Supplementary Material (ESI) for Dalton Transactions

Supporting information

Highly trans-1,4 Selective (co-)Polymerization of Butadiene and Isoprene with Quinolyl Anilido Rare-earth Metal Bis(alkyl) Precursors

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Legends

sFigure 1. ^{1}H NMR spectrum of L^{1}Lu(CH_2SiMe_3)$_2$(THF) (**4**) (25 °C, C_6D_6).
sFigure 2. ^{13}C NMR spectrum of L^{1}Lu(CH_2SiMe_3)$_2$(THF) (**4**) (25 °C, C_6D_6).
sFigure 3. ^{1}H-^{1}H COSY spectrum of L^{1}Lu(CH_2SiMe_3)$_2$(THF) (**4**) (25 °C, C_6D_6).
sFigure 4. ^{1}H-^{13}C COSY spectrum of L^{1}Lu(CH_2SiMe_3)$_2$(THF) (**4**) (25 °C, C_6D_6).
sFigure 5. ORTEP drawing of complex **3** with 35% probability of thermal ellipsoids.
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sFigure 8. ^{13}C NMR spectra (400 MHz) of the resulting polymers.
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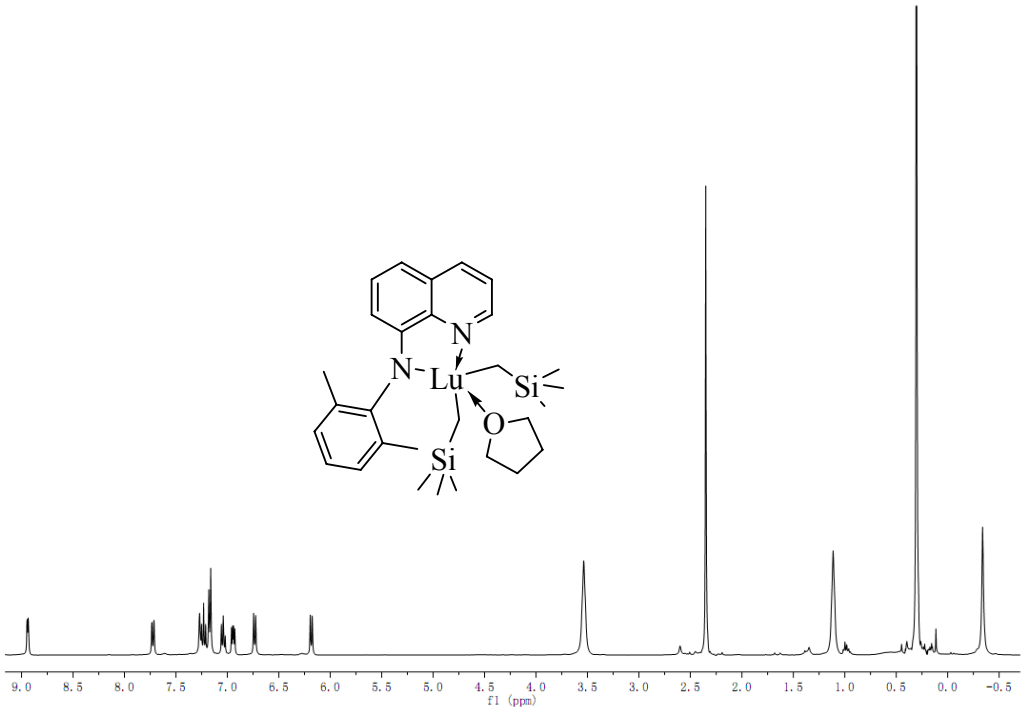
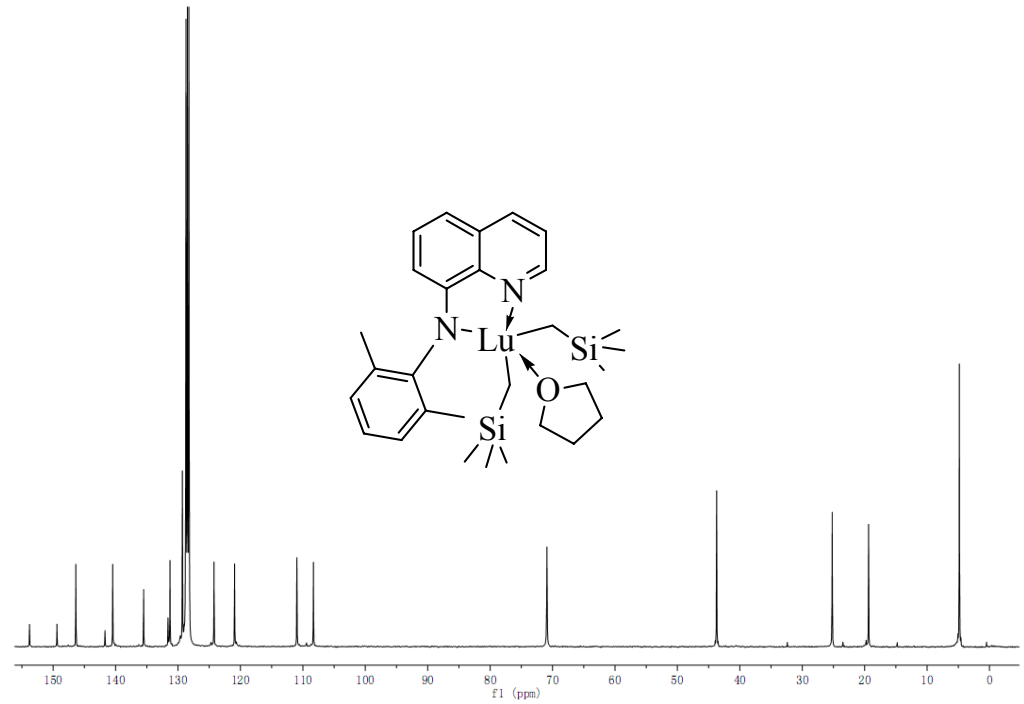
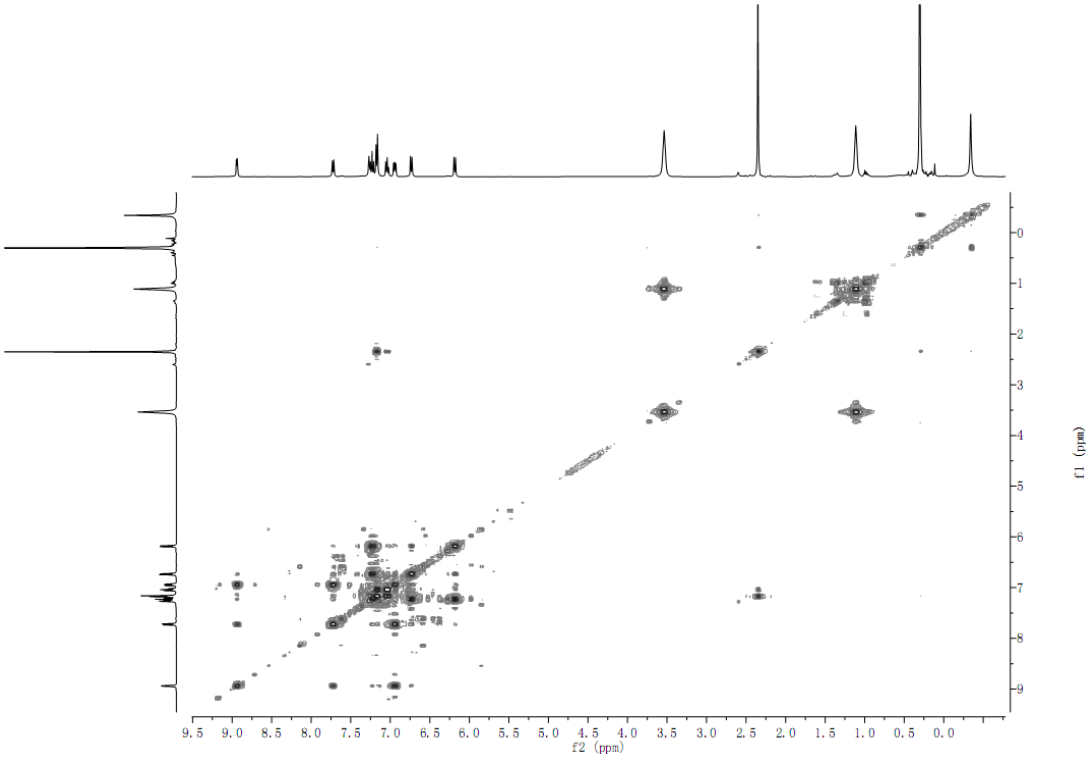
sFigure 10. A) ^{1}H NMR spectrum of complex **1** (25 °C, C_6D_6). **B)** ^{1}H NMR spectrum of complex **1** / $[PhNMe_2H][B(C_6F_5)_4]$ (25 °C, C_6D_6).
STable 1. Summary of Crystallographic Data for complexes **1, 2, 3, 5**



