

New Mineral Names*

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CENTROSYMMETRIC ANALOGUE OF LABYRINTHITE

K.A. Rosenberg, R.K. Rastsvetayeva, N.V. Chukanov, I.A. Verin (2004) Centrosymmetric modular structure of an analogue of labyrinthite. Dokl. Akad. Nauk, 399, 791–794 (in Russian); Dokl. Chem., 399, 253–256 (in English).

An apparently new member of the eudialyte group has been found in the central zone of an alkaline pegmatite at Mt. Koashva, Khibiny massif, Kola Peninsula, Russia. The mineral occurs in tabular grains intimately intergrown with villiaumite, in associations with lomonosovite, barytolamprophyllite, aegirine, and microcline. The authors infer from this assemblage that the formational conditions included relatively high temperature and high sodium and fluorine activity. The mineral is dichroic brown-gray to raspberry-pink. It is reported to have a unique IR spectrum and unusual physical properties. Microprobe analysis gives the empirical formula: $\text{Na}_{15}\text{Ca}_{6.1}\text{K}_{0.7}\text{Sr}_{0.2}\text{Y}_{0.2}\text{REE}_{0.3}\text{Fe}_{1-1.2}\text{Mn}_{0.7-0.9}\text{Zr}_{3.0}\text{Ti}_{0.3}\text{Nb}_{0.2}\text{Si}_{26}\text{O}_{72}\text{FCl}_{0.5}\cdot n\text{H}_2\text{O}$ ($Z = 6$). The crystal structure of the mineral, $R\bar{3}m$, a 14.243(3), c 60.907(8) Å has been solved to R_{aniso} 0.066 using 1659 independent [$F > 3\sigma(F)$] single-crystal $\text{MoK}\alpha$ X-ray diffraction data. As with other eudialyte-group minerals, the basic structure consists of three- and nine-membered Si-O rings and six-membered Ca-O rings, all united into a heterogeneous body with discrete Zr-O octahedra. The detailed structure can be described as consisting of modules of various structural end-members of the eudialyte group: kentbrooksit-eudialyte modules are interspersed with alluaivite modules.

Discussion. The full, official description of the potentially new mineral species “labyrinthite” has not yet been published, so it is odd to see the authors publishing a structural description of a potentially new analogue of “labyrinthite”, when their efforts would be better put to getting the official description of “labyrinthite” out in print. Nonetheless, the selection of the name “labyrinthite” has introduced an unnecessarily ambiguity into scientific terminology: the *exact* spelling of the mineral name in both French and Russian also corresponds to a viral or bacterial inflammation of the inner ear, thought to be responsible for approximately 15% of all cases of vertigo (*labyrinthitis* in English). **T.S.E.**

* 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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NALDRETTITE*

L.J. Cabri, A.M. McDonald, C.J. Stanley, N.S. Rudashevsky, G. Poirier, B.R. Durham, J.E. Mungall, V.N. Rudashevsky (2005) Naldrettite, Pd_2Sb , a new intermetallic mineral from the Mesamax Northwest deposit, Ungava region, Québec, Canada. Mineral. Mag., 69, 89–97.

Naldrettite occurs as anhedral grains from 10 to 239 μm (average 74.4 μm). Grains were liberated and isolated from the matrix by hydroseparation. It is often found attached to sulfide minerals and commonly associated with clinocllore. The mineral is metallic and opaque. It does not show cleavage, has an irregular fracture, a ductile behavior (flexibly inelastic), and has a Mohs hardness of 4 to 5 (average VHN50 load of 393 in the range 358–418 kg/mm^2). Naldrettite is bright creamy white in plane-polarized reflected light, does not show internal reflections, shows weak birefringence, no pleochroism, and distinct anisotropy in shades of deep bright blue, lemon-buff, and mauve to pale pink. Reflectance percentages for R_{min} and R_{max} in air/oil are 49.0, 50.9/35.9, 37.6 (470 nm), 53.2, 55.1/40.3, 42.1 (546 nm), 55.4, 57.5/42.5, 44.3 (589 nm), 58.5, 60.1/45.4, 47.2 (650 nm), respectively.

