

Sittichoke Tabthong 2009: Single-Site Catalysts for the Ring-Opening Polymerization of *rac*-Lactide. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Miss Pimpa Hormnirun, Ph.D. 49 pages.

Achiral *Bis*(pyrrolidene) Schiff base Aluminum complexes were synthesized. In the first step, ligands **59-64** were synthesized by the condensation reaction between 2-carboxaldehyde and coresponding diamine. All ligands were obtained in high yield. Then, ligands were reacted with trimethylaluminium to obtain desired aluminum catalysts. All ligands and complexes were characterized by ¹H-NMR spectroscopic technique. Aliminum complexes **1-6** in the presence of 2- propanol were used for polymerization of *rac*-lactide. Resulting polymers from polymerization using complexes **3** and **5** are isotactic polymers ($P_m \approx 0.8$), while resulting polymers from polymerization using other complexes are atactic polymers ($P_m \approx 0.5$).

Aluminum methoxide based on *N,N'*-bis(1H-pyrrole-2-ylmethylene)-1,2-ethylenediamine was used as a catalyst for the theoretical study. The ring-opening mechanism of *D*- and *L*-LA has investigated using a B3LYP density functional theory employing a 6-31G(d,p) basis set. The ring-opening of lactide occurs *via* a coordination insertion mechanism with two transition states (TS1 and TS2). From the energy profiles it found that the second transition state (TS2), the state that the lactide ring-opening can be readily activated through the octahedral transition that involves the C_{carbonyl}-O_{acyl} and Al-O_{carbonyl} bond dissociation, is rate determining step for both *D*- and *L*-LA. In comparison, the ring-opening of *L*-lactide occurs more readily than that of *D*-lactide.

Student's signature

Thesis Advisor's signature

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