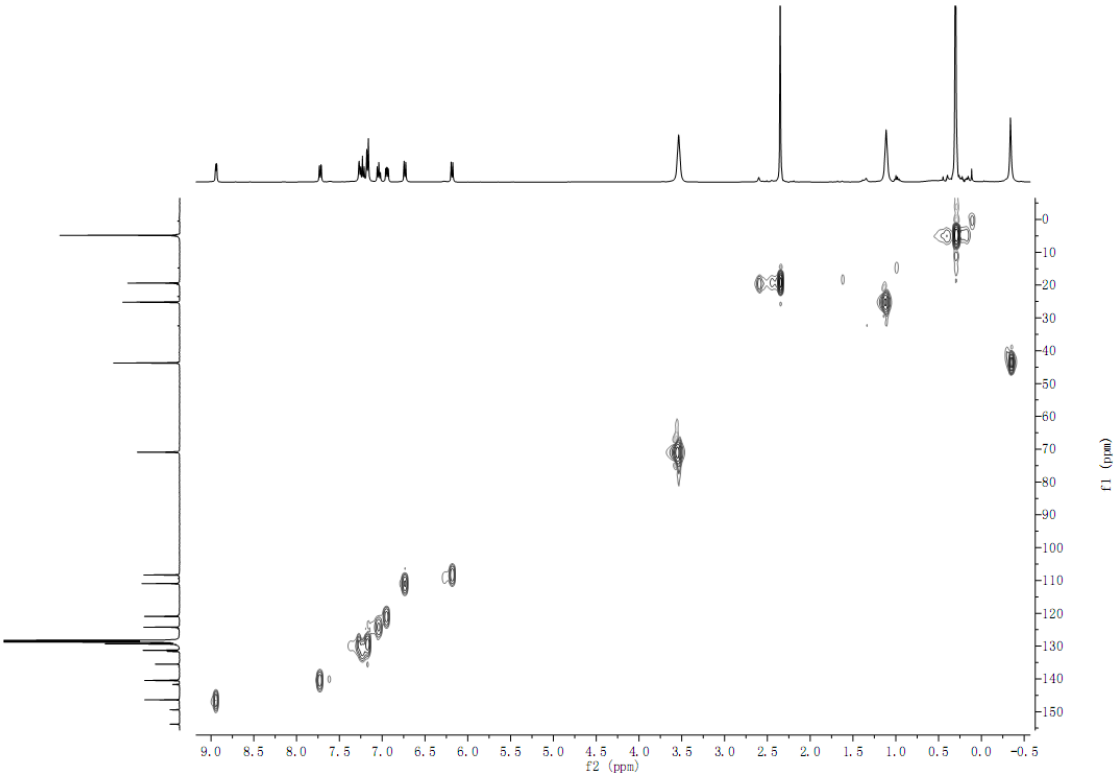
sFigure 1. ^{1}H NMR spectrum of L^{1}Lu(CH$_2$SiMe$_3$)$_2$(THF) (**4**) (25 °C, C$_6$D$_6$).



