Electronic Supplementary Information

Titanium and Zirconium Complexes Bearing New Tridentate [OSO] Bisphenolato-based Ligands: Synthesis, Characterization and Catalytic Properties for Alkene Polymerization

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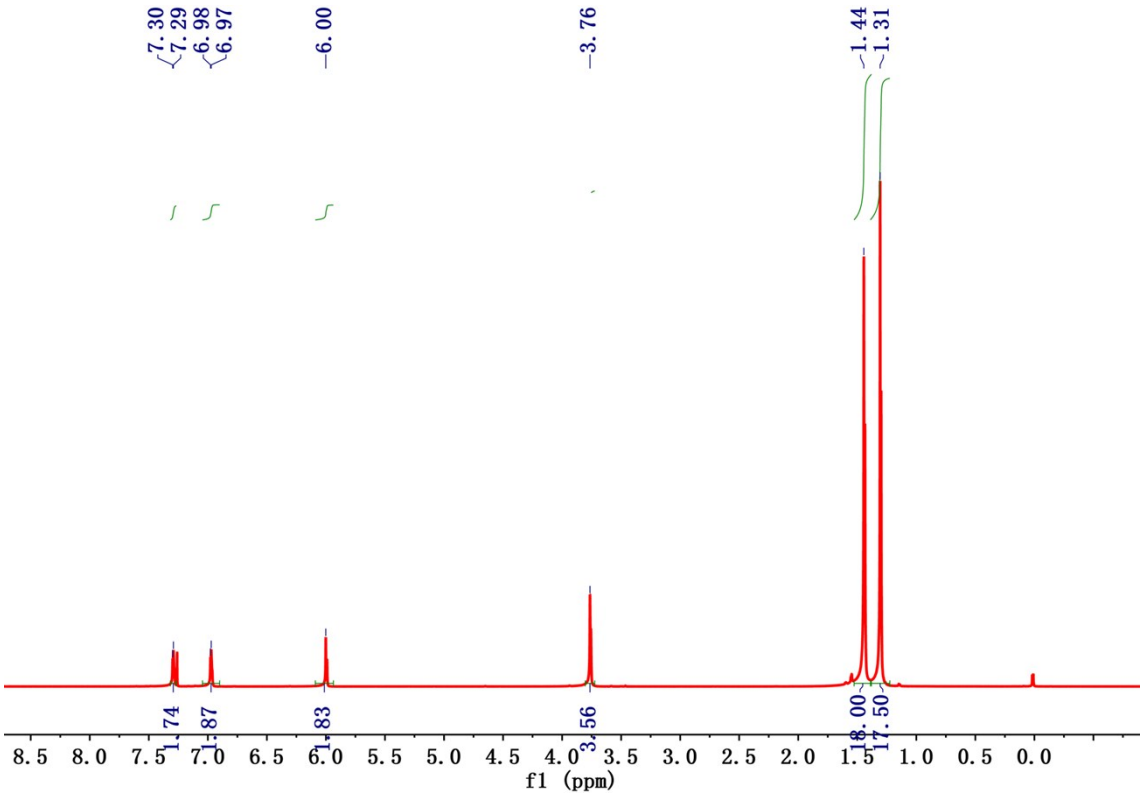

Figure S1 ^{1}H NMR spectrum of ligand H_2**L1** (400 MHz, $CDCl_3$, 25 °C)**.**

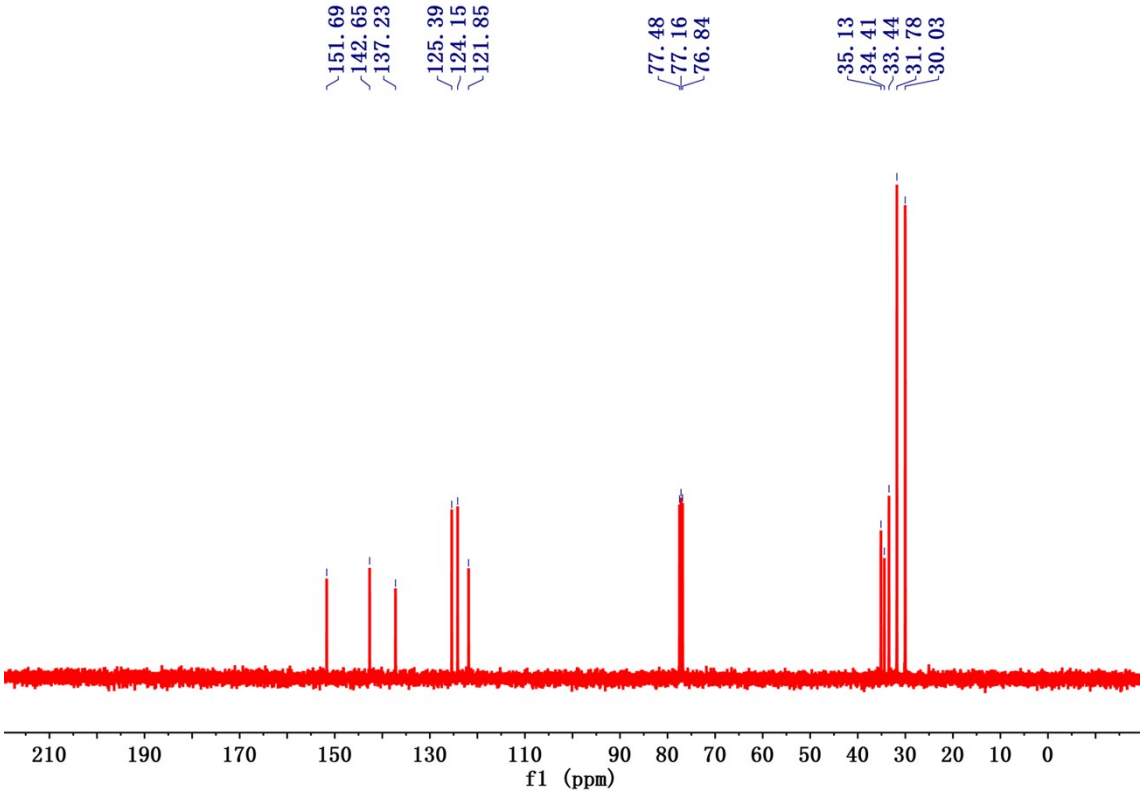

Figure S2 ^{13}C NMR spectrum of ligand H_2**L1** (100 MHz, $CDCl_3$, 25 °C)**.**

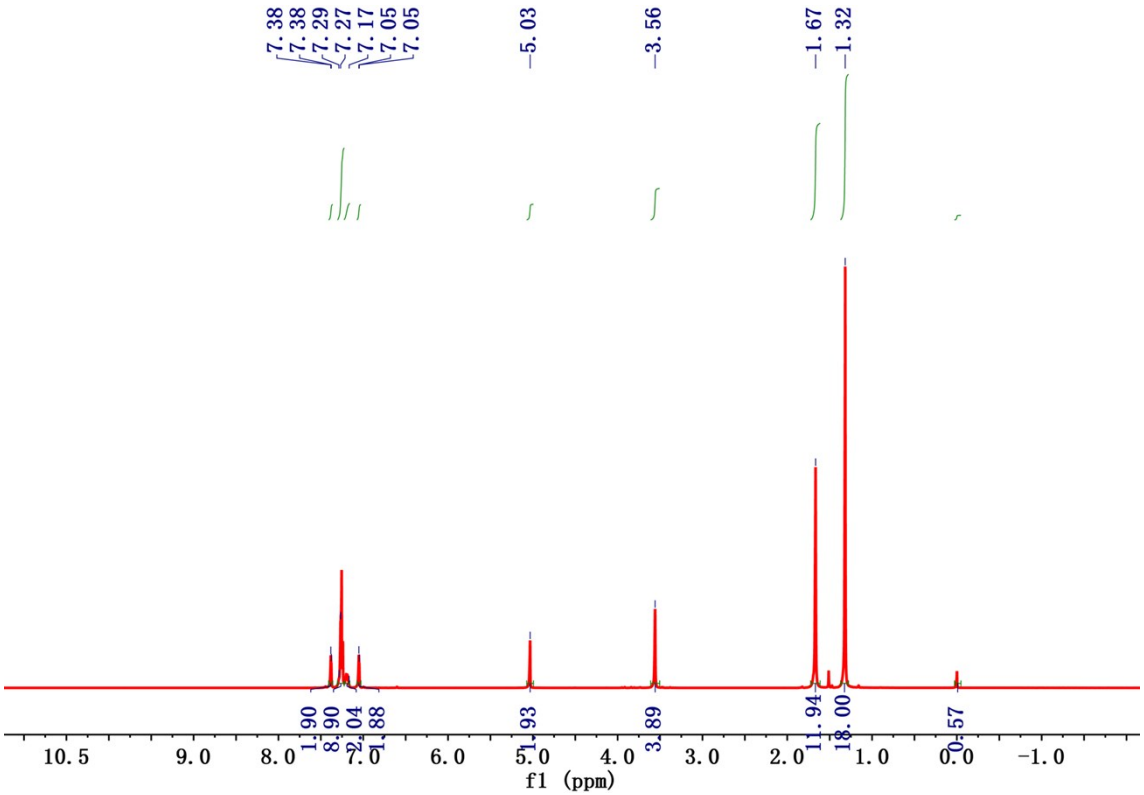

Figure S3 ^{1}H NMR spectrum of ligand H_2**L2** (400 MHz, $CDCl_3$, 25 °C)**.**

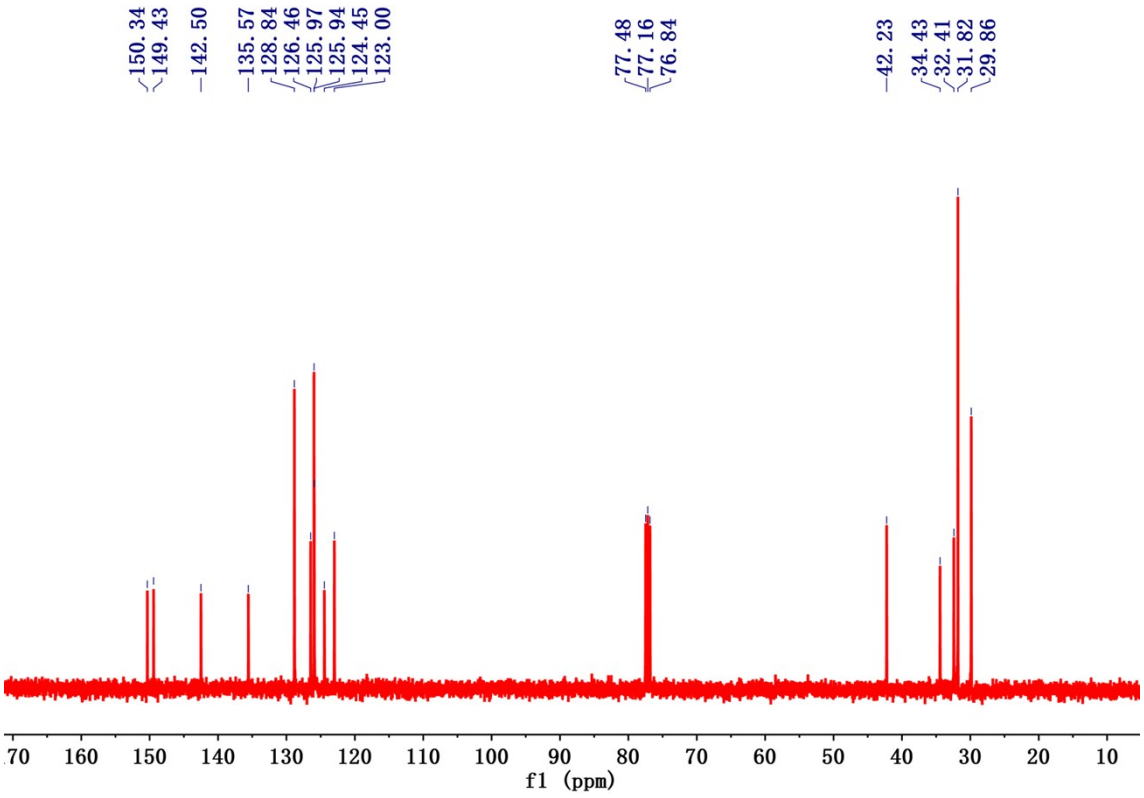

Figure S4 ^{13}C NMR spectrum of ligand H_2**L2** (100 MHz, $CDCl_3$, 25 °C)**.**

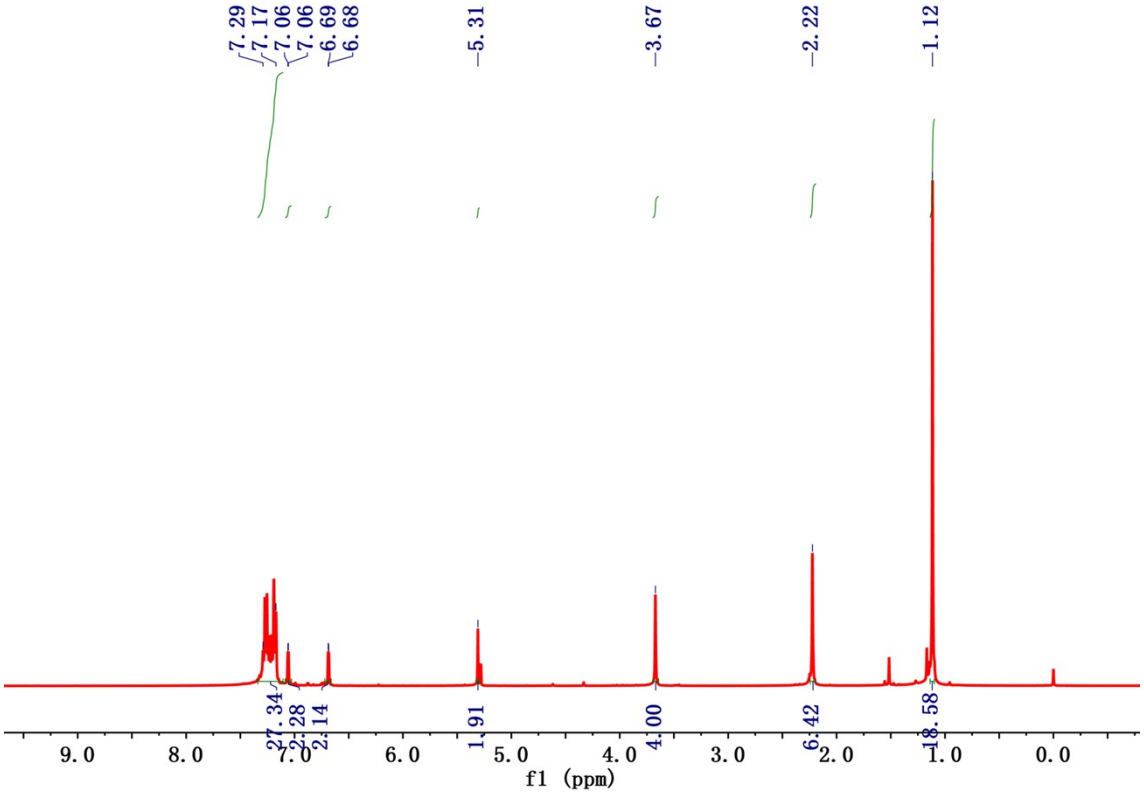

Figure S5 ^{1}H NMR spectrum of ligand H_2**L3** (400 MHz, $CDCl_3$, 25 °C)**.**

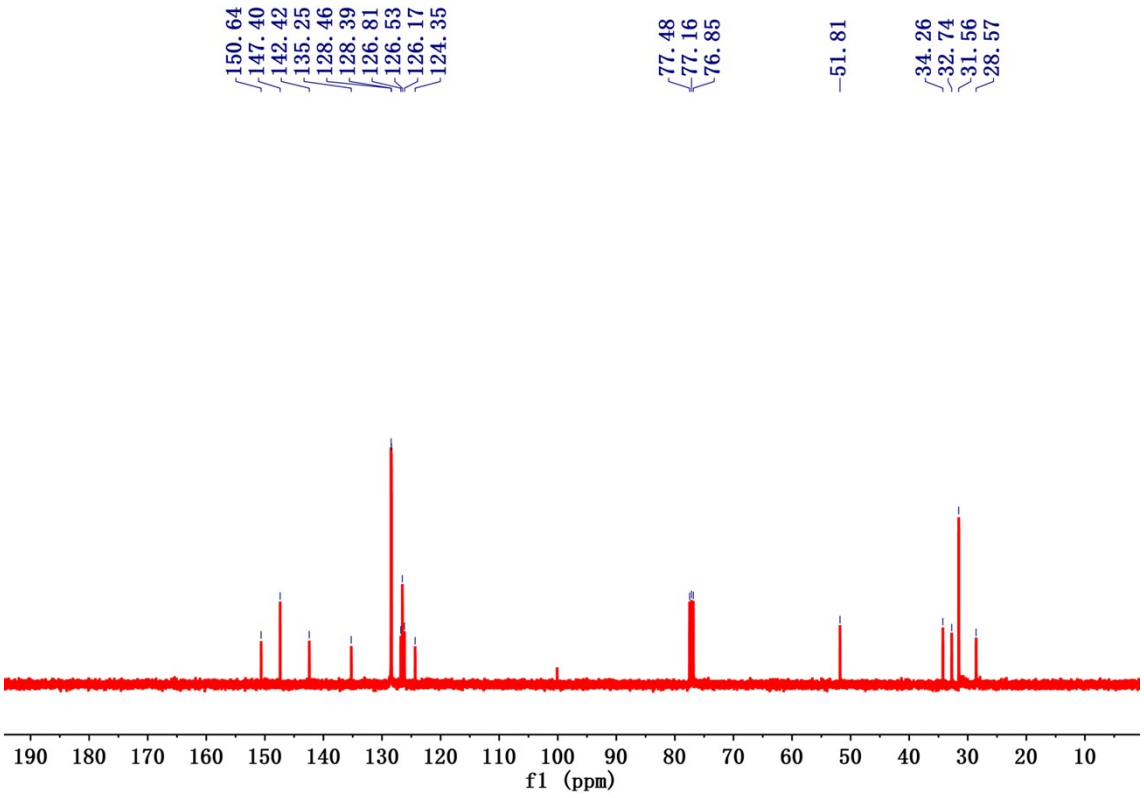

Figure S6 ^{13}C NMR spectrum of ligand H_2**L3** (100 MHz, $CDCl_3$, 25 °C)**.**

