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Al, Si, and Mg occupancies in tetrahedrally and octahedrally coordinated sites in synthetic aluminous tremolite

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ABSTRACT

A series of aluminous tremolites was synthesized at 800–850 °C and 6–13 kbar along the join $Ca_{1.8}Mg_{5.2}Si_8O_{22}(OH)_2$-$Ca_{1.8}(Mg_{4.2}Al)(AlSi_7)O_{22}(OH)_2$ by means of the Mg-Tschermaks substitution. Although the amphibole yields were high (97–99 wt%), traces of orthopyroxene, clinopyroxene, amorphous silica, and, for the most aluminous mixture, corundum, were identified in some synthesis products. The samples were characterized by electron microprobe (EMP), X-ray diffraction Rietveld structure refinement (XRD), Fourier-transform infrared (FTIR) spectroscopy, and magic-angle-spinning nuclear magnetic resonance (MAS NMR) spectroscopy for the purpose of identifying the extent of Al, Mg, and Si order-disorder in the octahedral and tetrahedral sites. Both EMP and ^{27}Al NMR verify that the Mg-Tschermaks substitution, with even distribution of Al between tetrahedral and octahedral sites, is obeyed in these amphiboles up to a limit of 1.9 total Al atoms per formula unit (apfu).

^{29}Si MAS NMR spectra indicate that Al substitutes essentially equally into both the T1 and T2 sites. For octahedral sites, the FTIR spectra indicate the presence of Al on the M1, M3, or both sites (presently indistinguishable) by the presence of an (MgMgAl)-OH band at 3652 cm^{-1}, which increases steadily with increasing Al content. The FTIR and ^{27}Al MAS NMR spectra show that Al is always present in the M1-M3 sites as well as the M2 site but partitioned among these sites in ways that are not clearly resolved at present. It is clear in this study that Al is more widely distributed over the octahedral and tetrahedral sites in synthetic aluminous tremolite with only a moderate Al content (<2.0 Al apfu) than has been traditionally thought.