

## CHAPTER VI

### CONCLUSION

The prepared ferrocenyl derivatives; *N, N*-dimethylaminomethylferrocene, *N, N*-dimethylaminomethylferrocene methiodide,  $\alpha$ -methylferrocenylmethylamine, ferrocenylethylamine, *N, N*-diphenylaminomethylferrocene, Schiff base derivative, reduced Schiff base derivative, 6-ferrocenyl-2, 2'-bipyridine, 2-( $\alpha$ ,  $\alpha$ -diphenylhydroxyl methyl) dimethylaminomethylferrocene, acetylferrocene, ferrocenylmethylalcohol,  $\alpha$ -hydroxyethylferrocene were used to make inclusion compound with  $\beta$ -cyclodextrin. The inclusion compounds obtained are thermally stable. Elemental analyses showed that ferrocenyl derivative forms inclusion with  $\beta$ -cyclodextrin in 1:1 stoichiometry. The result from  $^1\text{H}$  NMR technique revealed that H(3) and H(5) that located in cyclodextrin cavity were downfield shifted from anisotropic effect of cyclopentadienyl ring while H(1), H(2) and H(4) that located in the exterior of cyclodextrin cavity were unchanged. FTIR technique showed vibrational frequency change of  $-\text{CH}_2$  in inclusion compounds. UV-Visible spectroscopy showed that ferrocenyl derivatives absorb visible light at the same wavelength as the inclusion compounds but the molar absorptivity is hypochromic shift. X-Ray powder diffraction showed a diffraction pattern, which is different from that of mixture. The catalytic activity of ferrocenyl derivatives and its inclusion compounds in alkylation reaction was tested. Using hexane as solvent, room temperature, 24 hr reaction time, 2 mol % of catalyst revealed that ferrocenylamine derivatives were good catalyst especially Schiff base (96% yield). Ferrocenylalcohol and carbonylferrocene did not act as catalyst. Inclusion compounds of ferrocenyl derivatives gave lower yields but higher selectivity than free ferrocenyl derivatives. Studied enantioselectivity of catalyst by derivatization chiral alcohol with MTPA-Cl gave two diastereomeric esters. The diastereomers was analyzed using gas chromatographic and nuclear magnetic resonance techniques. The observation of different interaction of anisotropic  $\alpha$ -phenyl substituent on the chiral acid moiety with the alkyl substituent was explained. Integration data indicated ratio of R, S isomer in

good agreement with the result from gas chromatographic technique. Using inclusion compounds as catalyst gave more enantiomeric excess than free complexes. The mechanism of alkylation of inclusion compound was proposed.

1-Phenyl-1-propanol, product from the alkylation was derivatized with MTPA-Cl to give diastereomers, which were analyzed using GC and NMR techniques. The results from both techniques gave similar % e.e.s. The data from this work revealed that inclusion compounds gave higher enantioselectivity compared with free complexes, even though the % yields of the inclusion compounds are lower. The intermediate from the reaction between diethylzinc and inclusion compound was proposed.

#### **Suggestions for Future Works:**

Future work should be focused on:

- 1) The structures of inclusion compounds should be determined with single crystal X-ray crystallography, which is the most acceptable technique for structure determination.
- 2) The determination of R, S isomers of chiral alcohol should be supported with circular dichroism, chiral column GC and chiral column for HPLC. These instruments should be provided.
- 3) Using inclusion compound in other asymmetric reactions should be pursued.
- 4) Since MTPA-Cl is very sensitive to moisture, severe precaution has to be taken, such as using nitrogen atmosphere. Attempt to find a less expensive chemical to replace MTPA-Cl should be made.