ABSTRACT

Thesis Tittle : Theoretical Studies on the Intermolecular Potentials for Monte Carlo Simulations of Hydrogen Bonded Systems (Model Potentials for Protein-Water Interaction)

Student's Name : Pol.Capt. Supaporn Chaiyapongs

Degree Sought : Master of Science

Major : Applied Chemistry Academic Year 1994

Advisory Committee : 1. Assoc.Prof.Dr.Kritsana Sagarik Chairperson

2. Asst.Prof.Dr.Sunant Rochanakij

Intermolecular potentials to describe interaction between water and model molecules of amino acids were constructed using Test-particle model (T-model). The molecules considered in the study were N-Methylformamide (NMF), Acetamide (ACT) and Glycine Zwitterion (GLYZ). The computed T-model potentials were tested in the calculations of the equilibrium geometries of 1:1 complexes, formed from a water molecule and a model molecule. The solvation structures were tentatively studied using iso-energy contour maps. The transferability of the T-model potentials was investigated. It has been shown that the repulsion parameters of the T-model potentials could be transferred from small molecules to larger molecules. The T-model potentials were further applied to the study of solvation behavior of NMF, ACT and GLYZ at 298 K, using Monte Carlo (MC) simulations. The

hydration structures were represented by probability density distribution maps for oxygen (PDO) and hydrogen (PDH) of water. The average solute-solvent and solvent-solvent interaction energies were represented by energy diagrams, AWPD and WWPD, respectively. The results were not discussed extensively due to the lack of theoretical and experimental results on similar systems.