CHAPTER VI

CONCLUSIONS AND SUGGESTIONS

To study the polymerization of 1-hexene by iron-based non-metallocene catalysts, two diamine ligands [RHN(CH$_2$)$_3$NHR]; ligand (**a**) and RHN(CH$_3$)C=C (CH$_3$)C=NR; ligand (**b**) (R = 2,6-^{i}Pr$_2$C$_6$H$_3$)] and a Schiff's base ligand (salen); ligand (**c**) can be prepared and characterized readily by ^{1}H-NMR, ^{13}C-NMR, FT-IR and UV-visible spectrophotometry and employed to prepare some iron (III) complexes via reaction with FeCl$_3$. Four iron (III) complexes were synthesized; **cpx 1a**, **cpx 2b** and **cpx 3c**. They were characterized by elemental analysis, FT-IR and UV-visible spectrophotometry. These complexes served as catalyst precursors for the polymerization of 1-hexene. A variety of cocatalysts (MAO, [Ph$_3$C][B(C$_6$F$_5$)$_4$] and [PhNMe$_2$H][B(C$_6$F$_5$)$_4$]) and alkylating agents (TIBA, MeMgBr and PhMgCl) can be used to activate the complexes. When activated with MAO; only **cpx 1a** and **cpx 2b** are active. Optimum conditions for 1-hexene polymerization using **cpx 1a**/different cocatalyst: MAO and borate were investigated. For **cpx 1a**/MAO system; the optimum condition found was 10.0x10^{-6} mole catalyst, 39.98 mmol 1-hexene, Al/Fe mole ratio 1000, T$_p$ 50°C, t$_p$ 24 h. For **cpx 1a**/[Ph$_3$C][B(C$_6$F$_5$)$_4$] system, the condition found was 10.0x10^{-6} mole catalyst, 1 equivalent of [Ph$_3$C][B(C$_6$F$_5$)$_4$], Al/Fe mole ratio 400, T$_p$ 0°C, t$_p$ 24 h. Three chain termination pathways have been proposed using ^{1}H-NMR and FT-IR techniques: (1) β-H transfer to metal resulting in vinylidene end group, (2) rearrangement resulting in internal double bond and (3) chain transfer to aluminum resulting in saturated end group. The information from GC-MS and ^{13}C-NMR identified that the iron catalyst systems: **cpx 1a** and **2b** produced dimer, trimer, pentamer and hexamer of 1-hexene with atactic tacticity. For comparison, *rac*-Et(Ind)$_2$ZrCl$_2$ catalyst has been used in 1-hexene polymerization with [PhNMe$_2$H][B(C$_6$F$_5$)$_4$] cocatalyst. The polymerization condition was 5.0x10^{-6} mole catalyst, 1 equivalent of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$], Al/Fe mole ratio 200, T$_p$ 30°C, t$_p$ 24 h. The results from ^{13}C-NMR, GPC and DSC techniques identified that the white rubber-like product was isotactic poly(1-hexene) with molecular weight (Mw) of 48,600, molecular weight distribution (Mw/Mn) of 2.33 and glass transiton temperature (T$_g$) at –47°C.

SUGGESTIONS

The suggestions for future work are:

-   Polymerization of ethylene using **cpx 1a** and **cpx 2b** as catalyst should be attempted.
-   Using ligand (**a**) to synthesize Ni complex and use for other olefin polymerization should be tried.