

New Mineral Names*

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BOROMULLITE*

I.S. Buick, E.S. Grew, T. Armbruster, O. Medenbach, M.G. Yates, G.E. Bebout, and G.L. Clarke (2008) Boromullite, $\text{Al}_9\text{BSi}_2\text{O}_{19}$, a new mineral from granulite-facies metapelites, Mount Stafford, central Australia: a natural analogue of a synthetic "boron-mullite". *Eur. J. Mineral.*, 20, 935–950.

The type locality of boromullite, Mount Stafford, is situated about 170 km northwest of Alice Springs, central Australia (22°01'S, 132°40'E). The Mount Stafford area comprises Proterozoic metasedimentary and metagranitic rocks of the Arunta Region. Boromullite formed during anatexis of B-rich pelitic rocks under granulite facies conditions (810 °C $\approx$ $T \geq 775$ –785 °C, $P = 3.3$ –4 kbar), possibly due to a shift in bulk composition to lower SiO_2 and B_2O_3 contents associated with melt extraction. Sekaninaite-cordierite, potassium feldspar, biotite, werdingite, and its Fe-dominant analogue, hercynite, and ilmenite are other commonly associated minerals, whereas ominelite-grandidierite, plagioclase, and alusite, and tourmaline are much subordinate. The most widespread accessories are monazite-(Ce), an apatite-group mineral, and zircon.

For the structure analysis, the same grain of boromullite (section a/area 2/grain 2) was mounted on a Bruker PLATFORM three-circle goniometer equipped with a 1 K SMART CCD detector and a crystal-to-detector distance of 5.4 cm. Single-crystal X-ray diffraction gives orthorhombic symmetry, $Cmc2_1$, $a = 5.7168(19)$ Å, $b = 15.023(5)$ Å, $c = 7.675(3)$ Å, $V = 659.2(7)$ Å³, calculated density 3.081 g/cm³, $Z = 2$. X-ray powder-diffraction data were obtained from boromullite (section a/area 4/grain 2) with a 57.3 mm diameter Gandolfi camera and $\text{CuK}\alpha$ radiation at the Ruhr-Universität Bochum. The strongest lines in the powder pattern [d in Å, ($I_{\text{obs}}\%$, hkl)] are 5.37(50,021), 3.38(100,022,041), 2.67(60,042), 2.51(60,221,023), 2.19(80,222), 2.11(50,043), 1.512(80,263).

Boromullite is colorless and transparent, biaxial (+), $n_x = 1.627(1)$, $n_y = 1.634(1)$, $n_z = 1.649(1)$ (589 nm), $2V_z$ (meas) = 57(2)°, $2V_z$ (calc) = 69(12)°. In the type specimen boromullite tends to form prisms or bundles of prisms up to 0.4 mm long, typically as fringes or overgrowths on aggregates of sillimanite or as narrow overgrowths around embayed werdingite prisms. In other samples boromullite and sillimanite are intergrown on

a fine scale (from <1 μm to >10 μm). No cleavage is evident in boromullite, which is brittle. The density calculated with empirical formula is 3.081 g/cm³. Other physical properties could not be determined. No dispersion or pleochroism could be detected.

Boromullite was analyzed with a Cameca SX-100 electron microprobe at the University of Maine using wavelength-dispersive spectroscopy (WDS). Electron-microprobe analysis of the holotype prism is SiO_2 19.01, TiO_2 0.01, B_2O_3 6.52, Al_2O_3 74.10, MgO 0.07, CaO 0.00, MnO 0.01, FeO 0.40, total 100.12 wt%, which gives $\text{Mg}_{0.01}\text{Fe}_{0.03}\text{Al}_{8.88}\text{Si}_{1.93}\text{B}_{1.14}\text{O}_{18.94}$ (normalized to 12 cations), ideally $\text{Al}_9\text{BSi}_2\text{O}_{19}$. Additional analyses of boromullite were obtained at the Electron Microscopy Unit, The Australian National University, using a JEOL 6400 SEM and energy dispersive spectrometry (EDS; Oxford ISIS EDXA detector).

