ABSTRACT

Thesis Title   :   Model Potentials for Monte Carlo

Simulations of Nucleic Acid

Base-Water Systems

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Degree Sought   :   Master of Science (Applied Chemistry)

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Intermolecular potentials to describe the interaction between nucleic acid bases and water were constructed based on the test-particle model (T-model). The T-model was tested in the first place by considering the interaction between hydrogen fluoride (HF) molecules. The equilibrium interaction energies and geometries of HF dimers and trimers derived from the T-model potential were in good agreement with all reported experimental and theoretical results. The hydration patterns of nucleic acid bases: guanine, cytosine, adenine and thymine, were tentatively studied based on the information of 1:1 complexes. The most favorable binding features for the DNA base-water interaction were represented by the structures in which

water acts as proton donor and acceptor, or both at the same time. The guanine-cytosine complementary pair was confirmed in the present study to be the most stable. The stacking configurations and the Donohue pairs were also found to be rather stable. The hydration patterns of the bases computed from Monte Carlo (MC) simulations at 298 K were quite different from those inferred from the 1:1 complexes. This is due to the fact that the solvent-solvent interaction was omitted in the 1:1 complex calculations. The T-model has been proved in the present thesis to be suitable for theoretical investigation on large chemical systems such as biologically active molecules.