

## Scottyite, the natural analog of synthetic $\text{BaCu}_2\text{Si}_2\text{O}_7$ , a new mineral from the Wessels mine, Kalahari Manganese Fields, South Africa

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### ABSTRACT

A new mineral species, scottyite, ideally  $\text{BaCu}_2\text{Si}_2\text{O}_7$ , has been found in the Wessels mine, Kalahari Manganese Fields, Northern Cape Province, South Africa. The mineral appears to have formed as a result of a hydrothermal event and is associated with wesselsite, pectolite, richterite, sugilite, and lavinskyite. Scottyite forms blocky grains with striations parallel to the *c* axis. Crystals are found up to  $0.4 \times 0.3 \times 0.3$  mm. No twinning is observed. The mineral is dark-blue in transmitted and under incident lights, transparent with pale blue streak and vitreous luster. It is brittle and has a Mohs hardness of 4–5; cleavage is perfect on {100} and {010} and no parting was observed. The calculated density is  $4.654 \text{ g/cm}^3$ . Optically, scottyite is biaxial (–), with  $\alpha = 1.750(1)$ ,  $\beta = 1.761(1)$ , and  $\gamma = 1.765(1)$ ,  $2V_{\text{meas}} = 66(2)^\circ$ . It is insoluble in water, acetone, or hydrochloric acid. An electron microprobe analysis produced an average composition (wt%) (8 points) of CuO 36.98(31), BaO 35.12(16),  $\text{SiO}_2$  27.01(61), SrO 0.28(5), and  $\text{Na}_2\text{O}$  0.06(2), and total = 99.45(65), yielding an empirical formula (based on 7 O apfu)  $\text{Ba}_{1.00}\text{Sr}_{0.01}\text{Na}_{0.01}\text{Cu}_{2.04}\text{Si}_{1.97}\text{O}_7$ .

Scottyite is the natural analog of synthetic  $\text{BaCu}_2(\text{Si,Ge})_2\text{O}_7$ , which exhibits novel one-dimensional quantum spin-1/2 antiferromagnetic properties with tunable super-exchange interactions. It is orthorhombic, with space group *Pnma* and unit-cell parameters  $a = 6.8556(2)$ ,  $b = 13.1725(2)$ ,  $c = 6.8901(1)$  Å, and  $V = 622.21(6)$  Å<sup>3</sup>. The structure of scottyite is characterized by flattened  $\text{CuO}_4$  tetrahedra sharing corners with one another to form chains parallel to the *c* axis. These chains are interlinked by  $\text{Si}_2\text{O}_7$  tetrahedral dimers and  $\text{Ba}^{2+}$ . The  $\text{Ba}^{2+}$  cations are bonded to seven O atoms in an irregular coordination. The average Si-O, Cu-O, and Ba-O bond lengths are 1.630, 1.941, and 2.825 Å, respectively. Scottyite is topologically related to a group of compounds with the general formula  $\text{BaM}_2^3\text{Si}_2\text{O}_7$ , where M = Be (barylite and clinobarylite), Fe (andrémeyerite), Mg, Mn, Co, and Zn.

**Keywords:** Scottyite,  $\text{BaCu}_2\text{Si}_2\text{O}_7$ , crystal structure, X-ray diffraction, Raman spectra