$ ), 2.98(26, 021), 2.85(100,  $\bar{1}21$ ), 2.56(46,  $\bar{2}21$ ), 2.21(33, 112), 1.976(30,  $\bar{1}22$ ), 1.771(28, 041), and 1.663(21, 241). The structure of hingannite-(Y) was determined by single-crystal X-ray diffraction:  $0.10 \times 0.07 \times 0.05 \text{ mm}^3$  crystal,  $R_1 [I > 2\sigma(I)] = 0.0329$ ,  $R_1$  (all 1299 unique reflections) 0.0448,  $R_{\text{int}}$  0.0330,  $\text{GoF}$  1.151,  $a = 9.8830(16)$ ,  $b = 7.6091(9)$ ,  $c = 4.7423(9)$  Å,  $\beta = 90.342(14)^\circ$ ,  $V = 356.62$  Å<sup>3</sup>. The strongest lines on the powder X-ray diffraction pattern (114.6 mm Gandolfi camera and imaging plate,  $\text{CuK}\alpha$  radiation) include [ $d$  in Å (1%,  $hkl$ )]: 6.01(33, 110), 3.73(32,  $\bar{1}11$ ), 3.55(22, 120), 3.43(35,  $\bar{2}01$ ), 3.12(100,  $\bar{2}11$ ), 2.97(28, 021), 2.84(84,  $\bar{1}21$ ), 2.55(70,  $\bar{2}21$ ), 1.972(35,  $\bar{1}22$ ), 1.768(15, 041), and 1.662(23, 241).

Hingannite-(Ce) is isostructural with hingannite-(Y). The substitution of Ca for Ce in hingannite-(Ce) suggests a solid solution with calciogadolinite or datolite. REE distribution patterns in single, zoned grains of hingannite-(Ce) and hingannite-(Y) show varying Ho anomalies. Type material of hingannite-(Ce) (IMA no. 2004-004) has been deposited at the National Science Museum, Tokyo, Japan (NSM-M28552).

Comment: No detailed description of either the geology of the type locality or the structure is given. **P.C.P.**

### OSAKAITE\*

M. Ohnishi, I. Kusachi, and S. Kobayashi (2007) Osakaite,  $\text{Zn}_4\text{SO}_4(\text{OH})_6 \cdot 5\text{H}_2\text{O}$ , a new mineral species from the Hirao Mine, Osaka, Japan. *Can. Mineral.*, 45, 1511–1517.

Osakaite was discovered during a survey of secondary minerals from the gallery walls and in cracks in shale at the Hirao Mine, Osaka prefecture, Japan. The Hirao mine is one of a number of

small Cu, Zn, Pb, Fe, and Mn deposits found in Jurassic shales north of Osaka. The ore minerals are predominantly sphalerite with lesser amounts of chalcopyrite, pyrite, and galena. Within the mine a variety of secondary minerals including smithsonite, hydrozincite, schulenbergite, the Zn-dominant analogue of schulenbergite, brianyoungite, hemimorphite, brochantite, ramsbeckite, aurichalcite, malachite, azurite, posnjakite, and ktenasite are found in the altered shales. Osakaite is found either as hexagonal platy crystals (0.05 mm in width and 0.01 mm thick) or as stalactitic aggregates up to 2 cm in length. Associated minerals are hydrozincite, smithsonite, "chlorite," and "limonite" (author's quote marks).

Osakaite is white or pale blue to colorless with a pearly luster and a white to pale blue streak. Crystals have a perfect {001} cleavage and are fairly flexible. It is biaxial (−) with  $\alpha = 1.532(2)$ ,  $\beta = 1.565(2)$ ,  $\gamma = 1.567(2)$ ,  $2V_{\text{calc}} = 27.2^\circ$ , and positive elongation.  $D_{\text{meas}} = 2.70(1)$  g/cm<sup>3</sup>, comparable with  $D_{\text{calc}} = 2.75$  g/cm<sup>3</sup> based on empirical formula and unit-cell parameters. VHN is 20.3 kg/mm<sup>2</sup> (Mohs hardness = 1). It is not fluorescent and easily dissolves in dilute hydrochloric or nitric acids.

The strongest lines from X-ray powder diffraction are [ $d$  in Å ( $I\%$ ,  $hkl$ )] 10.96(100,001), 2.717(21,311), 1.574(18,533,245,523), 3.642(17,003), and 5.47(16,002).