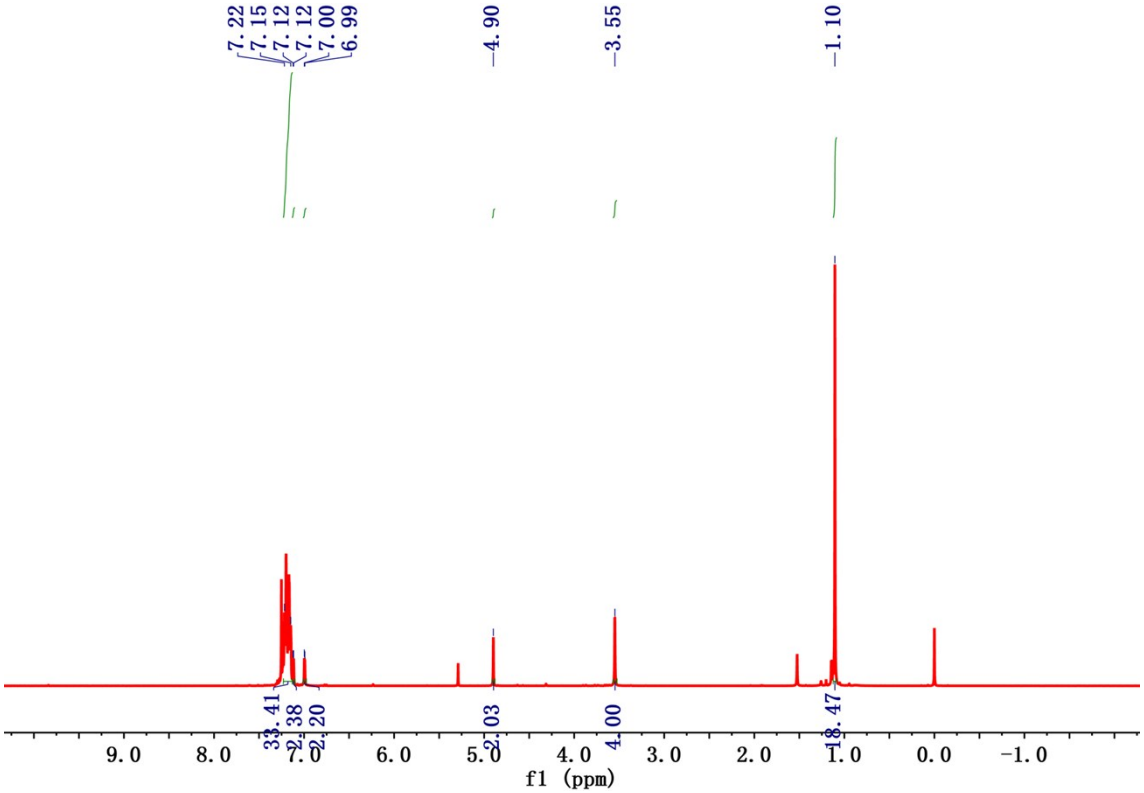

Figure S7 ^{1}H NMR spectrum of ligand H_2**L4** (400 MHz, $CDCl_3$, 25 °C)**.**

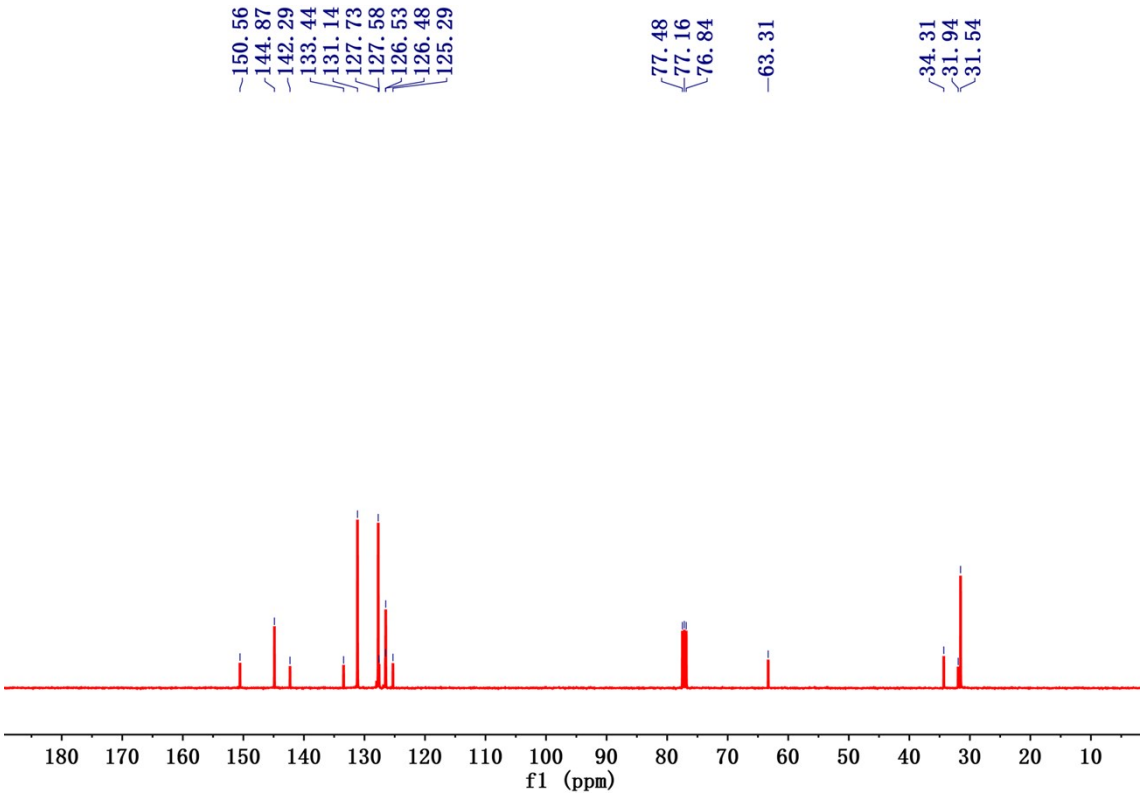

Figure S8 ^{13}C NMR spectrum of ligand H_2**L4** (100 MHz, $CDCl_3$, 25 °C)**.**

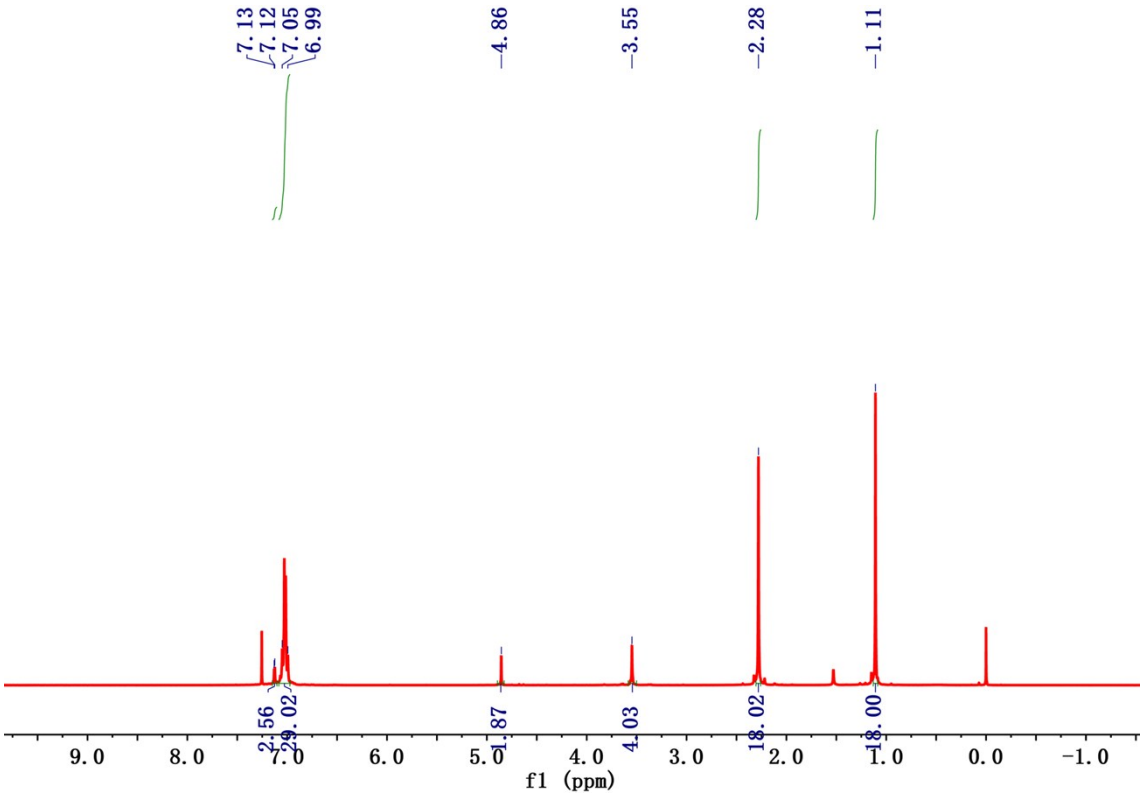

Figure S9 ^{1}H NMR spectrum of ligand H_2**L5** (400 MHz, $CDCl_3$, 25 °C)**.**

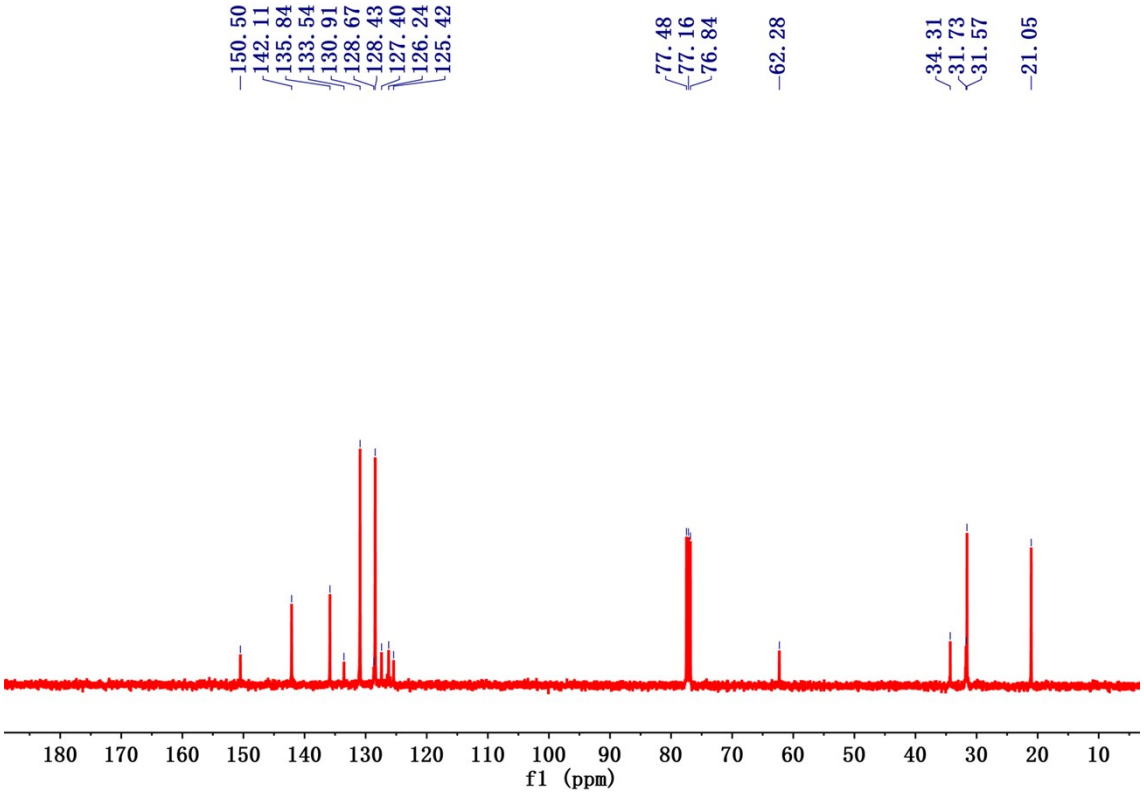

Figure S10 ^{13}C NMR spectrum of ligand H_2**L5** (100 MHz, $CDCl_3$, 25 °C)**.**

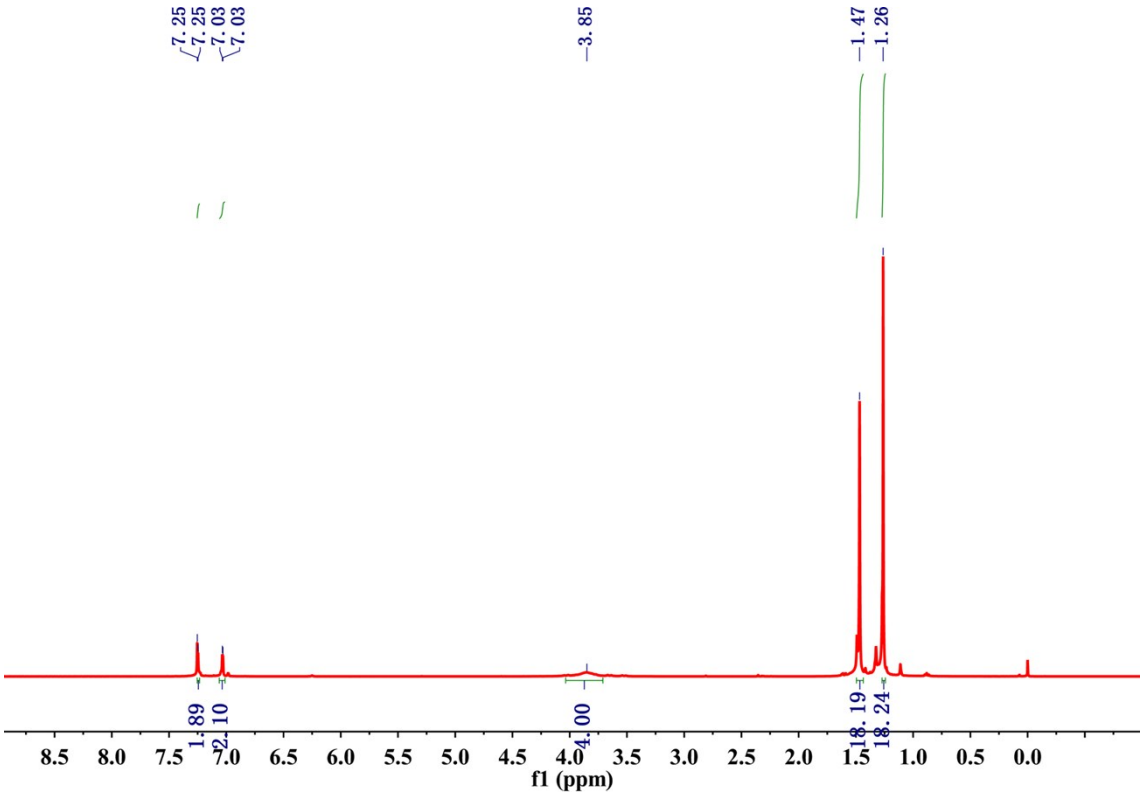

Figure S11 ^{1}H NMR spectrum of complex **1** (400 MHz, $CDCl_3$, 25 °C).

