## Synthesis and structure of a stuffed derivative of α-quartz, Mg<sub>0.5</sub>AlSiO<sub>4</sub>

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## ABSTRACT

A structural derivative of quartz with the composition  $Mg_{0.5}AlSiO_4$  has been grown from glass and characterized using synchrotron X-ray diffraction (XRD), transmission electron microscopy (TEM), and <sup>29</sup>Si nuclear magnetic resonance (NMR) spectroscopy. Rietveld analysis of the XRD data indicates that the framework of  $Mg_{0.5}AlSiO_4$  is isostructural with  $\alpha$ -quartz, rather than  $\beta$ -quartz, as is consistent with previous theoretical modeling (Sternitzke and Müller 1991). Al and Si exhibit long-range disorder over the framework tetrahedral sites, indicated by the absence of the superlattice reflections corresponding to the doubling of *c* relative to that of quartz. Nevertheless, <sup>29</sup>Si NMR measurements show that Al and Si exhibit partial short-range order with an ordering degree of 56%. Electron diffraction reveals superlattice reflections indicative of doubled periodicities along the **a**-axes. Fourier electron density maps show that Mg occupies channel sites that each are bonded to six O atoms, in contrast to the tetrahedral coordination of Li in the  $\beta$ -quartz-type framework for  $\beta$ -eucryptite, LiAlSiO<sub>4</sub>. Furthermore, the concentrations of Mg in adjacent channels are different, resulting in framework distortions that generate the superstructures along **a**.

**Keywords:** Quartz, eucryptite, stuffed derivative, synthesis, crystal structure, synchrotron X-ray diffraction, transmission electron microscopy, nuclear magnetic resonance spectroscopy