Refinement of powder diffraction data give the following unit-cell parameters:  $a = 8.358(5)$ ,  $b = 8.337(4)$ ,  $c = 11.027(2)$  Å,  $\alpha = 94.79(2)$ ,  $\beta = 83.16(2)$ ,  $\gamma = 119.61(4)^\circ$ ,  $V = 663.0(4)$  Å<sup>3</sup>, and  $Z = 2$ . The space group is inferred to be  $P1$  by analogy to the synthetic phase. Single-crystal X-ray studies were not carried out.

Infrared spectroscopy was carried using a KBr pellet. Absorption bands at 3420 cm<sup>−1</sup> (strong) and 1620 cm<sup>−1</sup> (weak) are attributed to O-H stretching and H-O-H bending, respectively. Absorption bands at 1120, 1070, and 960 cm<sup>−1</sup> are attributed to  $\nu_3$  and  $\nu_1$  SO<sub>4</sub> bending, while bands at 650 and 460 cm<sup>−1</sup> are attributed to  $\nu_4$  and  $\nu_2$  SO<sub>4</sub> bending.

The mineral was not suitable for microprobe analysis due to dehydration in vacuum and instability under the electron beam. The composition was determined using a combination of ICP-AES and thermogravimetric analyses (volatile components). The resultant composition is ZnO 55.30, CuO 3.44, SO<sub>3</sub> 14.66, and H<sub>2</sub>O 26.01. This gives an empirical formula of (Zn<sub>3.75</sub>Cu<sub>0.24</sub>)<sub>23.99</sub>(SO<sub>4</sub>)<sub>1.01</sub>(OH)<sub>5.96</sub>·4.99H<sub>2</sub>O on the basis of 15 oxygen atoms.

Dehydration of osakaite by radiation or heating in a dry atmosphere produces namuwite. Rehydration occurs after immersion in water. Powder diffraction patterns of this rehydrated material show broader reflections than the original material.

The authors believe that osakaite crystallized at around 20 °C from Zn-, Cu-, and SO<sub>4</sub>-bearing groundwater derived from sulfides in the host rock. The name is for the prefecture. The holotype specimen is deposited at the National Science Museum, Tokyo, (NSM-M28983). **G.P.**

#### SELENOPOLYBASITE\*

L. Bindi, M. Evain, and S. Menchetti (2007) Selenopolybasite, [(Ag,Cu)<sub>6</sub>(Sb,As)<sub>2</sub>(S,Se)<sub>7</sub>][Ag<sub>2</sub>Cu(S,Se)<sub>2</sub>Se<sub>2</sub>], a new member of the pearceite–polybasite group from the De Lamar Mine, Owyhee County, Idaho, USA. Can. Mineral., 45, 1525–1528.

In accordance with new nomenclature rules (Bindi et al. 2007) for the pearceite–polybasite group, this mineral, which has more Sb than As and two S sites dominated by Se, is named selenopolybasite (the selenium dominant analogue of polybasite). A structure determination of this mineral (Evain et al. 2006) indicates that it has the 111 unit-cell type and thus is properly named selenopolybasite-*Tac*.

The new species was found in a sample from the De Lamar Mine, Owyhee County, Idaho. Mineralization at this mine consists of mineralized northwest trending veins in a mid-Miocene rhyolite porphyry. Mineralization from heated brines occurred at shallow depths. Selenopolybasite forms subhedral to anhedral grains associated with naumanite and covellite. Grain size is typically several hundred micrometers.

Selenopolybasite is opaque with a black streak and metallic luster. It is brittle without cleavage or fracture. Small grain size precluded density measurement;  $D_{\text{calc}} = 6.548$  g/cm<sup>3</sup>. Measured VHN is 131 kg/mm<sup>2</sup>, corresponding to a Mohs hardness of 3–3.5. Selenopolybasite is light gray in plane-polarized reflected light, with weak to moderate bireflectance, and weakly pleochroic gray to violet blue gray. There are no rotation tints or internal reflections in cross polarized reflected light. Reflectance percentages ( $R_{\text{min}}$ ,  $R_{\text{max}}$ ) for the four standard COM wavelengths are 32.8, 34.1 (471.1 nm), 31.0, 32.9 (548.3 nm), 30.2, 31.8 (586.6 nm), and 29.3, 30.0% (652.3 nm), respectively.