The refined average structure model indicates two superimposed modules. Module 1 has the topology and stoichiometry of sillimanite and carries all the Si but none of the B, i.e., $\text{Al}_4\text{Si}_2\text{O}_{10}$. Module 2 is a type of mullite defect structure in which Si is replaced by B in triangular coordination and by Al in tetrahedral coordination, i.e., Al_5BO_9 . Instead of the uninterrupted tetrahedral Si-Al chains filling the channels between the columns of edge-sharing Al octahedra as in sillimanite, every other Al tetrahedron flips into the adjacent channel in domain 2. In the investigated grain, module 1 and module 2 are present in equal proportions. Module 2 is structurally identical to the synthetic compound Al_5BO_9 described previously to this study.

The mineral and name were approved by the Commission on New Minerals, Nomenclature and Classification, International Mineralogical Association (2007-021). Boromullite is named for boron being an essential constituent and for its relationship to mullite. Type material is deposited in the South Australian Museum, Science Centre, Morgan Thomas Lane (off Kintore Avenue), Adelaide, South Australia 5000, Australia; registration numbers SAM G31520 (holotype) and SAM G31521 (2 pieces of cotype); these are fragments of sample 2006-MST22. **K.T.T.**

F-RICH HIBSCHITE

A.R. Chakhmouradian, M.A. Cooper, L. Medici, F.C. Hawthorne, and F. Adar (2008) Fluorine-rich hibschite from silicocarbonatite, Afrikanda complex, Russia: crystal chemistry and conditions of crystallization. *Can. Mineral.*, 46, 1033–1042.

Fluorine-rich hibschite was found in a calcite-amphibole-diopside silicocarbonatite from the Afrikanda Complex, Kola Peninsula, Russia. The hibschite is found as colorless, isotropic

* All minerals marked with an asterisk have been approved by the IMA CNMMN.

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grains 10 to 50 μm in diameter with a consistent backscatter and optical zoning resulting from variations in Fe and Al content. Associated minerals include titanite, chlorite, calcic catapleite and calcite.

Chemical composition was determined by WDS using a 1 μm spot size. H_2O contents were calculated on the basis of stoichiometry. Analyses show that the main cause of the zoning is the substitution of Fe^{3+} for Al the Y site. Fluorine content varies from 4.25 wt% in the core to 5.82 wt% on the rims. The maximum recorded F content is 6.0 wt%. The F content is weakly correlated to Al content. Using Fgr to represent the hypothetical $\text{Ca}_3\text{Al}_2\text{F}_{12}$ end-member, the compositional range is Grs_{57–63}Kt_{21–27}Fgr_{8–11}Adr_{0–13}. Raman spectroscopy verified the presence of OH-stretching modes, but could not be used to measure H_2O due to small crystal size.

Diffraction data was collected in situ using with a microdiffractometer and graphite monochromated $\text{CuK}\alpha$. The strongest seven lines in the diffraction pattern [d in $\text{\AA}$ ($I\%$, hkl)] are 2.690(100,420), 1.611(51,642), 1.953(36,116), 2.197(30,521), 1.439(20,653), 2.362(18,431), and 1.738(18,444). A single-crystal study was carried on a small ($8 \times 14 \times 16 \mu\text{m}$) fragment extracted from a polished thin section. Data was collected using a four-circle diffractometer with a $\text{MoK}\alpha$ radiation and Apex 4k CCD detector. R_1 for the refinement was 2.84%, with 71 unique reflections and 54 reflections with $|F| > 4\sigma_{F_o}$. F-rich hibschite has space group $Ia3d$ with $a = 12.037(3) \text{ \AA}$, $V = 1744.0(13) \text{ \AA}^3$, and $Z = 8$. Refinement of the Z site gave a Si content of 2.05(5) apfu, compared with 1.97 apfu calculated for the bulk chemical composition. The authors estimate that the F-rich hibschite crystallized at a temperature of approximately 200–250 $^\circ\text{C}$ with $\log a(\text{H}^+)_{\text{aq}} \approx \log a(\text{F}^-)_{\text{aq}} \approx -5$. **G.P.**

MARIANOITE*

A.R. Chakhmouradian, R.H. Mitchell, P.C. Burns, Y. Mikhailova, and E.P. Reguir (2008) Marianoite, a new member of the cuspidine group from the Prairie Lake silicocarbonatite, Ontario. *Can. Mineral.*, 46, 1023–1032.

