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Gatedalite, a new Zr-rich braunite group mineral from Långban, Sweden

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A new Zr-rich braunite group mineral, gatedalite $ZrMn^{2+}_2Mn^{3+}_4SiO_{12}$, occurs as very rare, small (≤ 60 μm), rounded, grains in hausmannite-impregnated skarn at the Långban Fe-Mn deposit, central Sweden. Associated minerals are Mn-bearing calcite, hausmannite, jacobsite, Mn-bearing phlogopite, tephroite, långbanite, pinakiolite and oxyplumboromeite.

Gatedalite crystals are grey-colored opaque with a submetallic luster, brittle tenacity and greyish brown streak. The mineral has a Mohs hardness of approximately 6, and a calculated density of 4.78 g/cm^3. It is tetragonal, space group $I4_1/acd$, with the unit cell-parameters a = 9.4668(6) Å, c = 18.8701(14) Å, V = 1691.1(2) Å^3, Z = 8. The crystal structure of gatedalite (Figure 1) was refined to an R1 index of 3.53% using 1339 unique reflections collected with MoKα X-radiation. The strongest lines of the calculated powder diffraction pattern are [d, Å (hkl) I]: 2.730 (224) 100, 2.367 (040) 12, 2.155 (235) 6, 1.6735 (440) 12, 1.6707 (048) 29, 1.4267(264) 16, 1.4233 (2.2.12) 10.

Crystal chemical analysis of the holotype gatedalite (IMA 2013-091) resulted in the empirical formula: $(Zr^{4+}_{0.49}Mn^{2+}_{0.47}Ca_{0.02}Zn_{0.01}Ce^{3+}_{0.01})_{\Sigma 1.00}(Mn^{3+}_{4.44}Fe^{3+}_{0.59}Mn^{2+}_{0.50}Mg_{0.48}Al_{0.01})_{\Sigma 6.01}Si_{0.99}O_{12}$. Gatedalite is related to braunite $(Mn^{2+}Mn^{3+}_6SiO_{12})$ by the coupled substitution $^{M1}Zr^{4+}{}_1{}^{M2\text{-}4}Mn^{2+}{}_2{}^{M1}Mn^{2+}{}_{-1}{}^{M2\text{-}4}Mn^{3+}{}_{-2}$. The mineral is named in honour of the Swedish amateur mineralogist Kjell Gatedal (b 1947).

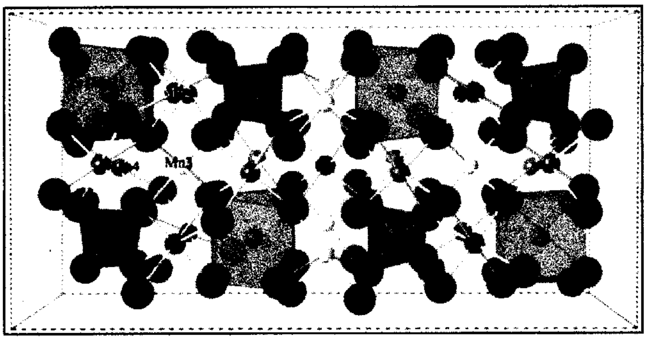

Figure 1: The crystal structure of gatedalite projected on [100]

A new nomenclature scheme for the alluaudite supergroup

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The alluaudite supergroup consists of phosphates and arsenates, divided in two groups: The alluaudite group, characterized by monoclinic species with unit-cell parameters *a* ~ 12, *b* ~12.5, *c* ~ 6.5 Å, β ~ 114°, space group *C*2/*c*, and the wyllieite group, in which phosphates show similar unit-cell parameters with space group $P2_1/n$. Alluaudite-type phosphates, as well as minerals of the wyllieite group, occur in rare-element granitic pegmatites, whereas alluaudite-type arsenates are more frequently observed in ore deposits or in volcanic fumaroles.

The alluaudite structure is based on kinked chains of edge-sharing octahedra stacked parallel to {101}. These chains are formed by a succession of M(2) octahedral pairs linked by highly distorted M(1) octahedra. Equivalent chains are connected in the b direction by the $P(1)O_4$ and $P(2)O_4$ tetrahedra, to form sheets perpendicular to [010]. These interconnected sheets produce channels parallel to the *c* axis, which contain large sites generally occupied by large Na of Ca atoms. The wyllieite structure is topologically identical to the alluaudite structure, but due to an ordering provoked by significant amounts of Al, the space group is modified and the M(2) and X(1) (=A(1)) sites are split into M(2a)-M(2b) and X(1a)-X(1b) positions, respectively.

The crystal-chemical formula of alluaudites is $A(2)'A(1)M(1)M(2)_2[(P,As)O_4]_3$; it becomes $X(2)X(1a)X(1b)M(1)M(2a)M(2b)(PO_4)_3$ in wyllieites. In pegmatites, the large X and A sites are generally occupied by Na and Ca, while the octahedral M sites contain Mn, Fe^{2+}, Mg, Fe^{3+}, or Al. In arsenates, more exotic cations occur in the structure, as for example Zn or Cu, due to the unusual geochemistry of the environment in which these minerals crystallize.

The nomenclature of phosphates of the alluaudite group [1] uses the content of the M(2) site to determine the root name: alluaudites (Fe^{3+} dominant), hagendorfites (Fe^{2+} dominant), and varulites (Mn dominant). A prefix ferro- or mag- is then added to indicate if Fe or Mg are dominant on the M(1) site, instead of Mn.

A careful re-calculation of ca. 100 analyses of natural phosphates of the alluaudite group indicates that this nomenclature scheme is very difficult to apply. In pegmatites, many samples are completely oxidized, leading to a composition $[]NaMnFe^{3+}_2(PO_4)_3$ corresponding indeed to alluaudite. But compositions for which Fe^{2+} or Mn are predominant on M(2) are extremely rare; even the chemical analyses of type hagendorfite and varulite show a significant amount of Fe^{3+} on M(2).

Since alluaudite is produced by oxidation of hagendorfite, following the mechanism $Na^+ + Fe^{2+} = [] + Fe^{3+}$, we can easily obtain the ideal formula of parent hagendorfite: $Na_2MnFe^{2+}Fe^{3+}(PO_4)_3$. The ideal composition of varulite becomes $Na_2Mn_2Fe^{3+}(PO_4)_3$. In this new nomenclature scheme, we allow a valency-imposed double site occupancy on M(2), in order to take into account the extremely complex crystal chemistry of this group. Several new root-names will be defined in the near future, in order to complete the existing nomenclature of the alluaudite supergroup.

[1] Moore P.B. and Ito J. (1979). Alluaudites, wyllieites, arrojadites: crystal chemistry and nomenclature. *Mineralogical Magazine*, 43, 227-235.