

MM8: The eudialyte group: A case study on mineral nomenclature

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Eudialyte-group minerals are Na-rich zirconosilicates with varying amounts of Ca, Fe, Mn, REE, Sr, Nb, K, Y, Ti, H and W. They are trigonal, $a \approx 14 \text{ \AA}$, $c \approx 30 \text{ \AA}$ (rarely 60 Å), crystallizing in $R\bar{3}m$, $R3m$ or $R3$. In order to encompass all substitutions known thus far, the general formula of eudialyte (s.l.) is $[N(1)N(2)N(3)N(4)N(5)]_1[M(1a)M(1b)]_1M(2)_1M(3)M(4)Z_3[Si_{23}O_{72}]O'_4X_2$; $Z = Zr, Ti$; $X = Cl, F$ or OH ; $Z = 3$.

The number of species in the group has increased rapidly within the last few years after systematic studies have explored the chemical and structural diversity. In order to avoid a proliferation of unique names within the group, CNMMN appointed a subcommittee with the mandate of creating a nomenclature system. Such a system should be applicable for known species and take into account foreseeable future species. This presentation is a report from this subcommittee.

Three different principles of naming minerals have been tested: (i) a hierarchical system with root names modified by use of modifiers and Levinson suffixes; (ii) a unique-name system with use of modifiers +/- Levinson suffixes; and (iii) a system based on the Linnean principle used in the biological world.

It is concluded that a hierarchical nomenclature system does not work for eudialyte-group minerals. Such a system would be either a multi-level system that would become either a very complicated and cumbersome system with disproportionately many root names or a more flat system with fewer root names but monstrously long names with formula-like endings, e.g. eudialyte-NaNaNaNaNaCaMnNbSiF for kentbrooksite. Names with highly extended Levinson modifiers would be very difficult to remember, would have a high risk for misspelling and complete revisions of the system would frequently become necessary.

Conventional unique names with a maximum of one cation prefix are recommended for the eudialyte-group minerals, and this prefix should refer to the M(2) site as in ferrokentbrooksite. Unique names are relatively easy to remember and misspelling is usually not critical. This scheme is relatively flexible and future revisions of the group can presumably take place without laborious renaming.

A Linnean name is composed of a genus name with a species suffix, e.g. eudialyte khomyakovite. In this binary system the non-specialist is instantly informed about the type of mineral in question and the flexibility of the system is simply unsurpassed. However, there is no tradition for binary names in mineralogy and the system is not endorsed.

MM9: New investigations of the adelite–descloizite group

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More than a dozen minerals and some synthetic compounds (arsenates, vanadates, silicates, and molybdates) are known to belong to the adelite-descloizite structure type. They have the formula $M1^{1+,2+}M2^{2+,3+}(OH)(X^{4+,5+,6+}O_4)$, $M1 = Na, Ca, Pb$; $M2 = Mg, Al, Mn, Fe, Co, Ni, Cu, Zn$; $X = Si, P, V, As, Mo$. Compounds with accurate structure refinements exhibit space-group symmetry $Pnam$ or $P2_12_12_1$. The parental structure is centrosymmetric. The deviation from the centrosymmetric parental structure is moderate. The type structure exhibits $M2O_6$ octahedra (elongated tetragonal dipyramids in case of divalent Cu atoms due to Jahn-Teller distortion) edge linked to chains parallel to [001]. Each of the XO_4 tetrahedra link two such chains to a three-dimensional net-work. Cavities house the M1 atoms. Their coordination varies from [7] to [8] depending on the space group symmetry. Centrosymmetric compounds exhibit a mono-capped trigonal prism for the coordination polyhedron around the M1 atoms (descloizite type). In the acentric structure variant (adelite type) the M1 cation is co-ordinated by a square antiprism. A tendency is observed that the centrosymmetric symmetry goes along with lead-vanadates whereas calcium, arsenate and silicate favour the acentric symmetry.

Single-crystal X-ray structure investigations were performed for adelite, $CaMg(OH)(AsO_4)$, and cobaltaustinite, $CaCo(OH)(AsO_4)$. The acentric space group $P2_12_12_1$ was proved for both minerals: $a = 7.468(1) / 7.475(1)$, $b = 8.953(2) / 8.976(2)$, $c = 5.941(1) / 5.916(1) \text{ \AA}$. During investigations in the Cd(II)-Cu(II)-arsenate(V) system under hydrothermal conditions a new Cd member was synthesized. Single-crystal X-ray structure investigations proved that this compound is a centrosymmetric $Pmma$ member of the adelite-descloizite group: $a = 7.415(1)$, $b = 5.890(1)$, $c = 9.016(2) \text{ \AA}$.

MM11: High-Hydrated Si-Deficient Vesuvianite ('Hydrovesuvianite') From Yakutia, Russia

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The high-hydrated, Si-deficient vesuvianite ($Si \approx 15 \text{ a.p.f.u}$) was discovered on the Wiluy deposit - the type-location of grossular and wiluite. The Si-deficient vesuvianite, occurring as split, sheaf-like, yellowish {110}+{111} crystals up to 50 μm in size and as {001}+{111}+{110} light-cream spherulites up to 200 μm in size, is found in hollows in achtarandite – tetrahedral hibschite pseudomorphs after wadalite. In addition, the Si-deficient vesuvianite forms very thin zones in complex hydrogrossular-wiluite-vesuvianite pseudomorphs after melilite and wadalite. Such zones are rarely observed in big crystals of wiluite.

The formula of high-hydrated Si-deficient vesuvianite is commonly given as $Ca_{10}(Al_9Mg_3Fe_{0.8-1}Mn_{0.0-0.2})_{13}B_{2-4.4}(Si_2O_7)_4(SiO_4)_{10-x}(OH)_{4x}(O,OH,F,Cl)_{10}$ where $x = 0.67-2.89$. Spherulites formed by crystals of pinacoidal habit are enriched in Mn. The Si-deficient vesuvianite is characterized by increased unit-cell parameters ($a=15.69 \text{ \AA}$, $c=11.85 \text{ \AA}$) and a lower refractive index ($n=1.691$, $\omega=1.668$) compared with vesuvianite of similar composition from rodingites. Structural investigations of monocrystals indicate that the Si-deficient vesuvianite probably has $P4$ or $P4/n$ symmetry.

FTIR spectra on the OH-region of the high hydrated Si-deficient vesuvianite sharply differ from the spectra of low-temperature vesuvianite from rodingites and display a similarity with the spectra of hibschite. The line near 3618 cm^{-1} indicates that hydrogrossular type of substitution occurs only in the isolated tetrahedra.

The concentration of hydrogrossular defects in the Si-deficient vesuvianite formed during $(SiO_4)^4- \rightarrow (H_4O_4)^+$ substitution in the isolated tetrahedra allows it to be considered as an analogue of hibschite in the hydrogrossular series. This vesuvianite is a member of the hypothetical series of vesuvianite - 'hydrovesuvianite' with the content of the 'hydrovesuvianite' molecule

$Ca_{10}(Al, Mg, Fe)_{13}(B, Al)_{0.5}(Si_2O_7)_4(OH)_{40}(O, OH, F)_{10}$ ranging up to 30%. In hibschite, the content of the "hydrogrossular" molecule is 6.6–50%.

The formation of the unusual high-hydrated vesuvianites is connected with mass hydration (serpentinization and rodingitization) of primary skarns under non-equilibrium conditions by mineral-forming solutions at with high Al/Si and Ca/Si and at high P_{H_2O} and $T < 300-350^\circ\text{C}$.

MM12: The crystal chemistry of double-ring silicates: a new natural silicate with $[Si_6O_{15}]$ rings

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There have been two types of tetrahedral double-rings previously known for silicates. Four-membered double-rings, ideally $[Si_8O_{20}]$, occur in three minerals with the general formula $[^{8}A]^{[8]}B_2^{[12]}C [Si_8O_{20}] \cdot nH_2O$, where $A = Th, REE$; $B = Ca, Na$; $C = K$; : steacyite, irakite-(La) and turkestanite. Six-membered double-rings, ideally $[Si_{12}O_{30}]$, occur in the 18 minerals of the milarite group with the general formula $[^{6}A_2]^{[9]}B_2^{[12]}C^{[18]}D^{[4]}T(2)_3^{[4]}T(1)_2O_{30}$, where $T(1) =$

Si, Al; T(2) = Li, Be, B, Mg, Al, Si, Mn²⁺, Zn; A = Al, Fe³⁺, Sn⁴⁺, Mg, Zr, Fe²⁺, Ca, Na, Y, REE; B = Na, H₂O, K; C = K, Na, Ba; D = .

The first occurrence of a three-membered double-ring [Si₆O₁₅]⁶⁻ is described for a new natural silicate, Na₂ K (Y,REE) [Si₆O₁₅], from the moraine of the Dara-I-Pioz glacier, the Alai mountain range, the Tien-Shan mountains, Northern Tajikistan. The structure is orthorhombic, *a* 10.623(2), *b* 14.970(2), *c* 8.553(1) Å, *V* 1359.8(4) Å³, space group *Ibmm*, *Z* = 4, *D* (calc.) = 2.850 g.cm⁻³. The crystal structure was solved by direct methods and refined to an *R*_i index of 1.7% based on 936 observed $|F_o| > 4\sigma(F_o)$ unique reflections. In the crystal structure of Na₂ K (Y,REE) [Si₆O₁₅], there are two tetrahedrally co-ordinated *T* sites occupied by Si with $\langle Si-O \rangle = 1.623$ Å. The (SiO₄) tetrahedra form a three-membered double-ring: [Si₆O₁₅]⁶⁻. There are two [6]-co-ordinated sites, one occupied by (Y_{0.77} + REE_{0.23}) with $\langle (Y,REE)-O \rangle = 2.255$ Å, and the other by Na with $\langle Na-O \rangle = 2.438$ Å. There is a [10]-co-ordinated site occupied by K with $\langle K-O \rangle = 3.062$ Å. [(Y,REE)O₆] and (NaO₆) octahedra share common edges to form sheets parallel to (010). These sheets are connected through [Si₆O₁₅] double-rings to form a framework. Channels extend along [010] and contain K atoms. The topology of the Na₂ K (Y,REE) [Si₆O₁₅] framework is identical to that of synthetic Na₃ Y [Si₆O₁₅] (*a* 10.468(2), *b* 15.247(1), *c* 8.385(1) Å, *V* 1338.3 Å³, space group *Ibmm*, *Z* = 4), but the arrangement of the channel cations is quite different.

MM13: Glauconite and celadonite: a nomenclature review

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Glauconite and celadonite are ^{VI}Fe³⁺-rich dioctahedral mica-type layer silicates. In the last 20 years, three nomenclature proposals were published about them by the IMA-CNMMN (Rieder *et al.*, 1998) and by the AIPEA (Bailey, 1980, 1986). In our work, we tested their viability on a range of chemical analyses carried out on Central European samples, as well as on analytical data of some references, generally considered essential. The samples included in the database represent various geological backgrounds and chemical compositions.

