The site preference and distribution of low concentration elements in forsterite as determined by NMR

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The olivine crystal structure can accommodate a wide variety of minor and trace elements. However, the short range ordering and site preference of these elements remains uncertain. While advanced theoretical models exist, the limited sensitivity of many experimental techniques has reduced the accuracy with which these models can be confirmed. Compatible elements, such as divalent transition metals, may behave similarly at low and high concentrations. Fewer observations of the distribution and substitution mechanisms of structurally incompatible elements exist. For both compatible and incompatible elements, nuclear magnetic resonance (NMR) provides a nuclide specific, sensitive observation of the coordination environment, allowing quantitative inferences on site preference to be determined.

To investigate the distribution of compatible elements, ^{29}Si NMR spectra have been collected on otherwise pure synthetic forsterite with minor amounts of Fe, Co, or Ni. The transition metal's unpaired electrons produce small, additional peaks whose frequencies are "contact shifted," and which are geometrically dependent on the relationship between the silicon site and neighboring sites occupied by paramagnetic cations. Analyses of these data place further constraints on the site preferences and distributions of these elements at low concentration.

A number of incompatible elements can be observed directly by NMR to determine coordination and substitution mechanisms. Promising observations have been made on Al- and Sc-doped forsterite samples. Electron microprobe analysis was used to determine sample homogeneity, the abundance of the doping element in the bulk forsterite, and the presence of impurity phases. Long ^{27}Al or ^{45}Sc NMR acquisitions were then used to identify the coordination and distribution of the trace element. Plans to continue the study with other sensitive nuclides such as Li, B, Na, and P should further expand these results.