Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Supporting Information for

Half-sandwich rare-earth-metal derivatives bearing pyrrolidinyl-functionalized cyclopentadienyl ligand: synthesis, characterization and catalysis in syndiospecific polymerization of styrene

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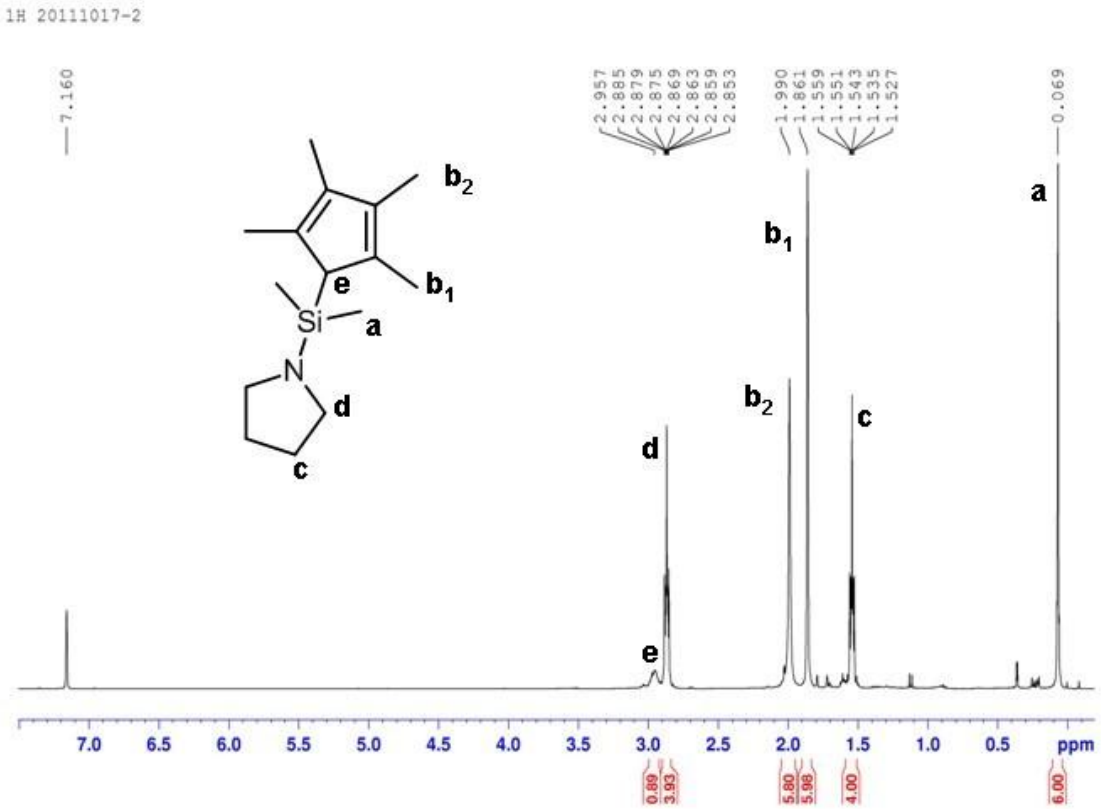