Marianoite was discovered in the Tantalum Pit, south of Anomaly Lake in the Prairie Lake intrusive complex. The rock in which the marianoite was discovered consists of phlogopite, U-rich pyrochlore, titanite, and marianoite (which makes up approximately 1 vol% of the rock) in a mesostasis of calcite. Marianoite crystallized early in the history of the rock, predating the phlogopite, calcite, and most of the pyrochlore.

Marianoite is pale yellow, translucent with luster ranging from vitreous on cleavage surfaces to greasy on resorbed surfaces. There is a distinct cleavage on {010}, an uneven fracture, with Mohs hardness of 6. Specific gravity is greater than 3.32 g/cm^3 [$D_{\text{calc}} = 3.45(2)$]. Marianoite is colorless and non-pleochroic in plane-polarized light, with lamellar twinning in crossed-polars. It is biaxial (–) with $\alpha = 1.700$, $\beta = 1.715$, $\gamma = 1.725$, $2V_{\text{meas}} = 80^\circ$, $2V_{\text{calc}} = 78^\circ$, and weak optic-axis dispersion ($r < v$). Optical orientation is $Z = b$, $X \wedge c = 45^\circ$ in acute β .

WDS analyses gave an average composition ($n = 18$) of (wt%, range) of Na_2O 7.45 (7.18–7.62), CaO 27.92 (27.49–28.86), MgO 0.14 (0.08–0.23), MnO 0.37 (0.31–0.45), FeO 0.72 (0.41–1.27), TiO_2 0.94 (0.55–1.82), ZrO_2 13.80 (11.42–14.77),

HfO_2 0.15 (0.03–0.32), Nb_2O_5 16.01 (14.94–16.59), Ta_2O_5 0.08 (0.00–0.26), SiO_2 29.68 (29.31–30.17), F 2.54 (2.27–2.81), total 98.73 wt%. This gives an empirical formula on the basis of 18 anions of: $\text{Na}_{1.930}(\text{Ca}_{3.996}\text{Mn}_{0.042})_{\Sigma 4.038}(\text{Nb}_{0.967}\text{Zr}_{0.899}\text{Ti}_{0.094}\text{Fe}_{0.080}\text{Mg}_{0.028}\text{Hf}_{0.006}\text{Ta}_{0.003})_{\Sigma 2.077}(\text{Si}_{3.965}\text{O}_{14})\text{O}_{2.927}\text{F}_{1.073}$. The simplified formula is: $\text{Na}_2\text{Ca}_4(\text{Nb,Zr})_2(\text{Si}_2\text{O}_7)_2(\text{O,F})_4$.

X-ray diffraction data was collected using a Gandolfi camera and Ni-filtered $\text{CuK}\alpha$ radiation. Line intensities were estimated visually from film and are given only as “weak,” “medium,” and “strong”. The 5 strongest lines are [d_{obs} in $\text{\AA}$, (hkl)] 3.04($\bar{1}31$, 031), 2.98(102,302), 2.85(320,230), 2.02(232,432). The structure of marianoite was solved by direct methods on single-crystal X-ray intensity data obtained using a three-circle goniometer, a 1 K SMART CCD and monochromatic $\text{MoK}\alpha$ radiation. Corrections were needed to remove the effect of {100} twinning. Final R_1 was 4.94% for 6188 unique reflections (5905 where $|F_o| > 4\sigma F$). Marianoite has space group $P2_1$ with $a = 10.8459(15)$, $b = 10.2260(14)$, $c = 7.2727(10) \text{ \AA}$, $\beta = 109.332(3)^\circ$, $V = 761.1(3) \text{ \AA}^3$. It is isostructural with wöhlerite, but Nb shows a strong preference for the smallest octahedrally coordinated sites in the structure.

The name is for Anthony Nicola Mariano in recognition for contributions to the study of alkaline rocks and carbonatites. Type material is held in the collection of the R.B. Ferguson Museum of Mineralogy, Winnipeg (M 7425). **G.P.**

WAKEFIELDITE-(La)*

T. Witzke, U. Kolitsch, J.M. Wamsloh, and J. Göske (2008) Wakefieldite-(La), LaVO_4 , a new mineral species from the Glücksstern Mine, Friedrichroda, Thuringia, Germany. *Eur. J. Mineral.*, 20, 1135–1139.

