

Supporting Information for

Amidomagnesium cations

Sumanta Banerjee,^a Ankur,^a Alex P. Andrews,^a Babu Varghese^b and Ajay Venugopal^{*,a}

^a *School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Vithura, Thiruvananthapuram 695551, India. E-mail: venugopal@iisertvm.ac.in*

^b *Sophisticated Analytical Instrument Facility, Indian Institute of Technology Madras, Chennai 600036, India.*

Table of Contents

Spectroscopic characterisation of 1	2-4
Spectroscopic characterisation of 2a,b	5-8
Variable Temperature ¹ H NMR of 2b	9
Spectroscopic characterisation of 3	10-11
NMR scale reaction of 2b with Ph ₂ C=O	12
Spectroscopic characterisation of 4	13-14
¹ H NMR of 5	15
¹ H NMR of 6	16
Single crystal XRD structure of [Mg(THF) ₆] ₂ [B(C ₆ H ₃ Cl ₂) ₄]	17

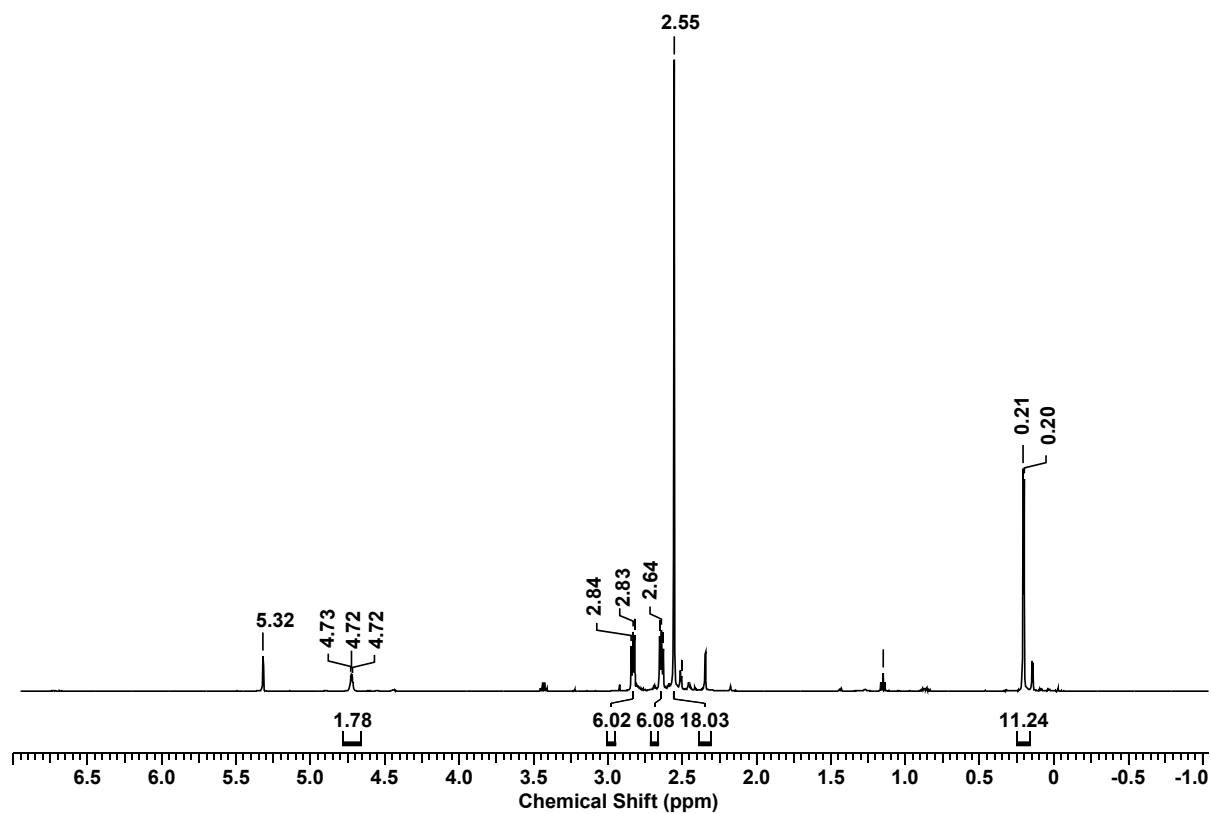


Figure S1. ¹H NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiHMe}_2)_2][\text{B}(\text{C}_6\text{F}_5)_4]$ (1) in CD_2Cl_2

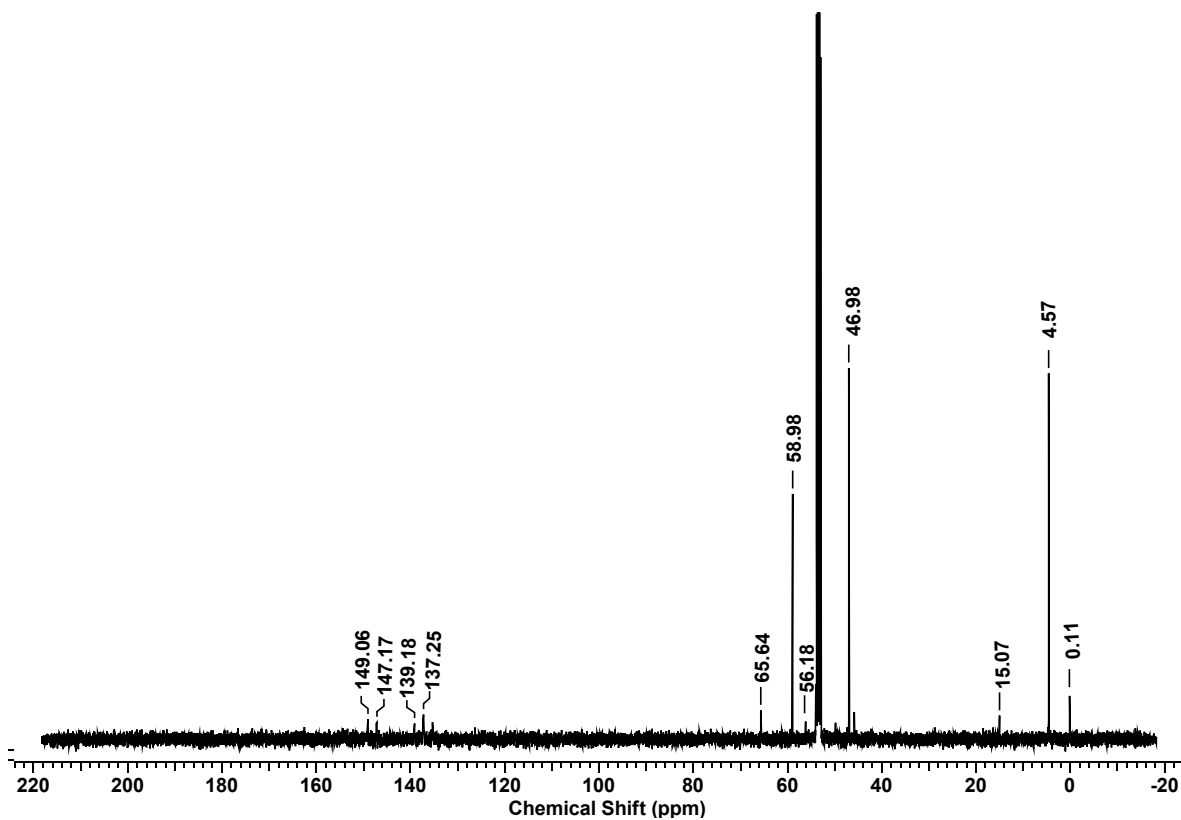


Figure S2. ¹³C NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiHMe}_2)_2][\text{B}(\text{C}_6\text{F}_5)_4]$ (1) in CD_2Cl_2

