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Crystal Chemistry of Wyllieite-Type Phosphates.

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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 $P2_1/n$ 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, 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 or Mn replacing Na on the X(2), X(1a) and X(1b) sites, Mg replacing Fe on the M(2a) site, and Mg or Fe^{3+} replacing Al on the M(2b) site, where represents a lattice vacancy. The name wyllieite corresponds to $Na_2MnFe^{2+}Al(PO_4)_3$, while 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)°), 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)°), of wyllieite from the Buranga pegmatite (R_1 = 2.74 %, a = 11.954(2), b = 12.439(2), c = 6.406(1) Å, β = 114.54(1)°), and of qingheiite from the Santa Ana pegmatite, Argentina (R_1 = 2.65 %, a = 11.878(3), b = 12.448(2), c = 6.438(2) Å, β = 114.49(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 structural features of rosemaryite, ferrorosemaryite, wyllieite, and qingheiite 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.

Keywords: phosphate minerals; wyllieite group; crystal chemistry

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Holtite from Szklary, Poland.

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Holtite is very rare borosilicate mineral with a complex and a various chemical composition. It has been found in pegmatites in only three places in the world: Greenbushes - Australia [1]; Kola Penisula – Russia [2] and Szklary - Poland [3]. The crystal structure has been already determined for single crystals originated from two of these occurrence (Australia [4], Russia [5, 6]), whereas the preliminary crystal structure for the holtite from Poland was announced in 2008 [7]. Recently three types of holtite from Szklary were isolated (yellow, amber, brown). For the amber, needle-shaped holtite crystals two kinds of the unit cell could be recognized: orthorhombic one with the lattice parameters a=40.980(2), b=23.6661(8), c=4.6979(2) Å and hexagonal one: a=23.6944(7), c=4.7012(2)Å. The holtite, isostructural with $Si_3B[Al_{6.75}\square_{0.25}O_{17.25}(OH)_{0.75}]$ (dumortierite), has SiO_4 tetrahedra partially replaced by SbO_3 or AsO_3 triangular pyramids. Additionally, Al cations in the octahedral positions are partially substituted by Ta or Ti cations. The characteristic features of the holtite structure is the presence of both cation and anion vacancies. The structural work on the amber single crystals together with a possible twinning consideration is in progress.

[1] Pryce M.W., Mineral. Mag., **1971**, 38, 21. [2] Voloshin A.V., Gordienk V.V., Gelman E.M., Zorina M.L., Elina N.A., Kulchitsaya E.A., Menshikov Y.P., Polejaeva L.I., Ryijova R.I., Sokolov P.B., and Utochkina G.I., *Zap. Vses. Mineral. Obshch.*, **1977**, 106, 337 (in Russian). [3] Pieczka A., Marszałek M., *Mineral. Polonica*, **1996**, 27, 3. [4] Hoskins B.F., Mumme W.G., Pryce M.W., *Mineral. Mag.*, **1989**, 53, 457. [5] Kazantsev S.S., PushcharovskY D.Yu., Pasero M., Merlino S., Zubkova N.V., *Crystal. Rep.*, **2005**, 50, 42. [6] Kazantsev S.S., Zubkova N.V., Voloshin A.V., *Crystal. Rep.*, **2006**, 51, 412. [7] Groat L.A., Grew E.S., Ercit T.S., Pieczka A., *Goldschmidt Conference Abstracts* **2008**, A330.

Keywords: holtite; mineral crystal structure; crystal twinning

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Layered Brownmillerites in the System of Manganese-Containing Alumino-Ferrites.

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The system $Ca_2Fe_2O_5$-"$Ca_2Mn_2O_5$"-"$Ca_2Al_2O_5$" was investigated by many authors (see [1] and citations therein), due to its relevance for the chemistry of cements. Single-