Wakefieldite-(La) is a new mineral species from the long abandoned Glücksstern Mine near the Gottlob quarry, northern slope of the Gottlob hill, Friedrichroda, Thuringia, Germany. The mine was a source of Mn and Fe ores until 1855. Wakefieldite-(La) occurs in hydrothermal barite veins cross-cutting a Lower Rotliegend conglomerate and is associated with hausmannite, barite, and gottlobite. It occurs as freestanding crystals in small vugs in pseudo-octahedral hausmannite, the result of crystallization from low-temperature hydrothermal fluids. Wakefieldite-(La) is very rare—only 10 crystals have been found to date. It occurs as light pink to brown crystals, elongated along [001], 0.1–0.5 mm in length, showing the pinacoids {001}, the prism {100}, and possibly a dipyrmaid. Wakefieldite-(La) has a white streak, an adamantine luster, is transparent to translucent, brittle, has uneven fracture, and a Mohs hardness of ~4. A cleavage was not observed, but the mineral shows preferred orientation by X-ray powder diffraction on {100}, suggesting a possible cleavage. It is not fluorescent in long- nor short-wave UV. The calculated density ($Z = 2$) for the measured composition is 4.703 g/cm^3 , and 4.727 g/cm^3 . Wakefieldite-(La) is uniaxial (+), ω and $\epsilon > 1.90$, medium birefringence, pleochroism $E = \text{pale pink}$, $O = \text{pale pink yellow}$, $E > O$.

The chemical composition of wakefieldite-(La) was determined by EDS and WDS, with an average of 10 analyses giving La_2O_3 43.87, Ce_2O_3 0.31, Nd_2O_3 9.49, Pr_2O_3 6.65, Sm_2O_3 0.58, Y_2O_3 0.31, CaO 0.10, UO_2 0.03, V_2O_5 34.91, As_2O_5 0.06,

P₂O₅ 0.02, SiO₄ 0.04, total 96.37 wt%, corresponding to an empirical formula calculated on the basis of 4 oxygen atoms of (La_{0.71}Nd_{0.15}Pr_{0.11}Sm_{0.01}Y_{0.01})_{Σ0.99}V_{1.01}O_{4.00} and an ideal composition of LaVO₄, which requires La₂O₃ 64.18, V₂O₅ 35.82, total 100 wt%.

The crystal structure of wakefieldite-(La) was solved by direct methods from single-crystal intensity data (crystal size 0.07 × 0.07 × 0.12 mm³) to $R_1 = 1.04\%$, $wR_2 = 2.68\%$ for 209 observed reflections with $F_o > 4\sigma(F_o)$ (422 total reflections), GooF = 1.207. Wakefieldite-(La) is tetragonal, $I4_1/amd$, with unit-cell parameters determined by the single-crystal structure refinement $a = 7.432(1)$, $c = 6.521(1)$ Å, $V = 360.18(9)$ Å³. Powder X-ray diffraction data were collected using a Siemens D500 diffractometer (CuKα₁ radiation) giving unit-cell parameters of $a = 7.406(6)$, $c = 6.504(8)$ Å, $V = 356.8(6)$ Å³. The strongest lines on the diffraction pattern [d_{obs} Å ($I_{\text{obs}}\%$, hkl)] include 3.707(100,200), 2.759(10,112), 2.623(7,220), 1.902(4,312), and 1.853(19,400). The powder X-ray diffraction pattern shows preferred orientation on {100}, either due to sample preparation or an undetermined cleavage on {100}. Wakefieldite-(La) is a member of the xenotime group and has the zircon-type structure, isostructural with wakefieldite-(Ce) and wakefieldite-(Y).

The mineral is named in accordance with wakefieldite-(Ce) and wakefieldite-(Y), and was approved by the IMA CNMNC (no. 89-035a) prior to publication. Type material has been deposited in the Mineralogical Collection of the Bergakademie Freiberg, Germany (no. 81876).

