

## **Magnesium coordination environments in glasses and minerals: New insight from high-field magnesium-25 MAS NMR**

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### **ABSTRACT**

A comparison of  $^{25}\text{Mg}$  magic angle spinning (MAS) NMR spectra of crystalline and glassy diopside ( $\text{CaMgSi}_2\text{O}_6$ ) reveals that the chemical shift in the disordered phase corresponds to that of the mineral, suggesting that sixfold coordination is essentially retained upon vitrification. Likewise, a crystalline leucite analogue ( $\text{K}_2\text{MgSi}_3\text{O}_{12}$ ) known to possess fourfold-coordinated Mg has the same peak position as the corresponding glass. In addition to being a sensitive probe of local structure by analogy with crystalline phases, these data may be understood in terms of the effect of competing cation field strengths: competing network modifier cations with higher field strength induce higher magnesium coordination numbers, with a consequent increase in bond length and decrease in chemical shift. This work demonstrates the utility of NMR at 14.1 Tesla for probing the coordination environment of Mg in glasses and minerals, and suggests great potential for high-field NMR investigations of quadrupolar nuclides with low resonance frequencies in amorphous systems.