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# Dense hydrous magnesium silicates, phase D, and superhydrous B: New structural constraints from one- and two-dimensional $^{29}$Si and $^{1}$H 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) $^{1}$H 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 $^{1}$H 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 $^{1}$H 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 *Pnn*2.

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