

The role of modifier cations in network cation coordination increases with pressure in aluminosilicate glasses and melts from 1 to 3 GPa

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ABSTRACT

Previous studies have shown that both NBO content and modifier cation field strength play important roles in increasing the network cation coordination with increasing pressure. It has been observed in previous studies that the increase in average Al coordination with pressure in alkali aluminosilicates depends on NBO concentration, where large increases in Al coordination with pressure have been observed for compositions containing significant concentrations of NBO and little or no Al coordination increase observed in glasses containing negligible NBO at pressures ranging from 1 to 3 GPa. Similarly, in NBO rich aluminosilicates and aluminoborosilicates containing different modifier cations, it was reported that the increase in average Al coordination followed a steeper rise with increasing pressure in compositions containing higher field strength modifiers. In this study, we look at Ca- and Mg-aluminosilicate glasses across all three compositional regimes (peralkaline, metaluminous, and peraluminous) to study the effect of both oxygen speciation and modifier cation field strength on network cation coordination changes with pressure. Our study shows that in Mg aluminosilicate glasses (both peralkaline and metaluminous), the increase in average Al coordination can be quite large and show no significant impact from differences in oxygen speciation (NBO content). In contrast, in Ca-aluminosilicate glasses, the oxygen speciation has a notable impact with the average Al coordination following a steeper rise with increasing pressure in a peralkaline composition and less steep for a metaluminous composition.

Keywords: High pressure, glasses and melts, NMR spectroscopy, aluminum coordination, non-bridging oxygen, cation field strength, densification, aluminosilicate