

# Supplementary Information

## Synthesis, Characterization and Ethylene Oligomerization Studies of Chromium Complexes Bearing Imino-Furfural Ligands

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**Table S1.** Crystal data and structure refinement for imino-furfural **L**<sup>1</sup> and **L**<sup>2</sup>

Imino-furfural proligand	<b>L</b> <sup>1</sup>	<b>L</b> <sup>2</sup>
Empirical formula	C <sub>14</sub> H <sub>15</sub> N O <sub>2</sub>	C <sub>18</sub> H <sub>15</sub> N O <sub>2</sub>
Formula weight	229.27	277.31
Temperature / K	150(2)	150(2)
Wavelength / Å	0.71073	0.71073
Crystal system	Monoclínico	Monoclínico
Space group	P 2 <sub>1</sub> /a	P 2 <sub>1</sub> /a
Unit cell dimensions	a = 9.1725(5) (Å); α = 90° b = 13.5288(7) (Å); β = 108.135(2)° c = 10.4894(5) (Å); γ = 90°	a = 8.719(2) (Å); α = 90° b = 5.8846(15) (Å); β = 97.925(7)° c = 28.239(7) (Å); γ = 90°
Volume / Å <sup>3</sup>	1237.00(11)	1435.0(6)
Z	4	4
Density / (g cm <sup>3</sup> )	1.231	1.284
Absorption coefficient / mm <sup>-1</sup>	0.082	0.084
F (000)	488	584
Crystal size / mm	0.5 × 0.19 × 0.08	0.34 × 0.24 × 0.09
Theta range for data collection	3.64-27.48°	2.91-27.48°
Index ranges	-10 ≤ h ≤ 11; -15 ≤ k ≤ 17; -13 ≤ l ≤ 13	-11 ≤ h ≤ 8; -7 ≤ k ≤ 7; -36 ≤ l ≤ 36
Reflections collected/ independ. [R <sub>int</sub> ]	10591 / 2821 [R(int) = 0.039]	10118 / 3289 [R(int) = 0.048]
Completeness to theta	99.8%	99.8%
Max. and min. transmission	0.993; 0.856	0.992; 0.809
Refinement method	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2821 / 0 / 155	3289 / 0 / 191
Goodness-of-fit (GOF) em F <sup>2</sup>	1.045	1.054
Final R indices [I > 2σ(I)]	R <sub>1</sub> <sup>a</sup> = 0.0388; wR <sub>2</sub> <sup>b</sup> = 0.0912	R <sub>1</sub> <sup>a</sup> = 0.0468; wR <sub>2</sub> <sup>b</sup> = 0.1195
R indices (all data)	R <sub>1</sub> <sup>a</sup> = 0.0546; wR <sub>2</sub> <sup>b</sup> = 0.0994	R <sub>1</sub> <sup>a</sup> = 0.0696; wR <sub>2</sub> <sup>b</sup> = 0.1322
Largest diff. peak and hole	0.151 and 0.189 (e Å <sup>-3</sup> )	0.23 and 0.196 (e Å <sup>-3</sup> )

