

Dense hydrous magnesium silicates, phase D, and superhydrous B: New structural constraints from one- and two-dimensional ^{29}Si and ^1H NMR

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ABSTRACT

To gain new structural insights into phase D and superhydrous B, two phases of potential mantle water reservoir, we have applied a range of one- (1D) and two-dimensional (2D) ^1H and ^{29}Si NMR techniques, as well as Raman spectroscopy, to samples synthesized at 24 GPa and 900–1100 °C. These data have revealed that phase D is characterized by disordered and varying local structures around both Si and H. The ^{29}Si NMR spectra of phase D contain a nearly symmetric, broad peak near -177.7 ppm, attributable to octahedral Si with local structural disorder. The high-resolution ^1H CRAMPS spectra of phase D contain a main broad peak near 12.6 ppm with shoulders near 10 and 7 ppm, suggesting a distribution of hydrogen bonding distances. For superhydrous B, our comprehensive 2D ^1H and ^{29}Si NMR results have clearly revealed that it contains dissimilar hydrogen (H1-H2) pairs and one tetrahedral Si site, consistent with space group *Pnn2*.

Keywords: Phase D, superhydrous B, NMR, Raman, order/disorder, space group