

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

KIMBERLY E. KELSEY,^{1,*} JONATHAN F. STEBBINS,¹ LIN-SHU DU,^{1,†} AND BEN HANKINS²

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

²U.S. Geological Survey, 345 Middlefield Road, Menlo Park, California 94025, U.S.A.

ABSTRACT

The ^{17}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}Al and ^{6}Al , thus these high-pressure glasses must contain oxygen bonded to high-coordinated aluminum. The ^{17}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}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 (CaAl_4O_7) and suspected triclusters in glasses. We also present ^{27}Al NMR spectra for pyrope, grossular, and mullite.

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