

Molecular Simulation of the Shear Viscosity and Phase Behavior of Dendrimers

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Dendrimers are a new class of highly branched polymers consisting of short chain units with multifunctional groups at both ends. Starting from an initiator core, the successive reaction of the functional groups with other units generates a highly branched chain molecule, which resembles a Cayley tree. Dendrimer molecules are characterized by the number of generations they contain (g), the functionality of the end groups (b), and the number of monomer segments or separator length (n) between the functional groups. The number of monomers (N) in a dendrimer grows rapidly with each successive generation obeying the relationship, $N = nb[(b - 1)g - 1]$. We have used non-equilibrium molecular dynamics to examine the viscosity behavior of dendrimers under shear. The results for dendrimers up to generation number 4 show that there are quantitative differences in the viscoelastic properties of dendrimers compared with linear systems of equivalent size. A particular feature of the work was the examination of mixtures of dendrimers plus linear chains and a complete shape analysis. We have also used a molecular dynamics implementation of the Gibbs Ensemble to examine the phase equilibria properties of both pure dendrimers and mixtures composed of dendrimers plus linear systems.