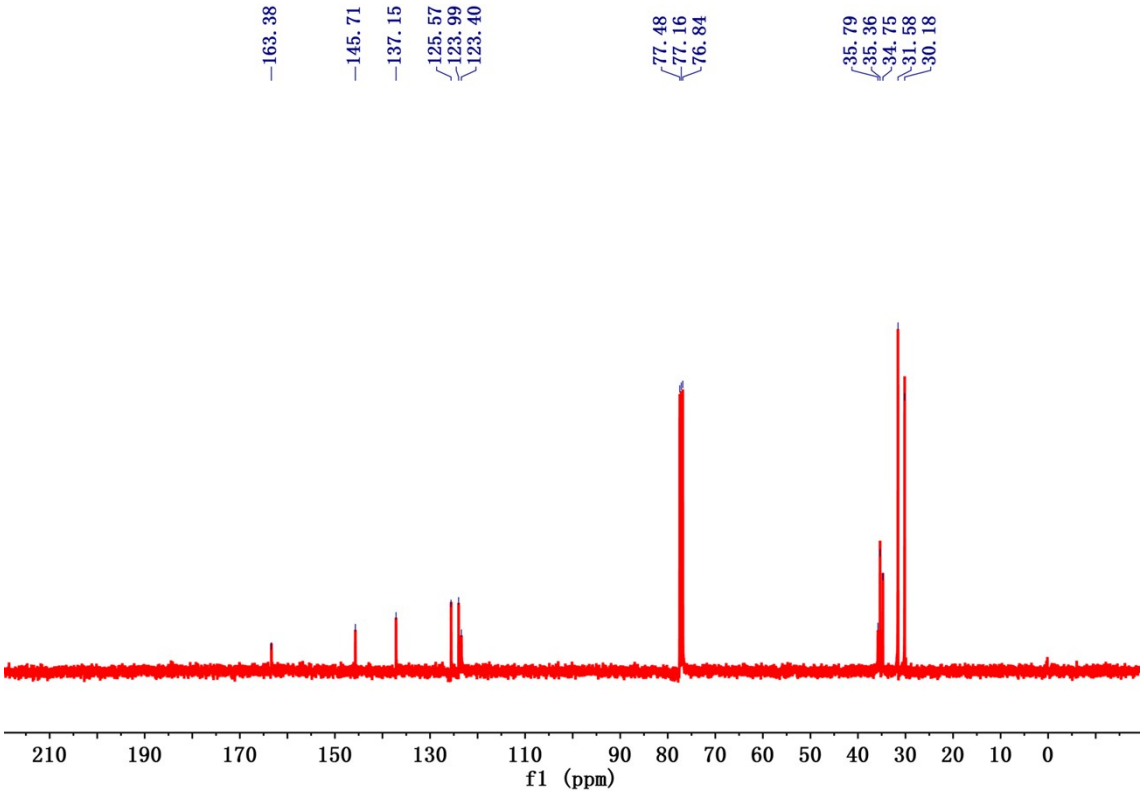

Figure S12 ^{13}C NMR spectrum of complex **1** (100 MHz, $CDCl_3$, 25 °C).

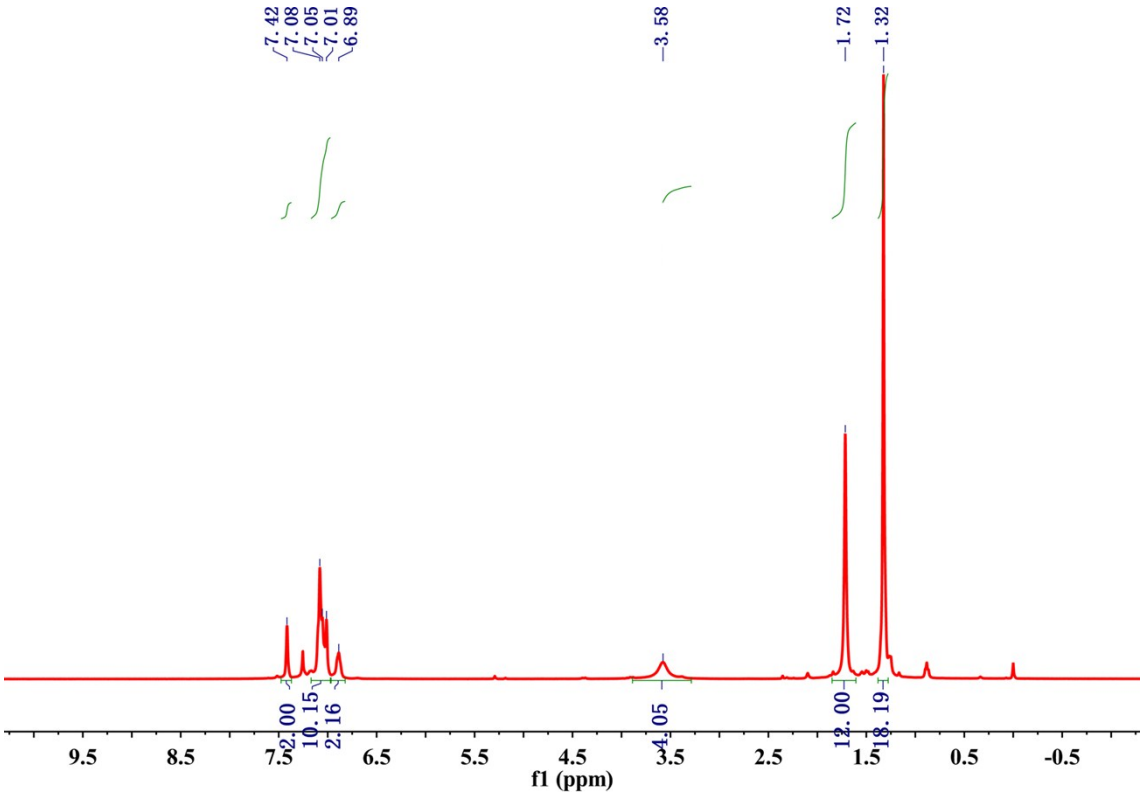

Figure S13 ^{1}H NMR spectrum of complex **2** (400 MHz, $CDCl_3$, 25 °C).

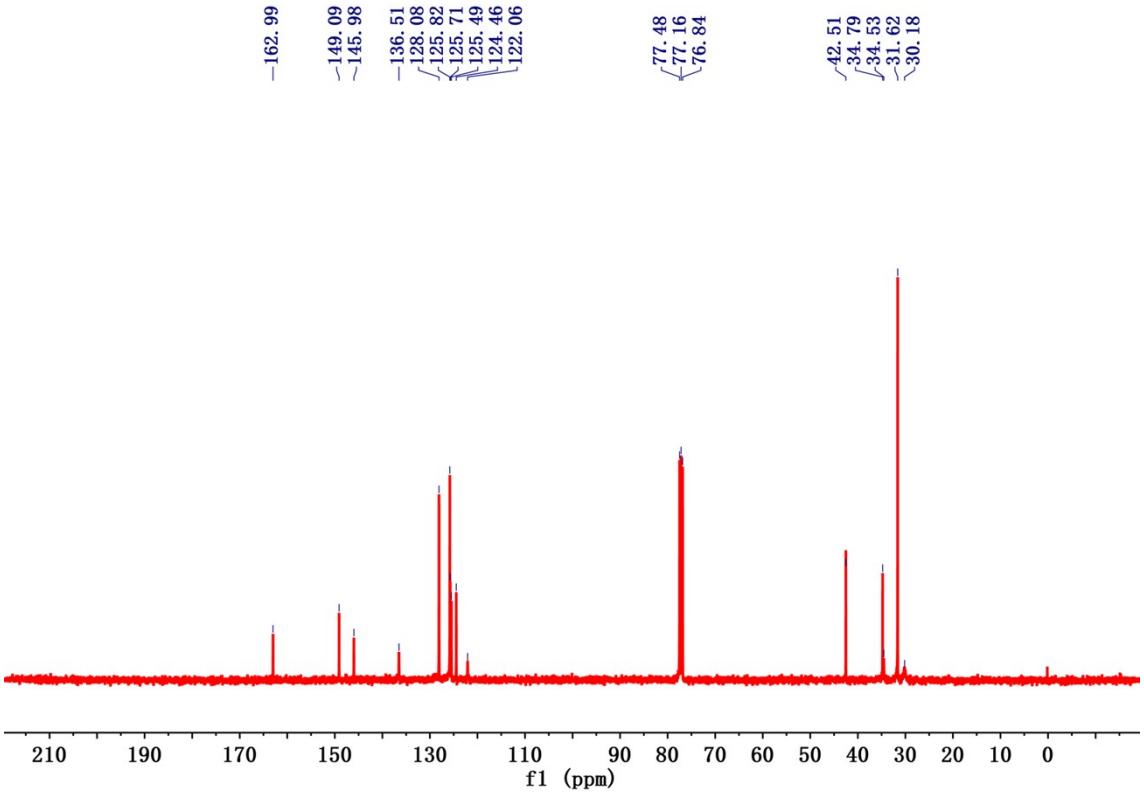

Figure S14 ^{13}C NMR spectrum of complex **2** (100 MHz, $CDCl_3$, 25 °C).

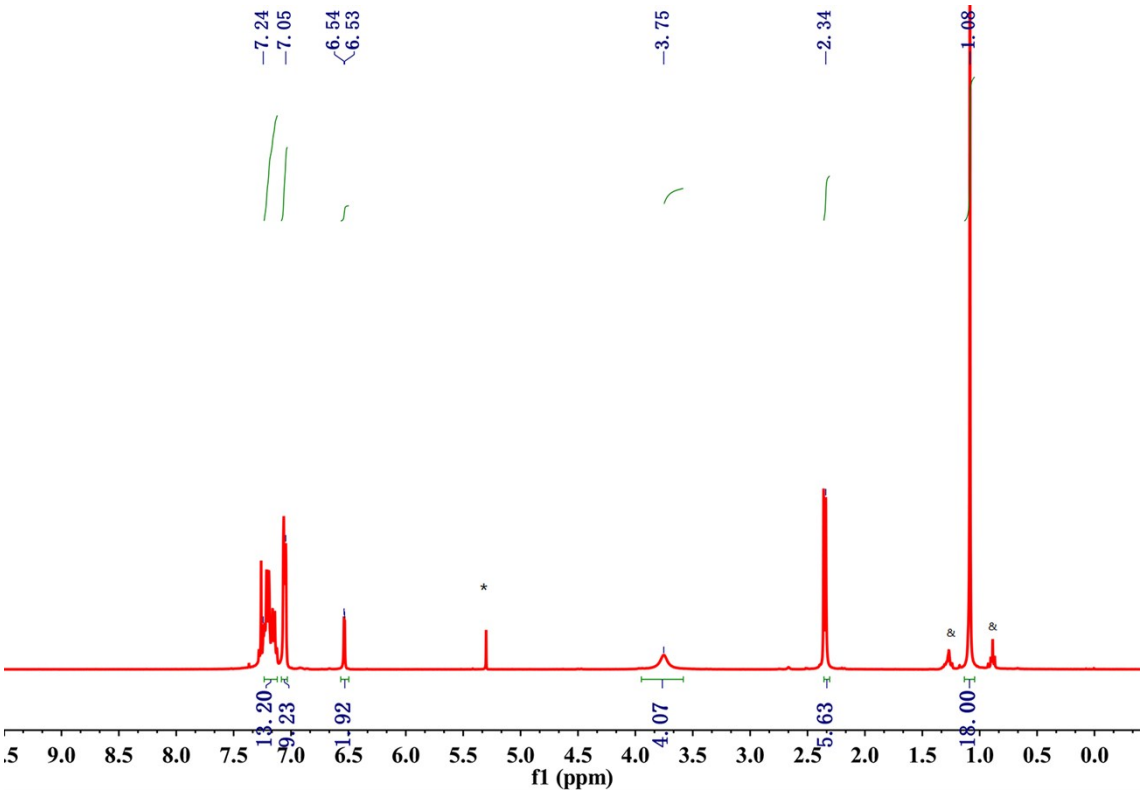

Figure S15 ^{1}H NMR spectrum of complex **3** (400 MHz, $CDCl_3$, 25 °C)**.** * and & stand for residual signals of CH_2Cl_2 and hexane, respectively.

