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Structural transitions in water under extreme conditions: implications for hydrothermal fluids.

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Although the microscopic structure of water has been thoroughly investigated, a conclusive picture that spans a wide range of thermodynamic conditions remains elusive. Many proposed water models predict the coexistence of two distinct structural forms—low-density water (LDW) and high-density water (HDW)—with the transition between these forms occurring between approximately 0.2 and 0.4 GPa. This liquid–liquid phase transition (LLPT) is thought to involve the collapse of the second coordination shell via the breaking or strengthening of hydrogen bonds between water molecules.

This research aims to elucidate this structural transitions in liquid water and their effects on the thermodynamic properties of aqueous fluids under extreme pressure conditions. We precisely control the pressure of an aqueous fluid–mineral mixture using a diamond anvil cell (DAC) and probe the system with Raman spectroscopy to monitor water's compressibility and bond dynamics. Preliminary results obtained from an aqueous sulfate system confirm that the transition from LDW to HDW indeed occurs between 0.2 and 0.4 GPa. These observations are in agreement with previous studies, suggesting that the LLPT influences the equilibrium sulfate concentration in solution. Moreover, variations in the chemical composition of the fluid appear to serve as a sensitive indicator of this phase transition. This correlation between chemical composition and phase behaviour provides a powerful tool for probing the interplay between solute–solvent interactions under variable mantle conditions.

These results can have implications for hydrothermal fluids that are of immense importance in geochemical processes, particularly in the Earth's mantle, where they play a key role in heat and mass transport. In subduction zones, for example, hydrothermal fluids can disrupt mineral bonds in the mantle, thereby lowering melting points and facilitating magma generation and the formation of volcanic arcs. Their efficiency in permeating rocks also allows them to dissolve and transport large amounts of salts and metal-bearing complexes, which is critical to the genesis of ore deposits.

Our findings not only provide valuable insights into the complex behaviour of water under extreme conditions but also offer essential benchmarks for evaluating water models and improving our understanding of the role of hydrothermal fluids in geologic processes.