Fig. S1 ^{1}H NMR spectrum of $C_5Me_4HSiMe_2NC_4H_8$

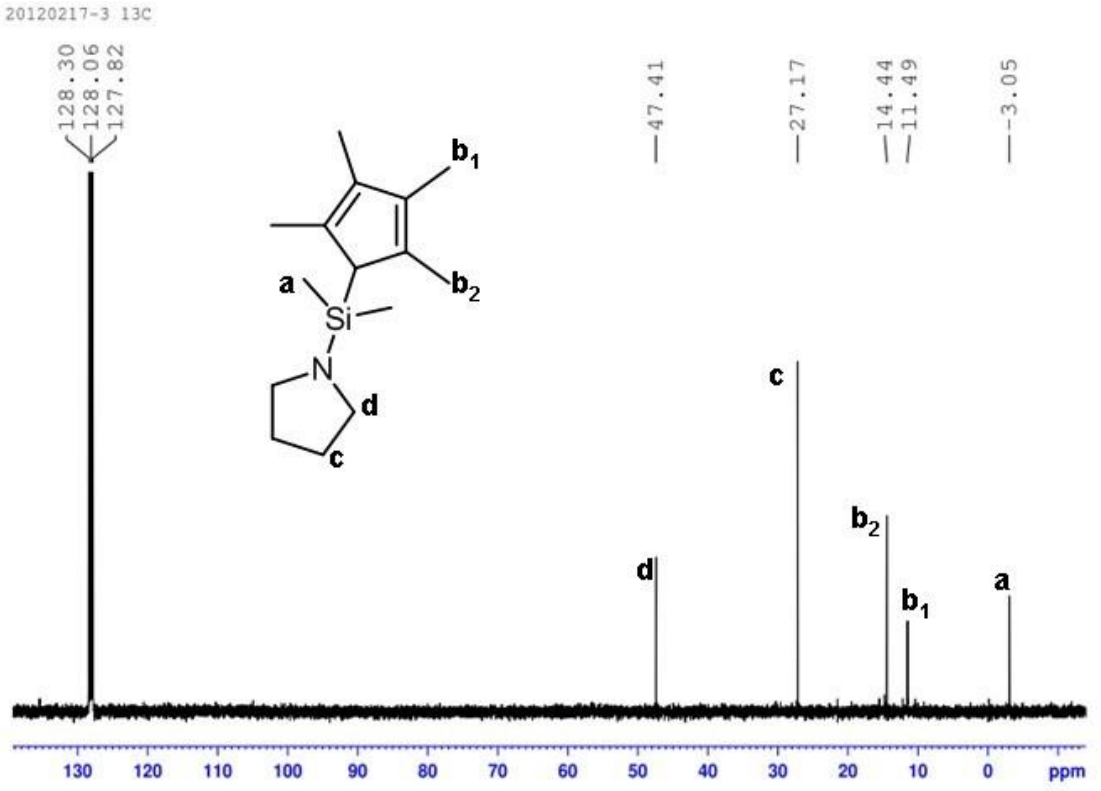

Fig. S2 ^{13}C NMR spectrum of $C_5Me_4HSiMe_2NC_4H_8$

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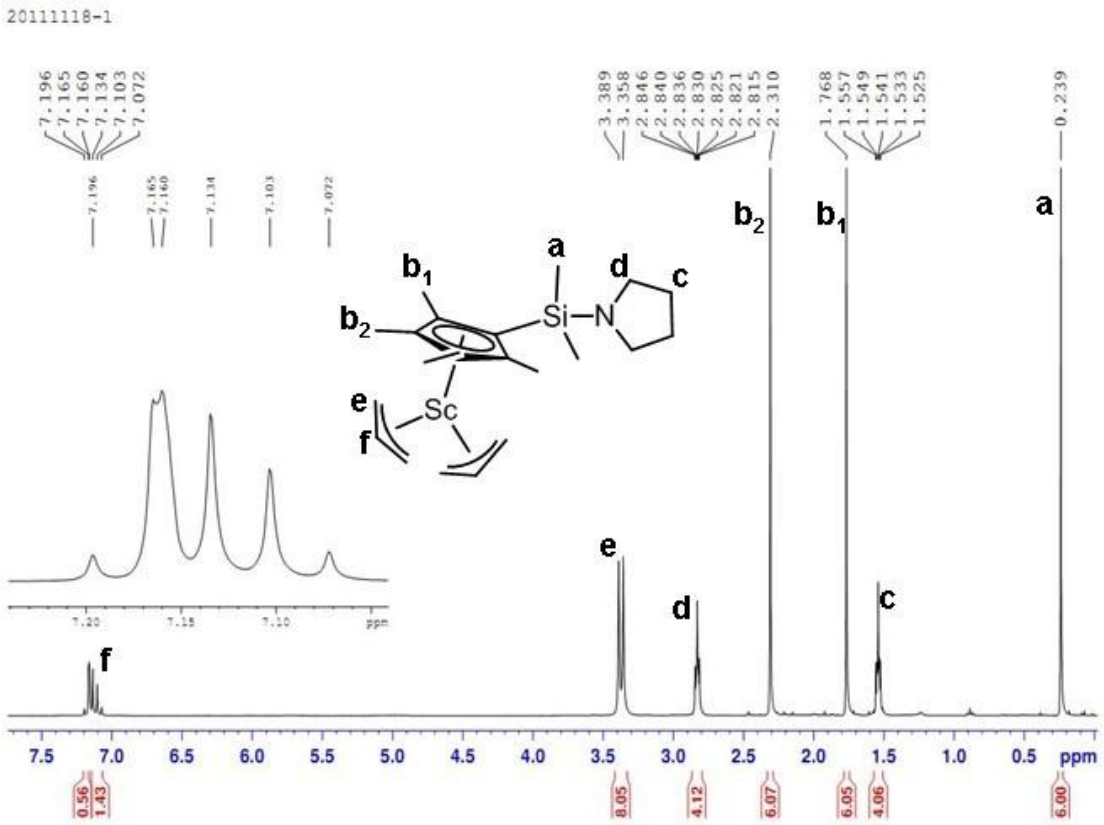