Based on the three possible cation positions in these minerals, a positive charge diagram $X_T - X_O - X_{IL}$ was designed for the interpretation of both the species definitions and the chemical data. In the diagram, the following charge ranges were plotted (using a formula unit based on 11 oxygen atoms): 0–1 for the interlayer charge, 5–6 for the octahedral layer charge and 15–16 for the tetrahedral layer charge, respectively.

In the IMA terminology, celadonite is described in terms of four true mica end-members while glauconite represents a series of interlayer-deficient micas. The decisive discrimination between celadonite and glauconite is the interlayer charge, with the dividing value of 0.85 per formula unit. In the AIPEA nomenclature of 1980, discriminative is the tetrahedral layer charge with a value of 15.8 (this corresponds to 0.2 ^{IV}Al per formula unit). The 1986 recommendation used however, the octahedral layer charge, and the discriminative value was this time 5.3 per formula unit.

Celadonite and glauconite have thus been distinguished by the charge values of all the three possible cation positions. The three classification schemes are partly overlapping, partly divergent. Relating the plotted analytical data to the three nomenclatures, we try to evaluate their suitability for differentiating between celadonite and glauconite.

It should be noted however, that in practice chemistry-based nomenclatures have their own serious limitations because of the problems of preparation of chemically "pure" and "homogeneous" samples. The effect of typical analytical uncertainty on the classification is discussed.

The indirect methods (XPD, IR) used in daily routine for discrimination between celadonite and glauconite are also evaluated.

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The bright canary-yellow and orange-yellow needles and hollow prismatic hexagonal crystals of this new hydrous Ca-bearing titanate of uranyl were found in cavities and fractures within rhyolite in a few small areas of Thomas Range. The size of needles and crystals is up to 0.4x10 mm but most are much smaller. The mineral occurs on fracture surfaces or as an intergrowth with hematite flakes, red beryl crystals and topaz crystals. Some crystals are covered with a dark purple crust of small fluorite crystals. Other associated minerals are pseudobrookite, bixbyite, sanidine, quartz. Visually, the mineral looks exactly like the U-Ti-Ca-HREE mineral reported by E. Foord *et al.* from the same locality. Moreover our X-ray data are very close to those published by Foord and colleagues. The strongest lines are (Å): 9.46 s; 4.60 s; 3.77 w; 3.38 w; 3.05m; 2.90 s; 2.35 w; 2.12 w; 1.870 m; 1.747 m; 1.211 m. According to X-ray and electron diffraction data the mineral is hexagonal, with *a* = 10.8 Å, *c* = 7.5 Å. Very poor diffraction data from a single crystal did not allow us to solve the crystal structure. The mineral is partly metamict. The chemical composition and physical properties are more than significantly different from data for the Foord sample (given in brackets after our data). The set of microprobe analysis gave (wt.%): UO₃ 76.03 (UO₂ 18.5); TiO₂ 11.89 (45.5); CaO 2.29 (3.25); HREE was not detected (EHREE 10.03). H₂O 10.0 (22.0). There were no significant variations in the chemical composition for different parts of the same crystal of from crystal to crystal. The empirical formula is U_{1.79}Ca_{0.27}Ti_{1.00}O_{7.64}*3.64H₂O. Since the IR spectrum shows U in uranyl form the idealized formula is close to (UO₂Ca)₂TiO₄*4H₂O. The mineral is uniaxial positive No=1.835(8); Ne=1.910(8) (uniaxial negative all refractive indexes <1.7 for the Foord mineral). Density >4.22, calculated 5.95. (2.62–2.64 for the Foord mineral). Thus, in spite of visual and diffraction similarity, a different mineral was investigated by E. Foord *et al.*

The mineral was crystallized from fumarole gases before most of the beryl and hematite and after most of the topaz. It probably grew originally as a U^{IV} mineral and then U oxidized to U^{VI}. No other U mineral with such a U/Ti ratio (~2:1) is known.

A12-2: Isomorphous series: eudialyte–alluaivite

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Eudialyte is one of the few well-known zirconium silicates, which have titanium analogues. Its titanium analogue, alluaivite, was discovered by A.P. Khomyakov, in one of the pegmatites of Alluaiv Mt. (Lovozero alkaline massif, Kola Peninsula) and until recently, it had been found in no other locality. The Lovozero alluaivite was found in epitaxial intergrowth with eudialyte, with clear phase borders, which initially caused researchers to come to a conclusion about the discontinuity of isomorphous miscibility between these minerals and about important role of the epitaxis in the crystallization of alluaivite.

We found alluaivite in the Khibiny alkaline massif, Kola Peninsula, as an accessory mineral in massive coarse-grained urites (Rasvumchorr Mt.) in association with ordinary eudialyte and forming either knots on the surface of eudialyte grains or as isolated crystals. The empirical formulae of eudialyte and the alluaivite associated with it are provided below:

Eudialyte

(Na_{14.42}K_{0.15}Sr_{0.37}Ba_{0.09})_{15.03}(Ca_{5.74}Mn_{0.26})₆(Fe_{1.16}Mn_{0.39})_{1.55}(Zr_{2.62}Ti_{0.35}Nb_{0.03})₃ × (Si_{25.87}Al_{0.05}Zr_{0.06}W_{0.02})₂₆O_{72.59}Cl_{1.49}S_{0.04}

Alluaivite

(Na_{18.42}K_{0.03}Ba_{0.12})_{18.57}(Ca_{5.23}Mn_{0.59}Ti_{0.11})_{5.93}Fe_{0.07}(Ti_{2.42}Nb_{0.58})_{3.00} × (Si_{25.80}Nb_{0.20})₂₆O_{72.95}Cl_{0.39}S_{0.59}

In one of the studied samples, gradual transitions have been found between alluaivite and eudialyte, which are of a great interest, because they indicate the possibility of absolute isomorphous miscibility between these minerals. Series of electron microprobe chemical analyses done every 100 μm in the transitional zone show the gradual change of composition from eudialyte to alluaivite. Besides the natural leaning of composition by Zr and its enriching by Ti, a natural changing of compositions has been found in almost all chemical elements of these minerals: gradual leaning by Zr, K, Sr, Fe, Cl, and also by Mn, Al, W, Hf, La, Ba, and enriching by Ti, Nb, Na, Si, S, Ce, Nd. An enrichment of the composition by sulphur in alluaivite excites a special interest, because this element is unusual for the minerals of the eudialyte group and it has not been found yet in such quantities.

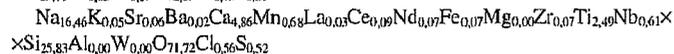
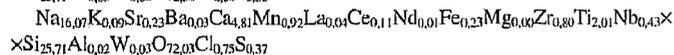
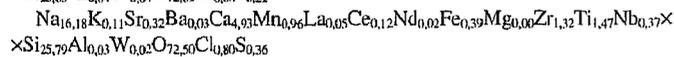
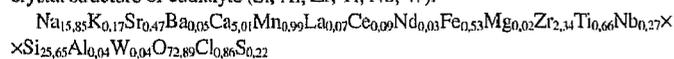
POSTERS for Session 12

A12-1: A new hydrous uranium titanate from Thomas Range, Utah, USA

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Below are the empirical formulae of eudialyte (1), alluaivite (4) and its some transitional varieties (2, 3), calculated for 29 atoms, that form a 'hard' carcass of a crystal structure of eudialyte (Si, Al, Zr, Ti, Nb, W):



The crystallization of eudialyte took place under conditions of decreasing alkalinity-basicity of medium of mineral formation, which is shown by enrichment of composition by less basic components in comparison with more basic components (increasing of proportions of ingredients - Ti/Zr, Na/K, Ca/Sr, Mn/Ca, Ce/La, S/Cl, Si/Al и т.д.) in individual positions of a crystal structure of mineral.

A12-3: MinAbs: An Online Mineral Database

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MinAbs was internationally introduced at the 16th General IMA Meeting in Pisa, 1994, [Abstracts page 399], as an offline version. It was programmed then in FORTRAN. An enhanced offline version, programmed in C/C++, was presented at the 17th General IMA Meeting in Toronto, 1998, [Abstracts page A62].

In the meantime, MinAbs was further improved, re-programmed in JAVA and placed in the World Wide Web.

MinAbs is based on the Mineralogical Abstracts, covering Vol. 1 (1920/23) up to Vol. 52 (2001). It is continuously being corrected, updated, and improved. One entry in MinAbs consists of the mineral name, the chemistry, symmetry, lattice constants, and literature reference.

A special feature of the new MinAbs edition is the extended symmetry information in form of ASCII adapted symbols. The use of subscript and superscript characters in space group and point group symbols is disadvantageous for printing as well as for electronic data processing. While preparing this edition of MinAbs, new symbols were designed consisting of a string of 5 ASCII characters for symbols after SCHOENFLIES, and of up to 7 characters for the symbols after HERMANN-MAUGUIN. It proved to be very useful to extend the new symbols to crystal systems as well.

For retrieving purposes in databases, the SCHOENFLIES symbols are useful because of their hierarchical nature and their independence of crystal settings. The advantage of HERMANN-MAUGUIN symbols is their more detailed symmetry information. The combination of both, using the new ASCII symbols, is being successfully applied in MinAbs.

A password is needed to access MinAbs. It will be granted, by request, to bona fide academics and students. The URL is: www.psusse.de/minabs/.

A12-4: Crystal structure of "redgillite", $\text{Cu}_{12}(\text{OH})_{20}(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$ from the Red Gill Mine, Caldbeck Fells, Cumbria, England

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"Redgillite" is the tentative name given to a phase as yet not submitted for formal mineral status. The crystal was obtained via Peter Braithwaite, Derbyshire, England and was found at the Old Dutch Level mine dump, also known as the No.2 Level mine dump, at Red Gill Mine, Caldbeck Fells, Cumbria, England. Oxidation processes presumably in the Tertiary produced the suite of supergene minerals for which the mine is famous. At other localities where redgillite occurs, it is clearly a dump oxidation product and is post-mining in origin. Crystals are emerald green, lath shaped, and seldom greater than 60 microns in length.

Single crystal intensity data were collected using synchrotron radiation ($\lambda = 0.6888 \text{ \AA}$) at ChemMatCARS, Sector 15, at the Advanced Photon Source, Argonne, IL using a tiny $60 \times 20 \times 4 \text{ \mu m}$ crystal. Monoclinic unit-cell dimensions were $a = 3.1521(13)$, $b = 10.495(5)$, $c = 19.515(10) \text{ \AA}$, $\beta = 90.09(2)^\circ$. The crystal structure

was determined using direct methods and refined to a final $R = 0.09$. Diffractions showed constant d streaking and speckling suggesting that even a sample of this size was polycrystalline. The crystal was also refined as a twin with ~ 80% - 20% split of twin components related by $(1\ 0\ 0, 0\ -1\ 0, 0\ 0\ -1)$. Electron microprobe analyses were consistent with the derived structural composition.

