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LETTER

Forsterite, wadsleyite, and ringwoodite (Mg_2SiO_4): ^{29}Si NMR constraints on structural disorder and effects of paramagnetic impurity ions

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ABSTRACT

We present here high-resolution ^{29}Si MAS NMR data for synthetic samples of forsterite (α-Mg_2SiO_4), wadsleyite (β), and ringwoodite (γ). Enrichment to >99% ^{29}Si provides greatly enhanced signal-to-noise ratios and thus great sensitivity to small features in the spectra. At a detection limit of 0.1 to 0.5%, no six-coordinated Si (^{VI}Si) is observed in any of the polymorphs, although these results could be consistent with theoretical predications of 1 to 2% Mg-Si site disorder in ringwoodite if re-ordering occurs rapidly during cooling. Several small ^{IV}Si peaks in ringwoodite samples may be related to residual defects from this process. In forsterite and wadsleyite, several very small "extra" peaks are observed, many of which are at positions far outside the known range of chemical shifts for ^{29}Si in silicates. These may be caused by "pseudo-contact" shifts from dipolar interactions with unpaired electron spins on trace impurities of paramagnetic transition metal cations.

Keywords: NMR spectroscopy, forsterite, ringwoodite, wadsleyite, high-pressure studies