Fig. S3 ^{1}H NMR spectrum of **1**

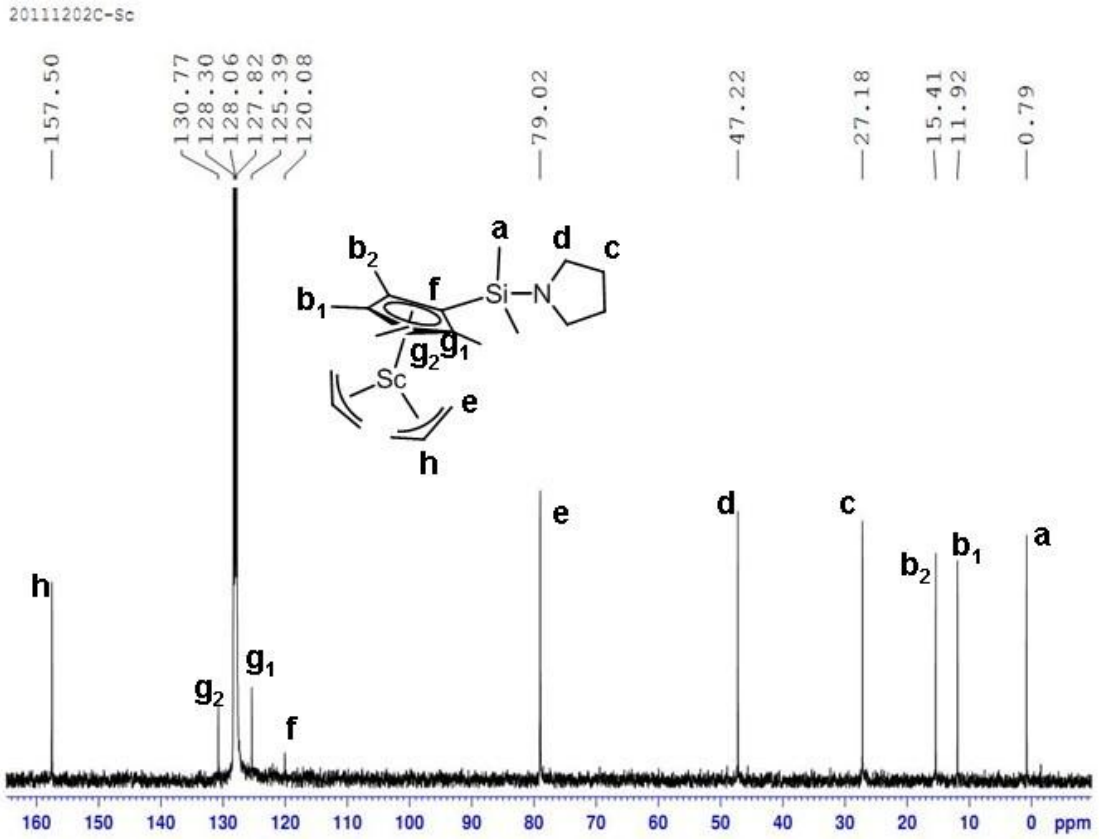

Fig. S4 ^{13}C NMR spectrum of **1**

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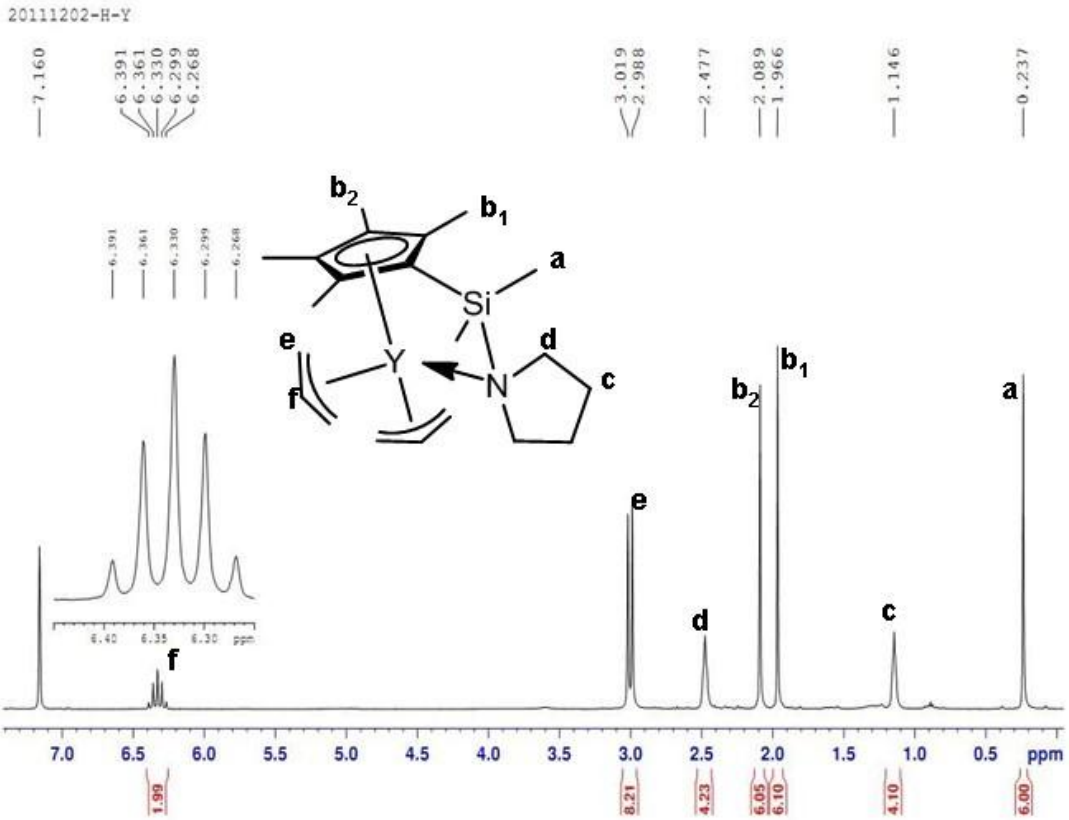

