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Conformation of Randomly Sulfonated Pentablock Ionomers in Dilute Solution: Molecular Dynamic Simulation Study DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — As part of our efforts to define the factors that control the structure and dynamics of structures ionic polymers, the conformation of a pentablock copolymer that consists of randomly sulfonated polystyrene, an ionomeric block, bound to poly-ethylene-r-propylene end caped by poly-t-butylstyrene has been studied in dilute solutions using molecular dynamic simulations. Multi-block copolymers offer a means to tailor several properties into one molecule, taking advantage of their rich phase diagram together with unique properties of specific blocks. We varied the solvent quality for the different blocks and followed the changes in conformation. The spatial configuration of the pentablock as well as the dynamics of the polymer was studied. We find that, independent on the solvent, the higher the sulfonation level, the lower R_g. The static and dynamic structure factors were calculated and compared in an implicit poor solvent, water and a common solvent. These data are compared with results obtained from neutron scattering.

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