Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
This journal is © The Royal Society of Chemistry 2017

Electronic Supplementary Information for

Efficient chromium-based catalysts for ethylene tri-/tetramerization switched by silicon-bridged/N, P-based ancillary ligands: A structural, catalytic and DFT study

Le Zhang[a, b], *Wei Wei*[a], *Fakhre Alam*[a], *Yanhui Chen*[a], *Tao Jiang*[a, *]

[a]College of Chemical Engineering and Material Science, Tianjin University of Science and Technology, Tianjin 300457, China

[b] Handan Key Laboratory of Organic small molecule materials, Handan University, Handan 056005, China

*E-mail: jiangtao@tust.edu.cn

Table S1. The data of molecular orbital energies for analysis.

Entry	Cyclic intermediates	Energies of LUMO+1 (kcal/mol)	Energy gaps (kcal/mol)
1	**C1a**	-99.05	68.78
2	**C2b**	-94.31	73.51

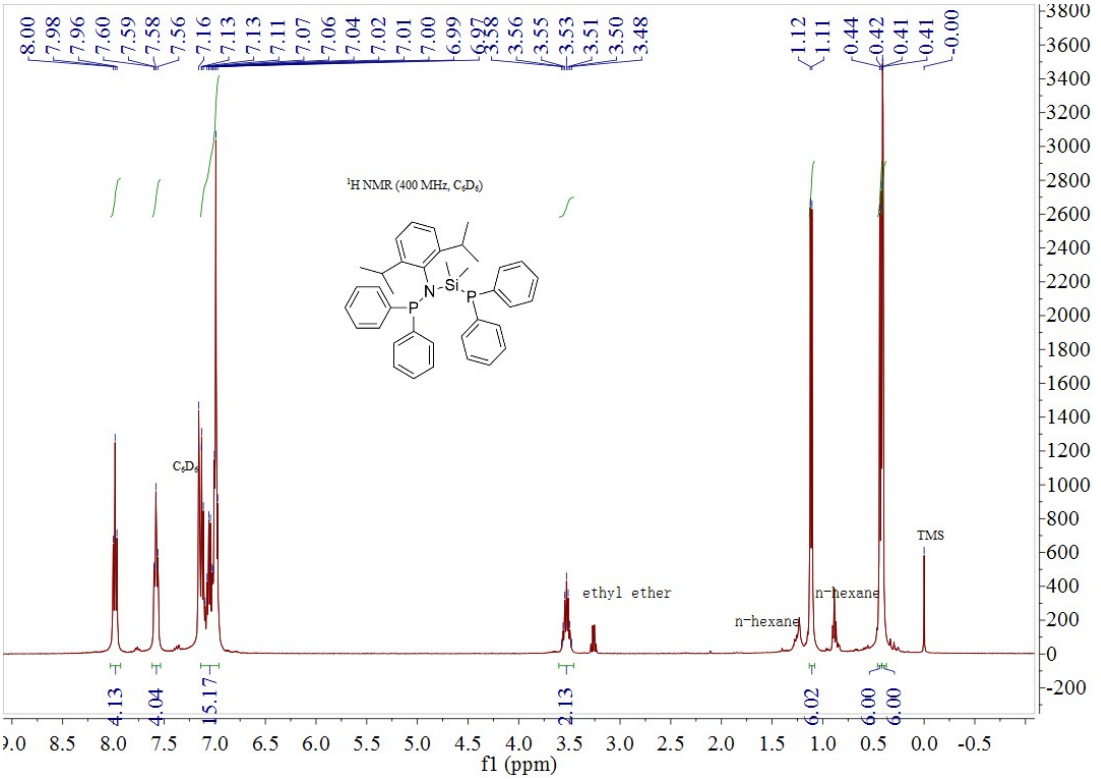

Figure S1. ^{1}H NMR spectrum of **L1** (400MHz, C_6D_6)

