

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Computational titrations of linear and branched polyethyleneimine JESSE ZIEBARTH, YONGMEI WANG, University of Memphis — Despite a great deal of interest in polyethyleneimine (PEI) for its potential use as a gene therapy vector, the protonation state of this polycation is currently not well understood. PEI is rare among polyelectrolytes as every third atom along the backbone of the polymer is a protonable nitrogen. The closeness of these potentially charged sites can lead to high electrostatic repulsion and a large shift in the effective pKa of the amine groups as the degree of protonation increases. Previous experimental and theoretical estimates of the degree of protonation of PEI under physiological conditions have ranged from 0.15 to 0.80. Here, we perform computational titrations on coarse-grained models of both branched and linear PEI under various conditions. Chain length, degree of branching, salt concentration, and the solvent dielectric constant are varied to determine how these factors influence the protonation of PEI.

Jesse Ziebarth
University of Memphis

Date submitted: 30 Nov 2008

Electronic form version 1.4