The redgillite structure consists of CuO_6 octahedra and SO_4 tetrahedra. The CuO_6 octahedra have four short distances of ~2.0 Å and two longer distances ranging from ~2.3-2.8 Å . The octahedra share edges to form sheets that are zig-zag in cross section when viewed down the a axis and are stacked perpendicular to the c axis. Each leg of the zig-zag is four octahedra in length and repeats after every 7 octahedra. SO_4 tetrahedra, that reside in the space between the Cu layers, form columns parallel to the a axis. The S site is only half occupied implying that only every other site in the column is filled. One O in SO_4 is also bonded to Cu, and the remaining three that occupy the space between Cu layers are bonded only to S. A valence balance calculation suggests that 20 out of 30 oxygen atoms are actually OH and that two are H_2O . An oxygen atom is either bonded to Cu and S or exists as H_2O when SO_4 is absent. The geometry is correct for this oxygen to bridge two SO_4 groups by forming hydrogen bonds. The remaining SO_4 oxygen link adjacent Cu sheets via hydrogen bonds.

A12-5: Crystal structure of ajoite, $\sim(\text{Na}+\text{K})_3\text{Cu}_{20}\text{Al}_3\text{Si}_{29}\text{O}_{76}(\text{OH})_{16}\sim 8\text{H}_2\text{O}$ from the Arizona porphyry copper/hydrothermal deposits

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Ajoite occurs rarely in the oxidized zone of porphyry copper deposits in Arizona. It was first described by Schaller and Vlissidis in 1958 and again by Chao in 1981, but the crystal structure was never determined. Data was collected at GeoSoilEnviro and Chem-Mat -CARS at the Advanced Photon Source at Argonne IL using a $60 \times 15 \times 5 \text{ \mu m}^3$ green crystal, from the type locality Ajo, AZ. Data quality was poor due to the nature and size of the crystal, but enough intensity was obtained from streaked diffractions to solve and refine the crystal structure to a final $R=0.145$ and 2-sigma accuracy ~ 0.01 Å for (Si,Al)-O. Ajoite is triclinic P-1, with unit-cell dimensions $a\ 13.638(2)$, $b\ 13.691(2)$, $c\ 14.518(2)$, $\alpha\ 110.765(4)$, $\beta\ 106.825(3)$, $\gamma\ 105.828(5)$. Electron microprobe showed variable Na and K, but is consistent with the reported composition.

The ajoite structure consists of sheets of edge-shared octahedrally-coordinated Cu atoms at $c\sim 0.5$. Sandwiched between two Cu layers are layers of Si,Al tetrahedra with most of the vertices shared with those of the Cu-O octahedra, and some shared with the adjacent tetrahedral layer to generate an octahedral-tetrahedral 3D framework. The 3D net contains a 2D channel system defined by elliptical 12 rings along a and circular 8-rings along b . As is typical of Cu (II)-O linkages, each Cu atom has 4 short distances to adjacent oxygen atoms in a square, and 2 longer distances to generate opposing vertices of a distorted octahedron. Eight tetrahedra are larger than the other 24 tetrahedra consistent with half occupancy by Si and Al. Valence balance estimates indicate that 16 oxygen atoms out of 92 are hydroxyl. Ajoite contains a total of 3 (K,Na) of which ~25% is Na from the electron probe analysis. One (K,Na) site, located in the (Si,Al) framework part of the structure, has distorted octahedral co-ordination. The remaining 2 (K,Na) and non-hydroxyl water from the chemical analysis presumably reside in the channels as disordered molecules as in zeolites and are not detected.

The crystal structure of ajoite opens up a further window into zeolitic (microporous) materials. Ion exchange experiments are needed to determine the selectivities and possible industrial use. Removal of the zeolitic water molecules may permit molecular sorption or catalysis. A theoretical study of polygonal linkages may allow invention of new octahedral-tetrahedral frameworks, and a family of copper silicate zeolitic materials may ensue.

A12-6: Labuntsovite group minerals with gutkovaite-type structure

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In recent years the minerals of the labuntsovite group have attracted interest because of their wide range of cation isomorphism, a number of structural types and their ion-exchange properties. The labuntsovite group contains 18 minerals, which are divided into 8 subgroups. Three minerals of the labuntsovite group with a new structural type were recently discovered in hydrothermally-altered pegmatites in the alkali massifs (the Kola Peninsula).

The crystal structure of conventional labuntsovite is based on a framework consisting of chains of (Ti,Nb)O-octahedra that are linked by tetrahedral four-membered rings [Si₄O₄]. Extra-framework cations (Na, K, Ca, Ba, Sr) and H₂O are situated in the cavities of this framework. There are three extra-framework cation positions – A, B, C. The chains of (Ti,Nb)O-octahedra are additionally linked by DO-octahedra, where D is usually a bivalent cation such as Mn, Fe, Mg and Zn.

Recently-discovered gutkovaite-Mn is a representative of a new structural type, which differs from labuntsovite by occupancy of the A-position. In the latter there are two related by axis 2 A-positions occupied by Na. In gutkovaite one of these positions (A(1)) is occupied by Ca and another is vacant. Because of this the symmetry of gutkovaite is lowered to Cm.

A new mineral with gutkovaite type structure and high K content ((Na_{0.7}K_{1.3})[K_{2.2}(H₂O)_{0.8}][K_{0.72}Ba_{0.48}][Fe_{0.66}Mg_{0.44}(H₂O)_{2.2}][Ti_{4.8}Nb_{3.2}(OH_{5.27}O_{2.73})]S₄O₁₂] 2.92H₂O, (Z=1); here and further, the composition of A, B, C and D – sites is shown in square brackets, correspondingly) was discovered soon after gutkovaite-Mn. In this mineral the same A(1) position is occupied by Na, but the split A(2)-position, which is occupied by water molecules in gutkovaite and labuntsovite, is occupied by K (with a 0.3 Å shift).

The third discovered mineral with gutkovaite-type structure – alsharovite-Zn ((Na_{0.7}Ca_{0.7})(Sr_{1.7}Na_{0.3})_{2.2}[(H₂O)₂K₁][Ba_{0.2}][Zn_{1.64}(Mn,Fe)_{0.18}(H₂O)_{3.64}][Ti_{5.68}Nb_{2.32}(O_{5.18}OH_{2.82})]Si₄O₁₂] 3.3H₂O, (Z=1)) is a bright example of cation order, it contains five alkali elements (K, Na, Sr, Ca, Ba) which are distributed among four structural positions. The A(1)-position contains Ca and partially Na, A(2) position contains Sr and the rest Na, B-position contains K, and Ba is sited in the C-position. Small bivalent cations with Zn prevailing occupy D-octahedra.

The distinctive feature of gutkovaite structural type is ordered occupancy of non-equivalent sites A(1) and A'(1), that results in lowering the symmetry to Cm. In some cases the split A(2) position (which is occupied by water molecules in other minerals of labuntsovite group) is occupied by large cations (K, Sr). These features make minerals with gutkovaite-type structure effective separators of alkali cations.

A12-7: Sewardite, CaFe³⁺₂(AsO₄)₂(OH)₂, the Ca-analogue of carminite, from Tsumeb, Namibia

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Sewardite, ideally CaFe³⁺₂(AsO₄)₂(OH)₂, is the Ca-analogue of carminite and is orthorhombic, Cccm (66), with unit-cell parameters derived from crystal structure: *a* = 16.461(2), *b* = 7.434(1), *c* = 12.131(2) Å, *V* = 1484.5(6) Å³, *a*:*b*:*c* = 2.2143:1:1.6318, *Z* = 8. The strongest nine lines of the X-ray powder-diffraction pattern [*d* in Å (*hkl*)] are: 4.874(90)(202), 3.473(50)(113), 3.389(60)(220), 3.167(100)(022), 3.015(50)(510), 2.988(50)(313), 2.919(70)(511), 2.503(90)(422, 314) and 1.775(50)(533, 026). The mineral occurs within a small 3 cm-sized vug on a single specimen collected from the 31st level of the Tsumeb mine, Tsumeb, Namibia, as platy to tightly bound anhedral-subhedral masses. These masses, which do not exceed 0.3 mm in maximum size, are intimately intergrown with a very dark green-black botryoidal tsumcorite supergroup mineral. Individual fragments tend to be between 50–100 μm in size with no obvious forms and {100} and {011} imperfect cleavages. Sewardite has physical properties which are very similar to those of carminite: colour is dark red in masses to a much lighter red-orange on thin edges of small fragments; streak reddish brown; lustre vitreous; translucent (masses) to transparent (on thin edges); nonfluorescent; hardness (Mohs) 3½; brittle; splintery (in [011] direction) to uneven fracture; calculated density 4.156 g/cm³ (for empirical formula). In polished section, it is light bluish grey in plane-polarized reflected light in air, with ubiquitous very bright pink to red internal reflections; the phase is very

weakly birefractant, non-anisotropic and with no pleochroism. Averaged results of eight electron-microprobe analyses yield CaO 11.77, ZnO 1.68, CuO 0.28, Fe₂O₃ 31.65, As₂O₅ 48.81, H₂O [4.04], total [98.23] wt.%. The empirical formula is Ca_{0.99}(Fe³⁺_{1.87}Zn²⁺_{0.10}Cu²⁺_{0.02}Fe³⁺_{0.09}As⁵⁺_{2.01})O₈[(OH)_{1.88}(H₂O)_{1.12}], on the basis of 10 anions. The infrared-absorption spectra show bands for structural (OH), substituting (H₂O) and arsenate. The mineral name honours Terry M. Seward, Professor of Geochemistry, ETH, Zurich, Switzerland, who self-collected the mineral specimen in 1982. The crystal structure (*R* = 6.1%) clearly shows that sewardite is the Ca-analogue of carminite: tetrahedra fully occupied by As⁵⁺ and an octahedron principally occupied by Fe³⁺. Mean bond lengths for the two minerals are virtually the same.

A12-8: Crystal structure of two hydrated minerals of the eudialyte group with doubled cell at –163°C

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Eudialyte is trigonal zeolite-like zirconosilicate of very complicated and variable composition. Depending on the number of extraframework positions, there can be up to 21 A atoms (Na and some other elements: K, Sr, Ba, Ca, REE, Mn) for 3 Zr atoms. In previously studied minerals this number is 12 to 19. Substantial deficiency of positive charges due to A-cation depletion is compensated by oxonium groups, which cannot be interpreted as neutral water molecules. The presence of these groups is also confirmed by the IR spectra of hydrated specimens. Using our previously studied minerals, we have compared 5 structures with different degrees of depletion. Two of them are potentially new analogues of eudialyte minerals with ordered A-cation distribution and doubled *c* parameter. Both of them were recently found in alkaline pegmatites of the Khibina massif (Kola Peninsula, Russia) as crystals up to 1 cm in diameter with a perfect (001) cleavage. Highly decationated member (I): *a* = 14.254(1) Å, *c* = 60.329(7) Å, space group R3, *R* = 4.4%, H₂O/A = 0.85. Moderately decationated member (II): *a* = 14.266(1) Å, *c* = 60.326(7) Å, space group R3*m*, *R* = 5.5%, H₂O/A = 0.45. The X-ray data were collected with a Bruker SMART CCD diffractometer at –163°C.

