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Short-range order in synthetic aluminous tremolites: An infrared and triple-quantum MAS NMR study

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ABSTRACT

Fourier-transform infrared spectra (FTIR) were recorded on a series of synthetic amphiboles along the join $Ca_{1.8}Mg_{5.2}Si_8O_{22}(OH)_2$–$Ca_{1.8}(Mg_{4.2}Al)(Si_7Al)O_{22}(OH)_2$. The spectra were fitted by up to six component bands by optimization and non-linear least-squares techniques. ^{27}Al MAS NMR and triple-quantum (3Q) MAS NMR spectra were recorded for the synthetic amphibole $Ca_{1.8}(Mg_{4.8}Al_{0.4})(Si_{7.6}Al_{0.4})O_{22}(OH)_2$. The fitted FTIR and NMR spectra show that ^{VI}Al occurs at the M2 site and at the M1 or M3 sites; by analogy with previous crystal-structure refinement results on natural amphiboles, ^{VI}Al occupancy of M2 and M3 is presumed. The fine structure present in the FTIR spectra indicates that they are also affected by NNN (next-nearest-neighbor) interactions. There are two types of NNN arrangements: (1) SiSi or SiAl at adjacent T1T1 dimers; (2) permutation of Mg/Al over M2M2M3 sites. Discounting those arrangements unlikely on bond-valence grounds, there are two arrangements that give rise to five distinct bands in the infrared spectra. There are two principal conclusions: (1) infrared spectra of amphiboles in the principal OH-stretching region can be affected significantly by NNN effects; (2) the small number of bands due to NNN effects indicates that amphiboles show strong short-range order.