New Mineral Names*

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NEW MINERALS

AFMITE*

A.R. Kampf, S.J. Mills, G.R Rossman, I.M. Steele, J.J. Pluth, and G. Favreau (2011) Afmite, $Al_3(OH)_4(H_2O)_3(PO_4)(PO_3OH) \cdot H_2O$, a new mineral from Fumade, Tarn, France: description and crystal structure. Eur. J. Mineral., 23, 269–277.

Afmite is found at Fumade, Castelnau-de-Brassac, Tarn, France (43°39′30″N, 2°29′58″E). The phosphates occur in fractures and solution cavities in shale/siltstone exposed in ploughs in a farmer's field. Afmite is rarely associated with the Al-phosphates matulaite and variscite, but usually it is not directly associated with any other well-crystallized phosphate minerals. Afmite sometimes occurs on todorokite and other, poorly defined, manganese oxides. Other secondary phosphate species noted at the locality include wavellite, cacoxenite, beraunite, and strengite.

The Cambrian age shale/siltstone was mildly metamorphosed during the Hercynian age intrusion of the Sidobre granite. Because of the limited exposures at the locality, it has not been possible to determine the source of the phosphate; however, it is presumed to have been present in the original sediments. While some recrystallization of phosphates probably occurred during Hercynian metamorphism, the formation of afmite and the other secondary phosphate minerals is probably largely the result of remobilization and crystallization during more recent low-temperature hydrothermal activity and/or weathering and ground water activity.

Crystals are thin diamond-shaped tablets on {001} with [010] elongation. Forms observed are {001}, {100}, {110}, and {010}. Crystals exhibit ubiquitous contact twinning on {001}. Individual twinned tablets are up to 0.40 × 0.25 × 0.02 mm. Tablets are also commonly twinned by rotation on [010] with {010} and {1̄10} composition planes, forming star-like sixlings, which are slightly concave/convex (dish-like). Tablets and sixlings commonly occur in cockscomb aggregates up to 1 mm across.

Crystals typically exhibit a dull white to cream to yellowish surface, presumably from weathering. Freshly broken aggregates exhibit {001} faces that are colorless to white with a pearly luster.

The streak is white and the Mohs hardness is estimated to be about 1½. Thin crystal fragments are flexible, but not elastic. The fracture is irregular and there are three cleavage directions: {001} perfect, {010} and {1̄10} good. The mineral is non-fluorescent under all wavelengths of ultraviolet radiation. The density measured by sink-float in aqueous solution of sodium polytungstate is 2.39(3) g/cm^3. The calculated density, based on the empirical formula and single-crystal cell, is 2.391 g/cm^3 and that for the ideal formula is 2.394 g/cm^3.

Electron microprobe analyses provided Al_2O_3 40.20 and P_2O_5 38.84 wt% and CHN analyses provided H_2O 25.64 wt%, total 103.68 wt%. Normalized EMP analyses and water based on the structure yield Al_2O_3 36.41, P_2O_5 35.17, and H_2O 28.42, total 100.00 wt%. The infrared spectra of afmite and related minerals kobokoboite and planerite were obtained with a Nicolet Magna860 FTIR and a SensIR DuraScope Attenuated Total Reflection (ATR) accessory and enough powdered mineral to cover a 1 mm diameter spot on the diamond ATR plate. All three spectra are dominated by phosphate bending modes in the 550–600 cm^{-1} region and phosphate antisymmetric stretching modes in the 900–1200 cm^{-1} region. Also obvious are OH bands in the 3000–3600 cm^{-1} range and water bending modes around 1600 cm^{-1}. The afmite spectrum has multiple bands in the OH region, both sharp and broad. The sharp bands more likely represent the OH groups associated with the aluminum, and the broad, underlying component comes from the molecular water. The successively higher contents of molecular water in planerite, afmite, and kobokoboite are reflected in successively greater absorptions in the 3000–3600 and 1600 cm^{-1} ranges for each phase.

Powder X-ray diffraction data were obtained on a Rigaku R-Axis Rapid II curved-imaging-plate microdiffractometer utilizing monochromatized MoKα radiation. The strongest powder X-ray diffraction lines are [d_{hkl} in Å (I_{obs}%,hkl)]: 11.089(100,001), 5.484(79,002,101), 4.022(30,102,1̄12), 6.826(23,010), 3.540(81,01̄3,1̄1̄2), 3.089(33,1̄13,201), and 2.918(60,1̄22). Ubiquitous fine-scale polysynthetic twinning and the general warping of crystals made the selection of a crystal fragment suitable for structure data collection very challenging. Data obtained on a small single-crystal fragment (50 × 40 × 5 mm) using synchrotron radiation were not of sufficient quality for structure determination. Data were subsequently collected on a larger crystal (100 × 80 × 10 mm), consisting of two individuals twinned by reflection on {001}, using a Rigaku R-Axis Rapid II instrument. The Rigaku CrystalClear software package, and

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specifically the TwinSolve program, was used for processing the structure data, including the application of an empirical absorption correction. A unit cell consistent with the synchrotron single-crystal cell was obtained. The relatively high R factor, 10.4%, is attributed to poor crystal quality and the imperfect nature of refinement using a twinned data set.

The structure of afmite consists of chains of AlO_6 octahedra parallel to [110] in which edge-sharing octahedral dimers share corners with individual octahedra. Both PO_4 and PO_3OH tetrahedra link the chains into sheets parallel to {001} and the PO_4 tetrahedra further serve to link two sheets together into a thick slab in which tetrahedral (T) and octahedral (O) layers alternate, forming a T-O-T-O-T sandwich. The linkage between these sandwiches in the c direction is via hydrogen bonding with isolated H_2O groups in the interlayer region. Afmite is closely related structurally to the turquoise-group minerals and specifically to planerite. The recently described mineral kobokoboite probably has a closely related sheet structure.

The current paper reports the results of a second submission in 2010 (IMA2005-025a) in which concerns with the first submission were addressed and, most importantly, a crystal structure determination was reported, clearly defining the ideal formula of afmite, clarifying its relationship to planerite and shedding light on the likely relationship of kobokoboite. The name "afmite" is for the Association Française de Microminéralogie (AFM) which is one of the most active amateur associations in the domain of micro-minerals. The holotype specimen has been deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, U.S.A., catalog number 55425. **K.T.T.**

Hydroniumpharmacosiderite*

S.J. Mills, A.R. Kampf, P.A. Williams, P. Leverett, G. Poirier, M. Raudsepp, and C.A. Francis (2010) Hydroniumpharmacosiderite, a new member of the pharmacosiderite supergroup from Cornwall, U.K.: structure and description. Mineral. Mag., 74, 863–869.

Hydroniumpharmacosiderite was described from a crystal that Buerger et al. had identified as K-deficient pharmacosiderite in 1967. The general locality given by Buerger et al. (1967) is Cornwall, U.K., and is probably from the St. Day group of mines. The new mineral is a single elongated cubic crystal 0.17 × 0.14 × 0.14 mm in size. It is yellowish-green, vitreous, and transparent with a cleavage on {001}. It has a Mohs hardness of 2–3, is brittle with an irregular fracture, D_{calc} = 2.559 g/cm^3 and does not fluoresce. The mineral is isotropic but displays an anomalous birefringence with n_{min} = 1.690(2) and n_{max} = 1.692(2).

