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Description and crystal structure of cabalzarite $Ca(Mg,Al,Fe)_2(AsO_4)_2(H_2O,OH)_2$, a new mineral of the tsumcorite group

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ABSTRACT

Cabalzarite, $^{M1}Ca^{M2}(Mg,Al,Fe^{3+})_2(^{X}AsO_4)_2(H_2O,OH)_2$, is a new mineral of the tsumcorite group occurring in altered Mn ore at the abandoned Falotta mine (Swiss Alps). Together with other arsenates, cabalzarite documents the mobility of As during the retrograde stage of the Tertiary Alpine metamorphism under lowest to sub-greenschist facies conditions. Cabalzarite crystals vary in morphology from hatchet-like to fibrous and tabular. The color is light-brownish to salmon pink or orange brown, and the average refractive index is around 1.7. Cabalzarite is chemically inhomogeneous, with the main variations occurring on the octahedral M2 site occupied by Mg, Al, Fe^{3+}, and Mn^{3+}. Al and Mg are the dominant M2 cations, with Al/(Al + Mg) ratios varying between 0.31 and 0.59 (92 analyses). Cabalzarite is the first member of the tsumcorite group with octahedral Mg and Al as major constituents. Single-crystal X-ray structure refinements were performed on two different crystals. Cabalzarite is monoclinic, space group *C*2/*m*, Z = 2. The cell parameters for the type crystal CABA11.5, of composition $(Ca_{1.00}Sr_{0.02})(Al_{0.80}Mg_{0.77}Fe_{0.23}Mn_{0.03})_{\Sigma 1.83}(AsO_4)_2(H_2O_{1.26}OH_{0.74})_2$, are $a = 8.925(2)$ Å, $b = 6.143(1)$ Å, $c = 7.352(1)$ Å, $\beta = 115.25(3)^\circ$, $\rho_{calc} = 3.73$ g/cm^3. The structure of cabalzarite is isomorphic with that of tsumcorite. The site M1 (Ca) is eightfold-coordinated (6 + 2) with average M1-O = 2.549 Å; M2 is octahedral with an average M2-O = 2.010 Å; and the average As-O distance of the arsenate group is 1.689 Å. Charge balance for the simultaneous occupation of M2 by two- and three-valent cations is achieved by H_2O as well as OH contributing to the M2 coordination.