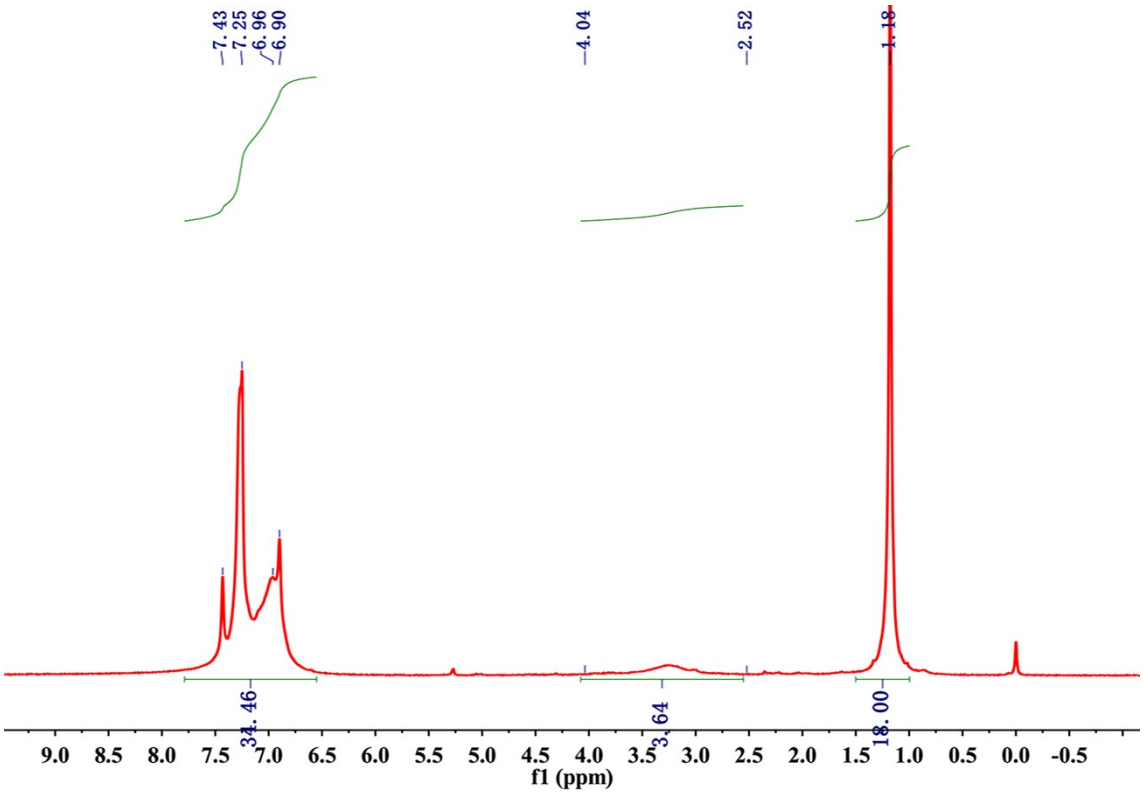

Figure S16 ^{1}H NMR spectrum of complex **4** (400 MHz, $CDCl_3$, 25 °C)**.**

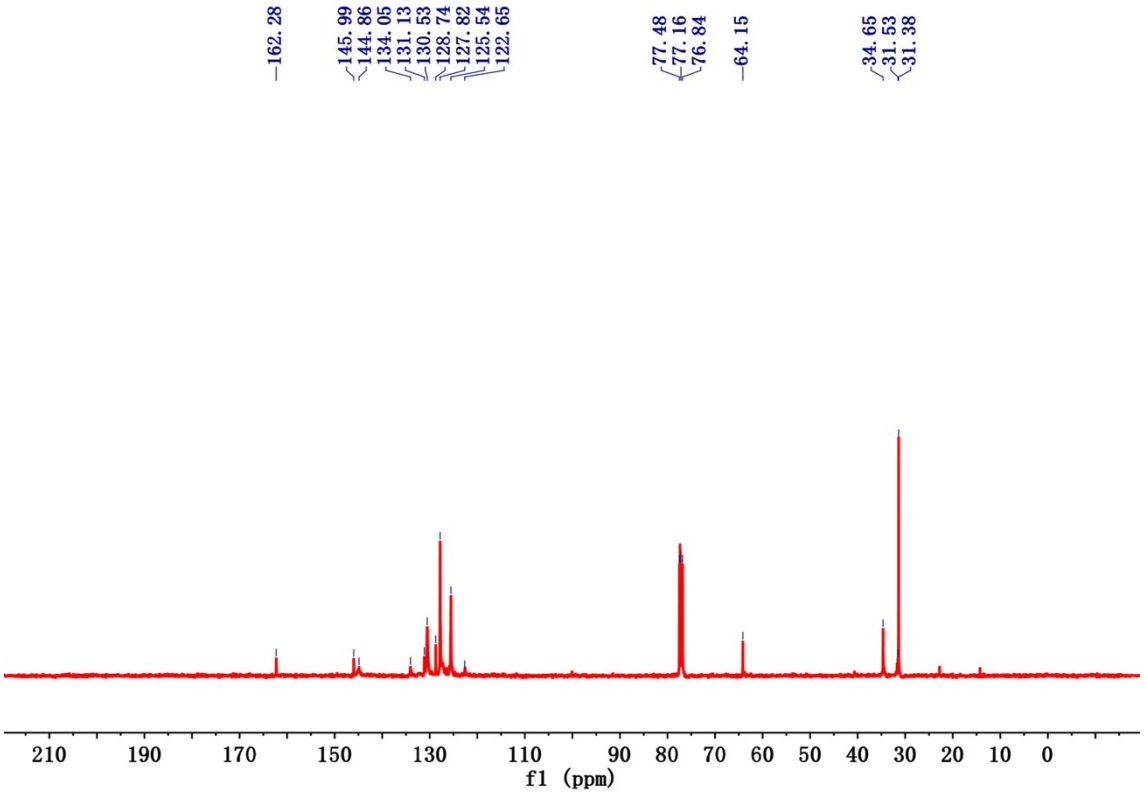

Figure S17 ^{13}C NMR spectrum of complex **4** (100 MHz, $CDCl_3$, 25 °C)**.**

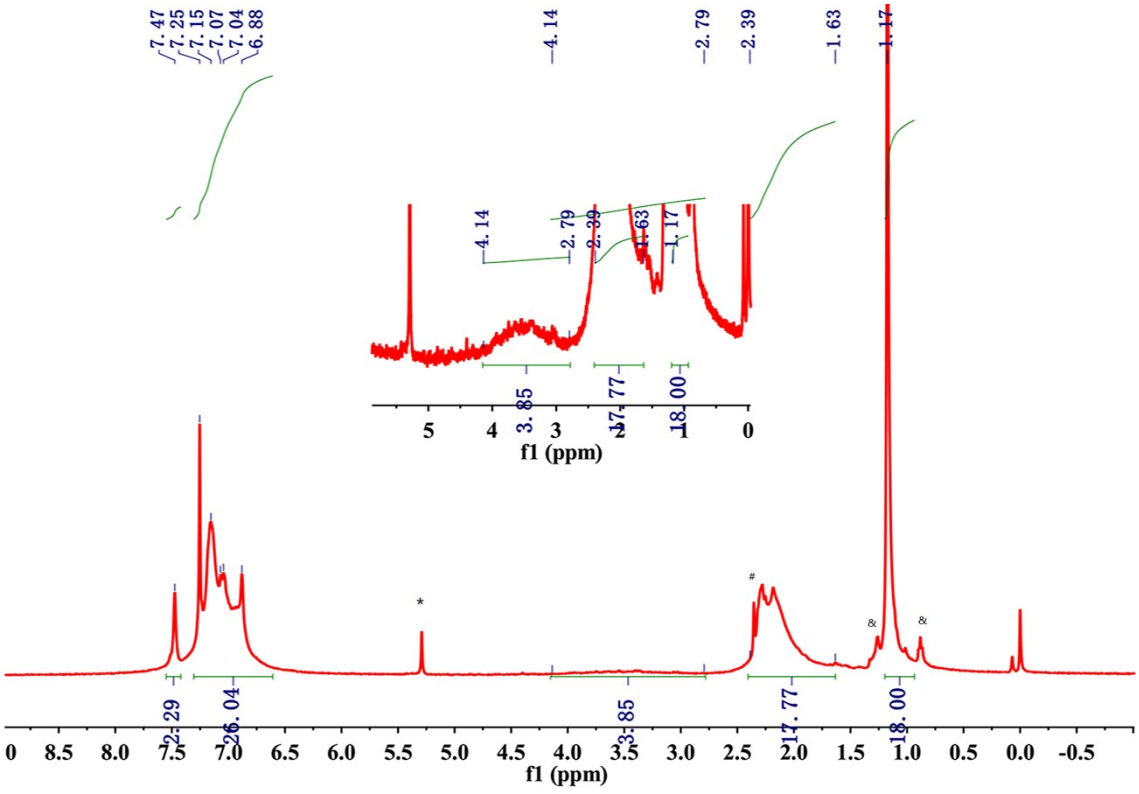

Figure S18 ^{1}H NMR spectrum of complex **5** (400 MHz, $CDCl_3$, 25 °C)**.** *, # and & stand for residual signals of CH_2Cl_2, toluene and hexane, respectively.

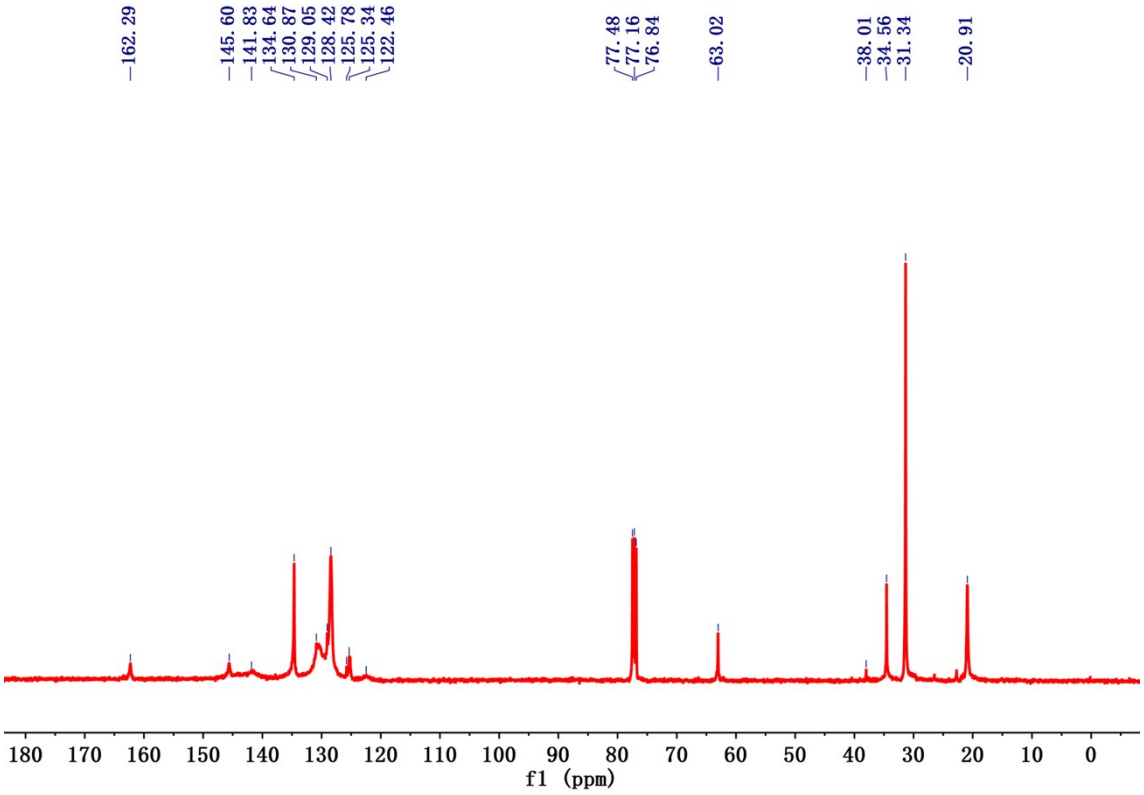

Figure S19 ^{13}C NMR spectrum of complex **5** (100 MHz, $CDCl_3$, 25 °C).

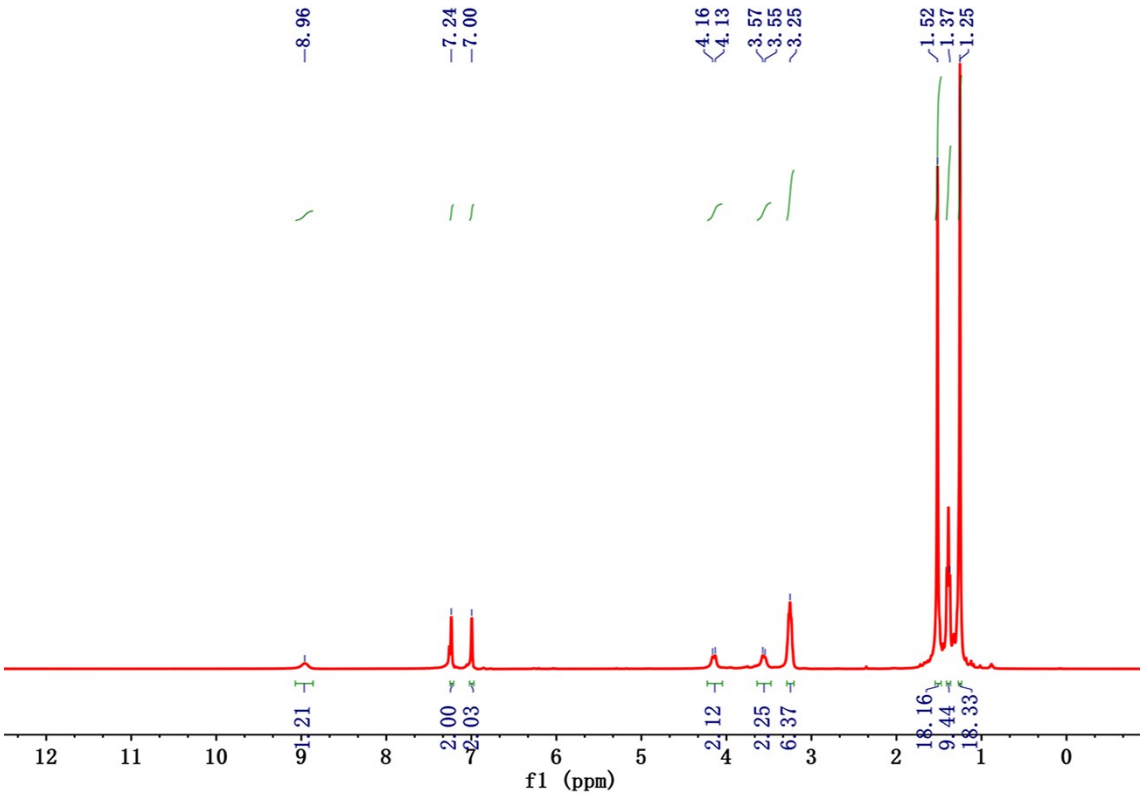

Figure S20 ^{1}H NMR spectrum of complex **6** (400 MHz, $CDCl_3$, 25 °C).

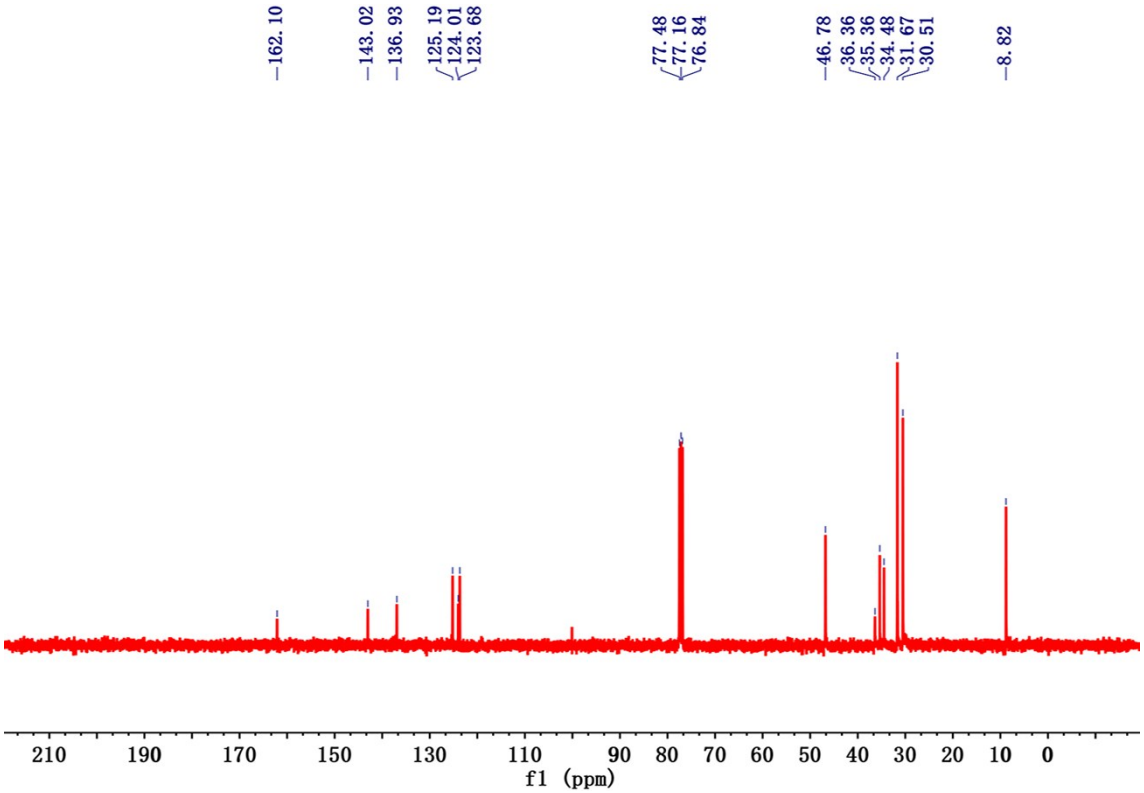

Figure S21 ^{13}C NMR spectrum of complex **6** (100 MHz, $CDCl_3$, 25 °C).

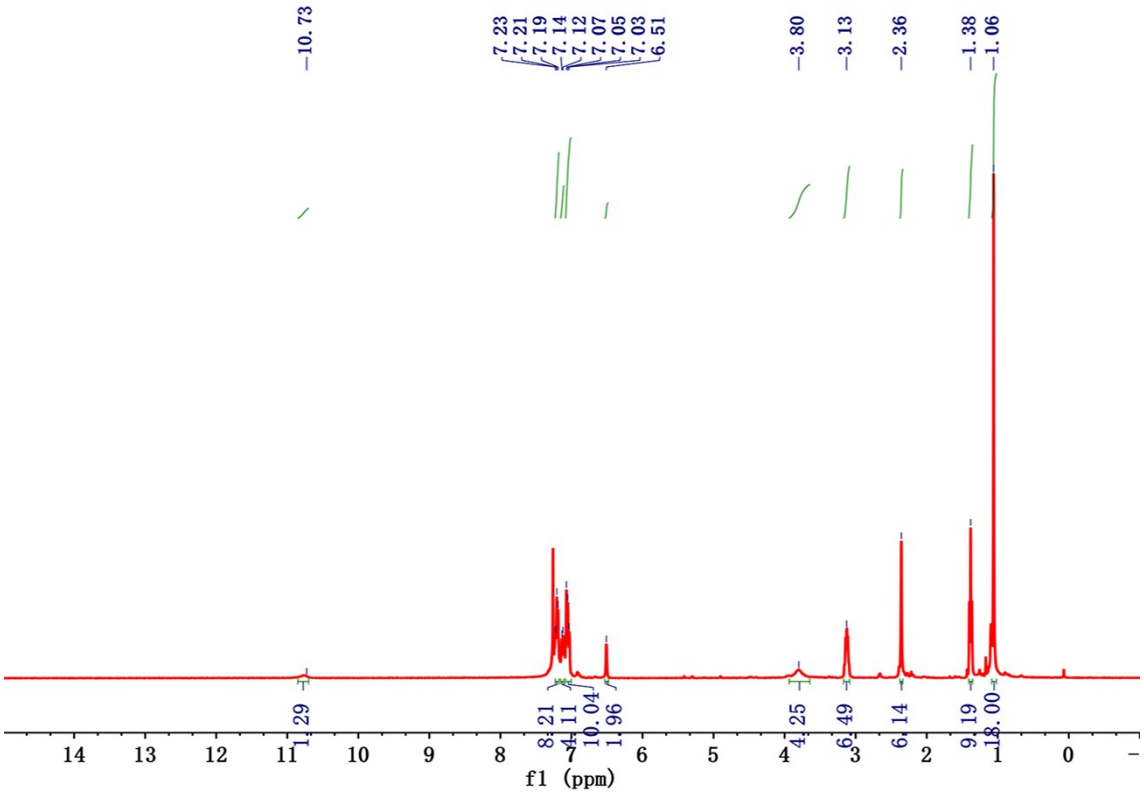

Figure S22 ^{1}H NMR spectrum of complex **7** (400 MHz, $CDCl_3$, 25 °C).