Electron microprobe analyses gave Na_2O 0.25, K_2O 2.84, Al_2O_3 1.45, Fe_2O_3 38.33, P_2O_5 1.30, As_2O_5 39.80, H_2O(calc) 16.03, sum 100 wt% corresponding to $[(H_3O)_{0.5}K_{0.48}Na_{0.06}]_{1.04}$ $(Fe_{3.79}Al_{0.22})_{4.01}[(As_{2.73}P_{0.15})_{2.88}O_{12}](OH)_4·4H_{2.14}O$ based on 20.5 O atoms. The ideal formula is $(H_3O)Fe_4(AsO_4)_3(OH)_4·4H_2O$.

The structure of hydroniumpharmacosiderite was solved using a Bruker X8 ApexII single-crystal diffractometer and refined to a R_1 = 4.81% and wR_2 = 13.58% for 540 reflections with $I > 2σ(I)$. The mineral is cubic, $P\overline{4}3m$ with refined unit cell using powder diffraction data a = 7.993(6) Å, V = 510.7(6) Å^3. The strongest lines on the powder diffraction pattern (24 lines, Rigaku R-Axis Rapid II curved-imaging-plate microdiffractometer, Mo$K\alpha$ radiation) [d_{obs} in Å (I_{obs}%, hkl)] include 8.050(100,001), 4.628(22,111), 4.005(14,002), 3.265(35,112), 2.830(23,202), 2.666(10,003), 2.528(19,013), 2.412(30,113), 1.787(14,024), and 1.412(10,044). The mineral is part of the pharmacosiderite supergroup. It is the H_3O analog of pharmacosiderite, where H_3O^+ replaces K^+ in the structure.

The mineral was named as the hydronium end-member of the pharmacosiderite group. Both mineral and name were approved by the Commission on New Minerals and Mineral Names, IMA 2010-014. The holotype crystal in a probe mount was deposited at the Harvard Mineralogical Museum in Cambridge, Massachusetts with catalog number 142784. **R.R.**

Kerimasite*

A.N. Zaitsev, C.T. Williams, S.N. Britvin, I.V. Kuznetsova, J. Spratt, S.V. Petrov, and J. Keller (2010) Kerimasite, $Ca_3Zr_2(Fe^{3+}_2Si)O_{12}$, a new garnet from carbonatites of Kerimasi volcano and surrounding explosion craters, northern Tanzania. Mineral. Mag., 74, 803–820.

Kerimasite is a new Zr garnet from the Kerimasi nephelinite/carbonatite volcano and Loluni, Kisete, and Loolmurwak explosion craters in Tanzania. The mineral was found in five samples of carbonatite and occurs as spherical, subhedral to euhedral crystals up to 100 μm in diameter, enclosed in calcite and rarely fluorapatite and magnesioferrite. Heavy mineral fractions from eluvial deposits of the carbonatite agglomerates have yielded large (up to 180 μm), subhedral to euhedral crystals of kerimasite, along with diopside, schorlomite, andradite, magnetite, magnesioferrite, perovskite, fluorapatite, pyrochlore, calzirtite, baddeleyite, and cerianite-(Ce). Kerimasite occurs as trapezohedra {211} and is light to dark brown in color, transparent with a vitreous luster, brittle but does not have a cleavage or a parting, with a Mohs hardness of ~7 and a calculated density of 4.104(1) g/cm^3. In transmitted light, kerimasite is optically heterogeneous, isotropic to anisotropic, and characterized by a yellow-green color. The Raman spectrum of kerimasite indicates (OH)$^-$ groups in the structure, with low-intensity vibration bands between 3100 and 3700 cm^{-1}. Other bands in the Raman spectrum include 152, 243, 298, 414, 500, 573, 732, 785, 830, and 875 cm^{-1}, which are almost identical to those of kimzeyite.

The chemical composition of kerimasite was determined on three samples (98 analyses) using a Cameca SX50 and SX100 electron microprobe in WDS mode. Results for sample KZ-2 are presented here, which represent the sample on which the structure was determined (average of 5 analyses): Fe_2O_3 16.92, Al_2O_3 6.77, SiO_2 7.32, ZrO_2 27.93, TiO_2 1.04, Nb_2O_5 8.78, MgO 0.63, Y_2O_3 0.71, La_2O_3 0.18, Ce_2O_3 0.64, Pr_2O_3 0.10, Nd_2O_3 0.43, Sm_2O_3 0.13, Gd_2O_3 0.10, Dy_2O_3 0.11, Er_2O_3 0.06, HfO_2 0.16, CaO 25.86, MnO 0.33, total 98.20 wt%, corresponding to the empirical formula (calculated on the basis of 12 O) $(Ca_{2.89}Mn_{0.03}Ce_{0.02}Nd_{0.02}$ $La_{0.01}Sm_{0.01})_{Σ2.98}(Zr_{1.42}Nb_{0.41}Mg_{0.10}Y_{0.04}Hf_{0.01})_{Σ1.98}(Fe^{3+}_{1.33}Al_{0.83}Si_{0.76}$ $Ti_{0.03})_{Σ3.00}O_{12}$, with an ideal formula of $Ca_3Zr_2(Fe^{3+}_2Si)O_{12}$. The compositional range of kerimasite is wide, mainly as a result of Zr – Nb, Zr – Ti, Si – (Fe,Al) substitutions. Of particular note is the high Nb_2O_5 contents, up to 10 wt%, in some of the samples.

The crystal structure of kerimasite was determined on a $0.05 \times 0.06 \times 0.06$ mm crystal (KZ-2) using a Stoe IPDS II image plate diffractometer (Mo$K\alpha$ radiation). The structure was solved by direct methods and refined to $R1 = 0.045$, w$R2 = 0.093$, GoF $= 0.912$ for 107 unique observed reflections with $|F_o| > 4\sigma F$. Kerimasite is cubic, $Ia\bar{3}d$, $a = 12.5512(15)$ Å, $Z = 8$. Powder X-ray diffraction data were collected on a Stoe IPDS II image plate diffractometer using the Gandolfi method (Mo$K\alpha$ radiation). The strongest lines on the pattern (KZ-2) [d_{obs} in Å ($I_{obs}\%,hkl$)] include: 4.445(67,220), 3.141(89,400), 2.808(100,420), 2.563(89,422), and 1.677(75,642). Kerimasite is isostructural with other members of the garnet group.

The mineral is named for its type locality, the Kerimasi volcano in Tanzania. Both the mineral and name have been approved by the IMA CNMMN (no. 2009-029). Cotype material has been deposited at the Natural History Museum, London, U.K. [catalog nos. BM.1995,P6(47) and BM.1995,P6(22)]. A block of heavy mineral fractions has been deposited at the Mineralogical Museum, Department of Mineralogy, Faculty of Geology, St. Petersburg State University, St. Petersburg, Russia (catalog no. 1/19363).

Discussion: The original manuscript abstract provides chemical data for a crystal not used in the structure refinement. All chemical data here corresponds to the crystal used for the single-crystal structure refinement to maintain continuity. **P.C.P.**

KRIESELITE*

J. Schlüter, T. Geisler, D. Pohl, and T. Stephan (2010) Krieselite, $Al_2GeO_4(F,OH)_2$: A new mineral from the Tsumeb mine, Namibia, representing the Ge analogue of topaz. Neus Jb. Mineral. Abh., 187, 33–40.

