Electronic Supplementary Information

Half-Sandwich Rare-Earth Metal Complexes Bearing a C_5Me_4-C_6H_4-*o*-CH_2NMe_2 Ligand: Synthesis, Characterization and Catalytic Properties for Isoprene, 1-Hexene and MMA Polymerization

Tingting Song, Ning Liu, Xiaobo Tong, Feng Li, Xiaoyue Mu* and Ying Mu*

* The State Key Laboratory for Supramolecular Structure and Materials, School of Chemistry, Jilin University, 2699 Qianjin Street, Changchun 130012, People's Republic of China

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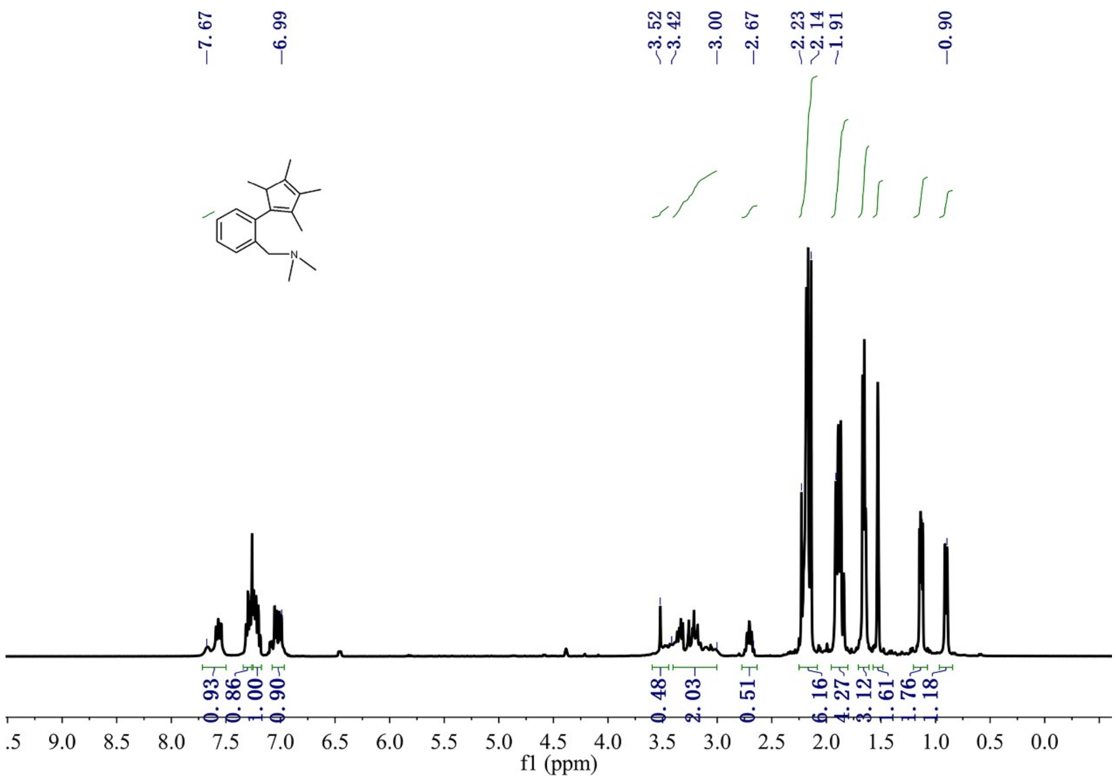

Figure S1 ^{1}H NMR spectrum of ligand H**L** (400 MHz, $CDCl_3$, 25 °C).

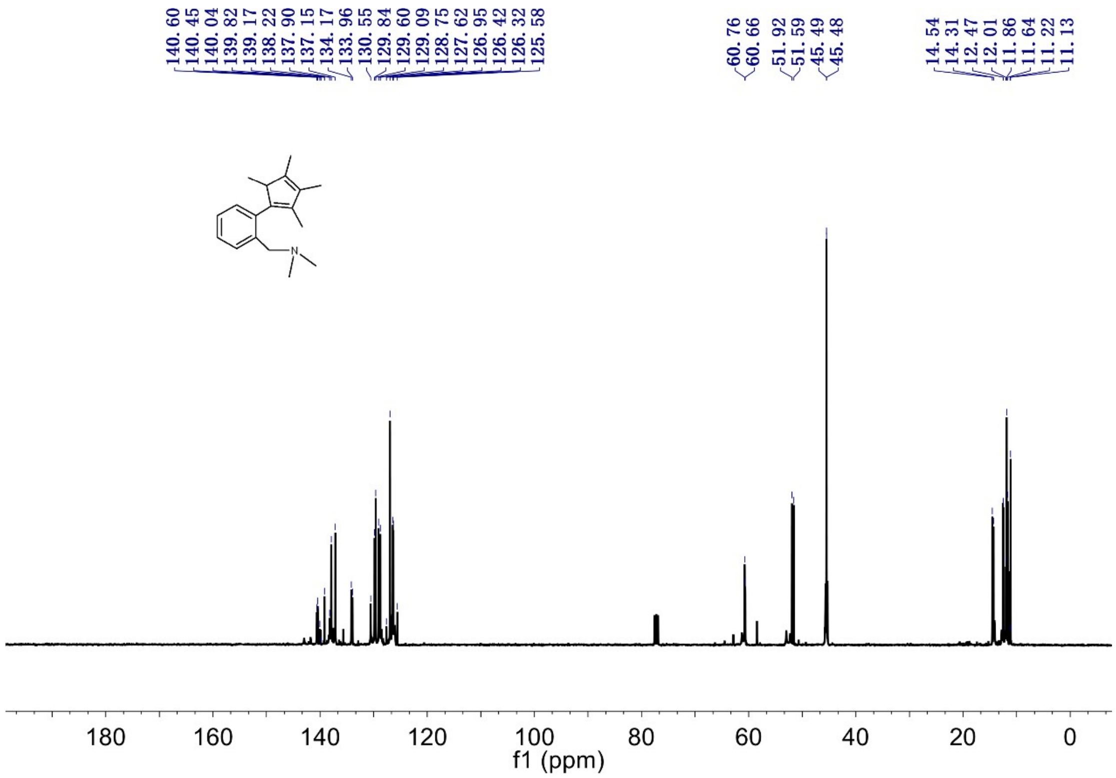

Figure S2 ^{13}C NMR spectrum of ligand H**L** (100 MHz, $CDCl_3$, 25 °C).

