

**LETTER**

**Aluminum coordination and the densification of high-pressure aluminosilicate glasses**

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**ABSTRACT**

To better understand the relationship between atomic-scale structures and densities of aluminosilicate glasses and liquids, we used <sup>27</sup>Al MAS NMR to determine the speciation of aluminum ions in K<sub>3</sub>AlSi<sub>3</sub>O<sub>9</sub>, Na<sub>3</sub>AlSi<sub>3</sub>O<sub>9</sub>, and Ca<sub>3</sub>Al<sub>2</sub>Si<sub>6</sub>O<sub>18</sub> glasses quenched from melts at 3 to 10 GPa. These data are a first approximation of high-pressure melt structure and illustrate the effects of the type of modifier cation. High field strength modifier cations (e.g., Ca) clearly induce more high-coordinated Al than lower field strength cations (e.g., Na and K). Measured glass densities show that, especially with rapid decompression, a significant portion of the total densification observed in-situ in melts is retained on return to ambient temperature and pressure. Observed increases in Al coordination are well correlated with decreased volume, which suggests that this structural change is a major part of the mechanism for recovered densification of high-pressure melts. Additionally, <sup>23</sup>Na MAS NMR, combined with the <sup>27</sup>Al MAS spectra and density determinations, reveal that other changes, such as the compression of modifier cation sites and/or decreased network bond angles, must also be significant, especially at low pressure.