Electron microprobe analyses (WDS, average of 69 analyses on 19 grains) gave S 0.02, Fe 0.11, As 0.31, Sb 35.75, Pd 63.49, sum 99.68 wt%, corresponding to $(\text{Pd}_{1.995}\text{Fe}_{0.007})_{\Sigma 2.002}(\text{Sb}_{0.982}\text{As}_{0.014}\text{S}_{0.002})_{\Sigma 0.998}$ based on three atoms. The ideal formula of naldrettite is Pd_2Sb , $Z = 8$, D_{calc} 10.694(1) g/cm^3 . Naldrettite is isostructural with synthetic Pd_2Sb [Bälz and Schubert (1969) *Less-Common Metals*, 19, 300–304] and is considered to be orthorhombic, $\text{Cmc}2_1$, $a = 3.906(1)$, $b = 17.5551(5)$, $c = 6.957(2)$ Å, $V = 414.097(3)$ Å³. The strongest lines on the powder X-ray diffraction pattern (114.6 mm Gandolfi camera, $\text{CuK}\alpha$ radiation, 155 lines given) include 2.7123(21,131), 2.441(17,150), 2.4067(34,112), 2.3029(35,151), 2.2454(100,132), 2.1971(27,080), 2.0979(28,081), 2.0567(52,043), 2.0009(40,152), 1.9058(30,113), 1.8226(22,133), 1.6857(17,200), 1.5229(22,202), 1.4983(15,134), 1.3674(35,193), 1.3513(23,223), 1.3332(19,1.11.2), 1.3049(23,243), 1.2842(42,115), 1.2565(27,135), 1.2122(50,204), 1.1466(23,2.10.2), 1.1199(25,0.12.4), 1.0784(21,2.10.3), 1.0434(15,156), 0.9982(15,333), 0.9665(16,047), 0.9506(17,226), 0.9478(28,314), 0.9335(17,2.12.4), 0.9089(30,266), 0.8658(17,3.13.0), 0.8584 (56,1.17.4), 0.8409(51,118). Determination of the crystal structure is underway.

Naldrettite was discovered in drill core from the Mesamax Northwest deposit, Cape Smith fold belt, Ungava region, Québec, Canada. The deposit consists of disseminated to net-textured sulfide mineralization hosted by amphibolite and serpentinite

replacing pyroxenite and peridotite, as well as a swarm of regionally extensive komatiitic basalt and basaltic komatiite dykes up to several hundred meters thick. The Mesamax Northwest deposit is located at the basal portion of a dyke where it intersected a silicate-facies iron formation ~20 m thick. Lead antimonide minerals are present in the contact zone that separates massive and disseminated sulfide mineralization. The mineral is associated with altaite, chalcopyrite, clinocllore, cobaltite, electrum, galena, magnetite, monoclinic pyrrhotite, pentlandite, sphalerite, and sudburyite with rare hessite, michenerite, petzite, sperryllite, and ungavaite. Palladium contents in the massive sulfide are low relative to other PGE and base metals as compared to the disseminated sulfide mineralization. This suggests removal of Pd from the massive sulfide body during a late magmatic event or regional metamorphism, followed by redeposition at the contact between the massive sulfide body and the ultramafic rock. The Sb is thought to have been derived from an external source that interacted with the high-Pd fluids, resulting in precipitation of a Pd-Sb assemblage. Naldrettite is named for Professor Anthony J. Naldrett (b. 1933), University of Toronto and past President of both the Mineralogical Association of Canada and the International Mineralogical Association. Type material has been deposited at the Natural History Museum, Cromwell Road, London, U.K. (BM 2004,34) and the Canadian Museum of Nature (CNMMN 84397). **P.C.P.**

Nb-DEFICIENT CARBONATE ANALOGUE OF FEKLICHEVITE

K.A. Rosenberg, R.K. Rastsvetayeva, N.V. Chukanov, I.A. Verin (2005) Crystal structure of the niobium-deficient carbonate analog of feklichevite. Dokl. Akad. Nauk, 400, 640–644 (in Russian).