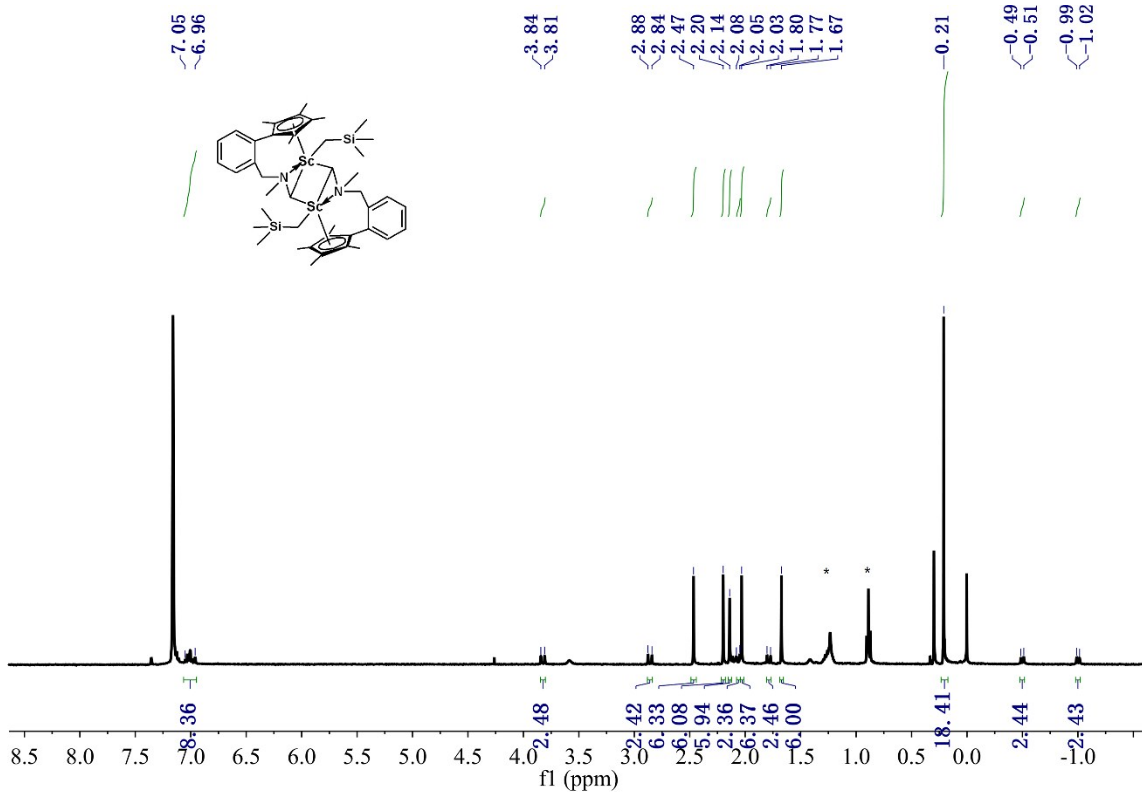

Figure S3 ^{1}H NMR spectrum of complex **1a** (400 MHz, C_6D_6, 25 °C). * stands for residual signals of hexane.

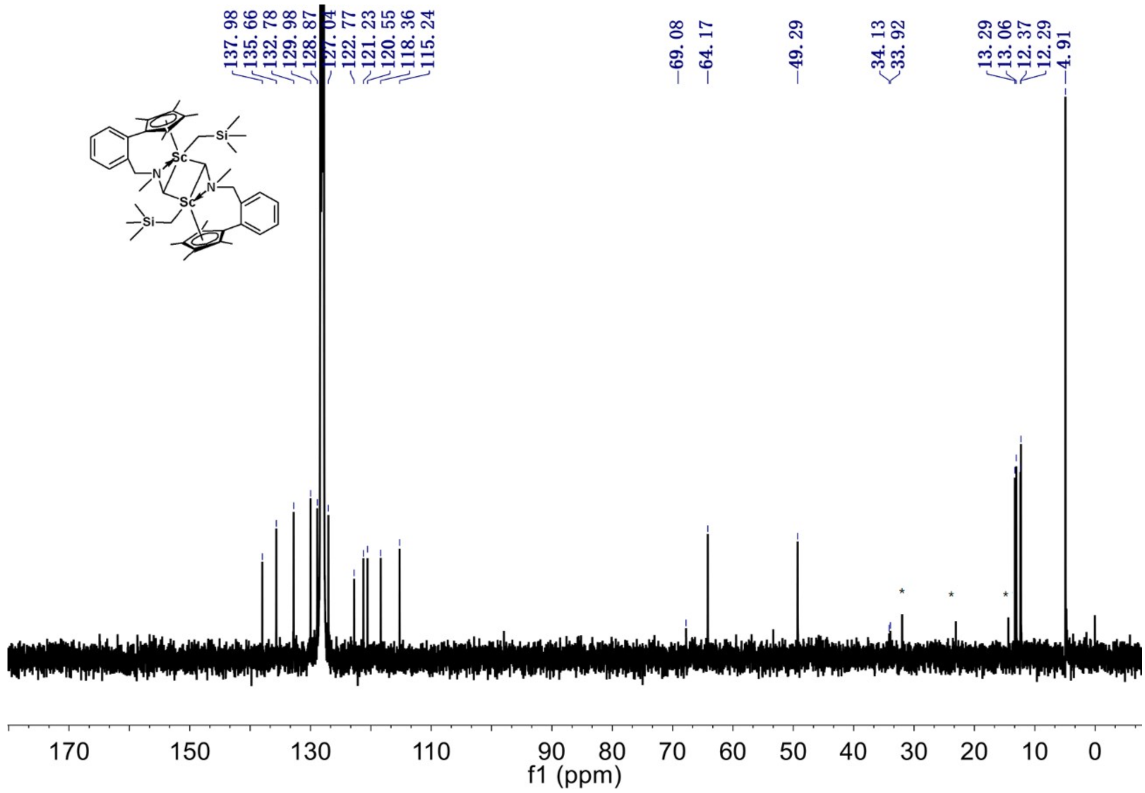

Figure S4 ^{13}C NMR spectrum of complex **1a** (100 MHz, C_6D_6, 25 °C). * stands for residual signals of hexane.