Discussion: A previous voting on a wakefieldite-(La) proposal (no. 89-035) was suspended and results were later published as a La-rich wakefieldite-(Ce). The IMA Chairman chose to use the same IMA number for the present mineral as it concerns the same mineral name. **P.C.P.**

NEW DATA

AENIGMATITE*

E.S. Grew, U. Hålenius, and M. Pasero (2008) The crystal-chemistry of aenigmatite revisited: electron microprobe data, structure refinement and Mössbauer spectroscopy of aenigmatite from Vesterøya (Norway). *Eur. J. Mineral.*, 20, 983–991.

A new structure refinement of aenigmatite from Vesterøya, Norway, has been reported with a new set of electron microprobe chemical analyses and with a Mössbauer spectrum, aimed at elucidating the structural role of Fe²⁺ and Fe³⁺. The new refinement has allowed a much better assessment of the extent of cation order than that was possible in either of the previous refinements, although our average bond distances differ little.

The structure of an untwinned aenigmatite crystal from Vesterøya, Vestfold district, Norway, having a composition (Na_{3.73}Ca_{0.27})_{Σ=4.00}(Fe_{8.55}²⁺Ti_{2.10}Mg_{0.46}Fe_{0.40}³⁺Mn_{0.40}Ca_{0.06}Zn_{0.01}Zr_{0.01})_{Σ=11.99}(Si_{11.10}Al_{0.64}Fe_{0.26}³⁺)_{Σ=12.00}O₄₀ was refined in space group $P\bar{1}$ to give $R_1 = 0.0277$ for 5515 unique reflections with $F_o > 4\sigma(F_o)$ and 0.0324 for all 6145 unique data; GooF 1.124. Least-squares refinement of 94 reflections accurately centered on the diffractometer gave: $a = 10.415(1)$, $b = 10.840(1)$, $c = 8.931(1)$ Å, $\alpha = 105.107(4)$, $\beta = 96.610(5)$, $\gamma = 125.398(4)^\circ$,

and $V = 746.8(1)$ Å³.

The aenigmatite structure consists of one sheet in (011) of winged chains of tetrahedra (T1–T6) parallel to a , with two octahedra (M1 and M2) alternating with a second sheet composed of walls of octahedra (M3–M7) also extending parallel to a and cross-linked by the larger M8 and M9 polyhedra. A ⁵⁷Fe Mössbauer spectrum of a bulk sample was obtained at room temperature using a conventional spectrometer system operated in constant acceleration mode, a 50mCi ⁵⁷Co/Rh source and a gas-filled proportional counter. Mössbauer spectroscopy of a bulk sample gave Fe³⁺/Fe_{tot} = 0.12(1) whatever was the initial fitting model, and ¹⁴Fe³⁺/Fe_{tot} = 0.04(2), which is consistent with ¹⁴Fe³⁺/Fe_{tot} = 0.018(1) obtained from occupancy of T3, the only T site to have Fe.

The structure refinement, together with the Mössbauer spectrum, shows an unexpected degree of ordering at cation sites, although one in many cases consistent with ordering reported in other minerals of the aenigmatite (Na >> Ca at M8 and M9) and rhönite (Ca >> Na) subgroups of the sapphirine group. For example, our Mössbauer refinement, taken in conjunction with the chemical data, gives 0.37 Fe³⁺ at each of M1 and M2, but only 0.11 Fe³⁺ at each of M3–M6. **K.T.T.**

BATISIVITE*

T. Armbruster, M. Kadiyski, L.Z. Reznitsky, E.V. Sklyarov, and E.V. Galuskin (2008) Batisivite, the first silicate related to the derbylite-hemloite group. *Eur. J. Mineral.*, 20, 975–981.

Recently batisivite has been described as a new mineral, which occurs as an accessory mineral in quartz layers from the metamorphosed Cr-V-bearing carbonate siliceous sediments of the Sludyanka complex, Southern Lake Baikal, Siberia, Russia. Batisivite [(Ti,V,Cr)₁₄Ba[Si₂O₇]O₂₂] is homeotypic with the members of the derbylite-hemloite group of minerals. The group consists of derbylite [Fe₄Ti₃SbO₁₃(OH)], tomichite [(V,Fe)₄Ti₃AsO₁₃(OH)], barian tomichite [Ba_{0.5}(As₂)_{0.5}Ti₂(V,Fe)₅O₁₃(OH)], hemloite [(Ti,V,Fe)₁₂(As,Sb)₂O₂₃(OH)], and graeserite [(Fe,Ti)₇As(O,OH)₁₄].