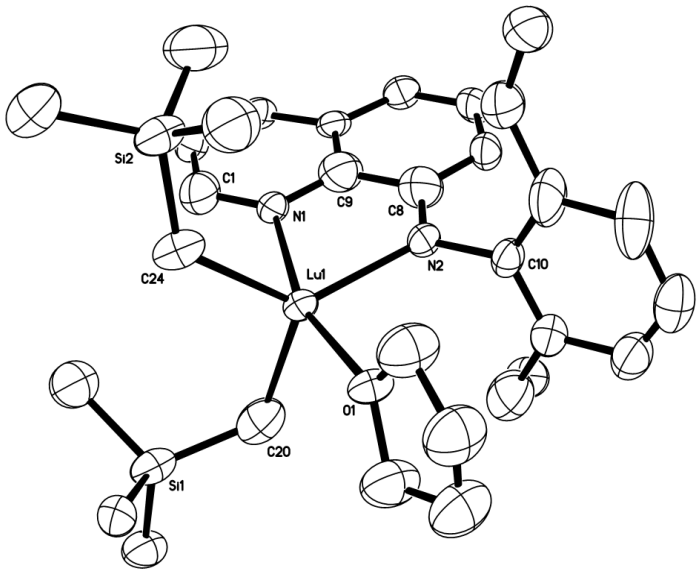
sFigure 2. ^{13}C NMR spectrum of L^{1}Lu(CH$_2$SiMe$_3$)$_2$(THF) (**4**) (25 °C, C$_6$D$_6$).



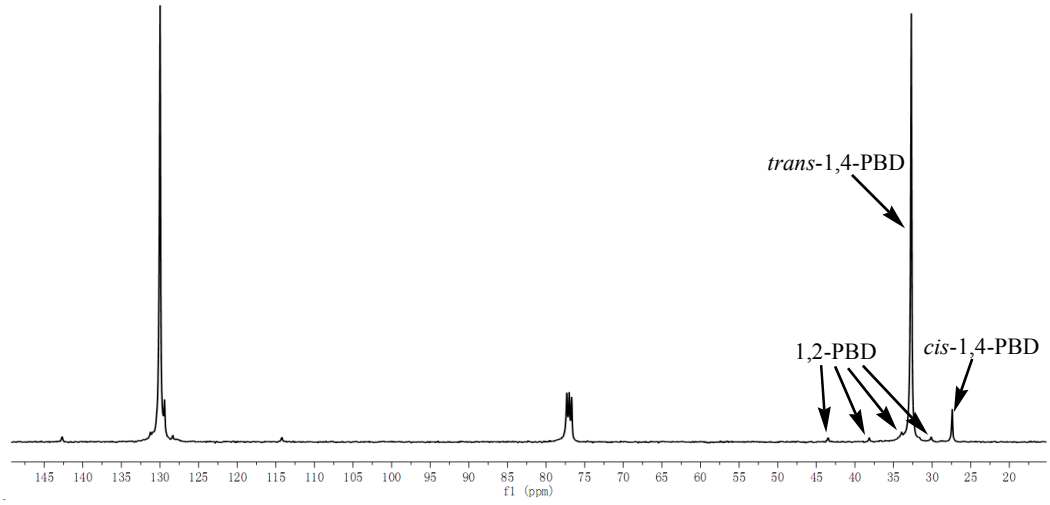
sFigure 3. ^{1}H-^{1}H COSY spectrum of L^{1}Lu(CH$_2$SiMe$_3$)$_2$(THF) (**4**) (25 °C, C$_6$D$_6$).



