

Supporting Information for

Rare-earth metal bis(alkyl) complexes bearing pyrrolidinyl-functionalized cyclopentadienyl, indenyl and fluorenyl ligands: synthesis, characterization and ligand effect on isoprene polymerization

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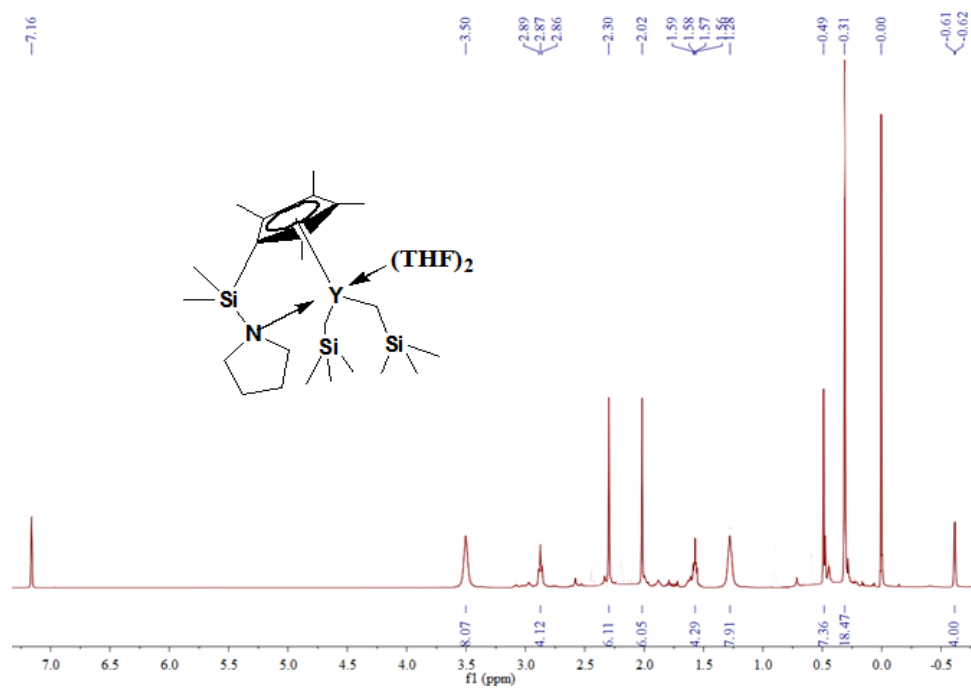


Fig. S1 ¹H NMR spectrum of (C₅Me₄SiMe₂NC₄H₈)Y(CH₂SiMe₃)₂(THF)₂ (1)

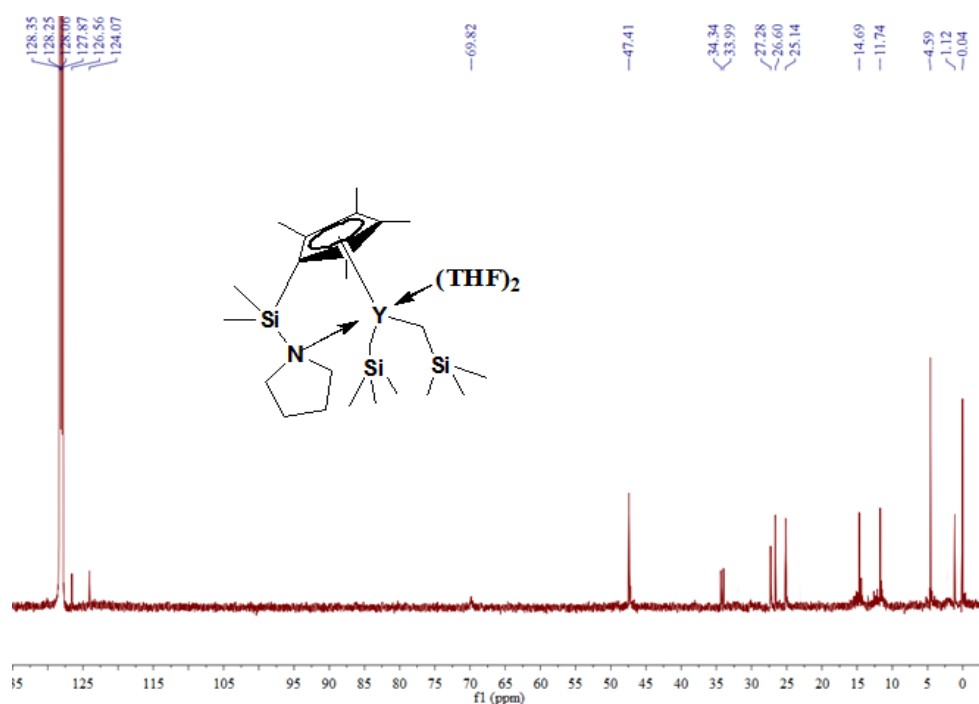


Fig. S2 ¹³C NMR spectrum of (C₅Me₄SiMe₂NC₄H₈)Y(CH₂SiMe₃)₂(THF)₂ (1)