Fig. S5 ^{1}H NMR spectrum of **2**

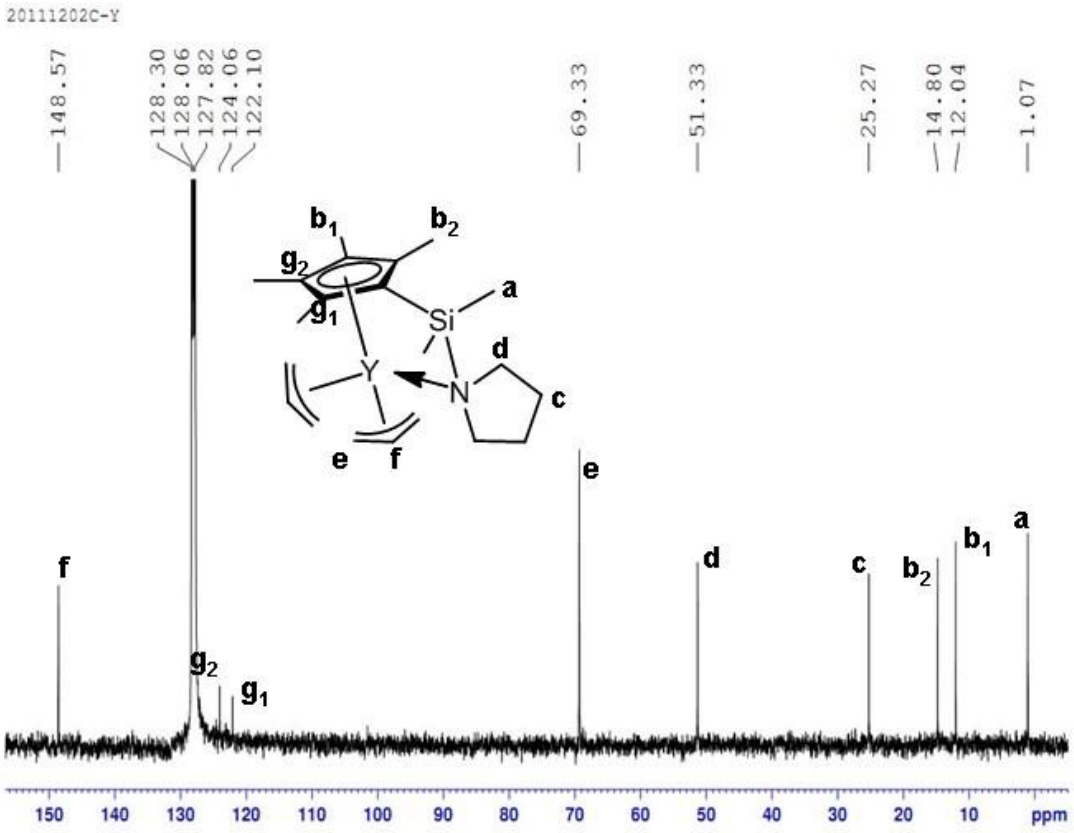

Fig. S6 ^{13}C NMR spectrum of **2**

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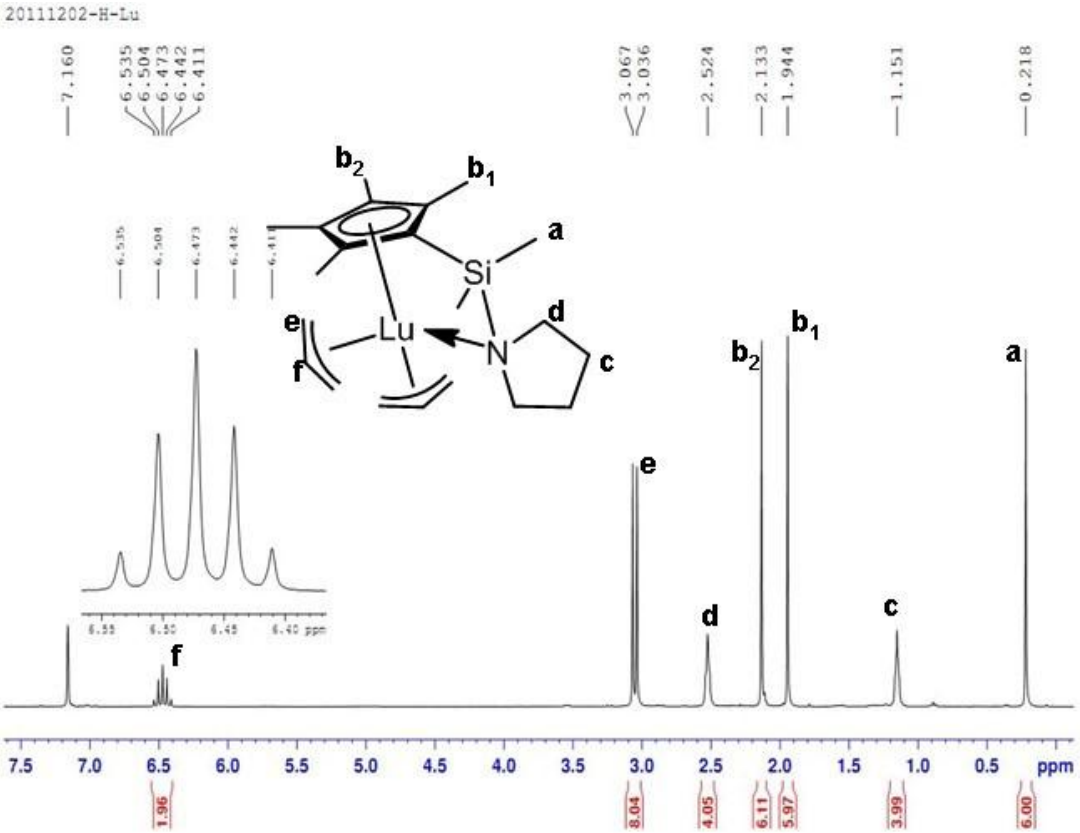

Fig. S7 ^{1}H NMR spectrum of **3**

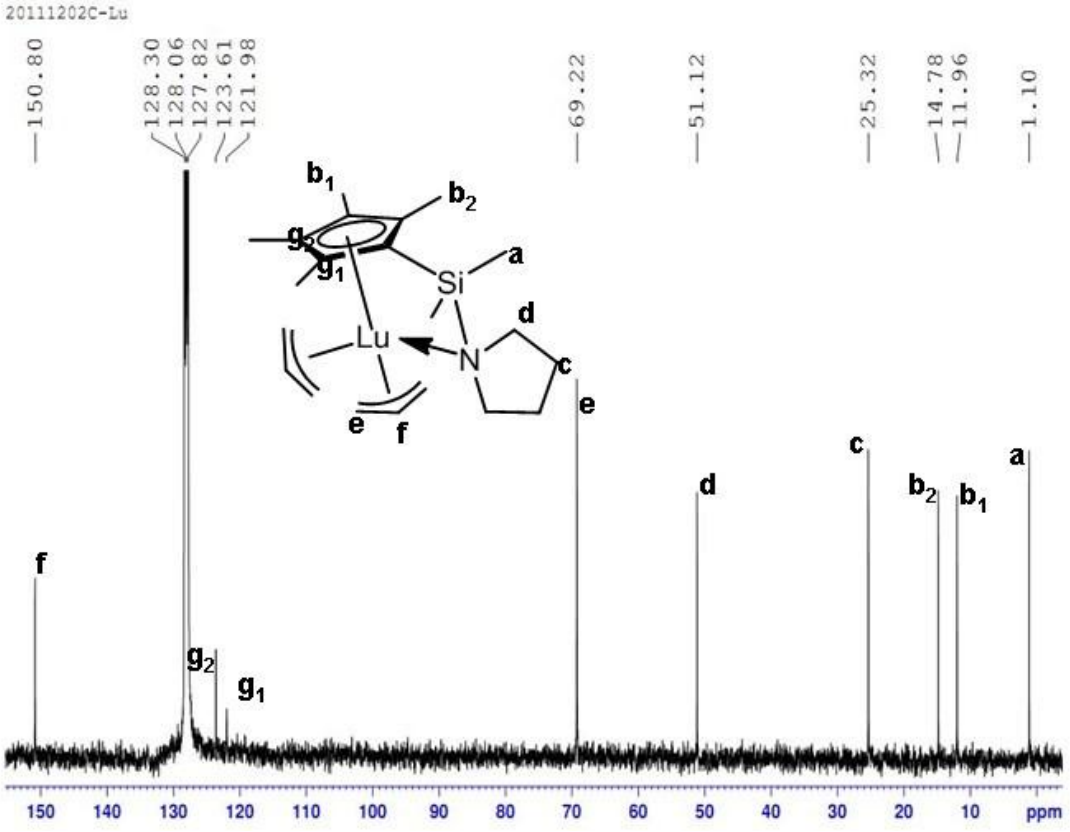

Fig. S8 ^{13}C NMR spectrum of **3**

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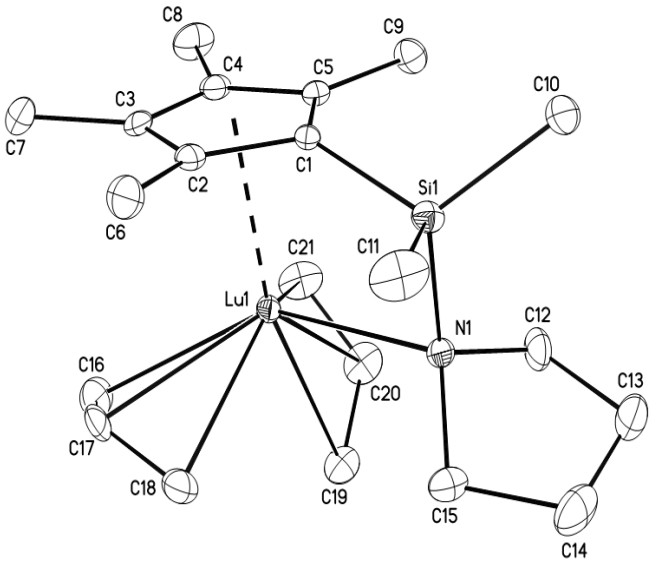

Fig. S9. Molecular structure of **3**. Selected bond distances (Å) and bond angles (°): Lu1-C1 = 2.523(4), Lu1-C2 = 2.637(4), Lu1-C3 = 2.728(4), Lu1-C4 = 2.647(4), Lu1-C5 = 2.528(4), Lu1-C16 = 2.596(4), Lu1-C17 = 2.564(4), Lu1-C18 = 2.539(5), Lu1-C19 = 2.633(4), Lu1-C20 = 2.592(4), Lu1-C21 = 2.506(4), $Cp_{centroid}$-Lu1 =2.320(10), C17-Lu1-C20 = 120.69(16), $Cp_{centroid}$-Lu1-N1 = 95.9(3).

