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Re-examination of the dumortierite group: A proposal for a new classification

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Currently, the dumortierite group comprises three minerals: dumortierite, $(Al,[])Al_6BSi_3O_{16}(O,OH)_2$, magnesiodumortierite, $(Mg,[])Al_6BSi_3O_{16}(O,OH)_2$, and holtite, $(Al,Ta,[])Al_6B(Si,Sb,As)_{\Sigma 3}O_{12}(O,OH,[])_{\Sigma 3}$, where [] denotes vacancies. Although the distinction between magnesiodumortierite and dumortierite, i.e., Mg vs. Al dominance at the partially vacant octahedral Al1 site, meets current criteria of the IMA Commission on New Minerals, Nomenclature and Classification (CNMNC) for distinguishing mineral species, the distinction between holtite and dumortierite does not, since Al and Si are dominant over Ta and (As,Sb) at the Al1 and two Si sites, respectively, in both minerals. Recent studies have revealed extensive solid solution between Al, Ta and Nb at Al1 and between Si, As and Sb at the two Si sites or nearly coincident (As,Sb) sites in dumortierite and holtite, further blurring the distinction between the two minerals. In addition, a mineral from the Szklary pegmatite (Lower Silesia, Poland) giving EBSD patterns consistent with the dumortierite structure is the first example of a dumortierite-group mineral with trivalent cations dominant at the Si-(As,Sb) sites. The analysis having the lowest SiO_2 content yields in weight %, SiO_2 12.34, Al_2O_3 50.66, Fe_2O_3 0.29, As_2O_3 16.89, Sb_2O_3 10.87, P_2O_5 0.48, Nb_2O_5 0.16, Ta_2O_5 below detection, TiO_2 0.27, $B_2O_{3(calc)}$ 5.37 (Σ97.32), corresponding to the composition

$$([]_{0.55}Al_{0.40}Fe_{0.02}Ti_{0.02}Nb_{0.01})_{\Sigma 1.00}Al_6B(Si_{1.33}As_{1.11}Sb_{0.48}P_{0.04}\ Al_{0.04})_{\Sigma 3.00}(O_{16.41}[]_{1.59})_{\Sigma 18.00}$$

with Si/(As+Sb) = 0.84. Other holtite-like minerals from Szklary have Ta, Nb or Ti dominant at Al1 if allowance is made for charge balance, which requires that Al^{3+} be replaced by $0.6(Ta^{5+}, Nb^{5+}) + 0.4[]$ and by $0.75Ti^{4+} + 0.25[]$, respectively. For example, from Nb-rich material the analysis with the highest Nb_2O_5 content (5.42 wt%) has the composition

$$([]_{0.45}Nb_{0.26}Ta_{0.02}Al_{0.20}Fe_{0.05}Ti_{0.01})_{\Sigma 1.00}Al_6B(Si_{2.01}Sb_{0.48}As_{0.37}Al_{0.10})_{\Sigma 3.00}(O_{17.15}[]_{0.85})_{\Sigma 18.00};$$

and from Ti-rich material, the analysis with the highest TiO_2 content (4.30 wt%) has the composition

$$([]_{0.36}Ti_{0.34}Al_{0.22}Fe_{0.01}Nb_{0.04}Ta_{0.03})_{\Sigma 1.00}Al_6B(Si_{2.32}Sb_{0.49}As_{0.14}Al_{0.04})_{\Sigma 3.00}(O_{17.35}[]_{0.65})_{\Sigma 18.00}.$$

Both these compositions show EBSD patterns consistent with the dumortierite structure. The holtite- and dumortierite-like material from Szklary is highly zoned, and all three compositions represent single point analyses. On the basis of these findings, we propose more specific end-member compositions for dumortierite and holtite together with a classification of a dumortierite supergroup based on occupancy of the Al1 site. The supergroup comprises 3 groups: (1) Dumortierite group, with Al1 = Al^{3+}, Mg^{2+}, and [] with charge balance provided by OH substitution for O; this includes dumortierite, $AlAl_6BSi_3O_{18}$ and magnesiodumortierite, $MgAl_6BSi_3O_{17}(OH)$, plus a hypothetical "hydroxydumortierite" end-member, $[]Al_6BSi_3O_{15}(OH)_3$; (2) Holtite group, with Al1 = Ta^{5+}, Nb^{5+}, Ti^{4+}, with [] created for charge balance and to reduce repulsion between highly charged cations; this includes holtite, $(Ta_{0.6}[]_{0.4})Al_6BSi_3O_{18}$ and its Nb analogue, $(Nb_{0.6}[]_{0.4})Al_6BSi_3O_{18}$ and Ti analogue, $(Ti_{0.75}[]_{0.25})Al_6BSi_3O_{18}$; and (3) a new group with Al1 = [] caused by loss of coordinating O due to replacement of Si^{4+} by As^{3+} or Sb^{3+}, which includes the new mineral from Szklary with an end-member formula $[]Al_6BAs^{3+}_3O_{15}$.