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Molecular Dynamics Simulations of Polyelectrolyte-Polyampholyte Complexes. Effect of Solvent Quality and Salt Concentration. JUNHWAN JEON, ANDREY DOBRYNIN, Polymer Program, Institute of Materials Science, Department of Physics, University of Connecticut — Using molecular dynamics simulations we have studied complexation in polyelectrolyte-polyampholyte mixtures in poor solvent conditions for the polyelectrolyte backbone. In a poor solvent a polyelectrolyte form a necklace-like structure. Upon forming a complex with both random and diblock polyampholytes a polyelectrolyte chain changes its necklace conformation by forming one huge bead. The collapse of the polyelectrolyte chain occurs due to neutralization of the polyelectrolyte charge by polyampholytes. In the case of the random polyampholyte the more positively charged sections of the chain adsorb on the surface of the globular bead while more negatively charged chain sections form loops surrounding the collapsed core of the aggregate. In the case of diblock polyampholyte the positively charged block and a part of the negatively charged block wraps around the collapsed polyelectrolyte with a substantial section of the negatively charged block sticking out from the collapsed center of the aggregate. These structures appear as a result of optimization of the net electrostatic energy of the complex and short-range attractive interactions between monomers of the polyelectrolyte chain.

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