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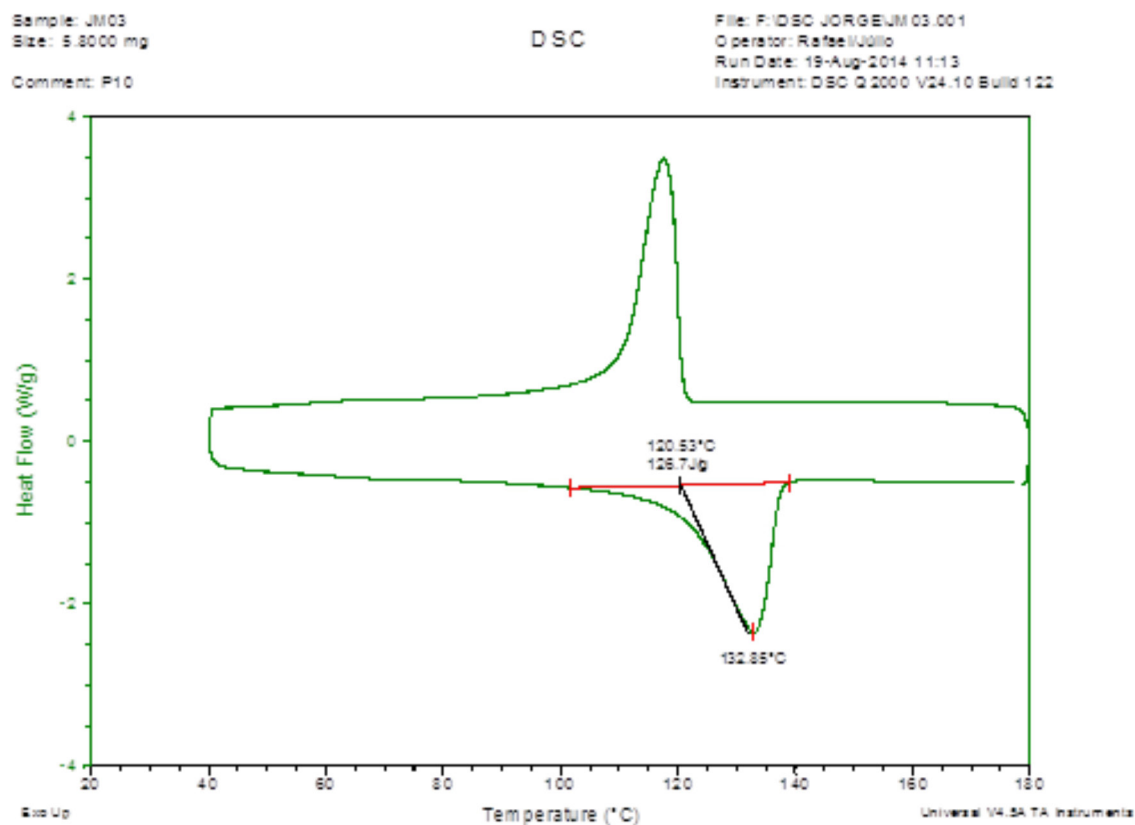


Figure S1. DSC curve of polyethylene produced by  $\text{CrCl}_3(\text{THF})_3/\text{L}^1/\text{MAO}$  (Table 2, entry 5).

