American Mineralogist, Volume 84, pages 1033–1040, 1999

^{23}Na, ^{29}Si, and ^{71}Ga MAS-NMR spectroscopy of synthetic gallian-fluor-amphiboles

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ABSTRACT

A magic-angle-spinning nuclear magnetic resonance (MAS NMR) spectroscopic study was done on the series of synthetic gallian-fluor amphiboles to identify the extent of Ga and Si ordering in the tetrahedral sites. Assignment of the peaks in the complex ^{29}Si MAS NMR spectra of pargasitic amphiboles is based on observations of the gradual change in peak intensity and position as well as by comparison with computer simulations of the relative intensities of the ^{29}Si MAS NMR spectra for the amphiboles along the compositional join. The ^{29}Si spectra agree best with models that allow Ga on both the T1 and T2 sites, which supports the previous cation distribution results obtained by Rietveld refinement of powder X-ray diffraction data. It was not possible, however, to discriminate between cation distribution models that allowed completely random mixing of Ga and Si vs. the presence of Ga-O-Ga avoidance on the tetrahedral sites. Comparison of the very high speed ^{71}Ga MAS NMR spectra (35 kHz) with the distribution of Ga in octahedral and tetrahedral sites shows that the ratio of tetrahedral to octahedral site occupancy is vastly overestimated from the NMR spectra due to the large quadrupolar effects of the asymmetrical octahedral site. The ^{23}Na MAS NMR spectra of tremolite and Ga-substituted pargasites show a shift to higher frequency and increasing peak width with Ga content that can be related to the reduction in magnetic shielding produced by the substitution of Ga for Si and Mg.