Supporting Information

Chromium Complexes Supported by the Bidentate PN Ligands: Synthesis, Characterization and Application for Ethylene Polymerization

Quande Zheng, Dejuan Zheng, Binghao Han, Shaofeng Liu,* and Zhibo Li

Key Laboratory of Biobased Polymer Materials, Shandong Provincial Education Department; College of Polymer Science and Engineering, Qingdao University of Science and Technology, Qingdao 266042, China

*E-mail: shaofengliu@qust.edu.cn (S.L.)

Table S1. Crystal data and structure refinement for **Cr3** and **Cr4**.

Complex	**Cr3**·2THF·H_2O	**Cr4**·2DCM·$2H_2O$
Empirical formula	$C_{31}H_{32}Cl_3CrNP$· $2C_4H_8O·H_2O$	$C_{54}H_{46}Cl_3CrNP$· $2CH_2Cl_2·2H_2O$
Formula weight	770.12	1102.11
Temperature / K	100	100
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	P-1
a / Å, b / Å, c / Å	20.439(2), 10.5810(10), 18.320(3)	12.196(2), 14.507(2), 17.197(3)
α/°, β/°, γ/°	90, 110.780(8), 90	109.393(3), 99.295(3), 102.656(3)
Volume / $Å^3$	3704.2(8)	2708.0(8)
Z	4	2
ρ_{calc} / mg mm^{-3}	1.381	1.352
μ / mm^{-1}	0.607	0.628
F(000)	1620.0	1138.0
Crystal size / mm^3	0.29 × 0.22 × 0.17	0.29 × 0.25 × 0.22
2Θ range for data collection	2.14 to 50°	4.96 to 50°
Index ranges	$-24 \le h \le 24$, $-9 \le k \le 12$, $-21 \le l \le 21$	$-14 \le h \le 14$, $-13 \le k \le 17$, $-20 \le l \le 18$
Reflections collected	18028	13695
Independent reflections	6514 [R(int) = 0.1076]	9428 [R(int) = 0.0344]
Data/restraints/parameters	6514/0/441	9428/0/611
Goodness-of-fit on F^2	1.083	1.081
Final R indexes [I>2σ (I)]	R_1 = 0.0618, wR_2 = 0.1122	R_1 = 0.0718, wR_2 = 0.1741
Final R indexes [all data]	R_1 = 0.0985, wR_2 = 0.1231	R_1 = 0.1078, wR_2 = 0.1890
Largest diff. peak/hole / e $Å^{-3}$	0.67/-1.17	1.97/-1.20

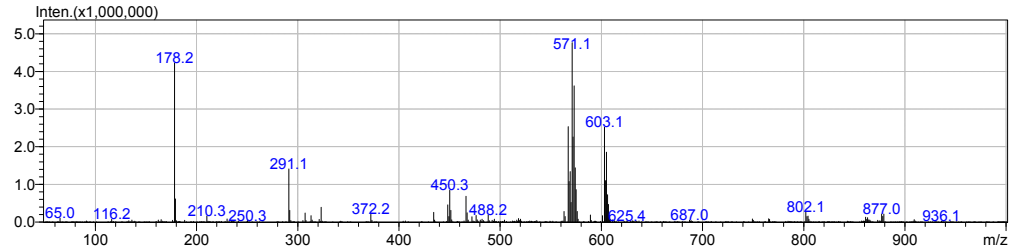

Figure S1. ESI spectrum of **Cr3** (m/z 571.1, $[M\text{-}Cl]^+$).

