

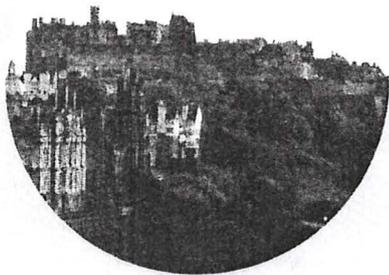
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Daniel Atencio - 2002

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The exchange mechanisms are:  $[(\text{Pb,Ca})^{2+} + \text{OH}]^+ \leftrightarrow [\text{Bi}^{3+} + \text{O}^{2-}]^+$  and  $[(\text{VO}_4\text{AsO}_4)^{3-} + \text{O}^{2-}]^{\pm} \leftrightarrow [(\text{SiO}_4)^+ + \text{OH}]^{\pm}$ ; consequently, a coupled substitution  $[(\text{Pb,Ca})^{2+} + (\text{VO}_4\text{AsO}_4)^{3-} + \text{OH}]^{\pm} \leftrightarrow [\text{Bi}^{3+} + (\text{SiO}_4)^+ + \text{OH}]^{\pm}$  makes it possible to maintain the number of OH<sup>-</sup> groups. A further exchange mechanism is  $(\text{VO}_4\text{AsO}_4)^{3-} \leftrightarrow (\text{SiO}_3\text{OH})^{3-}$  or, in an extended form,  $[\text{Pb}^{2+} + (\text{VO}_4\text{AsO}_4)^{3-} + (\text{OH})]^{2-} \leftrightarrow [\text{Bi}^{3+} + (\text{SiO}_3\text{OH})^{3-} + \text{O}^{2-}]^{2-}$ . 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  $Pnam$  M1O<sub>7</sub> is a mono-capped trigonal prism, whereas M1O<sub>8</sub> in space group  $P2_12_12_1$  is a square antiprism. The crystal-chemical role of the Bi<sup>3+</sup> cations and the parallel substitution of (OH)<sup>-</sup> groups by O<sup>2-</sup> atoms as well as their influences on the crystal structure is discussed: lone-electron pairs which are usually stereochemically active are expected for M1 = Bi<sup>3+</sup> 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)  $(\text{UO}_2)_2 \cdot \text{Si}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ . (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  $(\text{K}_{0.62}\text{Na}_{0.38})_2(\text{UO}_2)_2(\text{Si}_3\text{O}_{13}) \cdot 3\text{H}_2\text{O}$  and pseudo-haiweeite  $\text{Ca}(\text{UO}_2)_2[\text{Si}_3\text{O}_{12}(\text{OH})_2] \cdot 4\text{H}_2\text{O}$ , 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)<sub>4</sub>(UO<sub>2</sub>)<sub>4</sub>(Si<sub>2</sub>O<sub>5</sub>)<sub>5</sub>(OH)<sub>6</sub> · 11H<sub>2</sub>O, there is a some similarity between ursilite and gastunite (K,Na)<sub>2</sub>(UO<sub>2</sub>)<sub>4</sub>(Si<sub>2</sub>O<sub>5</sub>)<sub>5</sub> · 8H<sub>2</sub>O. (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  $\text{Ba}(\text{UO}_2)_2(\text{Si}_2\text{O}_5)_3 \cdot n\text{H}_2\text{O}$ , 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 CNMMN of IMA to approve of these names as well as pseudo-weeksite and pseudo-haiweeite.

### A12-24: Mcguinnessite [(Mg, Cu)<sub>2</sub>CO<sub>3</sub>(OH)<sub>2</sub>] in chromitite xenoliths from Onverwacht, Eastern Bushveld Complex, South Africa.

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Mcguinnessite [(Mg, Cu)<sub>2</sub>CO<sub>3</sub>(OH)<sub>2</sub>] 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  $d = 11.98 \text{ \AA}$  and  $d = 9.39 \text{ \AA}$  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 CNMMN – 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-

dominant), barionomicrolite, stannomicrolite, uranmicrolite and transitional species between stannomicrolite and uranmicrolite, and between barionomicrolite and stannomicrolite.

**A12-26: Tuperussuatsiaite from Poços de Caldas, Minas Gerais, Brazil**

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Tuperussuatsiaite has been reported and described as occurrences in veins or cavities in the Ilmaussaq alkaline intrusion in South Greenland, in the Aris phonolite in Namibia and in the Mont Saint-Hilaire and Saint Amable sill, in Canada. The Brazilian tuperussuatsiaite comes from an abandoned tinguaita quarry (Bortolan) in Poços de Caldas, State of Minas Gerais.

