

Supplementary Information

Article

Synthesis of High-Molecular-Weight Polypropylene Elastomer by Propylene Polymerization Using α -Diimine Nickel Catalysts

Lujie Gao ^{1,†}, Hegang Ren ^{2,†}, Yanhui Hou ^{3,*}, Linlin Ye ¹, Hao Meng ³, Binyuan Liu ¹ and Min Yang ^{1,*}

¹ Hebei Key Laboratory of Functional Polymers, Institute of Polymer Science and Engineering, Hebei University of Technology, Tianjin 300401, China; gaolujie0511@163.com (L.G.); yell_23@163.com (L.Y.); byliu@hebut.edu.cn (B.L.)

² School of Material Science and Engineering, Guangdong University of Petrochemical Technology, Maoming 525000, China; rhg@gdupt.edu.cn

³ State Key Laboratory of Separation Membranes and Membrane Processes, School of Material Science and Engineering, Tiangong University, Tianjin 300160, China; menghao@163.com

* Correspondence: houyanhui@tiangong.edu.cn (Y.H.); minyang@hebut.edu.cn (M.Y.); Tel.: +86-22-6020-4305 (M.Y.)

† These authors contributed equally to this work.

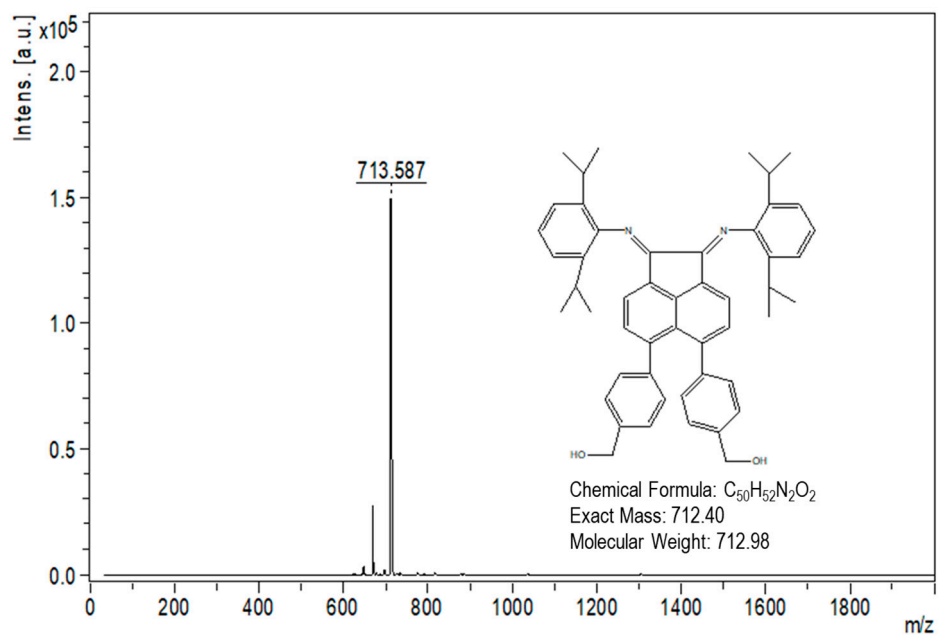


Figure S1 The MS(ESI) spectrum of **L1**

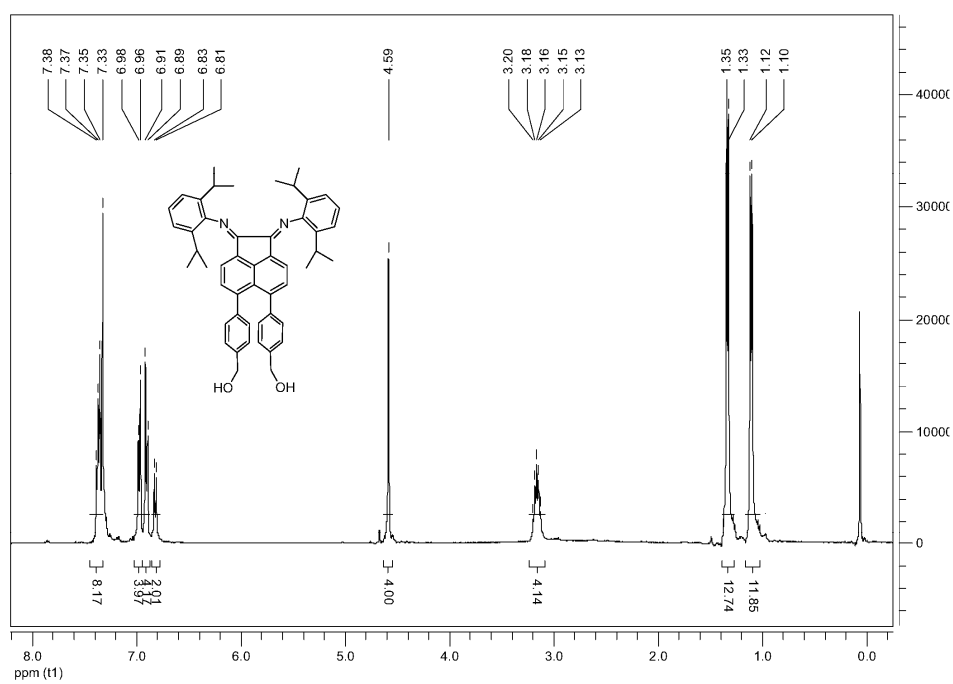


Figure S2 The ^1H NMR spectrum of **L1**

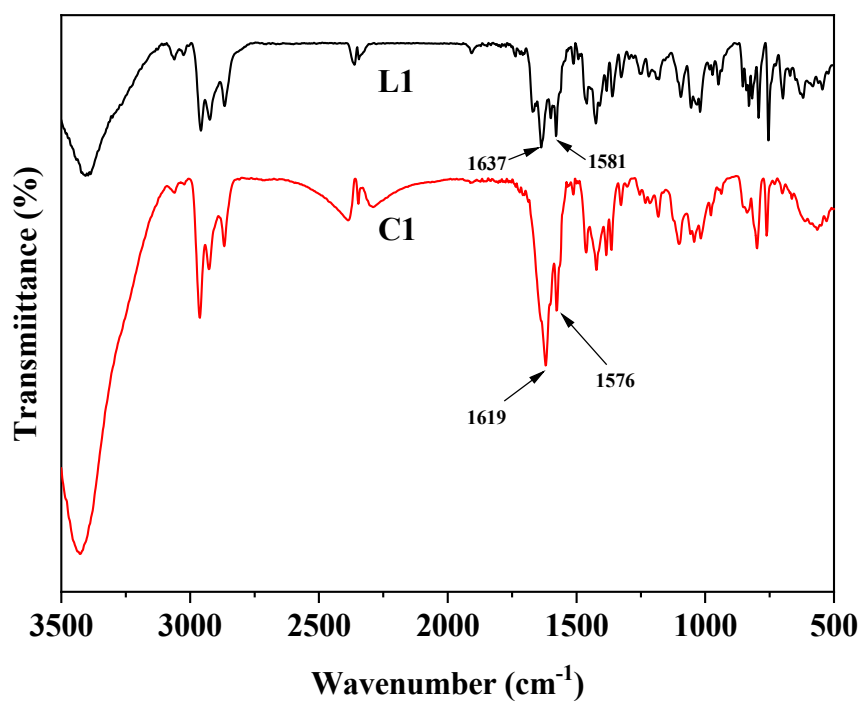


Figure S3 FT-IR spectra of L1 and corresponding complex C1

