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Crystal chemistry of trioctahedral micas-2M_1 from Bunyaruguru kamafugite (southwest Uganda)

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Abstract

The crystal chemistry of 2M_1 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, $Fe_{tot}/(Fe_{tot} + Mg)$, ranging from 0.15 to 0.22. Unit-cell parameters from single-crystal X-ray data are in the range: $5.3252(1) \le a \le 5.3307(1)$, $9.2231(3) \le b \le 9.2315(3)$, $20.1550(6) \le c \le 20.1964(8)$ Å, and $94.994(2) \le \beta \le 95.131(2)°$.

Anisotropic structure refinements, in the space group *C*2/*c*, converged to $2.77 \le R_1 \le 3.52\%$ and $2.91 \le wR_2 \le 4.02\%$. Mössbauer spectroscopy showed that the studied sample has: $^{VI}Fe^{2+} = 60(1)\%$, $^{VI}Fe^{3+} = 24(1)\%$, and $^{IV}Fe^{3+} = 16(1)\%$. 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 [$^{IV}Fe^{3+} \leftrightarrow {}^{IV}Al$]; Ti-oxy [$^{VI}M^{2+} + 2\ (OH)^- \leftrightarrow {}^{VI}Ti^{4+} + 2\ (O^{2-}) + H_2\uparrow$] and Al, Fe^{3+}, Cr-oxy [$^{VI}M^{2+} + (OH)^- \leftrightarrow {}^{VI}M^{3+} + O^{2-} + ½\ (H_2)\uparrow$]; Al, Fe^{3+}-Tschermak [$^{VI}M^{2+} + {}^{IV}Si^{4+} \leftrightarrow {}^{VI}M^{3+} + {}^{IV}Al$]; kinoshitalite [$^{XII}K + {}^{IV}Si^{4+} \leftrightarrow {}^{XII}Ba^{2+} + {}^{IV}Al$] and [$^{XII}K^+ + {}^{IV}Al^{3+} \leftrightarrow {}^{IV}Si^{4+} + {}^{XII}\square$].

The estimation of the OH^- content for Ugandan mica-2M_1 was obtained, for the first time, from the linear regression equation $c = 0.20(2) \times OH^-$ (gpfu) + 19.93(2) derived from literature data of 2M_1-samples with known OH^- content. The orientation of the O-H vector with respect to **c*** was found in the range from 2.0 to 6.9°.

Keywords: Kamafugitic 2M_1-phlogopites, crystal chemistry, substitution mechanisms, Mössbauer, FTIR