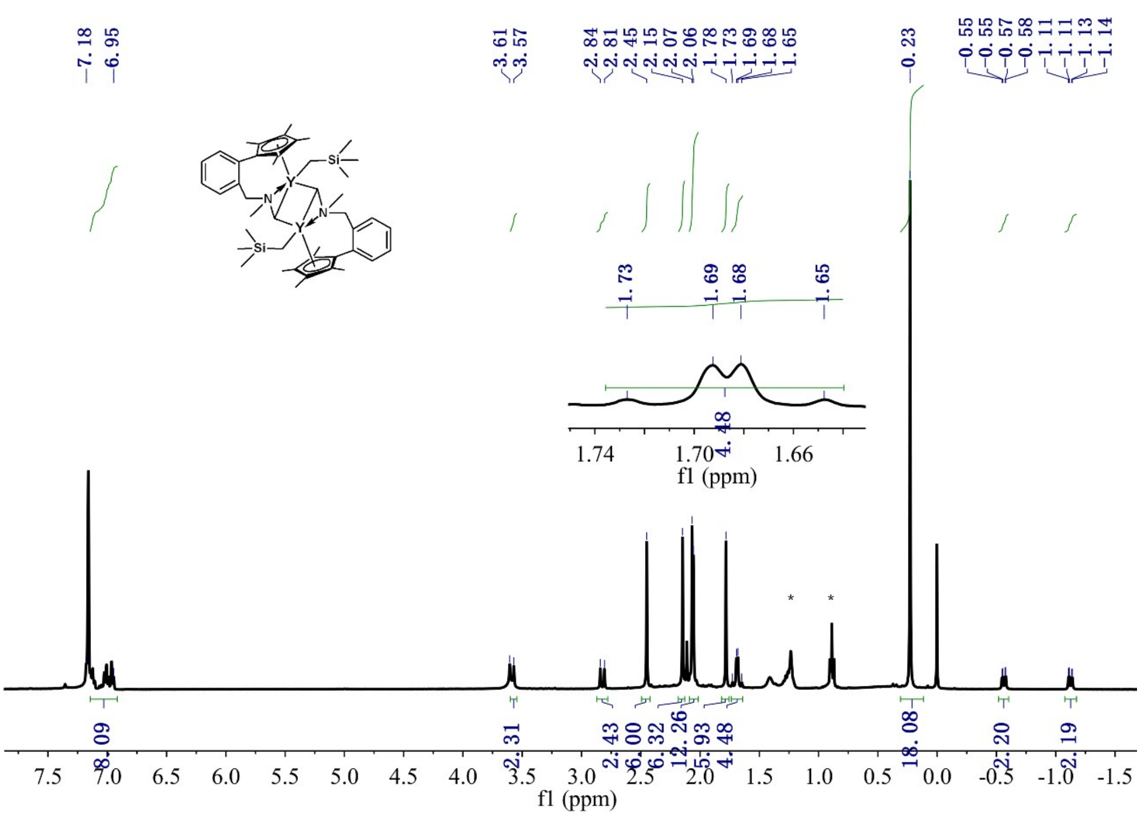

Figure S5 ^1H NMR spectrum of complex **1b** (400 MHz, C_6D_6, 25 °C). * stands for residual signals of hexane.

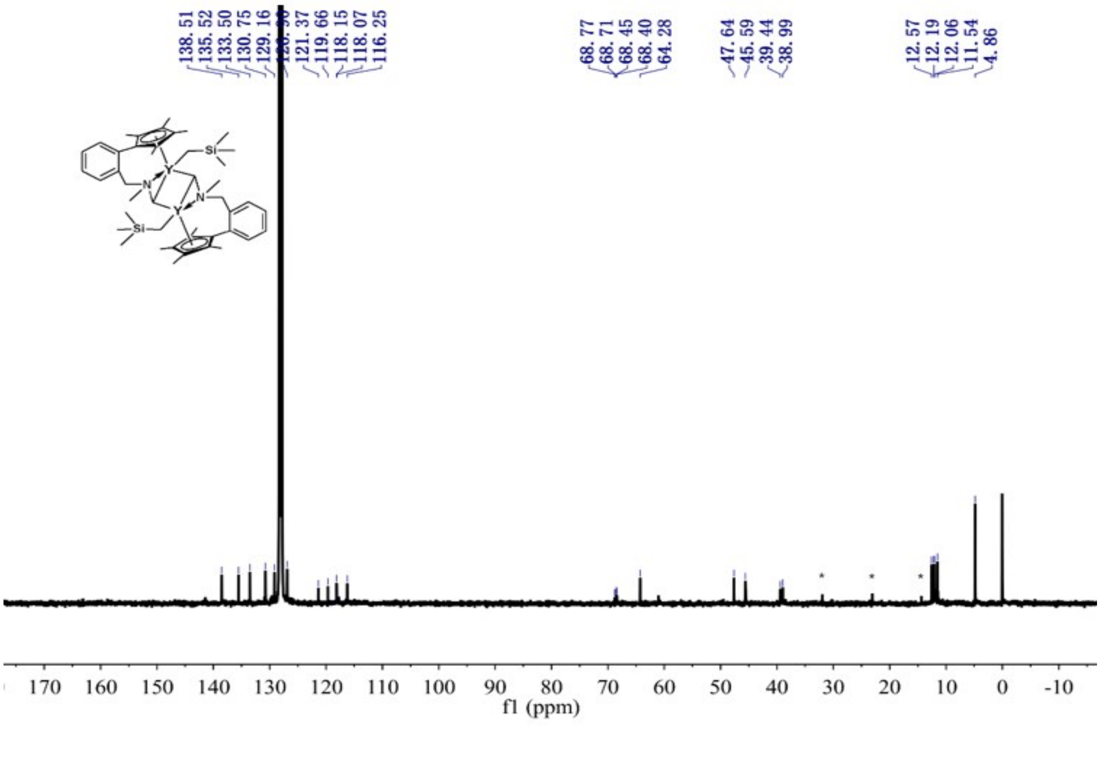

Figure S6 ^{13}C NMR spectrum of complex **1b** (100 MHz, C_6D_6,, 25 °C). * stands for residual signals of hexane.

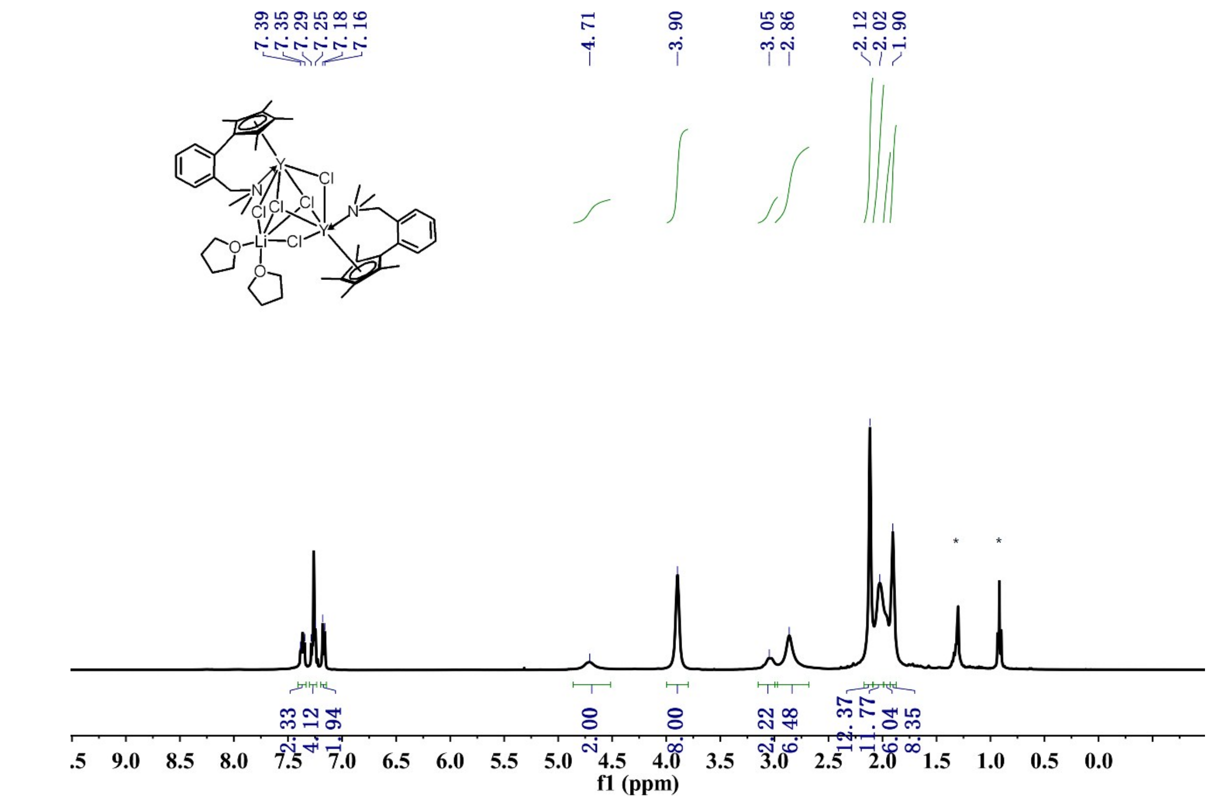

Figure S7 ^{1}H NMR spectrum of complex **2a** (400 MHz, $CDCl_3$, 25 °C). * stands for residual signals of hexane.

