

## **Al,Si order in the crystal structure of $\alpha$ -eucryptite ( $\text{LiAlSiO}_4$ )**

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### **ABSTRACT**

The crystal structure of  $\alpha$ -eucryptite,  $\text{LiAlSiO}_4$ , is reinvestigated by combining  $^{29}\text{Si}$  NMR spectroscopy and single-crystal X-ray diffraction. The silicon coordination in  $\alpha$ -eucryptite of three different samples (two of natural, one of synthetic origin) is shown to be identical on a local scale by means of  $^{29}\text{Si}$  MAS NMR spectroscopy. This method also suggests a well ordered arrangement of Si and Al within the crystal structure of  $\alpha$ -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  $R3$ .