

Electronic supplementary information

AN ORGANOMETALLIC APPROACH TO THE SYNTHESIS OF CATIONIC YTTRIUM BIS(ALKOXIDE) COMPLEXES

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Table S1. Crystal data and structure refinement parameters for complex **1**

	1
Empirical formula	C ₆₆ H ₅₄ BF ₂₀ O ₆ Y
Formula Weight	1422.81 g/mol
<i>T</i> , K	120
Crystal System	Monoclinic
Space Group	P2(1)/c
Unit Cell Dimensions	a = 20.9777(10)Å α = 90° b = 12.5628(6)Å β = 106.2510(10)° c = 26.2618(13)Å γ = 90°
<i>V</i> , Å ³	6644.5(6)
<i>Z</i>	4
<i>d</i> _{calc} , Mg/m ³	1.422
μ, mm ⁻¹	1.858
<i>F</i> ₀₀₀	2888
Crystal Size, mm	0.30x0.25x0.25
θ Range for Data Collection, °	1.011-27.000
Index Ranges	-26 ≤ h ≤ 26, -16 ≤ k ≤ 16, -33 ≤ l ≤ 33
Refl. Collected	14493
Independent Refl. (<i>R</i> _{int})	9337
Completeness to θ, %	99.3
Data / Restraints / Parameters	10290 / 90 / 511
<i>GOF</i> on <i>F</i> ²	0.982
Final <i>R</i> Indices (<i>I</i> > 2σ(<i>I</i>))	<i>R</i> ₁ = 0.0454, w <i>R</i> ₂ = 0.1025
<i>R</i> Indices (all data)	<i>R</i> ₁ = 0.0835, w <i>R</i> ₂ = 0.1131
Largest Diff Peak and Hole, e/Å ³	1.966 and -0.801

Table S2. SHAPE analysis for complex **1**

	HP	PPY	OC	TPR	JPPY
1	32.422	27.747	0.537	15.643	31.087

HP: Hexagon
 PPY: Pentagonal pyramid
 OC: Octahedron
 TPR: Trigonal prism
 JPPY: Johnson pentagonal pyramid (J2)

Figure S1. ^1H NMR spectrum (400 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^1OH