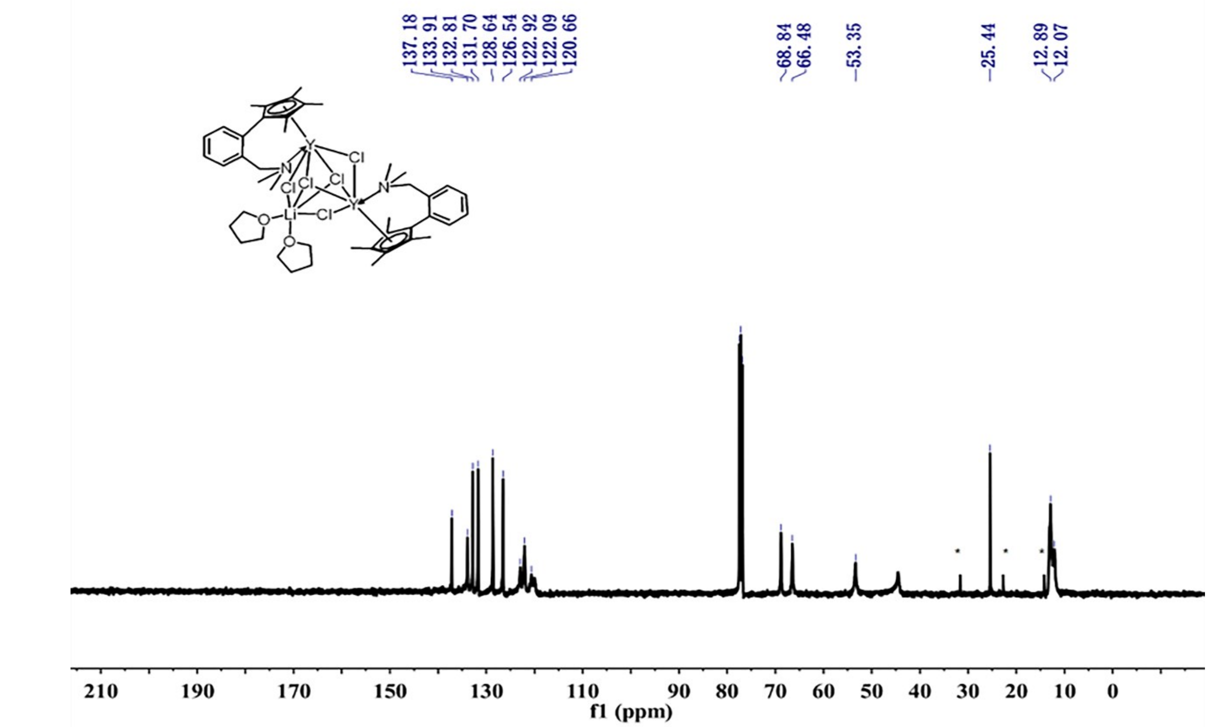

Figure S8 ^{13}C NMR spectrum of complex **2a** (100 MHz, $CDCl_3$, 25 °C). * stands for residual signals of hexane.

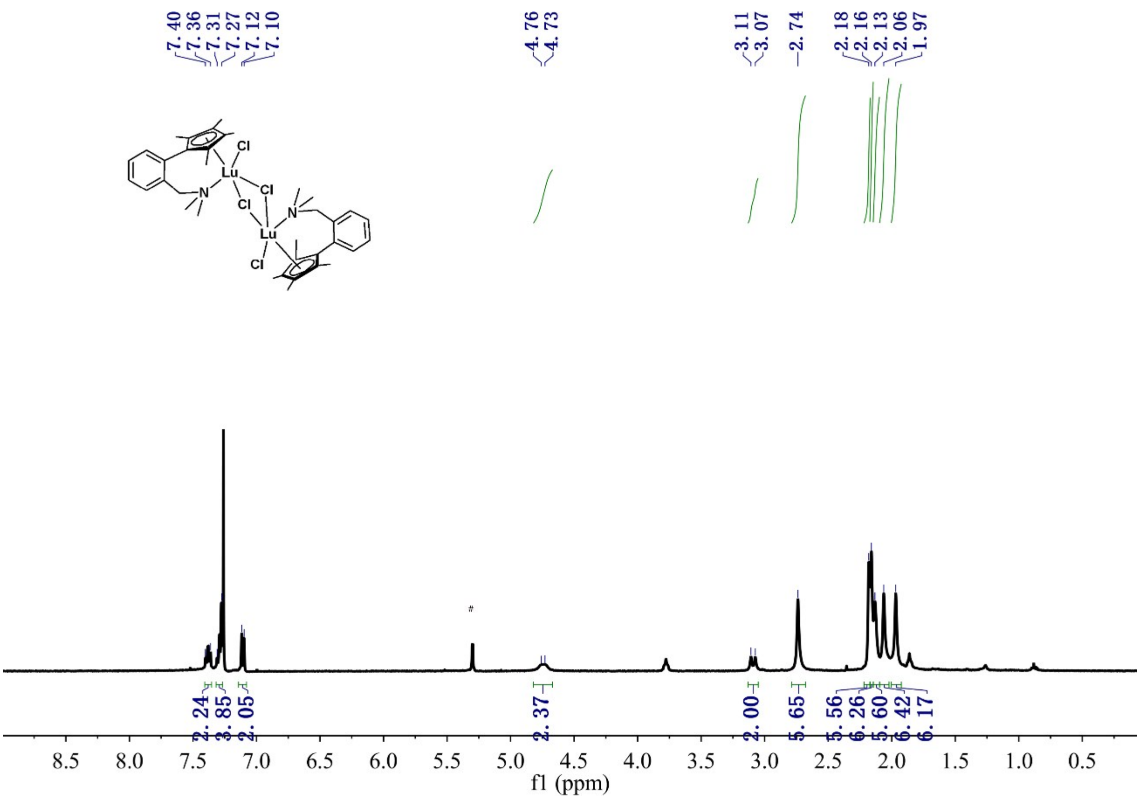

Figure S9 ^{1}H NMR spectrum of complex **2b** (400 MHz, $CDCl_3$, 25 °C). # stands for residual signals of CH_2Cl_2.

