

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

**NAMJUN KIM,<sup>1</sup> JONATHAN F. STEBBINS,<sup>1,\*</sup> SIMONA QUARTIERI,<sup>2,3</sup> AND ROBERTA OBERTI<sup>3</sup>**

<sup>1</sup>Department of Geological and Environmental Sciences, Stanford University, Stanford, California 94305-2115, U.S.A.

<sup>2</sup>Dipartimento di Scienze della Terra, Università di Messina, Salita Sperone 31, I-98166 Messina S. Agata, Italy

<sup>3</sup>CNR, Istituto di Geoscienze e Georisorse, unità di Pavia, via Ferrata 1, I-27100 Pavia, Italy

### **ABSTRACT**

Here we present <sup>45</sup>Sc and <sup>27</sup>Al NMR results on Sc-doped pyrope (Mg<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>), grossular (Ca<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>), 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 <sup>45</sup>Sc NMR is potentially a useful new method for studies of the site occupancies of Sc<sup>3+</sup> 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