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On the crystal chemistry of londonite [$(Cs,K,Rb)Al_4Be_5B_{11}O_{28}$]: A single-crystal neutron diffraction study at 300 and 20 K

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Abstract

The crystal chemistry of londonite, a rare Cs-bearing mineral [ideal chemical formula: $(Cs,K)Al_4Be_4(B,Be)_{12}O_{28}$; a = 7.3098(2) Å at 300 K, space group $P\bar{4}3m$] from the granitic pegmatites of the Antsongombato Gem Mine, Betafo district, Madagascar, has been reinvestigated by means of wavelength dispersive X-ray spectroscopy, laser ablation-inductively coupled plasma-mass spectroscopy, inductively coupled plasma-atomic emission spectroscopy, X-ray powder diffraction, and single-crystal neutron diffraction at 300 and 20 K. Single-crystal anisotropic structural refinement at 300 K gave a final agreement index $R_1 = 0.0479$ for 32 refined parameters and 416 unique reflections with $F_o > 4\sigma(F_o)$. The analysis of the difference-Fourier maps of the nuclear density discounts the presence of hydroxyl groups, as wrongly reported in some of the previous studies. The structural refinements and the chemical analyses suggested that: the tetrahedral 4*e* site (at $x \sim 0.258$) is mainly occupied by Be, but a low amount of B (~3%) likely occurs; the tetrahedral 12*h* site (at $x \sim 0.248$) is mainly occupied by B, but a significant fraction of Be (~12%) is present; the octahedral 4*e* site (at $x \sim 0.361$) is fully occupied by Al; and the 1*a* site (at $x = 0$, with CN = 12) is mainly occupied by Cs, with Rb and K. The significantly high amount of B_2O_3 (~50 wt%) and $Cs+Rb(CsO_2+RbO_2 \geq 8$ wt%) makes the synthetic counterpart of londonite of interest as a potential neutron absorber or a potential host for nuclear waste.

Keywords: Londonite, crystal chemistry, crystal structure, single-crystal neutron diffraction, low temperature