# Chapter 5

# Conclusion

A new non–empirical method is proposed which determines the potential functions suitable for the simulation including a highly–polarizable solute molecule. In this method, the *ab initio* MO method including the solvent effect by the continuum model using generalized Born formula was used to evaluate the interaction energy between polarized solute–solvent system, and a polarization effect by the solvation was incorporated into the potential function.

In application of this method to the ionic fragmentation reaction of $t$–BuCl, the solute–solvent potential functions were determined as a function of the C-Cl distance for the whole range of the dissociation. For a long C-Cl distance, the ionic state of $t$–BuCl is not the ground state in the gas phase, and the potential functions which are suitable for the simulation of the heterolysis of $t$–BuCl can not be determined by usual *ab initio* calculations. Present method provides EPPF which are applicable to the simulation for the solute molecule which is highly polarizable in solution. The calculated energy profile for the reaction of $t$–BuCl elucidated experimental facts qualitatively.

In application of this method to the intramolecular proton transfer in glycine, the solute–solvent potential functions were determined as a function of the N-H distance. The GLYZ does not exist as an energy minimum structure in the gas phase and it polarizes to a large extent in solution, although these effects can not be introduced

by the PF determination by usual *ab initio* calculations. The MC simulation with the determined EPPF was carried out for detail analysis of the intramolecular proton transfer in glycine, and elucidated the mechanism of the proton transfer reaction.

In these applications, the solute and solvent molecules polarizes to large extent in solution, and the incorporation of this effect into PF can not be realized by the conventional determination of potential function by using *ab initio* calculation in the gas phase. Thus, the method proposed in this study is very useful for determining the potential functions which can widely be employed in solution chemistry.