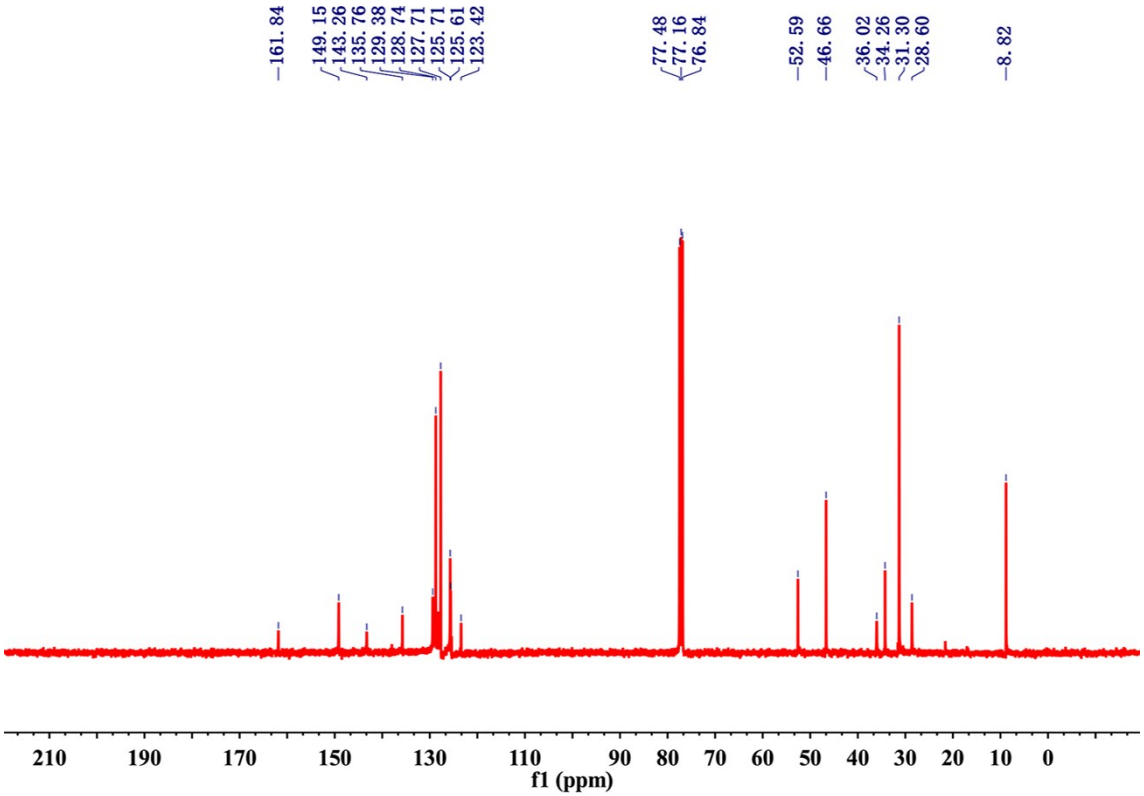

Figure S23 ^{13}C NMR spectrum of complex **7** (100 MHz, $CDCl_3$, 25 °C).

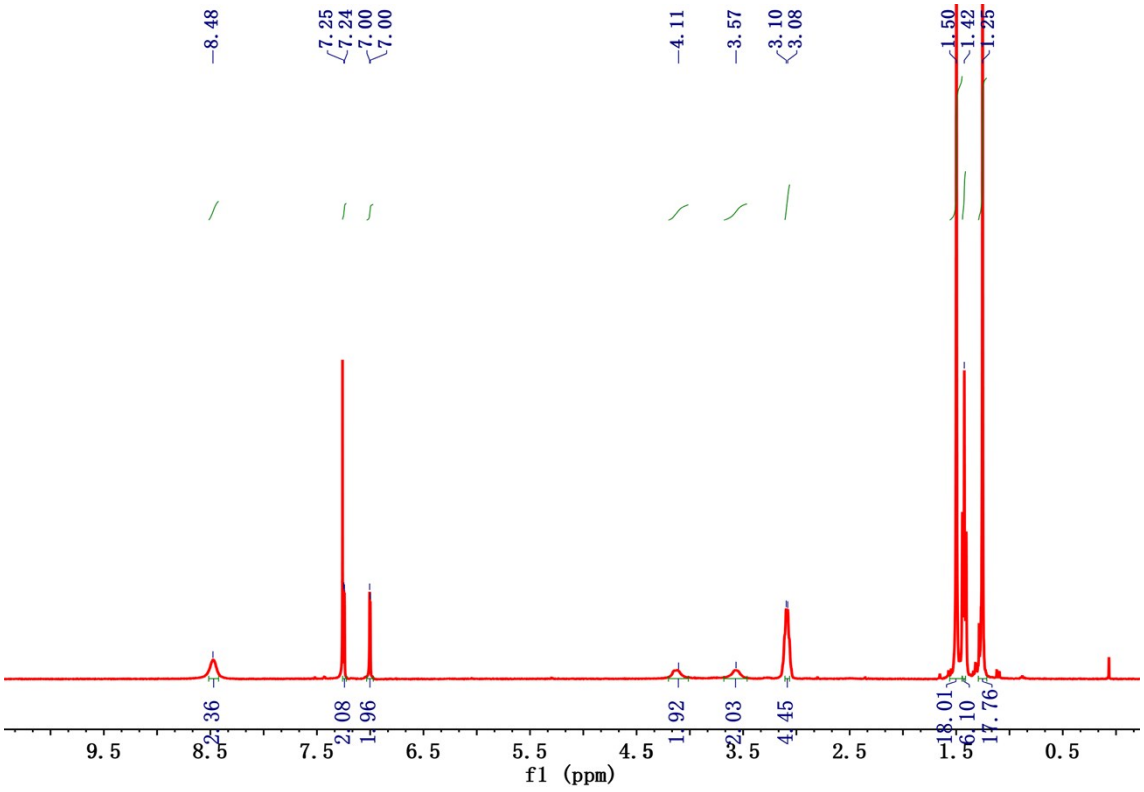

Figure S24 ^{1}H NMR spectrum of complex **8** (400 MHz, $CDCl_3$, 25 °C).

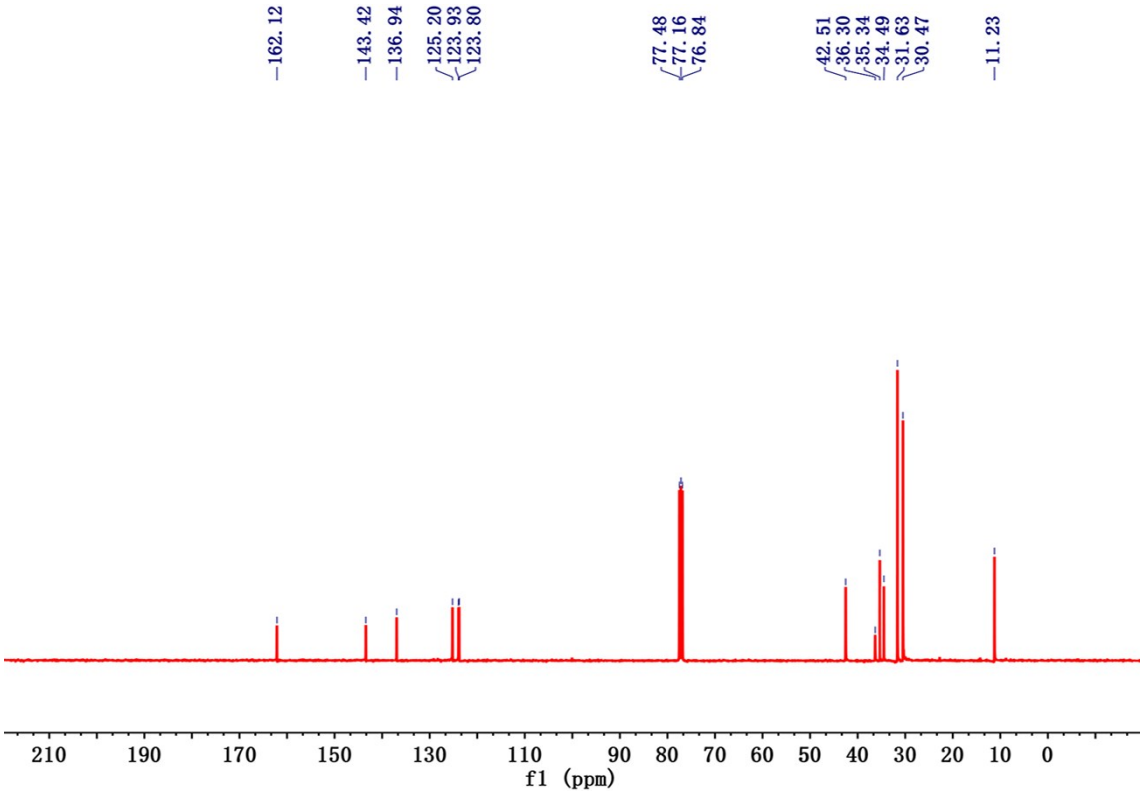

Figure S25 ^{13}C NMR spectrum of complex **8** (100 MHz, $CDCl_3$, 25 °C).

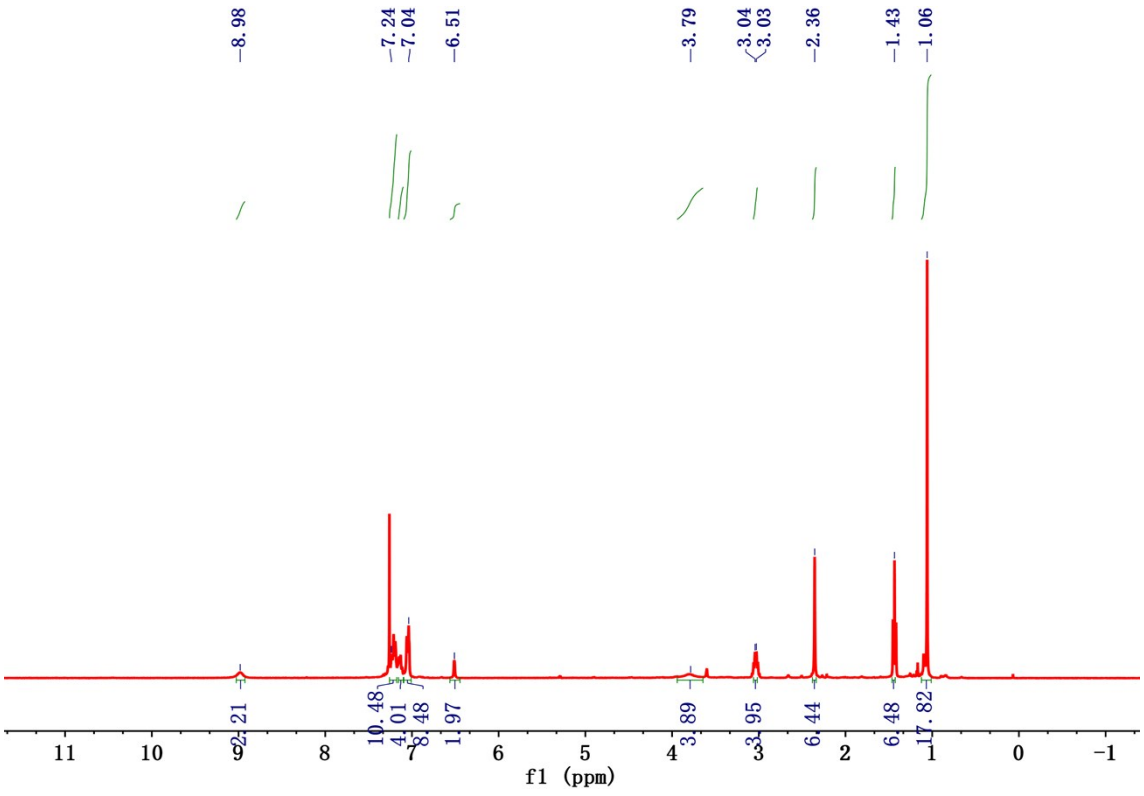

Figure S26 ^{1}H NMR spectrum of complex **9** (400 MHz, $CDCl_3$, 25 °C).

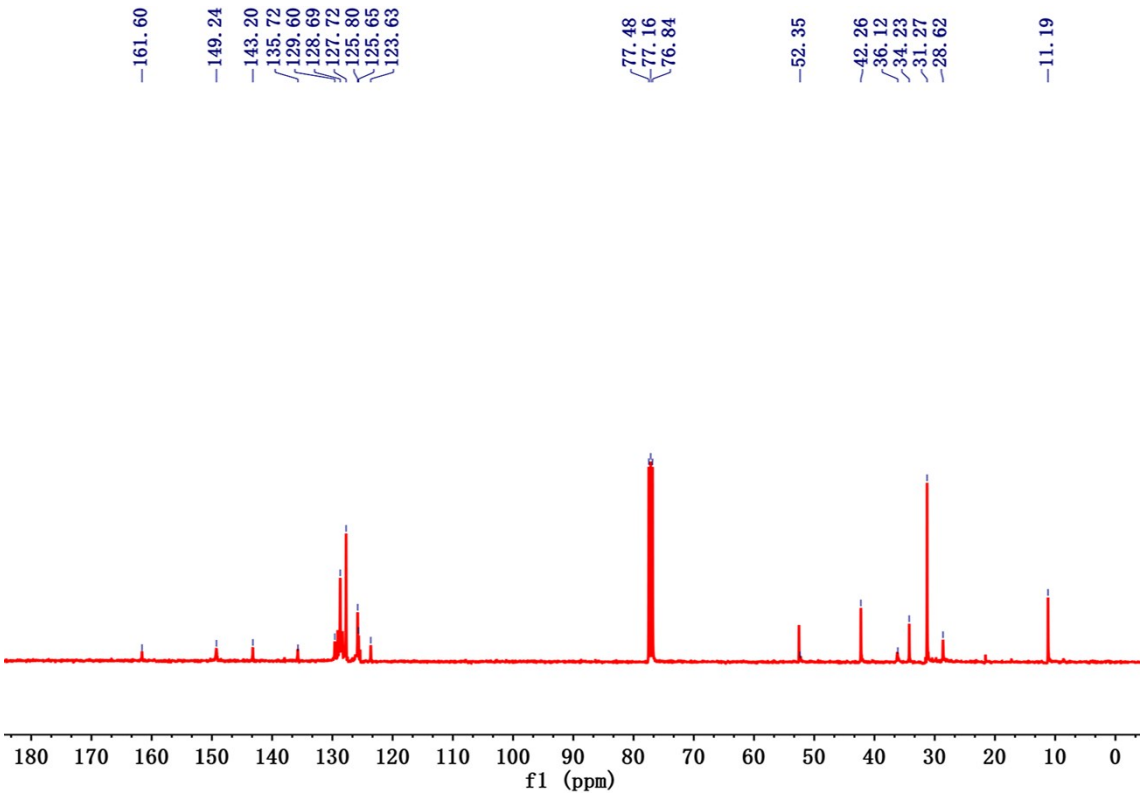

Figure S27 ^{13}C NMR spectrum of complex **9** (100 MHz, $CDCl_3$, 25 °C).