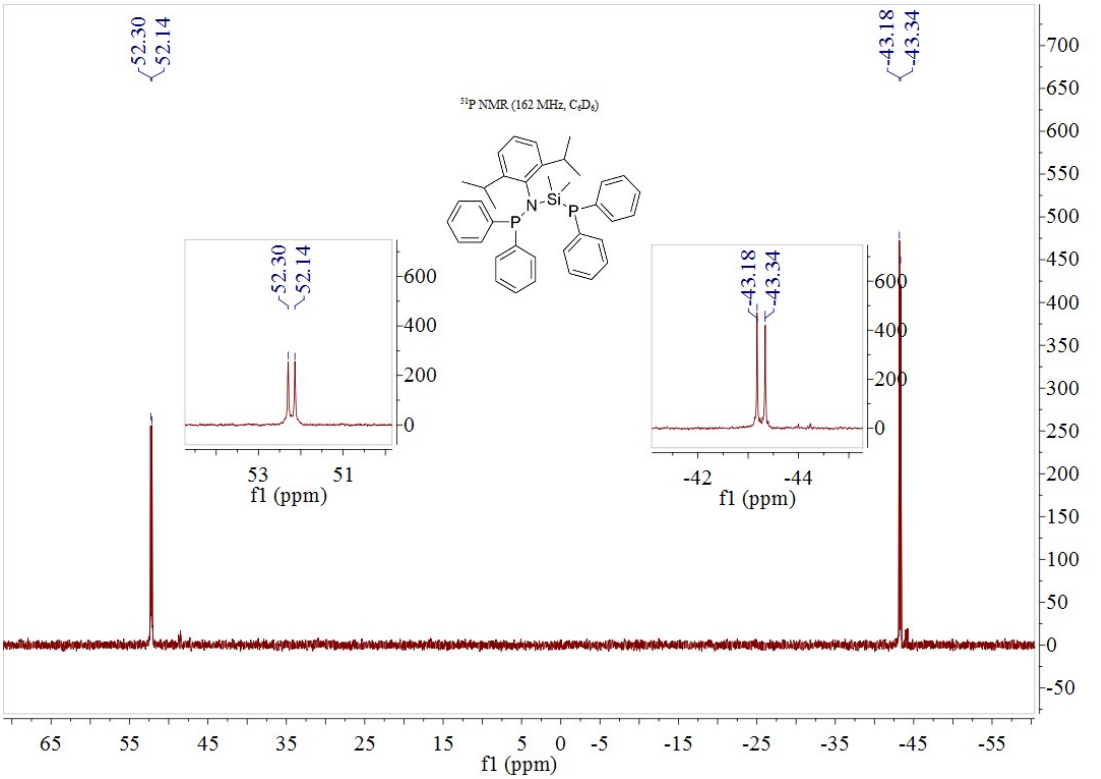

Figure S2. ^{31}P NMR spectrum of **L1** (162MHz, C_6D_6)

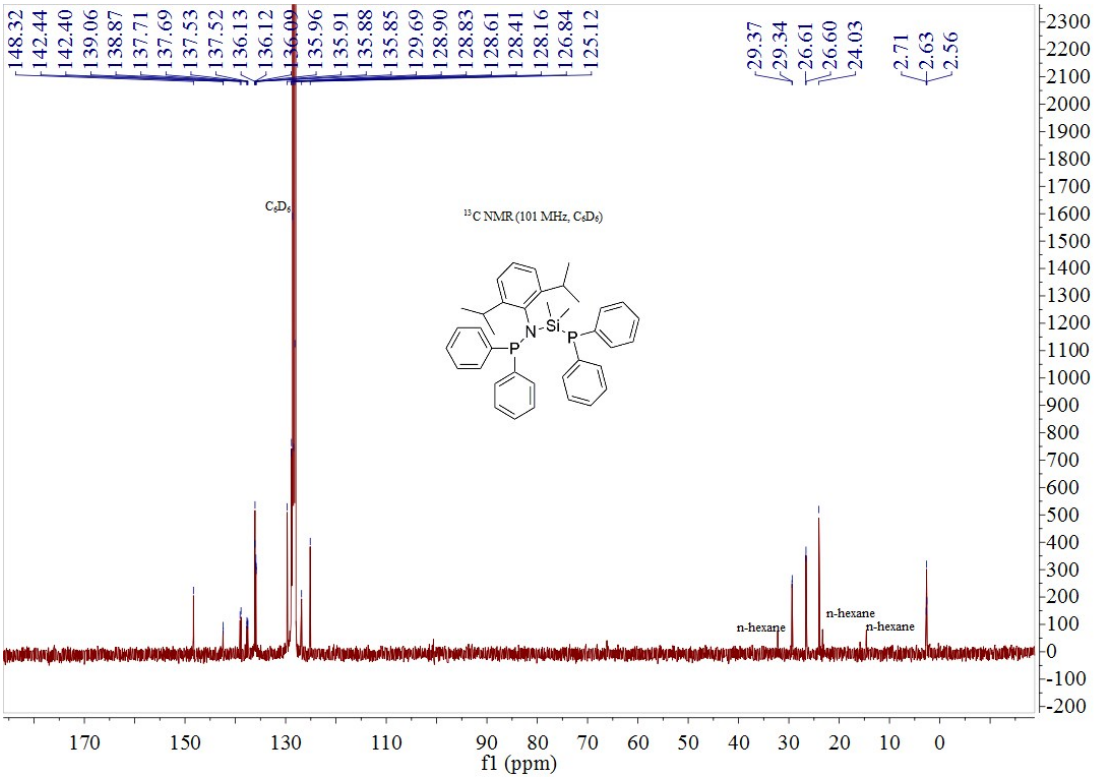

Figure S3. ^{13}C NMR spectrum of **L1** (101MHz, C_6D_6)