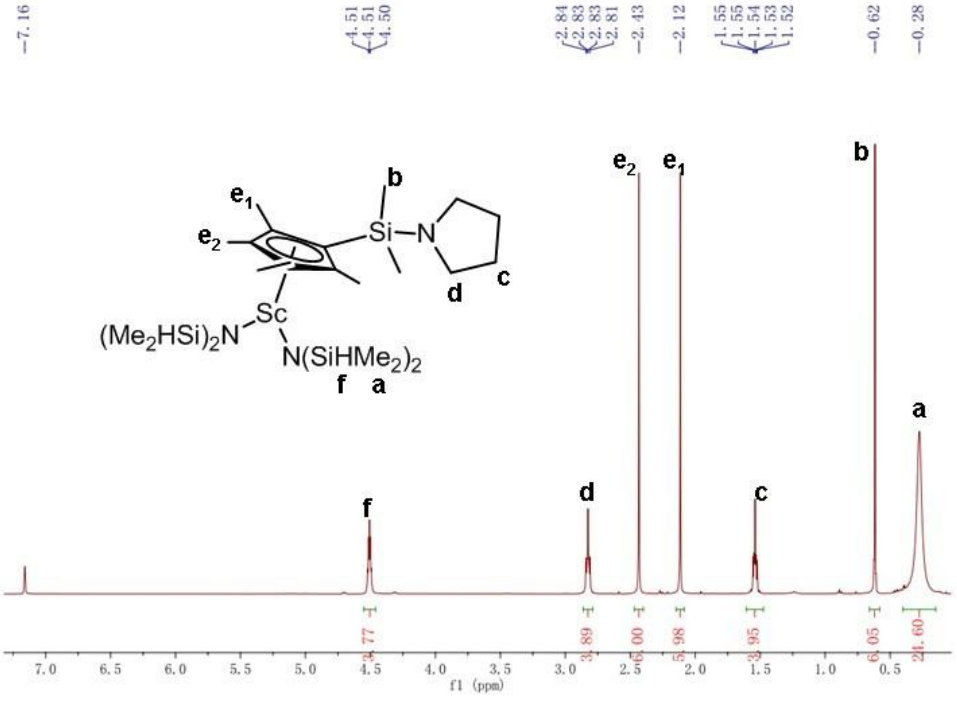

Fig. S10 ^{1}H NMR spectrum of **4**

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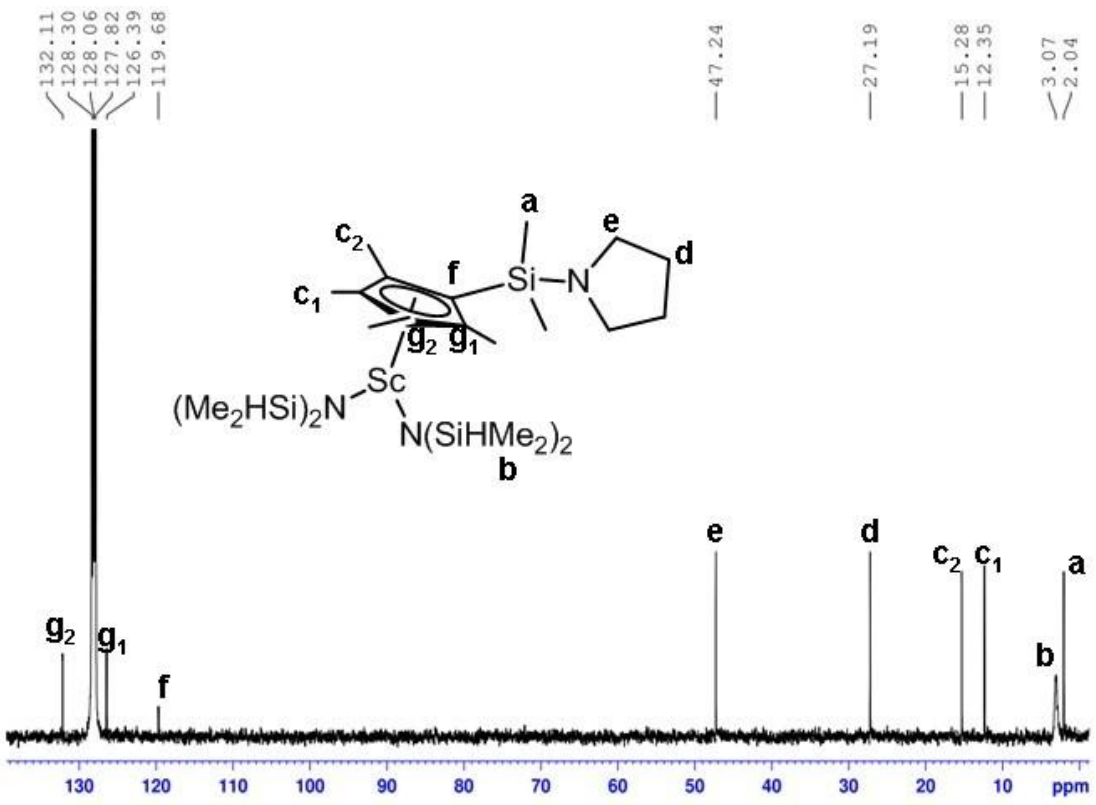