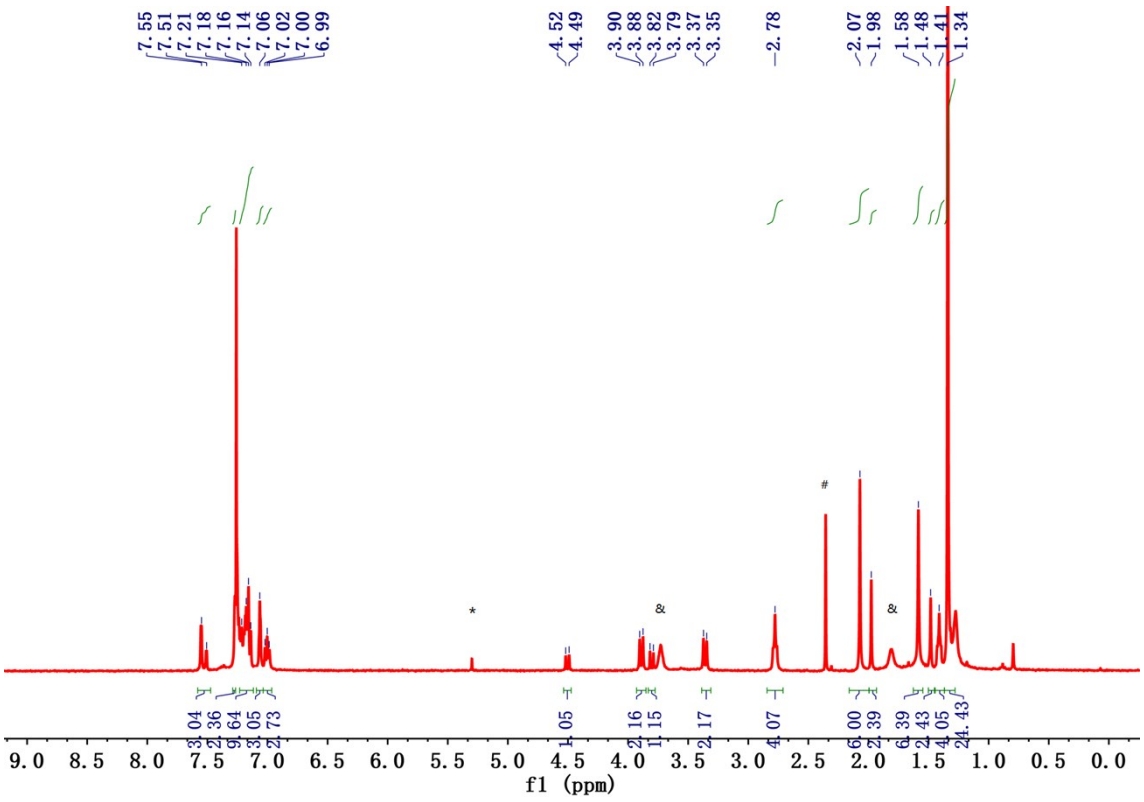

Figure S28 ^{1}H NMR spectrum of complexes **10** and **10**·THF (400 MHz, $CDCl_3$, 25 °C). *, & and # stand for residual signals of CH_2Cl_2, THF and toluene, respectively.

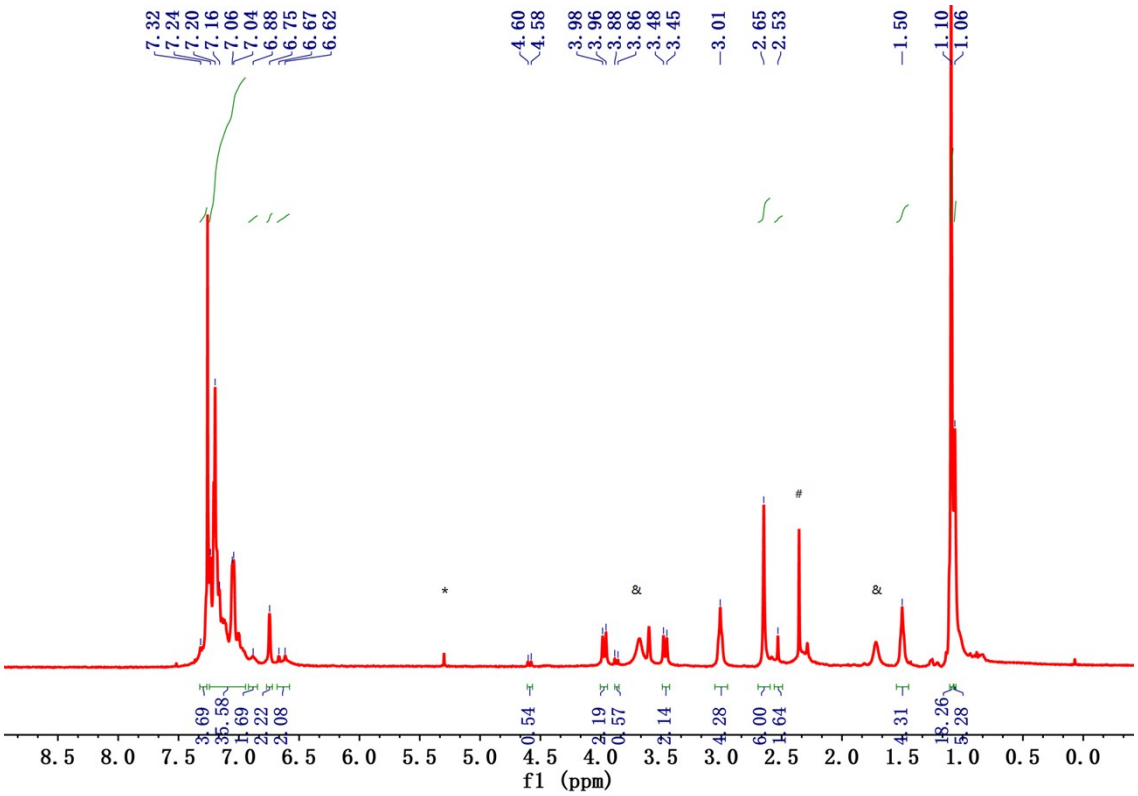

Figure S29 ^{1}H NMR spectrum of complexes **11** and **11**·THF (400 MHz, $CDCl_3$, 25 °C). *, & and # stand for residual signals of CH_2Cl_2, THF and toluene, respectively.

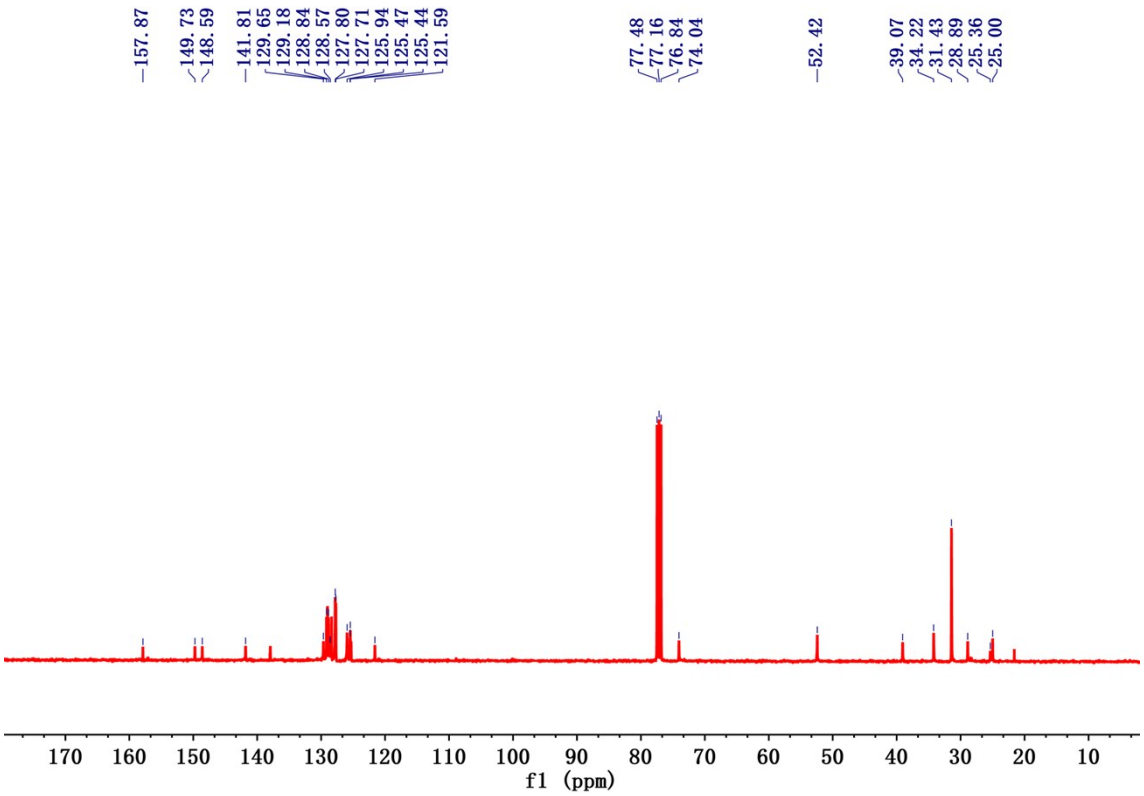

Figure S30 ^{13}C NMR spectrum of complex **11**·THF (100 MHz, $CDCl_3$, 25 °C).

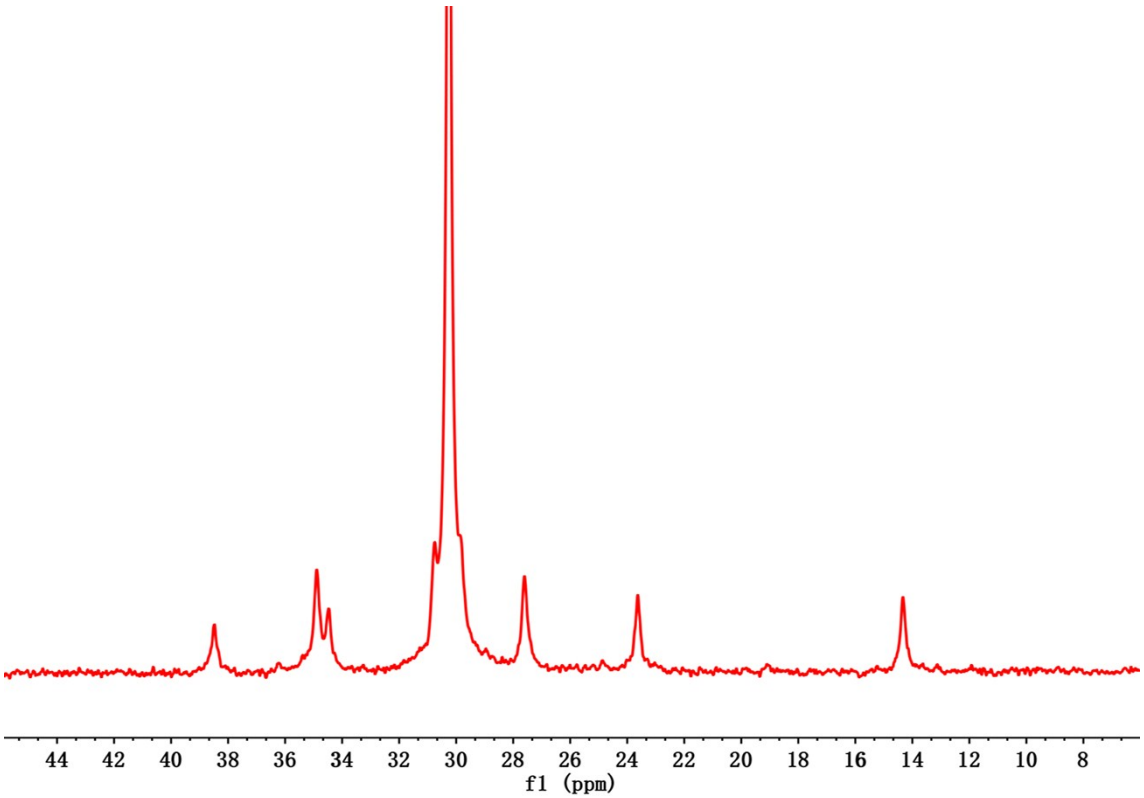

Figure S31 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 1, Table 2).

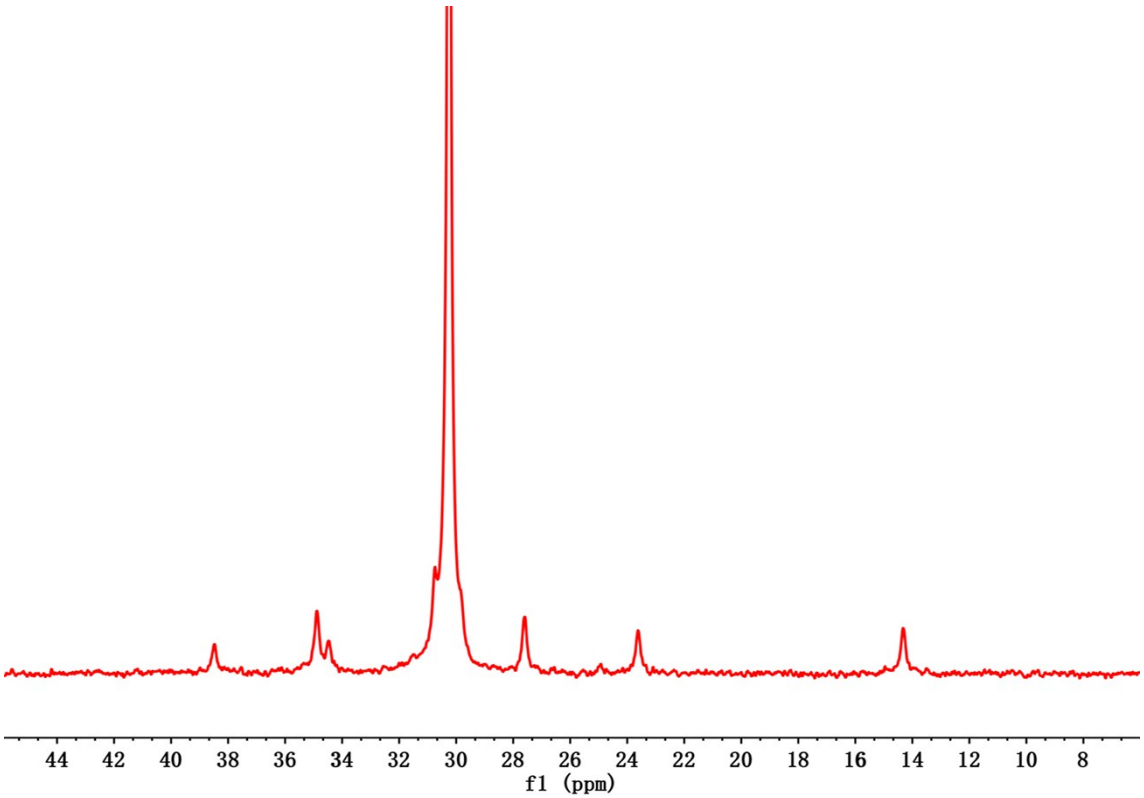

Figure S32 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 2, Table 2).

