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Incorporation of Fe and Al in $MgSiO_3$ perovskite: An investigation by ^{27}Al and ^{29}Si NMR spectroscopy

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ABSTRACT

We present ^{27}Al and ^{29}Si magic angle spinning nuclear magnetic resonance (MAS-NMR) spectra of Al- and Fe-bearing, high-pressure pyroxene and perovskite samples, synthesized in a multi-anvil apparatus at 26 GPa and 1900 °C at targeted compositions of $(Mg_{1-x}Fe_x)(Si_{1-x}Al_x)O_3$ ($x = 0.01$, 0.025, and 0.05). ^{27}Al MAS-NMR spectra of the perovskite samples indicate that Al^{3+} replaces both Si^{4+} in the octahedral site and Mg^{2+} in the larger 12-coordinated site. NMR signal loss caused by paramagnetic interactions is often a severe complication when performing NMR on materials containing $Fe^{2+,3+}$; however, careful measurement of signal loss and comparison to total Fe content in these samples sheds light on the nature of Al and Fe incorporation. NMR signal loss for the pyroxenes is linearly related to total Fe content as would be expected in the case of uncorrelated substitution of randomly distributed Al and Fe. However, ^{27}Al signal loss for the perovskite samples increases only slightly between samples with $x = 0.01$ and 0.025 indicating similar coordination of Al by Fe and non-random distribution. Complete signal loss at $Fe/(Fe + Mg) = 0.05$ suggests the upper limit of Fe^{2+} and Fe^{3+} concentration at which useful NMR data can be obtained for this system.

Keywords: NMR spectroscopy, perovskite, pyroxene, paramagnetic shifts, high-pressure studies