-01

iving names is not as easy as one thinks (J.W. von Goethe, 1807)

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The Commission on New Minerals and Mineral Names (CNMMN) of the International Mineralogical Association (IMA) was established in 1959 for the purpose of controlling and reviewing all proposed changes in nomenclature (new names, discreditations, changes in definitions) and of rationalising mineral nomenclature (international uniformity as far as may be practicable). The CNMMN has meanwhile taken a decision on more than 4000 minerals and mineral names, has brought order in many mineral groups (*e.g.*, micas, amphiboles, pyroxenes, zeolites, labuntsovites, eudialytes, sulphosalts, epidotes, tourmalines), and has formulated general principles (definition of a mineral, nomenclature of solid solutions, polytypes and synthetic substances).

From the classical period until today, there have been two problems in mineralogical nomenclature: what are proper names for minerals, and how should they be composed. From the start there has been a dichotomy in rational and irrational nomenclatures (in Greek-Roman times, *e.g.*, hematite and galena vs. nephrite and amethyst, nowadays, *e.g.*, arcubisite and phyllotungstite vs. mandarinoite and griceite).

Abraham Gottlob Werner was the first (at the end of the 18th century) to formulate clear guidelines for a rational naming of minerals, but he was also the first to disobey them by giving names after persons (prehnite, vivianite) and localities (vesuvianite, aragonite). From Werner until the formation of the CNMMN in 1959 there has been no control on mineralogical nomenclature, and the current CNMMN guidelines (most recent version: 1998) for naming minerals reflect the established historical diversity that grew during that period. A radical change of the nomenclature (as proposed, *e.g.*, by Povarennykh in the 1960-70s) would thus not only be undesirable, it certainly would be impracticable. Mineralogy will thus have to live with inconsiderate names (*e.g.*, bakhchisaraitsevite, pääkkönenite, uchacchacuaite, vandendriesscheite, zhemchuzhnikovite) and with 'double names' so despised by many (*e.g.*, henritermierite, theresemagnanite, thomasclarkite, jacquesdietrichite).

But the CNMMN should/could do something about schemes which lead to such improbabilities as sodic-ferri-clinoferroholmquistite, and to easily corrected inconsistencies in prefixes (sodicgedrite *vs.* natrotantite; alumotungstite *vs.* aluminoceladonite; arsendescloizite vs. arsenogoyazite *vs.* arseniosiderite), of two-word names (cobalt pentlandite, potassium alum, sodium boltwoordite), and of unnecessary hyphens (nickel-zippeite *vs.* nickelbischofite; hydroxyl-herderite *vs.* hydroxylellestadite). The use of prefixes in names (as desired by the CNMMN guidelines) for new minerals simply related to existing ones creates serious identification problems without chemical analyses, *e.g.*, the division of apatite into hydroxylapatite, fluorapatite and chlorapatite. Such problems have been avoided by using suffixes in groups like zeolites, labuntsovites, arrojadites and epidotes.

O31-02

Alkali and hydrous sulfide minerals: classification and genetic aspect of crystal chemistry