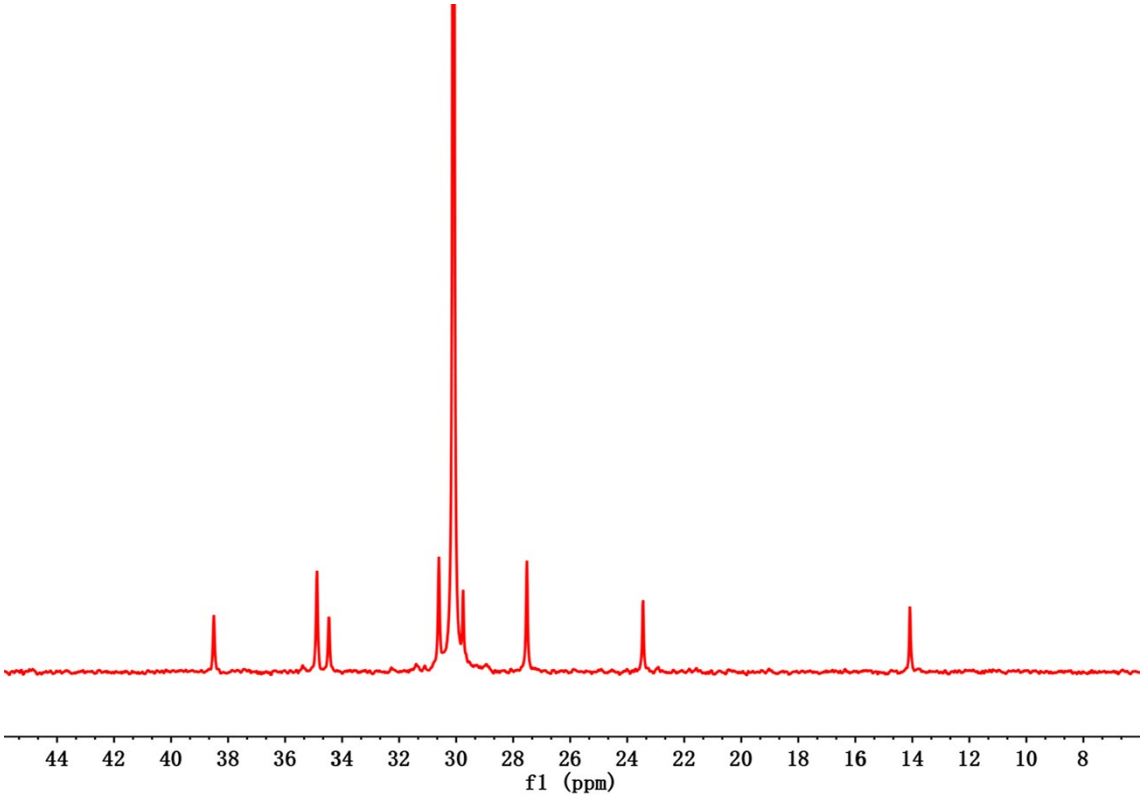

Figure S33 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 3, Table 2).

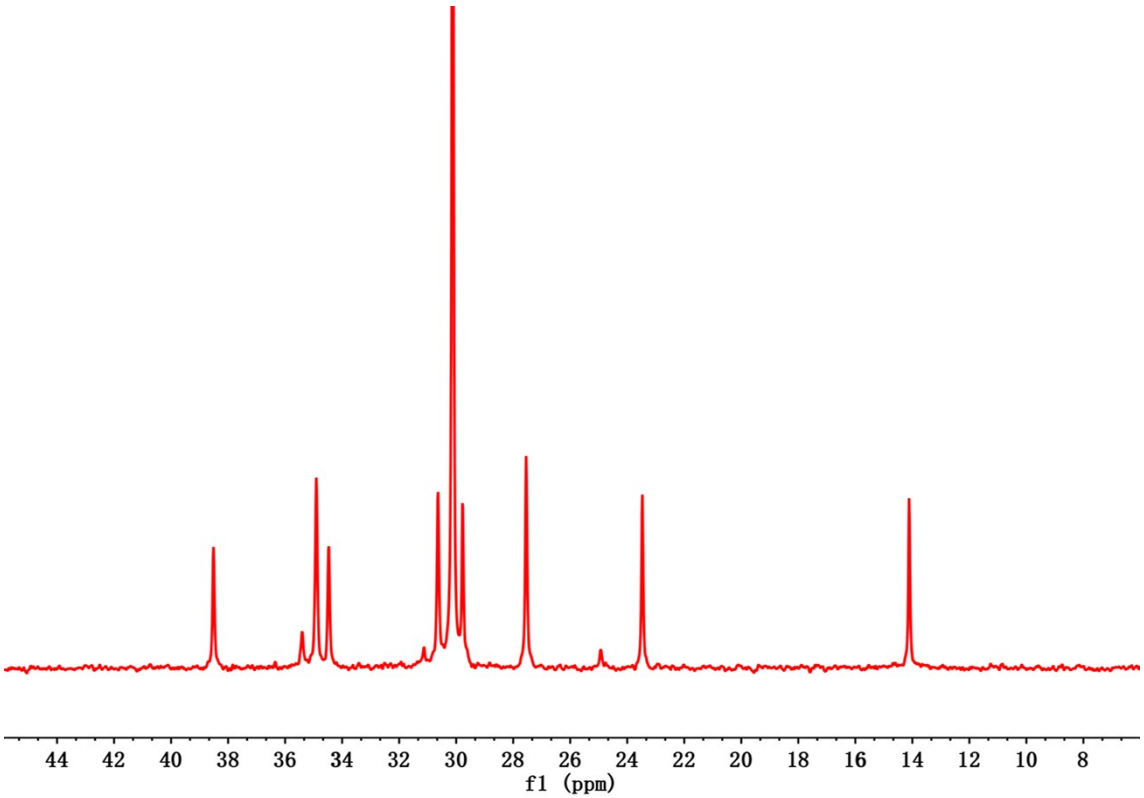

Figure S34 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 4, Table 2).

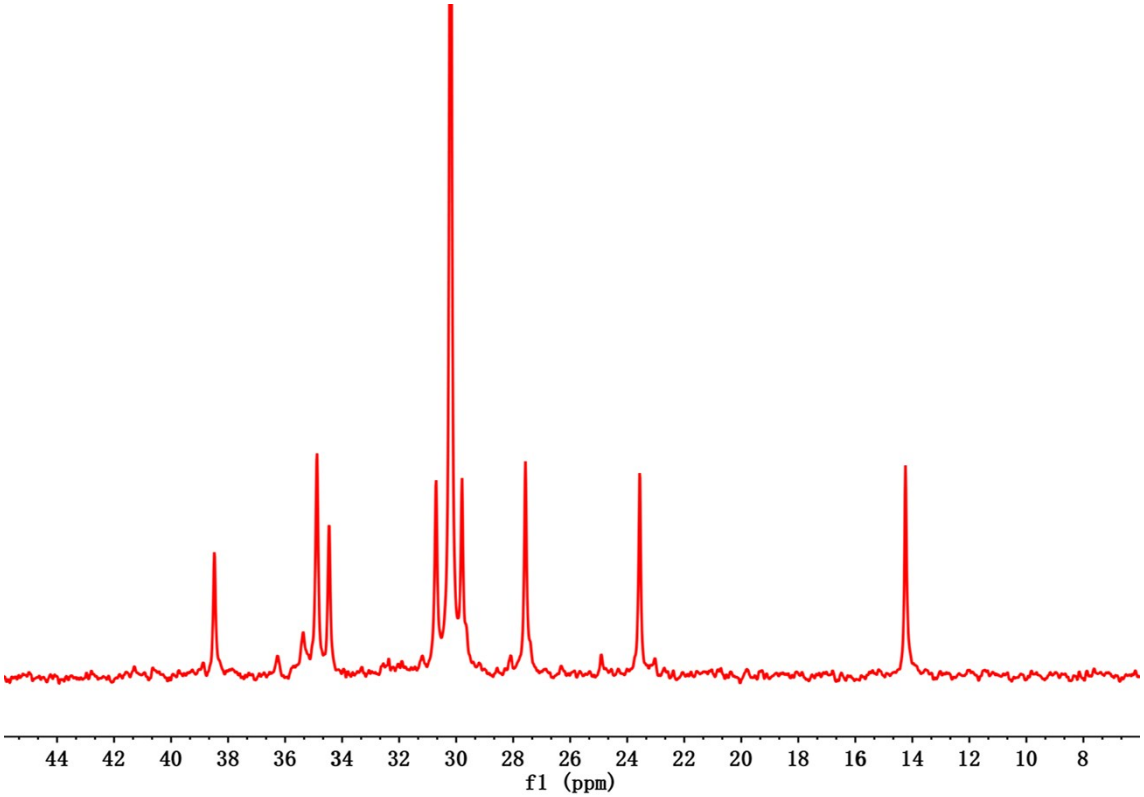

Figure S35 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 5, Table 2).

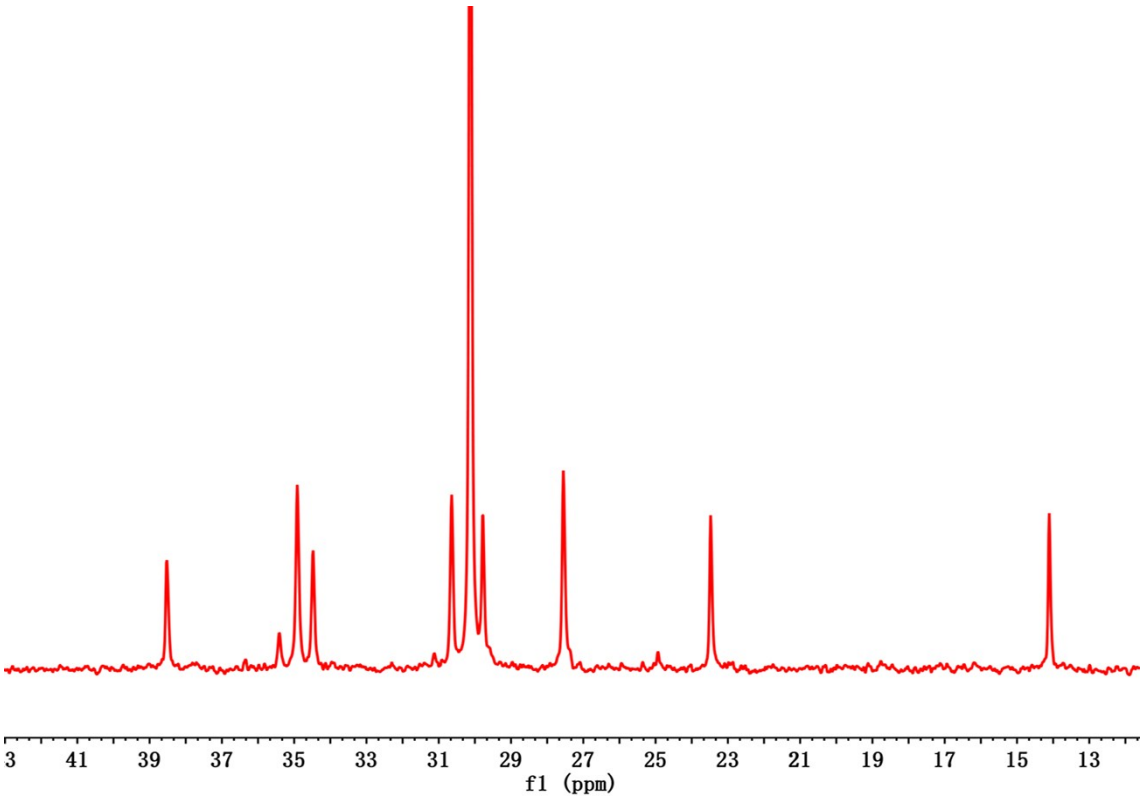

Figure S36 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 6, Table 2).

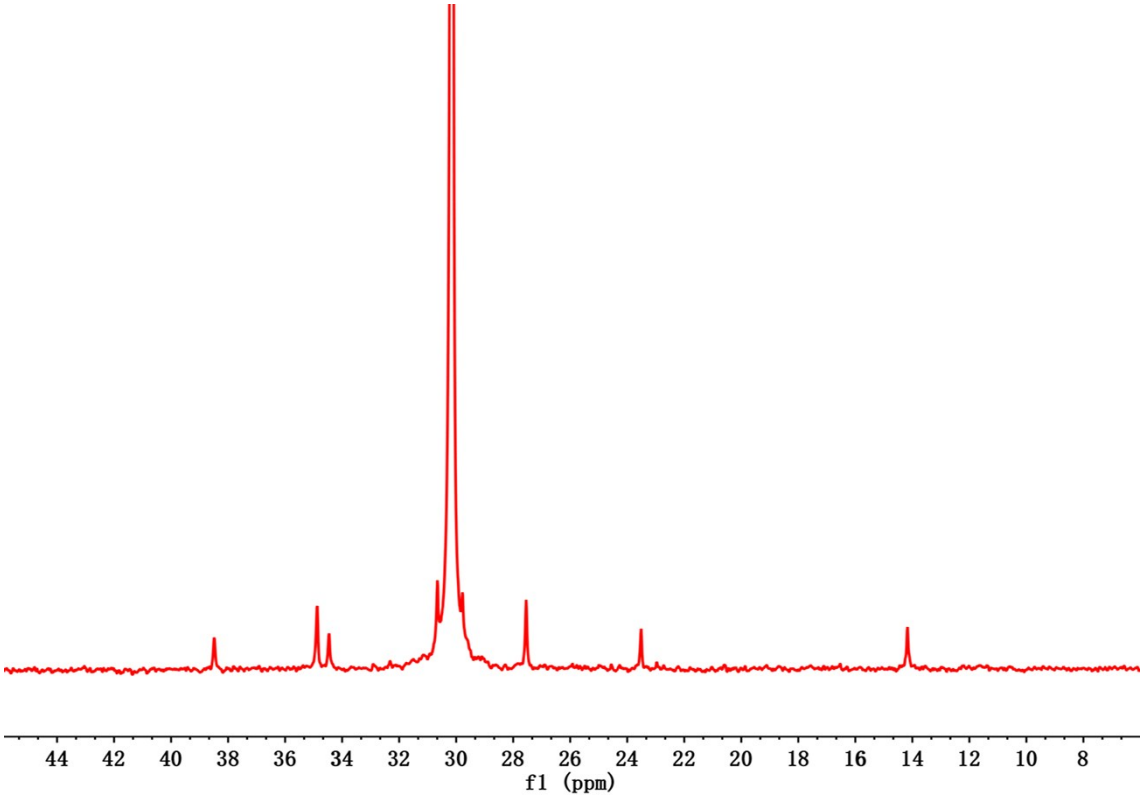

Figure S37 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 7, Table 2).

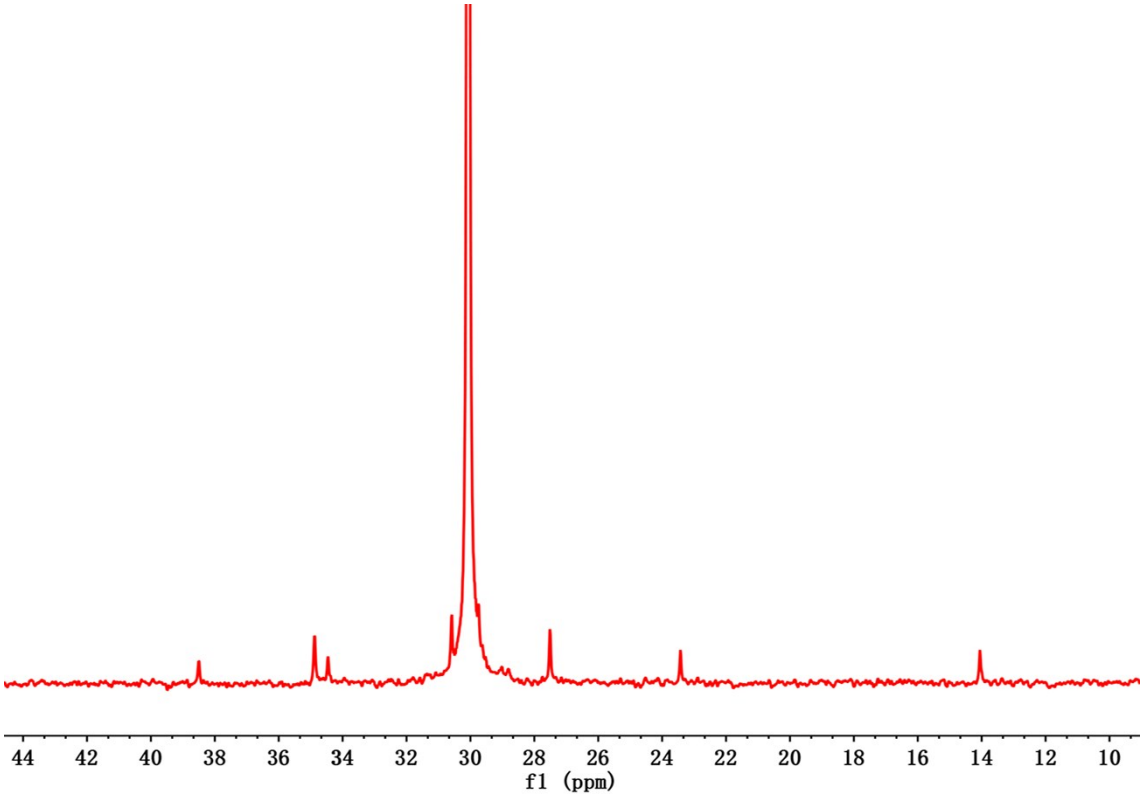

Figure S38 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 8, Table 2).