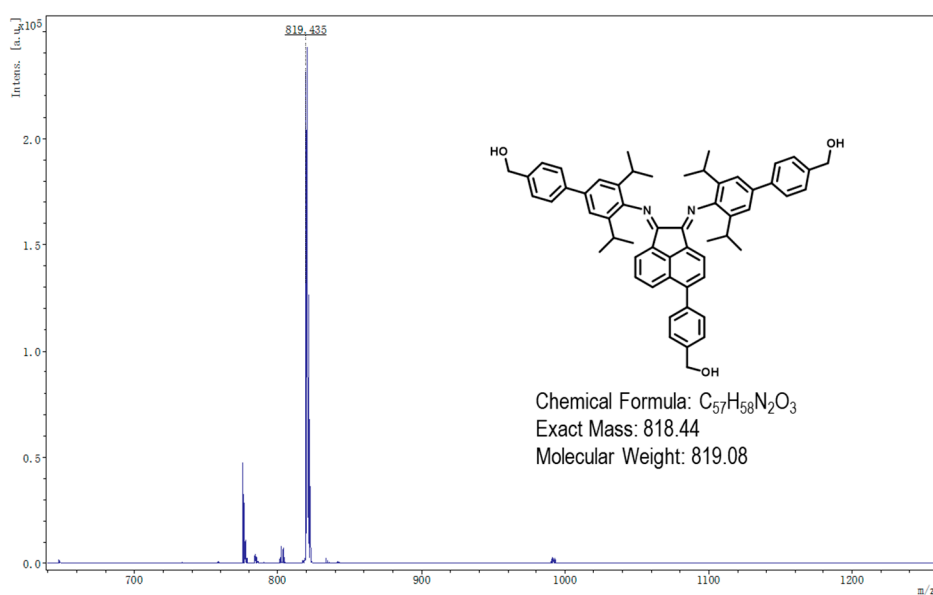


Figure S4 The MS(ESI) spectrum of L2

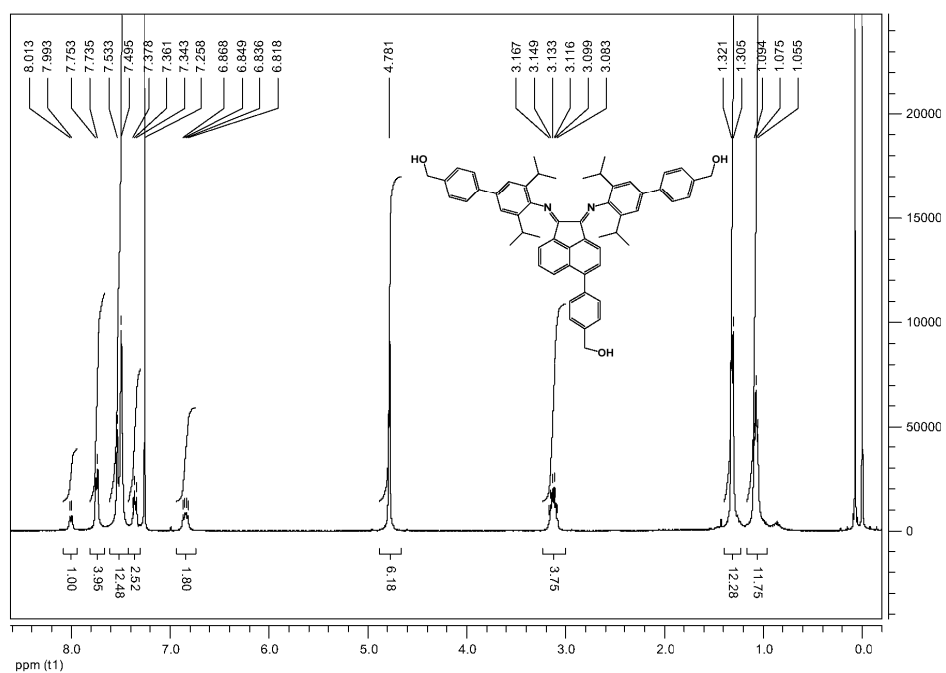


Figure S5 The ^1H NMR spectrum of L2

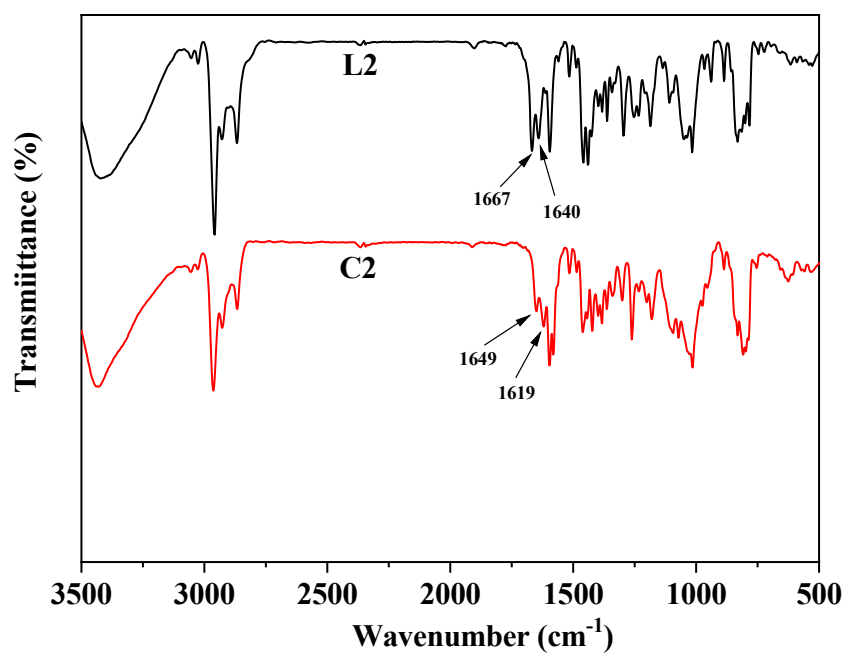


Figure S6 FT-IR spectra of L2 and corresponding complex C2

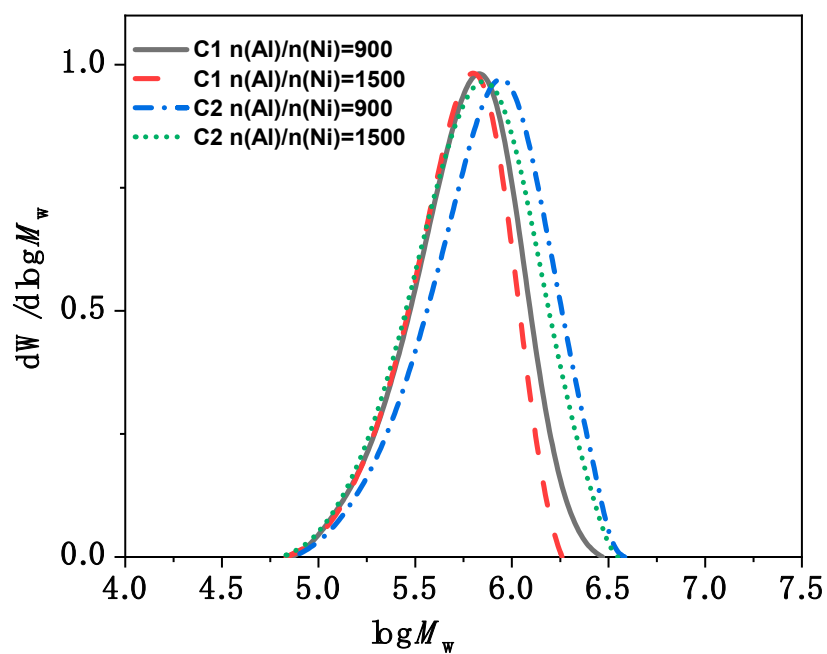


Figure S7 GPC curves of polypropylenes prepared by C1 and C2 (Entries 1, 3 in Table 1, Entries 11, 13 in Table 2)