A comparison of these two minerals with other oxonium-containing samples, as well as with a highly alkaline specimen (H₂O/A=0), allowed us to draw conclusions about the hydration process in minerals of the group. The full replacement of A cations by loose and mobile oxonium groups is probably impossible because of structure destabilization. An increasing degree of hydration is accompanied by increasing contents of K, Sr, Ba, Ca and REE stabilizing the structure. The isomorphic replacement of A cations by oxonium groups can be either statistical in the unit cells or ordered in the layers perpendicular to axis 3. Both of the new members are characterized by the presence of a H₂O-rich module and a Na-rich module. Thus, cationic ordering in these minerals leads to the doubling of the *c* parameter. The H₂O-rich layers are weaker and produce a parting. Replacement of A cations by H₂O groups in all minerals with different hydration states occurs in the Zr-Si-containing layer rather than in the layer with Ca-rings. Na atoms distributed in the Zr-containing layer in the cavity between two 9-membered Si₄O-rings are replaced partly or fully by H₂O groups in the most of the structures studied.

A12-9: Gjerdingenite-Fe, another new mineral of the labuntsovite group

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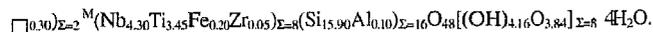
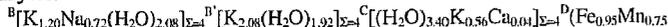
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The CNMMN (IMA) has recently approved a new nomenclature of the labuntsovite group. The idea is to keep the number of new mineral names to a minimum by combining root names with suffix modifiers according to the content of cations in specific structural sites. The labuntsovite minerals contain a variety of extra-framework sites in channels of a zeolite-like structure and,

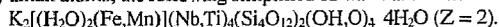
not surprisingly, the Commission has had several proposals for new root names lately.

The group includes Ti/Nb alkali silicates with general formula $A_2B_4[C_{2-2x}(H_2O,OH)_{2x}]D_x[M_8(Si_4O_{12})_4(OH,O)_8]nH_2O$. A and B are mainly alkalis; the C and D sites can contain several types of cations but exclude each other, their distance being only $\sim 2 \text{ \AA}$ (if the D site is occupied by cations, H_2O molecules or OH groups occur in C to complete the octahedral co-ordination of the D cations); M contains mainly Ti or Nb; there are two specific H_2O sites, W1 and W2.

In the case of the new mineral gjerdingenite-Fe: the A site is empty; unexpectedly, the site W1 (renamed B') contains about equal amounts of H_2O and K; the B site has K and Na plus an amount of H_2O equal to the content of K in B' (the content of B' is within the co-ordination sphere of B; if there is a cation in B', the site B must locally carry an oxygen atom or a vacancy); the content of Fe and Mn in site D is limited by the related content 2x of water in site C. In this way, the following crystal-chemical formula was derived, which compares well with the chemical analyses:



Unifying the contents of the sites C and D and the water molecules co-ordinated by alkali atoms, the following simplified formula is obtained:



Gjerdingenite (as a root name) has Nb > Ti in M and is an analogue of kuzmenkoite (root name) which has Ti > Nb. The species name is according to the prevailing D cation, i.e. gjerdingenite-Fe. The mineral is monoclinic $C2/m$ with $a = 14.529(2)$, $b = 13.943(2)$, $c = 7.837(2)$ Å, $\beta = 117.61(1)^\circ$. The crystal structure was refined to $R = 0.054$ for 1677 observed reflections. Twinning on {001} simulates an orthorhombic F-centred lattice with non-spacegroup absences.

Gjerdingenite-Fe occurs as yellow prisms or laths up to 1 mm long in miarolitic cavities of a soda granite (ekerite) at Gjerdingeslva, Lunner, Oppland, Norway.

A12-10: Gramaccioliite-(Y), a new entry in the crichtonite group

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The crichtonite group includes a set of minerals with the general formula $^{XII}A^{VI}B^{VI}C_{18}^{IV}T_2O_{38}$. Each mineral is characterized by a unique combination of dominating A and B cations, whereas C and T cations are mainly Ti and Fe in all minerals. The minerals so far known within the crichtonite group [with dominating A and B cations within brackets] are crichtonite [Sr, Mn], senaite [Pb, Mn], davidite-(La) [REE, La], davidite-(Ce) [REE, Ce], davidite-(Y) [REE, Y], loiveringite [Ca, Zr], landauite [Na, Mn], lindsleyite [Ba, Zr], mathiasite [K, Zr], dessauite-(Y) [Sr, Y]. Gramaccioliite-(Y), herewith described, is a new mineral of the group, recently approved by the IMA CNMNM. In the case of gramaccioliite-(Y) the dominant A and B cations are Pb and Y, respectively. The mineral was named in honour of prof. C.M. Gramaccioli (Milano). As a general rule for the nomenclature of minerals within the crichtonite group, Levinson suffixes are not given unless for REEs (and Y is considered as such).

Gramaccioliite-(Y) was found within quartz hydrothermal veins in a biotitic gneiss of the Hercynian Massif of Argentera, in the locality Pianche, close to Vinadio, Stura Valley, Piedmont, Italy.

Associated minerals are quartz, albite, anatase, brookite, rutile, pyrite. The mineral appears in prismatic tabular {001} crystals, up to 3 mm in length, black with black streak, opaque with metallic lustre, brittle with conchoidal fracture. Optically the mineral is opaque with very weak anisotropy and low birefractance. Reflectance measurements (% in air and oil) for the four critical wavelengths, are: 19.2, 6.7 (470 nm), 17.9, 5.9 (546 nm), 17.6, 5.7 (589 nm), 17.4, 5.8 (650 nm). The calculated density is 4.66 g/cm³.

EPMA analysis yielded (wt.%): V₂O₅ 0.22, Nb₂O₅ 0.32, TiO₂ 59.47, UO₂ 0.33, Fe₂O₃ 24.14, Y₂O₃ 3.03, La₂O₃ 0.14, Ce₂O₃ 0.70, Nd₂O₃ 0.20, CaO 0.12, MnO 1.45, ZnO 0.99, SrO 1.56, BaO 0.19, PbO 7.53, K₂O 0.01, Total 100.40, which gave the following formula: $(Pb_{0.61}Sr_{0.27}Ba_{0.02}U_{0.02})_{\Sigma=0.92}(Y_{0.49}Mn_{0.37}REE_{0.12}Nb_{0.04}Ca_{0.04})_{\Sigma=1.04}(Ti_{13.53}Fe_{3.82})_{\Sigma=17.35}(Fe_{1.67}Zn_{0.22}V_{0.04})_{\Sigma=1.93}O_{38}$. The simplified formula is $(Pb,Sr)(Y,Mn)(Ti,Fe)_{18}Fe_2O_{38}$.

As all the other members of the group, gramaccioliite-(Y) is trigonal, space group $R\bar{3}$, a 9.186(4) Å, α 68.82(4)°. The crystal structure of gramaccioliite-(Y) has been refined from single-crystal X-ray diffraction data to $R = 8.6\%$. The cation occupancy obtained from the structural data is in keeping with the chemical composition of the mineral.

A12-11: Pellouxite, a new Pb-Sb-Cu oxy-chloro-sulfosalt from Buca della Vena mine, Tuscany, Italy

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The new mineral pellouxite, $(Cu_{0.6}Ag_{0.3})Pb_{10.4}Sb_{11.6}S_{27}[Cl_{0.4}(OH)_{0.6}](OH)_{0.5}$, is the second oxy-chloro-sulfosalt after pillaitite, and the fifth halogeno-sulfosalt after dadsonite, ardaite, playfairite and pillaitite. Like pillaitite, pellouxite has been found at Buca della Vena mine, a small Fe-Ba ore deposit in the Apuan Alps, northern Tuscany, Italy. Pellouxite is present in small fractures of a dolomitic rock that hosts the massive Fe-Ba ore, together with many other Pb-Sb acicular sulfosalts, among which zinkenite, robinsonite, tintinaite, pillaitite and scainiite.

Pellouxite occurs as black acicular flattened crystals with metallic lustre, elongated // [010] and flattened on (100), up to 1 mm long and less than 0.05 mm thick. The mineral is brittle, flexible, opaque and present a good {100} cleavage; the density (calc.) is 5.95 g/cm³. In reflected light, it is weakly birefractant (white to white-grey); with crossed polars, anisotropy is distinct, without polarisation colours (no twinning observed); red internal reflections are frequent. Reflectance values (randomly oriented section, λ_c (nm), air/oil %): 470, 38.3/23.8; 546, 37.3/22.4; 589, 36.9/21.5; 650, 35.2/19.6. Electron microprobe analysis (mean of 15 spot analyses - wt.% - error σ): Pb 47.17(20), Sb 31.16(23), Cu 0.89(5), Ag 0.59(5), S 19.08(6), Cl 0.33(3), O 0.39(1.5), Sum 99.60(39). Empirical formula (based on Pb + Sb = 22): $Cu_{0.6}Ag_{0.3}S_{27.1}Pb_{10.4}Sb_{11.6}Cl_{0.4}O_{1.1}$.

Pellouxite is monoclinic, space group $C2/m$, $a = 55.824(11)$, $b = 4.0892(8)$, $c = 24.128(5)$ Å; $\beta = 113.14(3)^\circ$; $V = 5065(2)$ Å³. The strongest lines of the X-ray powder diffraction pattern are $[d(\text{\AA}), I_{obs}, (hkl)]$: 4.01, 25, ($\bar{0}$ 06); 3.423, 100, (605, 807); 2.779, 22, ($\bar{1}$ 16); 2.274, 32, ($\bar{1}$ 8, 517); 2.225, 43, ($\bar{1}$ 4,

13). According to the crystal structure study, there are specific sites for (Cu,Ag), Cl and O; bond valence calculations favour O as an hydroxyl group. Proposed structural formula: $(Cu_{0.6}Ag_{0.3})Pb_{10.4}Sb_{11.6}S_{27}[Cl_{0.4}(OH)_{0.6}](OH)_{0.5}$. Pellouxite is structurally related to scainiite, $Pb_{14}Sb_{30}S_{54}O_5$. It is an expanded monoclinic derivative of synthetic hexagonal $Ba_{12}Bi_{24}S_{48}$, belonging to the zinkenite group of lead sulfosalts with cyclically twinned structures.