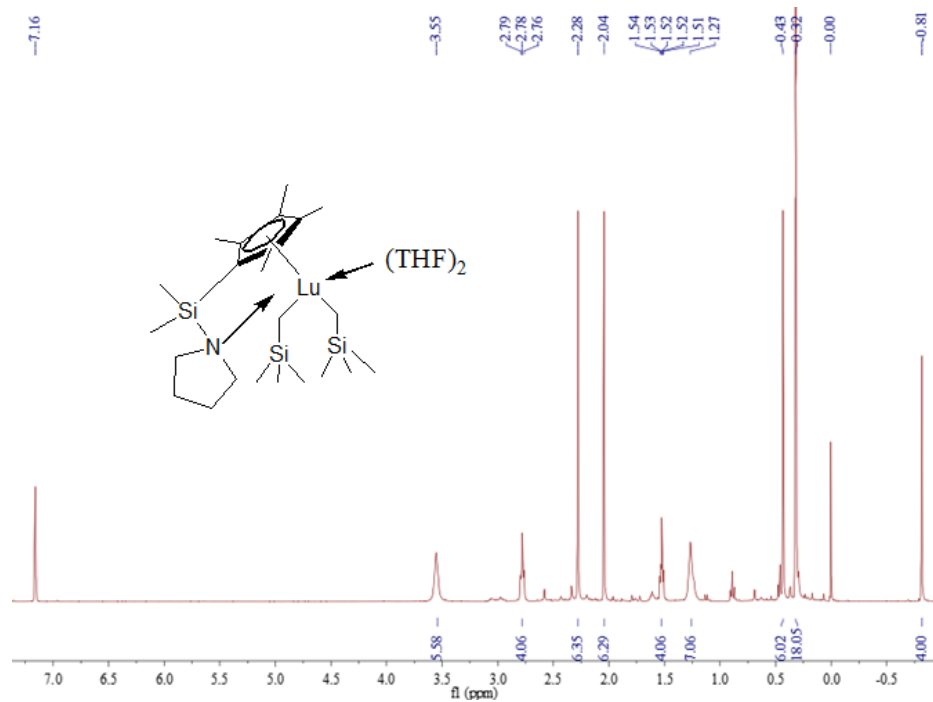


Fig. S3 ¹H NMR spectrum of $(C_5Me_4SiMe_2NC_4H_8)Lu(CH_2SiMe_3)_2(THF)_2$ (**2**)

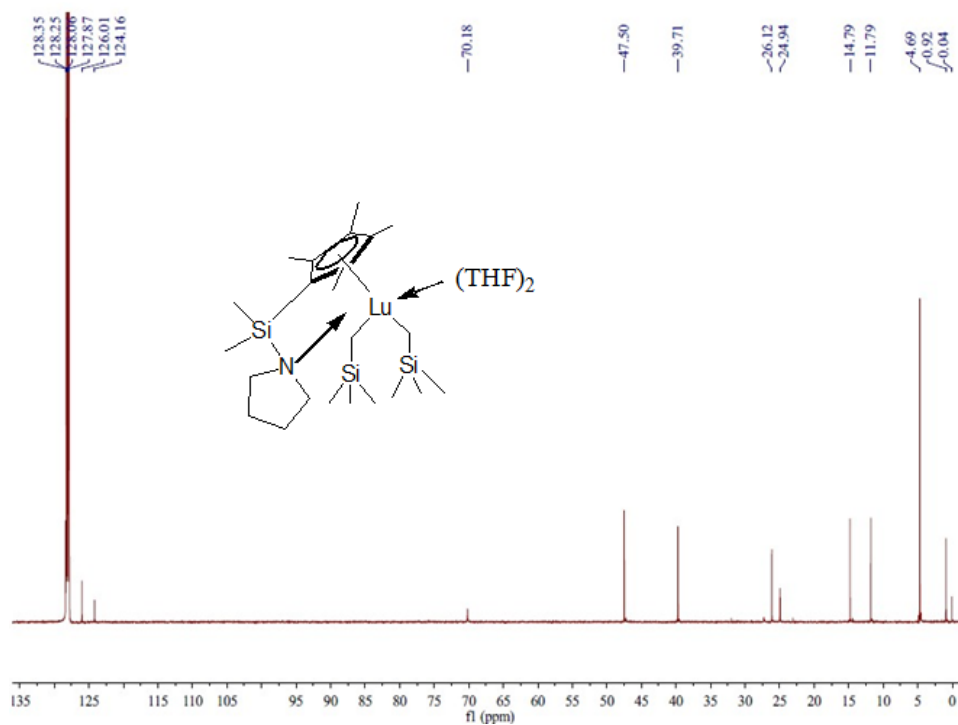


Fig. S4 ¹³C NMR spectrum of $(C_5Me_4SiMe_2NC_4H_8)Lu(CH_2SiMe_3)_2(THF)_2$ (**2**)