Krieselite is a new mineral described from vugs in tennantite-chalcocite-galena-germanite ore from the Tsumeb mine, Tsumeb, Namibia. The mineral occurs as hemispherical aggregates (up to 200 μm) and fibrous crusts associated with quartz, wulfenite, anglesite, and graphite. Fibers are up to 50×5 μm and form wedge-shaped aggregates of fine lamellae parallel to (110). The mineral is beige to white, has a white streak, is translucent with a greasy luster, is not fluorescent, has a Mohs hardness of 5.5–6.5, and a calculated density of 4.069 g/cm³.

The chemical composition of krieselite was determined by a combination of electron microprobe analyses, PIXE and INAA, with additional TOF-SIMS analyses to determine the presence/absence of trace elements. The combined, weighted average of 636 analyses is: GeO$_2$ 38.32, SiO$_2$ 0.33, Al$_2$O$_3$ 44.34, Ga$_2$O$_3$ 4.14, TiO$_2$ 0.12, Fe$_2$O$_3$ 0.43, CuO 0.05, ZnO 0.70, Sb$_2$O$_3$ 0.33, As$_2$O$_3$ 1.54, MgO 0.28, Na$_2$O 0.12, F 9.10, H$_2$O$_{calc}$ 3.51, F≡O 3.83, total 99.48 wt%, corresponding to an empirical formula based on 4 O + 2(F+OH) of: $(Al_{1.860}Ga_{0.102}As^{3+}_{0.036}Zn_{0.020}Mg_{0.016}Fe^{3+}_{0.012}Na_{0.009}Sb^{3+}_{0.005}Ti_{0.003}Cu_{0.001})_{\Sigma2.064}(Ge_{0.844}Al_{0.143}Si_{0.013})_{\Sigma1.000}O_4(F_{1.103}OH_{0.897})_{\Sigma2.000}$. The FTIR spectrum was acquired using the conventional KBr pellet method measured in a N$_2$ atmosphere with a Bruker Equinox 55 spectrometer. The observed IR vibrational frequencies are as follows: 421(w), 482(w), 522(w), 577(s), 733(vs) 869(sh,w), 993(w), 1135(s), 1185(vw), 1633(2), 3440(vb,s), and 3590(vb,s) cm⁻¹. The H$_2$O content of krieselite was determined by FTIR to be 2.83 ± 0.28 wt%, which agrees with the calculated value of

3.51 wt%. In addition, a Raman spectrum was acquired on a high-resolution Jobin Yvon HR800 Raman system with a He-Ne (632 nm) laser. The observed vibration frequencies include 224(w), 294(s), 718(vw), 802(sh,w), and 862 cm⁻¹. All vibrations in krieselite are broader than those observed for synthetic OH-Ge-topaz, as well as shifted to both higher and lower wavenumbers, indicating increased disorder at the cation positions, which is to be expected given the variety of substitutions occurring in the natural sample.

Powder X-ray diffraction data were collected using a Philips X'Pert powder diffractometer (Cu$K\alpha$ radiation). The strongest lines on the pattern [d_{obs} in Å ($I_{obs}\%,hkl$)] include: 3.811(78,111), 3.315(48,012), 3.121(20,022), 3.016(100,112), 2.576(20,130), 2.464(24,131,103), 2.417(27,023,200), 2.247(38,211), 2.128(23,220), and 1.398(29,303). The unit cell was refined using the Rietveld method in the orthorhombic space group $Pbnm$ ($R_B = 23.12$) with $a = 4.809(2)$, $b = 9.111(3)$, $c = 8.536(3)$ Å, $V = 374.0$ Å³, and $Z = 4$. Krieselite is the Ge-analogue of topaz and the F-dominant natural analogue of synthetic Al$_2$GeO$_4$(OH)$_2$.

The mineral is named for Friedrich Wilhelm Kriesel who was the chief chemist at the Tsumeb mine laboratory around 1920. Both the mineral and name have been approved by the IMA CNMNC (IMA no. 2000-043a). Type material has been deposited at the Mineralogical Museum of the University of Hamburg. **P.C.P.**

NATROPHARMACOALUMITE*

M.S. Rumsey, S.J. Mills, and J. Spratt (2010) Natropharmacoalumite, NaAl$_4$[(OH)$_4$(AsO$_4$)$_3$]·4H$_2$O, a new mineral of the pharmacosiderite supergroup and the renaming of aluminopharmacosiderite to pharmacoalumite. Mineral. Mag., 74, 929–936.

Natropharmacoalumite occurs as cubes up to 0.5 mm in size, often intergrown to form aggregates of a few millimeters in size in cavities or fractures within quartz. It exhibits step growth patterns on some faces. It is also associated with chenevixite, kaolinite, jarosite, and many other Fe and Sb oxyhydroxides. The specimen was recovered from a large Fe-rich silicified boulder. The type locality is the Maria Josefa mine, an abandoned gold mine in the Rodalquilar caldera near the town of Rodalquilar, Andalusia, Spain. Natropharmacoalumite is colorless, with a white streak, a vitreous to adamantine luster with an index of refraction $n = 1.556$. The Mohs hardness is around 2.5 with an average measured VHN of 267. Only the {100} form was observed with an imperfect cleavage along {100}, with a brittle tenacity and an irregular fracture. The calculated density based on the structure is 2.564 g/cm³.

A routine EDS analysis showed the mineral to be Na-dominant rather than K-dominant. Further electron microprobe analyses gave Na$_2$O 2.52, K$_2$O 1.49, Al$_2$O$_3$ 29.50, As$_2$O$_5$ 48.84, H$_2$O(calc) 16.28, sum 98.63 wt% corresponding to $[Na_{0.57}K_{0.22}(H_3O)_{0.21}]_{\Sigma1.00}Al_{4.05}(As_{2.97}O_{12})(OH)_4\cdot4H_2O$ based on 20.21 O atoms. The ideal formula is NaAl$_4$(AsO$_4$)$_3$(OH)$_4$·4H$_2$O.

The structure of natropharmacoalumite was solved on a $0.15 \times 0.15 \times 0.15$ mm single crystal with a Bruker X8 ApexII single-crystal diffractometer and refined to $R_1 = 5.92\%$ and w$R_2 = 16.57\%$ for 295 reflections [$F > 4\sigma(F_o)$]. It is cubic, space group

$P\overline{4}3m$ with unit-cell parameters refined using powder data to a = 7.740(3) Å, V = 463.723 Å^3. The diffraction data obtained using a Bruker D8 Discover powder diffractometer with Co$K\alpha$ radiation (11 lines) [d_{obs} in Å (I_{obs}%, hkl)] include 7.759(100,100), 4.473(40,111), 3.870(50,200), 2.446(9,301), and 2.331(12,113). Twinning on {100} was identified through single-crystal work, which was suspected based on the intergrowth pattern. The presence of H_3O^+ as a charge balance is a feature that was also identified in the structure of H_3O-exchanged pharmacosiderite and hydroniumpharmacosiderite. The structure of natropharmacoalumite is also characterized by large zeolite-like channels that host, in this case H_2O, H_3O, Na, and K. This type of channels is typical of the pharmacosiderite structure-type.