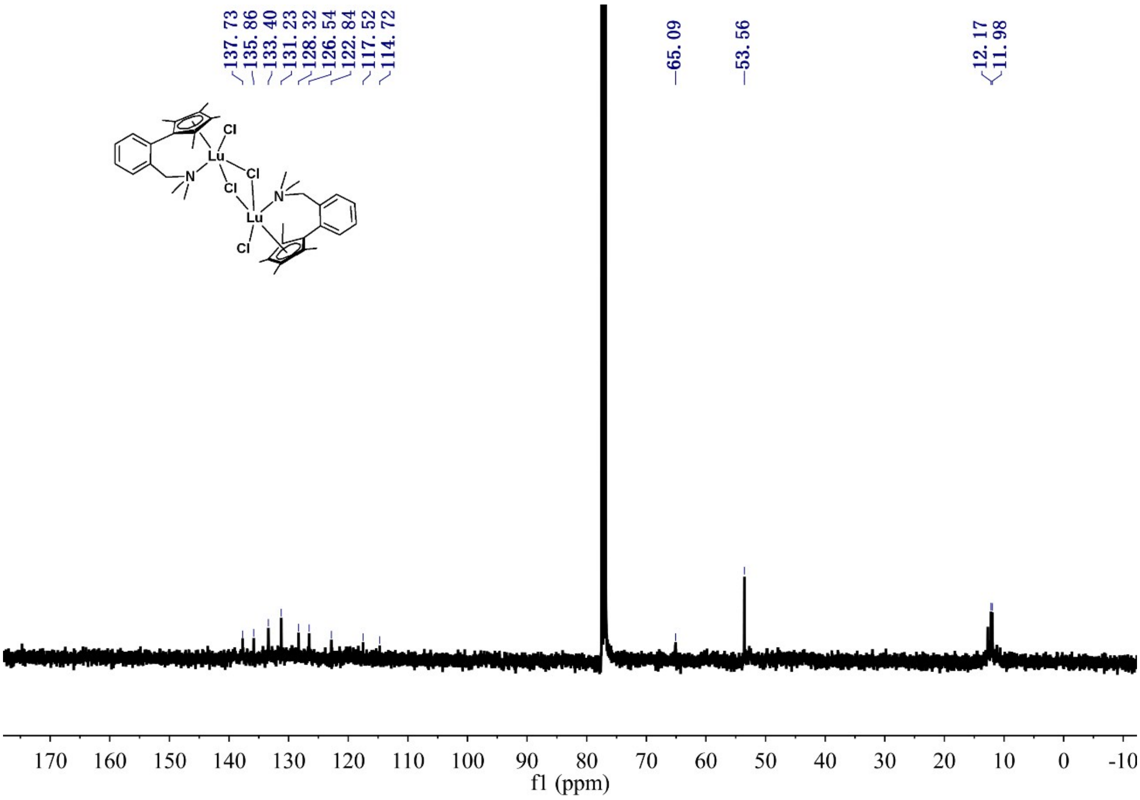

Figure S10 ^{13}C NMR spectrum of complex **2b** (100 MHz, $CDCl_3$, 25 °C).

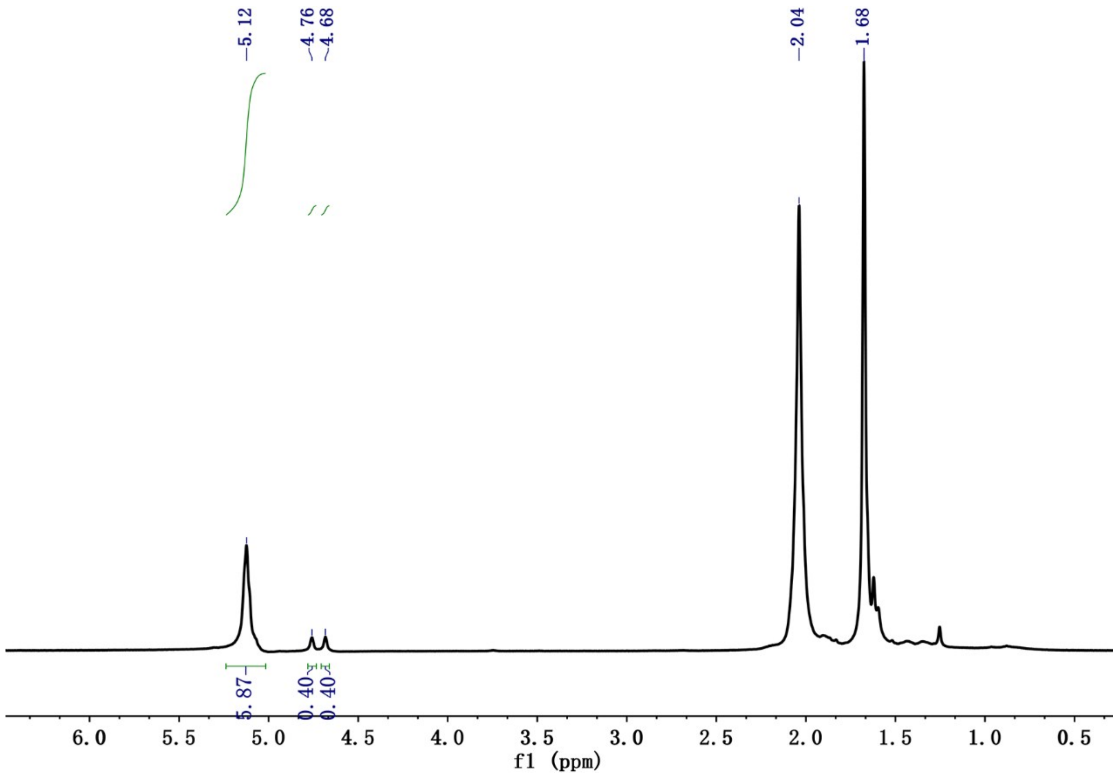

Figure S11 ^{1}H NMR spectrum of polyisoprene sample (Table 2, entry 8).

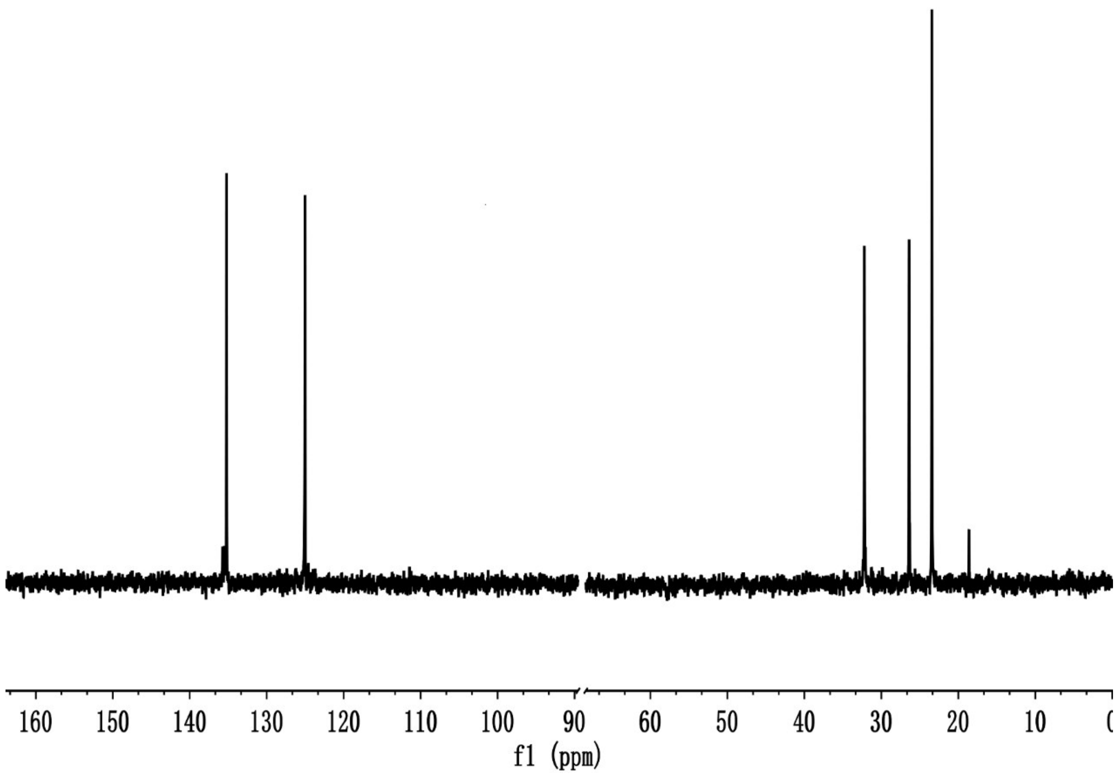

Figure S12 ^{13}C NMR spectrum of polyisoprene sample (Table 2, entry 8).

