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$2M_1$-phlogopite from Black Hills (South Australia): The first case of configurational polytype in micas

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ABSTRACT

The $2M_1$-phlogopite from the potassic gabbronorite (Black Hill, Australia) has been studied by electron microprobe and single-crystal X-ray diffraction analyses. The crystal-chemical formula was $(K_{0.95}Na_{0.01})(Al_{0.15}Mg_{1.27}Fe^{2+}_{1.16}Fe^{3+}_{0.04}Ti^{4+}_{0.38})(Si_{2.85}Al_{1.15})O_{10.76}F_{0.11}Cl_{0.03}OH_{1.10}$. The structural analysis has shown that the crystal has the cell parameters $a = 5.352(1)$, $b = 9.268(1)$, $c = 20.168(1)$ Å, and $\beta = 95.10(1)°$ and exhibits symmetry lowering from the ideal space group $C2/c$ to $C1$. An octahedral cation ordering pattern was revealed from the refined site-scattering powers. Specifically, using the scattering species Mg vs. Fe, it was found that the M1 site at $z = 0$ was occupied principally by Mg (~77%) and subordinately by Fe (~23%), whereas that at $z = 0.5$ was completely occupied by Fe; the M2 sites at $z = 0$ displayed ~88% Mg and ~12% Fe, whereas those at $z = 0.5$ were occupied by ~86% Fe and ~14% Mg. The analysis of geometrical features shows that the Ti uptake in the structure via the Ti-oxy mechanism induces structural distortions of different extents on the $z = 0$ and $z = 0.5$ layers, with stronger effects for the layer at $z = 0$. Minor chemical and structural differences, instead, affect the T sheets at $z = 0$ and $z = 0.5$.

Keywords: $2M_1$-phlogopite, octahedral cation ordering, symmetry lowering, structure refinement