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Phase Transitions and Helix Formation of a Fused Square-Well-Sphere[1] MICHAEL MROZ, MARK TAYLOR, Dept. of Physics, Hiram College — This study involves observing phase transitions of a flexible polymer chain made of N = 20 fused square-well-sphere monomers, with the hard-core diameter d and square-well diameter Rd, connected by bonds of fixed length L less than d. The density of states of the polymer is calculated using the Wang-Landau simulation technique. The density of states is utilized to compute thermodynamic and average structural properties of the chain. A temperature-interaction range (T-R) phase diagram was constructed for a chain of bond length L = 0.625d. With decreasing temperature this chain undergoes a coil-globule (i.e., collapse) transition followed by one or more low temperature transitions to an ordered ground-state structure. For R greater than 1.25 this ground state is a simple helix while for smaller R the ground state is a wrapped structure, in which one end of the chain forms a linear core about which the rest of the chain is helically wound. The low temperature transition takes on a first-order character for R less than 1.1.

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