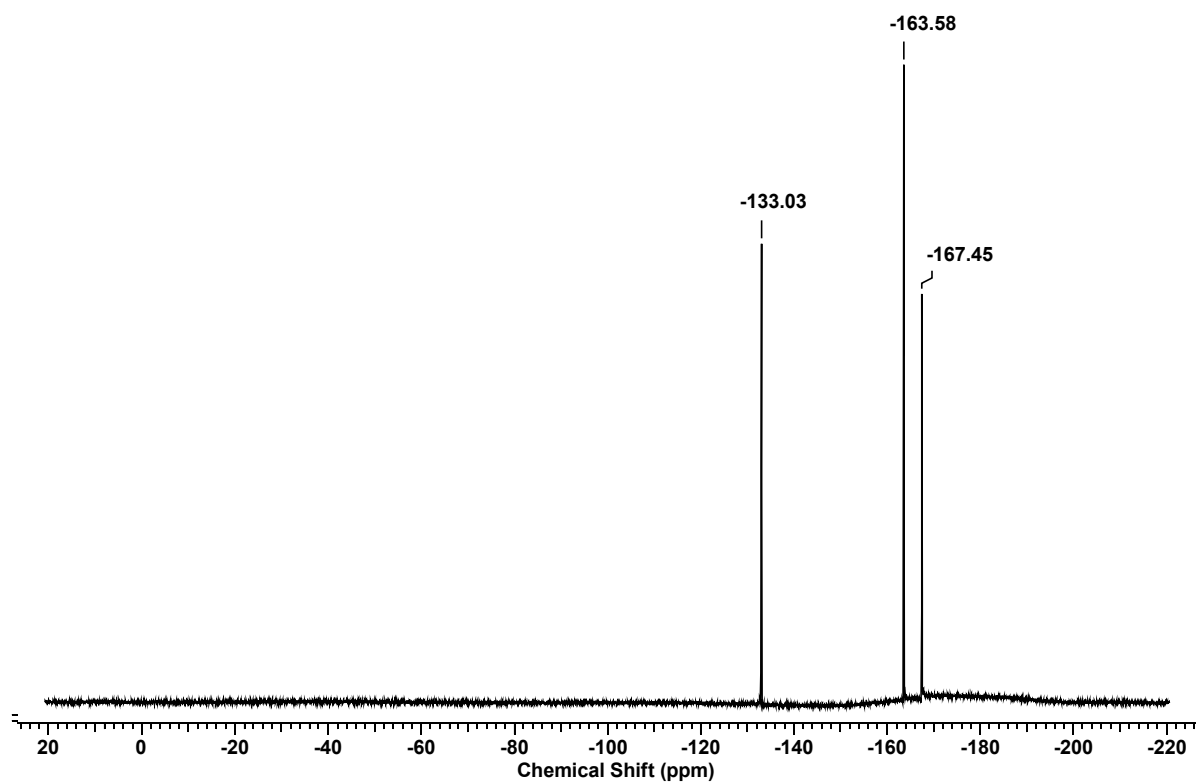


Figure S3. ^{19}F NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiHMe}_2)_2][\text{B}(\text{C}_6\text{F}_5)_4]$ (1) in CD_2Cl_2

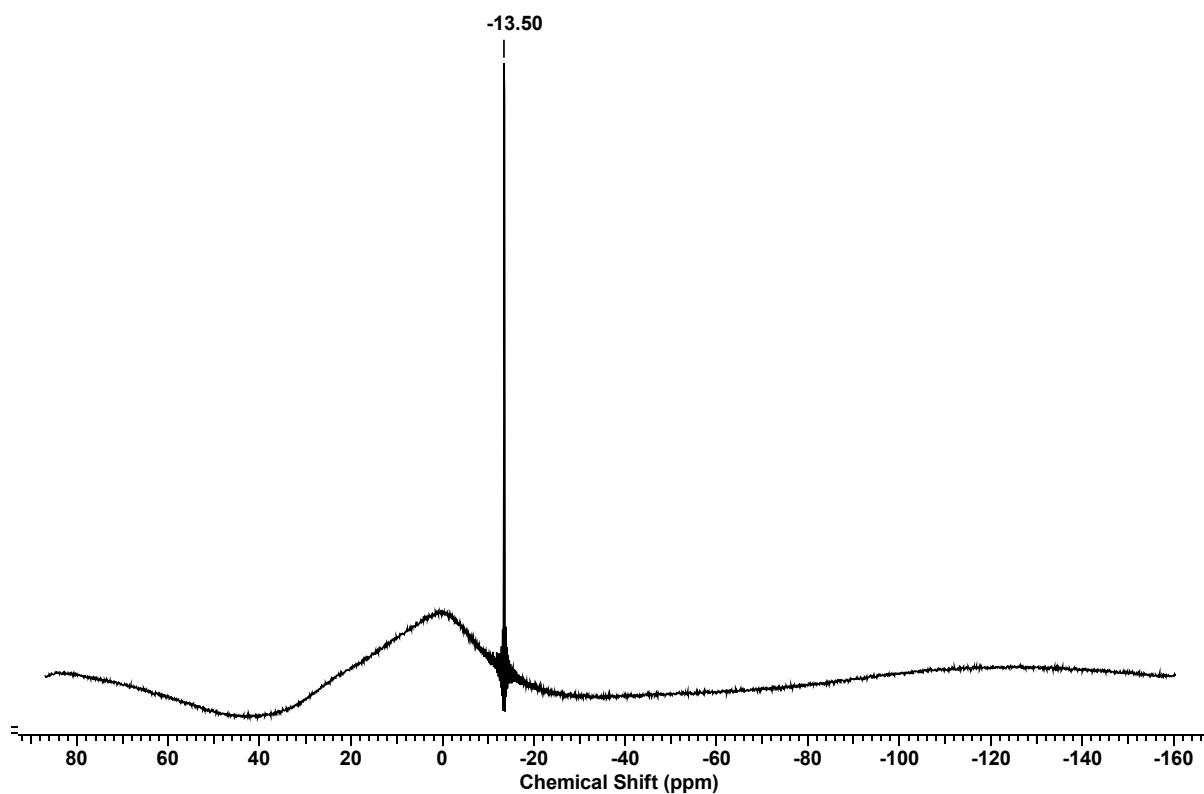


Figure S4. ^{11}B NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiHMe}_2)_2][\text{B}(\text{C}_6\text{F}_5)_4]$ (1) in CD_2Cl_2

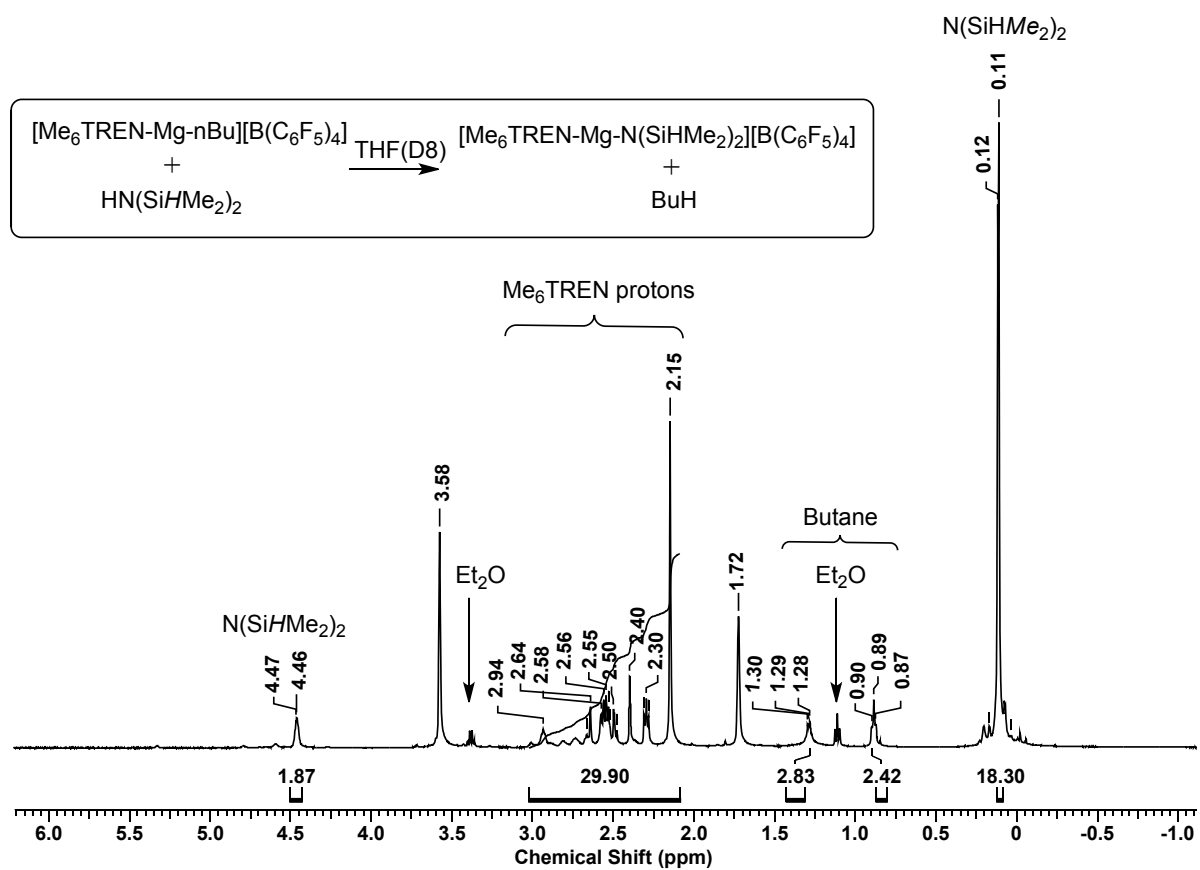


Figure S5. ^1H NMR spectrum of the reaction between $[\text{Me}_6\text{TREN-Mg-nBu}][\text{B}(\text{C}_6\text{F}_5)_4]$ (crystallised from Et_2O) and $\text{HN}(\text{SiHMe}_2)_2$ in THF(D8)

