

A Sc-Nb oxide from corundum pegmatites of the Krucze Skały in Karpacz (Karkonosze massif, Lower Silesia, Poland) – a potentially new mineral of the ScNbO₄ – FeWO₄ series

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The Sc-Nb oxide occurs as an accessory mineral in a peraluminous corundum pegmatite of the Krucze Skały in Karpacz–Wilcza Poręba, situated within the Karkonosze massif (Lower Silesia, SW Poland). Orthoclase, biotite, muscovite, albite, chamosite and corundum are the main rock-forming minerals of the pegmatite. Schorl, rutile, ilmenite and ferberite are accessories. The Nb-Sc oxide forms xenomorphic, more rarely idiomorphic, grains up to 30 µm in size (Fig. 1), inside rutile, Nb-bearing rutile and ilmenite grains. Grains showing complex zonation are composed of ferberite cores and Sc-Nb oxide in external parts.

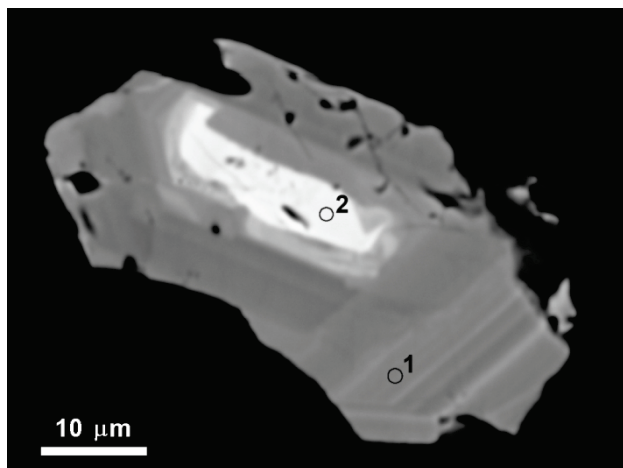


Fig. 1: Idiomorphic zoned grain of Sc-Nb oxides, BSE image; 1 and 2 are analysis sites.

The chemical formula of the zoned external part of a grain (Fig. 1) with maximum concentrations of Sc (1) is $(\text{Sc}_{0.55}\text{Fe}^{2+}_{0.15}\text{Ti}_{0.12}\text{Fe}^{3+}_{0.08}\text{Mn}_{0.05}\text{Zr}_{0.03})_{\Sigma 0.98}(\text{Nb}_{0.86}\text{W}_{0.07}\text{Sn}_{0.06}\text{Ta}_{0.03})_{\Sigma 1.02}\text{O}_4$. The core (Fig. 1) shows an intermediate composition, belonging to the ScNbO₄ – FeWO₄ series, with composition (2) $(\text{Fe}^{2+}_{0.39}\text{Sc}_{0.35}\text{Mn}_{0.13}\text{Ti}_{0.08}\text{Fe}^{3+}_{0.05}\text{Zr}_{0.02})_{\Sigma 1.02}(\text{Nb}_{0.48}\text{W}_{0.47}\text{Ta}_{0.01}\text{Sn}_{0.01})_{\Sigma 0.97}\text{O}_4$. The Sc-Nb oxide has a wolframite-type structure according to EBSD data. All analytical data point to the Sc-Nb oxide being a new mineral species with end-member composition ScNbO₄. Recently, the new mineral heftetjernite, ScTaO₄, was described [1], and is a Ta-analogue of the mineral from Krucze Skały. After detailed studies the new species will be submitted for approval to the IMA CNMNC.

[1] Kolitsch, U. et al. (2010) *Eur. J. Mineral.*, **22**, 309-316.

Ammineite, CuCl₂(NH₃)₂ – the first mineral containing an ammine complex

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The type locality of ammineite, CuCl₂(NH₃)₂, is Caleta Pabellon de Pica, Tarapaca, south of Iquique, Chile. It has been accepted as new mineral by CNMNC (2008-32).

Ammineite occurs as intense sky blue xenomorphic grains up to 4 millimetres in size in solution cavities in halite together with atacamite and darapskite. Ammineite is a reaction product of guano with copper mineralisation.

For ammineite Cu (37.60 wt.%) and Cl (41.67 wt.%) were analysed by EMP, N (16.54 wt.%) and H (3.32 wt.%) by CHNS analyser. O, S and C are below the detection limits. FTIR spectra give exclusively NH₃ frequencies at 3316, 3241, 3160, 1594, 1245, 711, 660 and 480 cm⁻¹.

Ammineite is orthorhombic, space group *Cmcm*, with *a* = 7.688(1), *b* = 10.645(2), *c* = 5.736(1) Å, *V* = 469.4(2) Å³ and *Z* = 4. The crystal structure was solved by direct methods and refined with SHELX-97 [1] to *R* = 0.024 [*F*_o > 4σ(*F*_o)] for 231 unique reflections.

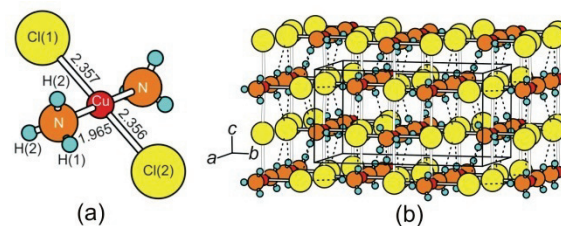


Fig. 1: The crystal structure of ammineite: (a) basic unit, (b) layers of CuCl₂(NH₃)₂ parallel (001). Dotted lines indicate hydrogen bonds.

The basic structural unit consists of a central Cu site with *trans* planar coordination of two NH₃ molecules and two Cl ions with Cu-N 1.965(3) Å and Cu-Cl distances of 2.356(2) and 2.357(2) Å (Fig. 1a). In the unit cell the complex forms layers parallel to (001) and oriented by Cl(1)-Cu-Cl(2) parallel to [010] (Fig. 1b). Along [001] Cu is connected to parallel layers nearly perpendicular by two long bonds (Cu-Cl(2) 2.868(1) Å), building orthorhombic dipyrramids connected by shared edges to form zigzag chains running along [001]. Some H...Cl distances ranging from 2.69(3) to 2.79(4) Å indicate the presence of weak hydrogen bonds, which connect the complexes within the (001) layers and also from one layer to the next.

X-ray powder data for ammineite and *trans*-diamminedichloro-copper(II), which was synthesized for comparison, are nearly identical. However, calculated powder data using parameters taken from the structure determination of synthetic Cu(NH₃)₂Cl₂ reported in [2] are completely different from our data.

[1] Sheldrick, G.M. (1997) *SHELX-97 programs for crystal structure refinement*. University of Göttingen, Germany. [2] Hanic, F. & Cakajdova, I.A. (1958) *Acta Crystallogr.*, **11**, 610-612.