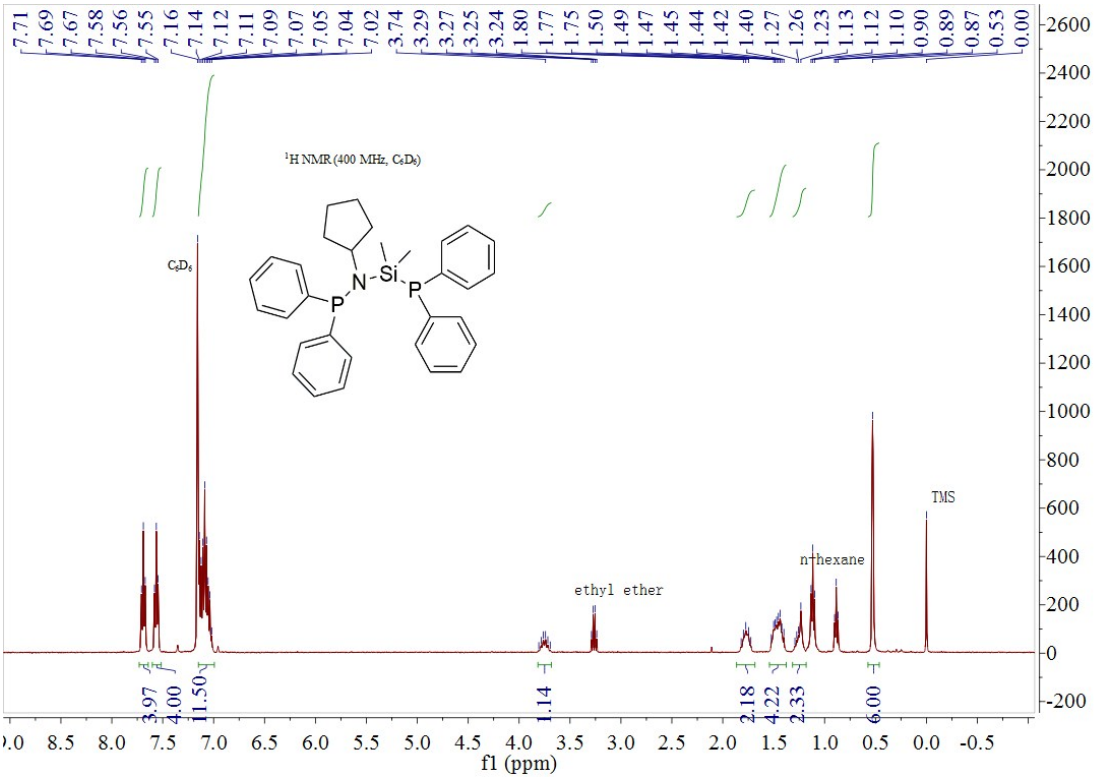

Figure S4. ^{1}H NMR spectrum of **L2** (400MHz, C_6D_6)