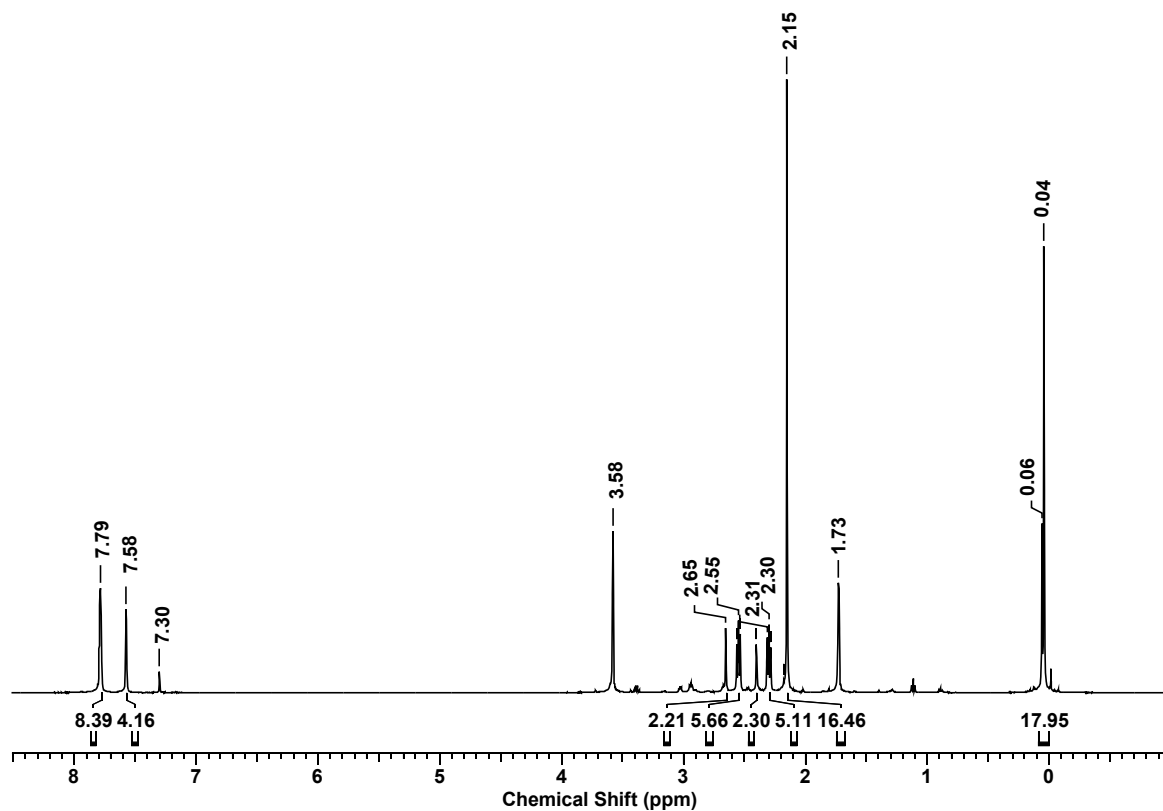


Figure S6. ^1H NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiMe}_3)_2][\text{B}\{\text{C}_6\text{H}_3(\text{CF}_3)_2\}_4]$ (2a) in THF(D8)

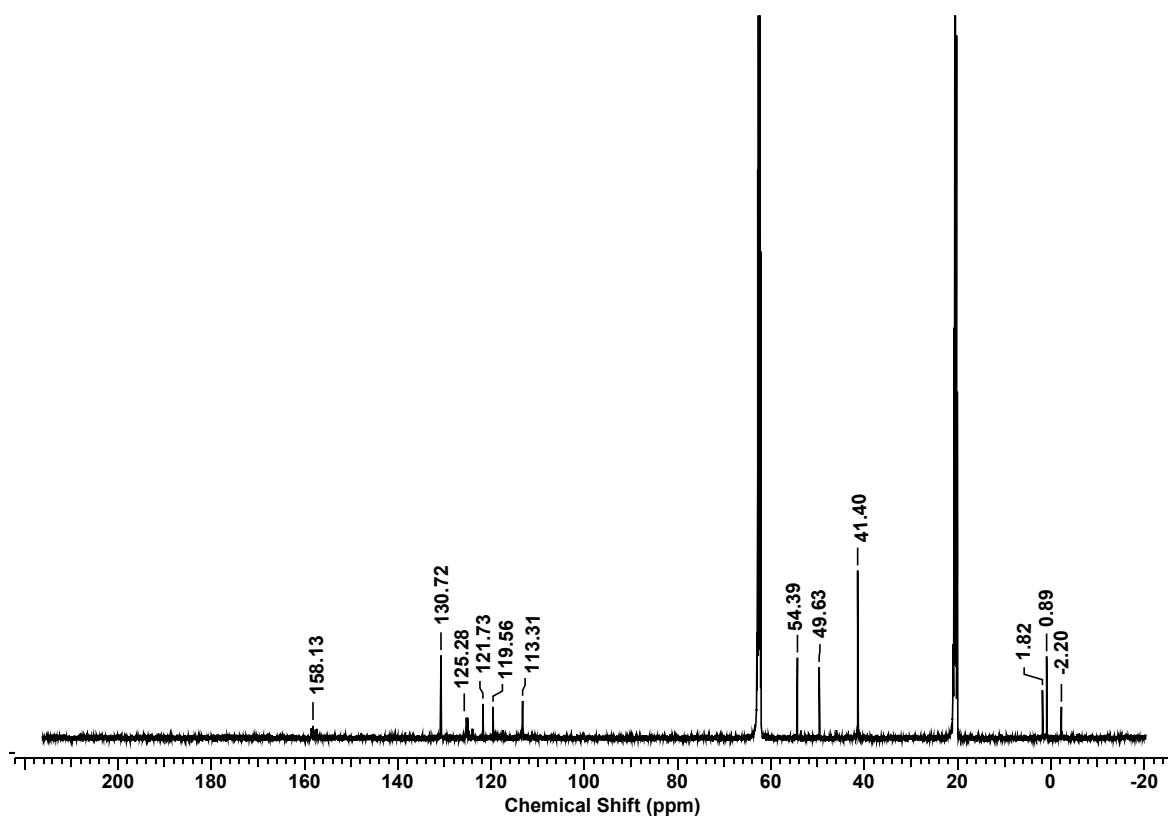


Figure S7. ^{13}C NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiMe}_3)_2][\text{B}\{\text{C}_6\text{H}_3(\text{CF}_3)_2\}_4]$ (2a) in THF(D8)

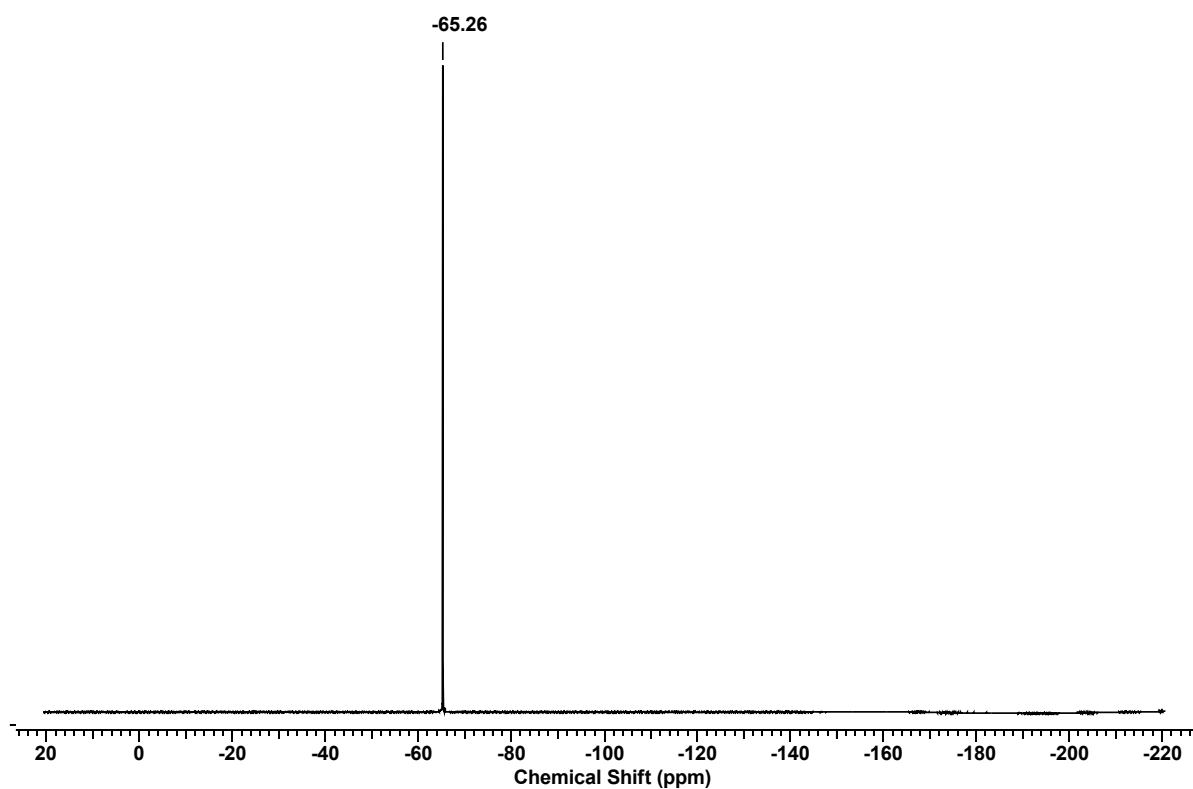


Figure S8. ^{19}F NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiMe}_3)_2][\text{B}\{\text{C}_6\text{H}_3(\text{CF}_3)_2\}_4]$ (2a) in THF(D8)

