

Synthesis of Half-Titanocene Complexes Containing π,π -Stacked Aryloxide Ligands, and Their Use as Catalysts for Ethylene (Co)polymerizations

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Table S1 Crystallographic data and refinement details for complex **Ti1** and **Ti3**.

	Ti1	Ti3
Empirical formula	C ₁₅ H ₁₂ Cl ₂ OTi	C ₂₂ H ₁₆ Cl ₄ OTi
Formula weight	327.05	486.05
Crystal color	Red	Red
Temperature (K)	273	187
Wave length (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	P2 ₁ /c	P2 ₁ /c
a (Å)	9.989 (6)	16.662(12)
b (Å)	7.039 (4)	10.291 (10)
c (Å)	19.978 (11)	12.087 (4)
α (°)	90	90
β (°)	92.25	101.1 (2)
γ (°)	90	90
Volume(Å ³)	1403.6	2033.6
Z	4	4
D calcd (mg m ⁻³)	1.548	1.588
μ (mm ⁻¹)	0.98	0.96
F (000)	664	984
Crystal size (mm)	0.17 × 0.16 × 0.15	0.21 × 0.18 × 0.11
θ range (°)	2.8–26.4	2.3–26.4
Limiting indices	-12 ≤ h ≤ 12 -8 ≤ k ≤ 8 -13 ≤ l ≤ 24	-20 ≤ h ≤ 20 -12 ≤ k ≤ 12 -8 ≤ l ≤ 15
No. of rflns collected	2848	12457
No. of unique rflns	2567	4135
R _{int}	0.037	0.029
Goodness-of-fit on F ²	1.05	1.03
wR2	0.091	0.122

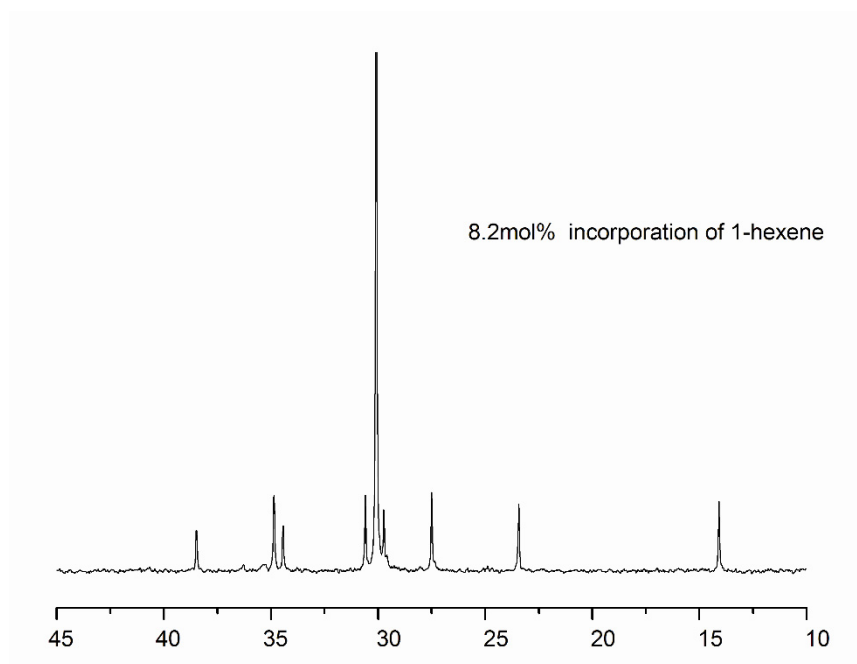


Figure S1 ^{13}C NMR spectrum of ethylene/1-hexene copolymer obtained with **1a**/MAO system (Table 2, Entry 9).

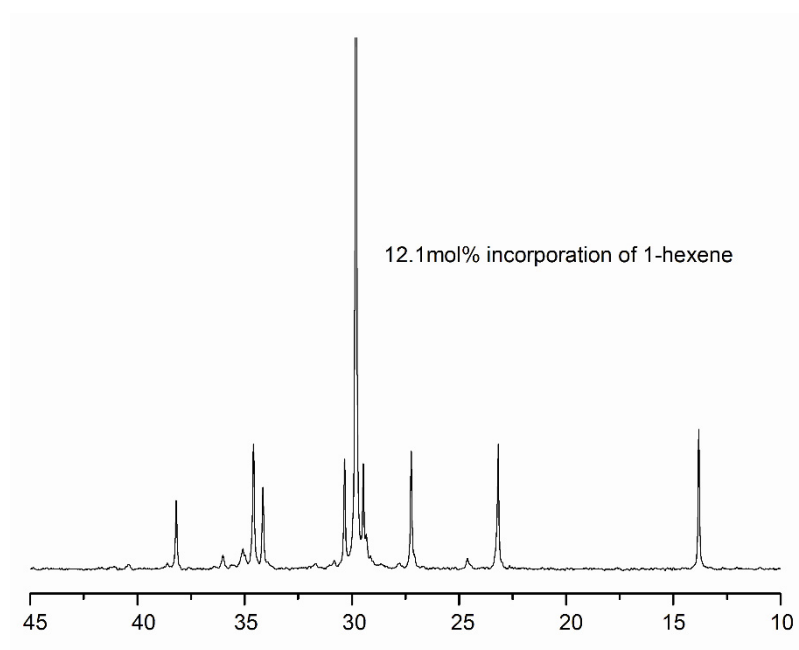


Figure S2 ^{13}C NMR spectrum of ethylene/1-hexene copolymer obtained with **1a**/MAO system (Table 2, Entry 10).