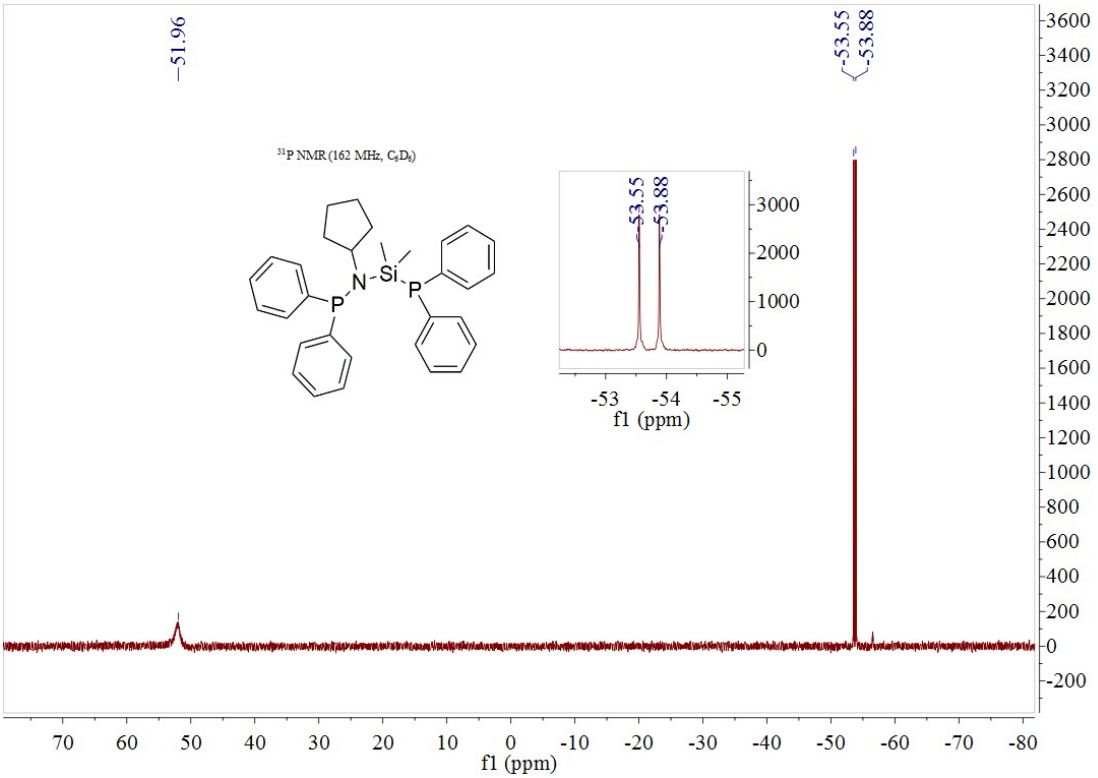

Figure S5. ^{31}P NMR spectrum of **L2** (162MHz, C_6D_6)

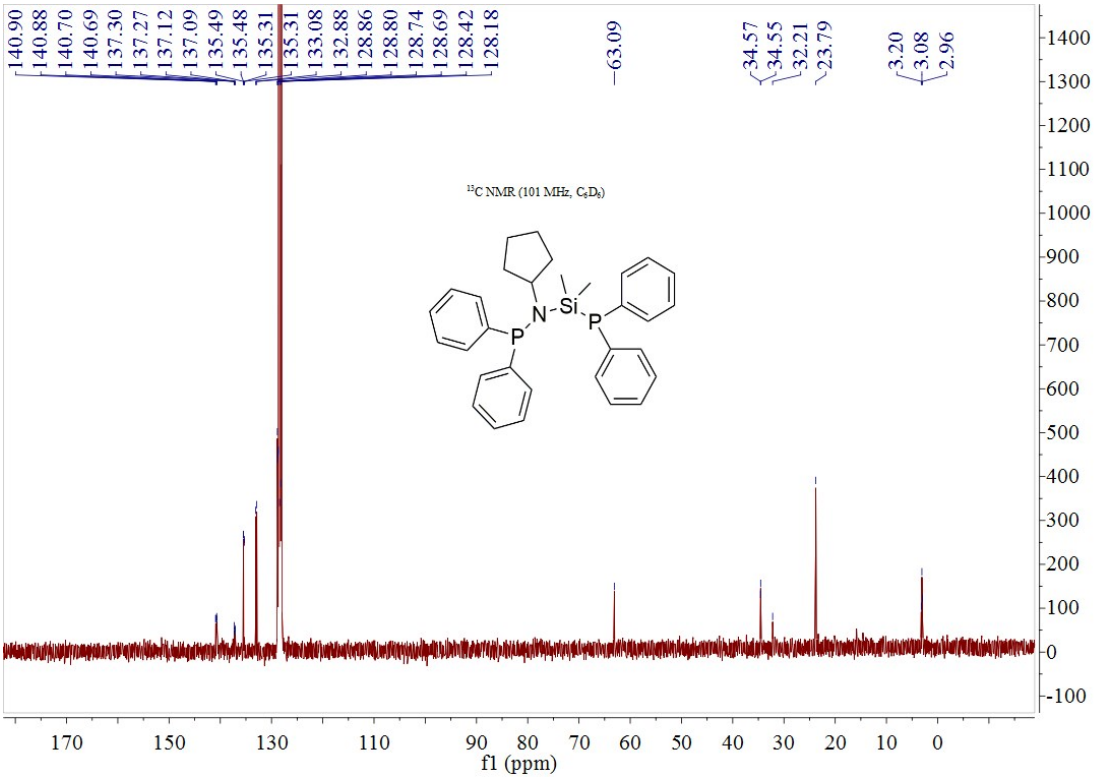

Figure S6. ^{13}C NMR spectrum of **L2** (101MHz, C_6D_6)

