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Unusual Al-Si ordering in calcic scapolite, $Me_{79.6}$, with increasing temperature

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ABSTRACT

A scapolite sample, $Me_{79.6}$, from Slyudyanka, Siberia, Russia, has been studied using in situ synchrotron powder X-ray diffraction (XRD) and Rietveld structure refinements on heating from 26 to 900 °C and on cooling to about 300 °C. The structure was modeled and refined in space group *I4/m*. An accurate room-temperature structure was also obtained by using synchrotron high-resolution powder X-ray diffraction (HRPXRD) data and Rietveld structure refinement. From HRPXRD, the cell parameters are $a = 12.16711(2)$, $c = 7.575466(5)$ Å, and $V = 1121.461(3)$ Å^3; <T1-O> and <T2-O> are 1.643(1) and 1.672(1), respectively, so the T1 ($Al_{0.25}Si_{0.75}$) and T2 ($Al_{0.46}Si_{0.54}$) sites are partially ordered at room temperature. On heating, the <T-O> distances indicate that the T1 and T2 sites become more Si- and Al-rich, respectively, and therefore, ordering increases unusually with increasing temperature. This increase in Al-Si ordering occurs from 892 to 900 °C. At 900 °C, the T1 site becomes fully ordered with only Si atoms, while the T2 site contains $Al_{0.51}Si_{0.49}$ and therefore, is fully disordered. On cooling, the sample does not fully revert back to the original partially ordered state. At 300 °C, all the cell parameters are smaller because of the increased Al-Si ordering that is quenched in.

Keywords: Scapolite, high-temperature crystal structures, Al-Si ordering