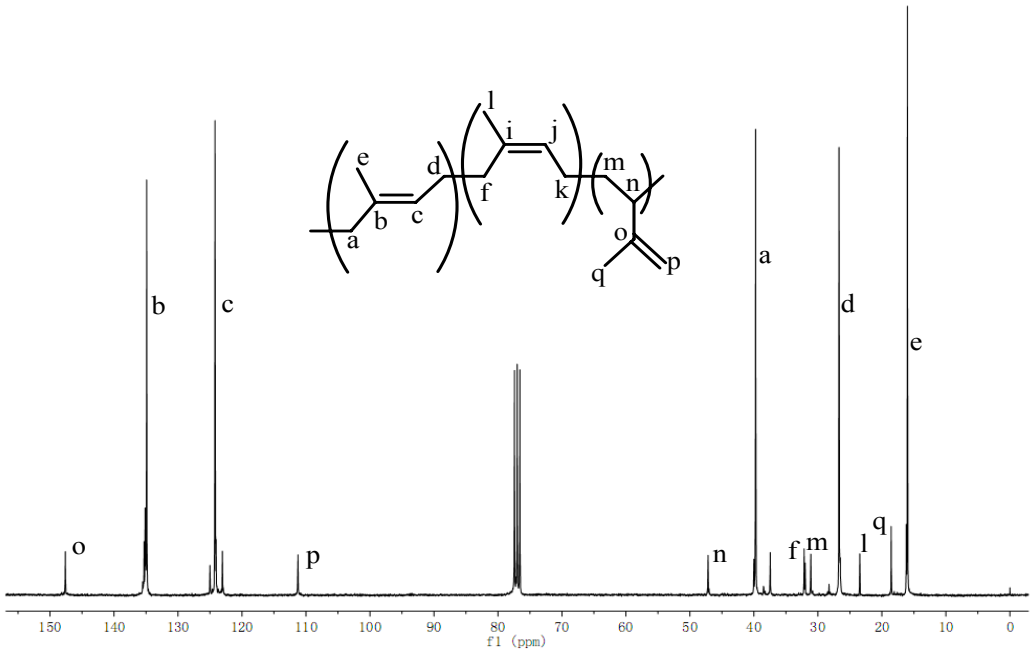
sFigure 4. ^{1}H-^{13}C COSY spectrum of L^{1}Lu(CH$_2$SiMe$_3$)$_2$(THF) (**4**) (25 °C, C$_6$D$_6$).



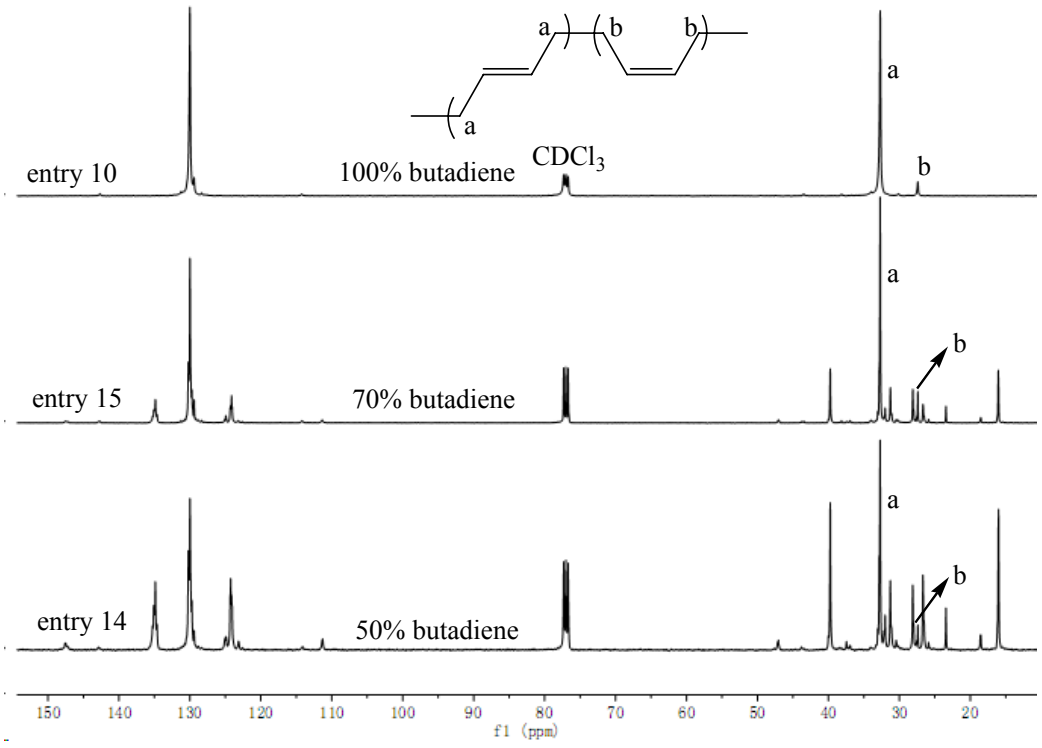
sFigure 5. ORTEP drawing of complex **3** with 35% probability of thermal ellipsoids. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (deg): Lu(1)–N(1) = 2.394(7), Lu(1)–N(2) = 2.260(8), Lu(1)–O(1) = 2.294(6), Lu(1)–C(20) = 2.327(14), Lu(1)–C(24) = 2.329(11), N(1)–C(9) = 1.367(16), N(2)–C(8) = 1.378(15), N(2)–C(10) = 1.431(11), O(1)–Lu(1)–N(1) = 163.1(2), C(20)–Lu(1)–C(24) = 111.6(5), N(2)–Lu(1)–N(1) = 70.3(2).



