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Natural kalsilite, $KAlSiO_4$, with *P*31*c* symmetry: Crystal structure and twinning

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Abstract

A new $KAlSiO_4$ polymorph was found in a granulite facies gneiss from the Punalur district, southern India. The structure was solved and refined on a twinned crystal to an *R* index value of 1.98% for 265 independent reflections. Metamorphic kalsilite is trigonal, space group *P*31*c* with $a = 5.157$ (1) Å, $c = 8.706$ (3) Å, $V = 200.52$ (9) Å^3, $Z = 2$. The overall diffraction symmetry 6/*mmm* exhibited from all the crystals examined arises from a {0001} twinning, related to a mistake in the ordered Al-Si-Al-Si sequence along the *c* axis. The crystal structure is a stuffed derivate of tridymite, and is characterized by six-membered tetrahedral rings with ditrigonal shape. Individual layers of this structure are the same as those of $P6_3$ kalsilite, but are stacked along the *c* axis in an eclipsed manner rather than in the staggered manner of the $P6_3$ structure.