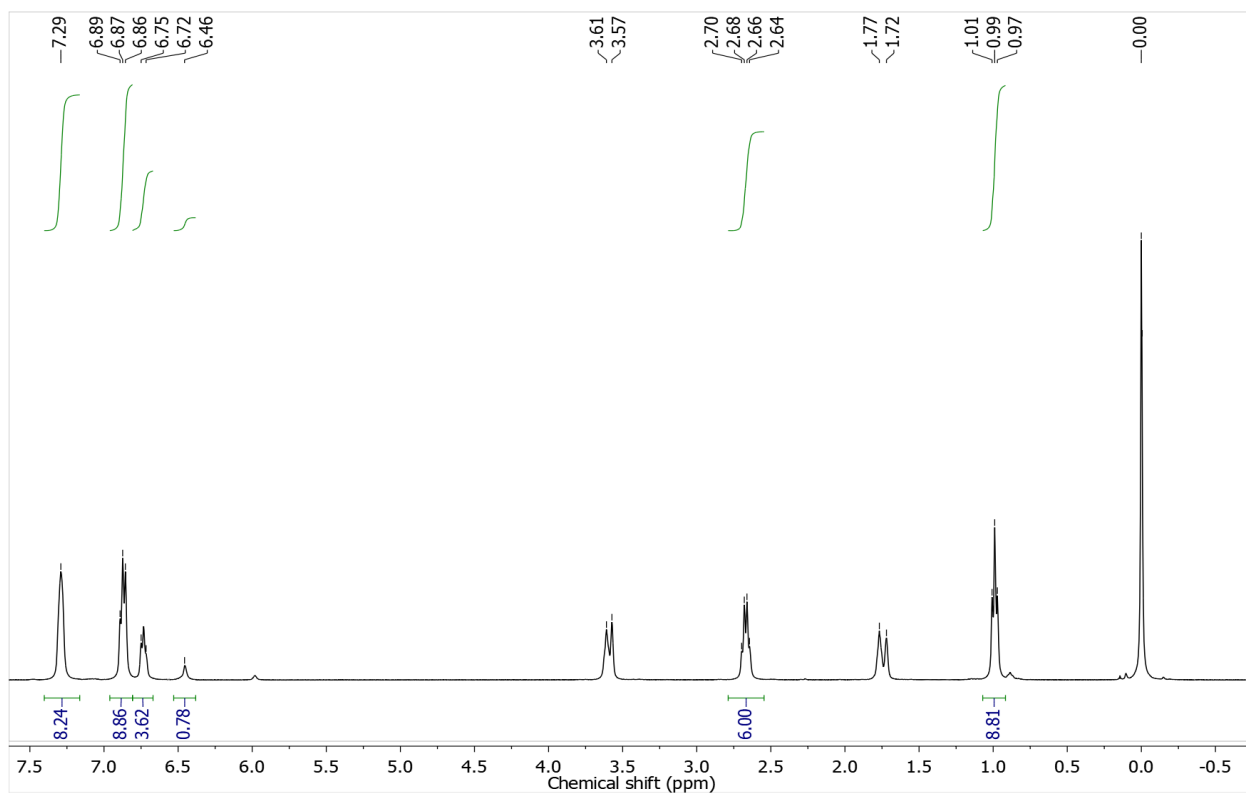


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^1OH

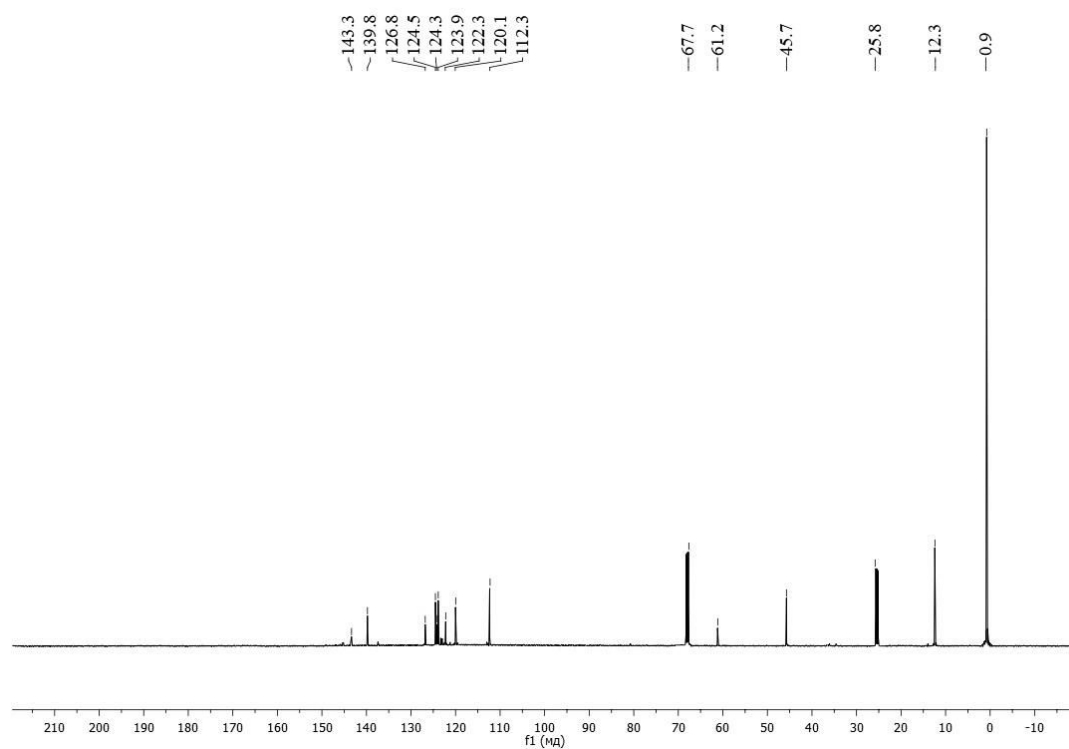


Figure S3. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^1OH

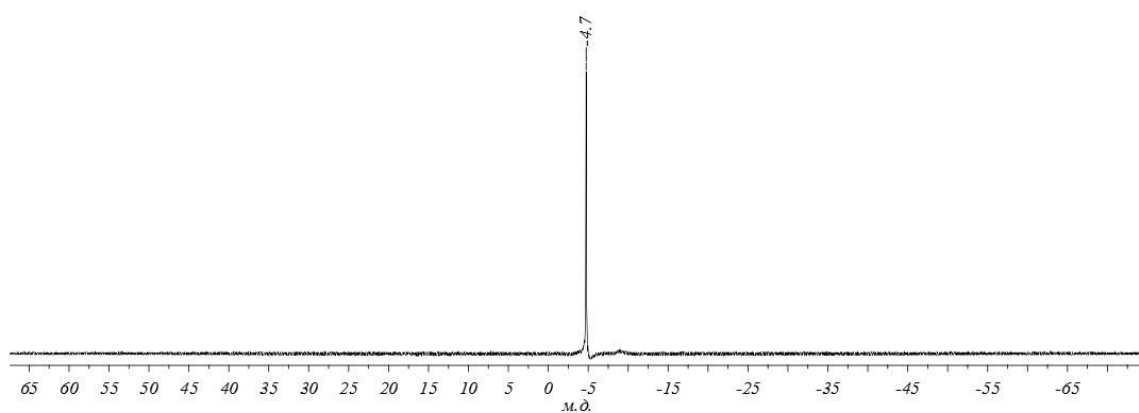


Figure S4. ^{19}F NMR spectrum (376 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^1OH