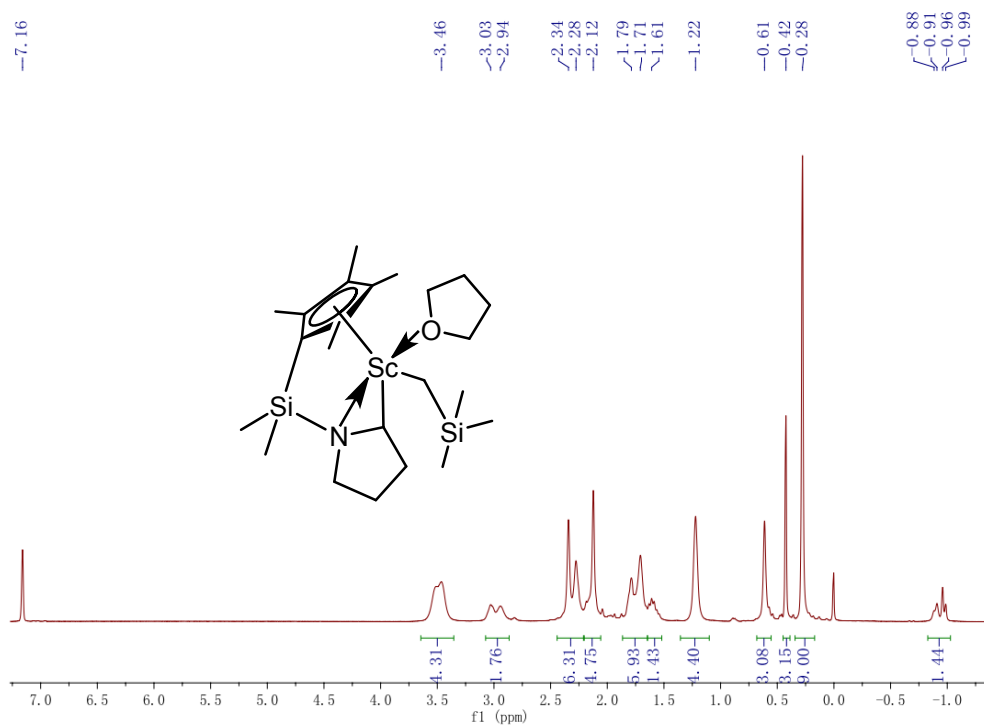


Fig. S5 ¹H NMR spectrum of (C₅Me₄SiMe₂NC₄H₇)Sc(CH₂SiMe₃)(THF) (**3**)

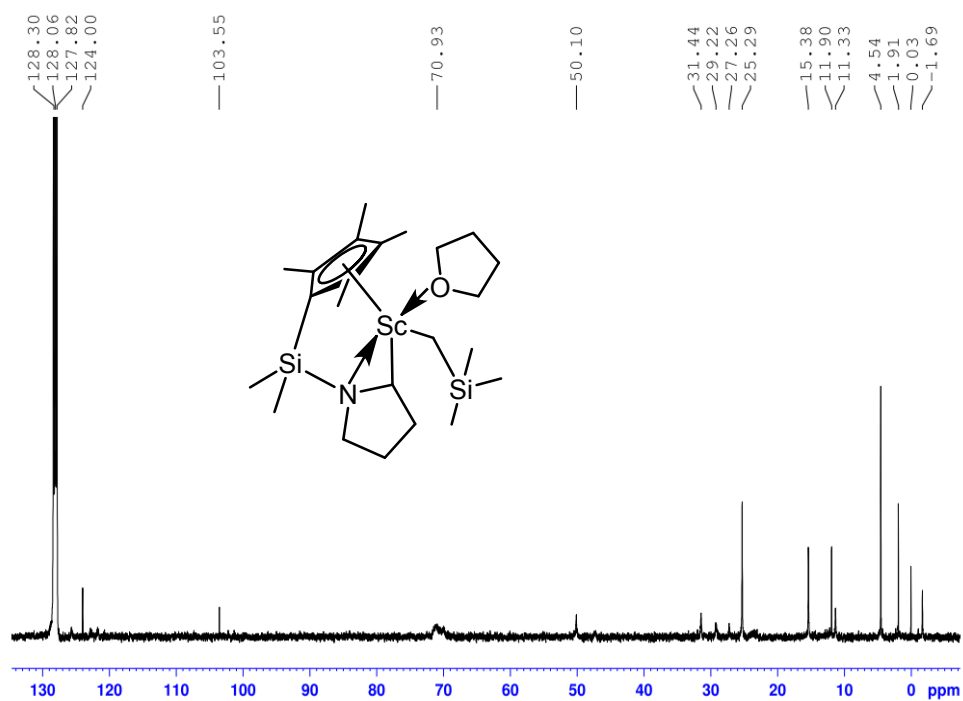


Fig. S6 ¹³C NMR spectrum of (C₅Me₄SiMe₂NC₄H₇)Sc(CH₂SiMe₃)(THF) (**3**)