Natropharmacoaluminite is named after its chemistry being the Na and Al end-member in the pharmacosiderite supergroup. The mineral and its name were approved by the commission on New Minerals and Mineral Names, IMA (2010-009). The type specimen was deposited at the Natural History Museum in London with catalog number BM2009,161 and the probe mount P16713.

Note: The authors revisited the nomenclature of the pharmacosiderite supergroup and proceeded to rename the mineral aluminopharmacosiderite, ideally $KAl_4[(AsO_4)_3(OH)_4\cdot6.5H_2O$ to pharmacoalumite since there is no iron in the formula and that Al occupies the same site in pharmacoalumite as Fe in pharmacosiderite. The new nomenclature properly shows that pharmacosiderite is the Fe end-member, whereas pharmacoalumite is the Al end-member. The name change was approved by the IMA (Proposal 2010-A). **R.R.**

NOONKANBAHITE*

Y.A. Uvarova, E. Sokolova, F.C. Hawthorne, R.P. Liferovich, R.H. Mitchell, I.V. Pekov, and A.E. Zadov (2010) Noonkanbahite, $BaKNaTi_2(Si_4O_{12})O_2$, a new mineral species: description and crystal structure. Mineral. Mag., 74, 441–450.

Noonkanbahite is a new mineral species discovered in Liley, Eifel Mountains, Germany (holotype) and Murun, Siberia, Russia (cotype). At Liley it occurs as straw-yellow sprays (pinkish orange as crystals) up to 8 mm in size, single prismatic crystals up to 4 mm in size and as larger anhedral grains on the walls of several cavities in igneous alkaline rocks. Noonkanbahite is fairly abundant in the Murun kalsilite syenite (up to 20–25% of the rock). There it occurs as mostly isolated brownish yellow to brown curved crystals reaching $0.05 \times 0.7 \times 1.5$ cm in size. In rare occasions, they will form clusters up to 2 cm in size. The mineral has a vitreous luster, is brittle, a Mohs hardness of 6, D_{obs} = 3.39(1), D_{calc} = 3.49 g/cm^3. It exhibit poor cleavage on {010} and {100} with a weak parting on {011}. The mineral does not fluoresce under UV light.

The chemical composition of the Liley noonkanbahite obtained with an electron microprobe gave SiO_2 37.82, Nb_2O_5 3.18, Al_2O_3 0.17, TiO_2 15.54, ZrO_2 0.42, Fe_2O_3 5.63 (re-calculated from FeO), MnO 0.32, MgO 0.53, BaO 20.60, CaO 1.36, K_2O 5.32. Na_2O 6.14, F 0.78, H_2O 0.58 (determined by SIMS), O=–F –0.33, sum 98.06 wt% corresponding to $(Ba_{0.85}K_{0.13})_{\Sigma0.98}(K_{0.59}Na_{0.26}Ca_{0.15})_{\Sigma1.00}$ $Na(Ti_{1.23}Fe^{3+}_{0.45}Nb_{0.15}Mg_{0.08}$ $Mn_{0.03}Zr_{0.02}Al_{0.01})_{\Sigma1.97}(Si_{3.99}Al_{0.01}O_{12})(O_{1.33}OH_{0.41}F_{0.26})_{\Sigma2.00}$, Z =

4, based on 14 anions (O + OH + F). The ideal formula is $BaKNaTi_2(Si_4O_{12})O_2$. The mineral is biaxial positive, $2V_{obs}$ = 75(2)°, $2V_{calc}$ = 72.7(9)°, α 1.730(5), β 1.740(5), and γ 1.765(5). It exhibits strong pleochroism; X colorless, Y yellow, and Z straw-yellow; X = a, Y = b, Z = c.

X-ray diffraction data (17 lines) were obtained with a 114.6 mm Gandolfi camera (Ni-filtered Cu$K\alpha$ radiation) and include [d_{obs} in Å (I_{obs}%,hkl)] 8.353(70,011), 3.377(30,031), 3.196(50,220), 2.907(100,222), 2.694(30,015), 2.304(30,233), 2.241(40,215), 2.179(40,035), 2.097(50,242), and 1.564(30,064). Refined unit-cell using powder diffraction data gave a = 8.102(17), b = 10.443(7), c = 13.950(14) Å, V = 1180(2.4) Å^3.

The structure of noonkanbahite was solved with a $0.16 \times 0.06 \times 0.02$ mm crystal using data collected with a Bruker P4 diffractometer equipped with a CCD detector to R_1 = 2.8% and WR_2 = 6.9% for 970 unique reflections [$Fo > 4\sigma F$]. It is orthorhombic, space group $Imma$, with refined cell a = 8.0884(4), b = 10.497(5), c = 13.9372(6) Å, V = 1183.3(1) Å^3, Z = 4. Noonkanbahite is a shcherbakovite group mineral, and is isostructrural to both batisite and shcherbakovite and, respectively their K and Ba analog. This is due to the tolerance of this structure-type for isomorphous substitutions at the cation sites.

The mineral is named after the first locality where it was found by Prider in 1965 but never approved as a new species until the new material from Liley, Germany, and Murun, Russia, was discovered. This locality is near the Noonkanbah sheep station, Wolgidee Hills, West Kimberley District, Australia. Both the mineral and mineral name were approved by the Commission on New Minerals and Mineral Names, IMA (2009-059) and the holotype material was deposited at the Royal Ontario Museum (catalog no. M54065). **R.R.**

NYHOLMITE*

P. Elliott, P. Turner, P. Jensen, U. Kolitsch, and A. Pring (2009) Description and crystal structure of nyholmite, a new mineral related to hureaulite, from Broken Hill, New South Wales, Australia. Mineral. Mag., 73, 723–735.

Nyholmite, discovered in ore mined from the Block 14 Opencut at Broken Hill, New South Wales, is only the third known natural Cd-bearing arsenate after keyite and andyrobertsite, and the second new Cd-dominant mineral to be described from the locality after birchite. The mineral occurs in cavities in a quartz-garnet-arsenopyrite matrix, associated with goldquarryite, lavendulan-sampleite, scorodite-strengite, and gypsum. Nyholmite occurs in isolated globules, tufted aggregates of fibrous crystals (up to 1 mm across), and radiating hemispheres of thin, bladed, colorless crystals (0.5 mm across) with individual crystals 0.2×0.05 mm. The mineral is transparent to translucent, nonfluorescent, has a white streak, vitreous luster, Mohs hardness of 3–3.5, is brittle and has an uneven fracture. No cleavage was observed and the mineral is slowly soluble in cold 10% HCl. The calculated density is 4.23 g/cm^3 for the empirical formula and 4.42 g/cm^3 for the ideal formula. Only one refractive index was determined, β ~ 1.70.