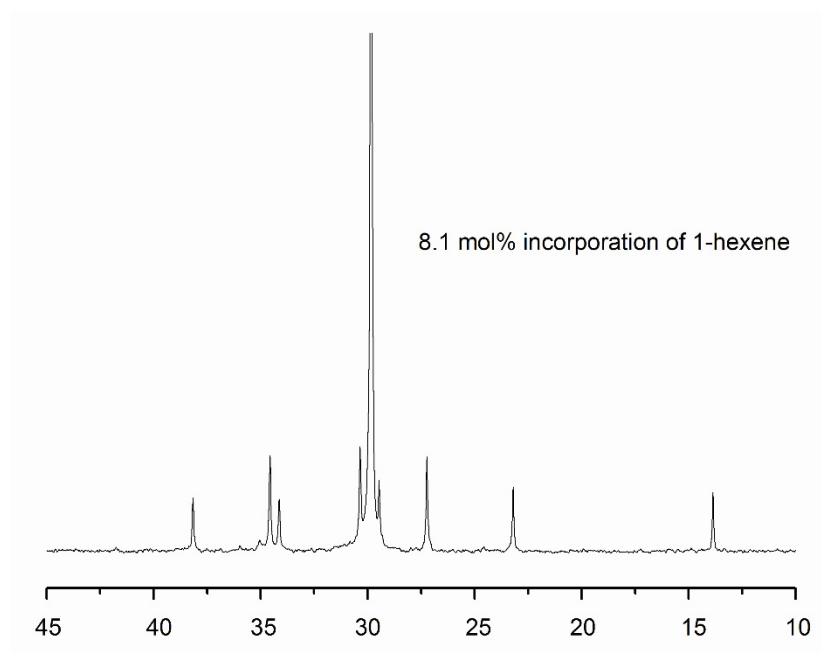


Figure S3 ^{13}C NMR spectrum of ethylene/1-hexene copolymer obtained with **2a**/MAO system (Table 2, Entry 11).

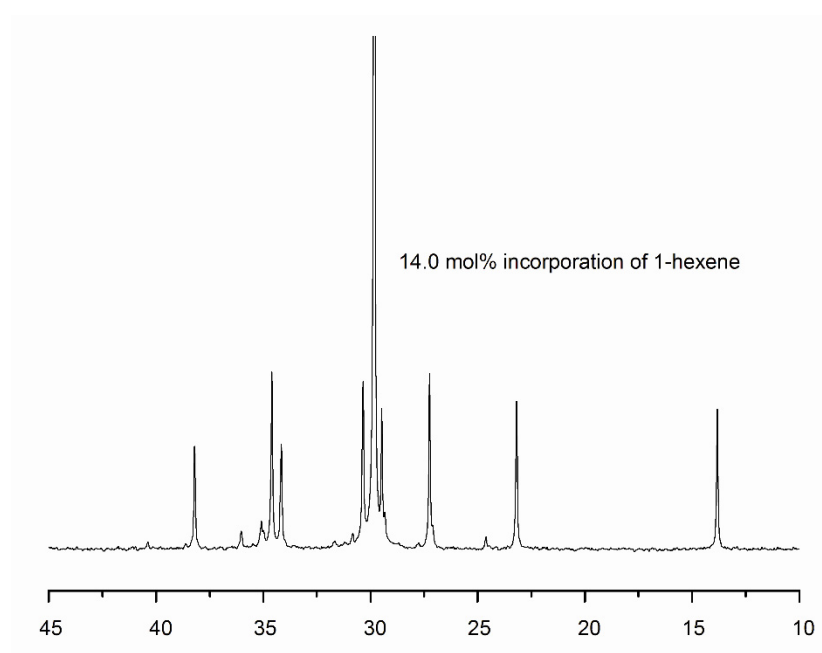


Figure S4. ^{13}C NMR spectrum of ethylene/1-hexene copolymer obtained with **2a**/MAO system (Table 2, Entry 11).

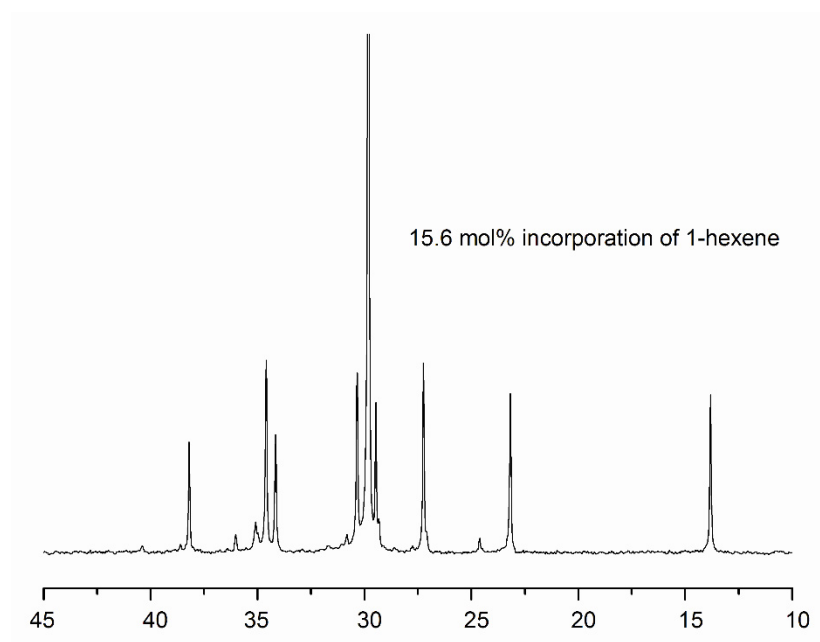


Figure S5 ^{13}C NMR spectrum of ethylene/1-hexene copolymer obtained with **2a**/MAO system (**Table 2, Entry 12**).