Like for pillaitite, the formation of pellouxite at the Buca della Vena mine is related to a high chlorinity of the hydrothermal solution, but also to the oxygen fugacity, like for scainiite. This new mineral species and its name have been approved by the IMA-CNMMN (vote n° 2001-033). The name of this mineral honours the late professor Alberto Pelloux (Crema 1868- Bordighera 1947), curator of the mineralogical Museum at the University of Genova.

A12-12: An experimental verification of alteration of lanthanite-(Nd) into kozoite-(Nd)

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Kozoite-(Nd), $Nd(CO_3)(OH)$, occurs in cavities and fissures of alkali olivine basalt exposed at Niikoba, Hizen-cho, Higashi Matsuura-gun, Saga Prefecture, Japan. The shape of aggregates of minute crystals of kozoite-(Nd) is usually platy, which corresponds to the crystal habit of lanthanite-(Nd), $Nd_2(CO_3)_2 \cdot 8H_2O$. This mode of occurrence suggests that kozoite-(Nd) is probably an alteration product of lanthanite-(Nd) in postmagmatic hydrothermal activity.

The alteration condition was examined using a chemical reagent of $Nd_2(CO_3)_2 \cdot 8H_2O$ [lanthanite-(Nd)] and sodium aqueous solutions under

hydrothermal conditions. The powder of starting material, $\text{Nd}_2(\text{CO}_3)_2 \cdot 8\text{H}_2\text{O}$, was sealed with sodium aqueous solution (0 – 0.5M NaHCO_3 or NaOH) in a Teflon vessel or a platinum capsule. The reaction containers were kept at 100, 150, 200 or 250°C. The reaction process was traced varying the duration of reaction up to 7 days. The reaction products were filtered, washed with distilled water, and dried overnight at room temperature. They were characterized by XRD.

The starting material, $\text{Nd}_2(\text{CO}_3)_2 \cdot 8\text{H}_2\text{O}$, decomposed within 30 minutes. A phase with the XRD pattern of $\text{Nd}_2(\text{CO}_3)_2 \cdot 2.5\text{H}_2\text{O}$ [ICDD #33-0932] was formed as a decomposition product. Subsequently, kozoite-(Nd) and hydroxylbastnäsité-(Nd), the polymorph of kozoite-(Nd), were crystallized. The higher reaction temperature and the higher pressure tend to promote the formation of hydroxylbastnäsité-(Nd) instead of kozoite-(Nd). Since kozoite-(Nd) is the less dense polymorph in comparison with hydroxylbastnäsité-(Nd), it is reasonable that kozoite-(Nd) crystallizes under lower pressure conditions. These observations suggest that kozoite-(Nd) is formed under relatively lower-temperature and lower-pressure conditions. On the other hand, the yield of kozoite-(Nd) reduced and hydroxylbastnäsité-(Nd) was the dominant product in the reaction runs using sodium solutions with higher concentration and in the runs with elongated reaction duration. These trends indicate that kozoite-(Nd) may be a metastable phase in the present reaction system.

A12-13: $^{[12]}K_2^{[6]}(\text{Mn,Fe,Mg})_4^{[4]}(\text{Be,Al})_6^{[4]}\text{Si}_{24}\text{O}_{60}$ – a new Mn-analogue of milarite from the Bellberg volcano, Eifel area, Germany

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The osumilite-type compounds, included under the title milarite group minerals, are classified as double-ring silicates with the general formula $^{[18]}D_2^{[12]}C_2^{[9]}B_4^{[6]}A_4^{[4]}T(2)_2^{[4]}T(1)_{24}O_{60}$, where $D = \text{H}_2\text{O}$; $C = \text{Na, K, Ca, Ba}$; $B = \text{Na, K, Ca, H}_2\text{O}$; $A = \text{Mg, Al, Ca, Mn, Fe, Sn, Ti, Zr}$; $T(2) = \text{Li, Be, B, Mg, Al, Fe}$, and $T(1) = \text{Si, Al}$. The compounds usually crystallize in space group $P6/mmc$ and, due to the chemical variability, wide ranges for a (10.0–10.4 Å) and c (13.5–14.4 Å) are reported. The main structural motif consists of a double six-membered ring of corner-linked $T(1)O_4$ tetrahedra, which is stacked along the c -axis and interconnected via the $T(2)O_4$ tetrahedra and the AO_6 octahedra. Accordingly, a channel along the c -axis exists, which may be occupied by large alkali- or alkaline-earth cations at the C -site.

The specimens of the new osumilite-type mineral were found in a quarry of the Bellberg volcano near Mayen, western Eifel area, Germany. They occur in cavities of silicate-rich xenoliths together with clinopyroxene, amphibole and tridymite. The sample material consists of semitransparent to clear, tabular {0001} hexagonal crystals (0.10–0.17 mm), and small anhedral grains (< 0.1 mm). The crystals are yellowish brown and have a glassy lustre. This appearance is similar to osumilite and roederite, both previously reported from this area. A preliminary single-crystal X-ray investigation revealed the cell parameters $a = 9.997(1)$ Å, $c = 14.090(1)$ Å and $V = 1219.5(2)$ Å³ indicating a sugilite-type member which should exhibit a purple to magenta colour.

The empirical chemical formula obtained from microprobe analyses and LAM-ICP-MS for the beryllium content can be given as $^{[12]}K_{1.8}^{[9]}Na_{0.4}^{[6]}(\text{Mn}_{2.0}\text{Fe}_{1.3}\text{Mg}_{0.7})^{[4]}(\text{Be}_{4.4}\text{Al}_{1.6})^{[4]}\text{Si}_{24}\text{O}_{60}$ with minor amounts of ZnO. All crystals investigated exhibit a distinct zoning due to chemical variations on the A-site, which are dominated by a $\text{Mn}^{2+} \leftrightarrow \text{Mg}^{2+}$ substitution. Only at the outermost rim of some grains can the presence of CaO be observed. The refinement of the single-crystal data ($wR = 0.045$, $R = 0.021$) confirmed these findings by crystal chemical calculations.

The new mineral is distinguished from the minerals of the osumilite group by the lack of Ca on the octahedral A site with a dominance of Mn^{2+} and Fe^{2+} over Mg^{2+} , as it is known for the lithium-bearing dusmatovite. The $T(2)$ -site chemistry, however, is very close to the calcium-rich milarite.

A12-14: Martinite, a new borosilicate mineral from Mont Saint-Hilaire, Quebec, Canada: description and crystal structure determination

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Martinite is a new mineral discovered as a rare, late-stage phase in sodalite syenite xenoliths at the Poudrette quarry, Mont Saint-Hilaire, Quebec, Canada. It occurs as thin (< 10 µm) lavender to colourless pseudohexagonal plates up to 50 µm across in vugs, associated with villiaumite, eudialyte group minerals, lovozerite group minerals, terskite and erdite. Results from single-crystal X-ray diffraction and EMP analyses indicate the ideal formula $(\text{Na}, \text{Ca})_{11}\text{Ca}_4(\text{Si}, \text{S}, \text{B})_{14}\text{B}_2\text{O}_{40}\text{F}_2 \cdot 4\text{H}_2\text{O}$. Martinite is triclinic, $P\bar{1}$, but is strongly pseudohexagonal [a 9.5437(7), b 14.0268(10), c 9.5349(6) Å, α 71.057(1), β 119.788(1), γ 105.846(1)°]. Its crystal structure, which is strongly layered parallel to [010], is dominated by silicoborate (S) layers composed SiO_4 tetrahedra joined into distorted hexagonal rings which in turn are cross-linked in the (010) plane by $(\text{Si}, \text{B})\text{O}_4$ and BO_4 tetrahedra. Two such layers (S_1, \bar{S}_2 , related by a centre of symmetry) are joined along [010] via shared corners and edges with interlayer $\text{Na}\Phi_5, \text{Na}\Phi_6$ ($\Phi =$ unspecified ligand) polyhedra and H_2O molecules. Weak bonding between the tetrahedral layers and the interlayer components produces a perfect {010} cleavage. Tetrahedra in the hexagonal silicate rings are oriented with their apices directed upward (away from the centre of symmetry) while the $(\text{Si}, \text{B})\text{O}_4$ and BO_4 tetrahedra have their apices directed downward (towards the centre of symmetry). Closest-packed $M\Phi_6$ ($M = \text{Ca, Na}$) octahedral layers (O) are joined to apical oxygens belonging to the distorted hexagonal silicate rings. The structure may be considered as a modular centrosymmetric structure with the stacking sequence, $O \bar{S}_2 \bar{S}_2 O$. Martinite is a member of the reyerite merotype series, which includes reyerite, gyrolite, fedorite, truscottite and tungusite. These minerals constitute a group of layered alkali/alkaline earth silicates containing single or double tetrahedral sheets that typically develop as late-stage phases in highly alkaline environments. Considering its environment of formation (vugs in sodalite syenite xenoliths that are located proximal to a biotite-muscovite-quartz hornfels unit), martinite may be the product of the interaction of late-stage hyperalkaline fluids and metasediments, the latter possibly being a source of B and SiO_2 .

A12-15: Cavoite, CaV_3O_7 , a new mineral from the Gambatesa mine, northern Apennines, Italy

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In Eastern Liguria, manganese ores occur near the bottom of chert sequences ("Diaspri di Monte Alpe" Formation) overlaying Jurassic ophiolites and consist of braunite-bearing layers within hematite-rich cherts. Tectono-metamorphic re-equilibration under prehnite-pumpellyite facies conditions affected ophiolites and their sedimentary covers; a complex vein system, mainly localized at the fold hinges, developed, inducing reaction processes responsible for the formation of Mn-silicate and/or Mn-carbonate assemblages, at the expense of braunite + quartz assemblages. Fluids circulating along later fractures, at decreasing metamorphic conditions, lead to the concentration of elements such as V, As, Ba, Sr and the precipitation of a great variety of uncommon minerals, included many new species.

Cavoite, CaV_3O_7 , occurs at the Gambatesa mine (Eastern Liguria, Italy) filling microcavities in massive bands of caryopilite + calcian rhodochrosite ± quartz. The formation of these assemblages, replacing tephroite + rhodonite veins within the braunite layers, is referred to the increased activity of CO_2 -bearing and Ca-rich hydrous fluids in the veins, which also induced V mobilization.

Cavoite has been found as very rare radiated aggregates of strongly elongated prismatic to acicular crystals up to about 0.28 mm in length, intimately associated with an unidentified silicate phase. The crystals vary in colour from colourless to olive green-brown; they are brittle, transparent and non-fluorescent, with vitreous lustre and near white streak; no cleavage, parting and twinning were observed.

The mean empirical formula from microprobe analyses, based on seven oxygen atoms, is $(\text{Ca}_{0.95}\text{Mn}_{0.03}\text{K}_{0.02})(\text{V}_{2.79}\text{Si}_{0.22})\text{O}_7$. It approaches the ideal formula, CaV_3O_7 , taking into account that the chemical determinations (presence of K and Si) are possibly affected by contamination due to intimate association with an unidentified silicate.