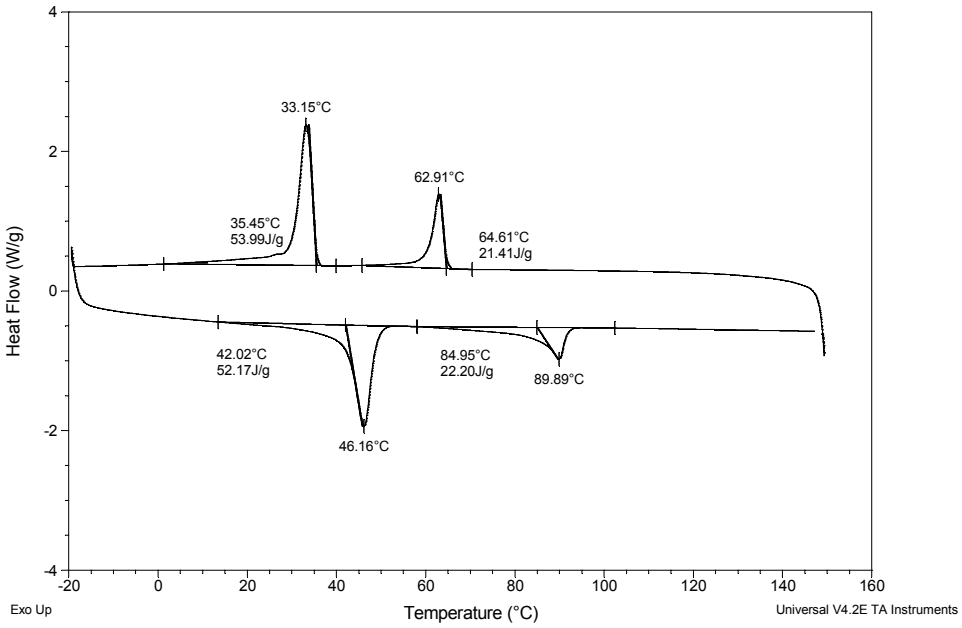
sFigure 6. ^{13}CNMR spectrum of polybutadiene prepared by use of **1** / $AlMe_3$ / $[Ph_3C][B(C_6F_5)_4]$ at 25 °C in toluene (91% *trans*-1,4) (Table 1, entry 3).