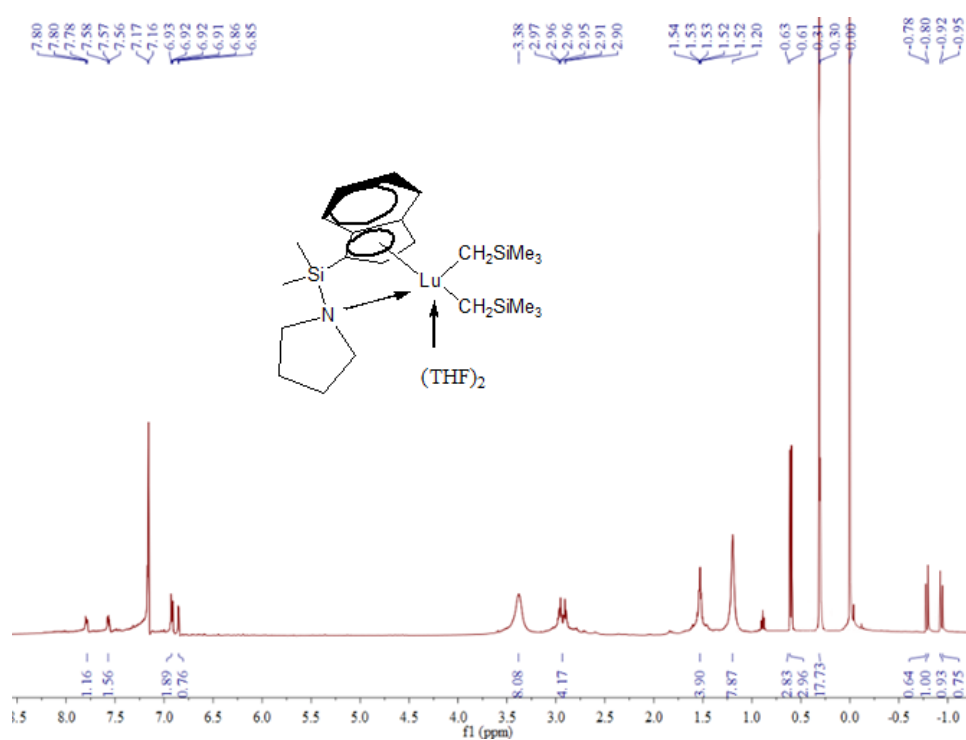


Fig. S7 1H NMR spectrum of $[C_9H_6SiMe_2NC_4H_8]Lu(CH_2SiMe_3)_2(THF)_2$ (4)

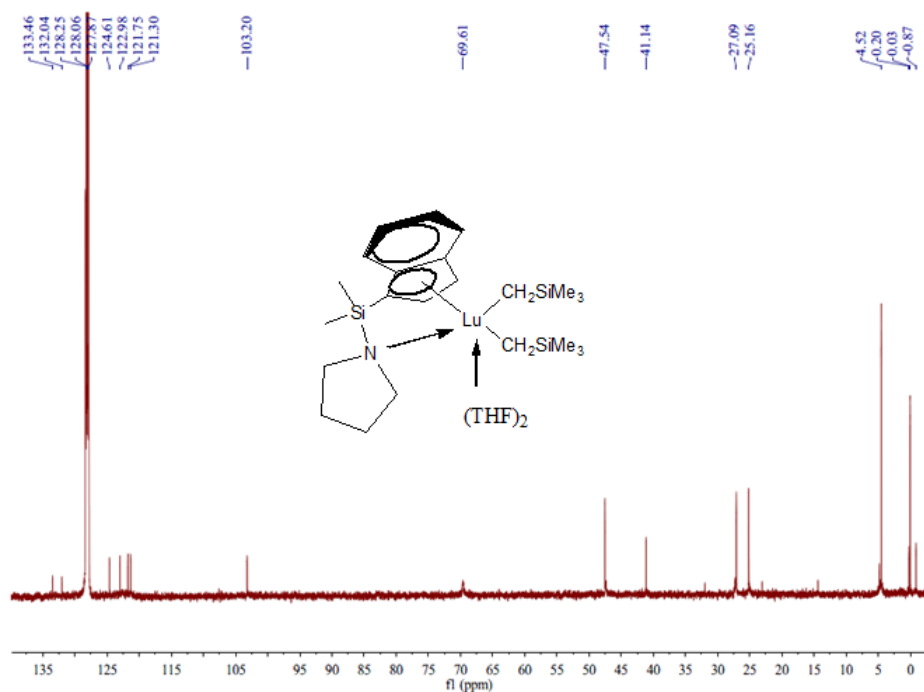


Fig. S8 ^{13}C NMR spectrum of $[C_9H_6SiMe_2NC_4H_8]Lu(CH_2SiMe_3)_2(THF)_2$ (4)

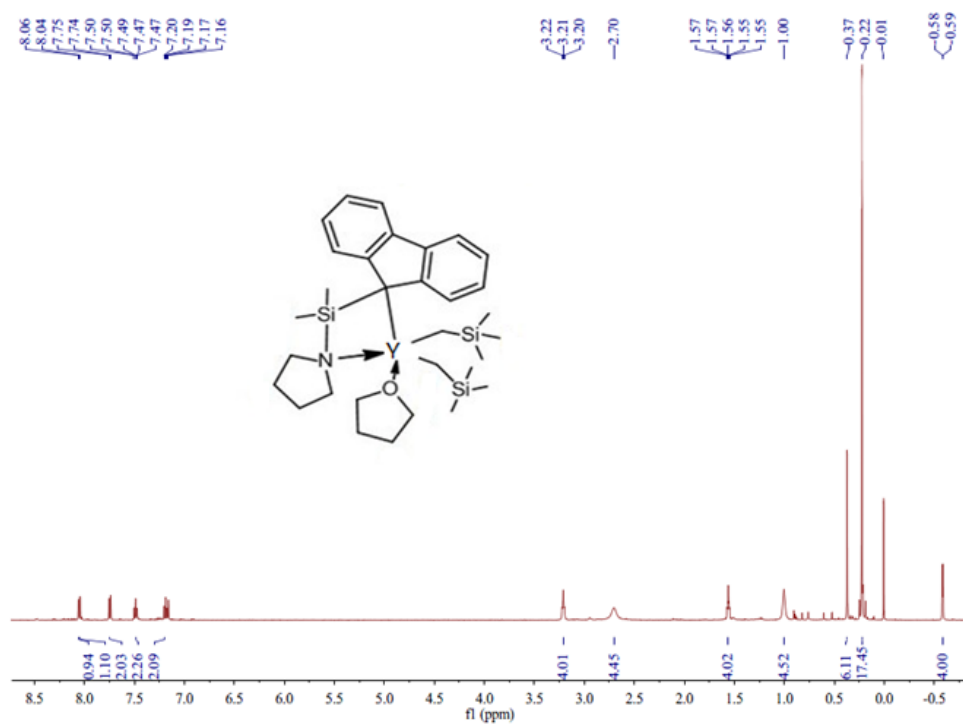


Fig. S9 1H NMR spectrum of $(C_{13}H_8SiMe_2NC_4H_8)Y(CH_2SiMe_3)_2(THF)$ (5)

