

### A Sc-Nb oxide from corundum pegmatites of the Krucze Skały in Karpacz (Karkonosze massif, Lower Silesia, Poland) – a potentially new mineral of the ScNbO<sub>4</sub> – FeWO<sub>4</sub> series

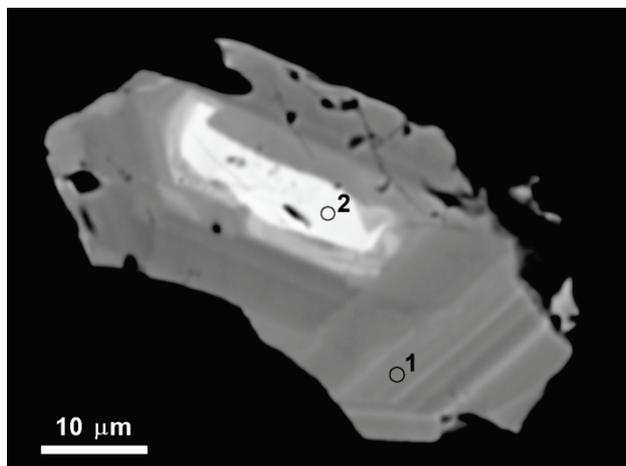
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The Sc-Nb oxide occurs as an accessory mineral in a peraluminous corundum pegmatite of the Krucze Skały in Karpacz–Wilcza Poręba, situated within the Karkonosze massif (Lower Silesia, SW Poland). Orthoclase, biotite, muscovite, albite, chamosite and 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 ScNbO<sub>4</sub> – FeWO<sub>4</sub> 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 ScNbO<sub>4</sub>. Recently, the new mineral heftetjernite, ScTaO<sub>4</sub>, 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, CuCl<sub>2</sub>(NH<sub>3</sub>)<sub>2</sub> – the first mineral containing an ammine complex

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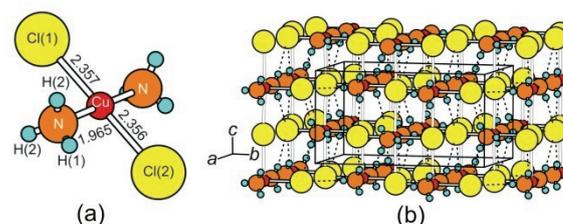
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The type locality of ammineite, CuCl<sub>2</sub>(NH<sub>3</sub>)<sub>2</sub>, is Caleta Pabellon de Pica, Tarapaca, south of Iquique, Chile. It has been accepted as new mineral by CNMNC (2008-32).

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 NH<sub>3</sub> frequencies at 3316, 3241, 3160, 1594, 1245, 711, 660 and 480 cm<sup>-1</sup>.

Ammineite is orthorhombic, space group *Cmcm*, with  $a = 7.688(1)$ ,  $b = 10.645(2)$ ,  $c = 5.736(1)$  Å,  $V = 469.4(2)$  Å<sup>3</sup> and  $Z = 4$ . The crystal structure was solved by direct methods and refined with SHELX-97 [1] to  $R = 0.024$  [ $F_o > 4\sigma(F_o)$ ] for 231 unique reflections.



**Fig. 1:** The crystal structure of ammineite: (a) basic unit, (b) layers of CuCl<sub>2</sub>(NH<sub>3</sub>)<sub>2</sub> parallel (001). Dotted lines indicate hydrogen bonds.

The basic structural unit consists of a central Cu site with *trans* planar coordination of two NH<sub>3</sub> 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 dipyramids 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(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> 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.