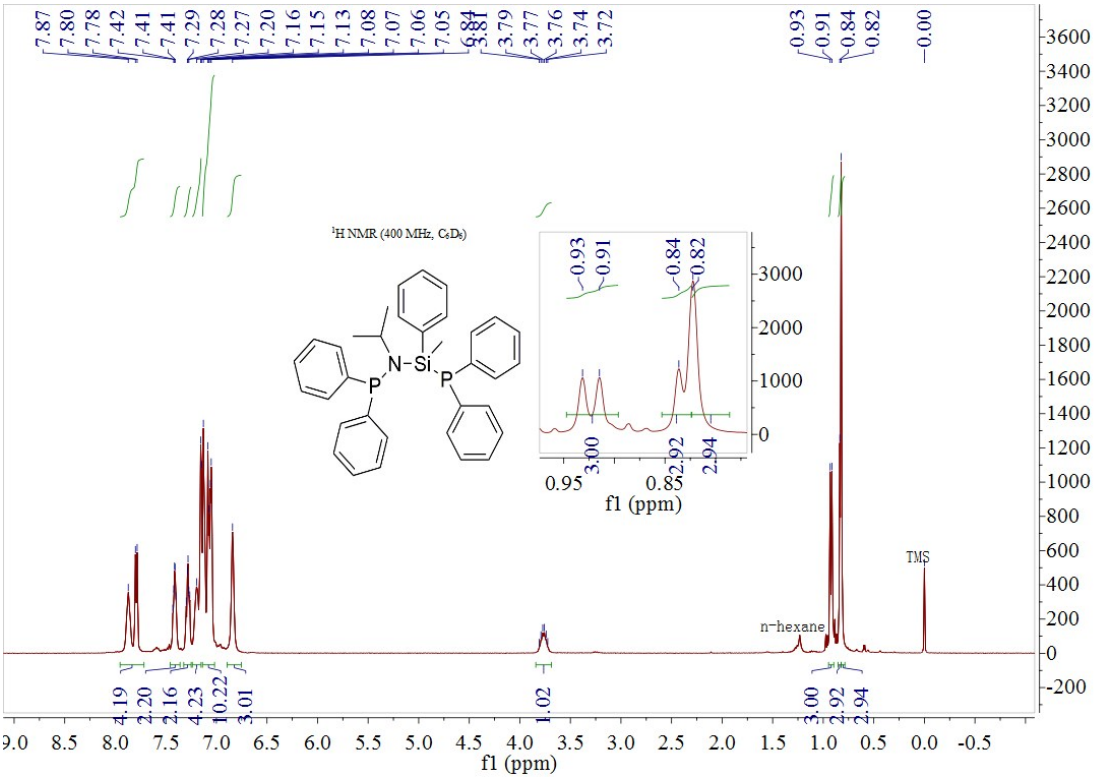

Figure S7. ^{1}H NMR spectrum of **L3** (400MHz, C_6D_6)

