

## **Constraining $^{17}\text{O}$ and $^{27}\text{Al}$ NMR spectra of high-pressure crystals and glasses: New data for jadeite, pyrope, grossular, and mullite**

**KIMBERLY E. KELSEY,<sup>1,\*</sup> JONATHAN F. STEBBINS,<sup>1</sup> LIN-SHU DU,<sup>1,†</sup> AND BEN HANKINS<sup>2</sup>**

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

<sup>2</sup>U.S. Geological Survey, 345 Middlefield Road, Menlo Park, California 94025, U.S.A.

### **ABSTRACT**

The  $^{17}\text{O}$  NMR spectra of glasses quenched from melts at high pressure are often difficult to interpret due to overlapping peaks and lack of crystalline model compounds. High-pressure aluminosilicate glasses often contain significant amounts of  $^{15}\text{Al}$  and  $^{6}\text{Al}$ , thus these high-pressure glasses must contain oxygen bonded to high-coordinated aluminum. The  $^{17}\text{O}$  NMR parameters for the minerals jadeite, pyrope, grossular, and mullite are presented to assist interpretation of glass spectra and to help test quantum chemical calculations. The  $^{17}\text{O}$  NMR parameters for jadeite and grossular support previous peak assignments of oxygen bonded to Si and high-coordinated Al in high-pressure glasses as well as quantum chemical calculations. The oxygen tricluster in mullite is very similar to the previously observed tricluster in grossite ( $\text{CaAl}_4\text{O}_7$ ) and suspected triclusters in glasses. We also present  $^{27}\text{Al}$  NMR spectra for pyrope, grossular, and mullite.

**Keywords:** NMR spectroscopy, pyrope, grossular, mullite, jadeite, aluminosilicate glasses, oxygen-17, aluminum-27