The powder diffraction data give the refined cell parameters: $a = 10.42(2) \text{ \AA}$, $b = 5.28(2) \text{ \AA}$, $c = 10.34(2) \text{ \AA}$ and $V = 568.2 \text{ \AA}^3$.

Micrometric crystals of cavotte were also investigated by means of transmission and analytical electron microscopy.

Cavotte is the natural analogue of the synthetic CaV_3O_7 , whose structural study is reported by Bouloux & Galy together with that of the isostructural phases SrV_3O_7 and CdV_3O_7 .

Both the mineral and the name, derived from the chemical composition, have been approved by the I.M.A. Commission on New Minerals and Mineral Names (ref. 2001-24).

A12-16: Pepprosiite-(Ce) as a new mineral from Campagnano in Italy: one decade later

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In the early 1990s, a new mineral from Campagnano in Italy with an ideal chemical formula $(\text{Ce,Lu})\text{Al}_2\text{B}_3\text{O}_9$, was announced: P62m space group, $a = 4.610(1) \text{ \AA}$, $c = 9.358(7) \text{ \AA}$, $D_{\text{meas}} = 3.45(5) \text{ g cm}^{-3}$, $n_o = 1.703(2)$ and $n_e = 1.711(5)$ (G. Della Ventura, 1993). However, its empirical composition is very complicated, although preliminary structural investigations resulted in the data geometrically similar to the synthetic metaborates.

On the other hand, for the first time, the neodymium representative of metaborate family with a general formula $\text{Re}_2\text{O}_3 \cdot 2\text{Al}_2\text{O}_3 \cdot 4\text{B}_2\text{O}_3$ (Re=La, Ce, Pr, Nd) was synthesized in the field of existing melts of the polycomponent system $\text{Nd}_2\text{O}_3\text{-Al}_2\text{O}_3\text{-B}_2\text{O}_3\text{-K}_2\text{O-MoO}_3$. An increase in concentration of B_2O_3 in the complex flux $\text{K}_2\text{O-MoO}_3\text{-Nd}_2\text{O}_3\text{-B}_2\text{O}_3$, which used for the crystal growth of $\text{NdAl}_3(\text{BO}_3)_4$, leads to the replacement of NdAl-orthoborate by the another Nd- and Al- and B-containing solid phase with reduced aluminium concentration. The structural determination shown that this compound belongs to the centrosymmetric P62m space group, and it is a new neodymium aluminium metaborate having tetrahedral co-ordination of boron atoms and a layered type of boron-oxygen polyanion $[\text{B}_4\text{O}_{10}]^{8-}$, i.e. $\text{NdAl}_{2.07}[\text{B}_4\text{O}_{10}]_{0.6}$. Consequently, single crystals of the La-, Ce- and Pr-metaborates have been grown from $\text{K}_2\text{Mo}_3\text{O}_{10}$ -based fluxed melts saturated with 50 wt.% of borate crystalline substances ($\text{Re}_2\text{O}_3\text{:Al}_2\text{O}_3\text{:B}_2\text{O}_3=1\text{:}1\text{:}5\text{:}4$, in molar ratio) by cooling slowly ($0.5\text{-}2^\circ\text{C/h}$) in the temperature range $1100\text{-}800^\circ\text{C}$. Five years ago, lanthanum aluminium borate, $\text{LaAl}_{2.05}(\text{B}_4\text{O}_{10})_{0.54}$, was found to be isostructural with hexagonal $\text{NdAl}_{2.07}[\text{B}_4\text{O}_{10}]_{0.6}$. It was obtained by cooling slowly an initial melt of La_2O_3 and Al_2O_3 over B_2O_3 , with $\text{PbF}_2\text{-B}_2\text{O}_3$ as a flux, from 1050°C to room temperature.

Thus, at least, four synthetic rare earth aluminium metaborates are known to date:

(1) LaAl: $a = 4.594(3) \text{ \AA}$, $9.340(6) \text{ \AA}$, $D_{\text{meas}} = 3.95 \text{ g cm}^{-3}$, $n_o = 1.725(2)$

and $n_e = 1.740(2)$

(2) CeAl: $a = 4.593(7) \text{ \AA}$, $9.320(5) \text{ \AA}$, $D_{\text{meas}} = 4.02 \text{ g cm}^{-3}$, $n_o = 1.767(2)$

and $n_e = 1.788(2)$

(3) PrAl: $a = 4.583(1) \text{ \AA}$, $9.310(5) \text{ \AA}$, $n_o = 1.730(2)$ and $n_e = 1.745(2)$

(4) NdAl: $a = 4.583(1) \text{ \AA}$, $9.291(2) \text{ \AA}$, $D_{\text{meas}} = 3.96 \text{ g cm}^{-3}$, $n_o = 1.755(2)$ and $n_e = 1.765(2)$.

Since no new results were published relating to the pepprosiite-(Ce), its composition as well structure need to be re-examined.

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A12-17: Zn analogue of rancieite, a new mineral from the Dongnam mine, Korea

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A new mineral, the Zn analogue of rancieite, has been discovered at the Dongnam mine, Korea. It occurs as compact subparallel fine-grained flaky or acicular aggregates in the massive manganese oxide ores which were formed by supergene oxidation of rhodochrosite-sulfide ores in the hydrothermal veins trending NS-N25E and cutting the Pungchon limestone of Cambrian age. The flakes of the Zn analogue of rancieite are 0.2 mm for the largest one but usually <0.05 mm. The acicular crystals are elongated parallel to and flattened on (001). This mineral shows gradation to rancieite constituting its marginal part, thus both minerals are found in one and the same flake. The colour is bluish black, with dull lustre and brown streak in globular or massive aggregates. The cleavage is perfect in one direction. The hardness ranges from 2.5 to 4. Under reflected light it is anisotropic and birefractant. It shows reddish brown internal reflection. Chemical analyses using JEOL Superprobe 733 give MnO_2 70.08, MnO 0.00, CaO 0.86, MgO 0.78, Fe_2O_3 0.27, ZnO 12.87, K_2O 0.13, Na_2O 0.93, H_2O 14.08 for a total of 100.00 wt.%. Chemical analyses of different parts of both minerals suggest that rancieite and its Zn analogue constitute a continuous solid solution series. The empirical chemical formula for the Zn analogue of rancieite has been calculated following the general formula, $R_{2x}\text{Mn}^{4+}_{9-x}\text{O}_{18} \cdot n\text{H}_2\text{O}$ for the 7□ phyllosilicate minerals. x varies from 0.81 to 1.28 in so far studied samples, thus averaging to 1.0. Therefore, the formula is close to the stoichiometric formula $\text{RMn}^{4+}_4\text{O}_9 \cdot 4\text{H}_2\text{O}$ by Bardóssy and Brindley (1978). The Zn analogue of rancieite from the Dongnam mine has the formula $(\text{Zn}_{0.78}\text{Na}_{0.15}\text{Ca}_{0.08}\text{Mg}_{0.01}\text{K}_{0.01})(\text{Mn}^{4+}_{3.98}\text{Fe}^{3+}_{0.02}\text{Al}_{0.04}\text{O}_9 \cdot 3.85\text{H}_2\text{O})$, thus the ideal formula is $(\text{Zn,Ca})\text{Mn}^{4+}_4\text{O}_9 \cdot 3.85\text{H}_2\text{O}$. The mineral has a hexagonal unit cell with $a = 2.840 \text{ \AA}$, $c = 7.486 \text{ \AA}$ and $a:c = 1:2.636$. The X-ray diffraction lines are 7.480 (vs) (001), 3.740 (s) (002), 2.45 (m) (100), 2.34 (m) (101), 2.06 (vw) (102), 1.76 (vw) (103), 1.42 (m) (110). The DTA curve shows endothermic peaks at 65, 180, 690 and 1020°C . The IR absorption spectrum shows absorption bands at 445, 500, 1630 and 3400 cm^{-1} .

A12-18: New chapter in the mineralogy and crystal chemistry of the eudialyte group

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The term *eudialyte*, which was introduced about 200 years ago to refer to a mineral species identified in Greenland, has in recent years been elevated to a higher rank to cover the entire rapidly expanding group of zircono- and titanosilicates of symmetries R3m, R3m, and R3 and of general formula $A(1)_3A(2)_3A(3)_3A(4)_3A(5)_3B_{3-6}CD[M_2Z_1[T_{23}O_{72}]](O,OH)_2 \cdot X_2$. Their basic structural array is an intricate framework (braces) whose cavities contain cations with valencies ranging from 1+ to 6+ (Na, K, Ca, Sr, Mn, Fe, REE, Si, Ti, Nb, W, etc.), additional anions (Cl, F, O, OH, SO_4 , CO_3), and water molecules. The mixed framework consists of (001) layers alternating along the c axis in the sequence (TZTM)(TZTM)... The layers are made up of mutually isolated $[\text{Si}_9\text{O}_{27}]$ and $[\text{Si}_3\text{O}_9]$ rings (T), discrete Zr(Ti) octahedra (Z), and six-membered rings of Ca or more complex octahedra (M). This structural array is characterized by extremely extensive isomorphous substitutions in most extraframework and some intraframework sites, giving the eudialyte group a unique wealth of potential mineral species. The currently-known members of the group are dominated by species with relatively low-ordered structures, such as eudialyte (*sensu stricto*) or kentbrooksite, described by a hexagonal cell with $a = 14$, $c = 30 \text{ \AA}$. With the recent discoveries of "mega-eudialytes" in the Lovozero and Khibina alkaline massifs, a "second chapter" has been opened in the mineralogy and crystal chemistry of the eudialyte group. Such discoveries include alluaivite $\text{Na}_{36}(\text{Ca,Mn})_{12}(\text{Ti,Nb})_6\text{Si}_{52}\text{O}_{148}\text{Cl}_2 \cdot 4\text{H}_2\text{O}$ ($a = 14.05$, $c = 60.60 \text{ \AA}$) and several minerals submitted to the IMA-CNMMN of compositions

$\text{Na}_{30}(\text{Ca,Na,Ce,Sr})_{12}(\text{Na,Mn,Ti,Fe})_6\text{Zr}_3(\text{Ti,Nb})_3\text{MnSi}_{51}\text{O}_{144}(\text{OH,H}_2\text{O,Cl})_8$ ($a = 14.15$, $c = 60.72 \text{ \AA}$), $\text{Na}_{27}\text{K}_8\text{Ca}_{12}\text{Fe}_3\text{Zr}_6\text{Si}_{52}\text{O}_{144}(\text{O,OH,H}_2\text{O})_6\text{Cl}_2$ ($a = 14.25$, $c = 60.97 \text{ \AA}$), and $(\text{Na,K,Sr})_{35}\text{Ca}_{12}\text{Fe}_3\text{Zr}_6\text{Ti}_{51}\text{O}_{144}(\text{O,OH,H}_2\text{O})_9\text{Cl}_3$ ($a = 14.24$, $c = 60.73 \text{ \AA}$). These species differ from the "first chapter" eudialytes in having more highly ordered structures and, as a consequence, a double c parameter. They have a different sequence of the structural layers: [(TZTM)(T'Z'T'M')] [(TZTM)(T'Z'T'M')]..., imparting a modular character to the structural array. There is a close correlation between the degree of structural ordering of the eudialyte-group minerals and the degree of alkalinity of their host rocks: eudialytes of low and high ordering are characteristic, respectively, of moderately and highly alkaline apatitic rocks. This, considered with the widespread occurrence of eudialytes in genetically different apatitic

complexes, makes them important indicators of the type of association of alkaline rocks and the conditions of their formation.

