

LETTER

Fivefold-coordinated aluminum in tectosilicate glasses observed by triple quantum MAS NMR

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ABSTRACT

Eight glasses with molar $\text{Mg}/2\text{Al} \approx 1$ in the system $\text{MgO}-\text{Al}_2\text{O}_3-\text{SiO}_2$ have been studied by magic angle spinning (MAS) NMR spectroscopy. Using triple quantum (3Q) NMR techniques we find evidence for significant concentrations of Al coordinated to five O atoms in all glasses, the proportion increasing with decreasing Mg/Al and decreasing silica content. In glasses with $\text{Mg}/2\text{Al} = 1$, up to 6% of the Al is estimated to be coordinated to five rather than four O atoms. Calculations of the polymerization state of these liquids made assuming that all aluminum is in tetrahedral coordination charge balanced by magnesium are thus seriously in error. Such errors may be of even greater importance at the high temperatures and pressures relevant to the Earth and materials sciences.