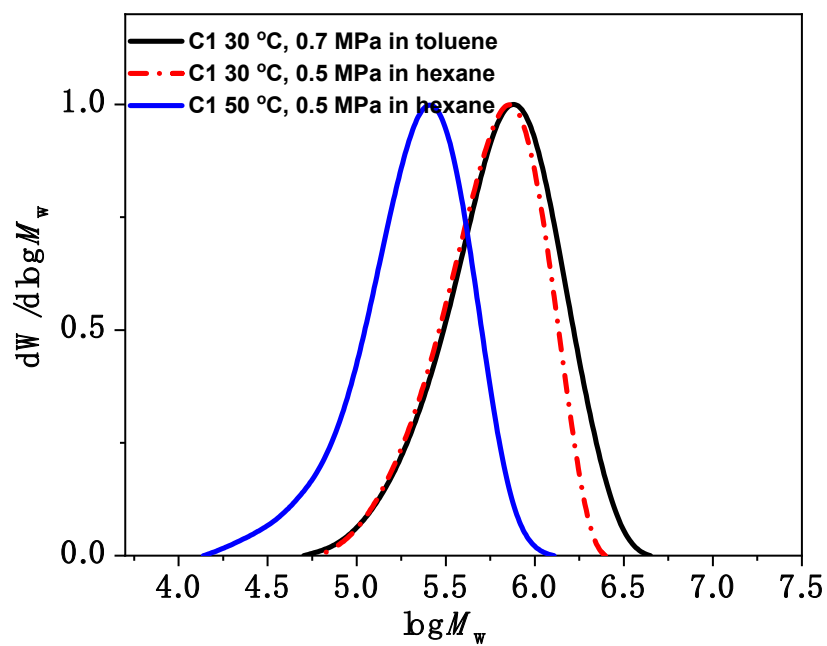


Figure S8 GPC curves of polypropylenes prepared by C1 (Entries 8, 9, 10 in Table 1)

