

Supporting Information
for

2,6-Dibenzhydryl-*N*-(2-phenyliminoacenaphthylenyl-idene)-4-methylbenzenamine

Nickel Dibromides: Synthesis, Characterization and Ethylene Polymerization

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Table S1. Selected bond lengths and angles for **C4** and **C5**

	C4	C5
Bond Lengths (Å)		
Ni(1)-N(1)	2.040(3)	2.039(2)
Ni(1)-N(2)	2.027(3)	2.010(3)
Ni(1)-Br(1)	2.3336(8)	2.3483(7)
Ni(1)-Br(2)	2.3426(8)	2.3176(9)
N(1)-C(12)	1.284(5)	1.291(4)
N(1)-C(13)	1.451(5)	1.444(3)
N(2)-C(1)	1.281(5)	1.286(4)
N(2)-C(46)	1.460(5)	1.439(4)
Bond Angles (°)		
N(2)-Ni(1)-N(1)	83.03(14)	83.25(10)
N(2)-Ni(1)-Br(1)	109.68(10)	105.18(8)
N(1)-Ni(1)-Br(1)	108.76(10)	105.43(7)
N(2)-Ni(1)-Br(2)	111.07(10)	110.94(8)
N(1)-Ni(1)-Br(2)	115.24(10)	115.76(7)
Br(1)-Ni(1)-Br(2)	122.20(3)	127.18(2)
C(12)-N(1)-C(13)	119.4(3)	122.5(2)
C(1)-N(2)-C(46)	119.4(3)	121.4(3)

Table S2. Crystal data and structure refinement for **C4** and **C5**

	C4	C5
formula	C ₅₄ H ₄₄ Br ₂ N ₂ Ni	C ₅₆ H ₄₈ Br ₂ N ₂ Ni
Formula weight	939.44	967.49
Temperature(K)	173(2)	173(2)
Wavelength(Å)	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	P2(1)/n	P-1
a (Å)	13.993(3)	10.685(2)
b (Å)	17.075(3)	12.489(3)
c (Å)	18.979(4)	18.069(4)
α (°)	90	75.13(3)
β (°)	105.35(3)	84.45(3)
γ (°)	90	79.63(3)
Volume (Å ³)	4372.9(15)	2289.4(8)
Z	4	2
Dcalc (Mg m ⁻³)	1.427	1.404
μ (mm ⁻¹)	2.310	2.209
F(000)	1920	992
Crystal size(mm)	0.17×0.14×0.13	0.27×0.15×0.14
θ range (°)	1.62-27.48	1.17-27.48
Limiting indices	-18 ≤ h ≤ 18, -21 ≤ k ≤ 22, -22 ≤ l ≤ 24	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -23 ≤ l ≤ 23
No. of reflections collected	35240	28271
No. of unique reflections	9800	10447
R_{int}	0.0558	0.0366
Completeness to θ (%)	97.8(θ =27.48°)	99.5(θ =27.48°)
No. of parameters	532	578
Goodness-of-fit on F ²	1.230	1.211
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0682 wR2 = 0.1674	R1 = 0.0516 wR2 = 0.1375
R indices (all data)	R1 = 0.0803 wR2 = 0.1811	R1 = 0.0631 wR2 = 0.1516

