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Computer simulation of supramolecular assembly by metal-ligand complexation[1] SHIHU WANG, CHUN-CHUNG CHEN, ELENA E. DORMIDONTOVA, Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OHIO 44106 — Monte Carlo simulations were employed to study the supramolecular assembly of oligomers end-functionalized by ligands capable of complexation with metal ions. The properties of these metallo-supramolecular polymers strongly depend on the oligomer concentration, strength of complexation, and metal-to- ligand ratio. At high oligomer concentration the average molecular weight exhibits a maximum near the stoichiometric composition and decreases for higher or lower metal content. On the other hand, at low oligomer concentration the molecular weight shows a local minimum around the stoichiometric composition. This unusual behavior is attributed to the larger population of small rings around the stoichiometric composition, which make up a significant fraction of the overall molecular weight at low oligomer concentration. This effect is especially pronounced at low temperature, where the fraction of rings is higher. The fraction of chains and rings for different concentrations, temperatures and oligomer lengths were calculated and compared with experimental data.

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Shihu Wang
Case Western Reserve University, Cleveland, OHIO 44106

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