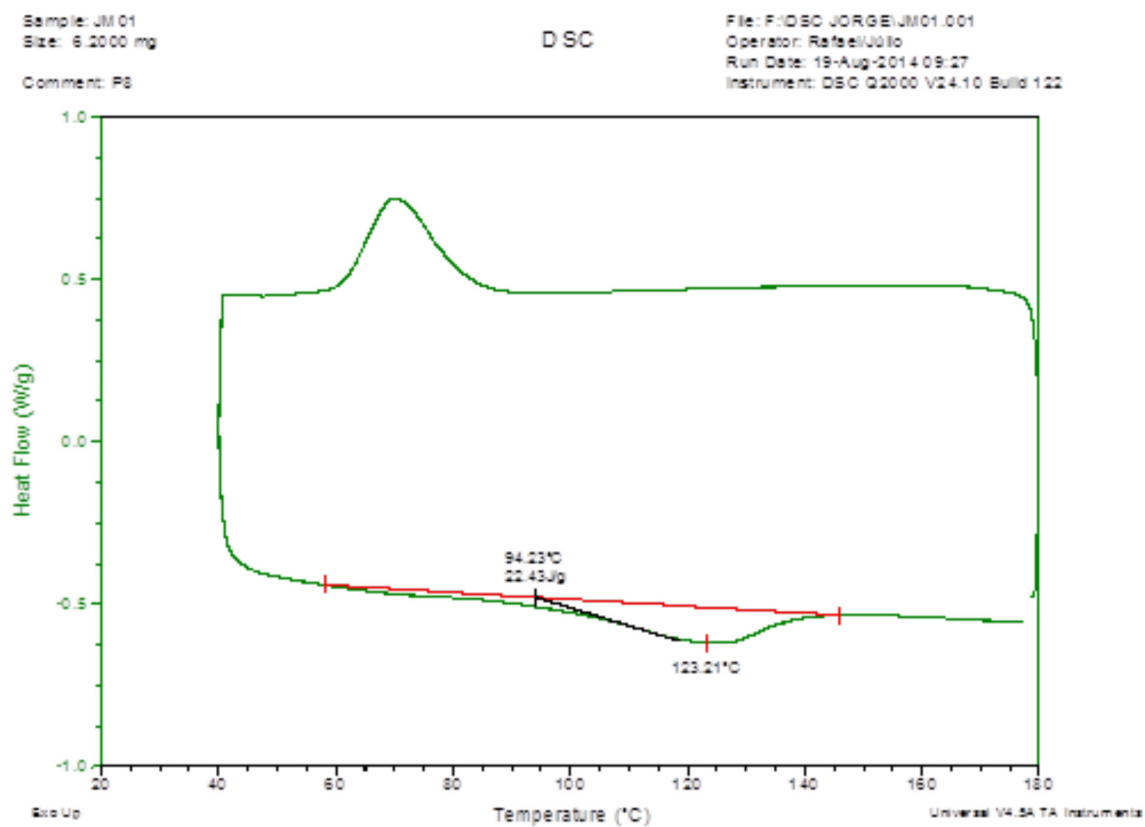


Figure S2. DSC curve of polyethylene produced by  $\text{Cr}(\text{acac})_3/\text{L}^1/\text{MAO}$  (Table 2, entry 6).

