SYNTHESIS AND CRYSTAL STRUCTURES OF NEW ALKALI-REE-FLUOROSILICATES

Manninger, T. & Kahlenberg, V.

University of Innsbruck, Institute of Mineralogy & Petrography, Innrain 52, A-6020 Innsbruck, Austria
e-mail: volker.kahlenberg@uibk.ac.at

During a systematic study on the crystal chemistry and the synthesis of REE-fluorosilicates by the flux-method using KF and RbF melts as solvents several new compounds were prepared. Therefore, mixtures with a nutrient:flux ratio of 1:1 were homo-genized, loaded in platinum capsules and welded shut. The containers were fired to 1100 °C in a resistance heated furnace, isothermed for 2 h, followed by slow cooling to 800 °C at 5 °C/h and finally quenched to ambient temperature. In all cases transparent crystals of good optical quality (up to several mm in size) could be easily retrieved by dissolving the flux in distilled water. Furthermore, the crystals were characterized by X-ray single-crystal diffraction (performed at 25 °C). The crystal structures of all phases could be solved by direct methods and difference Fourier synthesis. Structure solution was also employed to establish the chemical composition of the following three compounds:

(1) $K_9Y_3[Si_{12}O_{32}]F_2$, triclinic, space group *P*-1, a=6.8187(3) Å, b=11.3345(4) Å, c=11.3727(5) Å, α=87.846(3)°, β=89.747(3)°, γ=80.524(3)°, V=866.36(6)Å^3, Z=1. Salt inclusion compound based on silicate layers with 6-, 8- and 12-membered rings.

(2) $Rb_2Sc[Si_4O_{10}]F$, tetragonal, space group *I*4/*m*, a=11.2619(3) Å, c=8.3053(4) Å, V=1053.37(7)Å^3, Z=4. Tubular chain structure, isotypic with narsarsukite ($Na_2(Ti,Fe^{3+})Si_4O_{10}(O,F)$ (PEACOR & BUERGER (1962)).

(3) $Rb_2Lu[Si_4O_{10}]F$, monoclinic, space group $P2_1/m$, a=11.6695(3) Å, b=8.5238(2) Å, c=11.8165(3) Å, β=111.753(2)°, V= 1091.67(5) Å^3, Z=4. Tubular chain structure.

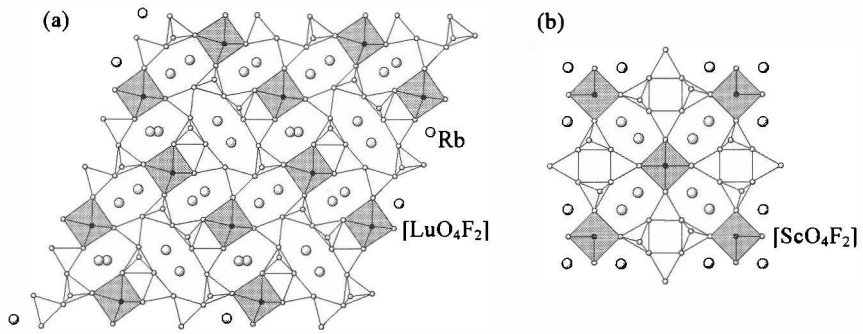

Figure 1. Projections of the crystal structures of (a) $Rb_2Lu[Si_4O_{10}]F$ and (b) $Rb_2Sc[Si_4O_{10}]F$ parallel to the directions of the tubular chains. Linkage between the silicate chains is provided by $(Sc,Lu)O_4F_2$-octahedra.

PEACOR, D.R., BUERGER, M.J. (1962): Am. Mineral. 47, 539-556.