Supporting Information

Termination Events in Sterically Hindered Metallocene-Catalyzed Olefin Oligomerizations: Vinyl Chain Ends in Oligooctenes

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Figure S1. $^1$H NMR Spectrum of Complex 1.

Figure S2. $^{13}$C NMR Spectrum of Complex 1.
2.0 Characterization of Oligomers

$^1$H NMR spectra were obtained on a Bruker DRX 500 MHz instrument operating at 500 MHz and 80 °C. The polymers were dissolved in C$_2$D$_2$Cl$_4$ and spectra referenced to residual C$_2$HDCl$_4$ at 6.98 ppm. $^{13}$C NMR spectra were obtained at 125.7 Hz and at 80 °C on a Bruker 500 MHz instrument. All samples were dissolved in C$_2$D$_2$Cl$_4$ and referenced to same at 74.9 ppm. $M_w$ and $M_n$ are measured by using a High Temperature Size Exclusion Chromatograph (either from Waters Corporation or Polymer Laboratories), equipped with a differential refractive index detector (DRI). Three Polymer Laboratories PLgel 10 mm Mixed-B columns were used. The nominal flow rate was 0.5 cm$^3$/min, and the nominal injection volume was 300 microliter. Solvent for the SEC experiment was prepared by dissolving 6 grams of butylated hydroxy toluene as an antioxidant in 4 liters of Aldrich reagent grade 1, 2, 4 trichlorobenzene (TCB). The TCB mixture was then filtered through a 0.7 micrometer glass pre-filter and subsequently through a 0.1 micrometer Teflon filter. The TCB was then degassed with an online degasser before entering the SEC. Polymer solutions were prepared by placing dry polymer in a glass container, adding the desired amount of TCB, then heating the mixture at 160 °C with continuous agitation for about 2 hours. All quantities were measured gravimetrically. The TCB densities used to express the polymer concentration in mass/volume units were 1.463 g/ml at room temperature and 1.324 g/ml at 135 °C. The injection concentration was from 1.0 to 2.0 mg/ml, with lower concentrations being used for higher molecular weight samples. Prior to running each sample the DRI detector and the injector were purged. Flow rate in the apparatus was then increased to 0.5 ml/minute, and the DRI was allowed to stabilize for 8 to 9 hours before injecting the first sample. The concentration, $c$, at each point in the chromatogram was calculated from the baseline-subtracted DRI signal, $I_{DRI}$, using the following equation:

$$c=K_{DRI}I_{DRI}/(dn/dc)$$

where $K_{DRI}$ is a constant determined by calibrating the DRI, and $(dn/dc)$ is the refractive index increment for the system. The refractive index, $n=1.500$ for TCB at 135 °C and $\lambda=690$ nm.

Units on parameters throughout this description of the SEC method are such that concentration is expressed in g/cm$^3$, molecular weight is expressed in g/mole, and intrinsic viscosity is expressed in dL/g.

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<th>Vinyls (%)</th>
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<th>$M_w$ (g/mol)</th>
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Table S1. aPP produced in a continuous reactor using catalyst 1. aDetermined by $^1$H NMR spectroscopy. bDetermined by GPC DRI analysis.
Figure S3. Comparison of $M_n$ from different techniques for the oligomerization of propylene catalyzed by 1.

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<th>[C8] (mol/L)</th>
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<th>Vinyldene$^a$ (%)</th>
<th>Trisub$^a$ (%)</th>
<th>$M_n^a$ (g/mol)</th>
<th>C8$^b$ (mol %)</th>
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Table S2. Results from co-oligomerization of octene and propylene catalyzed by 1. $^a$Determined by $^1$H NMR spectroscopy. $^b$Determined by $^{13}$C NMR spectroscopy.
Figure S4. $^1$H NMR spectrum of PO (propylene-octene) oligomer with 55 mol% octene.
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References