A12-19: Kimzeyite from aposkarn rodingites, Wiluy River, Republic Sakha -Yakutia (Russia)

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Zirconian schorlomite and kimzeyite garnets described in the geological literature are usually associated with rocks of the ultrabasic-alkaline complexes (carbonatite) or with basic magmatic rocks. Minerals of the kimzeyite-schorlomite series occur in aposkarn metarodingites in the Wiluy deposit of achtarandite, grossular and wiluite on the Wiluy River, Republic Sakha-Yakutia. The metarodingites of the deposit comprise unusually stratified rodingites that are part of a metasomatically-altered, volcano-sedimentary rock mass belonging to the Tungus Series, the formation of which was connected with the formation of Siberian trapps.

Garnets form metacrystals in rodingite-like, fine-grained rock consisting of tabular pseudomorphs of vesuvianite and hydrogarnet after melilite. The spaces between the pseudomorphs is filled by serpentine and chlorite. Relict metacrystals related to an early skarn stage are represented by wiluite, garnet and high-Al diopside. Perovskite and apatite occur as accessory minerals.

Garnets of the schorlomite ($\text{Ca}_3\text{Ti}_2\text{R}^{3+}_2\text{SiO}_{12}$)-kimzeyite ($\text{Ca}_3\text{Zr}_2\text{R}^{3+}_2\text{SiO}_{12}$) series are preserved as relicts in the central parts of an idiomorphic crystal of rhombododecahedron habit exhibiting complex zoning. The central part of the crystal is composed of Zr-schorlomite-morimotoite. Zr and Ti contents are constant with variation ranging from 0.48 to 0.52 a.p.f.u. and from 0.72 to 0.83 a.p.f.u. respectively. A reaction zone with increased Zr content varying from 0.78 to 0.82 a.p.f.u. (often $\text{Zr} > \text{Ti}$) follows. This zone is succeeded in turn by a homogeneous zone comprising Zr-bearing, Ti-andradite. The last zone overgrowing the metacrystal is composed of grossular with a proportion of the andradite molecule.

Most of the fine-grained, Zr-containing garnets are characterised by a different type of zoning. The composition of these garnets changes from kimzeyite (with a Zr content ranging up to 0.83 a.p.f.u.) - Zr-schorlomite in the centre through Zr-containing Ti-andradite to Fe-grossular in the marginal zone. The high concentration of divalent elements in these garnets indicates a significant presence of morimotoite ($\text{Ca}_3\text{Ti}^{4+}\text{R}^{2+}_2\text{Si}_3\text{O}_{12}$) and Zr-morimotoite ($\text{Ca}_3\text{Zr}^{4+}\text{R}^{2+}_2\text{Si}_3\text{O}_{12}$).

The discovery of schorlomite-kimzeyite series garnets in what are unusual aposkarn rodingites is unique. Firstly, the garnet described is a new genetic type of kimzeyite-Zr-schorlomite series garnet. Secondly, garnets are the main reservoir of Zr and Ti in rocks of this type. Thirdly, garnets with such a high content of ZrO_2 (19.02 wt.%) have not previously been described from Russia.

A12-20: Shirokshinite, $\text{K}(\text{NaMg}_2)\text{Si}_4\text{O}_{10}\text{F}_2$: first mica with octahedral Na (Kola Peninsula, Russia).

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Shirokshinite is a late mineral found within an alkaline pegmatite of the Kirovskii Mine (Kukisvumchorr Mt., Khibiny massif). The new species has been approved by the IMA. Minerals associated to shirokshinite are: microcline, kupletskite, aegirine, galena, natrolite, lorenzenite, calcite, remondite-(Ce), donnayite-(Y), mckelveyite-(Y). Colourless, biaxial (-), α 1.526(1), β 1.553(2), γ 1.553(2); chemical composition: $\text{K}_{0.90}(\text{Na}_{0.94}\text{Mg}_{1.97}\text{Fe}_{0.09}\text{Mn}_{0.01}\text{Ti}_{0.01})_{\Sigma 3.02}(\text{Si}_{3.98}\text{Al}_{0.02})_{\Sigma 4.00}\text{O}_{9.995}\text{F}_{2.01}$. From single-crystal X-ray diffractometry a 5.269(2), b 9.092(11), c 10.198(3) Å, β 100.12(7)°, $C2/m$ have been obtained.

The crystal structure of shirokshinite has been refined to R 0.13 for 715 observed reflections. In spite of a high R value (due to poor crystallinity), the refined number of electrons (e_{ref}) shows that the octahedral sites M cannot contain cations lighter than Na. The dimension of the site M1, larger than that of M2, and e_{ref} show that these two sites are occupied by Na and Mg, respectively. Thus, the ratio Na/Mg found by chemical analysis is confirmed by the structure refinement

IR spectroscopy played an important role in the characterization of the new mica. The IR spectrum of shirokshinite is unique but similar to that of tainiolite: the presence of the heavier Na⁺ instead of Li⁺ causes up to 40 cm⁻¹ shifts of some bands towards low frequencies.

It was reported an indirect evidence for octahedral Na in micas, but shirokshinite is the first reported mica with Na dominant in an octahedral site. Both octahedral and interlayer Na is instead quite common in the layer titanosilicates; the structure of these minerals is based on mica-like layers where rows of Si-tetrahedra are replaced by rows of 6(or 5)-co-ordinated Ti.

After the recent first description of a 2O mica polytype, the Khibiny massif becomes the type locality for two micas.

A12-21: Roedderite(?) from the Nagy Hill, Tarpa, NE Hungary: a problem with the classification based on electron microprobe analyses in the roedderite-merrihueite subgroup of the milarite group

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The Nagy Hill is an outcrop of a large early Sarmatian dacite body. Roedderite occurs at the contact of dacite and agglomerate, where it can be found on the joint surfaces and in the fissures of dacite as well as in agglomerate together with epidote. Roedderite forms greyish blue and blue, hexagonal, short prismatic crystals up to 1.5 mm, with forms {0001}, {1010}, {1120}, {2130}, {1012} and {1122}.

In the literature the chemical formula of roedderite is written as $(\text{Na}, \text{K})_2(\text{Mg}, \text{Fe})_3\text{Si}_{12}\text{O}_{30}$, while the formula of merrihueite is $(\text{K}, \text{Na})_2(\text{Fe}, \text{Mg})_3\text{Si}_{12}\text{O}_{30}$. The line is drawn at $\text{Fe}/(\text{Fe} + \text{Mg}) = 0.5$ between roedderite and merrihueite. The mineral is roedderite, if the above value is <0.5, but it is merrihueite, if >0.5. However, this approach is incorrect because the general structural formula of the minerals of the milarite group is $^{61}\text{A}_2^{62}\text{B}_3^{112}\text{C}^{118}\text{D}^{14}\text{T}(2)_3^{64}\text{T}(1)_{12}\text{O}_{30}$, so the formula of roedderite end-member should be written as $^{\text{B}}\text{Na}^{\text{C}}\text{K}^{\text{A}}\text{Mg}_2^{\text{D}}\text{Mg}_3^{\text{T}(2)}\text{Si}_{12}\text{O}_{30}$. Similarly, the formula of merrihueite end-member is $\text{NaKFe}_2\text{Fe}_3\text{Si}_{12}\text{O}_{30}$. Thus there are two unnamed, theoretical end-members of the roedderite-merrihueite subgroup, namely UN1 with composition $\text{NaKFe}_2\text{Mg}_3\text{Si}_{12}\text{O}_{30}$, and UN2, $\text{NaKMg}_3\text{Fe}_3\text{Si}_{12}\text{O}_{30}$.

Based on electron microprobe analyses the composition of Tarpa roedderite is the following: $(\text{K}_{0.94}\text{Na}_{0.74})_{\Sigma=1.68}(\text{Mg}_{3.69}\text{Fe}_{1.24}\text{Mn}_{0.09}\text{Al}_{0.07})_{\Sigma=5.09}\text{Si}_{12.02}\text{O}_{30}$. Because both of Mg and Fe can occupy the A and T(2) sites, we can not give the structural formula of Tarpa mineral. If the total iron goes to the T(2) sites, then the Tarpa mineral is roedderite, but if the total iron occupies the A sites, then our mineral represents the UN1 species. Merely based on electron microprobe analyses it is impossible to determine the distribution of Mg and Fe between A and T(2) sites.

A12-22: Duhamelite discredited

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Reinvestigation of duhamelite, originally described as $\text{Cu}_4\text{Pb}_2\text{Bi}(\text{VO}_4)_4(\text{OH})_3 \cdot 8\text{H}_2\text{O}$, has demonstrated that it is not a valid independent mineral species. Analyses of the type material and of additional samples by means of electron microprobe, X-ray powder and single-crystal diffractometry including structure refinements, and transmission electron microscopy have shown that duhamelite belongs to the adelite-desclowitzite-group, $\text{M1M2}(\text{XO}_4)(\text{OH})$ and corresponds to a bismuth- and calcium-bearing mottramite, $[\text{PbCu}(\text{VO}_4)(\text{OH})]$. The chemical formula is $(\text{Pb}, \text{Bi}, \text{Ca})\text{Cu}(\text{VO}_4)(\text{OH}, \text{O})$. Bi³⁺ is an essential component; however, Pb²⁺ dominates over Bi³⁺ with a strong variation in the Pb:Bi ratio. All duhamelite samples contain small but distinct Ca²⁺ contents; some also contain minor amounts of As⁵⁺ and Si⁴⁺.