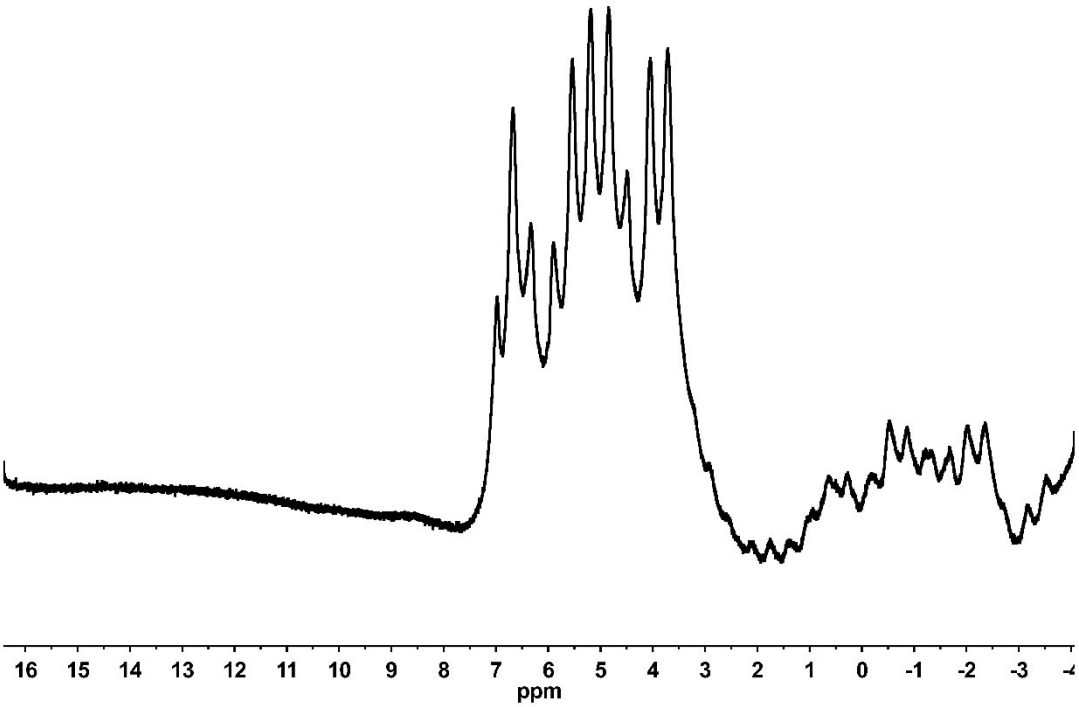

Figure S2. ^1H NMR spectrum of **Cr3** in $CDCl_3$.

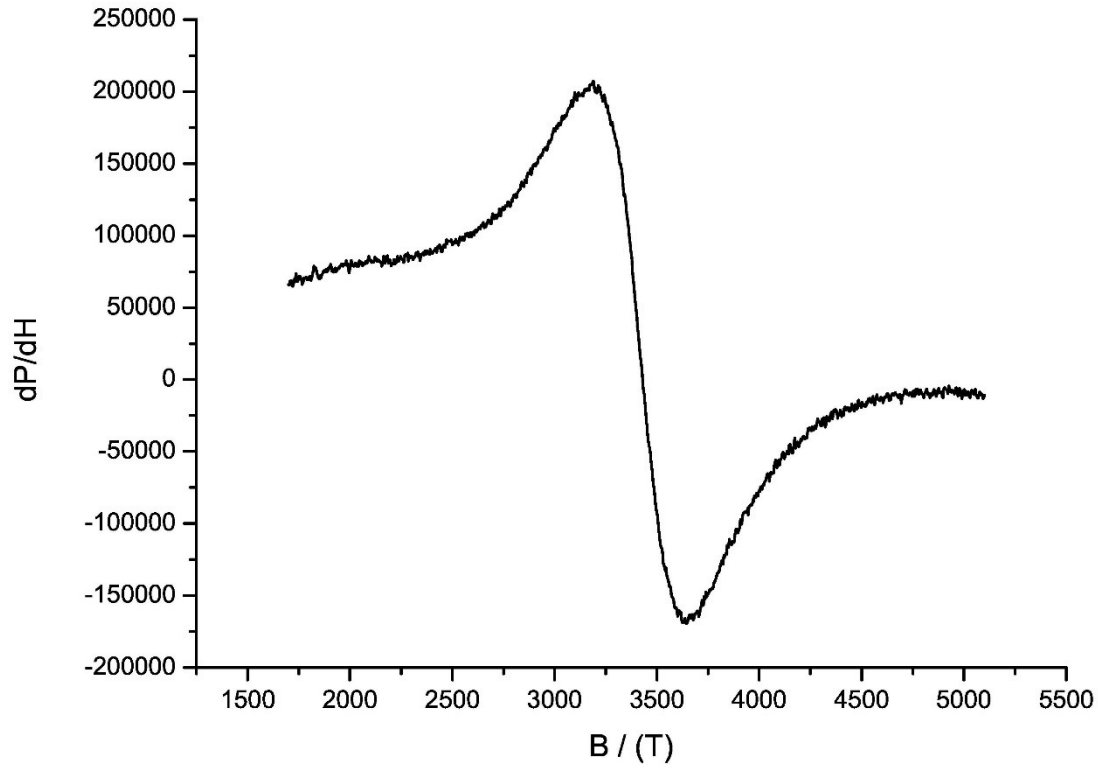

Figure S3. EPR spectrum of **Cr3**.

