

Al,Si order in the crystal structure of α -eucryptite (LiAlSiO_4)

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ABSTRACT

The crystal structure of α -eucryptite, LiAlSiO_4 , is reinvestigated by combining ^{29}Si NMR spectroscopy and single-crystal X-ray diffraction. The silicon coordination in α -eucryptite of three different samples (two of natural, one of synthetic origin) is shown to be identical on a local scale by means of ^{29}Si MAS NMR spectroscopy. This method also suggests a well ordered arrangement of Si and Al within the crystal structure of α -eucryptite and the presence of two symmetrically non-equivalent sites for silicon. The refinement of the structure of a natural crystal using single-crystal X-ray diffraction confirms these observations and demonstrates the presence of long-range Al-Si order and the acentric space group $R3$.