Chemical composition was determined by electron microprobe. The average of 10 analyses gives the following result [average(max–min)], Ag 66.17 (65.21–67.39), Cu 3.19 (2.88–3.81), Bi 0.09 (0.00–0.16), Pb 0.09 (0.02–0.20), Zn 0.03 (0.00–0.09), Fe 0.07 (0.00–0.12), Sb 9.47 (9.00–9.89) As 0.60 (0.23–0.99), S 11.36 (10.88–11.56), Se 8.42 (8.01–8.77), giving an empirical formula of [(Ag<sub>5.67</sub>Cu<sub>0.20</sub>Bi<sub>0.01</sub>Pb<sub>0.01</sub>Zn<sub>0.01</sub>Fe<sub>0.03</sub>)<sub>25.93</sub>(Sb<sub>1.86</sub>As<sub>0.19</sub>)<sub>22.05</sub>(S<sub>6.68</sub>Se<sub>0.34</sub>)<sub>27.02</sub>] [Ag<sub>9</sub>Cu(S<sub>1.79</sub>Se<sub>0.21</sub>)<sub>22.00</sub>Se<sub>2</sub>] on the basis of 29 atoms.

Selenopolybasite-*Tac* is trigonal with space group  $P3m1$  with  $a = 7.5950(4)$ ,  $c = 12.0731(6)$  Å,  $V = 603.12(5)$  Å<sup>3</sup>,  $c:a = 1.5896$ ,  $Z = 1$ . The eight strongest X-ray diffraction lines [ $d$  in Å ( $I\%$ ,  $hkl$ )] include 3.1731(48,201), 3.0183(84,004), 2.8880(48,022), 2.8880(100,202), 2.5466(23,023), 2.3629(34,114), 2.2237(28,024), and 1.8987(31,220). **G.P.**

#### NEW DATA

##### ISOKITE\*

H. Yang, J. Zwick, R.T. Downs, G. Costin (2007) Isokite, CaMg(PO<sub>4</sub>)F<sub>0.8</sub>(OH)<sub>0.2</sub>, isomorphous with titanite. Acta Crystallogr., C63, i89–i90.

The crystal structure of isokite, CaMg(PO<sub>4</sub>)F<sub>0.8</sub>(OH)<sub>0.2</sub>, a member of the titanite group, has been determined for the first time on a 0.06 × 0.05 × 0.05 mm<sup>3</sup> crystal from Kjorrestad, near Bamle, Norway. The average chemical composition of the mineral, as determined by electron microprobe methods, is CaMg(PO<sub>4</sub>)F<sub>0.8</sub>(OH)<sub>0.2</sub><sub>Σ=1.00</sub>. Intensity data were collected by single-crystal X-ray diffraction methods,  $R_{\text{int}} = 0.031$ ,  $R[F^2 > 2\sigma(F^2)] = 0.030$ ,  $wR(F^2) = 0.081$ ,  $S = 1.05$ , 801 independent reflections (3037 measured reflections). The mineral is monoclinic,  $C2/c$ ,  $a = 6.5109(3)$ ,  $b = 8.7301(5)$ ,  $c$

$a = 6.9046(5)$  Å,  $\beta = 112.246(2)^\circ$ ,  $V = 363.25(4)$  Å<sup>3</sup>,  $Z = 4$ . Isokite is homologous with other  $C2/c$  minerals of the titanite group, and topologically similar to minerals of the  $\text{Ca}$  amblygonite-montebrasite group. It is composed of kinked chains of corner-sharing  $\text{MgO}_4\text{F}_2$  octahedra cross-linked by isolated  $\text{PO}_4$  tetrahedra, forming a 3D polyhedral network, with Ca atoms in the interstitial sites coordinated by six O atoms and one F atom. **P.C.P.**

### KOLBECKITE\*

H. Yang, C. Li, R.A. Jenkins, R.T. Downs, and G. Costin (2007) Kolbeckite,  $\text{ScPO}_4 \cdot 2\text{H}_2\text{O}$ , isomorphous with metavariscite. *Acta Crystallogr.*, C63, i91–i92.