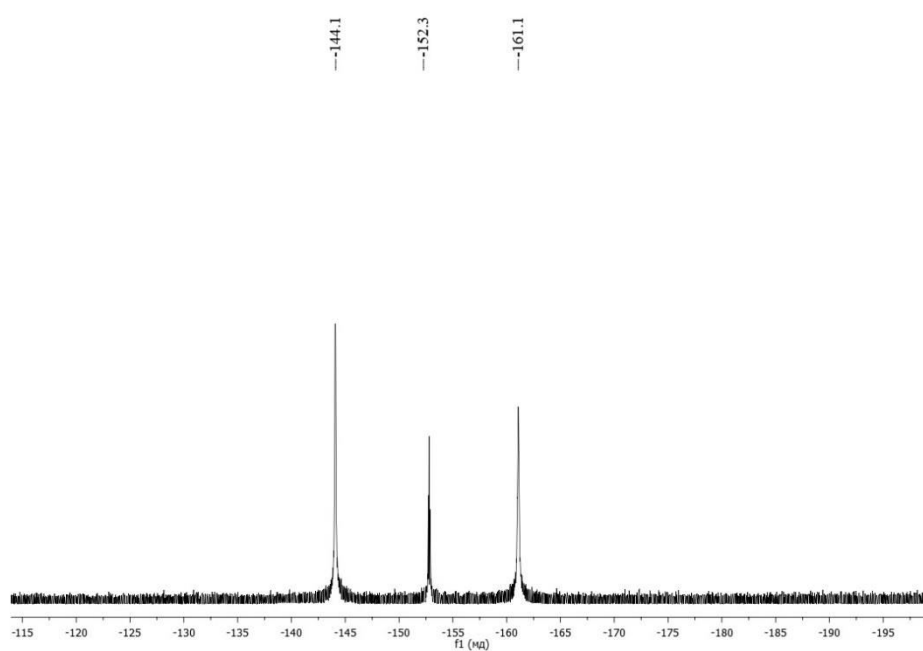


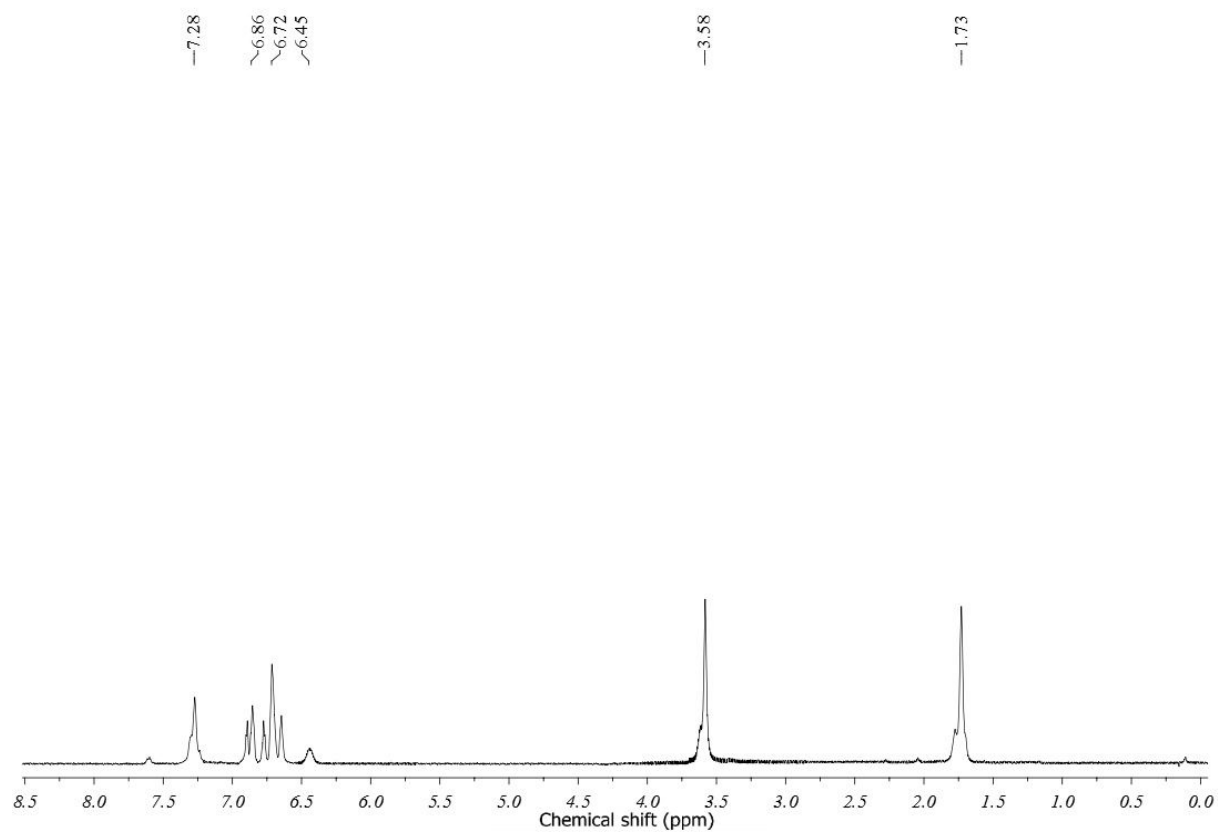
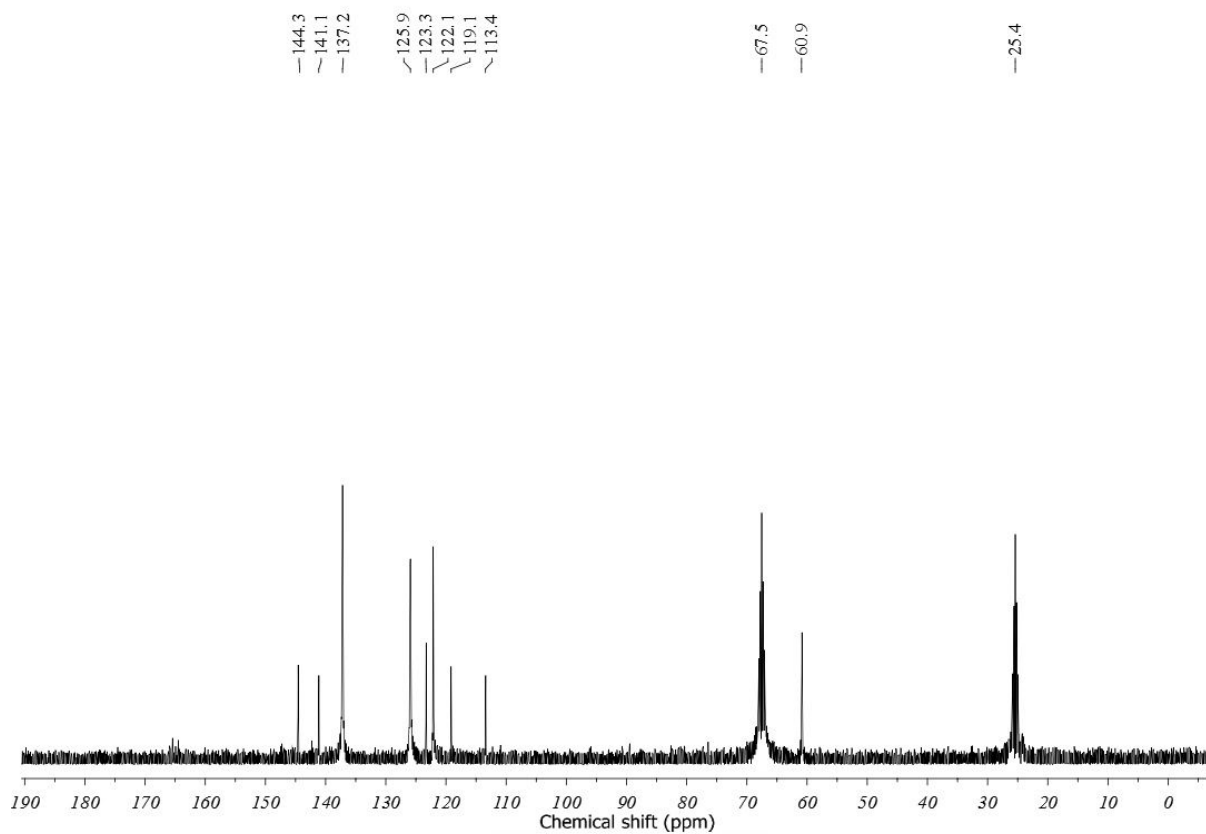
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Figure S7. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128 MHz, THF- d_8 , 293K) of complex **1**

