

Supporting Information

Synthesis of Early Transition Metal Bisphenolate Complexes and their Use as Olefin Polymerization Catalysts

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Table S1. Stereo-sequence distribution (at the pentad level) of PPs.

Pentad	1-VCl(THF) ₂	1-TiCl ₂ (THF)	1-TiBn ₂	2-TiBn ₂	1-ZrBn ₂	1-HfBn ₂	3-TiBn ₂	4-TiBn ₂
<i>mmmm</i>	0.036	0.471	0.165	0.197	0.131	0.40	0.030	0.015
<i>mmmr</i>	0.066	0.089	0.094	0.124	0.092	0.13	0.079	0.049
<i>rmmr</i>	0.062	0.029	0.035	0.034	0.045	0.07	0.068	0.065
<i>mmrr</i>	0.087	0.078	0.115	0.148	0.102	0.11	0.111	0.095
<i>mmrm/</i>	0.186	0.096	0.188	0.154	0.214	0.11	0.263	0.275
<i>rmrr</i>								
<i>rmrm</i>	0.172	0.054	0.105	0.091	0.126	0.04	0.147	0.157
<i>rrrr</i>	0.126	0.071	0.068	0.048	0.074	0.03	0.073	0.087
<i>mrrr</i>	0.142	0.060	0.120	0.096	0.126	0.04	0.150	0.172
<i>mrrm</i>	0.123	0.053	0.111	0.109	0.092	0.06	0.080	0.087

Note: the uncertainty is ± 0.004

Table S2. The results of varying the amount of MAO with **1-VCl(THF)₂** for propylene polymerization.^a

Entry	Catalyst Loading (μmol)	MAO (eq)	Yield (mg)	Activity ^b	M _w ^c	M _N	PDI
1	5.0	500	210	84.0			
2	5.1	500	313	122.7	1147347	497142	2.31
3	5.0	1000	478	191.2			
4	6.3	1000	559	177.5	1446521	641472	2.26
5	5.1	2000	698	273.7			
6	5.1	2000	894	350.6	1170922	578123	2.03
7	5.1	3000	1753	687.5			
8	5.1	3000	2038	803.1			
9	5.1	4000	1546	606.3			
10	5.1	4000	1606	629.8			

^aConditions: Propylene (5 atm, approx. 30 mL), toluene (2 mL), 0°C, 30 m. ^bActivity = kg PP · mol cat⁻¹ · h⁻¹. ^cThe omission of data indicated that the analysis was not performed.

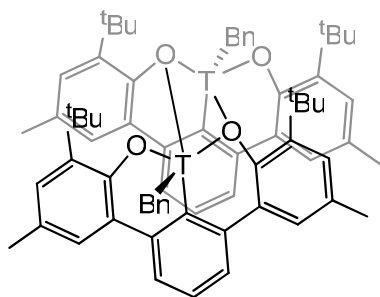


Figure S1. A schematic of the dimer obtained from **4-TiBn₂** in the presence of a sub-stoichiometric amount of activator.

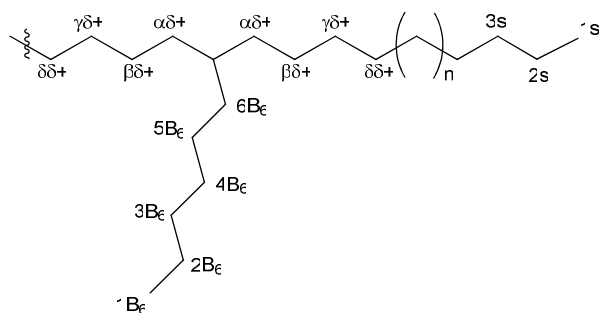


Figure S2. A schematic of an ethylene/1-octene copolymer.

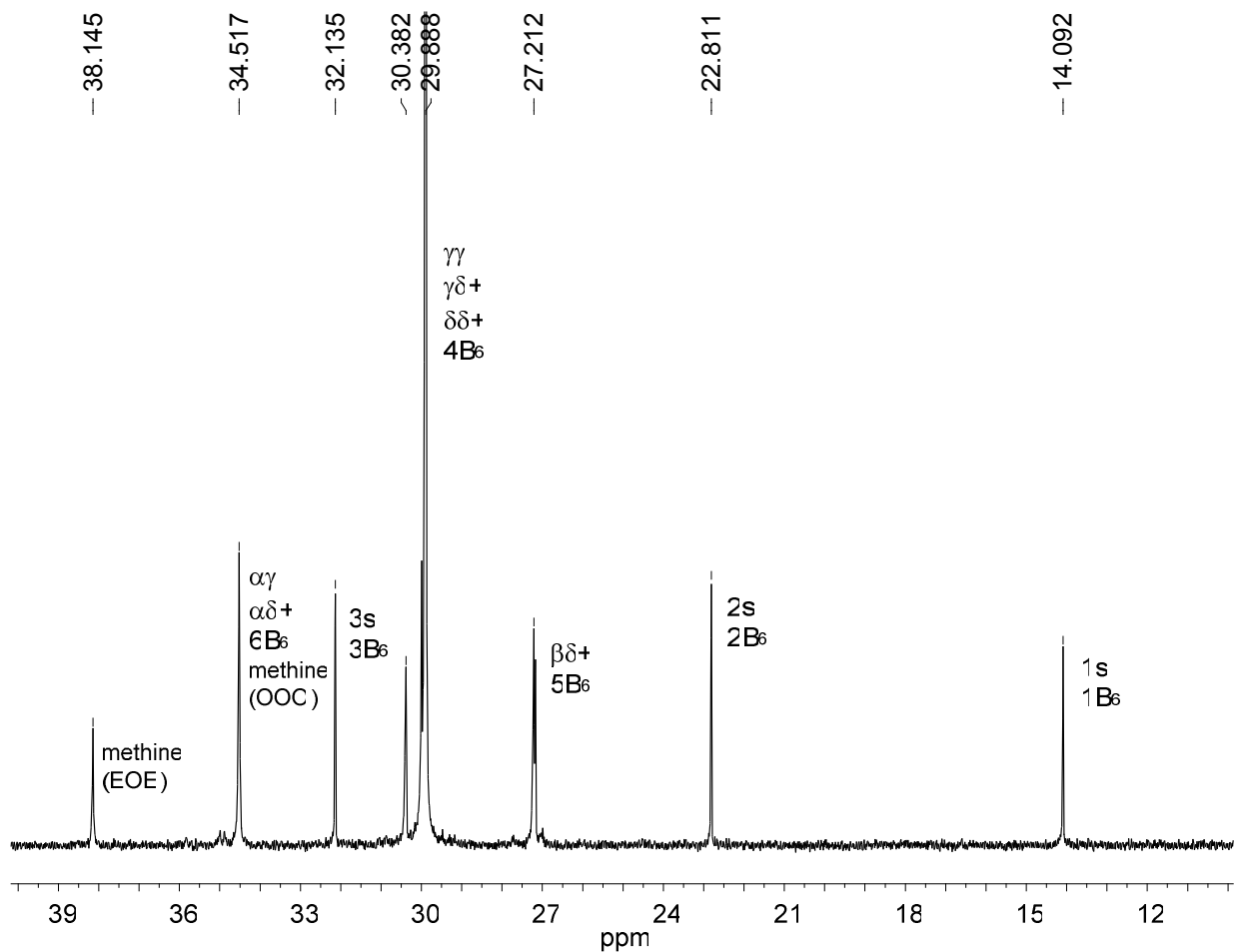


Figure S3. The ^{13}C NMR of the polymer produced by **1-VCl(THF)** in the presence of ethylene and 1-octene.