Fig. S11 ^{13}C NMR spectrum of **4**

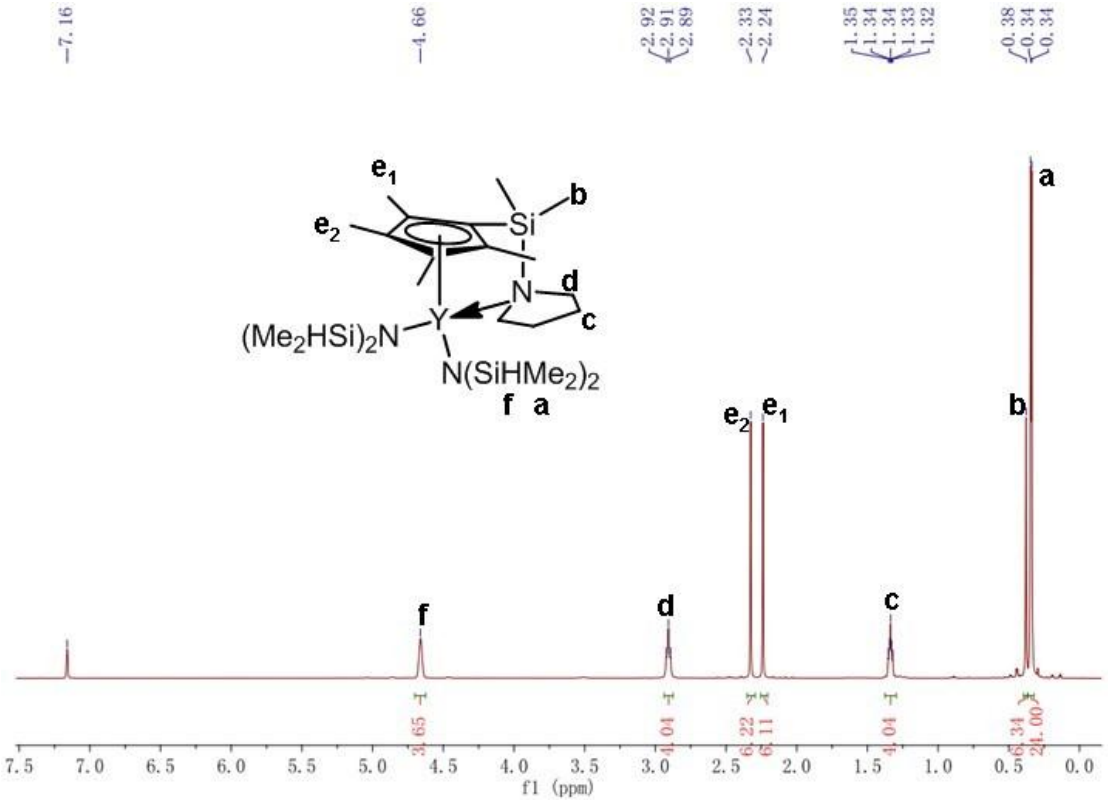

Fig. S12 ^{1}H NMR spectrum of **5**

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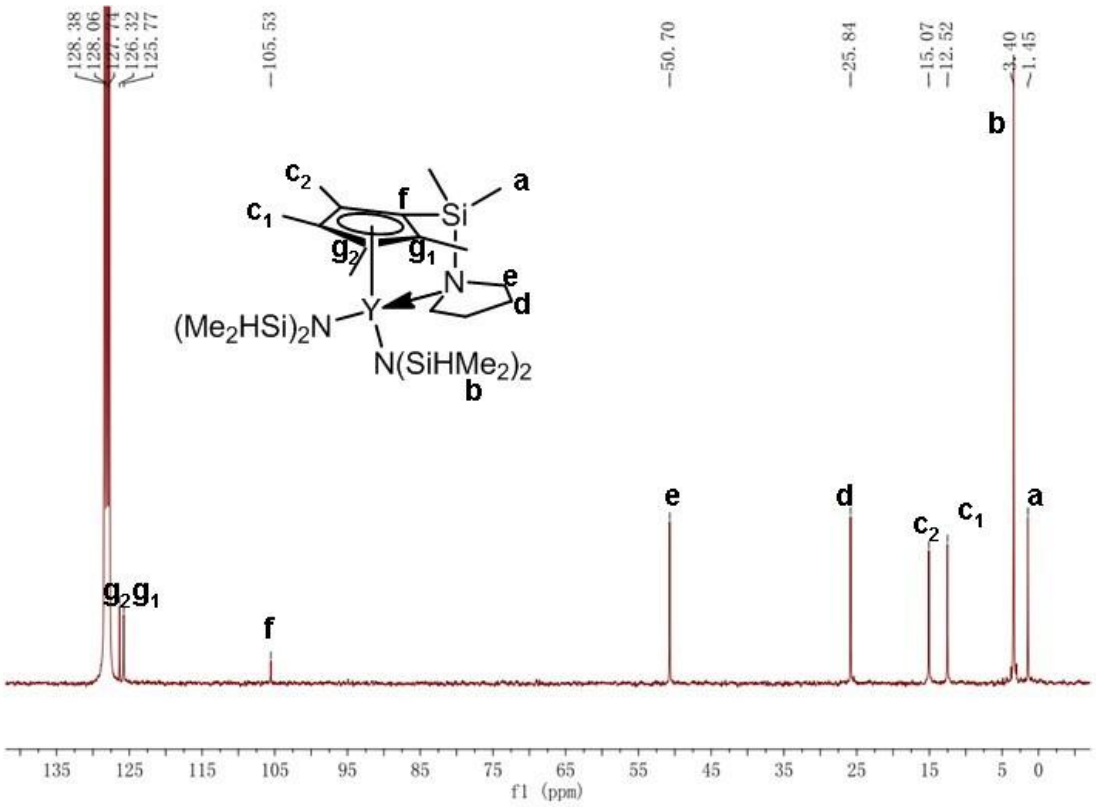

