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Temperature and Lengthscale Dependence of Solvophobic Solvation in a Water-like Liquid JOHN DOWDLE, PETER ROSSKY, University of Texas at Austin — Temperature and lengthscale dependence of the solvation of cavity solutes is investigated along the saturation curve of the Jagla liquid, a simple liquid consisting of particles that interact via a spherically symmetric potential combining hard and soft core interactions. The results are compared with an identical calculation for a model of a typical atomic liquid, the Lennard-Jones potential, and with predictions for cavity solubilities in water made by the recently developed cavity equation of state. We find that the Jagla liquid captures the qualitative thermodynamic behavior of hydrophobic hydration as a function of temperature for both small and large lengthscale solutes. The results suggest that a competition between two lengthscales that favors low-density, open structures as temperature is decreased is an essential interaction of a liquid that models hydrophobic hydration.

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