Small amounts of the mineral were collected as finely fibrous tufts, 1–3mm long needles or fan-shaped aggregates filling spaces between well formed crystals of Na-K-feldspar, sodalite, natrolite, aegirine and hainite, that project from the walls of miarolitic cavities. They are also associated with rare long needles of a still unidentified mineral, presently under study.

The mineral is monoclinic, space group  $C2/m$ . The 7 strongest X-ray powder diffraction lines are  $[d$  in Å  $(I/I_0)(hkl)$ ]: 10.96(100)(110), 5.433(3)(130), 4.490(3)(040), 3.736(3)(240), 2.641(1)(150), 2.313(4)(22-2), 2.263(3)(13-2).

Analysis by electron microprobe, on average of seven points, wt.%: SiO<sub>2</sub> 52.49 (45.00–58.60), Al<sub>2</sub>O<sub>3</sub> 0.30 (0.20–0.48), Fe<sub>2</sub>O<sub>3</sub> 25.10 (23.03–27.20), MnO 0.41 (0.35–0.51), MgO 0.15 (0.13–0.19), ZnO 0.20 (0.12–0.29), CaO 0.13 (0.10–0.19), Na<sub>2</sub>O 4.37 (2.54–5.66), K<sub>2</sub>O 0.73 (0.55–0.94), H<sub>2</sub>O 16.12 (Fe<sub>T</sub> as Fe<sub>2</sub>O<sub>3</sub>, H<sub>2</sub>O by difference): total 100%. The standards used were: Si, Mg, Mn, Fe: Mn-hortonolite; Al, Ca: anorthite; Ti: rutile; Zn: smithsonite; Na: albite; K: microcline. FeO, Fe<sub>2</sub>O<sub>3</sub> and H<sub>2</sub>O may be discriminated further by the gathering and analysis of larger sample amounts.

The empirical formula based on Si + Al = 8.00, is:

(Na<sub>1.28</sub> K<sub>0.14</sub> Ca<sub>0.02</sub>)<sub>Σ</sub> 1.44 (Fe<sup>3+</sup><sub>2.86</sub> Mn<sup>2+</sup><sub>0.05</sub> Mg<sub>0.03</sub> Zn<sub>0.02</sub>)<sub>Σ</sub> 2.96 (Si<sub>7.95</sub> Al<sub>0.05</sub>)<sub>Σ</sub> 8.00 O<sub>20</sub>(OH)<sub>2.19</sub>. 7.06 H<sub>2</sub>O. The suggested ideal formula is: Na Fe<sup>3+</sup><sub>3</sub> Si<sub>8</sub>O<sub>20</sub> (OH)<sub>2</sub>. 7 H<sub>2</sub>O

Needles measure at most 3x0.003 mm, a size exceedingly small for precise optical determinations. Two samples from two different miarolitic cavities furnished the data:

Cavity 1	Cavity 2		
Biaxial (+)	2V =	large	large
$\alpha \perp c$	= 1.556 (5) 1.548 (5)	pleocr.: colourless	
$\beta \perp c$	= 1.565 (5) 1.560 (5)	pleocr.: light green	
$\gamma \parallel c$	= 1.662 (3) 1.648 (3)	pleocr.: red brown	
$\gamma - \alpha$	= 0.106	0.100	

**A12-27: Stoichiometry-based estimates of ferric iron in calcic, sodic-calcic and sodic amphiboles: A comparison of various methods**

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One of the most notable drawbacks of the electron microprobe is its inability to quantify the different valence states of elements – particularly iron – in routine work. Although ferric/ferrous iron ratios are usually calculated considering electroneutrality and perfect stoichiometry, in the case of amphiboles, there is no unique criterion that can be applied to all compositions.

Using a dataset of 554 analysis of calcic, sodic-calcic and sodic amphiboles from A-type granites and syenites from southern Brazil, we assess the choices made by the method of Schumacher (1997, *The Canadian Mineralogist*, 35, 219–246), which uses the mean between selected maximum and minimum estimates. The maximum estimates selected with higher frequency are: 13 cations excluding Ca, Na and K (13eCNK – 66%); sum of Si and Al equal to 8 (8SiAl – 17%); and 15 cations

excluding K (15eK – 8%). These selections may be considered appropriate based on crystallographic considerations. The minimum estimates are mostly all iron as Fe<sup>2+</sup> (all Fe2 – 71%), which are too unrealistic for these amphiboles. Hence, the maximum estimates should better approximate the actual values.

