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Crystal chemistry of Mg-, Fe-bearing muscovites-2M_1

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Abstract

Phengitic muscovite-2M_1 crystals $[^{[12]}(K_{0.88-0.99}Na_{0.01-0.09}Ca_{0.00-0.06}Ba_{0.00-0.01})^{[6]}(Al_{1.64-1.88}Fe^{2+}_{0.06-0.29}Fe^{3+}_{0.01-0.16}Mg_{0.00-0.16}Mn_{0.00-0.07}Ti_{0.00-0.06})^{[4]}(Si_{2.87-3.30}Al_{0.70-1.13})(OH)_{1.56-2.07}F_{0.00-0.41}O_{9.91-10.25}]$ from pegmatites and peraluminous granites were refined to investigate the influence of phengitic substitution on the mica structure. Single-crystal X-ray diffraction data were collected for eleven crystals in the *C*2/*c* space-group (agreement factor 2.1% $\leq R_{obs} \leq$ 3.9%). Tetrahedral Si and Al cation disorder was found for each sample, with the mean tetrahedral cation-oxygen distances ranging from 1.639 Å $\leq$ <T1-O> $\leq$ 1.647 Å and 1.640 Å $\leq$ <T2-O> $\leq$ 1.646 Å. As phengitic substitution increases, the octahedral sheet expands and requires a less distorted (more hexagonal) tetrahedral ring (7.70° $\leq \alpha \leq$ 11.38°) and low corrugation of the basal O plane (0.1796 Å $\leq \Delta z \leq$ 0.2296 Å). The electron density at the M2 site is greater than that required for the ideal muscovite-2M_1 structure, and a small excess of electron density is found in the M1 site. The inner sixfold coordination of the interlayer (A) cation is elongated along **c***, which is consistent with the high α values and the long A-O11 bond length.