

Abstract Submitted
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Stiffening of Dilute Alcohol and Alkane Mixtures with Water¹

HANK ASHBAUGH, Tulane Univ — We probe the anomalous compressibilities of dilute mixtures of alcohols and alkane gases in water using molecular simulations. The response to increasing solute concentration depends sensitively on temperature, with the compressibility decreasing upon solute addition at low temperatures and increasing at elevated temperatures. The thermodynamic origin of stiffening is directly tied to the solute's partial compressibility, which is negative at low temperatures and rises above water's compressibility with increasing temperature. Hydration shell waters concurrently tilt towards clathrate-like structures at low temperatures that fade with heating. Kirkwood-Buff theory traces the solute's partial compressibility to changes in the solute-water association volume upon heating and incongruous packing of waters at the boundary between the more structured hydration shell and bulk water.

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