Table S3. Polyethylenes by the catalytic systems of **C1-C5** and the branches

Entry	Cat.	Cocat.	Al/Ni	T/°C	T/min	Branches/1000 C
1	C4	MAO	1000	20	30	47 ^a
2	C4	MMAO	1000	20	30	
3	C4	Et ₂ AlCl	200	20	30	46 ^a
4	C4	EASC	200	20	30	
5	C4	Et ₂ AlCl	400	20	30	72 ^a
6	C4	Et ₂ AlCl	600	20	30	64 ^a , 99 ^b
7	C4	Et ₂ AlCl	800	20	30	59 ^a
8	C4	Et ₂ AlCl	1000	20	30	48 ^a
9	C4	Et ₂ AlCl	500	20	30	77 ^a
10	C4	Et ₂ AlCl	700	20	30	61 ^a
11	C4	Et ₂ AlCl	600	40	30	90 ^a
12	C4	Et ₂ AlCl	600	60	30	120 ^a , 337 ^b
13	C4	Et ₂ AlCl	600	50	30	113 ^a
14	C1	Et ₂ AlCl	600	20	30	70 ^a
15	C2	Et ₂ AlCl	600	20	30	66 ^a
16	C3	Et ₂ AlCl	600	20	30	93 ^a
17	C5	Et ₂ AlCl	600	20	30	85 ^a
18	C4	Et ₂ AlCl	600	20	5	71 ^a
19	C4	Et ₂ AlCl	600	20	10	69 ^a
20	C4	Et ₂ AlCl	600	20	20	82 ^a
21	C4	Et ₂ AlCl	600	20	60	79 ^a
22	C4	MAO	2000	20	30	64 ^a
23	C4	MAO	3000	20	30	56 ^a
24	C4	MAO	4000	20	30	46 ^a
25	C4	MAO	2500	20	30	71 ^a
26	C4	MAO	3500	20	30	63 ^a
27	C4	MAO	3000	40	30	83 ^a
28	C4	MAO	3000	60	30	93 ^a
29	C4	MAO	3000	50	30	91 ^a
30	C1	MAO	3000	20	30	61 ^a
31	C2	MAO	3000	20	30	47 ^a
32	C3	MAO	3000	20	30	74 ^a
33	C5	MAO	3000	20	30	75 ^a
34	C4	MAO	3000	20	5	57 ^a
35	C4	MAO	3000	20	10	63 ^a
36	C4	MAO	3000	20	30	77 ^a
37	C4	MAO	3000	20	60	79 ^a

^a Determined by FT-IR. The number of branches were calculated according to the FT-IR spectra of the polyethylenes obtained according to the literature.¹ ^b Determined by ¹³C NMR (see Figure 3 in text and the following Figure 1S).

In general, the relative lower values were obtained by FT-IR spectra for the branch numbers for the obtained polyethylenes, compared to the values obtained by ¹³C NMR.

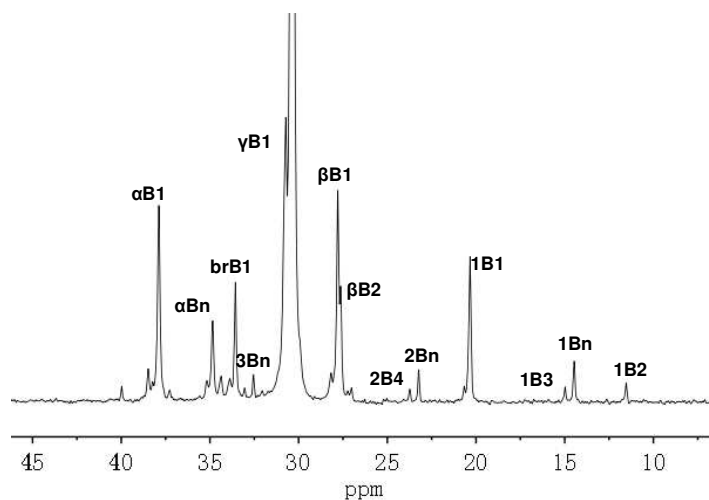


Figure S1. ^{13}C -NMR spectrum of polyethylene prepared with catalyst **C4**/ AlEt_2Cl (entry 3 in Table 2).

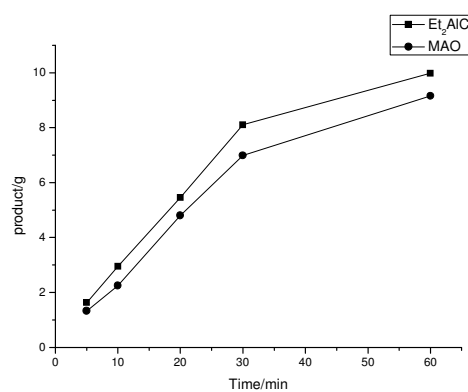
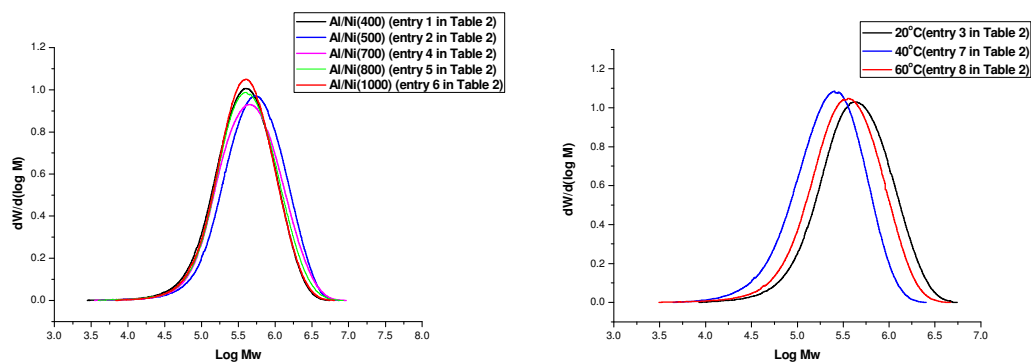
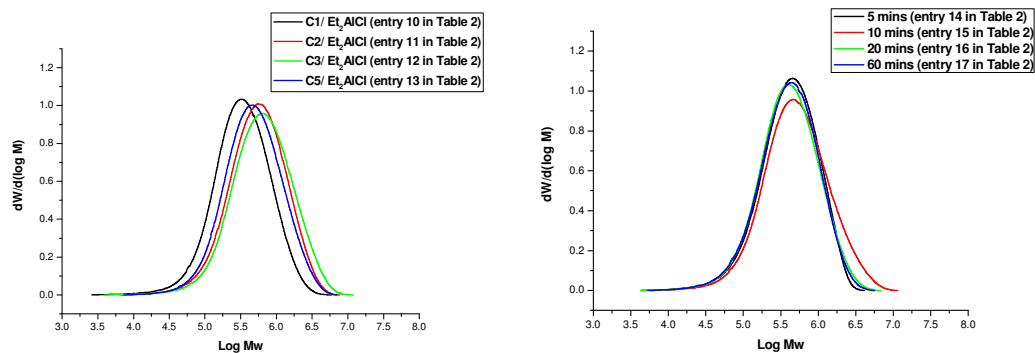