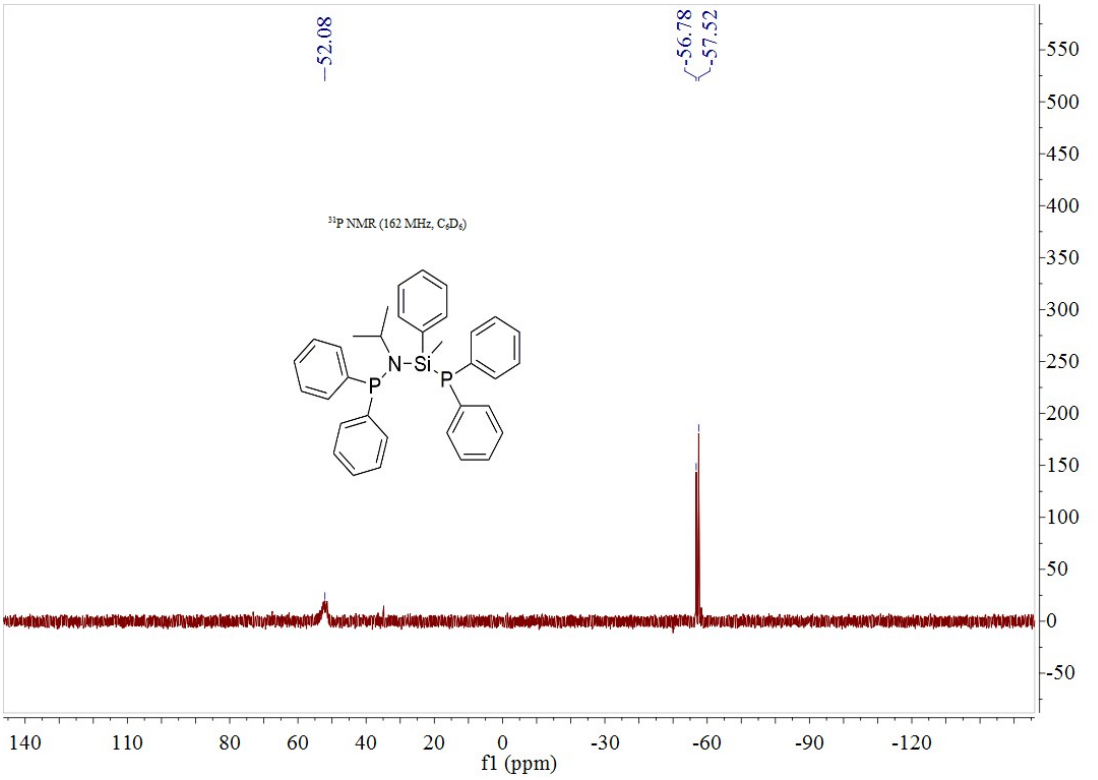

Figure S8. ^{31}P NMR spectrum of **L3** (162MHz, C_6D_6)

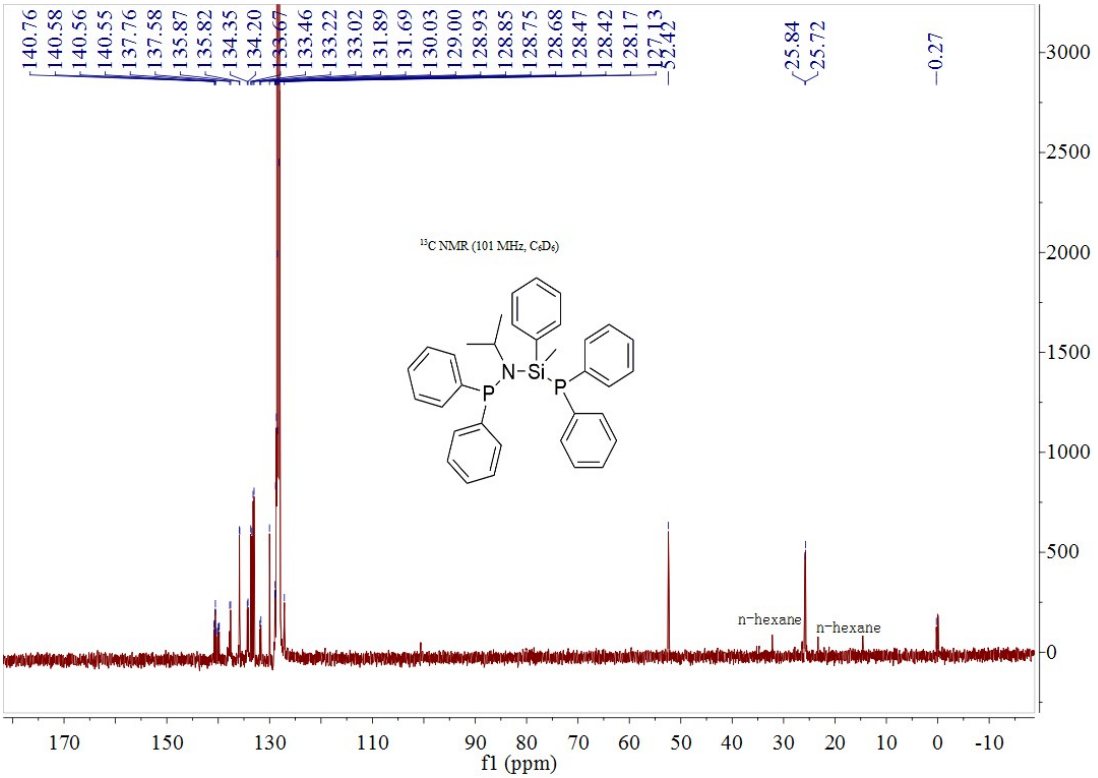

Figure S9. ^{13}C NMR spectrum of **L3** (101MHz, C_6D_6)