A Nb-deficient carbonate analogue of the mineral feklichevite has been found in an alkaline pegmatite in the Kovdor massif, Kola Peninsula, Russia, and is thought to have formed via interaction between an alkaline fluid and calcite carbonatite. The crystal structure of the mineral (eudialyte-group), $R3m$, a 14.232(3), c 30.210(3) Å has been solved to R_{iso} 0.031, R_{anis} 0.044 using 1494 independent [$F > 3\sigma(F)$] single-crystal $MoK\alpha$ X-ray diffraction data. The empirical formula ($Z = 3$; basis of 25 Si atoms) derived mainly from electron microprobe data is: $Na_{10-12}Ca_{9-10}K_{0.3}Ce_{0.1}Zr_{2.8-3.2}Nb_{0.36-0.45}Fe_{1.9-2.2}Mn_{0.2-0.3}Si_{25}O_{72}(CO_3)_{1\pm 0.1}Cl_{0.2-0.4}(OH, H_2O)_n$, and agrees well with the formula from the structural study: $(Na_{8.51}Ce_{0.11})(Ca_{1.8}Na_{0.96}K_{0.24})(Ca_{2.25}Na_{0.75})(Ca_6)(Zr_3)(^{14}Fe_{1.05})(^{15}Mn_{0.3})(^{15}Fe_{0.18})(^{15}Fe_{0.78})(Nb_{0.21}Si_{0.21-0.58})(Si_{0.5}Nb_{0.2}Ti_{0.1-0.2})(Si_3O_9)_2(Si_9O_{27})_2(OH)_{2.24}(CO_3)_{0.94}Cl_{0.49}(H_2O)_{0.54}$. The mineral shares common features with other members of the eudialyte group such as three- and nine-membered Si-O rings, sixfold Ca-O rings, all united into a heterogeneous body with discrete Zr-O octahedra. However, as the Ca- and CO_3 -richest member of the eudialyte group, the mineral has some unique structural features such as: (1) Ca in extra-skeletal positions; (2) Nb approximately evenly distributed between M3 and M4, but with vacancies dominant at M3; (3) X positions show different ordering patterns of Cl, C and H_2O than other carbonate-bearing members of the group. The IR spectrum of the mineral indicates minor distortion of the various CO_3 groups.

Discussion. On the basis of the composition and structural parameters this mineral would seem to correspond to IMA 2004-40 (see <http://sheba.geo.vu.nl/%7Eima-cnmmn/minerals2004.pdf>), the full description of which has not yet been published. **T.S.E.**

POTASSICARFVEDSONITE*

I.V. Pekov, N.V. Chukanov, Yu.S. Lebedeva, D.Yu. Pushcharovsky, G. Ferraris, A. Gula, A.E. Zadov, A.A. Novakova, O.V. Petersen (2004) Potassicarfvedsonite, $KNa_2Fe^{2+}_4Fe^{3+}Si_8O_{22}(OH)_2$, a K-dominant amphibole of the arfvedsonite series from agpaite pegmatites—Mineral data, structure refinement and disorder in the A site. N. Jb. Mineral. Mh., 12, 555–574.

Potassicarfvedsonite has been described from three agpaite complexes: Ilímaussaq, south Greenland (holotype), Lovozero and Khibina, Kola Peninsula, Russia (cotypes). The mineral occurs as euhedral, prismatic to acicular crystals from a few centimeters to 15×0.8 cm. It varies in color from black (Ilímaussaq, Khibina) to dark blue-green or blue-gray (Lovozero), is transparent to semitransparent with a pale blue streak and a vitreous luster. Potassicarfvedsonite has perfect {110} cleavage, a splintery fracture, is brittle and has a Mohs hardness of 5.5 to 6. The mineral is biaxial negative, $\alpha = 1.683(2)$, $\beta = 1.692(2)$, $\gamma = 1.699(2)$, $2V_{meas} > 60^\circ$, $2V_{calc} = 82^\circ$, the dispersion, $r > v$, is strong. The pleochroism is strong with X dark blue-green, Y gray-green, Z pale green-gray to pale green-brown, absorption $X \geq Y > Z$, $Z = b$, $X \wedge c = 20(10)^\circ$, $Y \wedge a = 30(10)^\circ$.