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Sixteen sulfide minerals containing species-forming K, Na, Cs or/and H_2O molecules are known: nine anhydrous alkali sulfides (djerfisherite, bartonite, chlorbartonite, galkhaite, rasvumite, pautovite, murunskite, chvilevaite, caswellsilverite), four sodium-hydrous sulfides (erdite, coyoteite, gerstleyite, schöllhornite) and three sulfides containing only H_2O but no alkali metals in their idealized formulae (orickite, wilhelmramsayite, cronusite). In fact, the latters also contain significant admixtures (0.*n* wt.%) of K or/and Na. Thus, alkali-free hydrous sulfides are unknown in nature for sure. Alkali and hydrous sulfide minerals are related also crystallochemically and genetically. The most important crystallochemical feature of alkali sulfides is arrangement of alkali atoms in structures. These minerals can be classified to three topological types using this sign: zero-dimensional (alkali atoms are isolated, *e.g.* djerfisherite, bartonites, galkhaite), unidimensional (alkali atoms form chains in tunnels, *e.g.* rasvumite, pautovite, erdite), and two-dimensional (alkali atoms form layers, *e.g.* murunskite, chvilevaite, caswellsilverite). The type determines properties: ability of leaching and exchange of alkali, conductivity character *etc.* All these sulfides are microporous minerals (Makovicky, 2005). Crystallochemical roles of larger K, Cs, Rb (and Tl) and smaller Na in sulfides are essentialy different. Anhydrous sulfide minerals show strong affinity to larger alkali atoms while hydrous sulfides "prefer" Na. Recent discoveries of sulfides extremely enriched by Cs and Rb, especially pautovite, $CsFe_2S_3$, demonstrate earlier-unknown feature of geochemistry of these elements in peralkaline formation. Strong fractionation of K, (Cs+Rb) and Tl between simultaneously crystallized alkali sulfides of different topological types takes place. In the Palitra peralkaline pegmatite in Lovozero complex, Kola, Russia, chlorbartonite contains 9.5 wt.% K and 0.2% Tl; pautovite: 36.1% Cs, 1.3% Rb, 0.5% Tl and 0.2% K; murunskite: 24.7% Tl and 7.4% K. Layered sulfides can loose alkali atoms with their substitution by H_2O molecules. An example is the evolution chain: caswellsilverite, $NaCrS_2$ → (Na leaching, hydration) schöllhornite, $Na_{0.3}CrS_2 \cdot H_2O$ → (cation exchange, hydration) cronusite, $Ca_{0.2}CrS_2 \cdot 2H_2O$ (Britvin *et al.*, 2001). It seems that hydrous sulfide minerals were formed mainly (only?) as a result of alteration of their alkali proto-phases. From this viewpoint, presence of alkali in all hydrous sulfides and occurrence of hydrous sulfides mainly in peralkaline assemblages become well-explainable. Galkhaite, $(Cs,Tl)_{<1}(Hg,Cu)_6(As,Sb)_4S_{12}$, is only cesium mineral in some ore deposits, sporadically major constituent of mercury ores. Because of its unique "broad-porous" structure galkhaite fixes mobile Cs and becomes principal geochemical indicator showing high activity of this element in the process of formation of mercury and gold deposits including very important Carlin-type objects.

O31-03

Crystal chemistry of the vicanite group

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A new mineral species from the Hundholmen granitic pegmatite, north Norway, can be added to the vicanite group, comprising okanoganite-(Y) and vicanite-(Ce). The chemical and structural data on the new mineral have significantly added to the understanding of the crystal-chemical properties of these rare minerals. There are three distinct layers parallel to (001) in the structures of these minerals (space group *R*3*m*):

- Layer A contains an octahedron with (Al,Fe^{3+},Ti) as the central atoms, sharing corners with six SiO_4 groups in the form of a pinwheel. $B(1)O_4$ tetrahedra form threefold rings, and each $B(1)O_4$ tetrahedron of the rings shares a corner with one SiO_4 tetrahedron, forming an $(Si_3B_3O_{18})^{15-}$ polyanion.
- Layer B contains a tetrahedron which may incorporate variable amounts of As^{5+}, P, Si (As1 site). This tetrahedron occurs in two orientations with the same probability of occurrence. In vicanite-(Ce), a $B(2)O_3$ triangle is also present in this layer.
- Layer C contains two very close polyhedra, of As^{3+} in three-coordination (As2 site) and (Na,Ca) in ten-coordination, which are mutually exclusive. The As2 site is empty in okanoganite-(Y).

A three-dimensional network of five different polyhedra with coordinations from eight to ten (M1 to M5) contains Y, REE, Th and Ca and provides connections among the three layers.

Okanoganite-(Y) [described in 1980, crystal structure published in 2004], has the simplified formula: $(Y,REE,Ca,Na,Th)_{15}(Fe^{3+},Ti)Na(P,Si)Si_6B_3(O,F,OH)_{48}$.

Vicanite-(Ce) [described in 1995, crystal structure published in 2002], has simplified formula: $(Ca,REE,Th)_{15}Fe^{3+}Na_xAs^{3+}_{1-x}(As^{5+},P)Si_6B_4(O,F)_{47}$ (x = 0.58).