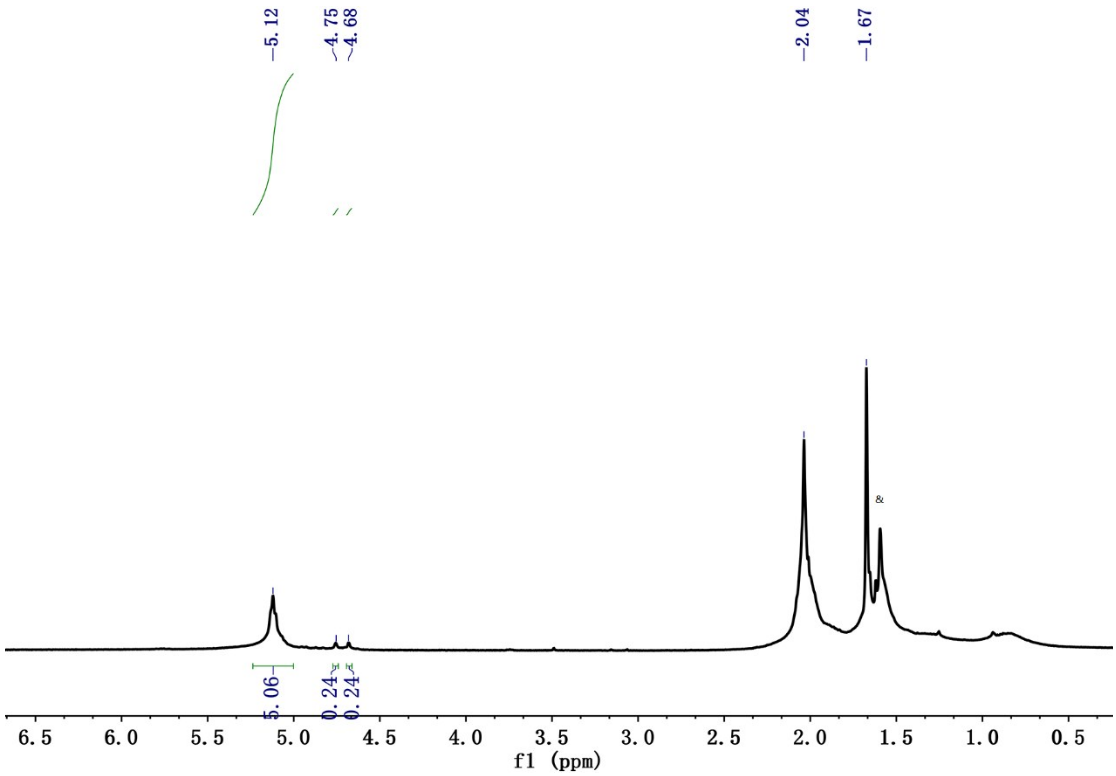

Figure S13 ^{1}H NMR spectrum of polyisoprene sample (Table 2, entry 11). & stands for residual signals of H_2O.

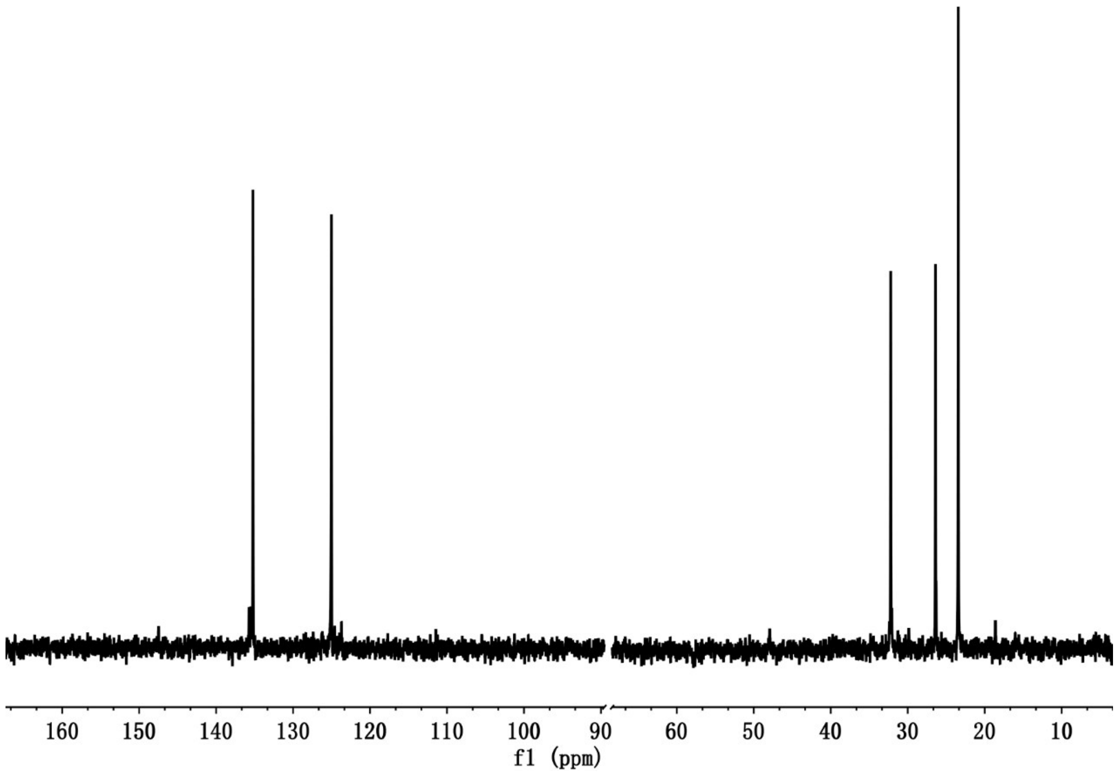

Figure S14 ^{13}C NMR spectrum of polyisoprene sample (Table 2, entry 11).