X-ray diffraction intensity-data were collected with an Enraf-Nonius CAD4 diffractometer using graphite monochromated MoKα-X-radiation. The diffraction pattern is characterized by strong, sharp reflections, defining a C-centered monoclinic lattice with $a = 4.9878(3)$, $b = 14.1899(16)$, $c = 7.0813(2)$ Å, $\beta = 103.598(4)^\circ$. These cell dimensions are characteristic for members of the derbylite group. However, there are additional weak reflections revealing a half-width about 30% greater (slightly diffuse) than the sharp reflections consistent with the monoclinic subcell. In reciprocal space these additional reflections are shifted $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$ relative to the reflections of the monoclinic subcell. However, this pseudo-monoclinic “supercell” has all axes doubled ($V = 3897$ Å³). Thus the volume is eight-times that of the triclinic cell. Triclinic cell dimensions were refined from the angular settings of 25 reflections ($23^\circ < \theta < 29^\circ$) where each reflection was centered for four diffracting positions (positive and negative θ) to reduce systematic errors.

The crystal structure [space group $P\bar{1}$, $a = 7.5208(4)$, $b = 7.6430(4)$, $c = 9.5724(4)$ Å, $\alpha = 110.204(3)$, $\beta = 103.338(6)$, $\gamma = 98.281(7)^\circ$, $V = 487.14(7)$ Å³, $Z = 1$] has been determined and

refined from single-crystal X-ray data to $R = 2.59\%$.

Stacking of α - PbO_2 double chains and columns as in the structure of V_3O_5 forming interstitial channels define the structure of the derbylite type. The channels may be described by chains of empty cube-octahedra running parallel to [011] in triclinic setting. Adjacent cube-octahedra are alternately occupied by Ba and disilicate units. This order pattern is responsible for the triclinic symmetry. However, Ba-disilicate order is not complete. One cube-octahedron is statistically filled by $\sim 3/4$ Ba and $1/4$ disilicate, the other is occupied by $\sim 3/4$ disilicate and $1/4$ Ba. This type of disorder is in qualitative agreement with the observed slight diffusivity of the super-structure reflections.

The refined composition of the studied crystal is $(\text{Ti,Cr,V})_{14}\text{Ba}_{1.02}[\text{Si}_2\text{O}_7]_{0.98}\text{O}_{22.12}$, which agrees nicely with the analytically determined composition of $(\text{V}_{4.955}^{3+}\text{V}_{0.600}^{4+}\text{Cr}_{2.157}\text{Fe}_{0.256}\text{Nb}_{0.032})_{\Sigma 8.0}(\text{Ti}_{5.687}\text{V}_{0.313}^{4+})_{\Sigma 6.0}[\text{Ba}_{1.042}\text{Mg}_{0.020}(\text{Si}_{1.467}\text{Al}_{0.533}\text{O}_7)_{0.953}]\text{O}_{22.283}$ and with empirical formula $(\text{V}_{4.77}^{3+}\text{V}_{0.75}^{4+}\text{Cr}_{2.20}\text{Fe}_{0.25}\text{Nb}_{0.03})_{\Sigma 8.0}(\text{Ti}_{5.41}\text{V}_{0.59}^{4+})_{\Sigma 6.0}[\text{Ba}_{1.01}\text{Mg}_{0.02}(\text{Si}_{1.49}\text{Al}_{0.51}\text{O}_7)_{0.94}]\text{O}_{22.38}$. **K.T.T.**

BRAITHWAITEITE*

F.C. Hawthorne, M.A. Cooper, and W.H. Paar (2008) The crystal structure of braithwaiteite. *J. Coord. Chem.*, 61, 15–29.

