Crystal chemistry of trioctahedral micas-2M₁ from Bunyaruguru kamafugite (southwest Uganda)

FERNANDO SCORDARI,* EMANUELA SCHINGARO, MARIA LACALAMITA, AND ERNESTO MESTO

Dipartimento di Scienze della Terra e Geoambientali, Università degli Studi di Bari, via E. Orabona 4, I-70125 Bari, Italy

ABSTRACT

The crystal chemistry of 2M₁ micas from Bunyaruguru kamafugite (southwest Uganda) was studied by electron probe microanalysis, single-crystal X-ray diffraction, Mössbauer and Fourier transform infrared spectroscopy. Chemical analyses showed that the studied crystals are Ti-rich, F-poor phlogopites with an annitic component, Fe_to(Mg), ranging from 0.15 to 0.22. Unit-cell parameters from single-crystal X-ray data are in the range: 5.3252(1) ≤ a ≤ 5.3307(1), 9.2231(3) ≤ b ≤ 9.2315(3), 20.1550(6) ≤ c ≤ 20.1964(8) Å, and 94.994(2) ≤ β ≤ 95.131(2)°.

Anisotropic structure refinements, in the space group C2/c, converged to 2.77 ≤ R₁ ≤ 3.52% and 2.91 ≤ wR₂ ≤ 4.02%. Mössbauer spectroscopy showed that the studied sample has: \( ^{57} \text{Fe}^{6+} = 60(1)\% \), \( ^{57} \text{Fe}^{3+} = 24(1)\% \), and \( ^{57} \text{Fe}^{2+} = 16(1)\% \). FTIR investigations pointed to the occurrence of Fe\(^{3+}\)-oxy substitutions and ruled out the presence of vacancy mechanisms. The overall crystal-chemical features are consistent with the following substitutions: tetraferriphlogopite \( [^{3+} \text{Fe}^{3+} ↔ ^{1+} \text{Al}] \); Ti-oxi \( [^{2+} \text{M}^{2+} + 2 \text{OH}^\text{−} ↔ ^{2+} \text{Ti}^{4+} + 2 \text{OH}^\text{−}] \) and Al, Fe\(^{3+}\), Cr-oxi \( [^{3+} \text{M}^{3+} + \text{OH}^\text{−} ↔ ^{2+} \text{M}^{3+} + \text{OH}^\text{−}] \); AI, Fe\(^{2+}\)-Tschermak \( [^{2+} \text{M}^{2+} + ^{2+} \text{Si}^{4+} ↔ ^{3+} \text{Al}^{3+} + ^{3+} \text{M}^{3+}] \); kinoshitalite \( [^{3+} \text{K} + ^{2+} \text{Si}^{4+} ↔ ^{3+} \text{Ba}^{2+} + ^{2+} \text{Al}] \) and \( [^{3+} \text{K} + ^{4+} \text{Al}] \) \( ↔ ^{2+} \text{Si}^{4+} + ^{2+} \text{Ba}^{2+} \).

The estimation of the OH\(^−\) content for Ugandan mica-2M₁ was obtained, for the first time, from the linear regression equation \( c = 0.20(2) \times \text{OH}^− \) (gpfu) + 19.93(2) derived from literature data of 2M₁-samples with known OH\(^−\) content. The orientation of the O-H vector with respect to e* was found in the range from 2.0 to 6.9°.

Keywords: Kamafugitic 2M₁-phlogopites, crystal chemistry, substitution mechanisms, Mössbauer, FTIR

INTRODUCTION

It is known that the mica structure arises from the stacking of T-O-T layers along the c-axis direction connected by I-cations where T, O, and I stand for tetrahedral-, octahedral-, and interlayer, respectively. The six standard mica polytypes, 1M, 2M₁, 2M₂, 2O, 3T, and 6H, theoretically derived by Smith and Yoder (1956), were subsequently classified on the basis of the mutual rotation between the two neighboring T-O-T layers, into three types: (1) subfamily A (1M, 2M₁, and 3T), with successive layers rotated by 2πn × 60°; (2) subfamily B (2M₂, 2O, and 6H) with successive layers rotated by (2πn + 1) × 60°; and (3) mixed polytypes in which both types A and B occur (Nespolo 1999).

In trioctahedral micas, polytype 2M₁ occurs less frequently than the 1M polytype (Bailey 1984a). For this reason, the trioctahedral 1M-polytype has been extensively studied to date, whereas studies on the 2M₁-polytype are relatively scarce.

In several cases, 2M₁-micas have been reported as coexisting with 1M-micas in the same rock sample. Takeda and Ross (1975), analyzed 2M₁ and 1M igneous oxybiotite from Ruiz Peak (New Mexico), and concluded that the unit layer of the 2M₁ polytype showed a shift of the upper and lower triads of octahedral O atoms along the ±b direction with respect to the 1M polytype. This caused the reduction in the unit layer symmetry from C2/m to C T.

Bohlen et al. (1980) carried out a full crystal-chemical characterization of a metamorphic 2M₁ biotite from Au Sable Forks, New York, and concluded that chemistry and structure were quite close to the Ruiz Peak specimen of Takeda and Ross (1975). Ohta et al. (1982) studied hydrogenated and hydrogen-depleted Fe\(^{3+}\)-rich 1M and 2M₁ igneous biotites from Ruiz Peak. The lack of hydrogen seemed to mainly affect the interlayer configuration, causing a decrease in the interlayer separation.

2M₁- and 1M-micas in plutonic rocks from Valle del Cervo and in ignimbrites and lavas from Mt. Sassetto, Italy, were studied by Bigi and Brigatti (1994) and Laurora et al. (2007), respectively. By comparing the two polytypic forms, Bigi and Brigatti (1994) concluded that, despite the similarity in the chemical composition, the 2M₁ polytype had the most pronounced tetrahedral and octahedral distortions. Laurora et al. (2007) found that the 2M₁ polytype had structural features compatible with the occurrence of Ti-oxy substitutions. Aldega et al. (2009) reported, through X-ray powder diffraction, the coexistence of 1M- and 2M₁-polytypes in phlogopite from altered volcanoclastic deposits in the Grotta del Cervo cave, Pietrasecca, Italy.

Other studies focused on the characterization of phlogopite-aninite 2M₁ micas with peculiar composition. For instance, Bigi et al. (1993) analyzed crystals from diorites with high Ti and \(^{3+}\text{Ba}\) content. The authors associated the decrement of the tetrahedral layer thickness to the entrance of \(^{3+}\text{Ba}\) by means of the \(^{3+}\text{Si} + ^{3+}\text{K} ↔ ^{3+}\text{Al} + ^{3+}\text{Ba}\) substitution mechanism. Brigatti et al. (2000) investigated a 2M₁, Al-rich biotite from a pluton of Northern...