

## **Network cation coordination, oxygen speciation, and modifier cation effects on silicate glass and melt structure**

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Recent spectroscopic (and other) studies of multicomponent oxide glasses have yielded details that often have required the re-thinking of “conventional wisdom” on both glass and melt structure. These include the presence of non-bridging oxygens in aluminosilicates even of peraluminous compositions, significant fractions of aluminum with coordination numbers greater than 4 even in highly peralkaline systems and even at ambient pressure, and partial ordering of both network forming and network modifying cations, the latter contrary to common solution models based on ideal mixing. All of these factors can or should enter into models of melt properties, whether based on empirical fits or theoretical considerations. Modifier cation field strength (e.g. Mg>Ca>Na>K) is now known to have large effects on equilibria among network species, involving both oxygen and cation coordinations, as smaller and higher charged cations promote the concentration of negative charge on anions, such as on non-bridging oxygens and on bridging oxygens shared by tetrahedral cations with charges less than 4+ (e.g. Al<sup>3+</sup> and B<sup>3+</sup>). When network cation coordination can readily change as a function of temperature, pressure, or composition, as in aluminoborosilicates of wide application in advanced glass technologies, interactions of such species can be quite complex and even surprising. We will discuss new results on such compositionally complex systems to explore implications for magmatic systems at high temperatures and pressures.