Electron microprobe analysis, atomic emission spectroscopy (Li), the Alimarin method (H_2O), and Mössbauer spectroscopy (Fe^{2+}/Fe^{3+}) of the Ilímaussaq material (average of 12 analyses) gave Li_2O 0.45, Na_2O 7.01, K_2O 3.29, CaO 0.30, MgO 0.04, MnO 1.37, ZnO 0.20, FeO 24.69, Fe_2O_3 11.60, Al_2O_3 0.58, SiO_2 48.63, TiO_2 0.43, H_2O 1.70, F 0.36, $O = F$ 0.15, sum 100.50 wt%, corresponding to $(K_{0.67}Na_{0.22})_{\Sigma 0.89}(Na_{1.95}Ca_{0.05})_{\Sigma 2.00}(Fe_{3.29}^{2+}Fe_{1.26}^{3+}Li_{0.29}Mn_{0.19}Ti_{0.05}Zn_{0.02}Mg_{0.01})_{\Sigma 5.11}(Si_{7.76}Fe^{3+}_{0.13}Al_{0.11})_{\Sigma 8.00}O_{22}[(OH)_{1.81}F_{0.18}]_{\Sigma 1.99}$ based on $O_{22}(OH,F)_2$. The ideal formula for potassicarfvedsonite is $KNa_2Fe_4^{2+}Fe^{3+}Si_8O_{22}(OH)_2$. The D_{calc} is 3.43 g/cm³ for $Z = 2$. The IR spectrum of potassicarfvedsonite contains bands (sh = shoulder) at 3700, 3675, 1134, 1076, 1025 sh, 990 sh, 957, 900 sh, 741, 692, 661, 643, 520 sh, 491, 445 and 430 sh. No identification of the bands is given.

The crystal structure of potassicarfvedsonite was solved and refined by direct methods using a $0.11 \times 0.08 \times 0.34$ mm crystal by single-crystal X-ray diffraction methods, $R_1 = 0.0229$ for 3296 reflections with $I > 2\sigma(I)$. Potassicarfvedsonite is monoclinic, $C2/m$, $a = 10.002(2)$, $b = 18.054(3)$, $c = 5.319(1)$ Å, $\beta = 103.90(3)^\circ$, $V = 932.4(3)$ Å³. The strongest lines on the X-ray diffraction pattern (DRON UM-1 diffractometer, $CoK\alpha$ radiation, 33 lines) include 9.02(28,020), 8.53(100,110), 3.419(12,131), 3.303(23,240), 3.184(40,310), 2.847(17,330), and 2.725(10,151). The structure of potassicarfvedsonite does not differ significantly from that determined for arfvedsonite. The distribution of cations over the five cation sites is presented and the absence of dehydroxylation at the O3 site has been confirmed.

Potassicarfvedsonite at Ilímaussaq was found in “Pegmatite Valley” in the Kangerluarsuk area. It occurs in pegmatite veins

(20 m long, 0.5 m thick) and is associated with coarse-grained analcime and fine-grained aegirine, epistolite, eudialyte, microcline, sodalite and steenstrupine-(Ce). At Lovozero, the mineral occurs in the Palitra (Palette) pegmatite at the underground Ioparite mine at Mt. Kedykmatite. The potassicarfvedsonite occurs as aggregates of acicular crystals up to 2×0.1 mm and as massive nodules up to 1.5 cm across in ussingite cavities associated with a suite of hyperalkaline minerals inside partially altered crystals of manaksite. In the peripheral zone of the pegmatite, potassicarfvedsonite occurs as an early mineral (crystals up to 15 cm) associated with aegirine, arfvedsonite, eudialyte, microcline, and nepheline, with minor lamprophyllite, lomonosovite, lorenzenite, and villiaumite. At Khibina, potassicarfvedsonite was found in the Hilairitovoye pegmatite at the Kirovskii apatite mine, Mt. Kukisvumchorr. It occurs in the peripheral zone of the pegmatite and is associated with aegirine, eudialyte, fluorapatite, fluorite, lamprophyllite, microcline, natrolite, nepheline, rinkite, sphalerite, and titanite. Potassicarfvedsonite crystallizes after arfvedsonite, and is an early mineral in K-rich complexes (Khibina) and a late-stage, hydrothermal mineral in Na-rich complexes (Ilímaussaq and Lovozero). The mineral is named for its chemistry as the K-dominant analogue of arfvedsonite. Type and cotype material has been deposited at the Fersman Mineralogical Museum, Russian Academy of Sciences, Moscow, Russia (catalogue no. 3137/1 for Ilímaussaq and 3137/2 for Lovozero). **P.C.P.**

Discussion. The original “arfvedsonite” studied by Hawthorne (1976, *Can. Mineral.*, 14, 346–356) is compositionally a potassicarfvedsonite.