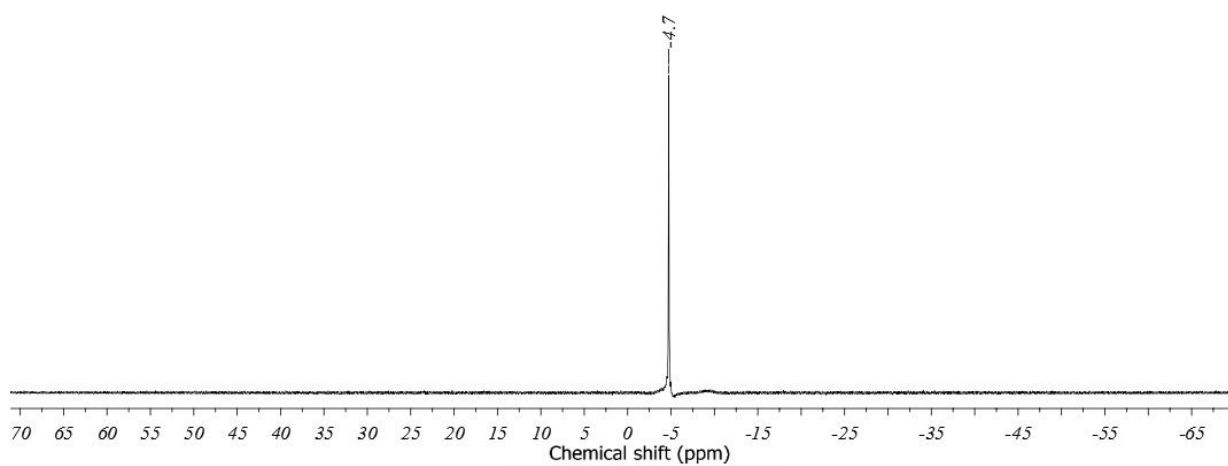


Figure S8. ^{19}F NMR spectrum (376 MHz, THF- d_8 , 293K) of complex **1**

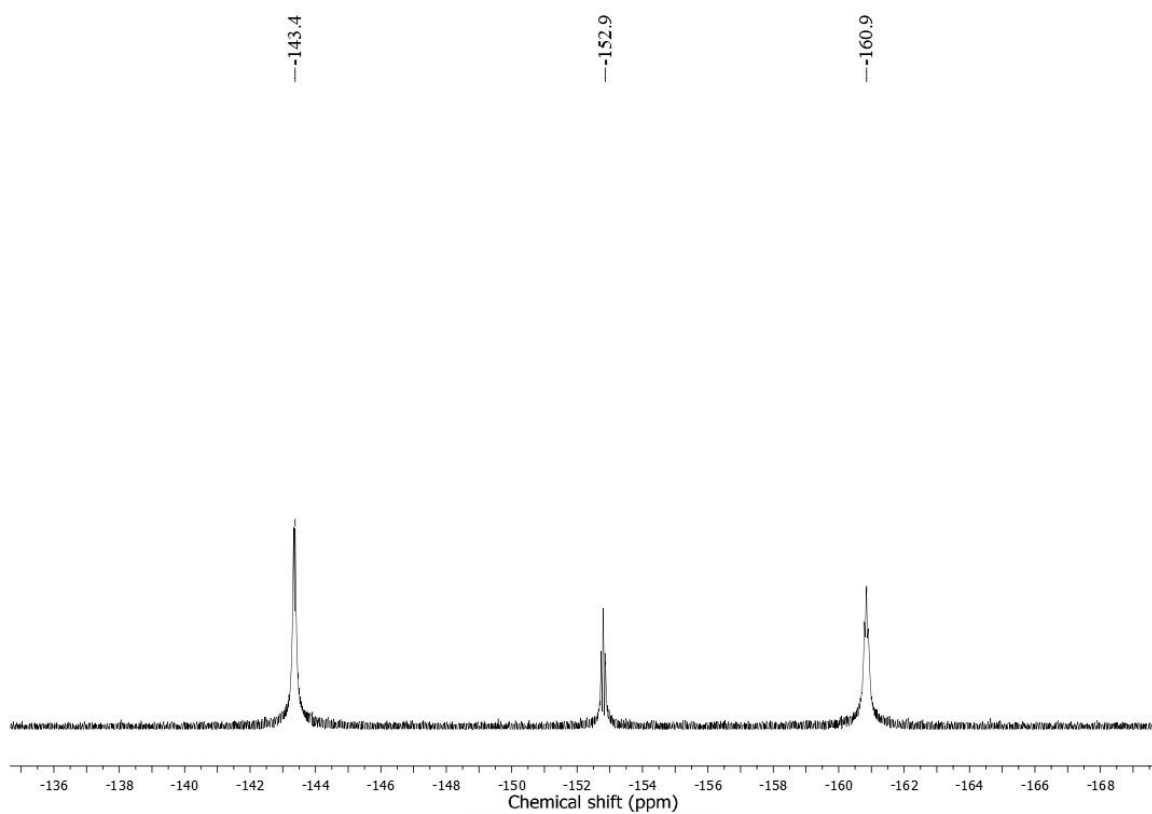


Figure S9. ^1H NMR spectrum (400 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^2OH