The exchange mechanisms are: $[(\text{Pb,Ca})^{2+} + \text{OH}]^+ \leftrightarrow [\text{Bi}^{3+} + \text{O}^{2-}]^+$ and $[(\text{VO}_4, \text{AsO}_4)^{3-} + \text{O}^{2-}]^+ \leftrightarrow [(\text{SiO}_4)^+ + \text{OH}]^{2-}$; consequently, a coupled substitution $[(\text{Pb,Ca})^{2+} + (\text{VO}_4, \text{AsO}_4)^{3-} + \text{OH}]^+ \leftrightarrow [\text{Bi}^{3+} + (\text{SiO}_4)^+ + \text{OH}]^{2-}$ makes it possible to maintain the number of OH⁻ groups. A further exchange mechanism is $(\text{VO}_4, \text{AsO}_4)^{3-} \leftrightarrow (\text{SiO}_3\text{OH})^{2-}$ or, in an extended form, $[\text{Pb}^{2+} + (\text{VO}_4, \text{AsO}_4)^{3-} + (\text{OH})^{1-}]^+ \leftrightarrow [\text{Bi}^{3+} + (\text{SiO}_3\text{OH})^{2-} + \text{O}^{2-}]^+$. The extended chemical formula is $\text{M1M2}[\text{X}(\text{O}_4, \text{O}_3\text{OH})](\text{OH}, \text{O}, \square)$.

Although the crystal structures of the Ca and Pb end-members are isostructural, their distinct space-group symmetries are $P2_12_12_1$ and $Pnam$, respectively. The structural change goes along with a change in the co-ordination number of the M1 atom: In space group $Pnam$ M1O₇ is a mono-capped trigonal prism, whereas M1O₈ in space group $P2_12_12_1$ is a square antiprism. The crystal-chemical role of the Bi³⁺ cations and the parallel substitution of (OH)⁻ groups by O²⁻ atoms as well as their influences on the crystal structure is discussed: lone-electron pairs which are usually stereochemically active are expected for M1 = Bi³⁺ atoms. X-ray film investigations show a splitting of the reflections along the *b** direction: two reciprocal lattices exhibit a superposition; they correspond with each other in the *a** and *c** directions (at least they are not resolvable) but exhibit a deviation with respect to [010] by ~15%. All investigations of bismuthian-calcian mottramite showed a superposition of two commensurate lattices.

A12-23: Systematics of the uranyl silicate minerals and their names

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The uranyl silicates are the most common uranyl minerals. There are no fewer than three groups of uranyl silicates according to U:Si ratios in the minerals. (1) The group with U:Si = 1:1 – uranophane $\text{Ca}(\text{H}_3\text{O})_2(\text{UO}_2)_2(\text{SiO}_4)_2 \cdot 3\text{H}_2\text{O}$, β-uranophane $\text{Ca}(\text{UO}_2)(\text{UOOH})(\text{SiO}_4)(\text{SiO}_3\text{OH}) \cdot 5\text{H}_2\text{O}$, boltwoodite $\text{K}(\text{H}_3\text{O})(\text{UO}_2)(\text{SiO}_4) \cdot 2.5\text{H}_2\text{O}$, Na boltwoodite $(\text{Na}_{0.7}\text{K}_{0.3})(\text{H}_3\text{O})(\text{UO}_2)(\text{SiO}_4) \cdot 2.5\text{H}_2\text{O}$, kasolite $\text{Pb}(\text{UO}_2)(\text{SiO}_4) \cdot \text{H}_2\text{O}$, sklodowskite $\text{Mg}(\text{H}_3\text{O})_2(\text{UO}_2)_2(\text{SiO}_4)_2 \cdot 3\text{H}_2\text{O}$, cuprosklodowskite $\text{Cu}(\text{UO}_2)_2(\text{SiO}_3\text{OH})_2 \cdot 5\text{H}_2\text{O}$, oursinite (Co,Mg) $(\text{UO}_2)_2 \text{Si}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$. (2) The group with U:Si > 1:1 – soddyite $(\text{UO}_2)_2(\text{SiO}_4) \cdot 2\text{H}_2\text{O}$ and swamboite $\text{U}^6\text{H}_6(\text{UO}_2)_6(\text{SiO}_4)_6 \cdot 30\text{H}_2\text{O}$. (3) These are the uranyl silicates with U:Si = 1:2.5; 1:2.55; 1:3 and 1:3. (A) U:Si=1:2.5 – calcium ursilite $\text{Ca}_4(\text{UO}_2)_4(\text{Si}_2\text{O}_5)_5(\text{OH})_6 \cdot 15\text{H}_2\text{O}$, magnesium ursilite $\text{Mg}_4(\text{UO}_2)_4(\text{Si}_2\text{O}_5)_5(\text{OH})_6 \cdot 15\text{H}_2\text{O}$, ranquillite $\text{Ca}_3(\text{UO}_2)_4(\text{Si}_2\text{O}_5)_5(\text{OH})_4 \cdot 22\text{H}_2\text{O}$, pseudo-weeksite $(\text{K}_{0.62}\text{Na}_{0.38})_2(\text{UO}_2)_2(\text{Si}_5\text{O}_{13}) \cdot 3\text{H}_2\text{O}$ and pseudo-haiweeite $\text{Ca}(\text{UO}_2)_2(\text{Si}_5\text{O}_{12})(\text{OH})_2 \cdot 4\text{H}_2\text{O}$, Al-containing calcium ursilite $\text{Ca}_3(\text{AlH}_3\text{O})_{0.5}(\text{UO}_2)_4(\text{Si}_2\text{O}_5)_5(\text{OH})_6 \cdot 15\text{H}_2\text{O}$. There is a some similarity between ranquillite and Al-containing calcium ursilite. (B) U:Si=1:2.55 – ursilite (Mg,Ca,Na,K)₄(UO₂)₄(Si₂O₅)₅(OH)₅·11H₂O, there is a some similarity between ursilite and gastunite (K,Na)₂(UO₂)₄(Si₂O₅)₅·8H₂O. (C) U:Si=1:3 – weeksite $\text{K}_2(\text{UO}_2)_2(\text{Si}_2\text{O}_5)_3 \cdot 4\text{H}_2\text{O}$, haiweeite $\text{Ca}(\text{UO}_2)_2(\text{Si}_2\text{O}_5)_3 \cdot 5\text{H}_2\text{O}$; synthetic Ba-weeksite $\text{Ba}(\text{UO}_2)_2(\text{Si}_2\text{O}_5)_3 \cdot \text{H}_2\text{O}$, where n = 2–13. (D) U:Si = 1:3 – uranosilite $\text{U}^{6+}\text{Si}_7\text{O}_{17}$.

The description of the distribution, properties, and cell constants of these minerals have been reported. Fleischer described ursilite, calcium ursilite and magnesium ursilite, but these minerals are not listed in the *Glossary of Mineral Species*. I propose to CNMNM of IMA to approve of these names as well as pseudo-weeksite and pseudo-haiweeite.

A12-24: Mcguinnessite [(Mg, Cu)₂CO₃(OH)₂] in chromitite xenoliths from Onverwacht, Eastern Bushveld Complex, South Africa.

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Mcguinnessite [(Mg, Cu)₂CO₃(OH)₂] is a member of the rosasite group carbonates found in few localities as secondary mineral phase in different rock-matrix such as gabbros, serpentinites, and massive dolomite. The reported chemical formulae show a relatively wide range of Mg/Cu ratio (mostly Mg > Cu) and trace amounts of Co, Ni, Zn, and Fe. Mcguinnessite crystal structure is unknown and unambiguous data about crystal structure of rosasite group minerals, except for malachite, are scarce. Mcguinnessite is considered (though with some reservations) as monoclinic with space group $P2_1/a$.

We have found mcguinnessite in a small chromitite xenolith sampled at Onverwacht, in the eastern part of the Bushveld Complex. The sample consists of amoeboid patches of chromite grains spotted with drop-like inclusions of clinopyroxene, amphibole and Na-rich phlogopite and partially rimmed and replaced by magnetite; gangue minerals are mainly serpentine, chlorites, Mg-Fe hydrous silicates and Fe hydroxides. Cu-bearing phases, suggestive of the original presence of sulfides, are scattered in the matrix. Mcguinnessite has been identified together with chrysocolla in a thin vein crosscutting the chromitite xenolith.

The veining can be related to that observed near the top of the pipe where reactions with acid ground-water produce magnesite and chrysocolla. Possibly minor sulphide in the rock becomes involved in this process and precipitates the mcguinnessite.

Mcguinnessite occurs in bluish green radial aggregates of elongated platy crystals (up to 150 μm long), together with chrysocolla. The X-ray powder pattern well agrees with those reported for the holotype from Red Mountain (California). However the reported weak peaks at *d* = 11.98 Å and *d* = 9.39 Å have not been observed. No crystal suitable for single-crystal X-ray analysis has been found. The X-ray powder diffraction pattern indexed in the same space group $P2_1/a$ of malachite, gives cell parameters in good agreement with those from Red Mountain. Following the hypothesis that mcguinnessite and malachite could be isostructural, calculated powder patterns for disordered and ordered distribution of Mg and Cu in the Cu-sites of the malachite structure indicate a possible preferred Mg-ordering in the Cu(2) malachite position for the mcguinnessite structure. EPMA and preliminary TEM-AEM analyses together with X-ray elemental maps show only Mg and Cu in significant amounts; Fe has been detected in subordinate amounts. The presence of Si has been observed as a consequence of the intimate intergrowth together with chrysocolla. The relation Mg > Cu previously observed in the other reported occurrences, seems to be confirmed.

A12-25: Microlite-subgroup minerals from Conceição do Mato Dentro and São João del Rei, Minas Gerais, Brazil.

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The type locality of uranmicrolite (originally “djalmaite”) is Posse farm (São José mine), 1 km from Brejaúba town, Conceição do Mato Dentro county, Minas Gerais, Brazil. This is also the type locality for dukeite. A second occurrence of “djalmaite” was described in the Volta Grande and Germinal pegmatites, in the area of São João del Rei, Minas Gerais, Brazil. The name “djalmaite” was officially discarded in favour of uranmicrolite, a name introduced to conform to the new nomenclature system for pyrochlore group minerals, approved by CNMNM – IMA. The new definition requires that uranmicrolite must contain U exceeding 20% of the total A-atoms. According to the original chemical analyses, the samples from São João del Rei are uranian microlite because U does not exceed 20% of the total A-atoms. The data on the ICDD 43-693 card (uranmicrolite) are actually for uranian microlite and the locality is also incorrect, because the sample is not from Posse farm, but from Germinal (Volta Redonda, Mortes river), Nazareno district, São João del Rei county, Minas Gerais. Only the original “djalmaite” specimen conforms to the uranmicrolite definition. However the original data were obtained from wet analyses and represent a mean of several compositions observed within an individual octahedra. Internal constitution of crystals is commonly heterogeneous. Complex zoning, or veining with diffuse boundaries, are rather common features. New material from both Conceição do Mato Dentro and São João del Rei was studied by X-ray powder diffraction and EDS. In terms of mineral species, microlite (Ca-dominant), plumbomicrolite and uranmicrolite were identified in Conceição do Mato Dentro samples. A transitional species qualifies for the status of both plumbomicrolite and uranmicrolite, with virtually equal atomic contents of Pb and U. The species observed in São João del Rei octahedra are microlite (Ca-