TOKYOITE*

S. Matsubara, R. Miyawaki, K. Yokoyama, M. Shimizu, H. Imai (2004) Tokyoite, $\text{Ba}_2\text{Mn}^{3+}(\text{VO}_4)_2(\text{OH})$, a new mineral from the Shiromaru mine, Okutama, Tokyo, Japan. *J. Mineral. Petrol. Sci.*, 99, 363–367.

Tokyoite occurs as small aggregates (250 μm) of irregular grains less than 15 μm . The mineral is red-black, translucent, has a vitreous luster and a dark brownish-red streak. Cleavage was not observed and the Mohs hardness is 4–4.5 (VHN25 363–390 kg/mm^2). In thin section, tokyoite is distinctly pleochroic reddish orange to dark brownish red. It has refractive indices higher than 1.99 and the mean calculated index is 2.03. Reflectance percentages for R_{\min} and R_{\max} in air/oil are 12.8, 13.2/3.3, 3.5 (470 nm), 12.3, 12.6/3.1, 3.4 (546 nm), 12.2, 12.5/3.1, 3.6 (589 nm), and 12.5, 12.6/3.6, 4.3 (650 nm), respectively.

Electron microprobe analysis by WDS gave an average (6 analyses) of 31.77 V_2O_5 , 0.15 SiO_2 , Al_2O_3 0.07, Fe_2O_3 2.33, Mn_2O_3 11.27, CaO 0.07, BaO 51.91, SrO 0.22 Na_2O 0.13, $\text{H}_2\text{O}_{\text{calc}}$ 1.59, total 99.51 wt%, corresponding to $(\text{Ba}_{1.92}\text{Na}_{0.02}\text{Sr}_{0.01}\text{Ca}_{0.01})_{\Sigma 1.96}(\text{Mn}_{0.81}^{3+}\text{Fe}_{0.17}^{3+}\text{Al}_{0.01})_{\Sigma 0.99}[(\text{V}_{1.99}\text{Si}_{0.01})\text{O}_{7.92}](\text{OH})_{1.00}$ on the basis of $\text{V} + \text{Si} = 2$ and $(\text{OH}) = 1$. The ideal formula for tokyoite is $\text{Ba}_2\text{Mn}^{3+}(\text{VO}_4)_2(\text{OH})$. The D_{calc} is 4.62 g/cm^3 .

The unit-cell parameters of tokyoite were refined using powder X-ray diffraction data and by analogy with its Fe-analogue, monoclinic gamagarite, $P2_1/m$: $a = 9.10(4)$, $b = 6.13(2)$, $c = 7.89(5)$ \AA , $\beta = 112.2(5)^\circ$, $V = 408(3)$ \AA^3 . The strongest lines on the powder X-ray diffraction pattern (114.6 mm Gandolfi cam-

era, $\text{CuK}\alpha$ radiation, 38 lines) include 7.26(6,001), 4.97(14,110), 3.73(15,111), 3.46(26,210), 3.31(100,112), 3.08(20,020), 3.00 ($301, \bar{2}12, 102$), 2.90(19,120), 2.80(62, $\bar{1}21, 300$), 2.71(40, $\bar{3}11$), 2.16(18, $\bar{3}21$), and 1.963(15, $\bar{2}04$). It is the Mn^{3+} -analogue of gamagarite and a member of the brackebuschite group.

Tokyoite was found in an outcrop of an abandoned Mn ore deposit in the Shiromaru mine, Okutama Town, Tokyo, Japan. The ore deposit occurs in chert blocks enclosed in middle to upper Jurassic sandstone of the accretionary Kanto Mountains complex. The mineral occurs in brecciated braunite or in veinlets associated with hyalophane or tamaite. The mineral is named after its type locality. Type material has been deposited at the National Science Museum, Tokyo (catalogue no. NSM-M 28569).