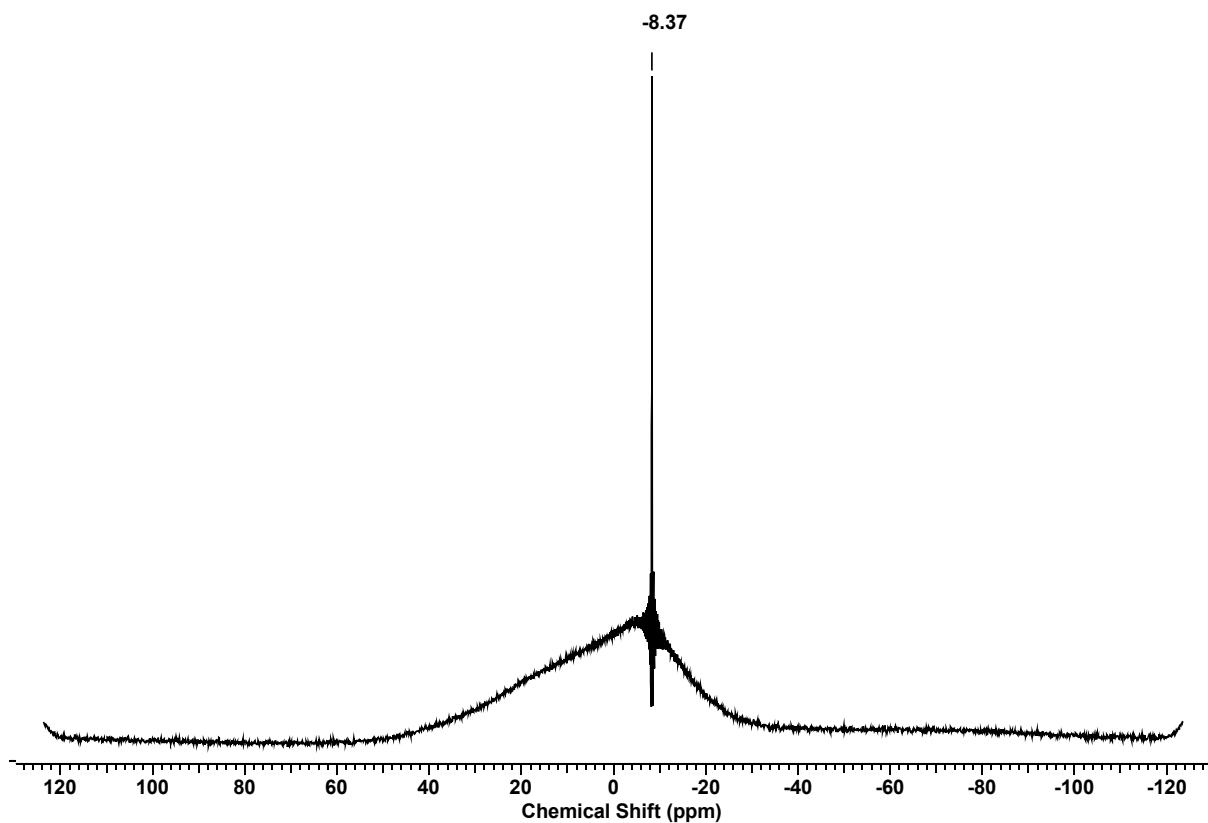


Figure S9. ^{11}B NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiMe}_3)_2][\text{B}\{\text{C}_6\text{H}_3(\text{CF}_3)_2\}_4]$ (2a) in THF(D8)

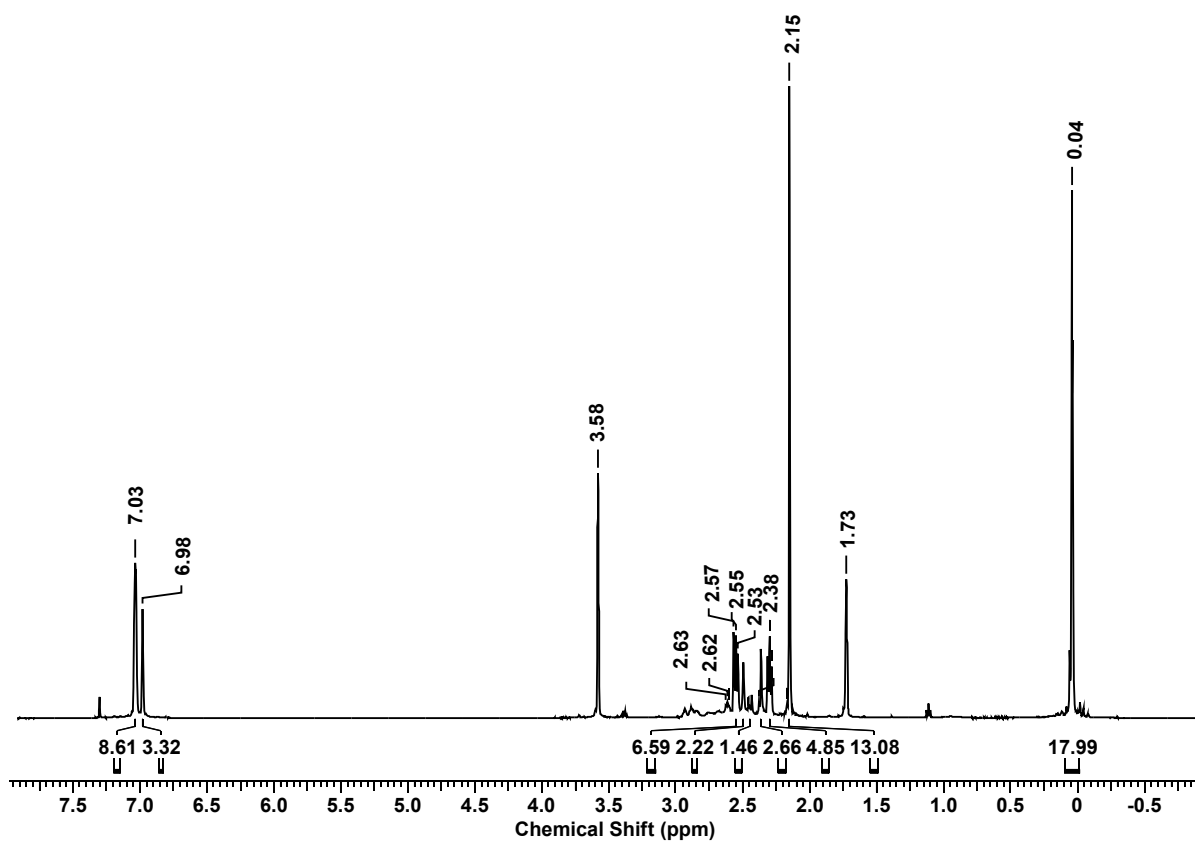


Figure S10. ¹H NMR spectrum of [Me₆TREN-Mg-N(SiMe₃)₂][B(C₆H₃Cl₂)₄] (2b) in THF(D₈)

