

Scandium-45 NMR of pyrope-grossular garnets: Resolution of multiple scandium sites and comparison with X-ray diffraction and X-ray absorption spectroscopy

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ABSTRACT

Here we present ⁴⁵Sc and ²⁷Al NMR results on Sc-doped pyrope (Mg₃Al₂Si₃O₁₂), grossular (Ca₃Al₂Si₃O₁₂), and an 80% grossular-20% pyrope garnet (grs80) that have recently been well-studied by X-ray diffraction and X-ray spectroscopies. Clearly distinct NMR peaks are observed for Sc in the eight-coordinated X site (pyrope and grs80) and in the six-coordinated Y site (grossular and grs80). X-ray and NMR data agree that only eight-coordinated Sc is present in pyrope and that six-coordinated Sc is predominant in grossular; however, the XRD results also indicated significant X and Z site (four-coordinated) Sc in the Ca-rich garnet. Possible reasons for this apparent discrepancy are discussed. We demonstrate that ⁴⁵Sc NMR is potentially a useful new method for studies of the site occupancies of Sc³⁺ in oxides and silicates, at least in experimental systems where its concentration is a few percent or greater.

Keywords: Crystal structure, pyrope-grossular garnet, scandium in garnet, NMR spectroscopy, pyrope-grossular garnet, scandium-45, aluminum-27