

Oxygen triclusters in crystalline CaAl_4O_7 (grossite) and in calcium aluminosilicate glasses: ^{17}O NMR

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ABSTRACT

We present ^{17}O MAS NMR data for crystalline calcium dialuminate (grossite), CaAl_4O_7 and monoaluminate, CaAl_2O_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 CaAl_2O_4 sample are distinct from those for NBO in Ca-aluminosilicate glasses, indicating that the latter are primarily bonded to Si, not Al.