Pressure Effects on Polymer Coil-Globule Transitions near an LCST

DAVID SIMMONS, ISSAC SANCHEZ, University of Texas at Austin — A model for the pressure - temperature behavior of the coil-globule transition (CGT) of a polymer in dilute solution is developed without adjustable parameters. The predicted pressure-temperature conformational behavior semi-quantitatively correlates with extant experimental data. The model yields a heating induced coil-to-globule transition (HCGT) temperature that increases with pressure until it merges with a cooling induced coil-to-globule transition (CCGT). The point at which the CCGT and HCGT meet is a hypercritical point that also corresponds to a merging of lower critical solution temperature (LCST) and upper critical solution temperatures (UCST). Theoretical results are discussed in terms of a generalized polymer/solvent phase diagram that possesses two hypercritical points.

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