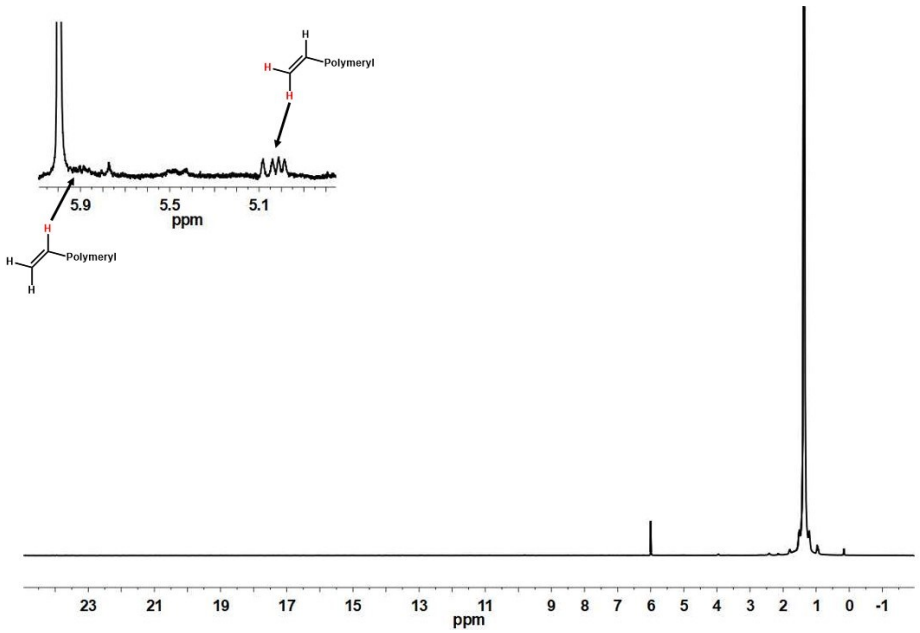

Figure S4. ^{1}H NMR spectra of PE sample obtain in Table 2 entry 7 in $C_2D_2Cl_4$.

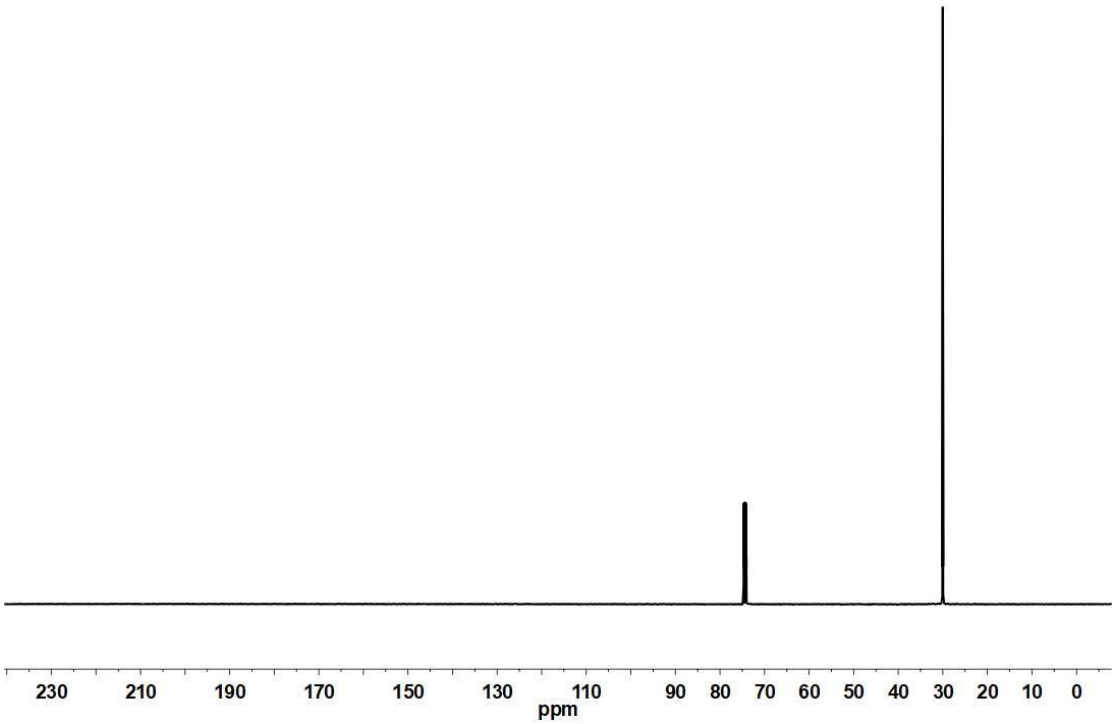

Figure S5. ^{13}C NMR spectrum of PE sample obtain in Table 2 entry 7 in $C_2D_2Cl_4$.

