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Molecular Dynamics Simulations of a Dendritic Polyelectrolyte with Flexible Spacers in Salt-free Solution QI LIAO, YONG LIN, XIGAO JIN, CHARLES C. HAN, PPCL, Joint Lab. of Polymer Science and Materials,Institute of Chemistry, Chinese Academy of Science, Beijing 100080, China — We present the results of molecular dynamics simulation of a dendritic polyelectrolyte in a dilute salt–free solution. The dendritic polyelectrolyte is modeled as an ensemble of bead spring regular-branched chain of charged Lernard-Jones particles with explicit counterions. The simulations were performed covering a wide range of molecular variables of the dendritic polyelectrolyte such as generation number, spacer length, and charge density. The relaxation time of dendrimer size, the conformation of spacers, the size depend of dendrimer on the generation and charge density are discussed and compared with a Flory-type theory. We determined the osmotic coefficients of the dilute dendritic polyelectrolyte solution, and compared with the prediction of cell model of charged sphere.

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