The crystal structure of kolbeckite,  $\text{ScPO}_4 \cdot 2\text{H}_2\text{O}$ , has been determined, for the first time, on a  $0.07 \times 0.06 \times 0.06$  mm<sup>3</sup> crystal from Hot Springs County, Arkansas. The average composition of the mineral (based on 15 analyses and determined by electron microprobe methods) is  $(\text{Sc}_{0.94}\text{V}_{0.03}^{3+}\text{Fe}_{0.02}^{3+}\text{Al}_{0.01})_{\Sigma 1.00}\text{P}_{1.00}\text{O}_{4.2}\text{H}_2\text{O}$ . Intensity data were collected by single-crystal X-ray diffraction methods,  $R_{\text{int}} = 0.042$ ,  $R[F^2 > 2\sigma(F^2)] = 0.052$ ,  $wR(F^2) = 0.168$ ,  $S = 1.11$ , 1858 independent reflections (8954 measured reflections). All crystals examined were twinned (twin axis along  $a$ ) and the twin law  $(100,0\bar{1}0,00\bar{1})$  was included in the refinement. Four H atoms were located on the difference Fourier map and their positions allowed to refine freely. Kolbeckite is monoclinic,  $P2_1/n$ ,  $a = 5.4258(4)$ ,  $b = 10.2027(8)$ ,  $c = 8.9074(7)$  Å,  $\beta = 90.502^\circ$ ,  $V = 493.08(7)$  Å<sup>3</sup>,  $Z = 4$ . The mineral is homologous with metavariscite, and consists of two basic polyhedral units:  $\text{PO}_4$  tetrahedra and  $\text{ScO}_4(\text{H}_2\text{O})_2$  octahedra. Each  $\text{PO}_4$  tetrahedron shares four vertices with four  $\text{ScO}_4(\text{H}_2\text{O})_2$  octahedra and vice versa, forming a 3D network of polyhedra. The two  $\text{H}_2\text{O}$  molecules are coordinated to  $\text{Sc}^{3+}$ . Kolbeckite, previously called eggonite or sterrettite, is a member of the metavariscite group of minerals, which are being investigated extensively because of the biological and geochemical importance of phosphorous and arsenic in soils, water, and waste management. In addition, recent studies have shown variscite- and metavariscite-group minerals to have interesting microporous and absorption properties. **P.C.P.**

### SCHULENBERGITE\*, ZN-DOMINANT SCHULENBERGITE

M. Ohnishi, I. Kusachi, S. Koyayashi, and J. Yamakawa (2007) Mineral chemistry of schulenbergite and its Zn-dominant analogue from the Hirao mine, Osaka, Japan. *J. Mineral. Petrol. Sciences*, 102, 233–239.

Schulenbergite,  $(\text{Cu},\text{Zn})_7(\text{SO}_4,\text{CO}_3)_2(\text{OH})_{10} \cdot 3\text{H}_2\text{O}$ , and its Zn-dominant analogue have been described and characterized from the Hirao mine (Lat. 34°50'N, Long. 135°28'E), Minoo complex, 17 km north of Osaka City, Japan. The host rock is hydrothermally altered shale and sandstone, with disseminated sphalerite as the dominant ore mineral. Schulerbergite and its Zn-dominant analogue are secondary Cu-Zn minerals, and occur as crusts on the mine wall and in cracks in the altered shale. The minerals are virtually indistinguishable from one another and occur as aggregates of hexagonal platy crystals up to 0.5 mm across and 0.05 mm thick. Schulerbergite is greenish

blue to blue-green, whereas the Zn-dominant analogue is pale blue in color. Associated minerals with schulerbergite include smithsonite, ramsbeckite, anatase, and limonite, and associated minerals with the Zn-dominant analogue include hydrozincite, brianyoungite, and limonite.

