

## Modeling of cationic polyelectrolyte solutions in water: influence of the hydrophobic groups on interaction with sodium halides

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We investigated the electrostatic and hydrophobic effects in aqueous solutions of charged chain-like polyions. An explicit water molecular dynamics simulation results for solutions of aliphatic 3,3 and 6,6 ionene oligocation (six monomer units long) in mixture with various low-molecular weight electrolytes are presented. Fluorine, chlorine, bromine, and iodine anions are chosen as the counterions, and sodium ion is the coion in all cases. Different numbers of methylene groups (three in 3,3 and six in 6,6 ionene) separate charged groups and regulate degree of electrostatic/hydrophobic impact of oligocations on the system properties. The explicit water approach reveals the ion-specific effects important for understanding counterion-polyion association. Due to the smaller charge density of the 6,6 ionene, less counterions are located around the oligoion. We also found that the presence of extra hydrophobic groups on the 6,6 ionene shifts the hydrating waters toward the larger distances in comparison with the corresponding 3,3 ionene molecule. The simulation helps us to understand the behavior of osmotic coefficients observed experimentally in aqueous solutions of ionenes with varying degree of hydrophobicity and different counterions. The study seem to explain low osmotic pressure measured in aqueous solutions of polyelectrolytes containing hydrophobic groups.