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XIV МЕЖДУНАРОДНАЯ НАУЧНАЯ КОНФЕРЕНЦИЯ «ПРОБЛЕМЫ СОЛЬВАТАЦИИ И КОМПЛЕКСООБРАЗОВАНИЯ В РАСТВОРАХ»

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СОДЕРЖАНИЕ

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XIV Международная научная конференция «Проблемы сольватации и комплексообразования в растворах»

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carbon atoms in the alkyl chain of AAIL = 4, 6, 8; X = Cl – chloride, Br – bromide, [Leu] – L-Leucinate, [Val] – L-Valinate, [Lys] – L-Lysinate) and K_2HPO_4 and K_3PO_4 as inorganic salts. L-tryptophan was chosen as a model solute due to its high hydrophobicity.

As a result, new data on partition coefficients of L-tryptophan in the selected ABSs were obtained. The results showed that in ABSs with some AAILs, higher distribution coefficients are observed than in the systems with halide ILs. Moreover, a correlation was established between the partition and phase behavior (the results were obtained by us earlier [3]) of ABSs. It was found that, in general, partition coefficients of L-tryptophan are larger for ABSs with a wider heterogeneous region.

It should be concluded that ABSs with AAILs are promising for the extraction of small biomolecules. The results can be useful for understanding the driving force of phase separation and distribution of the solutes.

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POLYMERIC IONIC LIQUIDS IN DILUTE AQUEOUS SOLUTION: MD SIMULATION OF POLY(DIMETHYL DIALLYL AMMONIUM) SALTS

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Polymeric ionic liquids (PILs) containing amino acid anions is an important new class of PILs that attract an increasing attention. The effect of the anion chemistry on the conformational behavior of the PIL chain is one of the key issues.

In this work we report the results of molecular dynamics simulations for dilute aqueous solutions of poly(dimethyl diallyl ammonium) chloride (PDADMAC) and poly(dimethyl diallyl ammonium) lysinate (PDADMALys). Evolution of the polycation chain from a compact globule into an expanded coil is examined and discussed in terms of theoretical models. The effect of presence of ionic pairs on the free energy of the chain is estimated from the theory of dipolar chains [1, 2]. Conformational and diffusive characteristics of PDADMAC and PDADMALys are compared, revealing the effects of size and shape of the counterion.

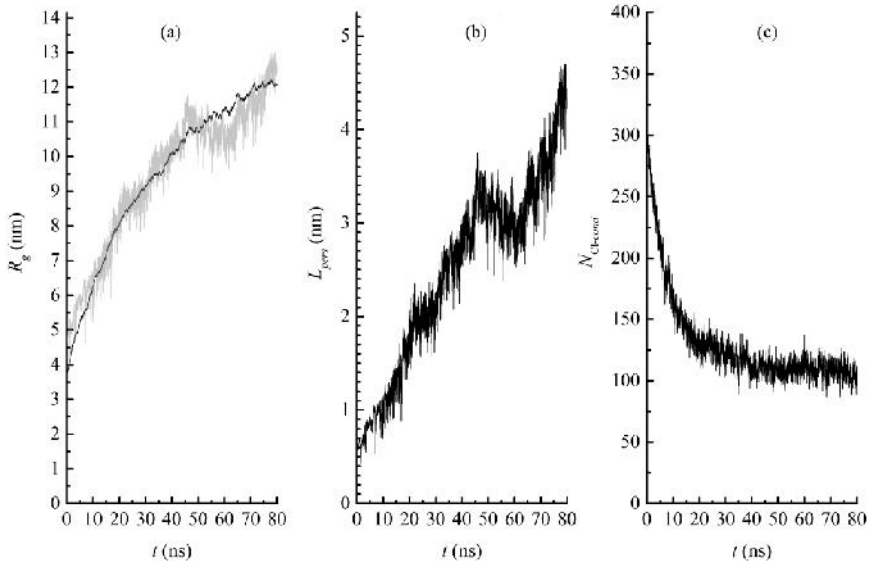

Figure 1. The gyration radius (a), the persistent length (b), and the number of Cl anions condensed on the chain (c) for a single poly(dimethyl diallyl ammonium) chain (400 monomers) in PDADMAC/water during its evolution from a globule to an expanded coil. Black, MD results; gray, the Benoit – Doty approximation for R_g using the persistent length from (b).

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