Chemical analyses of nyholmite were obtained on a Cameca SX51 electron microprobe in WDS mode: P_2O_5 6.29, As_2O_5 34.55, Al_2O_3 0.2, MnO 3.59, CaO 0.16, CuO 3.39, ZnO

9.72, CdO 34.58, PbO 0.37, H_2O_{calc} 8.21, total 101.06 wt%, corresponding to the empirical formula, calculated on the basis of 20 O atoms, of $Cd_{2.80}Zn_{1.24}Mn_{0.53}Cu_{0.44}Al_{0.04}Ca_{0.03}Pb_{0.02}$ $[(AsO_4)_{3.13}(PO_4)_{0.92}]_{\Sigma4.05}H_{1.91}\cdot3.79H_2O$, with a simplified formula of $Cd_3Zn_2(AsO_3OH)_2(AsO_4)_2\cdot4H_2O$, which requires CdO 35.09, ZnO 14.83, As_2O_5 41.88, H_2O 8.21, total 100.00 wt%.

Single-crystal X-ray intensity data were collected on a $0.050 \times 0.010 \times 0.003$ mm crystal at the ChemMatCARS facility, APS, Argonne National Laboratory, on a modified 3-circle diffractometer using a Bruker SMART-6000 CCD detector ($\lambda = 0.49594$ Å). The structure was refined in space group $C2/c$ using starting atomic coordinates of hureaulite and converged to $R1 = 0.0373$, $wR2 = 0.0861$, for 2045 observed unique reflections ($F_o > 4\sigma F$), GoF = 1.081, $a = 18.062(4)$, $b = 9.341(2)$, $c = 9.844(2)$ Å, $\beta = 96.17(3)°$, $V = 1651.2(6)$ Å^3, $Z = 4$. Powder X-ray diffraction data were collected on a 100 mm Guinier-Hägg camera ($CrK\alpha$ radiation) with intensities visually estimated. Unit-cell refinement gave $a = 18.042(2)$, $b = 9.315(1)$, $c = 9.797(1)$ Å, $\beta = 96.14(1)°$, $V = 1637.2(2)$ Å^3, which agree with those from the single-crystal refinement. The strongest lines on the pXRD pattern [d_{obs} in Å(I_{obs}%,hkl)] include: 8.985(30,200), 8.283(85,110), 6.169(25,111), 4.878(25,002), 3.234(100,2$\overline{2}$2,420), 3.079(65,222,511), and 2.976(45,113). The structure of nyholmite is characterized by short, kinked five-membered chains of $M_5\phi_{22}$ (where $\phi = O^{2-}$ or H_2O) that extend in the a direction. These chains share corners to form a sheet in the (001) plane, which are further linked by corner-sharing AsO_4 groups to form slabs in the (001) plane. Slabs link in the c direction by corner-sharing to form a densely packed heteropolyhedral framework with interstitial sites occupied by H atoms. Nyhomite is isostructural with minerals of the hureaulite group. It is a late-stage, supergene mineral that formed under low-temperature conditions along with a suite of secondary arsenate minerals.

The mineral is named for Sir Ronald Sydney Nyholm (1917–1971), who was born at Broken Hill, New South Wales, and was chair and professor of chemistry at University College, London, from 1955–1971. The mineral and name have been approved by the IMA CNMNC (IMA no. 2008-047). Type material has been deposited in the South Australian Museum, Adelaide, South Australia (G32511). **P.C.P.**

PARAERSHOVITE*

A.P. Khomyakov, F. Cámara, E. Sokolova, Y. Abdu, and F.C. Hawthorne (2010) Paershovite, $Na_3K_3Fe^{3+}_2(Si_4O_{10}OH)_2(OH)_2$ $(H_2O)_4$, A new mineral species from the Khibina alkaline massif, Kola Peninsula, Russia: description and crystal structure. Can. Mineral., 48, 279–290.

Paraershovite was first studied as part of an investigation of hyperagpaitic pegmatite of the Khibina alkaline massif in Russia, more precisely from Mount Yukspor area. The description of the new mineral was not completed for about 20 years due to the limited amount of material available. It was found associated to sodalite, aegirine, arfvedsonite, pectolite, shcherbakovite, lamprophyllite, lomonosovite, shafranovskite, villiaumite, and natrophosphate in the highly mineralized pegmatite. The mineral forms as equant (100), platy and [001] elongate prisms up to 0.5–1 mm with aggregates up to 2–3 mm scattered on a single

hand specimen from a pegmatite. Crystals are vitreous translucent or transparent, yellow with orange or pink shades, with a white streak. No fluorescence was observed under 240–400 nm UV radiation. Optically it is biaxial positive, $\alpha = 1.569(2)$, $\beta = 1.583(2)$, $\gamma = 1.602(2)$ ($\lambda = 589$ nm), $2V_{meas} = 80(3)°$, $2V_{calc} = 82°$. No pleochroism was observed, it has a dispersion $r > v$ (weak), and orientation $X \wedge c = 84°$, $Y \wedge c = 66°$, $Z \wedge c = 24°$. The mineral is brittle with a Mohs hardness of 3, a perfect cleavage along {100}, and a splintery step-like fracture. It readily dissolves in a 50% solution of HCl and HNO_3. $D_{meas} = 2.60(3)$, $D_{calc} = 2.584$ g/cm^3 and the compatibility index is excellent.

Electron microprobe analyses (average of 12 analyses) gave Na_2O 7.77, K_2O 14.07, MgO 0.24, MnO 0.73, Fe_2O_3 (Mössbauer spectroscopy) 11.29, Al_2O_3 0.58, SiO_2, TiO_2 3.32, F 0.39, H_2O (calc) 10.98, O=F –0.16, sum 98.88 wt%, corresponding to $(Na_{2.44}\square_{1.56})_{\Sigma4}K_{2.91}(Fe^{3+}_{1.38}Ti_{0.40}Al_{0.11}Mn^{2+}_{0.10}Mg_{0.06})_{\Sigma2.05}$ $Si_{8.05}O_{20}[(OH)_{3.80}F_{0.20}]_{\Sigma4}(H_2O)_4$, $Z = 1$, based on 28 (O + F). The ideal formula is $Na_3K_3Fe^{3+}_2(Si_4O_{10}OH)_2(OH)_2(H_2O)_4$. The presence of H_2O and OH groups is confirmed by absorption bands at 1600 and 3500 cm^{-1} in the IR spectrum.

The crystal structure was solved with data obtained from a $0.08 \times 0.18 \times 0.18$ mm crystal using a P4 automated four-circle diffractometer with a CCD 4K APEX detector, R_1 index = 4.28% and $wR_2 = 10.07$% for 2134 reflections [$F_o > 4\sigma(F_o)$]. Paraershovite is triclinic, $P\overline{1}$ with unit-cell parameters refined to $a = 10.244$, $b = 11.924$, $c = 5.276$ Å, $\alpha = 103.491$, $\beta = 96.960$, $\gamma = 91.945°$, $V = 620.8$ Å^3. The strongest line of the X-ray diffraction pattern [d_{obs} in Å (I_{obs}%,hkl)] include 11.778(100,010), 4.390(70,1$\overline{1}$1,0$\overline{2}$1), 3.012(70,230,$\overline{3}$20), 2.606(70,3$\overline{2}$1,131,0$\overline{1}$2,$\overline{1}$ $\overline{1}$2), 4.109(60,$\overline{1}$11,$\overline{1}$ $\overline{2}$1), and 2.730 (60,$\overline{3}$ $\overline{2}$1,$\overline{1}$ $\overline{4}$1,$\overline{1}$ $\overline{4}$1,3$\overline{1}$1,221). Paraershovite is isotructural and chemically related to ershovite $Na_4K_3(Fe^{2+},Mn,Ti)_2(Si_4O_{10}OH)_2$ $(OH)_2(H_2O)_4$ for which it is the Na-deficient, Fe^{3+}-dominant analog. The two species are considered to also be paragenetically related, where ershovite is the primary high-temperature phase and paraershovite the oxidized phase through epithermal alteration of ershovite. Their chemical relationship can be summarized by the following substitution: $\square + Fe^{3+}_2 \rightarrow Na^+ + M^{2.5+}_2$ ($M^{2.5+} = Fe^{2+}$, Mn^{2+}, Ti^{4+}).