Fig. S13 ^{13}C NMR spectrum of **5**

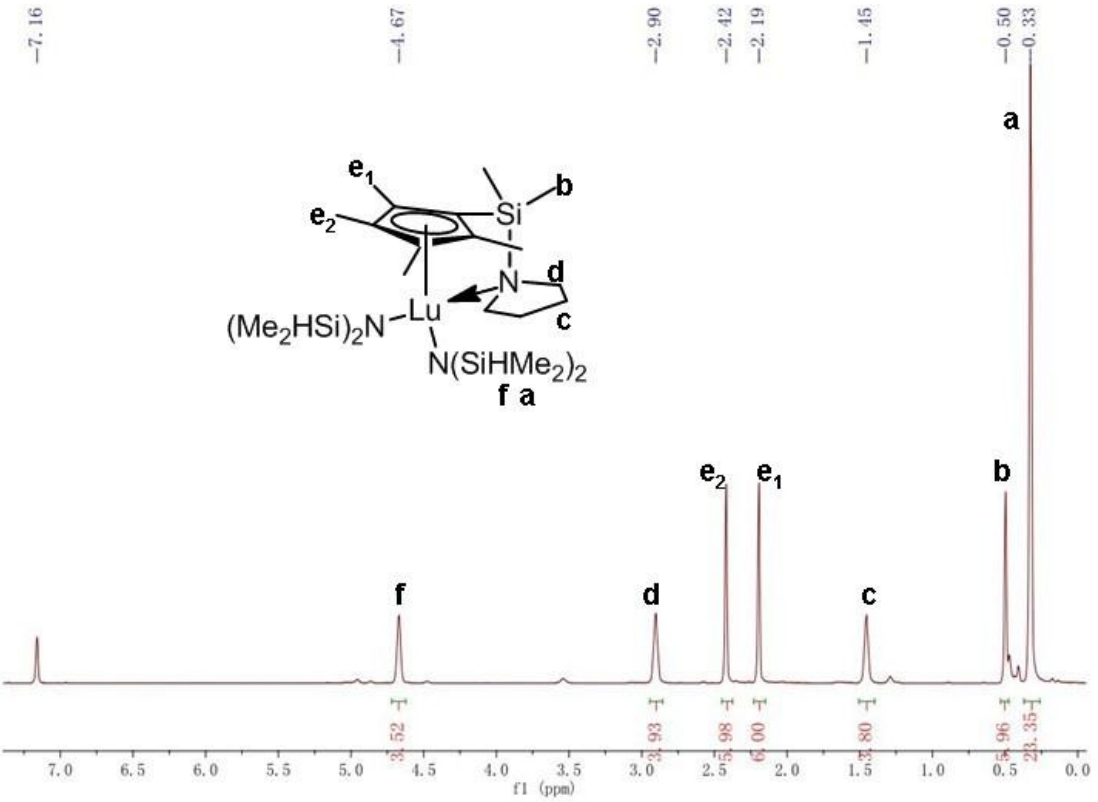

Fig. S14 ^{1}H NMR spectrum of **6**

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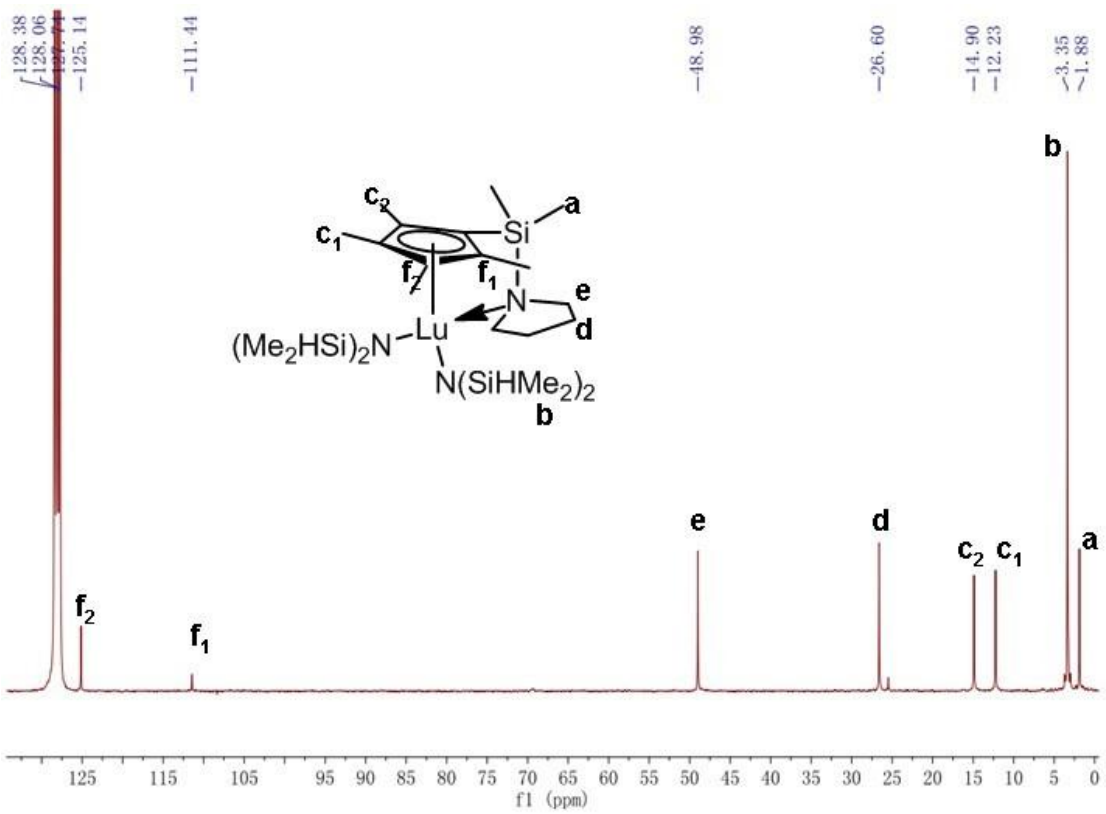

Fig. S15 ^{13}C NMR spectrum of **6**

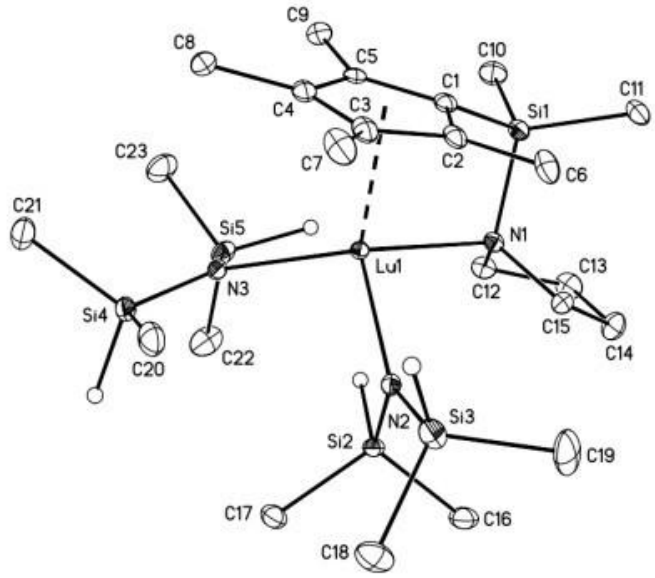

Fig. S16. Molecular structure of **6**. Selected bond distances (Å) and bond angles (°): Lu1-C1 = 2.550(4), Lu1-C2 = 2.612(4), Lu1-C3 = 2.708(4), Lu1-C4 = 2.707(4), Lu1-C5 = 2.618(4), Lu1–N2 = 2.216(3), Lu1–N3 = 2.237(3), $Cp_{centroid}$-Lu1 =2.347(9), N2–Lu1–N3 = 99.30(11), $Cp_{centroid}$-Lu1-N1 = 94.5(3).