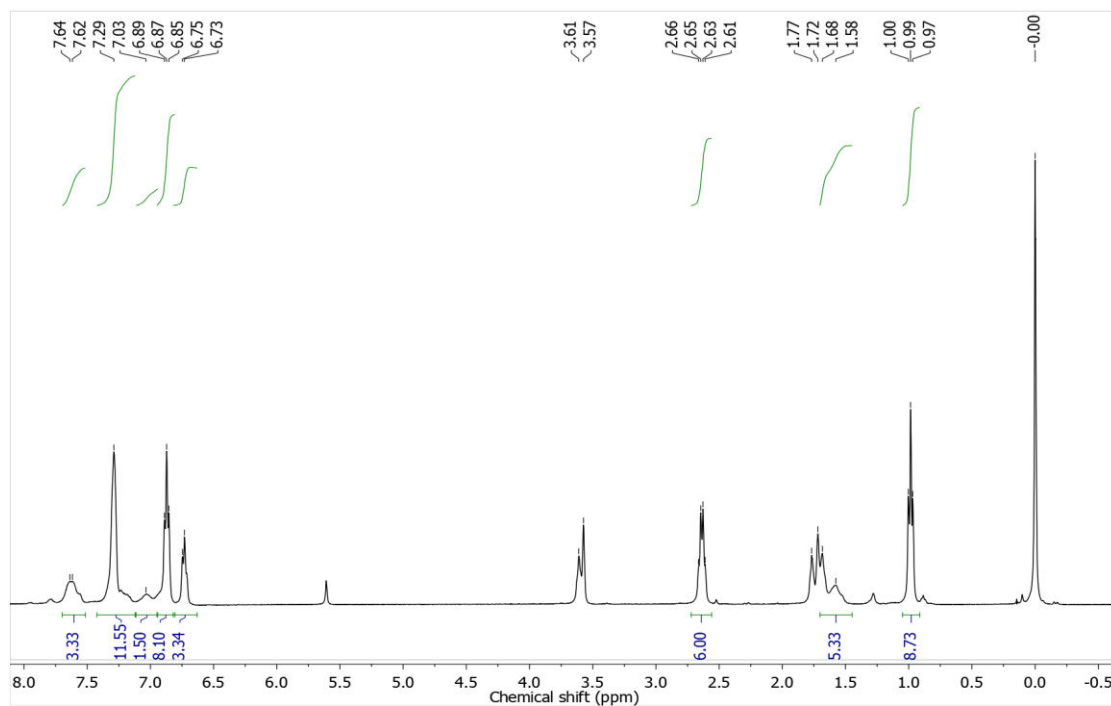


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^2OH

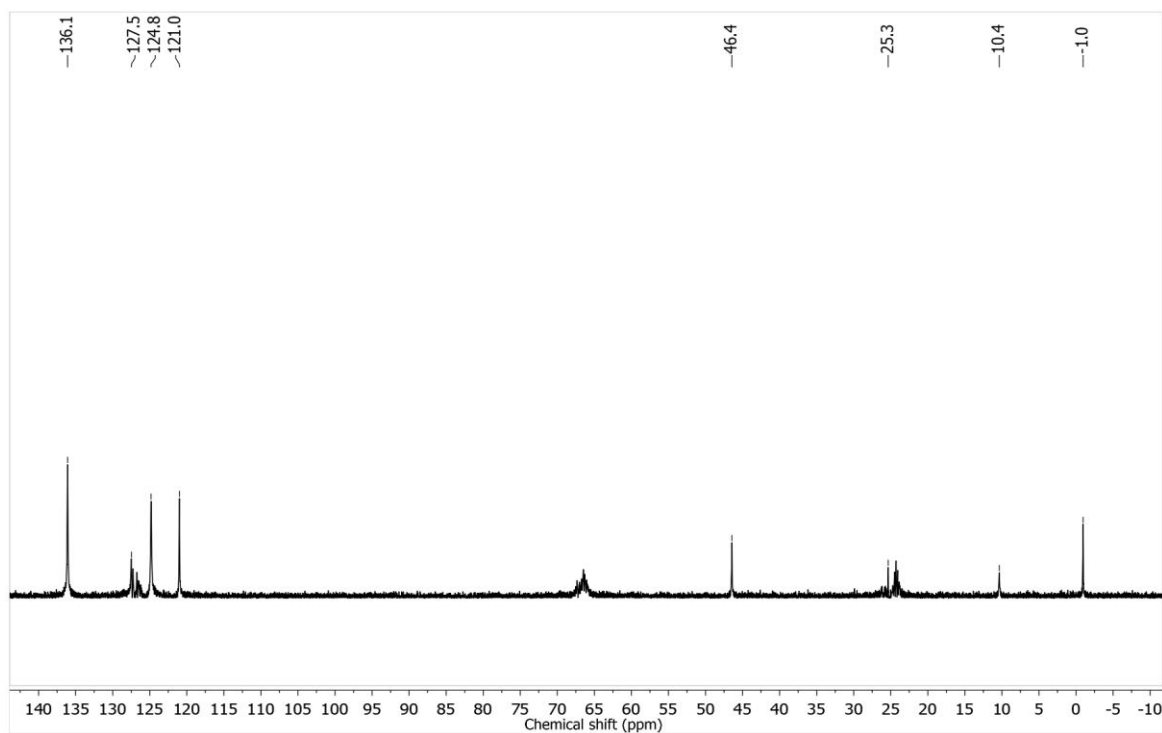


Figure S11. