ABSTRACT

Thesis Tittle	: Theoretical Studies on Solvation Behavior of Monovalent Metal ion Complexes.	
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Degree Sought	: Master of Science	
Major	: Applied Chemistry	Acadimic Year 1994
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Ab initio quantum chemical method was applied in the present thesis to construct intermolecular potentials by supermolecular approach. The calculations were made at the Hartree-Fock level of theory, with the basis set of double zeta with one polarization function (DZP) quality. The potentials were aimed at describing the interactions between Li^+ and ligands, as well as and Li^+/ligand and water. The ligands selected in the study were representatives of biologically active molecules, such as N-methylformamide (NMF), acetamide (ACT) and glycine zwitterion (GLYZ). The preferential binding positions and energies of Li^+ at various functional groups of NMF, ACT and GLYZ were optimized and illustrated by the iso-energy contour maps. It was concluded that Li^+ prefers to bind at oxygen atoms of all ligands considered. The Li^+/ligand complexes were confirmed in the present

thesis to be much more stable than the Li^+/H_2O complex. For all Li^+/ligand-H_2O complexes, water prefers to bind directly at Li^+. The H-bond structures and energies in Li^+/NMF-H_2O and Li^+/ACT-H_2O were shown to be not much different. However, the net stabilization of Li^+ on N-H..OH_2 H-bonds of NMF-H_2O and ACT-H_2O were found to be slightly different, depending on the position of the CH_3 group on the N-C=O backbone. The *ab initio* results have shown that the H-bond in GLYZ-H_2O is not much stabilized by Li^+. The hydration structures and energies of Li^+/NMF, Li^+/ACT and Li^+/GLYZ were studied at 298 K by Monte Carlo simulations, with the computed intermolecular potential energy functions. The hydration structures were represented in by the oxygen and hydrogen probability distribution maps (PDO and PDH, respectively). The forces responsible for the binding of water molecules at various functional groups of the Li^+/ligand complexes were discussed using the averaged solute-solvent and solvent-solvent interaction energies computed from MC. They were represented as solute-solvent and solvent-solvent interaction energy contour maps (AWPD and WWPD, respectively). The discussion on the effects of Li^+ on the hydration structures and energies of NMF, ACT and GLYZ cannot be made extensively due to the lack of the information on the hydrations of NMF, ACT and GLYZ.