Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Computer Simulation of Metallo-Supramolecular Networks[1]
SHIHU WANG, CHUN-CHUNG CHEN, ELENA DORMIDONTOVA, Department of Macromolecular Science and Engineering, Case Western Reserve University — Using Monte Carlo simulation we studied formation of reversible metallo-supramolecular networks based on 3:1 ligandmetal complexes between end-functionalized oligomers and metal ions. The fraction of 1:1, 2:1 and 3:1 ligand-metal complexes was obtained and analyzed using an analytical approach as a function of oligomer concentration, c and metal-to-oligomer ratio. We found that at low concentration the maximum in the number-average molecular weight is achieved near the stoichiometric composition and it shifts to higher metal-to- oligomer ratios at larger concentrations. Predictions are made regarding the onset of network formation, which occurs in a limited range of metal-to-oligomer ratios at sufficiently large oligomer concentrations. The average molecular weight between effective crosslinks decreases with oligomer concentration and reaches its minimum at the stoichiometric composition, where the high-frequency elastic plateau modulus approaches its maximal value. At high oligomer concentrations the plateau modulus follows a $c^{1.8}$ concentration dependence, similar to recent experimental results for metallo-supramolecular networks.

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Date submitted: 09 Dec 2008   Electronic form version 1.4