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^2OH

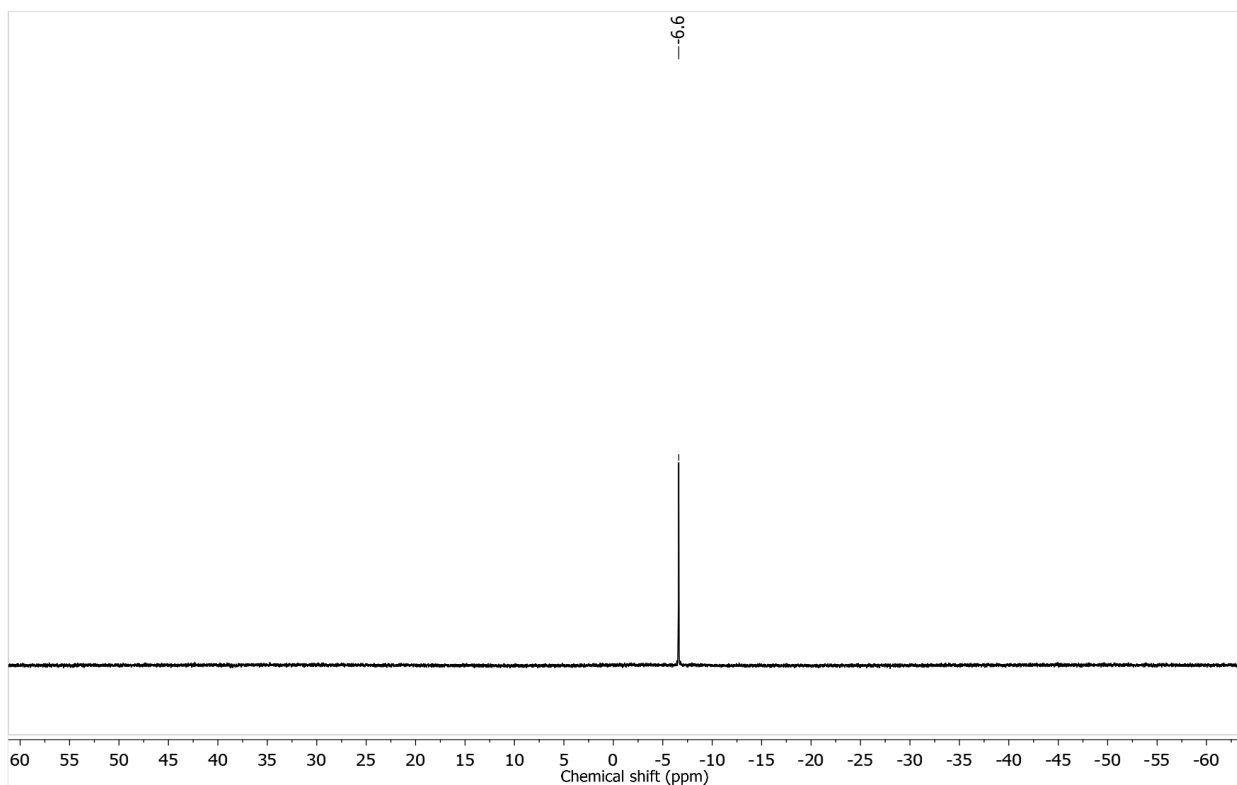


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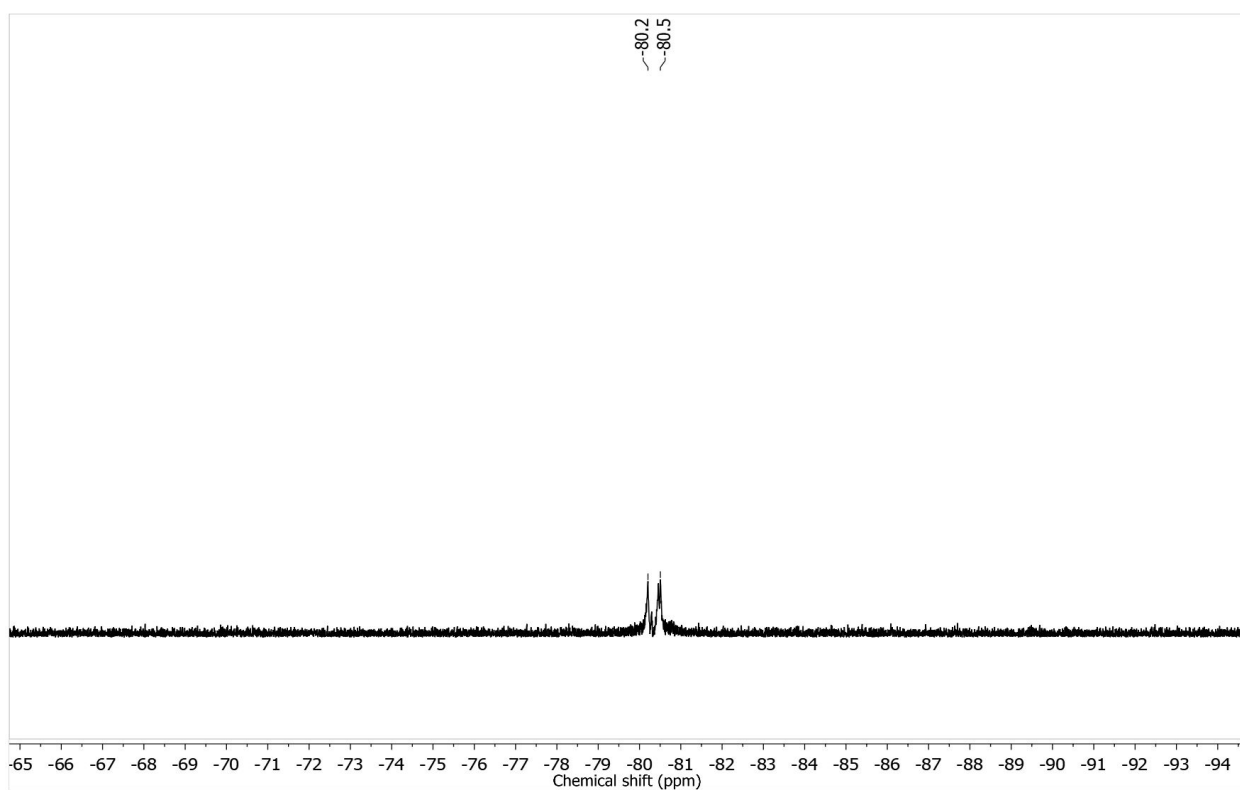


