

Crystal chemistry of Ti-rich fluorophlogopite from Presidente Olegario, Alto Paranaíba igneous province, Brazil

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ABSTRACT

Trioctahedral micas from kamafugitic lavas of Presidente Olegario (Brazil) are Ti-Fe-bearing fluorophlogopites. They were investigated using a combination of electron probe microanalysis (EPMA), single-crystal X-ray diffraction (SCXRD), and Mössbauer spectroscopy.

EPMA data yielded the following ranges: Al₂O₃ (8.7–10.1 wt%), MgO (19.6–20.6 wt%), FeO (5.7–6.5 wt%), TiO₂ (5.9–7.5 wt%), K₂O (8.9–9.7 wt%), Na₂O (0.4–0.6 wt%), and fluorine (3.4–4.1 wt%). Mössbauer investigation indicated: ⁵⁷Fe²⁺ ~ 60%, ⁵⁷Fe³⁺ ~ 10%, ⁵¹Fe³⁺ ~ 30%. X-ray analysis indicated the 1M polytype, with cell parameters in the range $a = 5.3208\text{--}5.3376$, $b = 9.2210\text{--}9.2464$, $c = 10.1227\text{--}10.155$ Å, $\beta = 100.157\text{--}100.194^\circ$. Structure refinements using anisotropic displacement parameters were performed in space group C2/m and converged to $2.01 \leq R_1 \leq 3.51$, $2.00 \leq wR_2 \leq 3.51\%$.

The micas have no ^{VI}Al³⁺ and Na is probably partitioned over both interlayer and octahedral sites. Major substitutions are OH⁻ ↔ F⁻, and the Ti-oxy substitution: ^{VI}M²⁺ + 2(OH)⁻ ↔ ^{VI}Ti⁴⁺ + 2O²⁻ + H₂↑. Accordingly, the structural features of the studied micas encompass those typical of both fluorophlogopites and micas affected by Ti-oxy substitution.

Keywords: Ti-fluorophlogopite, Mössbauer spectroscopy, crystal chemistry, substitution mechanisms