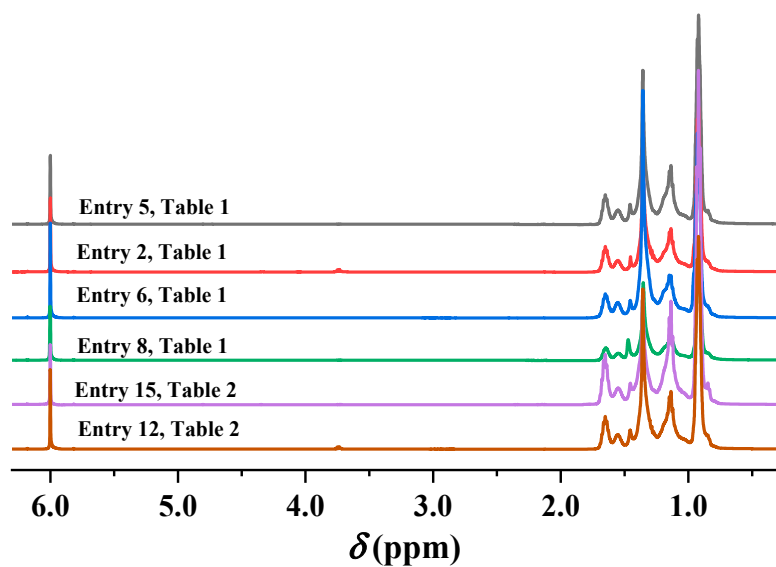


Figure S9 The ^1H -NMR spectra of polypropylenes

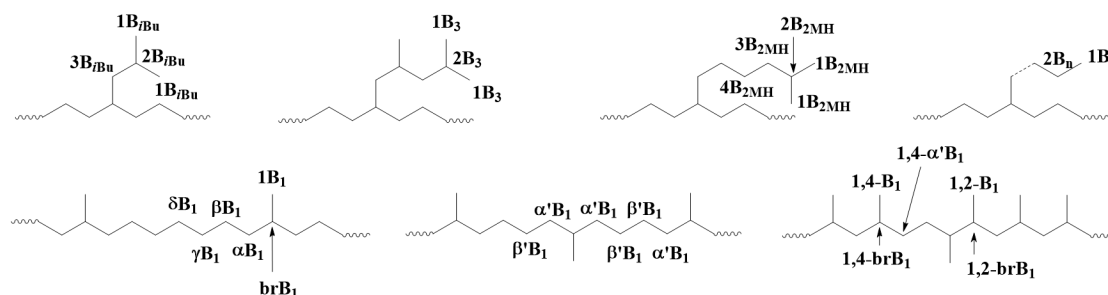


Figure S10 Branched units of polypropylenes

Table S1 Nuclear magnetic carbon spectroscopy of polypropylene

Peak Number	Chemical Shift Experiment (ppm)	Chemical Shift Calculation 1 (ppm)	Chemical Shift Calculation 2 (ppm)	Sequence	Carbon	
1	13.97	14.13	13.86	ELE	1B _n	
2	16.40	14.3-16.6	16.64	PP*P	1B ₁	P _{αγ}
3	16.68	16.72	17.13	PPP*	1B ₁	P _{αβ}
	16.91	17.01				
4	19.6-20.2	19.5-20.2	20.61	PPPr	1B ₁	P _{ββ}
	19.78	19.78		PPPPmrrm		
	19.90	12.92		PPPPmrrr		
	19.98					
	20.08	20.07		PPPPrrrr	1B ₁	P _{ββ}
5	20.3-20.5					
	20.42	20.43	20.61	PPPPmrrm	1B ₁	P _{ββ}

	20.48	20.57	20.12	<u>EPP</u> + <u>PPE</u> <u>P</u> * <u>PP</u>	1B ₁ 1,4-B ₁	P _{βδ} P _{βγ}
6	20.60	20.67	20.61	<u>PPPP</u> <u>mrmm</u> + <u>r</u> <u>mrr</u>	1B ₁	P _{ββ}
7	20.81	20.81	20.61	<u>PPPP</u> <u>mmrr</u>	1B ₁	P _{ββ}
8	21.0-21.7	20.95-22.0	20.61	<u>PPP</u> mm	1B ₁	P _{ββ}
#	22.58					
9	22.68	22.82	22.13	<u>E2MHE</u>	1B _{2MH}	
10	23.0-24.0	23.0-24.0	22.62	<u>EiBuE</u>	1B _{iBu}	
			22.65	<u>ELE</u>	2B _n	
11	24.4-24.8	24.0-25.0	24.58	<u>PEP</u>	β'B ₁	S _{ββ}
12	25.5-25.8					
	25.64	25.65	25.92	<u>EiBuE</u>	2B _{iBu}	
13	27.0-27.4	27.10-27.55	27.27	<u>E2MHE</u>	4B _{2MH}	
	27.27		27.27	<u>PEE</u> + <u>EEP</u>	βB ₁	S _{βδ}
14	27.4-27.8	27.51-27.81				
	27.47		27.51, 27.9			S _{βγ}
	27.64		27.77			
15	27.8-28.7					
	28.03	29.97	27.99	<u>E2MHE</u>	4B _{2MH}	
	28.16		28.4			T _{ββ} (mr+rr)
	28.23					
	28.59		28.7			T _{ββ} (mm)
16	29.38	29.58	29.71	<u>ELE</u>	4B _n	
17	29.84	30.00	29.96	<u>EEE</u>	δB ₁ , δB _n	S _{δδ}
18	30.21	30.35	30.21	<u>EEEP</u>	γB ₁	S _{γδ}
19	30.4-30.8	30.4-30.6	30.21	<u>ELE</u>	γB _n +(n-2)B _n	
				<u>E2MHE</u>	γB _{2MH}	
				<u>EiBuE</u>	γB _{iBu}	
			30.45	<u>P</u> * <u>PP</u>		T _{βγ}
	30.58	30.44	30.8	<u>EPP</u> + <u>PPE</u>	1,4-brB ₁	T _{βδ}
	30.62	30.52			brB ₁	
20	30.8-31.1	30.70	30.46	<u>PEEP</u>	1,4-α'B ₁	S _{βαβδ}
		30.79	31.53	<u>PP</u> * <u>P</u>	3B _n	
21	31.99	32.12	32.40	<u>ELE</u>	3B _n	
22	33.04	33.10	32.52	<u>EPE</u>	brB ₁	T _{δδ}
23	33.2-33.5	33.38	32.52	<u>EP</u> * <u>PE</u> + <u>EP</u> * <u>PE</u>	1,4-brB ₁ (between E)	T _{γδ} T _{γγ}
24	34.2-34.8					
		34.29	34.47	<u>P</u> * <u>P</u> * <u>PP</u> + <u>P</u> * <u>P</u> * <u>P</u> <u>P</u>	1,4-α'B ₁	S _{γαβδ}
		34.40-34.94	34.47	<u>ELE</u>	αB _n + nB _n	
				<u>E2MHE</u>	αB _{2MH} + 6B _{2MH}	
				<u>EiBuE</u>	αB _{iBu}	
			34.22	<u>EP</u> * <u>PE</u> + <u>EP</u> * <u>PE</u>	1,4-α'B ₁ (between E)	S _{δαβδ}
25	35.1-35.6					
		35.07	34.98	<u>EiBuE</u>	brB _{iBu}	
			34.99	<u>PPP</u> *	1,2-brB ₁	T _{αβ}
		35.2-35.8	34.72	<u>PP</u> * <u>PP</u>	1,4-α'B ₁	S _{γαβδ}
26	37.13-37.55					