Discussion. Although the authors state that Mn occurs as a trivalent cation, there is no supporting chemical or crystallographic evidence for this conclusion. **P.C.P.**

TOUNKITE-LIKE MINERAL

K.A. Rozenberg, A.N. Sapozhnikov, R.K. Rastsvetaeva, N.B. Bolotina, A.A. Kashaev (2004) Crystal structure of a new representative of the cancrinite group with a 12-layer stacking sequence of tetrahedral rings. *Crystallogr. Rep.*, 49, 635–642.

A tounkite-like mineral was discovered from the lazurite-bearing rocks of the Tultuiskoe deposit. The mineral forms bluish, columnar crystals up to 1 cm long. Analyses by electron microprobe gave an empirical formula of $(\text{Na}_{5.18}\text{Ca}_{2.58}\text{K}_{0.15})_{\Sigma 7.91}(\text{Al}_{6.01}\text{Si}_{5.99})_{\Sigma 12.00}\text{O}_{24}(\text{SO}_4)_{1.79}\text{Cl}_{1.33}$, based on 12 (Si + Al) and $Z = 6$. Single-crystal X-ray diffraction studies of the mineral (0.15 \times 0.3 \times 0.4 mm), $R_1 = 0.035$ for 3834 reflections with $F > 3\sigma(F)$, indicate it to be trigonal, $P3$, $a = 12.757(3)$, $c = 32.211(5)$ \AA , $V = 4539.75$ \AA^3 , $D_{\text{calc}} = 2.48$ g/cm^3 . The structure could not be solved by direct methods and therefore a model containing 114 independent atoms was constructed based on the tetrahedral frameworks of other cancrinite-group minerals. The crystal chemical formula is given as $[\text{Si}_{36}\text{Al}_{36}\text{O}_{144}][\text{Na}_{31.1}\text{Ca}_{3.94}\text{K}_{0.96}(\text{SO}_4)_{9.3}(\text{SO}_3)_{0.7}][\text{Ca}_{12}\text{Cl}_8]$ for $Z = 1$. The structure of the mineral is related to other cancrinite-group minerals and consists of layers of six-membered (Si,Al) rings of tetrahedra. These rings are packed in the sequence CACACBCBCACB, producing three types of cages made up of columns: the columns along [00z] are comprised of cancrinite cages, whereas two other columns along $[1/3\ 2/3\ z]$ and $[2/3\ 1/3\ z]$ are comprised of alternating cancrinite, bystrite, and liottite cages. This mineral is a 12-layer polymorph of tounkite and most closely related, structurally, to afganite.

Discussion. No additional information is provided on other optical or physical properties of this potentially new species.

NEW DATA

EVENKITE

E.N. Kotelnikova, S.K. Filatov, N.V. Chukanov (2004) Evenkite: Symmetry, chemical composition, identification and thermal behavior. *Zapiski Vseross. Mineral. Obshch.* 133(3), 80–92 (in Russian, English abstract).

The hydrocarbon and natural paraffin evenkite has been investigated by gas chromatography, infrared spectroscopy, and powder X-ray diffraction methods. Evenkite is orthorhombic, $Pbcm$, $a = 7.47(1)$, $b = 4.980(1)$, $c = 65.85(3)$ Å, $V = 2450(2)$ Å³, $Z = 4$. It is a polycomponent orthorhombic solid solution consisting of 10 normal paraffin homologues and n -numbers, C_nH_{2n+2} , ranging from 19 to 28 with $C_{23}H_{48}$ being the dominant homologue. Evenkite undergoes the same stages of thermal deformation and phase transformation as the binary orthorhombic solid solutions of synthetic paraffins; five condensed states were distinguished. **P.C.P.**

PARASCORODITE*

N. Perchiazzi, R. Ondruš, R. Skála (2004) *Ab initio* X-ray powder structure determination of parascorodite, $Fe(H_2O)_2AsO_4$. Eur. J. Mineral. 16, 1003–1007.

