

Supplementary Information

Rare-earth metal alkyl complexes bearing alkoxy N-heterocyclic carbene ligand: synthesis, characterization, catalysis for isoprene polymerization

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Table S1. Summary of crystallographic data and refinement for complexes **3a**, **3b**, **4a**, **4b**, **5**

Complexes	3a	3b	4a	4b	5
Formula	C ₃₆ H ₇₈ N ₄ O ₂ Sc ₂	C ₃₆ H ₇₈ N ₄ O ₂ Lu ₂	C ₄₀ H ₈₆ N ₄ O ₂ Y ₂	C ₄₀ H ₈₆ N ₄ O ₂ Lu ₂	C ₄₈ H ₉₀ N ₄ O ₂ Y ₂
	Si ₄	Si ₄	Si ₄	Si ₄	Si ₄
Formula weight	801.3	1061.32	945.3	1117.43	1045.42
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P2(1)/c	P2(1)/c	Cc	P2(1)/c	P2(1)/c
a (Å)	11.3570(7)	11.5311(7)	25.040(3)	11.5419(7)	13.3583(13)
b (Å)	11.8214(7)	11.8604(7)	10.6891(10)	17.7219(10)	14.9883(15)
c (Å)	19.0167(12)	19.0343(12)	20.951(2)	14.0192(8)	14.5687(15)
α (deg)	90	90	90	90	90
β (deg)	106.5510(10)	106.1820(10)	103.216(2)	106.3130(10)	91.521(2)
γ (deg)	90	90	90	90	90
V (Å ³)	2447.3(3)	2500.1(3)	5459.0(9)	2752.1(3)	2915.9(5)
Z	4	4	8	4	4
D _{calcd} (g/cm ³)	1.087	1.410	1.150	1.348	1.191
radiation (λ), Å	0.71073	0.71073	0.71073	0.71073	0.71073
μ (mm ⁻¹)	0.406	4.052	2.235	3.684	2.098
F(000)	872	1072	2016	1136	1112
θ range, (°)	1.87–26.04	1.84–25.99	1.67–26.05	1.90–25.00	1.95–26.01
no. of reflns colled	13465	13695	14999	9342	16164
no. of reflns unique	4811	4906	8697	3424	5696
R _{int}	0.0177	0.0163	0.0565	0.0367	0.0888
S	1.051	1.053	0.945	1.351	0.958
R	0.0361	0.0167	0.0552	0.0592	0.0553
R _w	0.0954	0.0430	0.0926	0.1322	0.0908
R (all data)	0.0414	0.0180	0.0946	0.0622	0.1091

<i>Rw</i> (all data)	0.0997	0.0438	0.1045	0.1331	0.1068
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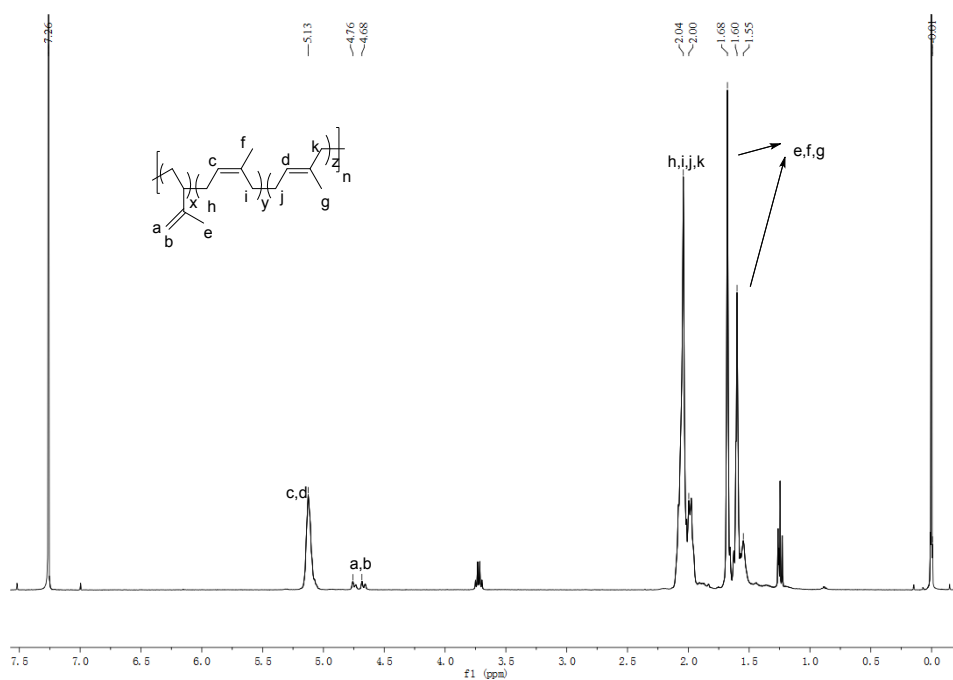


