

CHAPTER IV

CONCLUSION

The main focus of this research is to study for selective functionalization of saturated hydrocarbons catalyzed by six metal stearates. The study was carried out as followed: metal stearate 0.2 mmol, 70% tert-butylhydroperoxide 9.0 mmol as oxidant and reaction time of 24 hrs at 70°C. From this research, it was found that Cr(III) stearate was able to oxidize cyclohexane to cyclohexanone and cyclohexanol in high efficiencies and gave the best selectivity. The ratio of ketone/alcohol was 4.6.

The study of cocatalyst system for the selective oxidation of cyclohexane was observed that the total yield of product was higher than the use of Cr(III) stearate as catalyst alone, but the selectivity of ketone/alcohol was decreased. In terms of kinetic study the results displayed that the half-life for cyclohexane oxidation under this condition was approximately 4 hrs. In addition, the comparative kinetic study of cyclohexane catalyzed by cocatalyst (Cr(III) : Co(II) stearates) was investigated. The half-life of reaction on Cr(III) : Co(II) stearate system was approximately 8 hrs.

According to the regioselectivity investigation, the oxidation of *tert*-butylcyclohexane and methylcyclohexane displayed that the substituent on cyclohexane ring had profound effect on the reaction. The reaction preferentially took place at 3-position. The oxidation of *n*-hexane gave the yield of product taken place at 2-position and 3-position was main product. No reaction at 1-position was taken place. For the oxidation of adamantane was selectively transformed to 1-adamantanol. In the presence of appropriate trapping reagents, the formation of ketones was diverted to the production of monosubstitued alkyl derivatives. For instance, in the presence of carbon tetra chloride (CCl₄) or bromotrichloromethane (BrCCl₃), the formation of alkyl chlorides and alkyl bromides was detected instead of ketone. Addition, the kinetic study of effect of reducing agent such as triphenylphosphine (PPh₃) was observed that It could be reduced an intermediate in the process, cyclohexyl hydroperoxide to cyclohexanol. The study for the possible mechanistic pathway of this system was performed and confirmed to occur *via* free radical pathway supported by chemoselectivity study, regioselectivity study, the addition of trapping reagents

and reducing reagent. The route of mechanism of this system was believed to take place *via* a free radical pathway.

The modification of this system in the large scale experiments compared with other catalytic system referred, this process was more suitable for industrial use.

Suggestion for the future 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 variation of metal stearate catalysts for the functionalization of saturated hydrocarbons should be investigated. Moreover, other types of hydrocarbons: alkenes, aromatic hydrocarbons and alcohol should also be examined to see the regioselectivity and stereoselectivity of system.

