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Monte Carlo Simulation of Reversibly Associating Networks[1]
SHIHU WANG, CHUN-CHUNG CHEN, ELENA E. DORMIDONTOVA, Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OHIO 44106 — We applied Monte Carlo simulations to study the reversible network formation through oligomers end-functionalized by ligands capable of complexation in 3:1 ratio with metal ions acting as crosslinkers. By varying the oligomer concentration and metal-to-oligomer ratio, we studied the fractions of different associating species and the molecular weight distribution. The conditions for network formation (over the percolation threshold) were determined using three different criteria, which lead to similar results. The molecular weights of species in the corresponding sol and gel phases were obtained along with the fractions of small rings, dangling ends, and network mesh sizes. An analytical model based on the equilibrium among different associating species and classical gelation theory modified to account for unequal reactivity/cooperativity was developed. The predictions of the analytical model are in good agreement with the simulation results, which compare favorably with experimental observations.

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