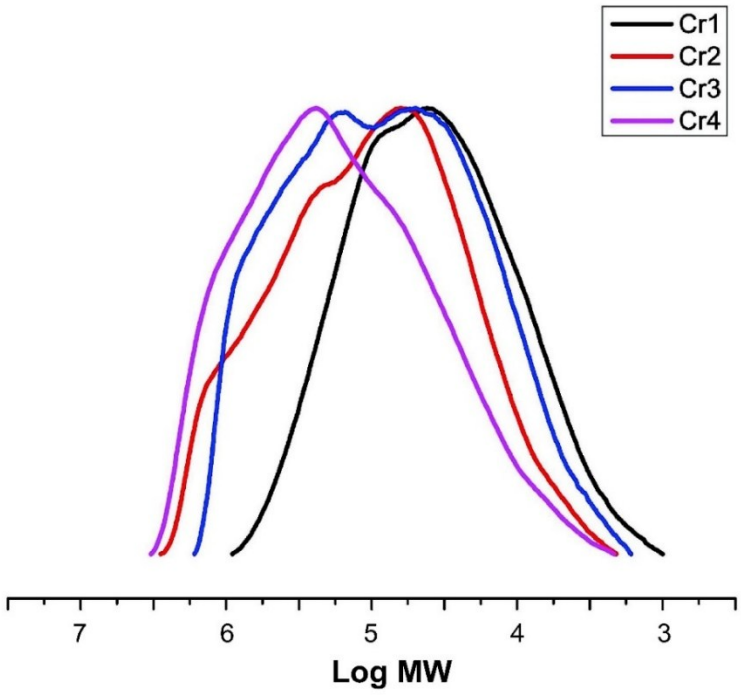

Figure S6. GPC curves of PE obtained by **Cr1-Cr4** in Table 3 entries 1-4.

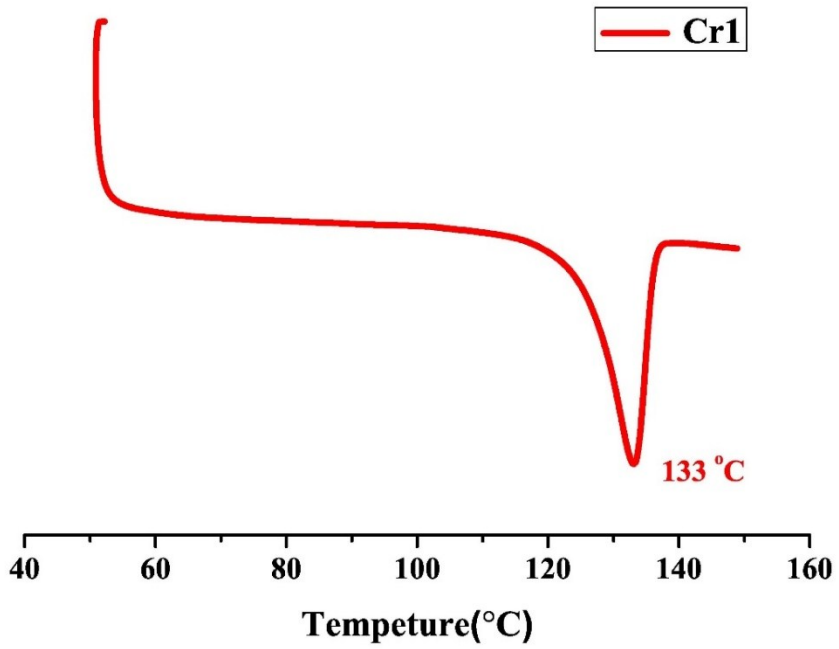

Figure S7. Thermal analysis (heating rate of 5 °C/min, 2nd scan) of PE prepared by **Cr1** in Table 3 entry 1.