Figure S2: Output of **C4**/ Et_2AlCl and **C4**/MAO systems over different reaction time.

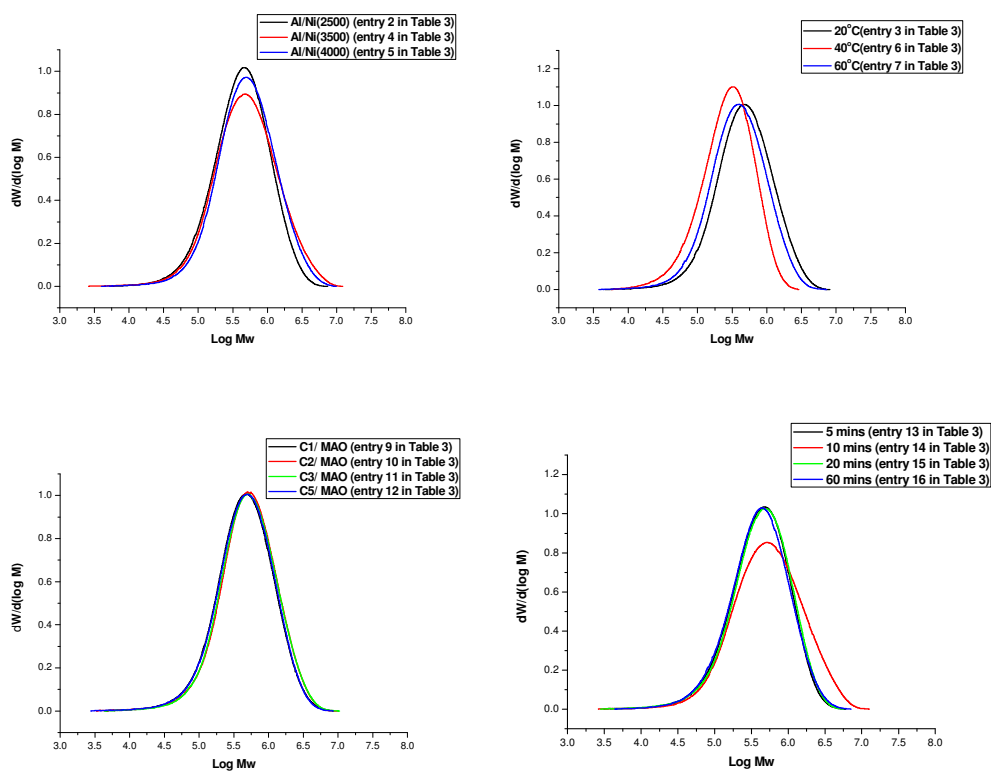
The GPC diagrams of corresponding polyolefins regarding individual tables.

The GPC diagrams of resultant PEs by the **C1-C5**/ Et_2AlCl systems (Table 2).





The GPC diagrams of resultant PEs by the C1-C5/ MAO systems (Table 3).



References

(1) Usami, T and Takayama, S. *Polym. J.*, **1984**, 16(10), 731.