The crystal structure of parascorodite was solved by *ab-initio* methods and refined by the Rietveld method ($R_p = 0.045$, $R_{Bragg} = 0.046$, $\chi^2 = 1.05$) from powder X-ray diffraction data (Stoe STADI diffractometer, $CoK\alpha_1$ radiation). The mineral is trigonal, $P\bar{3}c1$, $a = 8.9232(2)$, $c = 9.296(3)$ Å, $V = 687.71(3)$ Å³, $Z = 6$, $D_{calc} = 3.358$ g/cm³. Parascorodite is a dimorph of scorodite and its structure is composed of mixed octahedral-tetrahedral columns parallel to c that are interconnected in a 3D framework by the O1 oxygen between $[AsO_4]$ tetrahedra and Fe1 octahedra, as well as the OW-O2 hydrogen bond. **P.C.P.**

PERROUDITE*

Keller, P., Lissner, F., Schleid, T. (2005) Single-crystal structure determination of perroudite, $Hg_5Ag_4S_5(I,Br)_2Cl_2$, from Tsumeb (Namibia), and its structural relationship to other sulfide halides of mercury and cinnabar. N. Jb. Mineral. Abh., 181(1), 1–9.

The crystal structure of perroudite, ideally $Hg_5Ag_4S_5(I,Br)_2Cl_2$, has been solved and refined using a $0.13 \times 0.04 \times 0.01$ mm crystal by single-crystal X-ray diffraction methods (Nonius-κ-CCD diffractometer), $R_1 = 0.00521$ for 1070 reflections. Perroudite

is orthorhombic, $P2_12_12_1$, $a = 17.4198(9)$, $b = 12.2032$, $c = 4.2088(2)$ Å, $V = 903.20(8)$ Å³, $\mu = 51.20$ mm⁻¹, $Z = 2$, $D_{calc} = 6.928$ g/cm³. The structure is an improvement on previous determinations on fused bundles of several small crystals. The structure of perroudite is unique; structural relationships with capgaronnite, corderoite, cinnabar and $HgCuSCl$, β - $Hg_3S_2Br_2$ and $Hg_3S_3I_3$ are discussed. **P.C.P.**

WHEWELLITE AND CAOXITE*

T. Echigo, M. Kimata, A. Kyono, M. Shimizu, T. Hatta (2005) Re-investigation of the crystal structure of whewellite $[Ca(C_2O_4)]$ and the dehydration mechanism of caoxite $[Ca(C_2O_4) \cdot 3H_2O]$. Mineral. Mag., 69, 77–88.

The crystal structure of whewellite and the dehydration mechanism of caoxite has been determined by a combination of powder and single-crystal X-ray diffraction, differential thermal analysis and infrared analysis. The crystal structure of whewellite was refined by single-crystal X-ray diffraction methods (Rigaku RAXIS-RAPID, $MoK\alpha$ radiation) at 123 K on a $0.50 \times 0.40 \times 0.30$ mm crystal, $R_1 = 0.041$ for 1675 reflections with $I > 2\sigma(I)$. Starting parameters were taken from Tazzoli and Domeneghetti (*Am. Mineral.*, 65, 327–334) and the unknown H12 position was determined on the 3D difference-Fourier map. Whewellite is monoclinic, $P2_1/c$, $a = 6.250(1)$, $b = 14.471(2)$, $c = 10.114(2)$ Å, $\beta = 109.978(5)^\circ$, $V = 859.7(3)$ Å³, $Z = 8$, $D_{calc} = 2.258$ g/cm³, $\mu = 13.68$ cm⁻¹. Results indicate that all four hydrogen atoms in the crystal structure are involved in hydrogen bonding and that each water molecule occupies a distinct atomic position. Thermal analysis of synthetic caoxite was performed in a Rigaku Thermo plus TG8120 thermogravimetric analyzer. Four weight-loss steps were observed: 85.1, 166.9, 424.7, and 724.9 °C and end-products were identified by powder X-ray diffraction methods. The four weight-loss steps include (1) dehydration of caoxite to whewellite (25–100 °C), (2) dehydration of whewellite to anhydrous calcium oxalate (120–280 °C), (3) decarbonation of anhydrous calcium oxalate to calcite (280–550 °C), and (4) decarbonation of calcite to lime (550–1000 °C). Results confirm that caoxite transforms into whewellite by dehydration and not via weddelite.