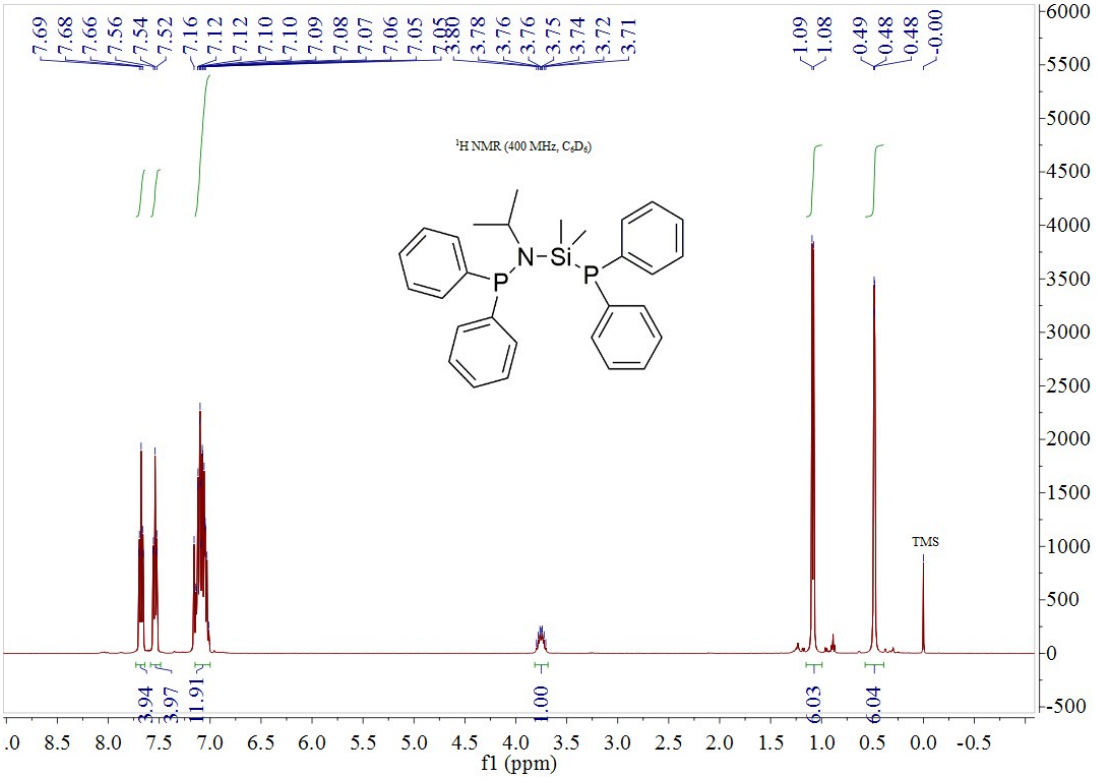

Figure S10. ^{1}H NMR spectrum of **L4** (400MHz, C_6D_6)