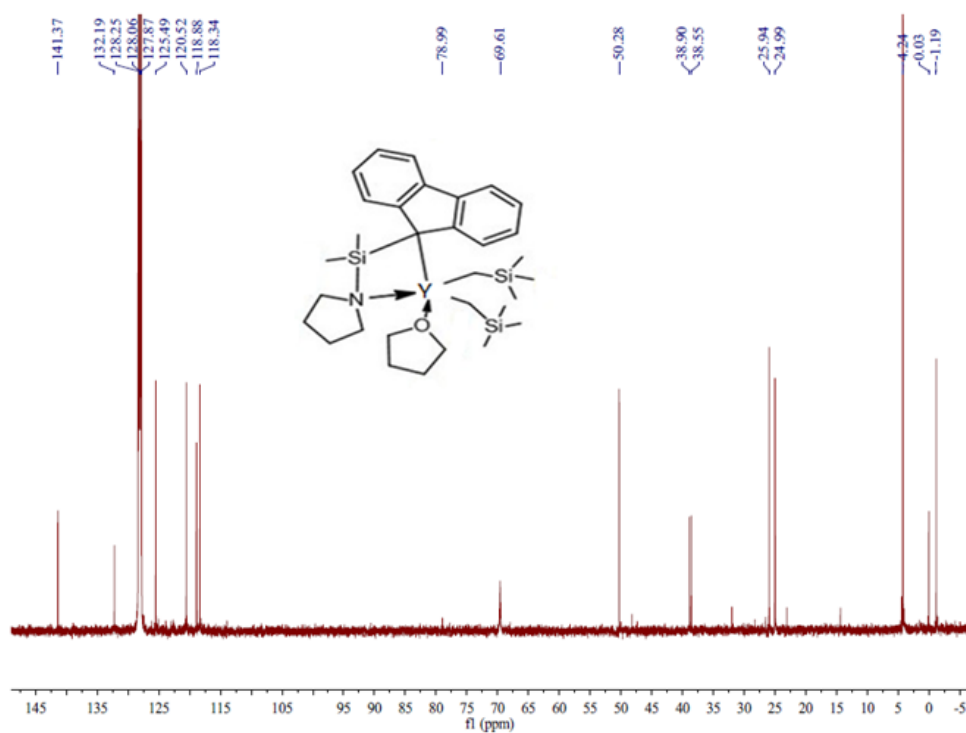


Fig. S10 ^{13}C NMR spectrum of $(C_{13}H_8SiMe_2NC_4H_8)Y(CH_2SiMe_3)_2(THF)$ (5)

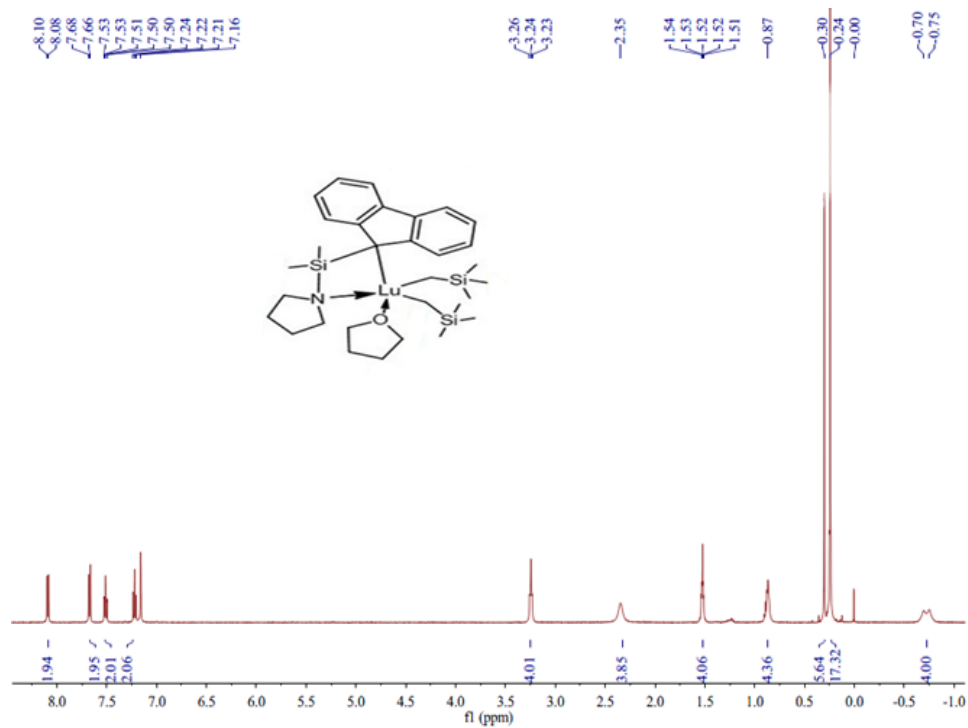


Fig. S11 ^1H NMR spectrum of $(\text{C}_{13}\text{H}_8\text{SiMe}_2\text{NC}_4\text{H}_8)\text{Lu}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (6)