The mineral is named for it structural and chemical relationship with the mineral ershovite. The IMA CNMMN has approved the mineral and its name (IMA 2009-025) and holotype material was deposited at Fersman Mineralogical Museum, Russian Academy of Sciences, Moscow, Russia (catalog no. 3793).

Note: A complete X-ray diffraction pattern was omitted in this paper, this list is from the abstract. **R.R.**

ROUMAITE*

C. Biagioni, E. Bonaccorsi, S. Merlino, G.C. Parodi, N. Perchiazzi, V. Chevrier, and D. Bersani (2010) Roumaite, $(Ca,Na,\square)_3(Ca,REE,Na)_4(Nb,Ti)[Si_2O_7]_2(OH)F_3$, from Rouma Island, Los Archipelago, Guinea: a new mineral species related to dovyrenite. Can Mineral., 48, 17–28.

Roumaite occurs in Albian (104 Ma) nepheline syenites, which make up a peralkaline complex whose outcrops form the Los Archipelago. The complex consists of agpaitic and miaskitic suites. The host rock of the type roumaite specimen

is part of suite of samples held in the collection of the Muséum National d'Histoire Naturelle of Paris. Roumaite is formed as a late-stage product of hydrothermal activity in the cavities of nepheline syenites. It is associated with aegirine, albite, analcime, arfvedsonite, catapleiite, a eudialyte-group mineral, microcline, sodalite, sphalerite, steacyite, and villiaumite. Roumaite occurs as acicular crystals up to 0.5 mm, elongate on [100] with a silky luster. Rare specimens tabular on (001) occur by parallel growth of individual fibers. Roumaite is brittle with a white streak and is non-fluorescent in ultraviolet light. Hardness and density could not be measured; calculated density is 3.33 g/cm³. The small size of roumaite crystals limited the optical data that could be collected. Crystals are colorless and nonpleochroic. Indices of refraction are between 1.652 and 1.654 both parallel and perpendicular, to the direction of elongation [100]. The maximum extinction angle on [100] is 4° with positive elongation and weak birefringence. The compatibility index is –0.007 (superior).

The composition of roumaite was determined using electron microprobe at 15 kV accelerating voltage, 20 nA beam current, and 5 μm spot size. The average composition (ranges in parentheses, n = 6) is SiO_2 29.78 (28.68–31.32), TiO_2 2.91 (2.57–3.43), ZrO_2 0.02 (0.00–0.02), ThO_2 0.07 (0.00–0.33) Y_2O_3 0.67 (0.41–0.80), Ce_2O_3 13.15 (11.97–13.67), La_2O_3 5.02 (4.37–5.40), Nd_2O_3 2.28 (1.97–2.51), CaO 20.61 (19.58–21.30), MnO 0.02 (0.00–0.05), Na_2O 7.83 (6.69–9.43) Nb_2O_5 10.51 (8.63–11.27), F 6.46 (5.78–7.25), O≡F –2.72, total 96.61 wt%. Consistently low analytical totals (94–99 wt%) are suggested to be due to either the presence of H_2O or a result of the beam diameter being close to the width of the acicular crystals. Raman spectroscopy of roumaite was unable to confirm the presence of water due to fluorescence effects caused by the presence of REE. The empirical formula (on the basis of four Si pfu) is $(Ca_{2.97}Na_{2.04}Ce_{0.65}La_{0.25}Nd_{0.11}Y_{0.05})_{\Sigma 6.07}(Nb_{0.64}Ti_{0.29})_{\Sigma 0.93}(Si_2O_7)_2F_{2.75}O_{0.38}$. The authors suggest that the low totals of octahedral cations (in comparison to other members the rinkite group) and low totals numbers of anions imply the presence of octahedral vacancies and some (OH)⁻ groups. This leads to a simplified formula of $(Ca,Na,REE,\square)_{\Sigma 7.00}(Nb,Ti)(Si_2O_7)_2(OH)F_3$.

A powder diffraction pattern was collected using a Gandalfi camera and Cu$K\alpha$ radiation. The pattern was indexed taking into account reflections observed during single-crystal data collection. The six strongest lines in the powder diffraction pattern [d_{hkl} in Å(I_{obs}%,hkl)] are: 2.790(40.1,041) 2.689(46.4,042,026), 2.567(44.4,223,043), 2.021(67.7,243), 1.680(60.1,$\overline{2}$61,065), and 2.004(32.5,226). Initial single-crystal X-ray diffraction data were collected using a 0.4 × 0.1 × 0.1 mm sample mounted on a SIEMENS P4 four-circle diffractometer with Mo$K\alpha$ radiation. Problems solving the structure caused by small sample size and weak reflections lead to a second structure refinement attempt using synchrotron radiation (λ = 0.7001 Å) and a MAR CCD detector. The structure was refined using 4558 independent reflections with $|F_o| \geq 4\sigma F_o$ and yielded a final R_1 = 0.08. Roumaite is monoclinic, space group Cc, with cell parameters a = 7.473(2), b = 11.294(2), c = 18.778(4) Å, β = 101.60(2)°, V = 1552.5(6) Å³, Z = 4. The structure of roumaite consists of stacks of tobermorite like layers, octahedral layers and disilicate layers parallel to (001). The tobermorite layers consist of columns of made of four edge-sharing, sevenfold coordinated polyhedra. The

columns are parallel to a, and are connected along b. In roumaite, these polyhedra are occupied by Ca, REE, and Na. The M5 site is probably dominated by Ce. The octahedral sheets consist of two types of columns running parallel to a. The first type is made up of M2 eightfold polyhedral alternating with smaller M1 octahedra occupied by Ti and Nb. The second column is formed by alternating M3 and M4 polyhedra. Disilicate groups attach to the M2 polyhedral on both sides of the octahedral sheet. The M1 sites are occupied by 55% Nb with the balance filled by Ti. The M2 site occupancies are $(Ca_{0.45}Na_{0.30}\square_{0.25})$, the M3 site occupancies are $(Ca_{0.60}Na_{0.15}\square_{0.25})$, and the M4 occupancies are $(Na_{0.60}Ca_{0.0.35}\square_{0.05})$. The tobermorite and octahedral layers are linked by disilicate groups attached to the Ca polyhedral of the tobermorite layer and M2 polyhedra of the octahedral layer. The formula based on the structural refinement is $(Ca,Na,\square)_3(Ca,REE,Na)_4(Nb,Ti)(Si_2O_7)_2(OH)F_3$. Roumaite is closely related to dovyrenite.