Braithwaiteite is a rare mineral that occurs on a specimen of Veta Negra (Black Vein) from Laurani, Bolivia, a high sulfidation epithermal deposit. It is a secondary mineral formed by oxidation of primary enargite by Na- and Ti-rich fluids in an arid environment. The crystal structure of braithwaiteite was determined by single-crystal X-ray diffraction methods on a crystal $0.015 \times 0.100 \times 0.150 \text{ mm}^3$ by direct methods. Braithwaiteite is triclinic, $P\bar{1}$, $a = 7.0308(4)$, $b = 9.8823(5)$, $c = 10.6754(6) \text{ \AA}$, $\alpha = 106.973(1)$, $\beta = 104.274(1)$, $\gamma = 93.839(1)^\circ$, $V = 679.76(11) \text{ \AA}^3$, $Z = 1$, $R_1 = 0.025$ for 3584 observed reflections. The chemical formula (EMPA analyses with OH and H_2O calculated from the single-crystal structure determination) gave the empirical formula $\text{Na}_{0.87}\text{Cu}_{5.17}(\text{Sb}_{1.15}\text{Ti}_{0.90})\text{O}_2(\text{As}_{0.98}\text{O}_4)_2[\text{AsO}_3(\text{OH})]_2(\text{H}_2\text{O})_8$, with an ideal chemical formula of $\text{NaCu}_5(\text{Sb}^{5+}\text{Ti}^{4+})\text{O}_2(\text{AsO}_4)_4(\text{AsO}_3\text{OH})_2(\text{H}_2\text{O})_8$. The braithwaiteite structure consists of $[(\text{SbTi})(\text{AsO}_4)_4\text{O}_2]$ chains that extend along the a direction and define the cell dimension. These chains are cross-linked in the b direction by $[\text{Cu}_2(\text{AsO}_4\text{OH})_2\text{O}_4]$ chains of edge-sharing Cu1 and Cu3 octahedra linked by AsO_4 tetrahedra, forming a sheet parallel to (001). These sheets are stacked along c and linked by Cu2 and Na octahedra and extensive hydrogen bonds. **P.C.P.**

KHINITE*

M.A. Cooper, F.C. Hawthorne, and M.E. Back (2008) The crystal structure of khinite and polytypism in khinite and parakhinite. *Mineral. Mag.*, 72, 763–770.

Khinite is a Pb-Cu tellurate originally discovered on the dumps of the Old Guard mine, Tombstone, Arizona. It is a rare secondary mineral associated with parakhinite, dugganite, quetzalcoatlite, tlappallite, tenorite, chlorargyrite, chrysocolla, gold, and quartz. Khinite forms by oxidation of gold-telluride ores in highly acidic minewaters.

The crystal structure of khinite was determined on a sample

($3 \times 60 \times 80 \text{ }\mu\text{m}$) from the dumps of the Empire mine, Tombstone, Arizona. It has excellent cleavage parallel to (001) and shows uniform extinction in cross-polarized light. Single-crystal X-ray diffraction data were collected on a Bruker P4 diffractometer equipped with a serial detector and graphite-filtered $\text{MoK}\alpha$ X-radiation. 1513 reflections were collected over a hemisphere of reciprocal space; 1321 remaining after standard corrections, with 926 unique and 636 observed ($F_o > 4\sigma F$). The structure was solved by direct methods, $R_1 = 0.032$ for ($|F_o| > 4\sigma|F_o|$). Khinite is orthorhombic, space group $Fdd2$, $Z = 8$, $a = 5.7491(10)$, $b = 10.0176(14)$, $c = 24.022(3) \text{ \AA}$, $V = 1383.6(4) \text{ \AA}^3$, $D_{\text{calc}} = 6.29 \text{ g/cm}^3$. The structure of khinite contains one six-coordinated Te site (TeO_6), three six-coordinated Cu sites ($\text{Cu}\phi_6$ where $\phi = \text{O, OH}$), and one eight-coordinated Pb site, $\text{Pb}\phi_8$. The original formula for khinite proposed by Williams (*Am. Mineral.*, 1978, 63, 1016–1019) has been revised and now given as $\text{Pb}^{2+}\text{Cu}_3^{2+}\text{Te}^{6+}\text{O}_6(\text{OH})_2$, based on the new crystal-structure refinement.

