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On how does the presence of hydrophobic groups influence the ion-specific effects in polyelectrolyte solutions

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The generic name ionene characterizes a class of cationic synthetic polyelectrolytes in which different numbers (x,y) of methylene groups separate quaternary ammonium groups located on the backbone. They are ideal molecules for studying the balance between hydrophobic and charge effects in water. The lecture will focus on thermodynamic and transport properties of aqueous solutions of 3,3-, 4,5-, 6,6-, and 6,9-ionene fluorides, chlorides, bromides and iodides. These counter-ions were chosen because they, from fluoride to iodide ion, widely differ in the way how they affect the surrounding water molecules. We have now a relatively complete set of data for thermodynamic and transport properties of these solutions. In the experimental part of this presentation I will review our own measurements of the osmotic coefficient, heat of dilution, conductivity and transference numbers, apparent partial molar volume and heat capacity, as also the dielectric relaxation spectroscopy in these solutions. Some of the data are new and have not been reported yet. From the theoretical side the results were, wherever possible, analyzed in view of the classical electrostatic theories. In addition I will report the results of the extensive explicit water molecular dynamics simulation of short 3,3- and 6,6-ionene oligoions with fluoride, chloride, bromide and iodide ions counter-ions and sodium ions as co-ions, performed by us in last years. We hope that studies of such model solutions can help in understanding the interactions in biologically relevant systems.

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