

Single-crystal X-ray diffraction of microlite-group minerals from Volta Grande pegmatites, Sao Joao del-Rei, Minas Gerais, Brazil.

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Pyrochlore-supergroup minerals research is being increased in the last years due to their physical and chemical properties. The prediction and development of pyrochlore-like structure materials expanded the number of technological applications such as oxide superconductors and nuclear-waste disposals. Unfortunately, Brazilian occurrences are only partially characterized. Microlite-group minerals belong to the pyrochlore-supergroup structure with $A_2B_2X_6Y$ stoichiometry. They crystallize in the cubic space group $Fd-3m$, $Z = 8$ with $a = 10.4$ to 10.6 Å. Selected samples from Volta Grande pegmatites, Nazareno pegmatite province, Sao Joao del-Rei, Minas Gerais, Brazil, were studied by electro microprobe and single crystal X-ray-diffraction. Chemical analyses were carried out by means of an electron microprobe (WDS mode, 15kV, 20 nA, 1 µm beam diameter). The crystal structure were studied using Mo $K\alpha$ ($\lambda = 0.71073$ Å) radiation on an Enraf-Nonius Kappa-CCD diffractometer. After this, the crystal structure has been solved and refined using X-ray reflections [$I_{obs} > 2\sigma(I)$] and compositional constraints from electron microprobe analyses as $(Ca,Na,Mn,Sr,Ba,Pb,Ce,U)_{0.35}(Ta,Nb,Si,As,Al)_2O_6$. The occurrence of H_2O at or in the vicinity of the A(16d) and Y(8b) sites due its vacancies was investigated too.

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