American Mineralogist, Volume 100, pages 2191–2198, 2015

Synthesis and structure of a stuffed derivative of α-quartz, $Mg_{0.5}AlSiO_4$

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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 ^{29}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 α-quartz, rather than β-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, ^{29}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 β-quartz-type framework for β-eucryptite, $LiAlSiO_4$. 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