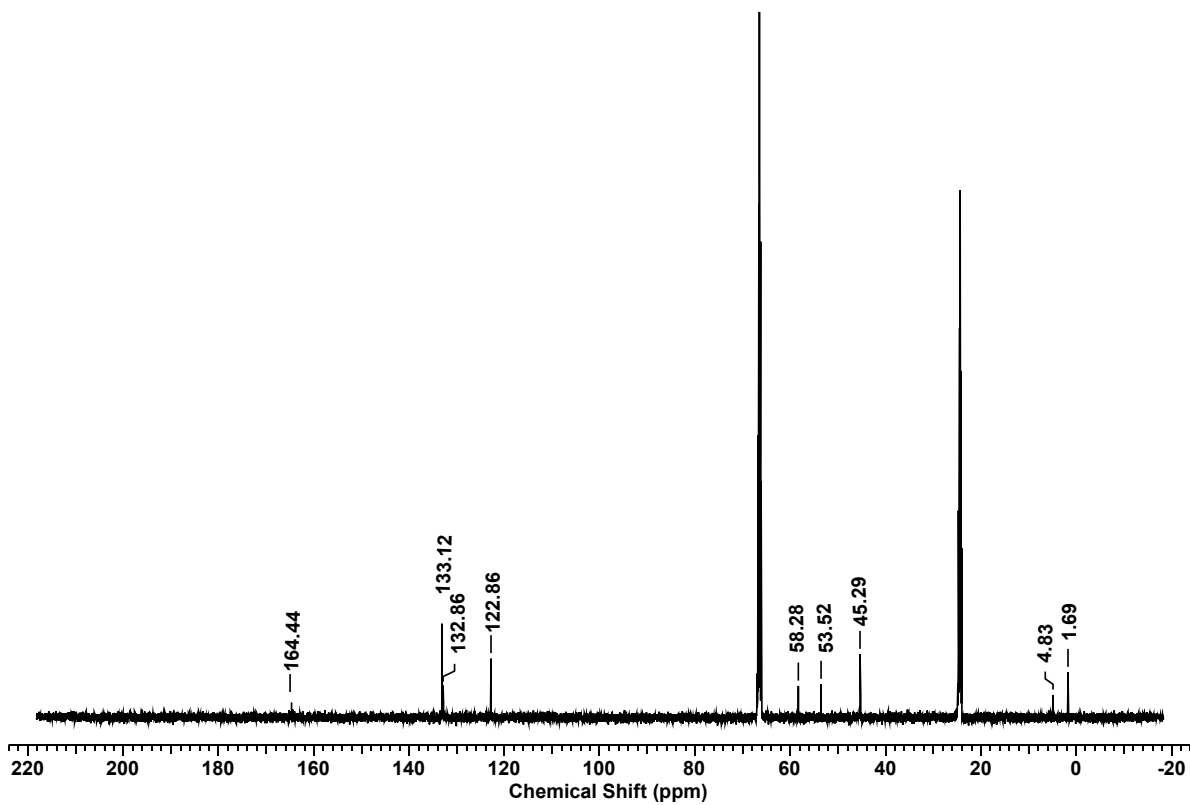


Figure S11. ¹³C NMR spectrum of [Me₆TREN-Mg-N(SiMe₃)₂][B(C₆H₃Cl₂)₄] (2b) in THF(D₈)

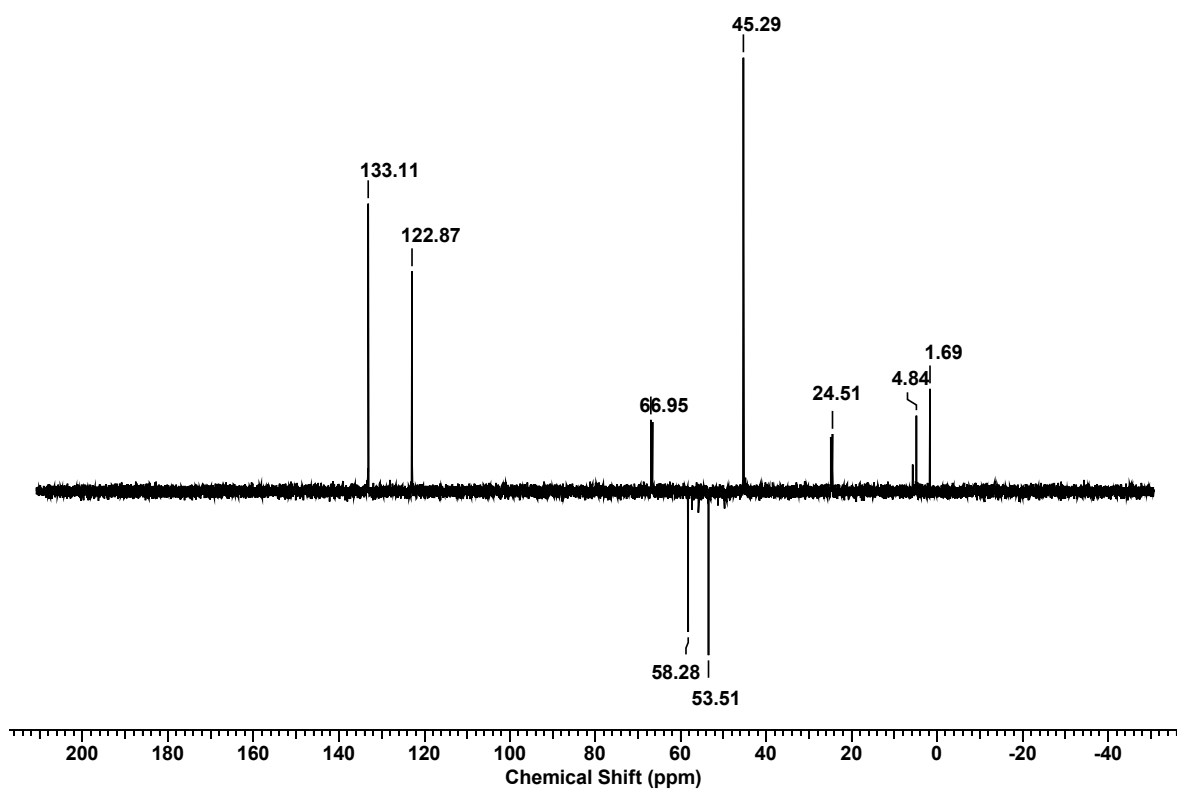


Figure S12. DEPT NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiMe}_3)_2][\text{B}(\text{C}_6\text{H}_3\text{Cl}_2)_4]$ (2b) in THF(D8)

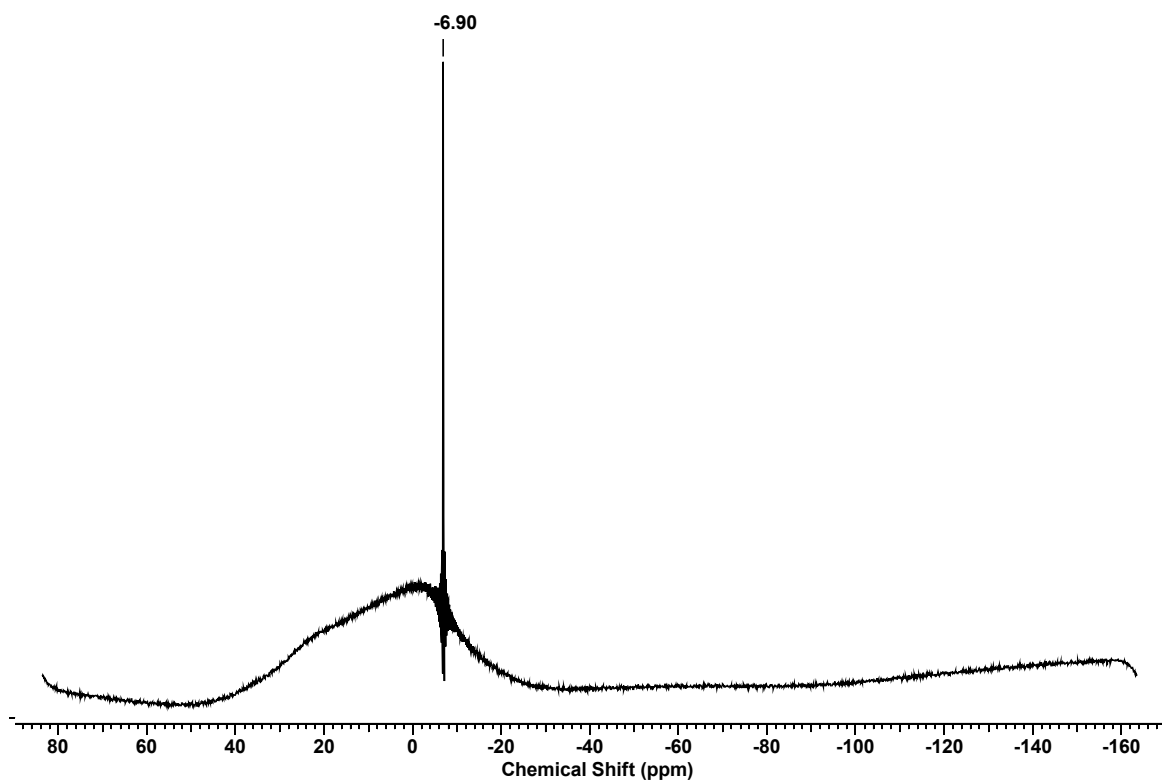


Figure S13. ^{11}B NMR spectrum of $[\text{Me}_6\text{TREN-Mg-N}(\text{SiMe}_3)_2][\text{B}(\text{C}_6\text{H}_3\text{Cl}_2)_4]$ (2b) in THF(D8)

