Supporting Information for the Manuscript entitled Sterically Hindered Aluminum Alkyls: Practical Scavenging Agents of Use in Olefin Polymerization

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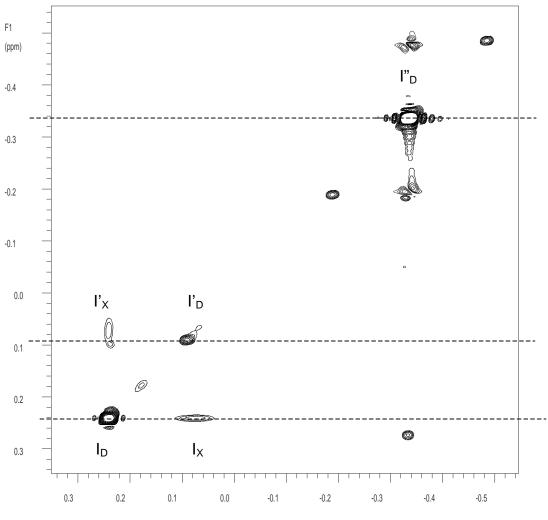
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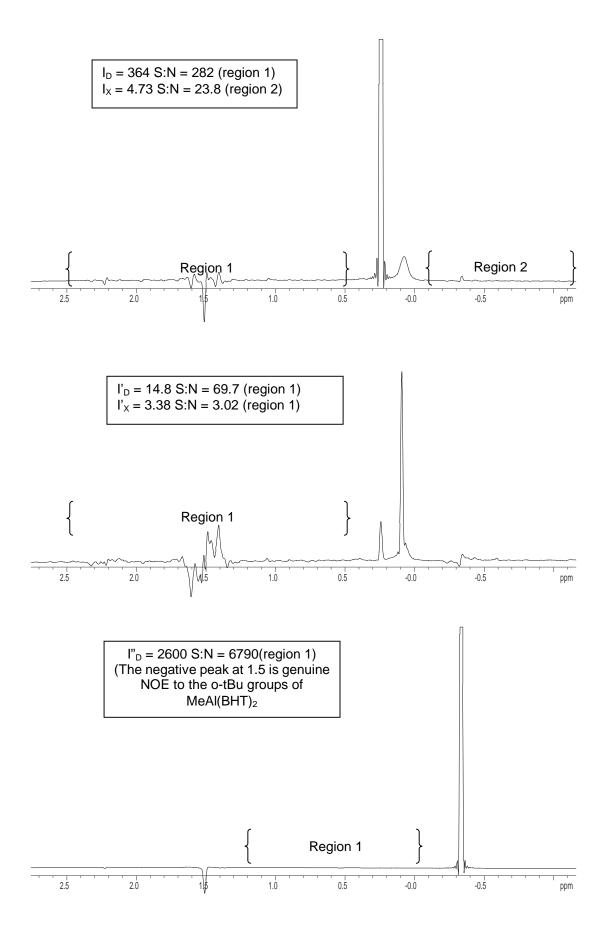
Figure S-1 - Partial ¹H-¹H (400 MHz) NOESY spectrum of [Cp₂ZrMe][MeB(C₆F₅)₃] (0.056 M) and MeAl(BHT)₂ (0.26 M) in C₆D₆ at 22 °C. Mixing time = 1.0 sec. Slices through diagonal and cross-peaks corresponding to spectra depicted in Figure S-2 are indicated with dashed lines. S-2 Figure S-2 - 1D slices through the 2D spectrum depicted in Figure S-1. Peak intensities and S:N ratios along with the regions used to determine noise are indicated. To determine an upper limit for k_{ex} between the Zr-Me signal (δ 0.24) and the Al-Me signal (δ -0.35), S:N values of 1830 (based on region 2 and I_D/I_X) and 6790, respectively were used to estimate $k_{ex} = \frac{1}{\tau_m} ln \left(\frac{r+1}{r-1}\right)$ where $r = \left(\frac{\Phi_D + \Phi_D''}{8}\right) = \left(\frac{1830 + 6790}{8}\right) = 1078$.¹ This gives an upper estimate for k_{ex} = 0.00186 s⁻¹ at 295 K.

