Modeling the interaction of a neutral polymer with small ions in solution. A theoretical study of ion binding to a neutral polymer

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The interaction between NaCl and 1,2-dimethoxyethylene is used to model ion binding to a neutral polymer. The relative binding energies involving different ion-polymer structures were calculated using minimal basis STO-3G and split valence 3-21G ab-initio and CNDO/2 semi-empirical wavefunctions. The results obtained are consistent with an adsorption model in which the cation is primarily adsorbed on the oxygen sites. The counter ion is then bound by the charged polymer in a form consistent with an ion pair structure. These results are consistent with recent experimental studies on polyoxyethylene (POE). Additional calculations were performed to include specific interactions with the liquid environment. Electrostatic solvation effects, introduced through the self-consistent reaction field (SCRF) model, appear to be significant in the stabilization of a solvent-separated ion-pair structure. However, the global stabilization produced by both specific and electrostatic solvations predicts