To test this hypothesis, three datasets of calcic, sodic-calcic and sodic amphiboles were selected from the literature and the calculated values are compared to those independently measured. In general, 13eCNK and the maximum estimates of the method of Schumacher (mainly 13eCNK but also 8SiAl and 15eK) are satisfactorily precise and accurate (concordance correlation coefficient –  $r_c$  = 0.83 and 0.85, respectively). Since the actual values are much closer to the maximum estimates than to the minimum ones, the averages between them yield poor estimates ( $r_c$  = 0.56).

Thus, it is recommended that, for calcic, sodic-calcic and sodic amphiboles, the maximum estimates of the method of Schumacher (1997) be used instead of the average ones.

Although ferric iron is underestimated when the oxy-amphibole component is present, the overall cationic distribution is correctly calculated. A correction procedure is conceived, but should be applied with caution.

**A12-28: Catalanoite, Na<sub>2</sub>H[PO<sub>4</sub>].8H<sub>2</sub>O, a new evaporite mineral from Santa Maria alkaline lagoon, Los Andes department, Salta province, Argentina.**

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Catalanoite, Na<sub>2</sub>H[PO<sub>4</sub>].8H<sub>2</sub>O – *lbca*, has been found at Santa Maria, a saline environment of white trona strata, about 5 km east of the Chile-Argentina border, in the Andcan Puna, Los Andes department, Salta province, Argentina (Lat. 24° 06' S, Long. 67° 23' W). In the lacustrine salt deposit of Santa Maria lagoon, 1,500 m long, 400 m wide and 4575 m above sea level, the associated minerals are major trona, with gaylussite, catalanoite and minor halite. Catalanoite origin is primarily from this desert playa lake, where the evaporate minerals are formed. Catalanoite crystal size ranges from less than 50 micrometers up to half a millimeter across. It is transparent and colourless, with vitreous to resinous luster, and no fluorescent under long or short-wave ultraviolet light. It has white streak, no cleavage or visible twinning, uneven fracture, and fragile tenacity. Hardness Mohs' 2. Density<sub>calc.</sub> 1.728 g/cm<sup>3</sup>. Orthorhombic symmetry *mmm*, *lbca* space group, with  $a = 11.4886(15)$ ,  $b = 11.6467(17)$ ,  $c = 16.4351(18)$  Å.  $Z = 8$ ,  $V = 2199.082(2)$  Å<sup>3</sup>. Cell parameters are refined from powder diffraction data. The  $a:b:c = 0.9863:1:1.4111$  (from unit cell parameters). The idiomorphic crystals show two contrasting habits: bipyramidal and tabular. Forms: a {100}, b {010}, d {hkl}, e {h'k'l'}. Main X-ray powder diffraction data<sub>obs.</sub>: 5.78 (4) {112}, 4.89 (4) {211}, 4.73 (6) {022}, 3.750 (8) {213}, 3.159 (3) {231}, 2.8763 (8) {400}, 2.7820 (10) {141}, 2.7443 (7) {042}, 2.7281 (4) {314}, 2.6008 (3) {116}, 1.9909 (4) {523}, 1.8017 (3) {255}. Also 4-circle studies were undertaken to solve the crystal structure. Optical refractive indices:  $\alpha = 1.443(1)$ ,  $\beta = 1.457(1)$ ,  $\gamma = 1.458(2)$ . Birefringence: 0.015. Biaxial negative (-). Optic axial angle:  $2V_{calc}$  29°42';  $2V_{meas}$  29°36' (Mallard), for wavelength 589 nm. Optical orientation:  $X = a$ ,  $Y = b$ ,  $Z = c$ . Pleochroism: none,  $X=Y=Z$ =colourless. Dispersion  $r > v$  strong. Chemical analyses were carried out by AAS (Atomic Absorption Spectroscopy) MOAS (Molecular Optical Absorption Spectroscopy) and microanalytical wet data: Na<sub>2</sub>O 22.37; P<sub>2</sub>O<sub>5</sub> 24.87; H<sub>2</sub>O 53.38; Total: 100.62 wt.%. Chemical empirical formula: H<sub>17</sub>Na<sub>2</sub>O<sub>12</sub>P (based on 12 O atoms). The Gladstone-Dale relationship compatibility  $(1 - (K_f/K_c) = 0.022)$ . Catalanoite lacks closely crystallochemical relationship to other species, but it is the third sodium phosphate after nahpoite, Na<sub>2</sub>[HPO<sub>4</sub>], and dorfmanite, Na<sub>2</sub>[HPO<sub>4</sub>].2H<sub>2</sub>O. Catalanoite is the first genuine evaporite mineral for the phosphate groups in the System of Mineralogy. Named after Luciano R. Catalano (1890-1970), Argentine economic geologist. The mineral form was submitted to CNMMN-IMA.