Figure S13. ^1H NMR spectrum (400 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^3OH

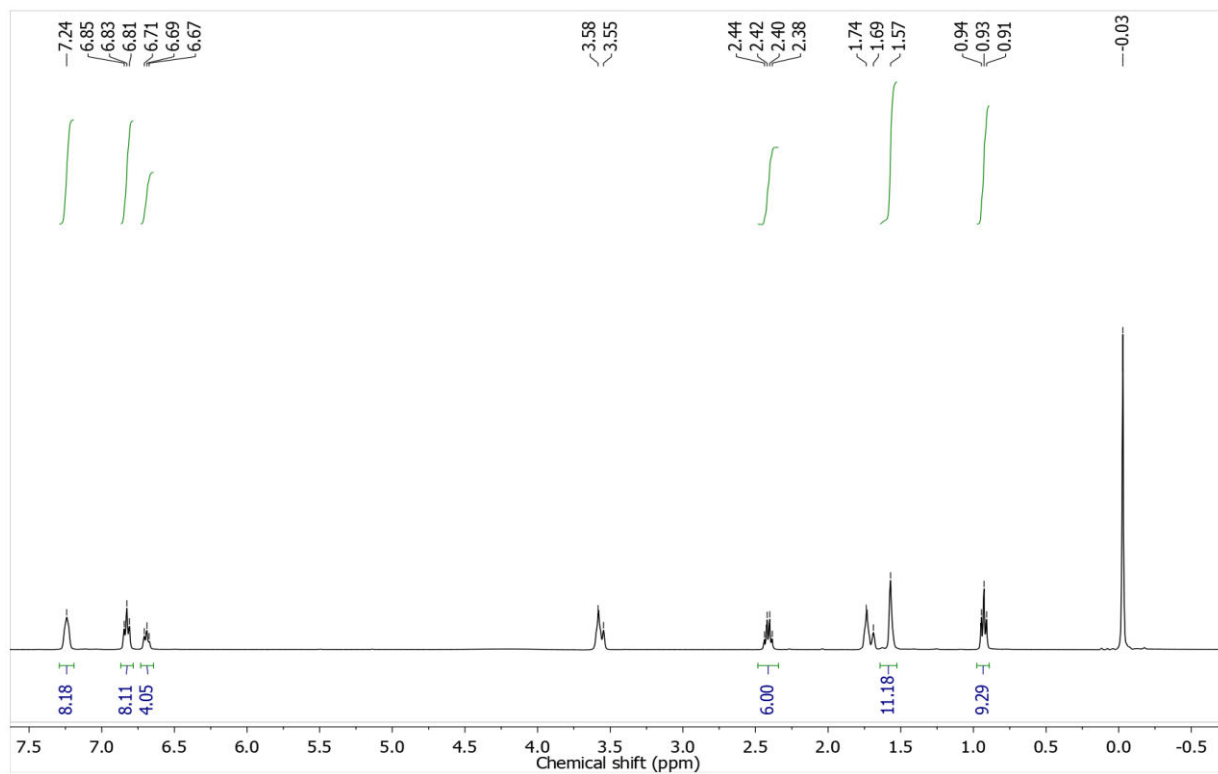


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^3OH

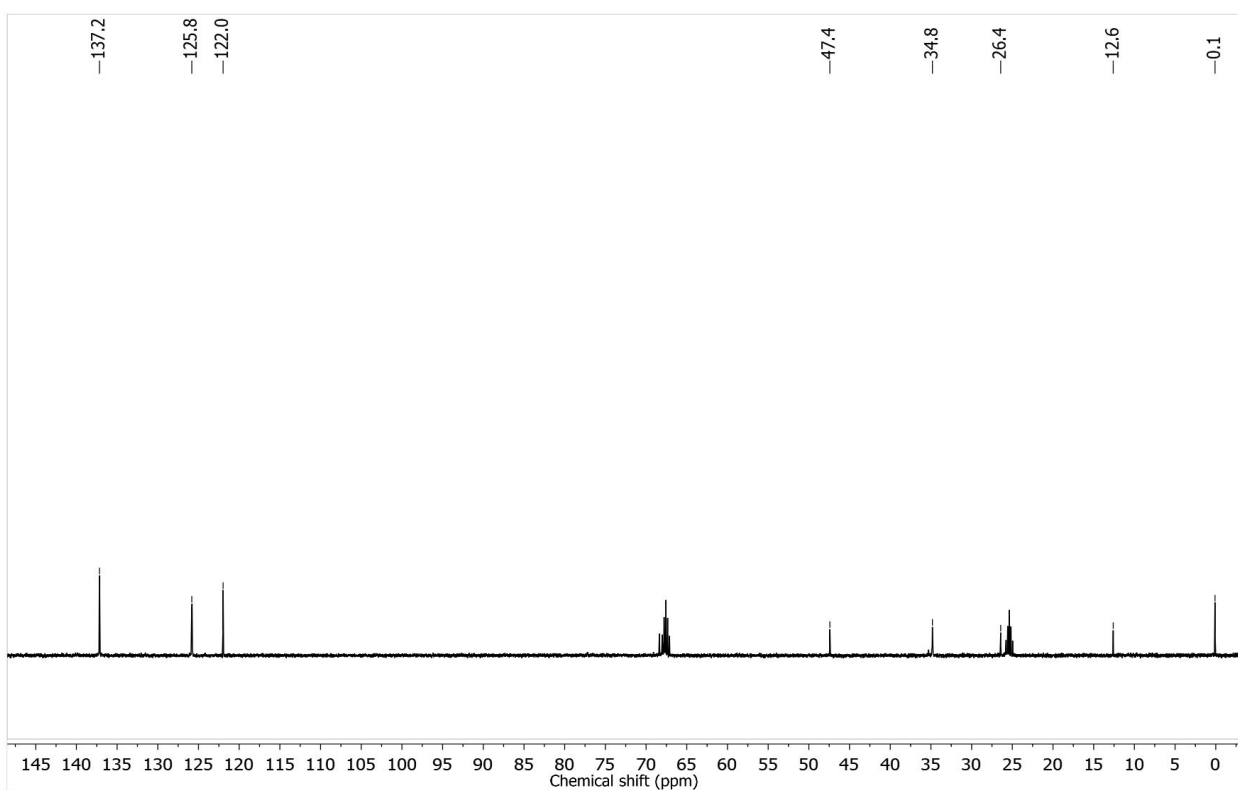


