CHAPTER IV

CONCLUSION

In this chapter, we summarize the ESPT reactions including the ESInterPT and ESIntraPT reactions in two systems of molecules having bifunctional groups (proton donor and acceptor) based on quantum dynamics simulations.

First, the ground-state structures of 7AI$(MeOH)_n$ clusters at RI-ADC(2)/ SVP-SV(P) level and 2-(iminomethyl)phenol derivatives at B3LYP/TZVP level in the gas phase were performed. Second, all these optimized structures were used to investigate the ESPT reactions using excited-state dynamics. From this study, the ESInterPT reactions for 7AI$(MeOH)_n$ (when n=1-3) clusters and the ESIntraPT reactions for 2-(iminomethyl)phenol derivatives exhibited ESPT reactions confirmed by no crossing between $S_{\pi\pi^*}$ and $S_{\pi\sigma^*}$ states. For 7AI$(MeOH)_n$ complexes, methanol assistance plays an important role in excited-state dynamics simulation. The intermolecular hydrogen bonds between 7AI and methanol molecules increase or become stronger when the number of methanol increases. The ESInterPT process is a cluster-size selective. Especially, two methanol molecules can assist and promote the ESTPT reaction with the most efficient one among the other complexes. Thus, 7AI$(MeOH)_n$ complexes can be used as a good prototype for studying of the ESInterPT process with an effective RI-ADC(2) method at sufficient small basis set. In addition, 2-(iminomethyl)phenol derivatives can also be used as a good representative for the ESIntraPT in the ultrafast reactions. To add methyl group into imino moiety, it is performed by modification of acid-base properties of the system by

changing the substitution as well as adding a substituent in phenol ring. These modifications should decrease the barrier in modulating the potential for the PT reaction in the ESIntraPT reaction in presence of strengthening of the intramolecular hydrogen bond. Especially, the 2-(*N*-methyl-α-iminoethyl)phenol (MIEP) is the most effective compound for the ESIntraPT reaction.

To this point, this thesis has been completely studied. The studies show the importance of the ESPT reactions in each system. However, we can apply other number of solvent or even change the protic solvent in assisting the ESInterPT reactions for $7AI(MeOH)_n$ complexes. We can vary the substituent on a phenol ring due to structural varieties of 2-(iminomethyl)phenol derivatives to investigate the ESIntraPT reactions. Moreover, these systems are model compounds of DNA bases which are surrounded by many molecules of solvents in our body so solvent effect is important parameter that can be used to describe the system in solvent more realistic than in the gas phase.