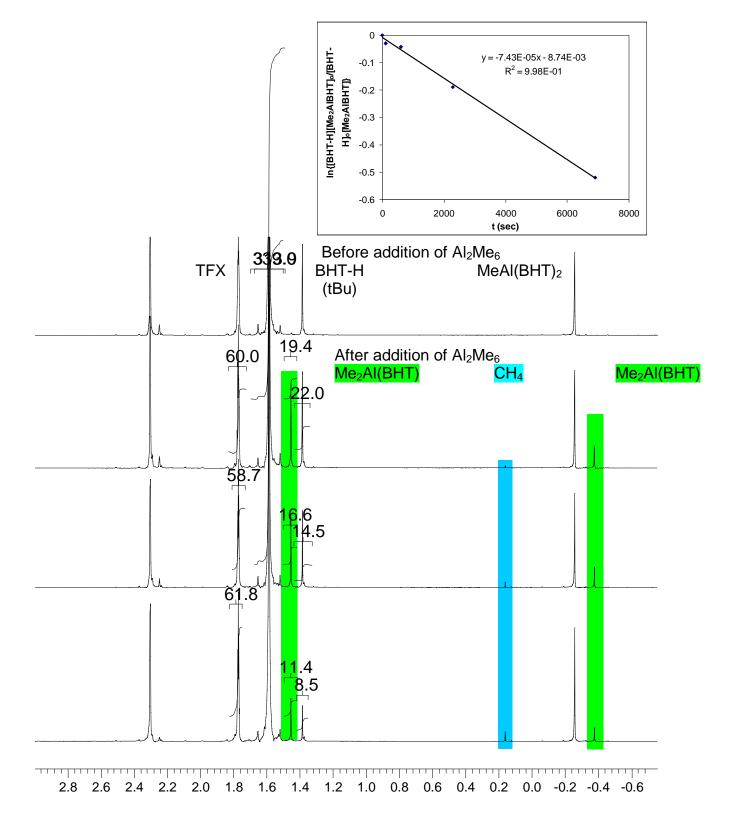
Figure S-3 Selected ¹H NMR spectra (300 MHz, C₆D₆, 25 °C) of a mixture of $[BHT-H]_0 = 0.0091$ M and MeAl(BHT)₂ before and after the addition of Al₂Me₆ $[Me_2Al(BHT)]_0 = 0.0080$ M. Inset is second-order kinetics plot for this reaction, monitoring the disappearance of BHT-H and Me₂Al(BHT). S-4

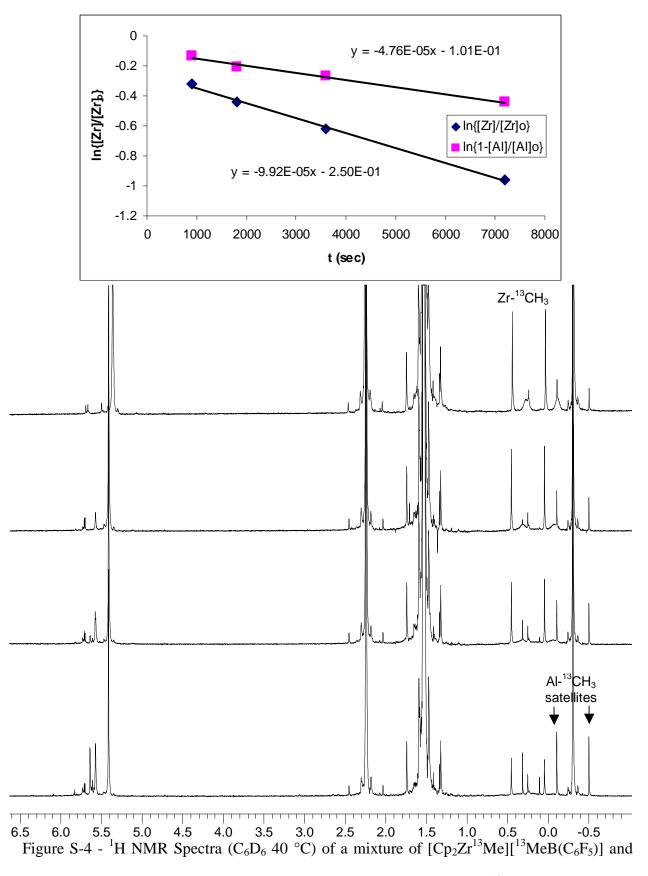
Figure S-4 - ¹H NMR Spectra (C_6D_6 40 °C) of a mixture of [$Cp_2Zr^{13}Me$][¹³MeB(C_6F_5)] and MeAl(BHT)₂ as a function of time. Plot of the rate of disappearance of Zr-¹³CH₃ and appearance of Al-¹³C satellites as a function of time. S-5



F2 (ppm)







MeAl(BHT)₂ as a function of time. Plot of the rate of disappearance of $Zr^{-13}CH_3$ and appearance of Al-¹³C satellites as a function of time.

1. Chen, M.-C.; Roberts J. A. S.; Marks T. J. J. Am. Chem. Soc. 2004, 126, 4605-25.