The name is for Rouma Island, a central island in the lagoon of the Los Archipelago. The current study did not allow a reliable distribution of REE among crystallographic sites; therefore a Levinson suffix is not used at this time. The mineral and name have been approved by IMA-CNMMN (2008-024). Holotype material is in the Muséum National d'Histoire Naturelle, 61, rue Buffon, F-75005 Paris, France (catalog no. MNHN208.1); cotype material is held in the collection of Museo di Storia Naturale e del Territorio, Università di Pisa, Via Roma 79, Calci (PI), Italy (catalog no. 18873). **G.P.**

SLAVKOVITE*

J. Sejkora, J. Plášil, P. Ondruš, F. Veselovský, I. Císařová, and J. Hloušek (2010) Slavkovite, $Cu_{13}(AsO_4)_6(AsO_3OH)_4\cdot 23H_2O$, a new mineral species from Horní Slavkov and Jáchymov, Czech Republic: description and crystal-structure determination. Can. Mineral., 48, 1157–1170.

Slavkovite was initially discovered in a supergene mineral assembly in an abandoned quarry near Horní Slavkov, Czech Republic. The material discovered here was not suitable for full characterization, which had to await the discovery of larger well-formed crystals in the Jáchymov ore district. Jáchymov ore district consists of medium-grade metasedimentary rocks of Cambrian to Ordovician age cut by Variscan granite plutons. The ore in the area is typical of Ag+As+Co+Ni+Bi and U hydrothermal mineralization and formed in the halo of the plutonic intrusions. Later supergene mineralization resulted in a wide variety of secondary mineralization.

In Jáchymov, slavkovite is found associated with lavendulan, geminite, lindackerite, and ondrušite; it is formed by the weathering of primary tennantite and chalcopyrite. In the Huber open pit near Horní Slavkov, slavkovite is found in an abandoned quarry that was mined for Sn and W. It is associated with amorphous Cu, Fe arsenates and clay minerals. Slavkovite form Jáchymov is pale-green in aggregates and colorless with a green tint as individual crystals. It occurs as rosettes up to 1 mm across and in spherical aggregates up to 5 mm across. Individual crystals are up to 1 mm long and 0.5 mm in width. Slavkovite from Krásno near Horní Slavkov occurs as light blue to blue-green coatings that are composed of very thin tabular crystals up to 50 μm in size. It is transparent (individual crystals) to translucent with a vitreous

luster and a white streak; it does not fluoresce in ultraviolet light. There is one perfect cleavage {011} and one good one {010}; the fracture is irregular, and it is very brittle. The Mohs hardness is 3.5–4, the measured density is 3.05(1) g/cm³, and the calculated density is 3.05 g/cm³. The optical properties were determined using material from Jáchymov. Slavkovite is biaxial positive; the exact positions of the individual optical orientations with respect to α, β and γ due to the presence of two cleavage planes in this triclinic mineral. The indices of refraction are α′ = 1.591(2), β′ = 1.620(2), γ′ = 1.701(2), and $2V_{calc}$ is approximately 64°. It is moderately pleochroic with X light gray to colorless, Y very light greenish gray, Z light green. Elongation on the (011) plane is negative with an extinction angle of 27°, on the (010) plane extinction is positive with an extinction angle of 17°.

The chemical composition was determined by WDS (Cameca SX-100, 15 kV, 5–10 nA, 5–10 μm spot size, PAP correction). Slavkovite is unstable under the electron beam. The average of six analyses of the Jáchymov material gives (ranges in parentheses) FeO 0.12 (0.00–0.21), CuO 39.93 (37.48–43.09), Al₂O₃ 0.13 (0.07–0.19), As₂O₅ 44.71 (43.77–45.60), H₂O 17.31 (from thermal analysis), total 102.20 wt%. This gives an ideal formula [on the basis of 63(O,OH,H₂O)] of $(Cu_{12.96}Al_{0.07}Fe_{0.04})_{\Sigma13.07}(AsO_4)_{6.11}$ $(AsO_3OH)_{3.93}\cdot22.83H_2O$. The average composition of material from Horní Slavkov (average of 3 points) is CaO 0.07, FeO 0.04, CuO 39.99, ZnO 0.12, Al₂O₃ 0.38, As₂O₅ 46.03, P₂O₅ 0.10, H₂O 18.2 (from structure considerations), total 104.93 wt%. The empirical formula for the Horní Slavkov sample [on the basis of 63(O,OH, H₂O)] is $(Cu_{12.51}Al_{0.19}Zn_{0.04}Ca_{0.03}Fe_{0.01})_{\Sigma12.78}$ $(AsO_4)_{5.70}(PO_4)_{0.04}(AsO_3OH)_{4.27}\cdot22.83H_2O$.

Thermogravimetric analysis of Jáchymov slavkovite showed that it dehydrates in seven steps; 11 H₂O molecules are lost between 20–100 °C, with a further five dehydration steps releasing 12 more H₂O molecules between 100–310 °C. A final two H₂O molecules are lost between 310 and 530 °C, with a total loss of 17.31 wt% (equivalent to 25 molecules of H₂O). Infrared absorption spectroscopy was performed using powder dispersed in a KBr disk and a Nicolet FTIR 740 spectrophotometer. An intense band at 3434 cm⁻¹ with a shoulder at 3265 cm⁻¹ is assigned to υ(OH) stretching. Bands at 1550–1750 cm⁻¹ are assigned to δ(H-O-H) bending of H₂O molecules. Bands in the range 1550 to 1000 cm⁻¹ are assigned to δ(As-OH) in plane bending. Shoulders at 896, 863, and the band at 798 cm⁻¹ are assigned to split triply degenerate antisymmetric stretching vibration υ3(AsO₄)³⁻.

A powder X-ray diffraction pattern was collected using a Phillips X'Pert powder diffractometer with graphite-monochromated CuKα radiation. The strongest eight lines in the pXRD pattern [d_{hkl} Å (I_{obs}%,hkl)] are as follows: 15.70(3,001), 11.98(100,0$\bar{1}$1), 6.992(3,0$\bar{2}$1,020), 5.992(6,0$\bar{2}$2), 3.448(5,040), 2.967(5,0$\bar{3}$5), 2.4069(4,1$\bar{5}$4), 2.4002(4,115,$\bar{1}$35,0$\bar{4}$6,0$\bar{6}$2). Single-crystal X-ray diffraction data were obtained using a 0.25 × 0.23 × 0.027 mm single crystal from Jachymov. Intensity data were collected using an Enraf Nonius Kappa CCD single-crystal diffractometer, using graphite-monochromated MoKα radiation. 7721 unique and 6613 observed reflections ([I > 2σ(I)]) were collected. The structure was solved by direct methods with final R_{obs} = 4.37%. Slavkovite is triclinic, space group $P\bar{1}$, a = 6.408(3), b = 14.491(5), c = 16.505(8) Å, α = 102.87(3), β = 101.32(5), γ = 97.13(3)°, V = 1442(1) Å³, Z = 1, a:b:c = 0.4422:1:1.1390.

The crystal structure of slavkovite consists of sheets made up of copper polyhedra linked by hydrogen arsenate and arsenate tetrahedra. These sheets are linked by Cu₆-Φ polyhedra.