The simplified formula of the new mineral species from Hundholmen (IMA 2006-005) is: $(Y,REE,Ca,Na)_{15}(Al,Fe^{3+})Ca_xAs^{3+}_{1-x}(Si,As^{5+})Si_6B_3(O,F)_{48}$ (x = 0.78).

Compared to the other two minerals, the Hundholmen mineral has $Al > Fe^{3+}$ at the Fe/Al site in layer A, has Si > As at the As1 site in layer B, and Ca > 0.5 at the Na site in layer C.

With 13 possible cation sites, the vicanite group might potentially comprise a large number of species, especially if the M1 to M5 sites are considered separately. For instance, vicanite-(Ce) has Th predominating at the M5 site. The correct distribution of Y, REE and Ca between the five M sites is not easily made on the basis of site-scattering values. Therefore, it might be wise to treat M1 to M5 as an entity for nomenclatural purposes.

O31-04

The wyllieite group of minerals: crystal chemistry, nomenclature and stability

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The wyllieite group of minerals consists of Na-Mn-Fe-Al-bearing phosphates which exhibit a crystal structure topologically similar to the alluaudite structure. However, the ordering of cations in the wyllieite structure induces a splitting of the M(2) and X(1) sites of alluaudite into the M(2a) M(2b) and X(1a) X(1b) positions. Consequently, the *C*2/*c* space group of alluaudite transforms into *P*2$_1$/*n* in wyllieite, with no significant change of the unit-cell parameters, and with a structural formula which corresponds to $X(2)X(1a)X(1b)M(1)M(2a)M(2b)(PO_4)_3$.

In granitic pegmatites, particularly in the beryl-columbite-phosphate subtype of the rare-element pegmatites, wyllieite-type phosphates display chemical compositions ranging from $Na_2(Mn,Fe^{2+})Fe^{2+}Al(PO_4)_3$ to $Na(Mn,Fe^{2+})Fe^{3+}Al(PO_4)_3$, with Ca^{2+} or Mn^{2+} replacing Na^+ on the X(2), X(1a) and X(1b) sites, Mg^{2+} replacing iron on the M(2a) site, and Mg^{2+} or Fe^{3+} replacing Al^{3+} on the M(2b) site, where represents a lattice vacancy. The name wyllieite corresponds to $Na_2MnFe^{2+}Al(PO_4)_3$, whereas the name rosemaryite designates the more oxidized compositions, such as $NaMnFe^{3+}Al(PO_4)_3$. The prefix ferro- is then added if Fe^{2+} dominates in the M(1) site, thus leading to ferrowyllieite, $Na_2Fe^{2+}_2Al(PO_4)_3$, and to ferrorosemaryite, $NaFe^{2+}Fe^{3+}Al(PO_4)_3$. The name qingheiite has been introduced for the Mg-rich equivalent of wyllieite, $Na_2MnMgAl(PO_4)_3$.

Single-crystal structure refinements of ferrorosemaryite from the Rubindi pegmatite, Rwanda (R_1 = 2.43 %, *a* = 11.838(1), *b* = 12.347(1), *c* = 6.2973(6) Å, *β* = 114.353(6)°), and of rosemaryite from the Buranga pegmatite, Rwanda (R_1 = 4.01 %, *a* = 12.001(2), *b* = 12.396(1), *c* = 6.329(1) Å, *β* = 114.48(1)°), indicate that Al is predominant on the M(2a) site, not on the M(2b) site as observed in ferrowyllieite. The morphologies of the X(1a) and X(1b) crystallographic sites correspond to a distorted octahedron and to a distorted cube, respectively. The [7+1]-coordinated X(2) site of rosemaryite is a very distorted gable disphenoid, similar to the A(2)' site of the alluaudite structure.

The infrared spectrum of rosemaryite shows absorption bands at 3450 and 1624 cm^{-1}, related to the vibrational modes of H_2O, and confirms the presence of molecular water in the channels of the wyllieite structure. A Mössbauer spectral investigation of rosemaryite and ferrorosemaryite also permits a comparison with the Mössbauer spectra of more disordered alluaudite-type phosphates.

Finally, the structural features of rosemaryite and ferrorosemaryite are compared to those of other natural and synthetic wyllieite-type phosphates, and the role played by Al to stabilize the wyllieite structure is discussed in detail.