

## **Oxygen triclusters in crystalline $\text{CaAl}_4\text{O}_7$ (grossite) and in calcium aluminosilicate glasses: $^{17}\text{O}$ NMR**

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### **ABSTRACT**

We present  $^{17}\text{O}$  MAS NMR data for crystalline calcium dialuminate (grossite),  $\text{CaAl}_4\text{O}_7$  and monoaluminate,  $\text{CaAl}_2\text{O}_4$ . The first of these contains an oxygen tricluster site and serves as a model compound for sites of this type in aluminosilicate glasses. Tricluster site NMR parameters are distinct from those of bridging O atoms (Al-O-Al), allowing partial resolution in triple quantum MAS NMR spectra. Such spectra for calcium aluminosilicate glasses are consistent with the presence of a small fraction of tricluster sites. Observed chemical shifts for non-bridging oxygen (NBO) atoms in an impurity phase in the  $\text{CaAl}_2\text{O}_4$  sample are distinct from those for NBO in Ca-aluminosilicate glasses, indicating that the latter are primarily bonded to Si, not Al.