Khinite is polytypic with parakhinite—both minerals contain TeO_6 and Cu_3O_6 octahedra that share trans edges to form rutile-like $[\text{MO}_4]$ chains parallel to [110]. The $\text{Cu}1\phi_6$ and $\text{Cu}2\phi_6$ octahedra link to form adjacent parallel $[\text{M}\phi_4]$ chains that share corners with the $(\text{TeCu}_3\text{O}_4)$ chains to form a $[\text{M}\phi_2]$ layer of composition $(\text{TeCu}_3\phi_8)$. The layers are stacked along c at $6 \text{ \AA}$ intervals and are linked by Pb atoms and hydrogen bonds. It is the relative stacking in the c direction that distinguishes the two structures. **P.C.P.**

ZIPPEITE GROUP

O.M. Peters, R. Vochten, and N. Blaton (2008) The crystal structures of synthetic potassium-transition-metal zippeite-group phases. *Can. Mineral.*, 46, 173–182.

Mn, Co, Ni, and Zn end-members of the potassium zippeite group were synthesized by mixing $\text{MeSO}_4 \cdot n\text{H}_2\text{O}$ with a solution of UO_2SO_4 and adjusting pH to 3.8 using KOH. The mixture was heated for 75 hours at 150°C (approximate pressure 3.5 MPa). The resulting crystals occur as monoclinic laths and plates. Monoclinic symmetry was confirmed by etch figures. Measured densities for the Mn, Co, Ni, and Zn phases were 4.7(2), 4.8(2), 4.9(2), and 4.9(2), respectively.

Chemical compositions (S, U, Mn, Co, Ni, and Zn) were determined by WDS, ICP-MS (K), and TGA (H_2O). The following compositions were found: K-Mn = UO_2 76.78, SO_3 10.57, MnO 6.32, K_2O 2.40, H_2O 6.20, total 102.27 wt%; K-Co = UO_2 75.94, SO_3 10.47, CoO 6.28, K_2O 2.78, H_2O 6.84, total 102.31 wt%; K-Ni = UO_2 75.98, SO_3 10.54, NiO 6.10, K_2O 2.85, H_2O 6.50, total 101.97 wt%; K-Zn = UO_2 75.90, SO_3 10.49, MnO 7.20, K_2O 2.64, H_2O 6.97, total 103.20 wt%.

Structure determinations were carried out using a four circle diffractometer and graphite-monochromated $\text{MoK}\alpha$ radiation. Structures were refined isotropically using starting parameters taken from previous zippeite refinements; $R_{\text{Mn}} = 0.0525$, $R_{\text{Co}} = 0.0459$, $R_{\text{Ni}} = 0.0383$, and $R_{\text{Zn}} = 0.0690$. The phases are monoclinic, space group is $C/2c$ with $Z = 8$. Cell dimensions are as follows: for Mn, $a = 8.661(6)$, $b = 14.375(8)$, $c = 17.705(12) \text{ \AA}$, $\beta = 104.12(5)^\circ$, $V = 2138(2) \text{ \AA}^3$; for Co, $a = 8.651(5)$, $b = 14.188(8)$, $c = 17.713(13) \text{ \AA}$, $\beta = 104.14(6)^\circ$, $V = 2108(2) \text{ \AA}^3$; for

Ni, $a = 8.662(5)$, $b = 14.095(8)$, $c = 17.770(9)$ Å, $\beta = 104.18(5)^\circ$, $V = 2103(2)$ Å³; and for Zn, $a = 8.650(6)$, $b = 14.180(12)$, $c = 17.709(13)$ Å, $\beta = 104.14(6)^\circ$, $V = 2106(3)$ Å³.

The interlayers in zippeite consist of two distinct transition metal sites (*Me*), one potassium atom, and water molecules. The *Me* sites are six-coordinated by oxygen to form distorted octahedra. In the *Me1* site, two of the O atoms form part of (UO₂)⁶⁺ from adjacent uranyl-oxo-sulfate layers. The remaining four O atoms are part of the water in the interlayer. The *Me2* site

has two of its O atoms as part of two equivalent positions of a water group with the remaining four forming part of the adjacent uranyl-oxo-sulfate layers.

This study demonstrates the ability to synthesize a zippeite group phase with mixed potassium and divalent cation transition metal interlayers, intermediate between synthetic zippeite and divalent-transition group metal zippeite phases. The preferred formula for the potassium-transition metal zippeite phases is $K_{0.5}Me_{0.75}[(UO_2)_2SO_4O_2] \cdot 3H_2O$. **G.P.**