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Crystal structures of Na and K aluminate mullites

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ABSTRACT

Mullite-type alkali aluminates $(K_yNa_{1-y})_{0.67}Al_6O_{9.33}$ were synthesized from amorphous Al and alkali nitrates by sol-gel techniques. Rietveld refinements of six members of the solid solution series (y = 0.0, 0.2, ..., 1.0), together with Fourier syntheses and grid search analyses show that the Na and K atoms reside in the vacant Oc sites, with K at 1/2, 0, 1/2 and Na on a split site off the special position. The number of alkali atoms is restricted to 2/3 atoms per unit cell due to crystal chemical constraints. Consequently, unlike the aluminosilicate mullites, alkali mullites do not form a solid solution series with varying oxygen composition. All compounds studied here crystallize in space group *Pbam* with lattice constants ranging from $a = 7.6819(4)$ Å, $b = 7.6810(4)$ Å, $c = 2.91842(8)$ Å for the Na aluminate to $a = 7.6934(3)$ Å, $b = 7.6727(3)$ Å, $c = 2.93231(7)$ Å for the K aluminate mullite.