

## 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:  $\text{Al}_2\text{O}_3$  (8.7–10.1 wt%),  $\text{MgO}$  (19.6–20.6 wt%),  $\text{FeO}$  (5.7–6.5 wt%),  $\text{TiO}_2$  (5.9–7.5 wt%),  $\text{K}_2\text{O}$  (8.9–9.7 wt%),  $\text{Na}_2\text{O}$  (0.4–0.6 wt%), and fluorine (3.4–4.1 wt%). Mössbauer investigation indicated:  ${}^{57}\text{Fe}^{2+} \sim 60\%$ ,  ${}^{57}\text{Fe}^{3+} \sim 10\%$ ,  ${}^{57}\text{Fe}^{3+} \sim 30\%$ . 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  ${}^{57}\text{Al}^{3+}$  and Na is probably partitioned over both interlayer and octahedral sites. Major substitutions are  $\text{OH}^- \leftrightarrow \text{F}^-$ , and the Ti-oxy substitution:  ${}^{57}\text{M}^{2+} + 2(\text{OH})^- \leftrightarrow {}^{57}\text{Ti}^{4+} + 2\text{O}^{2-} + \text{H}_2\uparrow$ . 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