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Theoretical investigation of the mechanism of syndiospecific propylene polymerization using *ansa*-dimethylsilylene(fluorenyl)(amido)titanium complexes

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KEYWORDS: Titanium catalyst, Theoretical study, Propylene polymerization

ABSTRACT: Theoretical study on the propylene polymerization using *ansa*-dimethylsilylene(fluorenyl)(amido)dimethyltitanium complexes were performed and related to the experimental results. The calculated activation energies for coordination-insertion of propylene via four different conformations after the first monomer insertion showed that propylene coordinates to the titanium center avoiding the steric repulsion of polymer chain, which was placed toward the amido group. The bulkiness of the amido groups was closely related to the frequency of the chain-migration without monomer insertion, probably because the bulky amido group would force the fluorenyl ligand to coordinate to the titanium center in η^1 -manner. These theoretical results well explained the experimental results.

1. Introduction

Syndiotactic polypropylene (*syn*-PP) has been recognized as a material with greater impact strength and higher transparency over isotactic polypropylene (*iso*-PP) because *syn*-PP has low crystallinity and elastic modulus compared with *iso*-PP.¹⁻³ To date, crystalline *syn*-PP is only accessible by early transition metal single-site catalysts⁴⁻¹⁴ and the thermal and mechanical properties of *syn*-PP can be varied by the random copolymerization¹⁵⁻¹⁷ or block copolymerization.¹⁸⁻²⁰ Therefore, the development of highly *syn*-

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