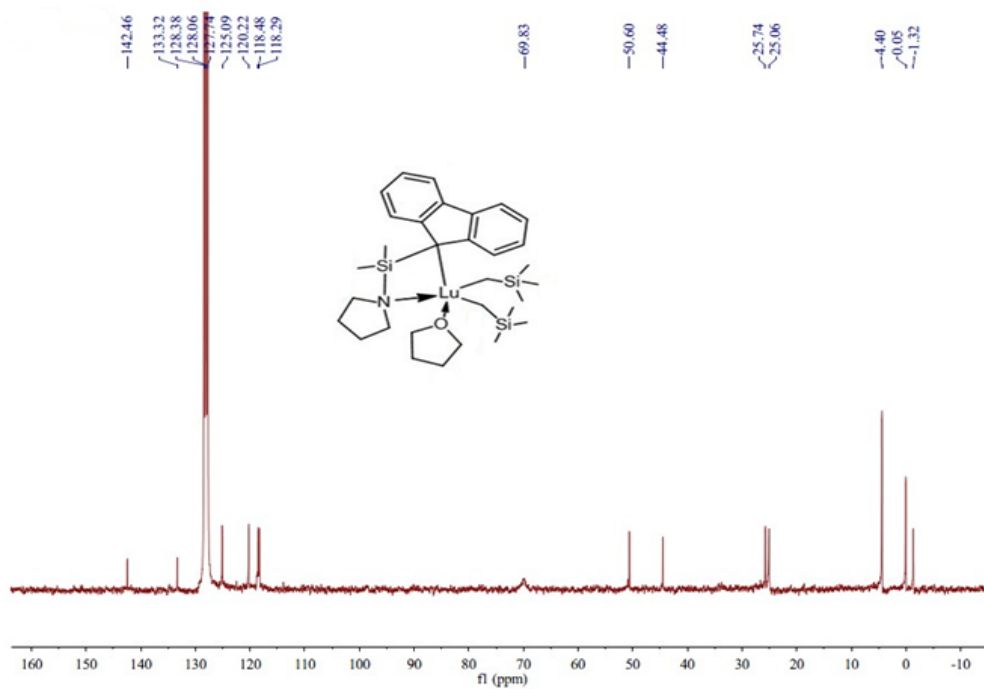


Fig. S12 ^{13}C NMR spectrum of $(\text{C}_{13}\text{H}_8\text{SiMe}_2\text{NC}_4\text{H}_8)\text{Lu}(\text{CH}_2\text{SiMe}_3)_2(\text{THF})$ (6)

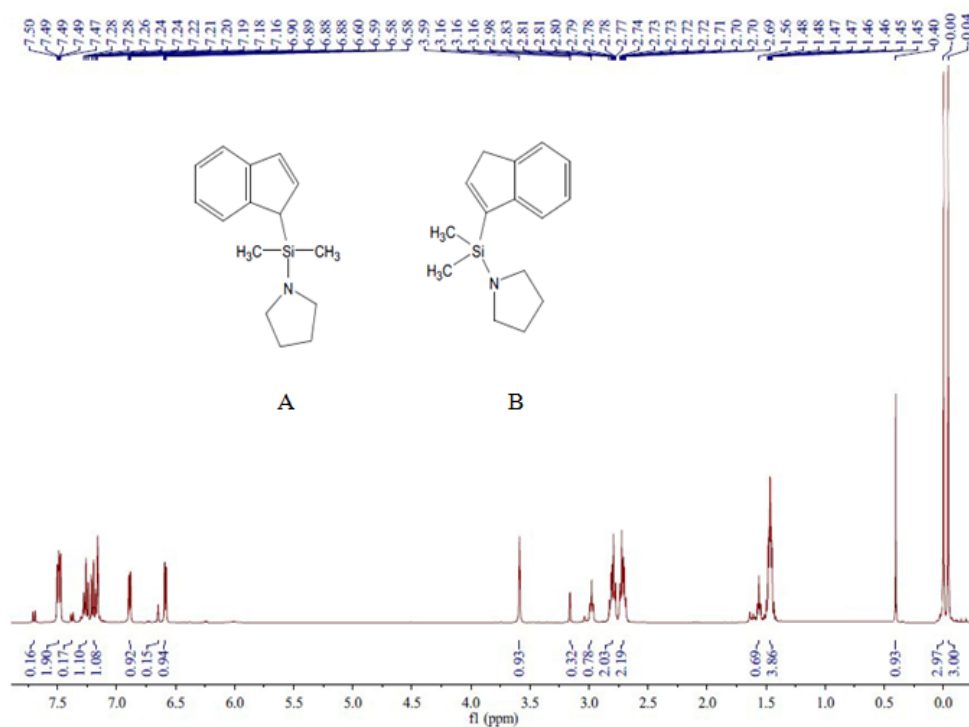


Fig. S13 ^1H NMR spectrum of $\text{C}_9\text{H}_6\text{SiMe}_2\text{NC}_4\text{H}_8$