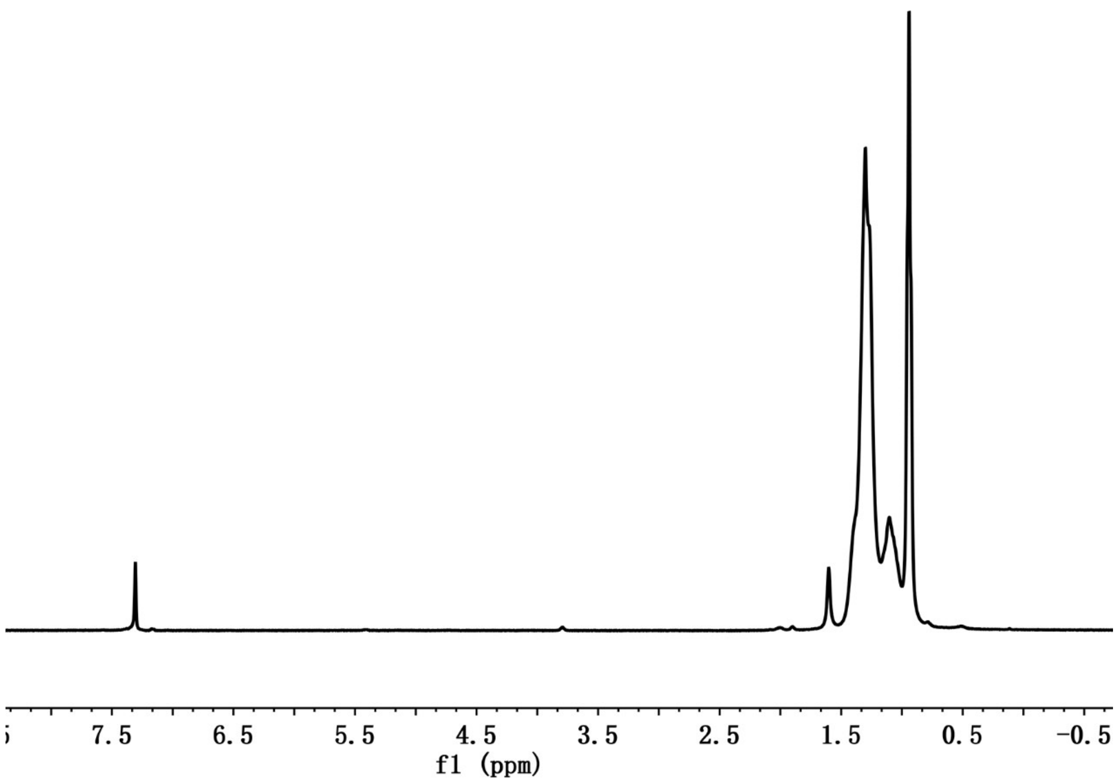

Figure S15 ^{1}H NMR spectrum of poly(1-hexene) sample.

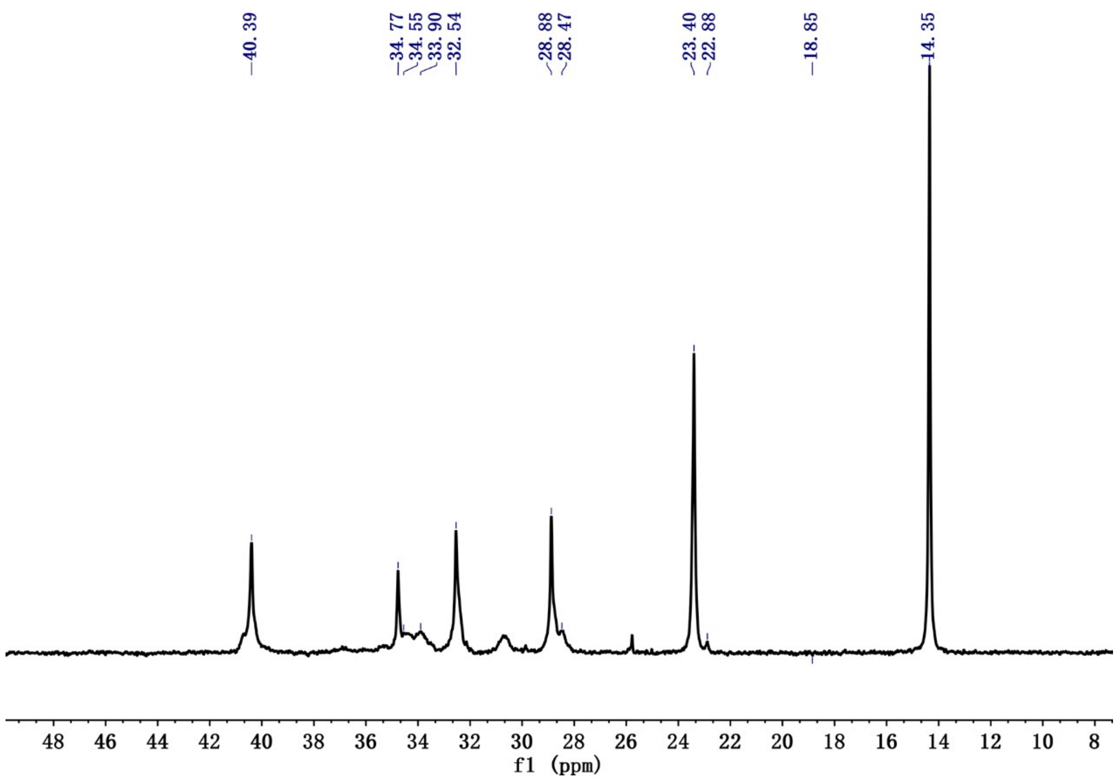

Figure S16 ^{13}C NMR spectrum of poly(1-hexene) sample.

Table S1. Crystal Data and Structure Refinements for Complexes **1a**, **1b**, **2a**, **2b**, **3a** and **3b**.

	1a	**1b**	**2a**	**2b**	**3a**	**3b**
Formula	$C_{44}H_{68}N_2Si_2Sc_2$	$C_{44}H_{68}N_2Si_2Y_2$	$C_{44}H_{64}LiN_2O_2Cl_5Y_2$	$C_{36}H_{48}N_2Cl_4Lu_2$	$C_{36}H_{64}B_4N_2Sm_2$	$C_{36}H_{64}B_4N_2Nd_2$
Mol wt	771.10	859.00	1014.98	1000.50	868.83	856.61
Cryst system	monoclinic	triclinic	monoclinic	orthorhombic	triclinic	monoclinic
Space group	$P2_1/c$	$P\bar{1}$	$P2_1/c$	Pccn	$P\bar{1}$	$P2_1/c$
a/ Å	9.8597(8)	9.2689(6)	20.3069(12)	12.5958(8)	8.6992(5)	8.732(6)
b/ Å	15.9005(13)	11.0330(8)	10.5790(6)	24.8514(15)	12.4170(7)	22.278(14)
c/ Å	14.3669(12)	11.9125(8)	24.3769(15)	12.0503(7)	21.8057(12)	24.533(16)
α/deg	90.00	77.1150(10)	90.00	90.00	92.1500(10)	90.00
β/deg	106.9240(10)	75.8990(10)	111.2640(10)	90.00	94.7390(10)	99.094(11)
γ/deg	90.00	72.1310(10)	90.00	90.00	96.5830(10)	90.00
V/ Å^3	2154.8(3)	1109.92(13)	4880.3(5)	3772.0(4)	2329.3(2)	4712(5)
Z	2	1	4	4	2	4
D_c/g cm^{-3}	1.188	1.285	1.381	1.762	1.239	1.207
F(000)	832.0	452.0	2096.0	1952.0	876.0	1736.0
abs coeff/mm^{-1}	0.402	2.686	2.675	5.514	2.518	2.200
No. of obsd reflns	4398	4409	9957	3863	9200	9621
No. of params refnd	238	238	517	205	449	473
GOF	1.037	1.206	1.052	1.043	1.102	1.027
$R_1(I > 2\delta)$	0.0507	0.0329	0.0426	0.0214	0.0360	0.0292
$wR_2(I > 2\delta)$	0.1268	0.0915	0.1144	0.0514	0.0989	0.0710