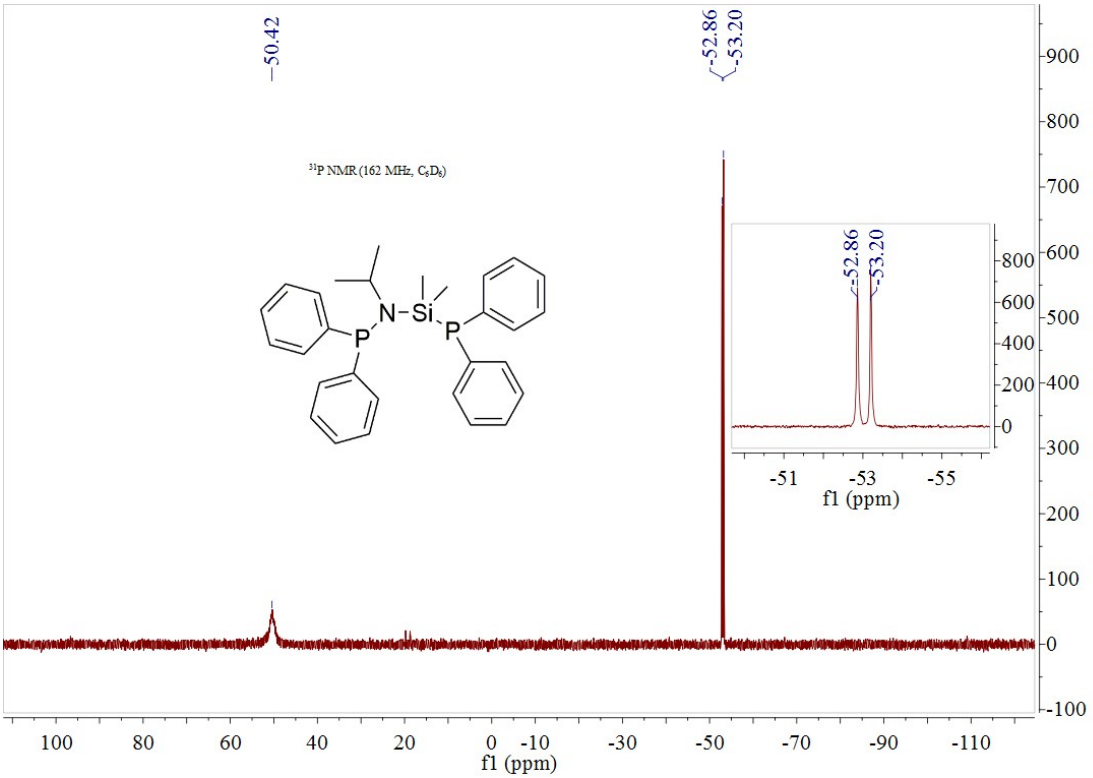

Figure S11. ^{31}P NMR spectrum of **L4** (162MHz, C_6D_6)

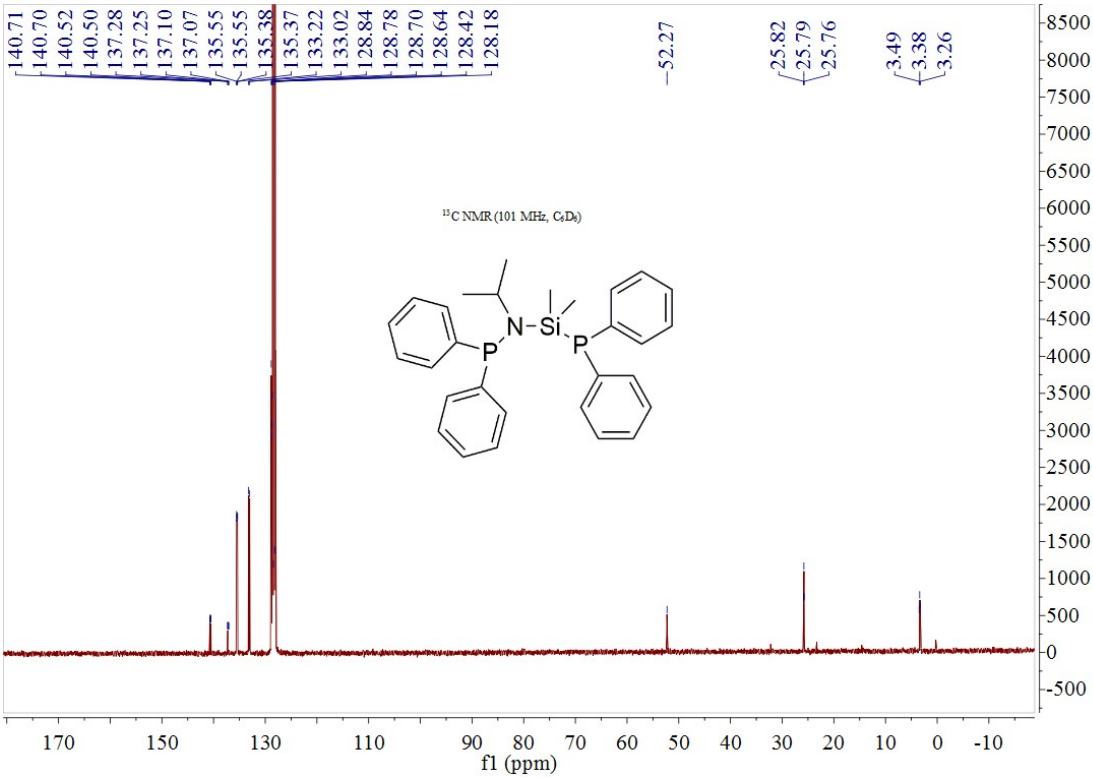

Figure S12. ^{13}C NMR spectrum of **L4** (101MHz, C_6D_6)

Table S1. Absolute energies in hartrees of the intermediates

	Intermediates					
	C1a	C1b	C1c	C2a	C2b	C2c
Absolute energies (hartrees)	-2744.33438	-2822.96657	-2901.58220	-2472.75898	-2551.42484	-2630.01498