Dialkoxy-Substituted, C_1 -Symmetric Metallocenes: Synthesis and Catalytic Behavior in the Propylene Polymerization Reaction

Martin Schlögl and Bernhard Rieger

University of Ulm, Department of Materials and Catalysis, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

Reprint requests to Prof. Dr. B. Rieger. Fax: +49 (0)731 5023039. E-mail: bernhard.rieger@chemie.uni-ulm.de

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The synthesis of a series of C_1 -symmetric metallocene complexes rac-[1-(5,6-dialkoxy-2-methyl-1- η^5 -indenyl)-2-(9- η^5 -fluorenyl)ethane]zirconium dichlorides (alkyl: n-butyl, n-hexyl, n-octyl, n-decyl) is described. These complexes are versatile catalysts in the polymerization of propylene after in situ activation with triisobutylaluminum (TIBA) and $Ph_3C[B(C_6F_5)_4]$ in toluene and heptane solution. All catalysts show higher solubility and improved polymerization properties in industrially used hydrocarbon solvents (e.g. heptane). However, the molecular weights and isotacticity values of the resulting polypropylene materials are decreased compared to the ethoxy-bridged analogue rac-[1-(5,6-ethylenedioxy-2-methyl- η^5 -indenyl)-2-(9- η^5 -fluorenyl)ethane]zirconium dichloride. A possible explanation is based on enhanced interaction of the active catalyst centers with Al(III) scavenger molecules even at low Al: Zr ratios, leading to reversible chain transfer.

Key words: Metallocene Catalysis, Dialkoxy Substitution, Propylene Polymerization