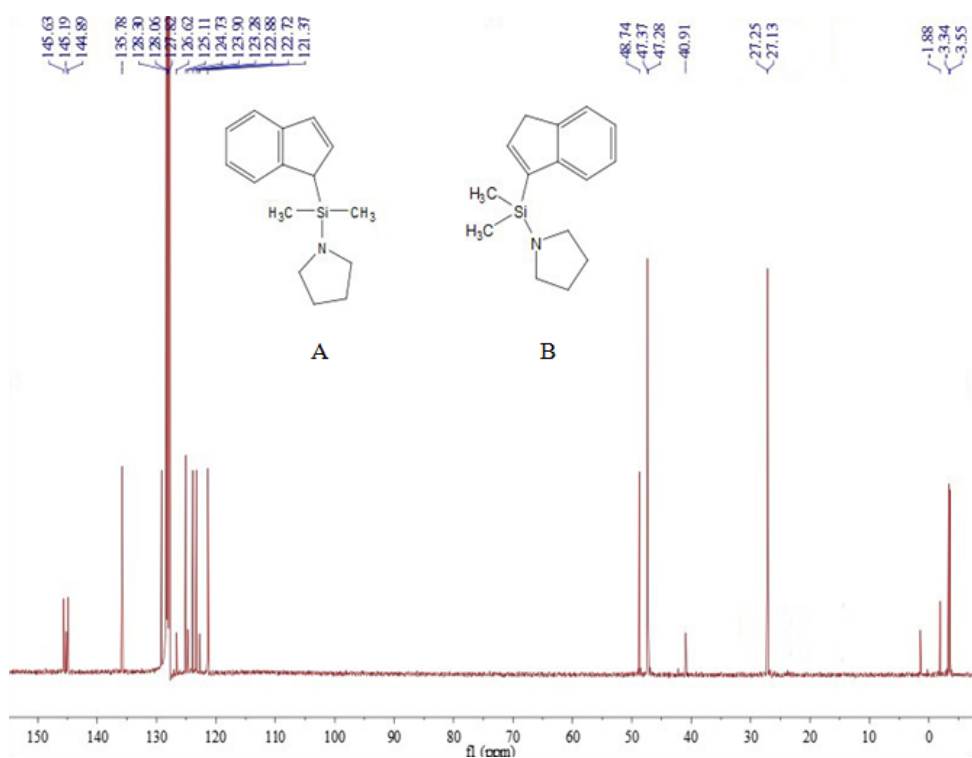


Fig. S14 ^{13}C NMR spectrum of $\text{C}_9\text{H}_6\text{SiMe}_2\text{NC}_4\text{H}_8$

