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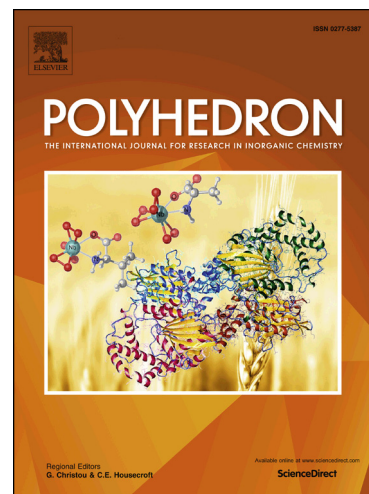
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Scandium and Gadolinium Complexes with Aryldiimine NCN Pincer Ligands: Synthesis, Characterization, and Catalysis on Isoprene and 1,5-Hexadiene Polymerization

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Abstract

Several scandium and gadolinium complexes bearing tridentate aryldiimine NCN pincer ligands $^{\text{Ar}}[\text{NCN}^{\text{H}}]\text{ScCl}_2(\text{THF})_2$ (Ar = Ph (**1a**); Ar = 2,6-Me₂C₆H₃ (**1b**), Ar = 2,6-Et₂C₆H₃ (**1c**), Ar = 2,6-ⁱPr₂C₆H₃ (**1d**), Ar = *p*-MeC₆H₄ (**1e**), Ar = 2,4,6-Me₃C₆H₂ (**1f**), $^{\text{Ar}}[\text{NCN}^{\text{Me}}]\text{MCl}_2(\text{THF})_2$ (M = Sc, Ar = 2,6-Me₂C₆H₃ (**2b**); M = Gd, Ar = 2,6-Me₂C₆H₃ (**3b**), Ar = 2,6-ⁱPr₂C₆H₃ (**3d**)), and ^{iPrPh}[NCN^{Me}] ScCl_2 (**2d**) were synthesized *via* lithiation of the corresponding ligands with ⁿBuLi and subsequent addition of ScCl₃(THF)₃ or GdCl₃(THF)₃ respectively. These complexes were well characterized by elemental analysis and the solid structures of **1c**, **1d**, **1f**, and **2b** were confirmed by X-ray diffraction analysis to be monomeric with *N,C,N*-tridentate ligands coordinating to the metal center in a typical meridional manner. In the presence of alkylaluminium and trityl borate, these well-defined complexes showed moderate to high activities in isoprene polymerization affording *cis*-1,4 enriched polymers (up to 98.3%). Moreover, the NCN pincer scandium complexes can also

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