Figure S15. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^3OH

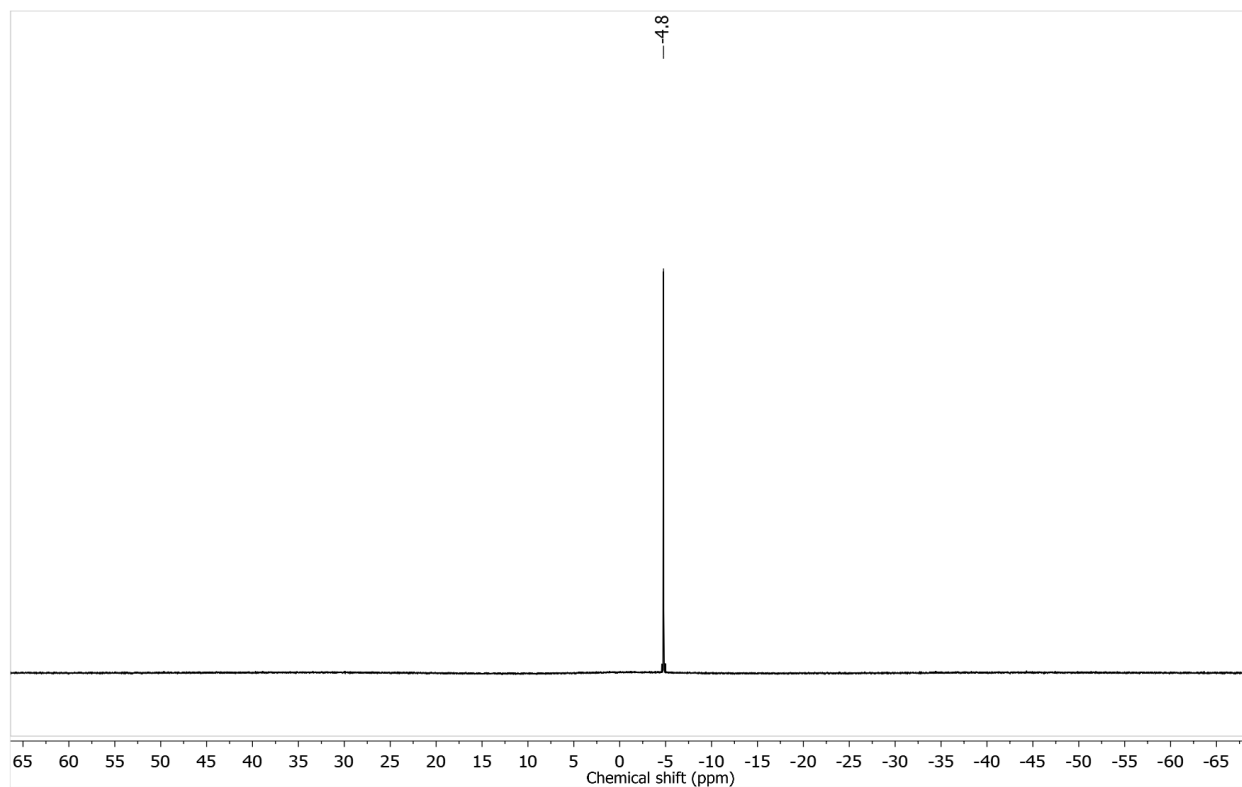


Figure S16. ^{19}F NMR spectrum (376 MHz, $\text{THF-}d_8$, 293K) of the reaction of $\text{Y}(\text{CH}_2\text{SiMe}_3)_3\text{THF}_2$ with $[\text{HNEt}_3][\text{BPh}_4]$ and L^3OH