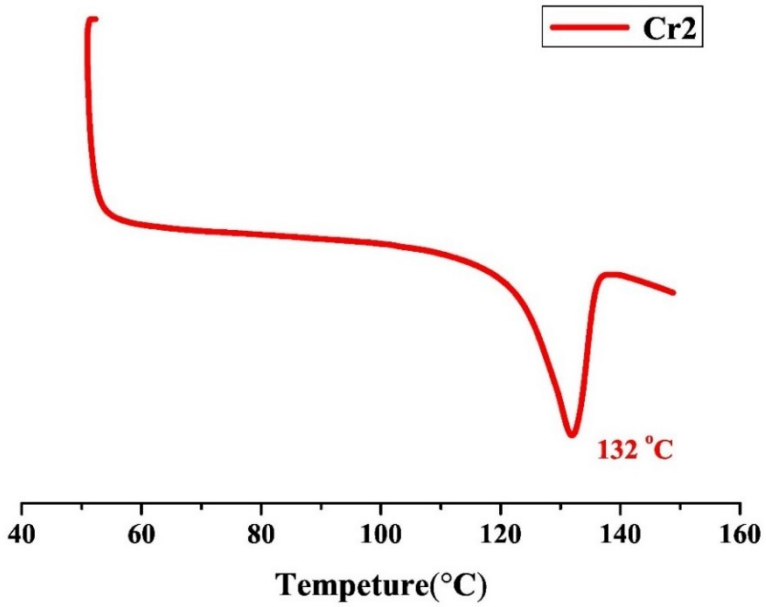

Figure S8. Thermal analysis (heating rate of 5 °C/min, 2nd scan) of PE prepared by **Cr2** in Table 3 entry 2.

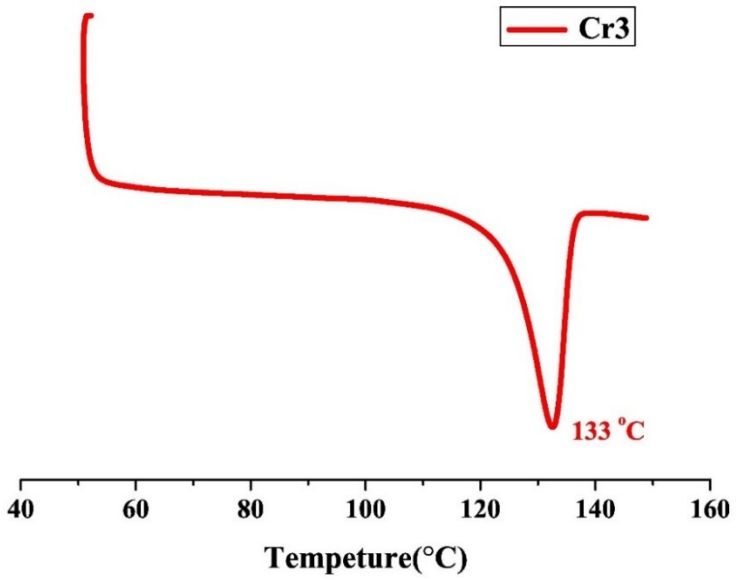

Figure S9. Thermal analysis (heating rate of 5 °C/min, 2nd scan) of PE prepared by **Cr3** in Table 3 entry 3.

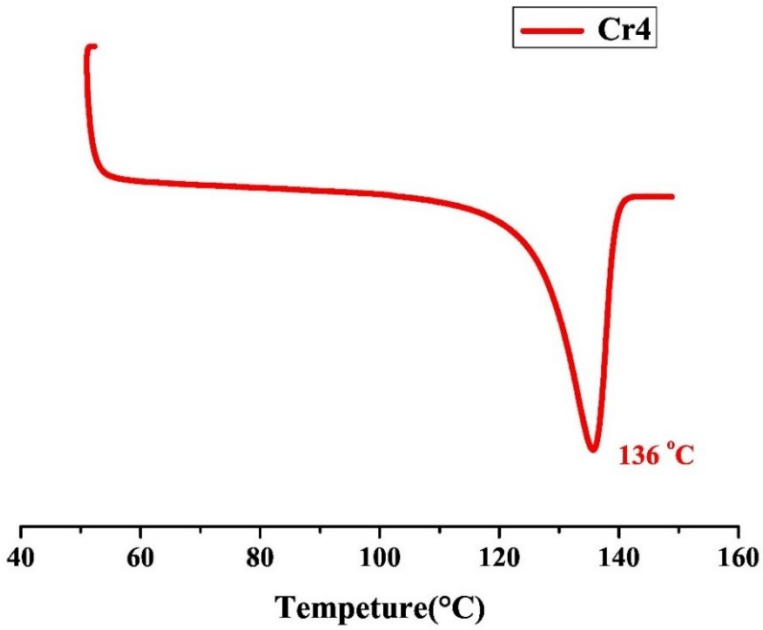

Figure S10. Thermal analysis (heating rate of 5 °C/min, 2nd scan) of PE prepared by **Cr4** in Table 3 entry 4.