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Single-crystal structure refinement of synthetic ^{M4}K-substituted potassic richterite, $K(KCa)Mg_5Si_8O_{22}(OH)_2$

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ABSTRACT

The crystal structure of a potassic richterite, $K(KCa)Mg_5Si_8O_{22}(OH)_2$ synthesized at 15 GPa and 1400 °C, was refined from single-crystal X-ray diffraction data. The unit-cell parameters are: a = 10.1926(5), b = 18.1209(3), c = 5.2736(2) Å, and β = 105.514(5)°. The refinement shows that the M4 site is occupied by K and Ca at a ratio of 1:1 with no site splitting. Entrance of K into the M4 site mainly affects the local environment: the M4-O2, M4-O4, and M4-O6 bond lengths in KK richterite are 3.4, 3.7, and 3.1% longer, respectively, than the corresponding ones in potassium richterite, whereas the M4-O5 distance is 1.2% shorter, giving rise to a more regular M4 polyhedron. Three major structural adjustments allow the M4 site to accommodate large K: a shift of the M4 cation along the two-fold b axis, a modification of the double silicate-chain configurations, and relative displacements of the two back-to-back tetrahedral chains. K at the A site is completely ordered at the Am position. The average of eight shortest A-O distances is 0.044 Å longer than that in potassium richterite, despite the A site being fully filled with K in both structures. The unpolarized Raman spectrum displays only one single band at 3735.5 cm^{-1} in the OH-stretching region.