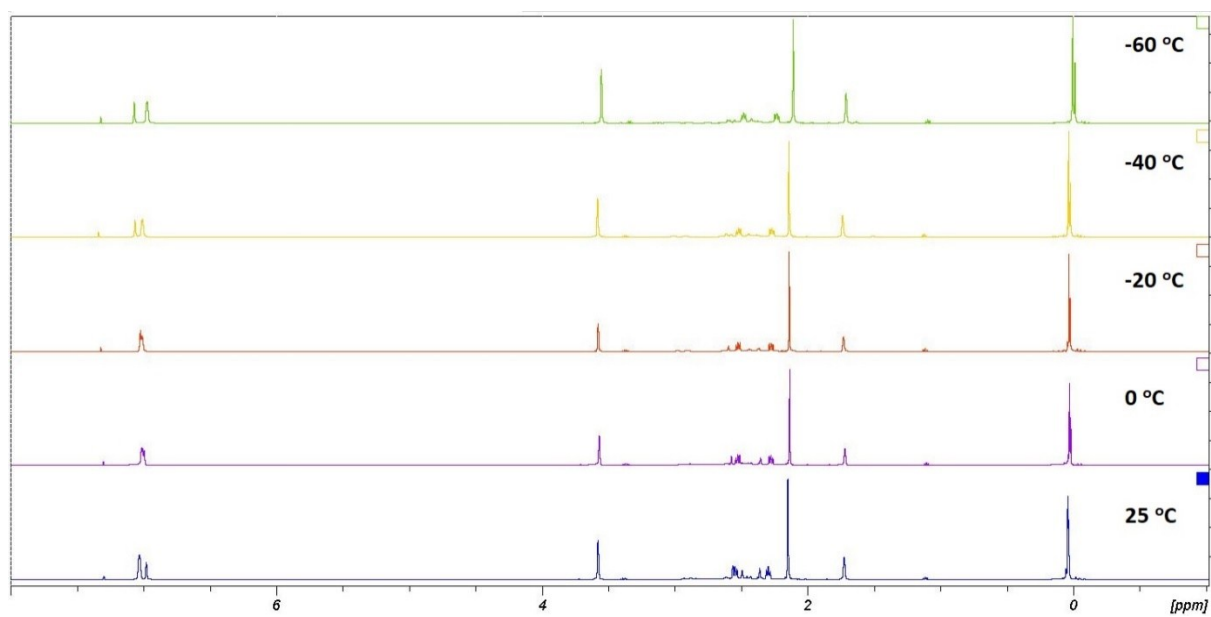
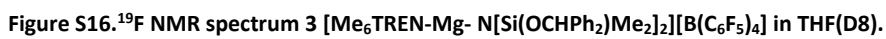


Figure S14. Variable Temperature ¹H NMR of [Me₆TREN-Mg-N(SiMe₃)₂][B(C₆H₃Cl₂)₄] (2b) in THF(D₈)



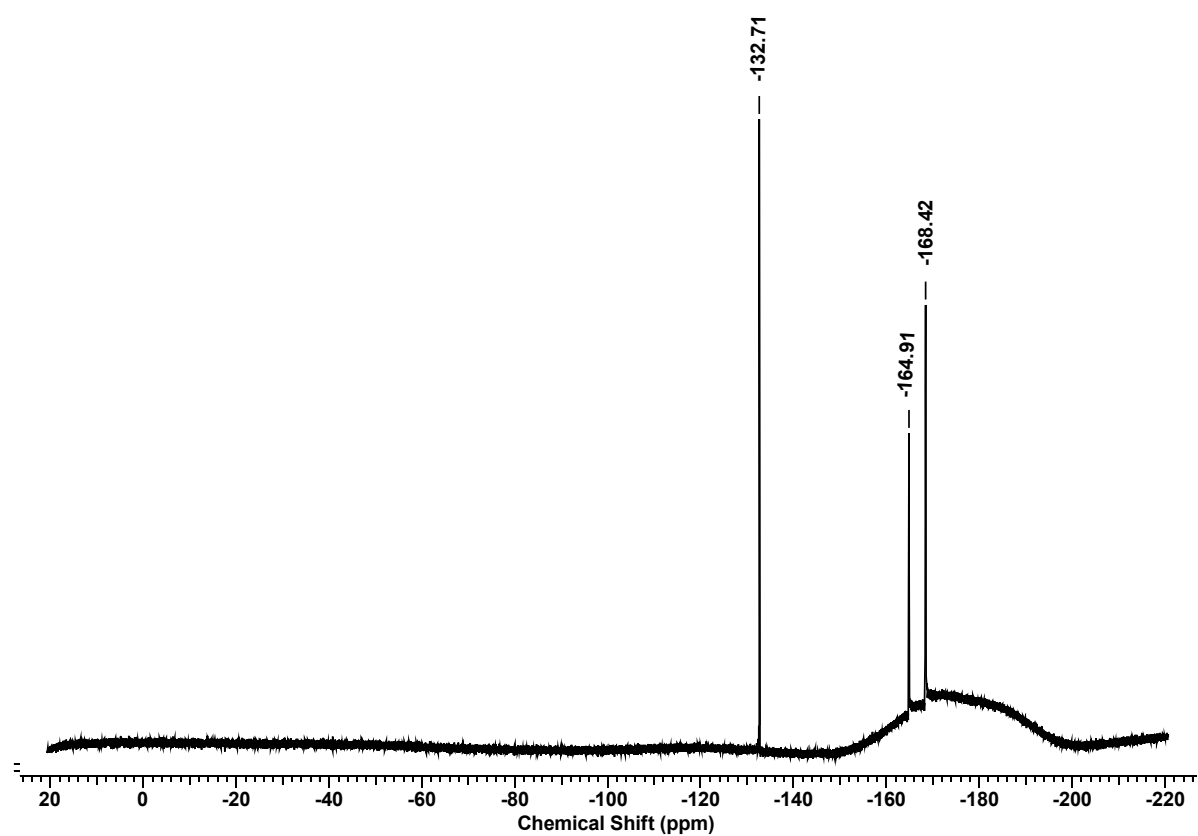


Figure S17. ^{19}F NMR spectrum 3 $[\text{Me}_6\text{TREN-Mg-N}[\text{Si}(\text{OCHPh}_2)\text{Me}_2]_2][\text{B}(\text{C}_6\text{F}_5)_4]$ in $\text{THF}(\text{D}_8)$.