The name is for the original discovery; name and mineral are approved by the IMA-CNMMN (IMA 2004-8). The holotype sample of slavkovite is held in the collection of the national Museum, Prague, Czech Republic (PIN 83.038). **G.P.**

Zigrasite*

F.C. Hawthorne, N.A. Ball, J.W. Nizamoff, and W.B. Simmons (2009) Zigrasite, MgZr(PO₄)₂(H₂O)₄, a new phosphate mineral from the Dunton Quarry, Newry, Oxford county, Maine, U.S.A. Mineral. Mag., 73, 415–420.

F.C. Hawthorne and W.B. Simmons (2010) The crystal structure of zigrasite, MgZr(PO₄)₂(H₂O)₄, a heteropolyhedral framework structure. Mineral. Mag., 74, 567–575.

Zigrasite is a new secondary phosphate mineral from the giant 1972 tourmaline-bearing pocket at the Dunton Quarry, Newry, Oxford County, Maine, U.S.A. It occurs as subhedral blocky grains in aggregates with its Ca-analogue and an unknown Zr phosphate mineral. Zigrasite was found on a tourmaline crystal and is associated with tourmaline, microcline, quartz, albite, beryl, amblygonite-montebrasite, childrenite-eosphorite, and apatite. The mineral is off-white to pale-yellow or light tan, translucent, has a white streak, a vitreous luster, Mohs hardness = 3, imperfect cleavage in two directions, no parting, is brittle, has a hackly fracture, and shows light blue to pale yellow cathodoluminescence. D_{meas} = 2.76(4) g/cm³, D_{calc} = 2.66 g/cm³. In transmitted light, zigrasite is colorless and non-pleochroic, biaxial (–) negative, α = 1.597(1), β = 1.622(1), γ = 1.635(1), $2V_{meas}$ = 65.5(4)°, $2V_{calc}$ = 71°.

The chemical composition of zigrasite was determined on a Cameca SX100 electron microprobe in WDS mode and gave the following results (average of six analyses): P₂O₅ 37.59, ZrO₂ 32.27, HfO₂ 0.34, FeO 0.20, MgO 10.37, ZnO 0.17, F 0.13, LOI_meas 18.60, O ≡ F 0.05, total 99.62 wt%, corresponding to the empirical formula (based on 12 anions with 4 H₂O) $(Mg_{0.97}Fe_{0.01}Zn_{0.01})_{\Sigma0.99}(Zr_{0.99}Hf_{0.01})_{\Sigma1.00}P_{2.00}O_8(H_2O)_4$, with the ideal formula of MgZr(PO₄)₂(H₂O)₄.

The structure of zigrasite was solved and refined using a 2560 × 100 μm crystal on a Bruker AXS SMART APEX diffractometer (MoKα radiation) to R1 = 0.0375, wR2 = 0.0872, on the basis of 2623 unique reflections ($F_o > 4\sigma F$). It is triclinic, P1, a = 5.3049(2), b = 9.3372(4), c = 9.6282(5) Å, α = 97.348(1), β = 91.534(1), γ = 90.512(4)°, V = 472.79(5) Å³, Z = 2. Powder X-ray diffraction data were collected on a 114.6 mm Debye-Scherrer camera (CuKα radiation) with a Gandolfi attachment, which gave the following refined unit-cell parameters: a = 5.321(7), b = 9.360(10), c = 9.660(8) Å, α = 97.38(10), β = 91.29(9), γ = 90.58(9)°, V = 477.0(5) Å³, which are in agreement with those determined from the single-crystal refinement. The strongest lines on the powder diffraction pattern [d_{obs} in Å (I_{obs}%,hkl)] include: 9.550(100,001), 4.589(40,110), 4.411(50,0$\bar{2}$1), 4.108(70,$\bar{1}$11), 4.008(50,111), 3.569(30,0$\bar{2}$2), 3.177(40,112), and 2.660(30,200).

Zigrasite is a heteropolyhedral framework mineral and is isochemical with mahlmoodite. There are two P sites, two Mg

sites occupied by Mg and octahedrally coordinated by two O anions and four (H_2O) groups, and one *Zr* site, occupied by Zr and octahedrally coordinated by six O anions. The (ZrO_6) octahedron shares corners with six (PO_4) tetrahedra, forming a [$Zr(PO_4)_2$] sheet parallel to (001). These sheets are stacked in the *c* direction and linked by [$MgO_2(H_2O)_4$] octahedra that share O atoms with the (PO_4) groups.

Zigrasite is named for James Zigras (b. 1981) of Paramus, New Jersey, U.S.A., a prominent mineral collector who discovered the mineral. The mineral and name have been approved by the IMA CNMNC (IMA no. 2008-046) and holotype material has been deposited in the mineral collection at the Royal Ontario Museum, Toronto, Ontario (catalog no. M53323). **P.C.P.**

NEW DATA

BILLINGSLEYITE*

L. Bindi, R.T. Downs, and S. Menchetti (2010) The crystal structure of billingsleyite, $Ag_7(As,Sb)S_6$, a sulfosalt containing As^{5+}. Can. Mineral. 48, 155–162.

Billingsleyite was originally described as orthorhombic on the basis of powder X-ray diffraction data. Subsequent studies of synthetic material believed to be analogous suggested the structure should be described as cubic. The current study presents a new single-crystal study of the cotype material from the North Lily mine, East Tintic district, Utah, U.S.A. It was obtained from the collection of the RRUFF project (deposition no. R070350; http://rruff.info/R070350). The sample consists only of pure billingsleyite, with no associated mineral or inclusions. It consists of fine-grained aggregates with a dark lead-gray to black color and a metallic luster.

The chemical composition of the sample was determined using WDS (JEOL 8600, 20 kV, 40 nA, 15 s counting time). The average of six analyses of a single grain gave the following results: Ag 72.84, Cu 0.25, Fe 0.06, As 6.32, Sb 1.53, S 18.73, Total 99.73. Se, Te, Au, Pb, and Bi were sought but not found. The sample was homogeneous within statistical error. The empirical formula on the basis of 14 atoms is $(Ag_{6.94}Cu_{0.04}Fe_{0.01})_{\Sigma6.99}$ $(As_{0.87}Sb_{0.13})_{\Sigma1.00}S_{6.01}$

Single-crystal data was collected using an Oxford Diffraction Xcalibur3 diffractometer using graphite monochromated Mo*K*α radiation and fitted with a Sapphire 2 CCD detector. The structure was refined on the basis of 902 independent reflections and 416 observed reflections where $|F_o| \geq 4\sigma F_o$. The *R* value for the observed reflection was 1.64%. Billingsleyite is cubic, space group $P2_13$, with a cell parameter a = 10.4760(8) Å, V = 1149.7(2) Å^3, and Z = 4. The structure of billingsleyite consists of $(As,Sb)S_4$ tetrahedra and Ag polyhedra. Silver polyhedra coordination's are linear, triangular or quasi-tetrahedral. Short bond lengths between Ag2 and Ag3 (2.969 Å) suggested Ag-Ag bonding. Electron-density analysis confirmed that Ag2 and Ag3 are indeed bonded and that As only bonds to four S atoms. The structure of billingsleyite is identical to synthetic Ag_7AsS_6. **G.P.**

ERRATUM

Garutiite (Ni,Fe,Ir) (2011) Am. Min., vol. 96, p. 941–942.

Note that the mineral name should have been written as Garutiite and not "Garutiite (Ni,Fe,Ir)" as written in the title and in the first sentence of the submission.