

## **Characterization of cation environments in polycrystalline forsterite by $^{25}\text{Mg}$ MAS, MQMAS, and QCPMG NMR**

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### **ABSTRACT**

Forsterite ( $\text{Mg}_2\text{SiO}_4$ ) is a silicate mineral frequently studied in the Earth sciences as it has a simple crystal structure and fast dissolution kinetics (elemental release rates under typical conditions on the order of  $10^{-7}$  mol/m<sup>2</sup>/s<sup>1</sup>). During the dissolution process, spectroscopic techniques are often utilized to augment solution chemical analysis and to provide data for determining reaction mechanisms. Nuclear magnetic resonance (NMR) is able to interrogate the local bonding arrangement and coordination of a particular nuclide to obtain structural information. Although previous NMR studies have focused on the silicon and oxygen environments in forsterite, studies focusing on the two nonequivalent magnesium environments in forsterite are limited to a few single-crystal studies. In this study, we present the results of  $^{25}\text{Mg}$  MAS, MQMAS, and static QCPMG experiments performed on a powdered sample of a pure synthetic forsterite. We also present spectral fits obtained from simulation software packages, which directly provide quadrupolar parameters for  $^{25}\text{Mg}$  nuclei occupying each of the two nonequivalent magnesium sites in the forsterite structure. These results are compared to calculations of the electric field gradient tensor conducted in previous ab initio studies to make definitive assignments correlating each peak to their respective magnesium site in the forsterite structure. Although previous NMR investigations of forsterite have focused on single-crystal samples, we have focused on powdered forsterite as the increased surface area of powdered samples makes them more amenable to laboratory-scale dissolution studies and, ultimately, the products from chemical weathering may be monitored and quantified.

**Keywords:** Forsterite, magnesium,  $^{25}\text{Mg}$ , NMR, MQMAS, QCPMG