

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

HEXIONG YANG,^{1,*} ROBERT T. DOWNS,¹ STANLEY H. EVANS,¹ AND WILLIAM W. PINCH²

¹Department of Geosciences, University of Arizona, Tucson, Arizona 85721-0077, U.S.A.

²19 Stonebridge Lane, Pittsford, New York 14534, U.S.A.

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 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), SiO_2 27.01(61), SrO 0.28(5), and Na_2O 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 $V = 622.21(6)$ Å³. The structure of scottyite is characterized by flattened CuO_4 tetrahedra sharing corners with one another to form chains parallel to the *c* axis. These chains are interlinked by Si_2O_7 tetrahedral dimers and Ba^{2+} . The 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