A new kristiansenite-like mineral from post-magmatic mineralization in the Szklarska Poręba granite?

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A mineral similar to kristiansenite, unusually highly enriched in scandium, was found in ore-mineralized granitic pegmatite at the Szklarska Poręba Huta quarry in Lower Silesia, SW Poland (latitude: 50.82778, longitude: 15.48944). Previously in the locality were discovered kristiansenite $Ca_4Sc_2Sn_2(Si_2O_7)_2(Si_2O_6OH)_2$, silesiaite $Ca_4Fe^{3+}{}_2Sn_2(Si_2O_7)_2(Si_2O_6OH)_2$ and kozłowskiite $Ca_4Fe^{2+}Sn_3(Si_2O_7)_2(Si_2O_6OH)_2$, forming the kristiansenite group [1-4].

It is a high-temperature mineral that crystallises from a Ca-bearing fluid phase, forming an inclusion in scheelite that is one of the mineral components of the polymetallic ore assemblage superimposed on this pegmatite. Cassiterite, Sc-bearing nioboixiolite-(Fe^{2+}), Sc-bearing nioboixiolite-(Mn^{2+}), scandiobabingtonite, kristiansenite, silesiaite, kozłowskiite and chamosite were recognized as the associated phases also occurring in the form of inclusions in scheelite.

The empirical formula calculated based on 16 cations and 28 (O,OH) anions is (all Fe as Fe^{3+}): $(Ca_{3.878}Mn_{0.121})_{\Sigma 3.999}(Sc_{2.385}Sn_{1.324}Fe^{3+}{}_{0.155}Nb_{0.058}Al_{0.051}Ti_{0.016}Zr_{0.008}Ta_{0.005})_{\Sigma 4.001}(Si_{7.982}Al_{0.018})_{\Sigma 8.000}O_{25.457}(OH)_{2.543}$. The formula shown in terms of the cation and anion valences is: $(2^+)_{3.999}(3^+{}_{2.591}4^+{}_{1.348}5+_{0.063})(4^+{}_{7.982}3^+{}_{0.018})(2^-{}_{25.457}1^-{}_{2.543})$.

This composition suggests the ideal formula $Ca_4Sc_3Sn(Si_2O_6OH)_3(Si_2O_7)$, which requires 20.59 calculated weight % CaO, 18.99 wt% Sc_2O_3, 13.83 wt% SnO_2, 44.12 wt% SiO_2, 2.48 wt% H_2O; Total 100 wt.%.

The mineral is isostructural with kristiansenite, silesiaite, and kozłowskiite, with the space group symmetry assigned as *C*1 with α and γ angles very close to 90°. Thus, as in the case of the other three minerals of the kristiansenite group, the structure of this new mineral is metrically monoclinic but structurally triclinic.

Crystal system: triclinic Space group: *C*1

a = 10.0753(5) Å b = 8.4542(2) Å c = 13.3605(4) Å

α = 90.002(3)° β = 109.395(2)° γ = 89.995(2)°

V = 1073.45(5) Å^3 Z = 2

The refinement of 278 structural parameters in *C*1 (positional and anisotropic displacement parameters for non-hydrogen atoms and positional parameters of hydrogen atoms) gave an R_1 index of 3.08 % [R_1(all) = 4.10 %], wR_2 index of 7.07 % and goodness of fit parameter S = 1.069.

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The research project was supported by program „Excellence initiative – research university" for the AGH University of Krakow