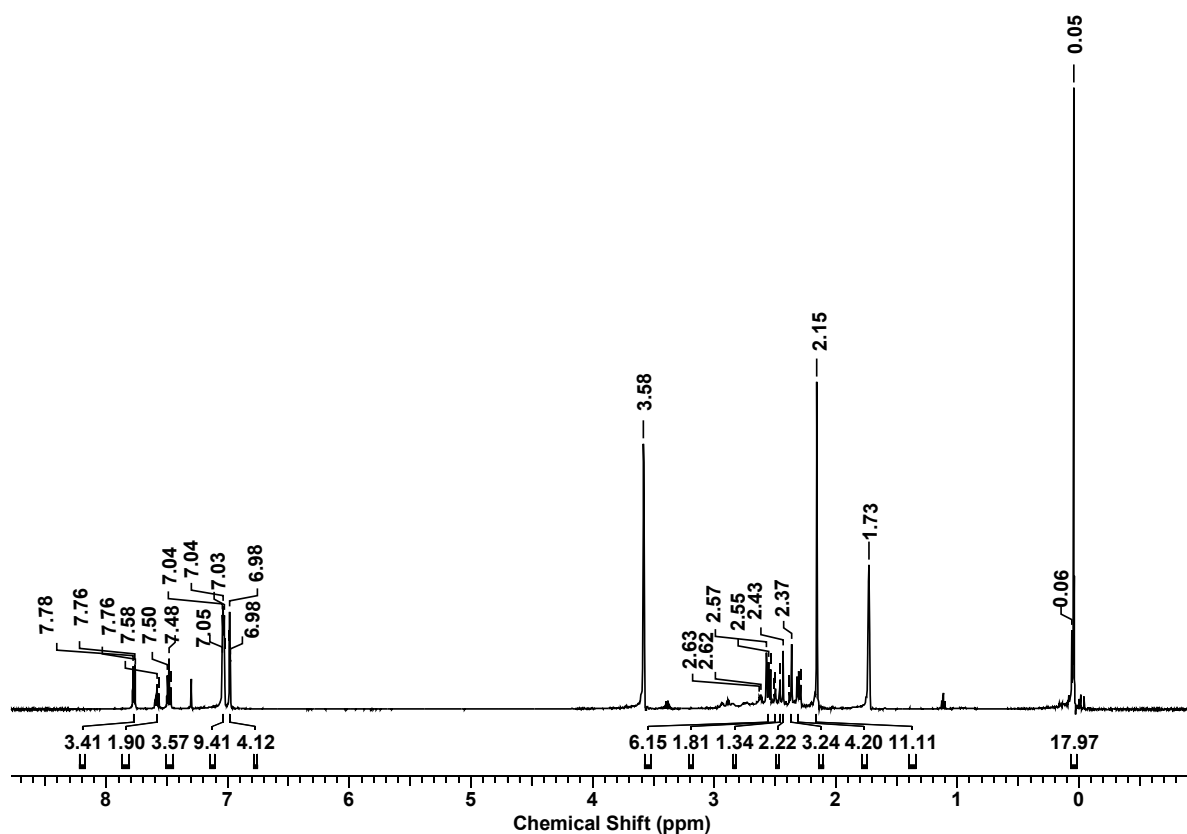


Figure S18. ¹H NMR spectrum in THF (D8) depicting no reaction of 2b with Ph₂CO

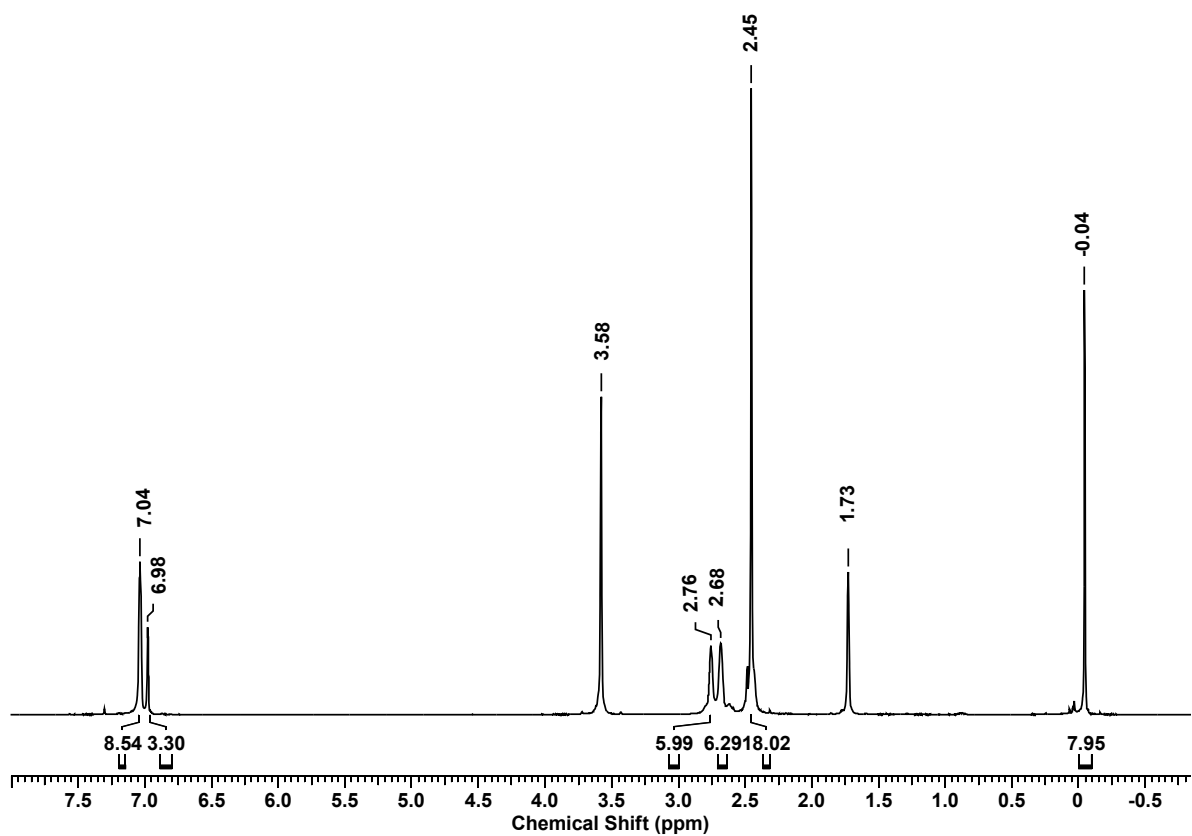


Figure S19. ¹H NMR spectrum of [Me₆TREN-Mg-OSiMe₃][B(C₆H₃Cl₂)₄] (4) in THF (D₈).

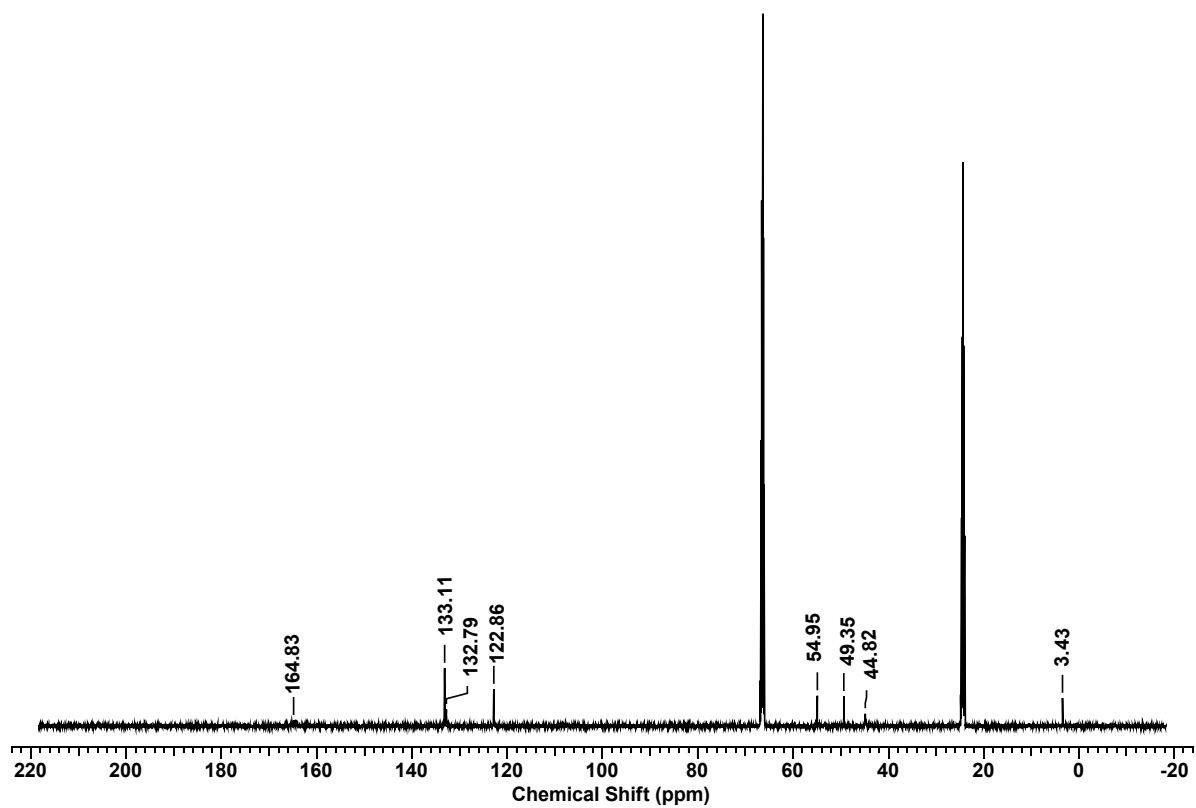


Figure S20. ¹³C NMR spectrum of [Me₆TREN-Mg-OSiMe₃][B(C₆H₃Cl₂)₄] (4) in THF (D₈).

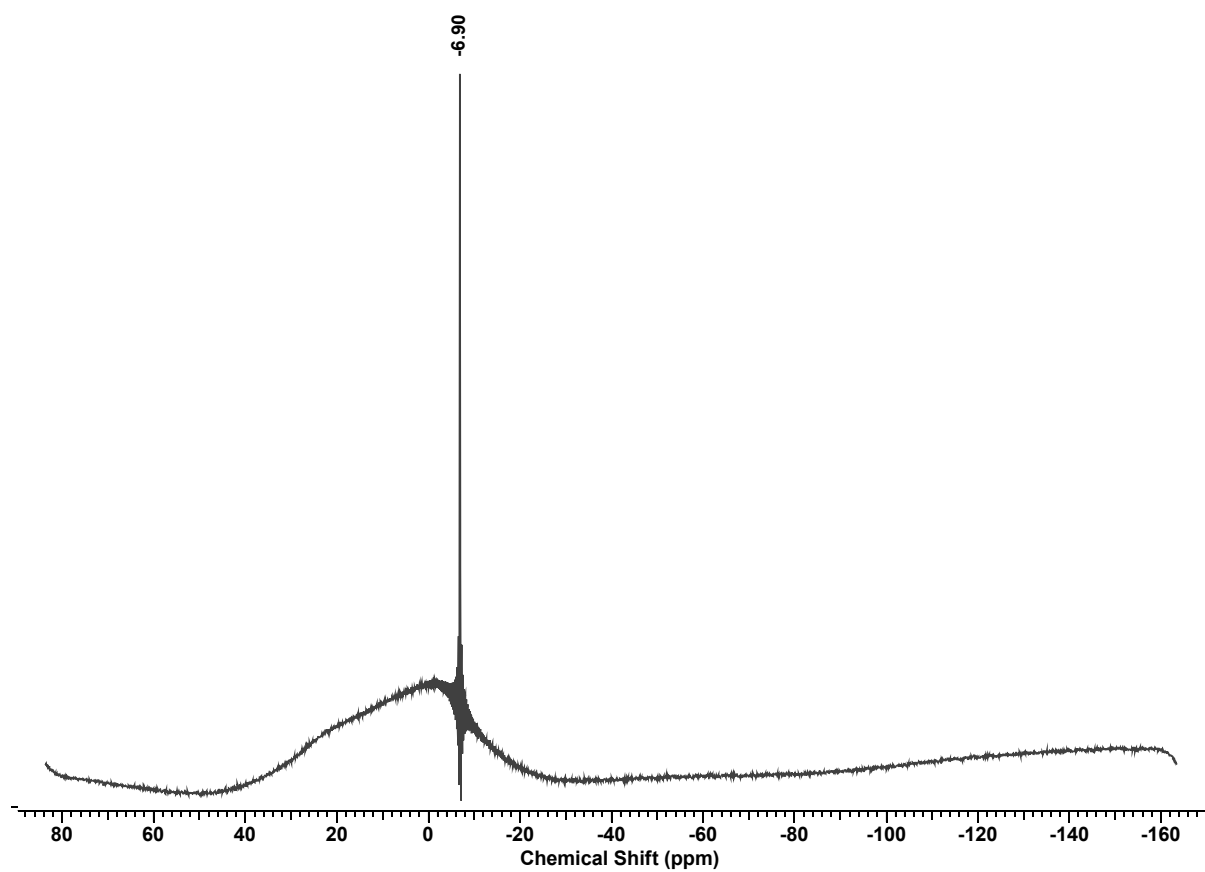


Figure S21. ^{11}B NMR spectrum of $[\text{Me}_6\text{TREN-Mg-OSiMe}_3][\text{B}(\text{C}_6\text{H}_3\text{Cl}_2)_4]$ (**4**) in THF (D_8).