Schulerbergite is translucent with a pearly luster, has a perfect {0001} cleavage,  $D_{\text{meas}} = 3.18(1)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.39$  g/cm<sup>3</sup> ( $Z = 1$ ), Vicker's microhardness 48.8 (30.4–76.2) kg/mm<sup>2</sup> (10 g load) and a Mohs hardness of 1–2. No fluorescence was noted under short- or longwave ultraviolet radiation. The mineral easily dissolves in dilute HCl and HNO<sub>3</sub> showing effervescence. The infrared absorption spectrum of schulerbergite was measured using the KBr pellet method and gave the following absorption bands: 3394 cm<sup>-1</sup> (strong, O-H stretching), 1637 cm<sup>-1</sup> (weak, H-O-H bending), 1104 and 1015 cm<sup>-1</sup> ( $v_3$  and  $v_1$  SO<sub>4</sub> stretching), 605 cm<sup>-1</sup> ( $v_4$  SO<sub>4</sub> bending), 1509 and 1321 cm<sup>-1</sup> (weak, CO<sub>3</sub> group vibrations), 881, 792, and 513 cm<sup>-1</sup> [(Cu,Zn)<sub>6</sub> octahedra vibrations]. Thermogravimetry and differential thermal analysis of schulerbergite resulted in a strong endothermic peak at 322 °C (loss of water molecules), an exothermic peak at 535 °C due to structural transformation of dehydrated Cu and/or Zn sulfate, and an endothermic peak at 823 °C due to decomposition of sulfate groups. At 1000 °C, tenorite and zincite appeared as crystalline phases. The mineralogical properties of the Zn-dominant analogue could not be measured due to the presence of Zn carbonate inclusions.

Refined powder X-ray diffraction data for schulerbergite and its Zn-dominant analogue (Rigaku RINT-2500V diffractometer,  $\text{CuK}\alpha_1$  radiation) gave hexagonal unit-cell parameters of  $a = 8.256(2)$ ,  $c = 7.207(3)$  Å for schulerbergite, and  $a = 8.292(2)$ ,  $c = 7.271$  Å for its Zn-dominant analogue. The strongest lines in the powder pattern of schulerbergite include [ $d$  in Å (I%,  $hkl$ )]: 7.21(100,001), 4.13(10,110), 3.590(30,002), 3.218(28,102), 2.704(34,210), 2.532(52,211), 2.164(14,212), and 1.795(12,213). The strongest lines in the powder pattern of the Zn-dominant analogue include [ $d$  in Å (I%,  $hkl$ )]: 7.28(100,001), 4.15(14,110), 3.636(36,002), 3.245(46,102), 2.715(52,210), 2.545(92,211), 2.175(34,212), 1.808(38,213), 1.567(30,410), 1.531(20,411), and 1.510(20,214).

Chemical analyses of the two minerals by electron microprobe gave the following results: (1) for schulerbergite (average of 17 analyses): CuO 35.43, ZnO 29.47, FeO 0.40, SO<sub>3</sub> 14.98, SiO<sub>2</sub> 0.94, CO<sub>2</sub> 2.09 (determined by CHNS/O analyzer), H<sub>2</sub>O<sub>calc</sub> 16.69, total 100.00 wt%, corresponding to  $(\text{Cu}_{3.85}\text{Zn}_{3.13}\text{Fe}_{0.05})_{27.03}[(\text{SO}_4)_{1.62}(\text{CO}_3)_{0.41}(\text{SiO}_4)_{0.14}]_{22.17}(\text{OH})_{9.44} \cdot 3.30\text{H}_2\text{O}$ , based on O = 21; (2) for the Zn-dominant analogue (average of 8 analyses): CuO 16.95, ZnO 50.18, FeO 0.37, SO<sub>3</sub> 11.28, SiO<sub>2</sub> 3.37, total 82.15 wt% (no H<sub>2</sub>O calculated or determined in these analyses due to the presence of impurities). Cu/(Cu + Zn) ratios in the two minerals from the Hirao mine range from 0.67 to 0.21, demonstrating the existence of extensive Cu-Zn substitution between the two minerals. In addition, there is a linear dependence between the Zn/(Cu + Zn) molar ratio and the length of the c-axis, a result of Cu-Zn substitution in the brucite-like layers of edge-sharing (Cu,Zn)<sub>6</sub> octahedra oriented parallel to the (0001) plane. **P.C.P.**

**SIBIRSKITE\***

H. Miura and I. Kusachi (2008) Crystal structure of sibirskite ( $\text{CaHBO}_3$ ) by Monte Carlo simulation and Rietveld refinement. *J. Mineral. Petrol. Sciences*, 103, 156–160.