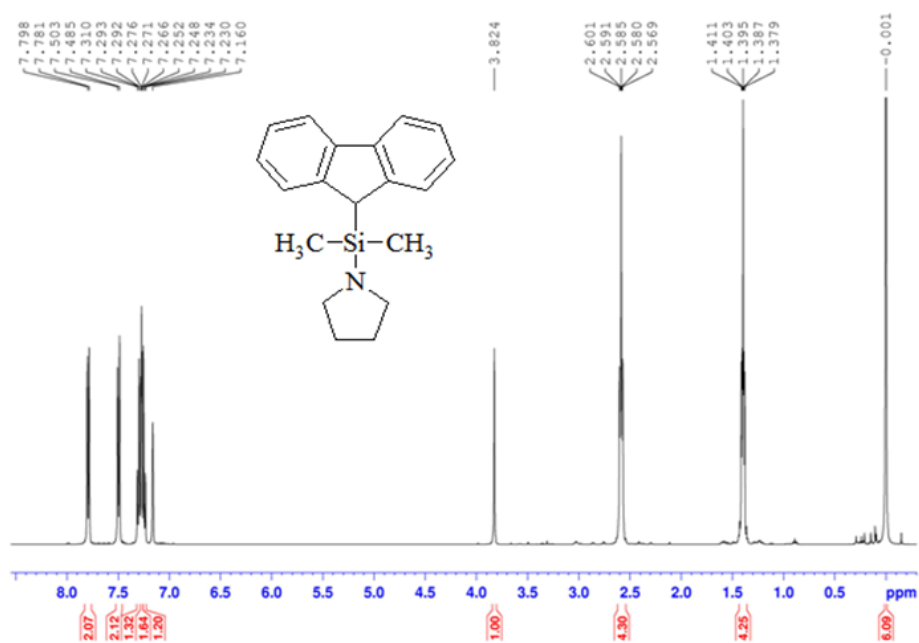


Fig. S15 ¹H NMR spectrum of C₁₃H₉SiMe₂NC₄H₈

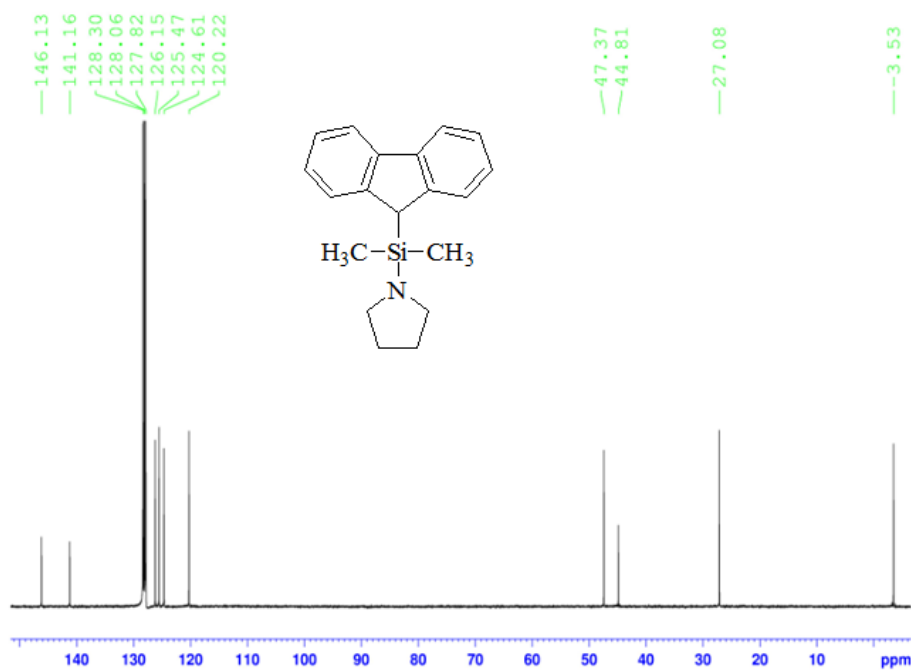


Fig. S16 ¹³C NMR spectrum of C₁₃H₉SiMe₂NC₄H₈

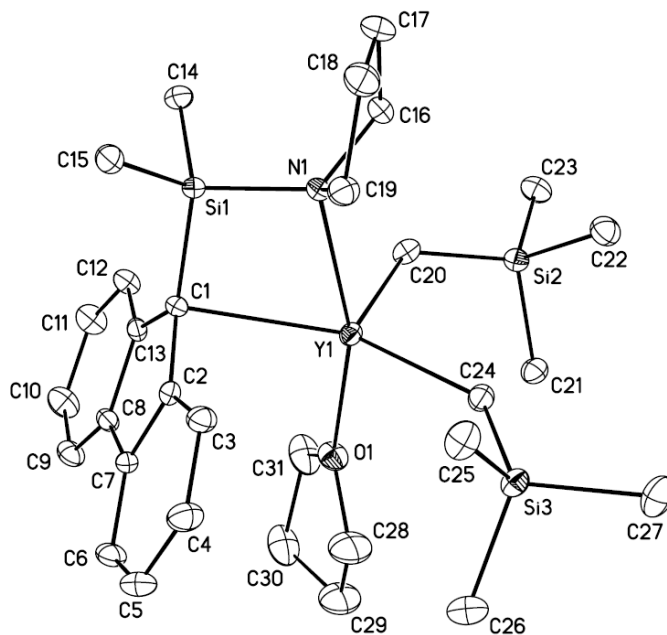


Fig. S17 Molecular structure of **5** with thermal ellipsoids at 20% probability. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and bond angles (°) for **5**: Y1-C1 = 2.564(3), Y1-C2 = 2.887(3), Y1-C20 = 2.386(3), Y1-C24 = 2.377(3), Y1-N1 = 2.525(2), Y1-O1 = 2.322(2), C24-Y1-C20 = 108.88(10), N1-Y1-C1 = 68.46 (8).

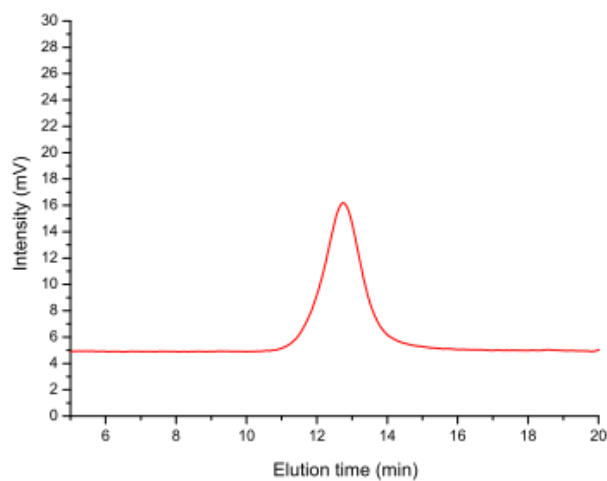


Fig. S18 GPC curve of the polymer sample

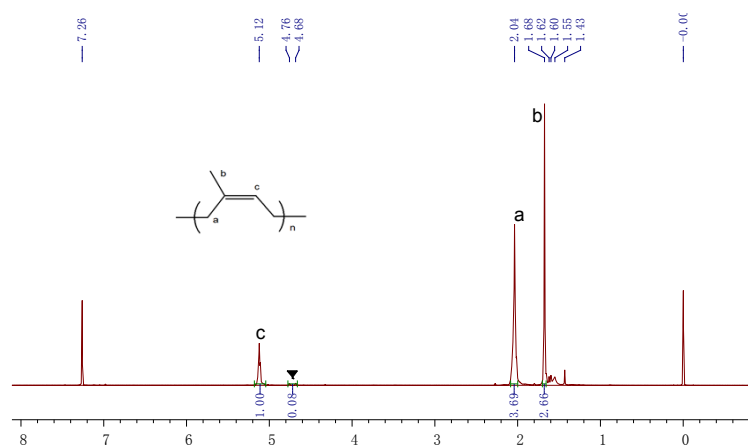


Fig. S19 ^1H NMR spectrum of the polymer sample

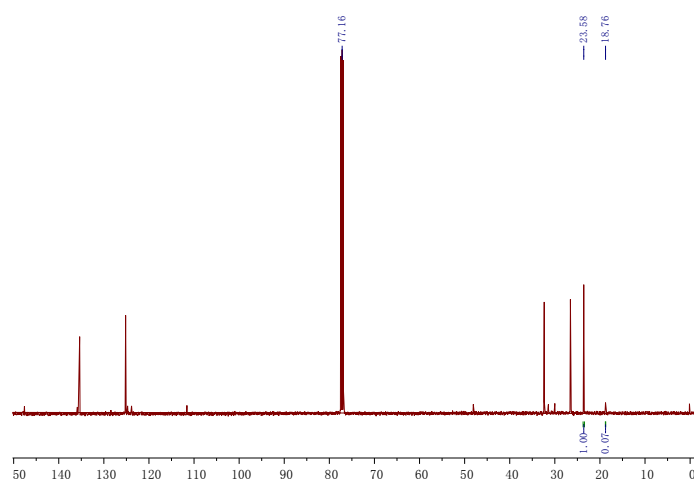


Fig. S20 ^{13}C NMR spectrum of the polymer sample