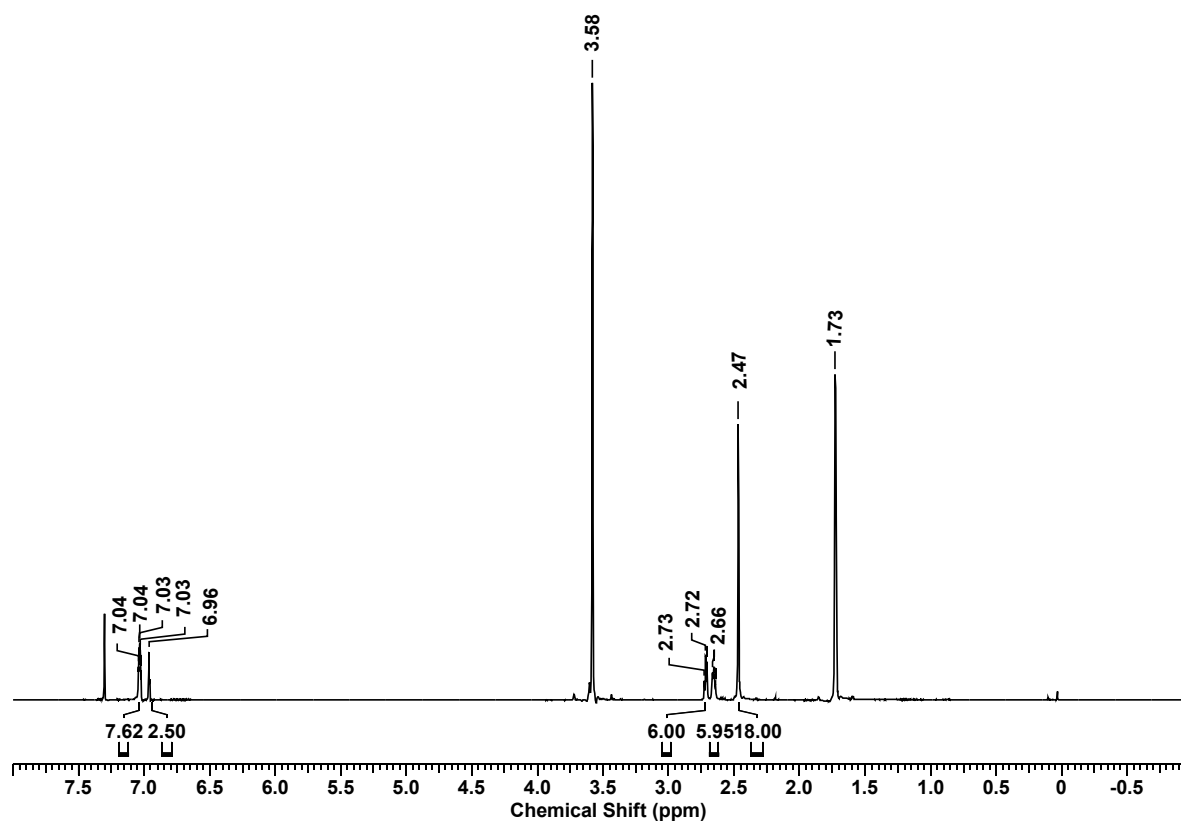


Figure S22. ^1H NMR of $[\text{Me}_6\text{TREN-Mg-OH}]_2[\text{B}(\text{C}_6\text{H}_3\text{Cl}_2)_4]_2(5)$ in $\text{THF}(d_8)$

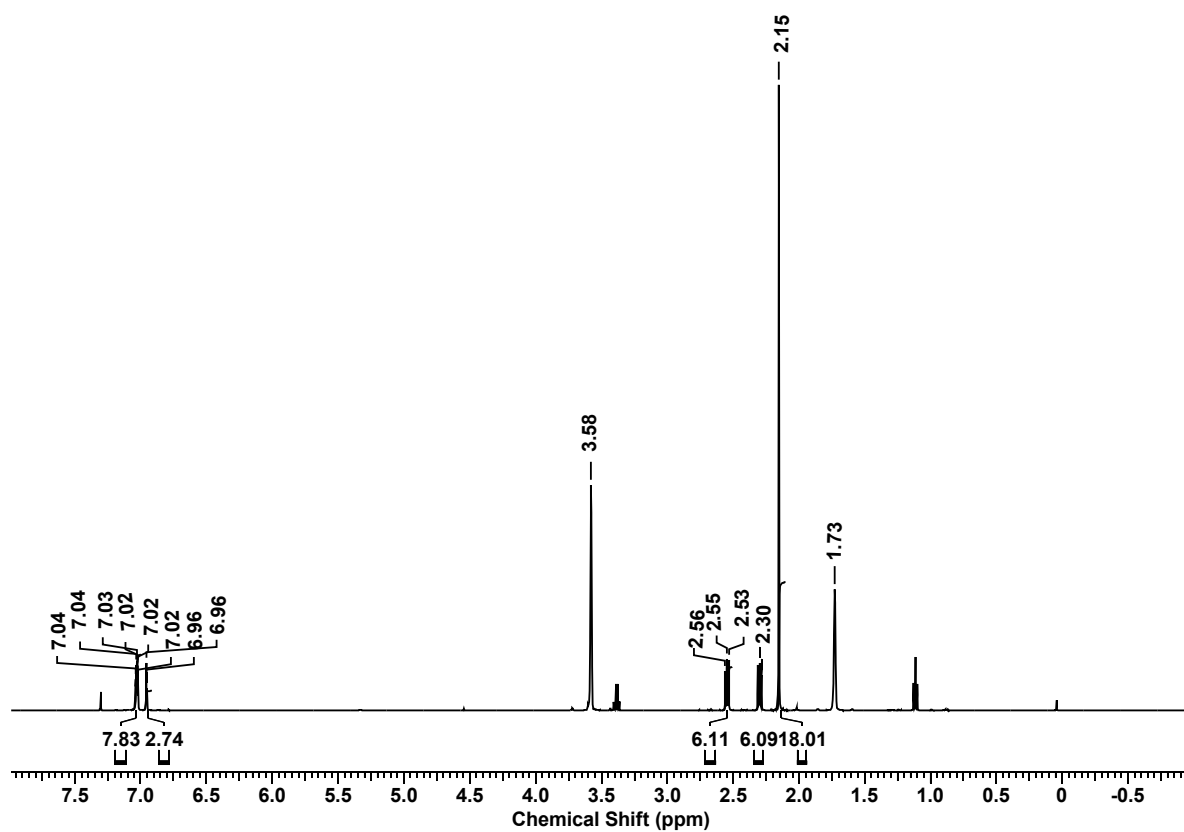


Figure S23. ¹H NMR of $[\text{Me}_6\text{TREN-K(THF)}_3][\text{B(C}_6\text{H}_3\text{Cl}_2)_4]_2(6)$ in THF(D₈)

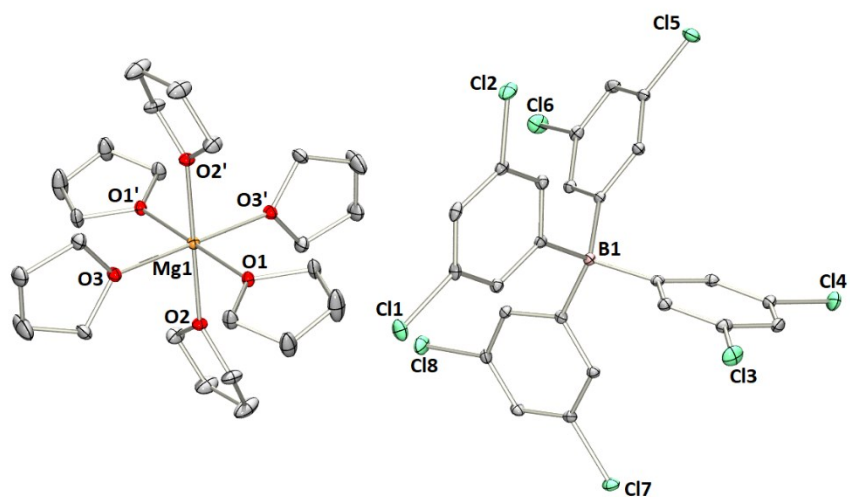


Figure S24. Molecular structure of $[\text{Mg}(\text{THF})_6]_2[\text{B}(\text{C}_6\text{H}_3\text{Cl}_2)_4]$ (CCDC 1886412). Hydrogen atoms have been omitted for clarity.