The crystal structure of sibirskite,  $\text{CaHBO}_3$ , was determined by Monte Carlo simulation using a set of  $d$  values and intensity data by Kusachi et al. (1997, *Japan Mineral. J.*, 19, 109–114), and further refined by the Rietveld method. Sibirskite is monoclinic,  $P2_1/a$ ,  $a = 8.643(6)$ ,  $b = 9.523(2)$ ,  $c = 3.567(3)$  Å,  $\beta = 119.23(3)^\circ$ ,  $Z = 4$ . The program used for the Monte Carlo simulation was the Structure Model-Assembly Program, developed by Miura and Kikuchi (1999), which automatically searches for the optimal structural model to satisfy the observed XRD data, unit-cell parameters, space group, chemical formula,  $Z$ , and interatomic distances. The  $R$  value for the final simulated structure is 0.243. A powder X-ray diffraction pattern was obtained (Mac Science MX-Labo diffractometer,  $\text{CuK}\alpha$  radiation) and the strongest peaks include [ $d$  (1%<sub>obs</sub>,  $hkl$ )]: 5.913(33,110), 4.762(29,020), 3.771(36,200), 2.959(72,011), 2.956(81,220), 2.727(33,221), 2.606(100,021), 2.223(25,320), 2.059(20,331), and 1.891(21,041). The final  $R$  values for the Rietveld refinement are  $R_{wp} = 7.75\%$ ,  $R_p = 5.93\%$ ,  $R_I = 4.22\%$ , and  $R_F = 4.68\%$ . The Rietveld refinement of sibirskite confirmed the crystal structure obtained by the Monte Carlo simulation. The final model obtained for sibirskite includes double chains of edge-shared  $\text{CaO}_6$  octahedra extending along the  $c$  axis, with  $\text{BO}_3$  polyhedra linked to one vertical and two shared oxygen atoms in the  $\text{CaO}_6$  double chain. The edge-sharing  $\text{CaO}_6$  double chains are analogous to edge-sharing  $\text{MgO}_6$  octahedra found in szaibelyite,  $\{\text{Mg}_2(\text{OH})$

$[\text{B}_2\text{O}_4(\text{OH})]\}$ . It was not possible to determine the position of the B or H atoms. **P.C.P.**

**TVALCHRELIDZEITE\***

H. Yang, R.T. Downs, G. Costin, and C.M. Eichler (2007) The crystal structure of tvalchrelidzeite,  $\text{Hg}_3\text{SbAsS}_3$ , and a revision of its chemical formula. *Can. Mineral.*, 45, 1529–1533.

The authors report on microprobe analyses and single-crystal structure analysis of tvalchrelidzeite from the type locality. The average of 15 point analyses gave an empirical formula of  $\text{Hg}_{3.03}\text{Sb}_{1.03}\text{As}_{1.00}\text{S}_3$  on the basis of 3 S atoms. A crystal-structure determination was carried out on a  $0.07 \times 0.07 \times 0.06$  mm<sup>3</sup> crystal using  $\text{MoK}\alpha$  radiation on a CCD diffractometer equipped with a graphite monochromator. Tvalchrelidzeite is monoclinic with space group  $P2_1/n$  and  $a = 11.5526(4)$ ,  $b = 4.3852(1)$ ,  $c = 15.6373(5)$  Å,  $\beta = 91.845(2)^\circ$ ,  $V = 791.79(5)$  Å<sup>3</sup>. Previous work on this mineral had not produced consistent structures or formulas.

The structure of tvalchrelidzeite consists of eight symmetrically distinct sites. Three of the sites are occupied by Hg, one each by As and Sb, and three by S. Unlike previous determinations for this mineral the present study shows no disorder between As and Sb. Sb behaves as a cation coordinated by six  $\text{S}^{2-}$  ions while As behaves as an anion and is coordinated by six  $\text{Hg}^{2+}$  ions. Hg is situated in strongly distorted octahedral sites distinguished by differing S:As ratios, specifically 5:1, 4:2, and 3: for the Hg1, Hg2, and Hg3 octahedra, respectively. The authors describe the structure of tvalchrelidzeite as sheets of  $[\text{Hg}_6\text{Sb}_2\text{As}_2\text{S}_6]$  units parallel to  $(\bar{1}01)$  linked by short Hg1-As bonds with the layers connected by weak Hg-S and Sb-S bonds. These weak interlayer bonds explain the perfect cleavage of this mineral. **G.P.**