Figure S1. ^1H NMR spectrum of Polyisoprene (Table 1, entry 2)

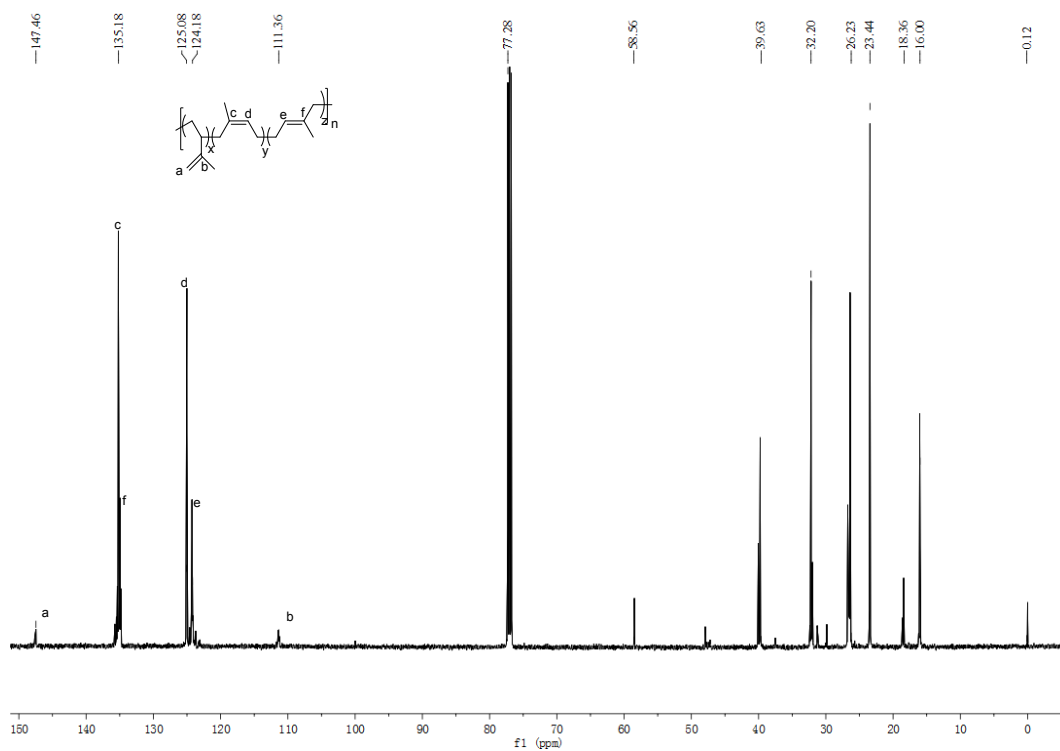


Figure S2. ^{13}C NMR spectrum of Polyisoprene (Table 1, entry 2)

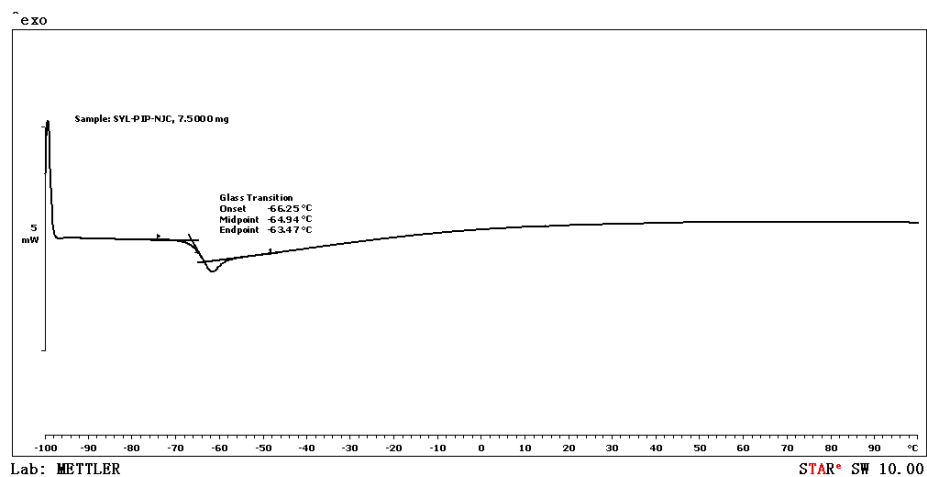


Figure S3 DSC thermograms of Polyisoprene (Table 1, entry 2)