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Composition and $I4/m$-$P4_2/n$ phase transition in scapolite solid solutions

YUSUKE SETO,* NORIMASA SHIMOBAYASHI, AKIRA MIYAKE, AND MASAO KITAMURA

Department of Geology and Mineralogy, Kyoto University, Kyoto, 606-8502, Japan

ABSTRACT

Scapolite is a metamorphic aluminosilicate mineral that can be described by the general formula $(Na,Ca,K)_4(Al,Si)_6Si6O_{24}(Cl,CO_3,SO_4)$. Two common end-members are called marialite ($Na_4ClSi_9Al_3O_{24}$) and meionite ($Ca_4CO_3Si_6Al_6O_{24}$). Variations in scapolite composition can be described by two independent substitutions, $NaSi(CaAl)_{-1}$ and $NaCl(CaCO_3)_{-1}$. Twenty eight natural scapolites in the present study exhibit a range of compositions from X_{EqAn} [(Al–3)/3] = 8% and X_{Me} [Ca/(Na+K+Ca)] = 7% to X_{EqAn} = 82% and X_{Me} = 90%. Several coupled exchange reactions can be identified in some inhomogeneous samples (e.g., $Na_{1.49}SiCl_{0.47}$ $[Ca_{1.44}Al(CO_3)_{0.43}]_{-1}$, $Na_{1.69}SiCl_{0.58}[Ca_{1.55}Al(CO_3)_{0.50}]_{-1}$, $Na_{1.91}SiCl_{0.79}[Ca_{1.75}Al(CO_3)_{0.69}]_{-1}$). The extent of coupling between the two substitutions is controlled by the crystallization environment (P, T, and mineral assemblages).

Electron diffraction patterns suggest that the symmetry of scapolite with X_{Me} up to 18% is $I4/m$, whereas that for intermediate scapolite from X_{Me} = 18% to at least X_{Me} = 90% is $P4_2/n$. Under dark-field observation (g = hkl, $h + k + l$ = odd) using a transmission electron microscope (TEM), the $P4_2/n$ samples have anti phase domains of various sizes, the presence of which provides evidence for an I-P phase transition. A wide compositional range of scapolite solid solutions should have an $I4/m$ symmetry at the time of formation.