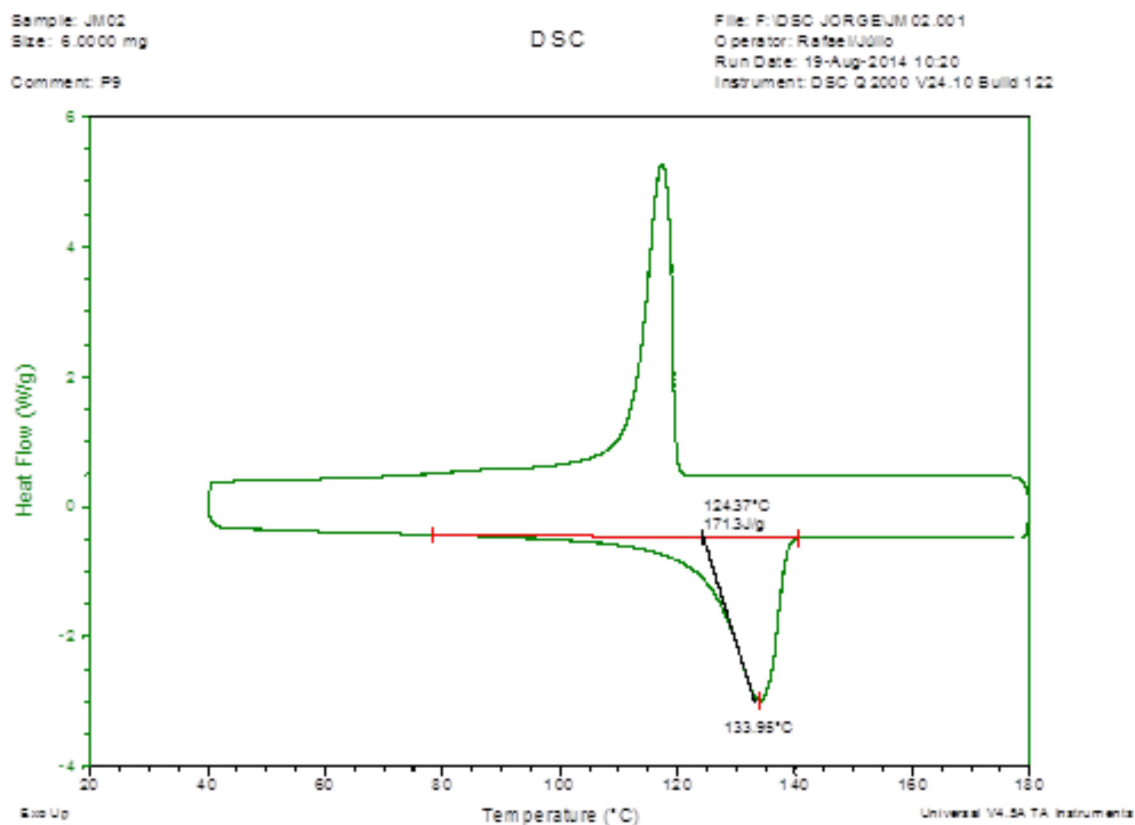


Figure S3. DSC curve of polyethylene produced by  $\text{Cr}(\text{acac})_3/\text{L}/\text{EASC}$  (Table 2, entry 7).

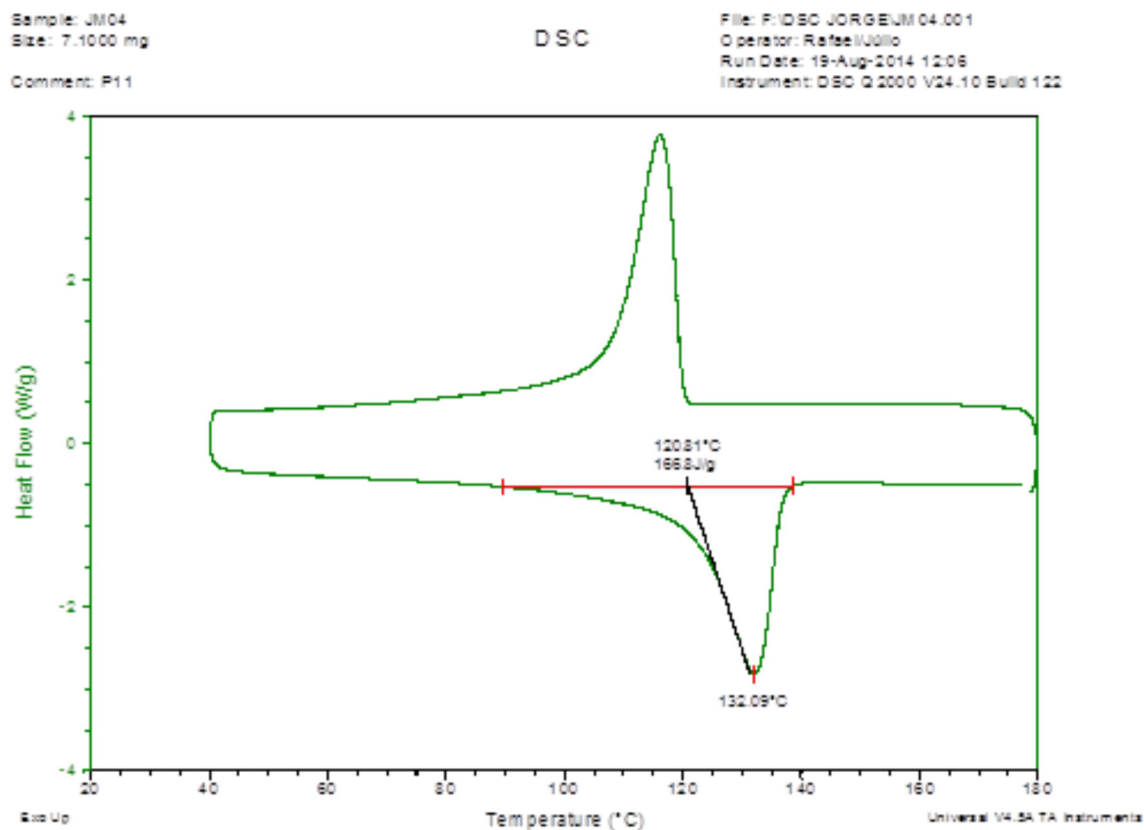


Figure S4. DSC curve of polyethylene produced by  $\text{Cr}(\text{acac})_3/\text{L}/\text{PMAO-IP}$  (Table 2, entry 8).