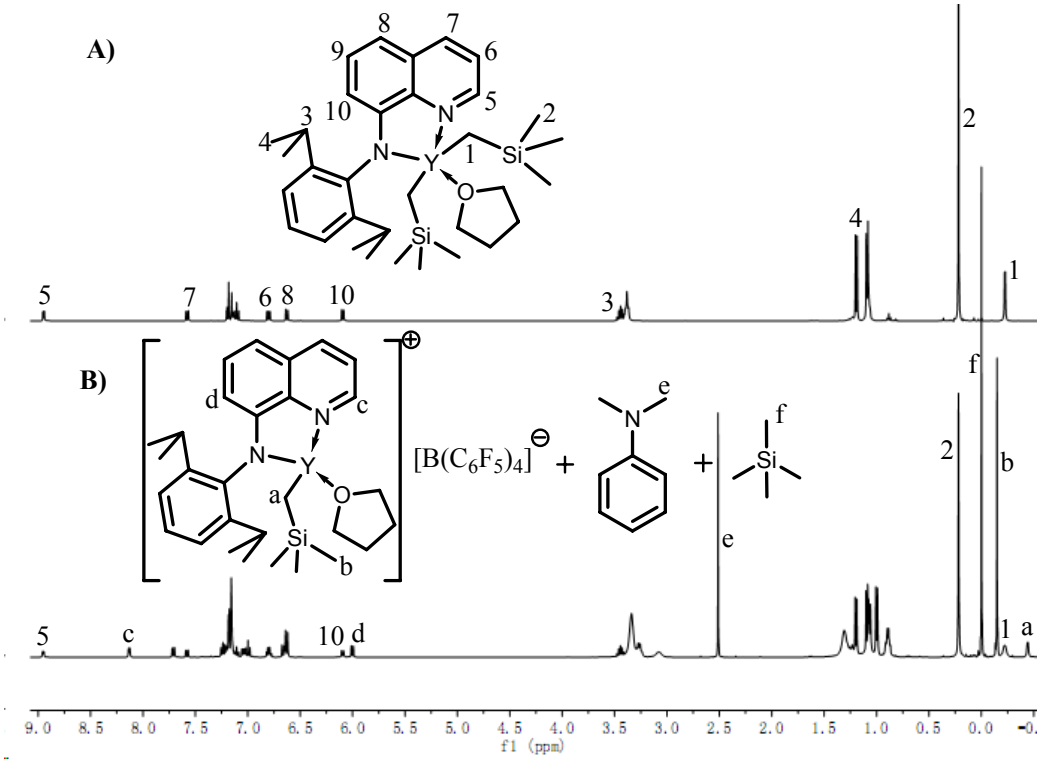
sFigure 7. ^{13}CNMR spectrum of polyisoprene prepared by use of **1** / $AlMe_3$ / $[Ph_3C][B(C_6F_5)_4]$ at 25 °C in toluene (87% *trans*-1,4) (Table 2, entry 11).



sFigure 8. ^{13}C NMR spectra (400 MHz) of the resulting polymers.



sFigure 9. DSC curve of polybutadiene prepared by use of **1** / $AlMe_3$ / $[Ph_3C][B(C_6F_5)_4]$ at 25 °C in toluene (91% *trans*-1,4) (Table 1, entry 3).



sFigure 10. A) ^{1}H NMR spectrum of complex **1** (25 °C, C_6D_6). **B)** ^{1}H NMR spectrum of complex **1** / $[PhNMe_2H][B(C_6F_5)_4]$ (25 °C, C_6D_6).

sTable 1. Summary of Crystallographic Data for 1, 2, 3, 5

Compound reference	**1**	**2**	**3**	**5**
Chemical formula	$C_{33}H_{53}YN_2OSi_2$	$C_{33}H_{53}LuN_2OSi_2$	$C_{31}H_{49}LuN_2OSi_2$	$C_{50}H_{65}NdN_4OSi$
Formula Mass	638.86	724.92	696.87	910.39
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
a/Å	11.4555(12)	11.3890(5)	9.7731(5)	11.0181(6)
b/Å	16.8260(18)	16.7980(8)	17.2591(9)	11.6008(7)
c/Å	18.987(2)	18.8840(9)	20.0423(10)	18.1909(10)
α/°	90.00	90.00	90.00	89.2590(10)
β/°	99.752(2)	99.7520(10)	90.2090(10)	89.7830(10)
γ/°	90.00	90.00	90.00	84.4310(10)
Unit cell volume/Å^3	3607.0(7)	3560.5(3)	3380.6(3)	2314.0(2)
Space group	*P2(1)/c*	*P2(1)/c*	*P2(1)/n*	*P-1*
No. of formula units per unit cell, *Z*	4	4	4	2
No. of reflections measured	19968	19474	18709	12109
No. of independent reflections	7105	7004	6643	8032
R_{int}	0.0621	0.0404	0.0271	0.0213
Final R_1 values ($I > 2\sigma(I)$)	0.0686	0.0356	0.0666	0.0385
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1655	0.0770	0.1738	0.0854
Final R_1 values (all data)	0.1159	0.0547	0.0810	0.0482
Final $wR(F^2)$ values (all data)	0.1898	0.0852	0.1865	0.0901
Goodness of fit on F^2	1.033	1.008	1.040	1.046