141h A Monte Carlo Study on Structural Properties of Dendrimer-Polymer Conjugates

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Structural properties of a neutral dendrimer-polymer conjugate are investigated by off-lattice Monte Carol simulations in near theta condition. The conjugate is a dendrimer with linear polymers grafted to its end segments. A bead-spring model along with Lennard-Jones potential is applied to simulate the structure of the conjugates. We find that the grafted polymers can expand the dendrimer moiety of a conjugate owning to the additional steric effect imposed. As a result, the core dendrimer has a more ordered structure and its terminal segments fold back to a lesser extent. Nevertheless, no clear boundary separates the dendrimer moiety and the polymer attachment. The grafted polymers with sufficient length show a scaling behavior of rodlike chains, and hence the conjugate is less compact than an unmodified dendrimer. The dendrimer swelling caused by the polymer attachment gives rise to more free space for drug encapsulation. The size expansion increases with the length of grafted chains until it gets saturated when the chain becomes sufficiently long.