	37.37	37.0-37.7	36.91	$\underline{EPE} \underline{EPEE}$	αB_1	$S_{\alpha\delta}$
27	37.71	37.77	37.41	$\underline{PPEPmm}$	$\alpha\gamma B_1$	$S_{\alpha\gamma}$
28	37.8-38.0			$\underline{PEPPmm}$		
		37.91	37.06	PP^*P	1,2-brB ₁	$T_{\alpha\gamma}$
		38.00	37.05	$\underline{ELE} + \underline{E2MHE}$	brBn+brB2MH	
29	38.05-38.25	38.23	37.16	$\underline{PEPEr}$	$\alpha'B_1$	$S_{\alpha\gamma}$
				$\underline{EEPPr}$	$\alpha'B_1$	
30	38.35	38.45	37.41	$\underline{PEPP} + \underline{PPEPmr} +$	$\alpha'B_1$	$S_{\alpha\gamma}$
				$\underline{mr}$		
				$\underline{PEPP} + \underline{PPEPr}$		
				$\underline{PEPPmr} + \underline{rm}$		
				$\underline{PEPPr}$		
31	39.27	39.35	39.35	$\underline{E2MHE}$	3B _{2MH}	
32	45.2-47.6	45.0-47.5				
			41.17	P^*PPP^*		$S_{\delta\alpha\alpha\beta}$
			41.42	$PPPP^*$		$S_{\gamma\alpha\alpha\beta}$
			43.86	$EPPE$		$S_{\alpha\alpha}$
			44.11	$PPPE$		
		46.74	44.36	$PPPrr$		
			43.86		3B _{iBu}	



Figure S11 The stretching of polypropylene

Table S2 Mechanical properties of polypropylenes prepared by **C1** (Entries 4, 5, 6 in Table 1)

Sample	T °C	Tensile Strength (MPa)	Young's Modulus (MPa)	Elongation Break (%)
1	0	1.03	2.19	218
2	30	0.75	1.46	317
3	50	0.29	1.20	403