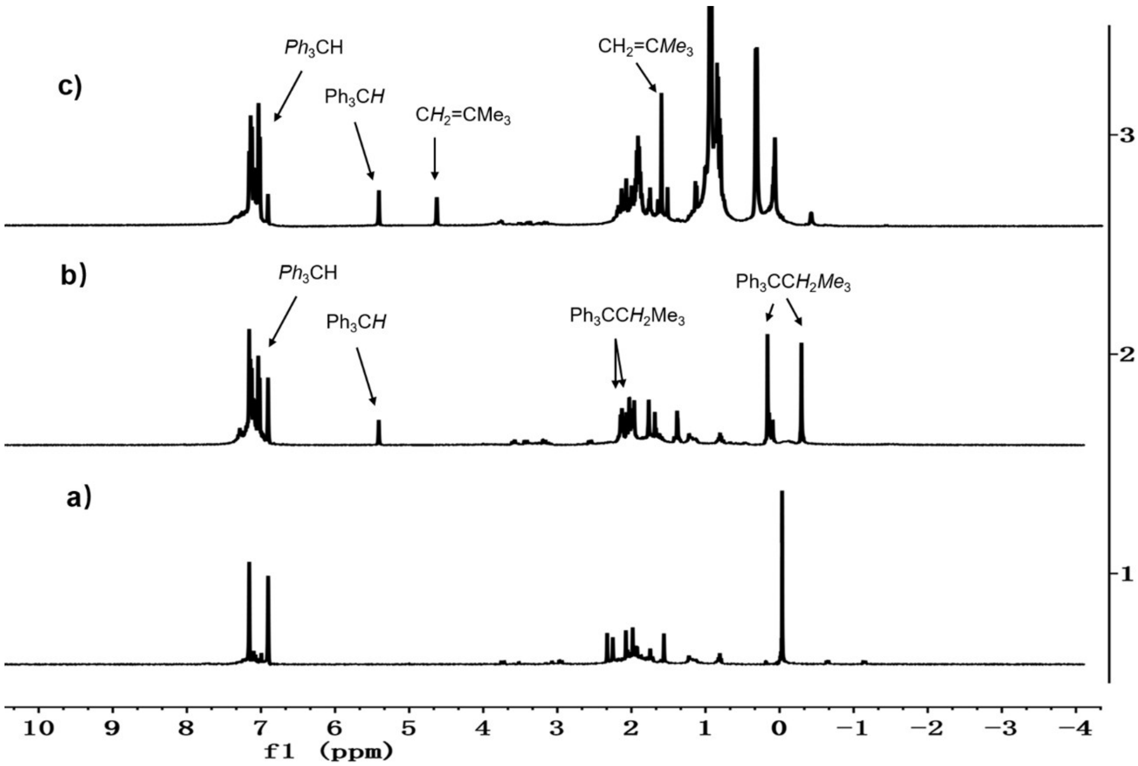

Figure S17 ^{1}H NMR spectra (400 MHz, *o*-$C_6D_4Cl_2$, 25 °C) of a) Complex **1a**, b) Complex **1a**/$Ph_3CB(C_6F_5)_4$, and c) Complex **1a**/Al^iBu_3/$Ph_3CB(C_6F_5)_4$.

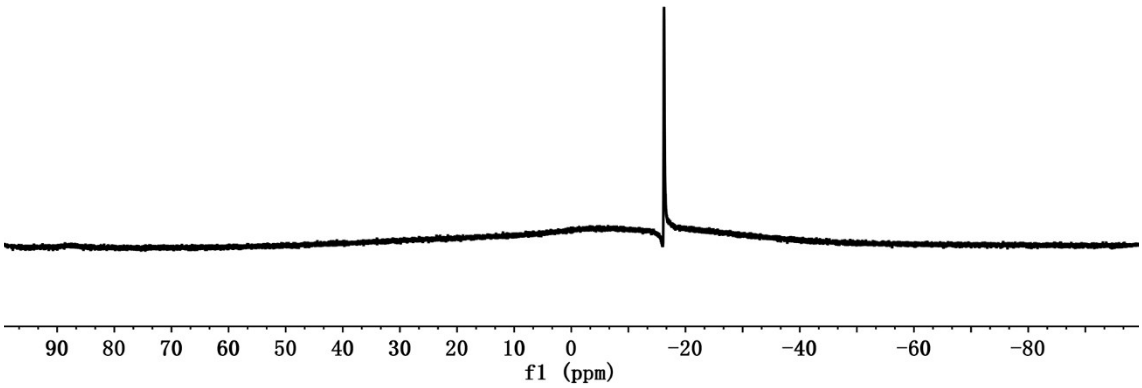

Figure S18 ^{11}B NMR spectra (161 MHz, *o*-$C_6D_4Cl_2$, 25 °C) of complex **1a**/Al^iBu_3/$Ph_3CB(C_6F_5)_4$.

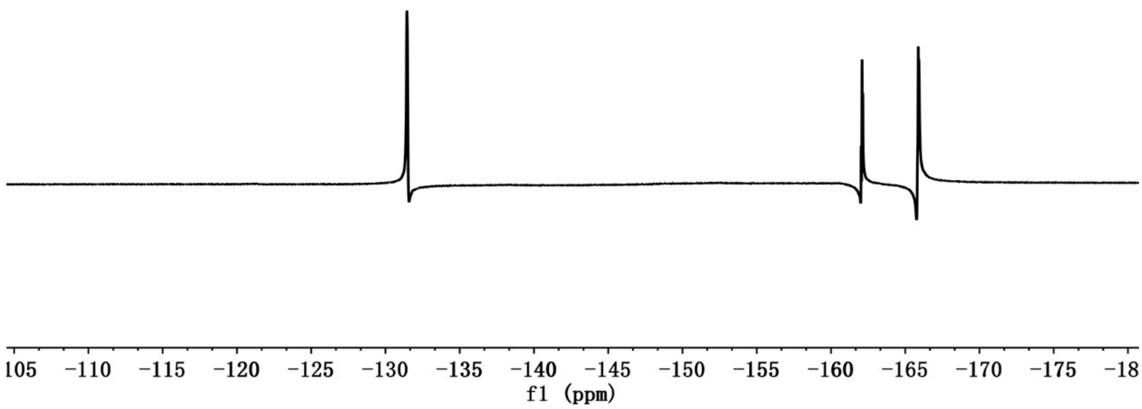

Figure S19 ^{19}F NMR spectra (471 MHz, *o*-$C_6D_4Cl_2$, 25 °C) of complex **1a**/Al^iBu_3/$Ph_3CB(C_6F_5)_4$.