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Interaction between composition and temperature effects on non-bridging oxygen and high-coordinated aluminum in calcium aluminosilicate glasses

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Abstract

The configurational changes that occur with temperature, and how these vary with composition, affect the thermodynamic and transport properties of aluminosilicate melts but are not well understood. We present here high-resolution ^{27}Al and ^{17}O NMR data on several calcium aluminosilicate glasses along two silica isopleths crossing the metaluminous (SiO_2-$CaAl_2O_4$) join, prepared with varying quench rates and thus with fictive temperatures spanning approximately 100 K. In all compositions, five-coordinated aluminum increases with increasing fictive temperature. For glasses along the 60 mol% SiO_2 isopleth, NBO also increases with increasing fictive temperature; this is less obvious for the glasses along the 30 mol% SiO_2 isopleth. The data suggest the mixing of bridging oxygen contributes to the magnitude of the observed temperature effect on NBO and continue to suggest the existence of multiple mechanisms that generate NBO and ^{V}Al.

Keywords: NMR spectroscopy, non-bridging oxygen, five-coordinated aluminum, temperature effects