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Refinements of the crystal structure of Li-bearing tetra-silicic fluoro micas

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1 Introduction

Potassium Tetra Silicic Fluoro Micas (K-TSFMs) are chemically related to yangzhumingite [$KMg_{2.5}Si_4O_{10}F_2$] [1] and tainiolite [$KMg_2LiSi_4O_{10}F_2$], and are synthesized as non-swelling mica for paint and lubricant materials. K-TSFM often contains Li in synthesized crystals as well as natural minerals. The Li^+ (0.76 Å) occupies the octahedral sites replacing the Al^{3+} (0.535 Å) in the di-octahedral micas to relax the misfit in dimensions between octahedral and tetrahedra sheets. On the contrary, the introduction of Li^+ (0.76 Å) into Mg^{2+} (0.72 Å) site must conduce a slight enlargement of the octahedral volume in K-TSFMs.

2 Experiment

The crystals of K-TSFMs were grown from melt in magnesia crucibles. Starting materials, K_2SiF_6, LiF, MgO, SiO_2, were melt, mixed and kept to 1450°C for 20 min. Electron microprobe showed the chemistry, with the stoichiometric estimation of Li, for 4 samples; $K_{1.0}Mg_{2.5}Si_4O_4F_2$ (I-YZM), $K_{0.8}Mg_{2.6}Si_4O_4F_2$ (V-YZM), $K_{0.7}Li_{0.3}Mg_{2.5}Si_4O_4F_2$ (Li-YZM), and $K_{0.9}Li_{0.5}Mg_{2.3}Si_4O_4F_2$ (TNL). I-YZM has the composition close to ideal formula of yangzhumingite. V-YZM shows the deficiency of K and excess of Mg. Li-YZM is synthetic equivalent of the type specimen of yangzhumingite suggesting a partial substitution of Li^+ for K^+. TNL is an intermediate between V-YZM and the ideal tainiolite.

Single crystal X-ray diffraction data were obtained by three ways; a Rigiku VariMax RAPID with curved IP detector employing Mo *K*α radiation monochromatized by a confocal multilayer optics, a Rigaku AFC7R conventional 4-circle diffractometer with monochromatized Mo *K*α radiation generated by a rotary anode, and a 4-circle diffractometer specially designed for synchrotron radiation at BL-10A, PF, KEK. The lattice parameters determined with synchrotron (λ = 1.00030 Å) data are given with avaraged interatomic distances in Table 1.

3 Results and Discussion

The refinements of the crystal structures suggest that the octahedral volumes are comparable to each other in these crystals. It is worth noting that the octahedral interatomic distances [Mg-(O,F) ≈ 2.06 Å] are smaller than those [Li-(O,F) ≈ 2.12 ~ 2.25 Å] in the Li-micas, such as polylithionite, trilithionite and norrishite.

References

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Table 1. Lattice parameters and mean interatomic distances of K-TSFMs.

	I-YZM	V-YZM	Li-YZM	TNL	I-YZM[2]	Yangzhumingite[1]
a (Å)	5.2472	5.2475	5.2526	5.2499	5.253(1)	5.249(4)
b (Å)	9.0871	9.0947	9.0917	9.0902	9.086(2)	9.095(5)
c (Å)	10.1484	10.1545	10.1480	10.1566	10.159(1)	10.142(5)
β (°)	99.871	99.932	99.887	99.888	99.89(3)	99.96(6)
V (Å^3)	476.73	477.36	477.43	477.50	477.7	476.9(5)
d_{060} (Å)	1.515	1.516	1.515	1.515	1.514	1.516
K-O (Å)	3.108	3.100	3.110	3.114	3.111	
Si-O (Å)	1.626	1.629	1.624	1.626	1.625	
Mg1-O,F (Å)	2.057	2.068	2.060	2.058	2.062	
Mg2-O,F (Å)	2.058	2.064	2.060	2.057	2.064	