CHAPTER IV

CONCLUSION

The aim of this research is to search for suitable methodology for functionalization of saturated hydrocarbon and to develop catalytic system for iron (II)-catalyzed oxidation reaction. The developed oxidation system was justified from the superior amount of the desired products obtained with high selectivity.

During the course of this study, it was found that the substituent at phenyl ring of ligand, transition metal that binds with ligand, solvent system, oxidizing agent, temperature and additive affected the oxidation reaction. The reaction system in this study could be smoothly proceeded using pyridine-acitic as solvent and zinc grit/air as an oxidant at room temperature and atmospheric pressure. The optimum conditions were cyclohexane (or other saturated hydrocarbons) 30 mmol, pyridine 28 mL, acetic acid 2.3 mL, zinc grit 1.31 grams and metal porphyrin complex 0.25 mmol. The oxidation of cyclohexane under this condition uniquely produced mainly cyclohexanone and small amount of cyclohexanol. The use of ascorbic acid or imidazole as an additive gave higher yield of the desired products. In asddition, the use of triphenylphosphine altered the production of cyclohexanone to cyclohexanol with almost the same amount of activation process taken place.

According to the efficiency of catalyst, Fe (II)-TPP (15) gave a little better yield than other metalloporphyrin from this experiment. In addition, iron (II) porphyrin catalyst 25 was selected to use in most oxidation reactions in this research. The utilization of iron (II) porphyrin complexes as a catalyst in saturated hydrocarbon oxidation using this solvent system has never been reported in the literature. The products observed and selectivity of the system were uniqued and similar to ironbased Gif-type systems. From the information derived from comparison of relative reactivity, the route of mechanism of cyclohexane oxidation was believed to take place *via* non-radical reaction. The addition of triphenylphosphine in cyclohexane oxidation was proved that the reaction took place *via* alkyl hydroperoxide as an intermediate. Moreover, the addition of carbon tetrachloride was also proved that there should have at least two distinct intermediates involved in this proposed mechanism.

In terms of the rate of reaction, the use of *tert*-butyl hydroperoxide as an oxidant at 70 0 C provided good yields of the desired products and the oxidation was faster than using zinc grit/air as an oxidant. Due to the selectivity, the investigation based upon regioselectivity study was proved that iron (II) porphyrin catalyst (25) could oxidize other saturated hydrocarbons selectively under this particular conditions.

Suggestion for further work

The modification of this catalytic system to the larger scale experiments that could be applied in a pilot scale of petrochemical industry may be the one of important things to carry out. The comparative study between iron (II) porphyrin catalysts and other catalysts such as Schiff-base complexes in cycloalkane oxidation should be done. In addition, the variation of iron (II) porphyrin catalysts for the functionalization of saturated hydrocarbons should be investigated. Moreover, other types of hydrocarbons : alkenes, aromatic hydrocarbons and alcohols should also be examined to see the regioselectivity and stereroselectivity of the system.