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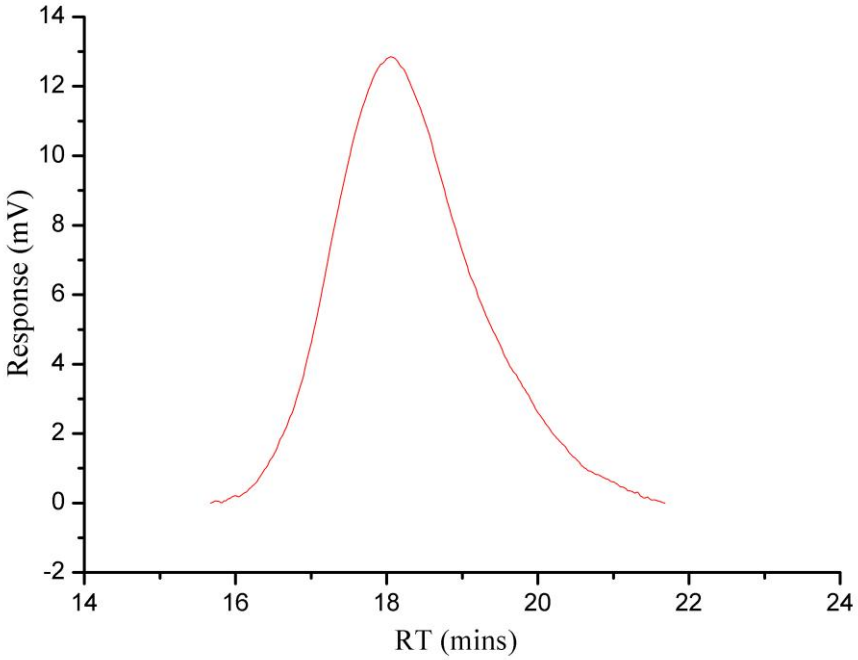

Fig. S17 GPC trace for polymer sample (Table 2, run 1)

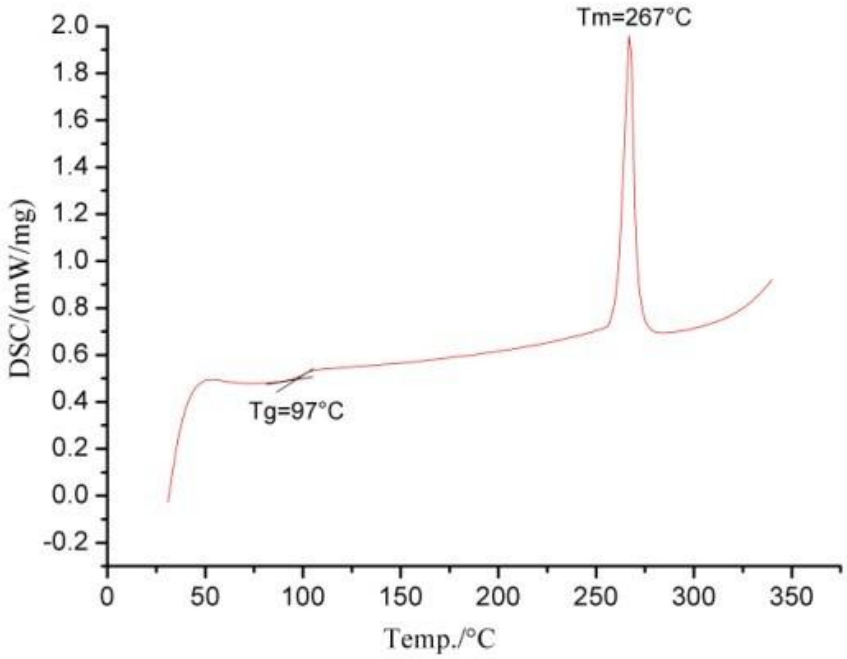

Fig. S18 DSC curve for polymer sample (Table 2, run 1)

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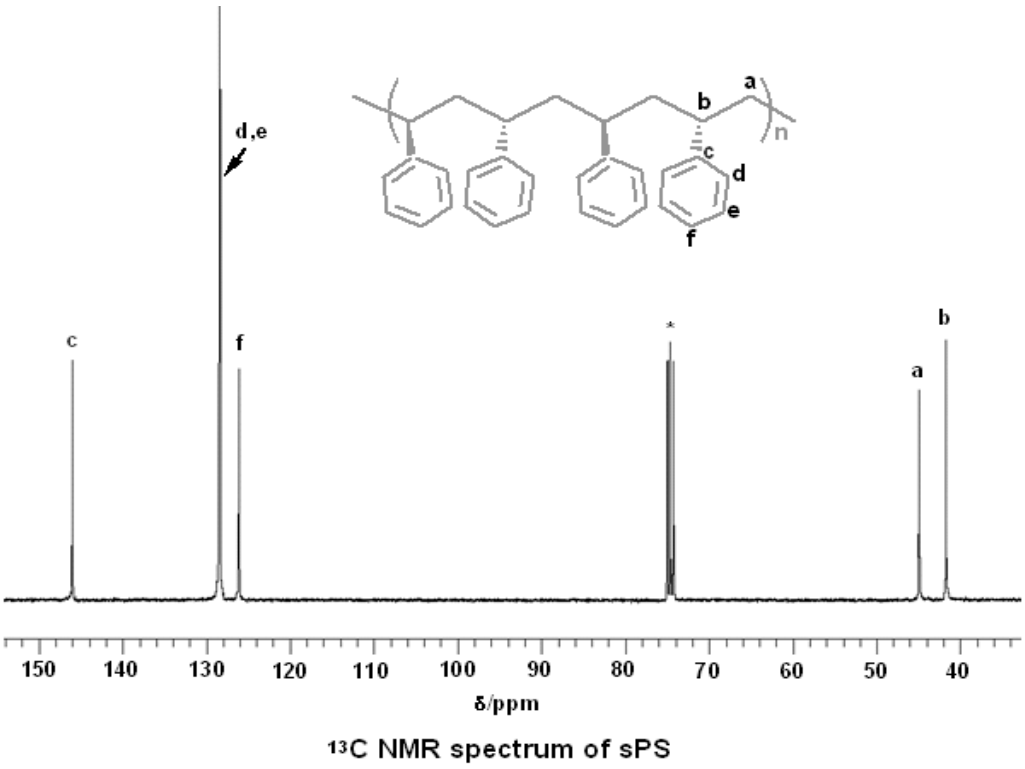

Fig. S19 ^{13}C NMR for polymer sample (Table 2, run 1)