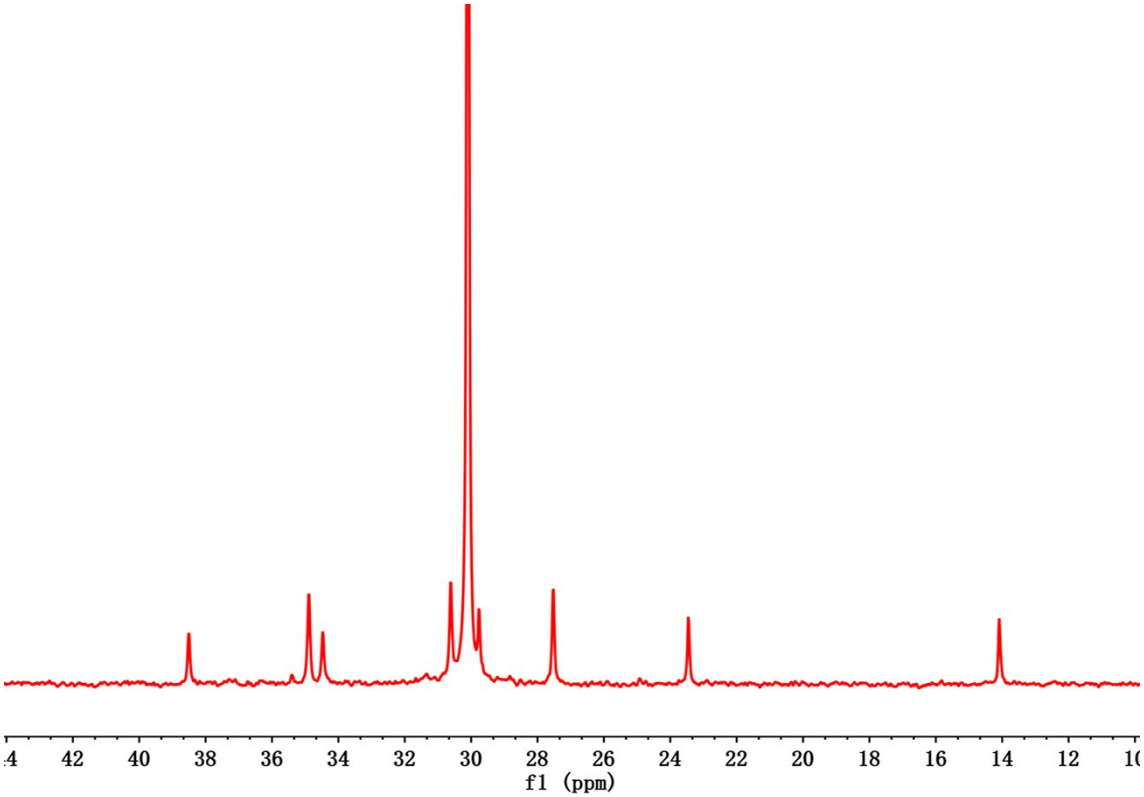

Figure S39 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 9, Table 2).

Figure S40 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 10, Table 2).

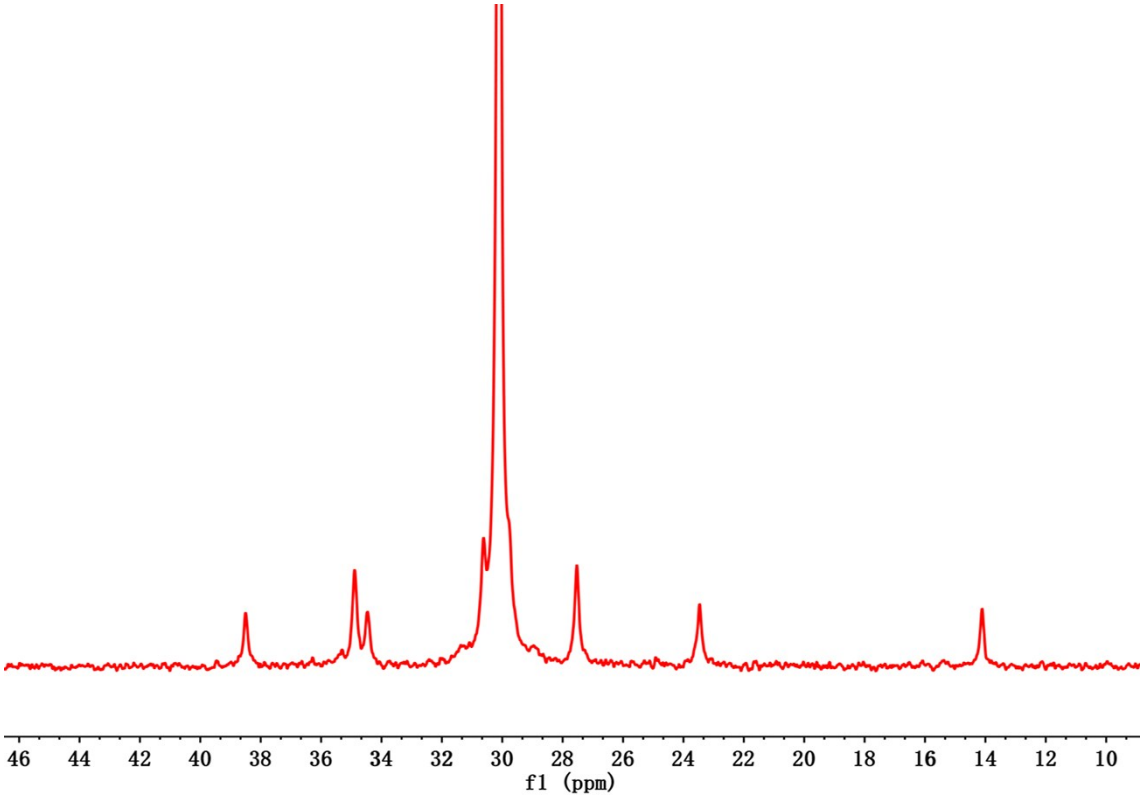

Figure S41 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 11, Table 2).

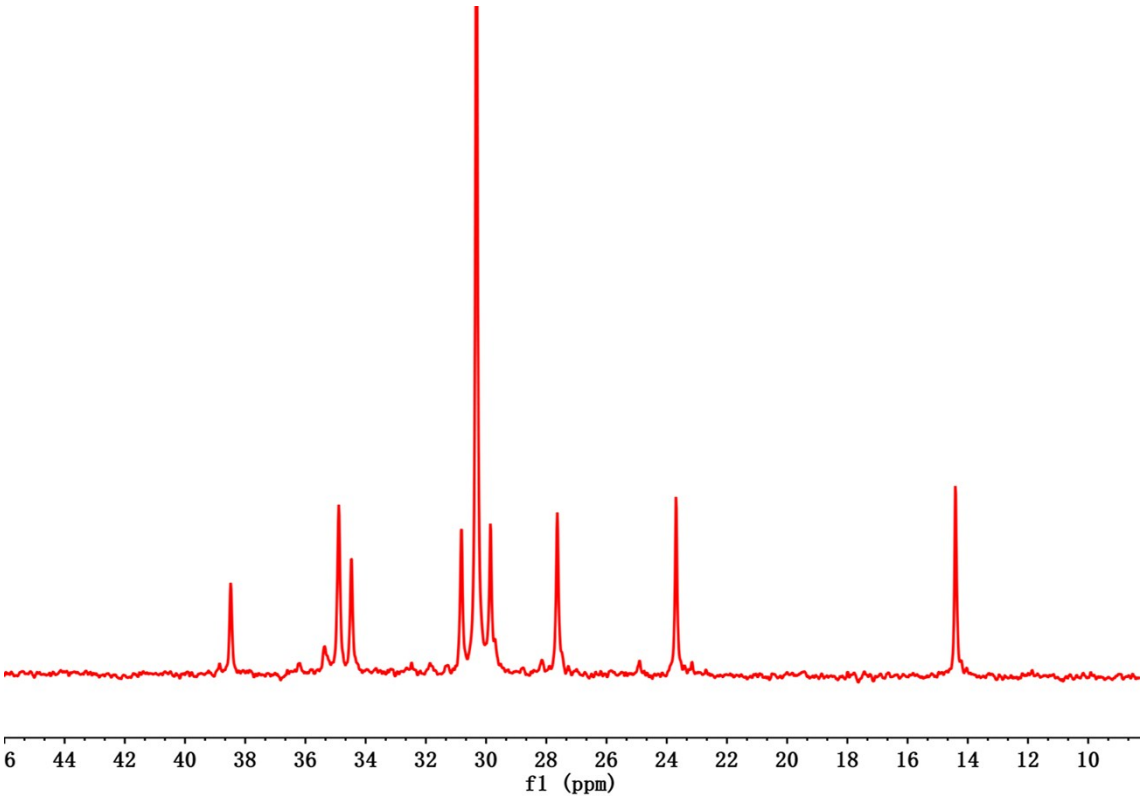

Figure S42 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 12, Table 2).

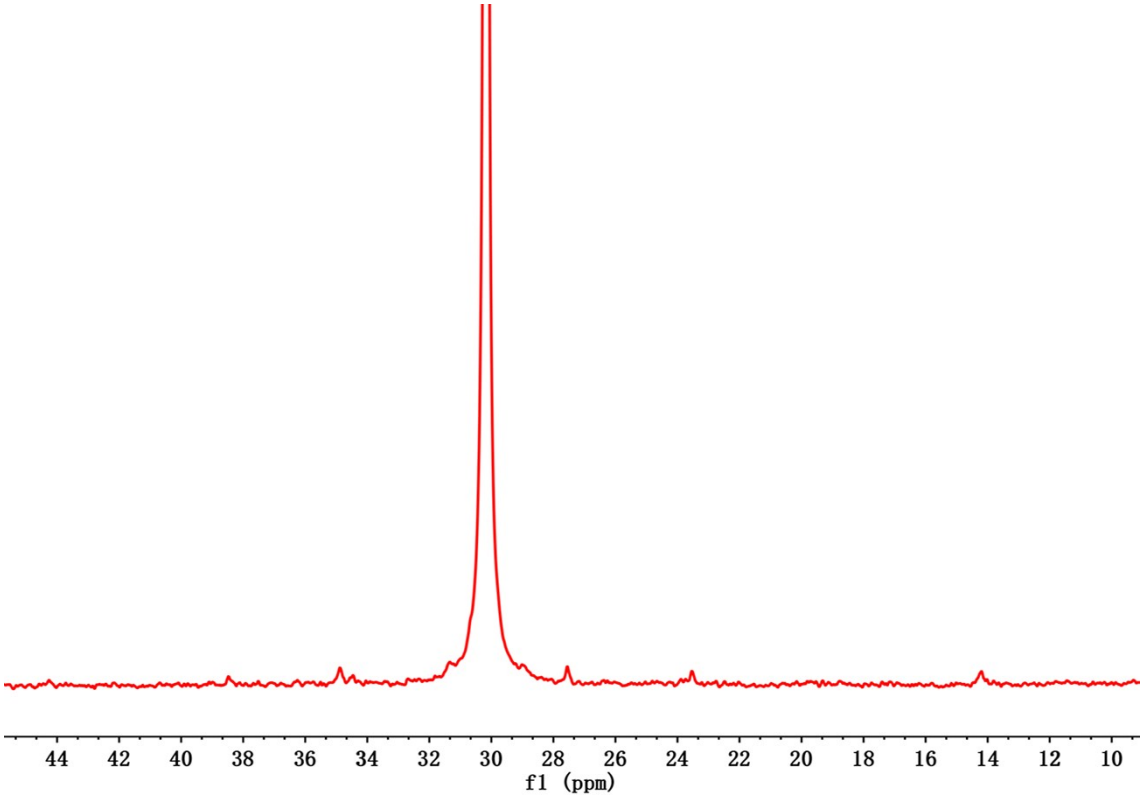

Figure S43 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 13, Table 2).

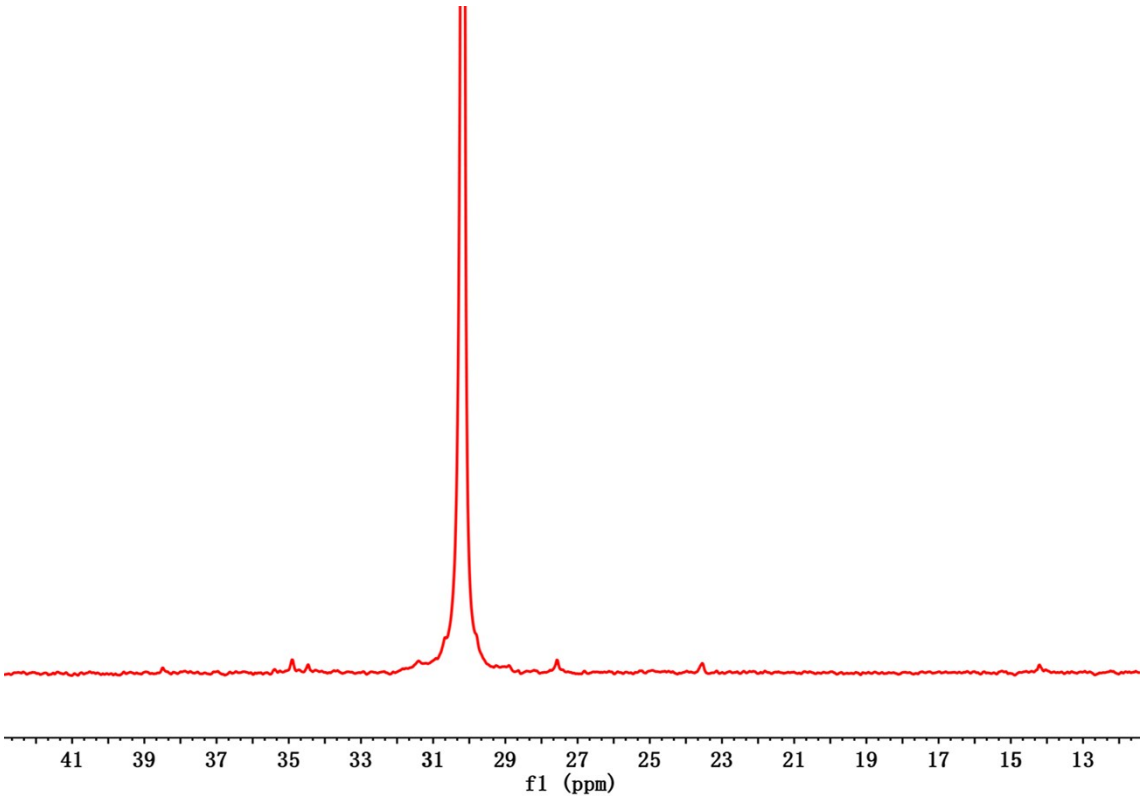

Figure S44 ^{13}C NMR spectra for poly(ethylene-co-1-hexene) sample (entry 14, Table 2).

Table S1. Crystal Data and Structure Refinements for Complexes **4**, **6** and **10**·THF

	4	**6**·CH_2Cl_2	**10**·THF·$2CH_2Cl_2$
Formula	$C_{60}H_{56}Cl_2O_2STi$	$C_{37}H_{62}Cl_5NO_2STi$	$C_{46}H_{60}Cl_6O_3SZr$
Mol wt	959.91	810.08	996.92
Cryst system	Triclinic	Monoclinic	Orthorhombic
Space group	$P\bar{1}$	$P2_1/c$	Ibam
a/ Å	10.142(3)	15.5858(11)	14.4804(4)
b/ Å	14.635(5)	18.7525(11)	25.1371(7)
c/ Å	17.205(5)	17.3122(12)	29.5376(7)
α/deg	86.535(6)	90.00	90.00
β/deg	89.821(6)	107.126(3)	90.00
γ/deg	77.971(6)	90.00	90.00
V/ Å^3	2493.0(14)	4835.5(6)	10751.5(5)
Z	2	4	8
D_c/g cm^{-3}	1.279	1.113	1.232
F(000)	1008	1720	4144
abs coeff/mm^{-1}	0.364	0.524	0.575
No. of obsd reflns	9521	8565	5415
No. of params refnd	601	443	270
GOF	0.987	1.057	1.081
R_1 ($I > 2\delta$)	0.0769	0.0565	0.0822
wR_2 ($I > 2\delta$)	0.1919	0.1187	0.2080