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Cation order and hydrogen bonding of high-pressure phases in the Al_2O_3-SiO_2-H_2O system: An NMR and Raman study

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ABSTRACT

Topaz-OH, phase egg, and δ-AlOOH are hydrous phases in the Al_2O_3-SiO_2-H_2O system that have been found to be stable at successively higher pressures up to those corresponding to the lower mantle, and thus they may be important water reservoirs in the deep mantle. We have applied ^{1}H, ^{29}Si, and ^{27}Al nuclear magnetic resonance (NMR) and Raman spectroscopy to shed new light on the structure of these phases. ^{29}Si and ^{27}Al NMR results clearly revealed that the Si-Al distribution in phase egg is partially disordered. The presence of structural disorder in topaz-OH was also confirmed. ^{1}H NMR and Raman data are both consistent with strong, but asymmetric hydrogen bonding in δ-AlOOH and phase egg, and a range of hydrogen bonding distances in topaz-OH. The observed structural disorder and hydrogen bonding could be responsible for the high upper temperature stability limits (1500~1700 °C) of phase egg and topaz-OH, and are also relevant to the incorporation mechanisms of water in nominally anhydrous stishovite.

Keywords: NMR spectroscopy, topaz, phase egg, δ-AlOOH, Raman spectroscopy, crystal structure, order-disorder