

Supplementary Data for:

Triple *para*-substitution reactions of $B(C_6F_5)_3$ and $[(C_6F_5)_3PF]^+$ with $P(SiMe_3)_3$

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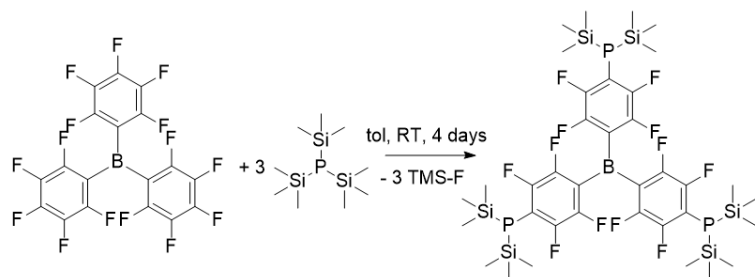
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General Considerations

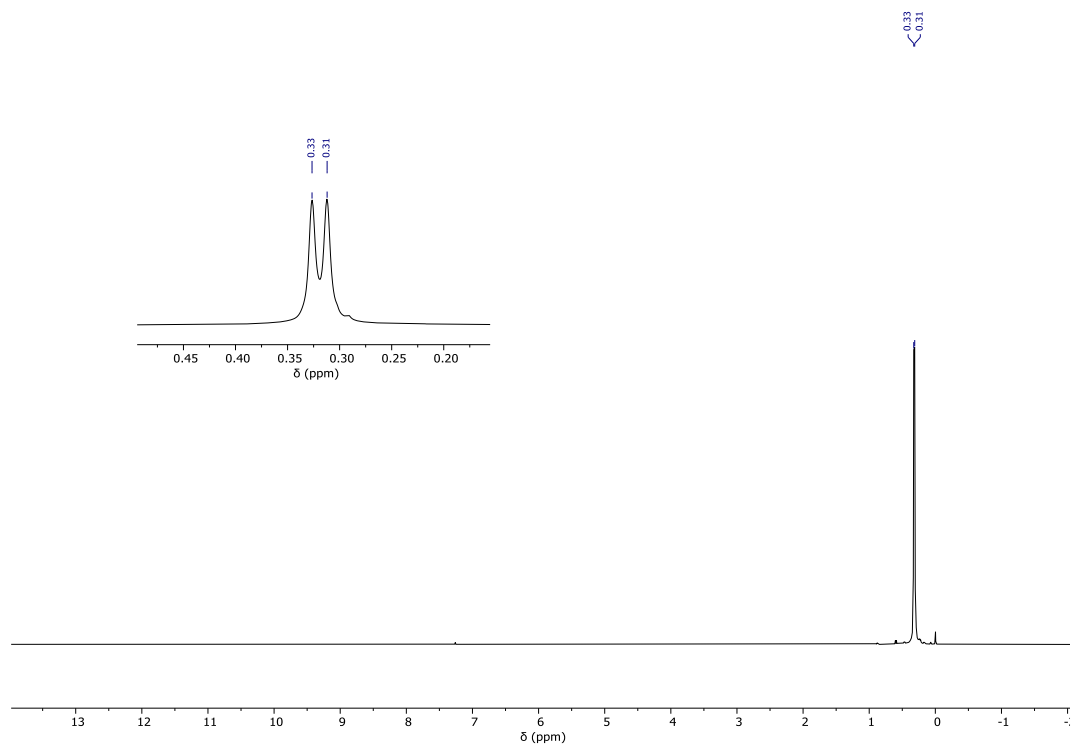
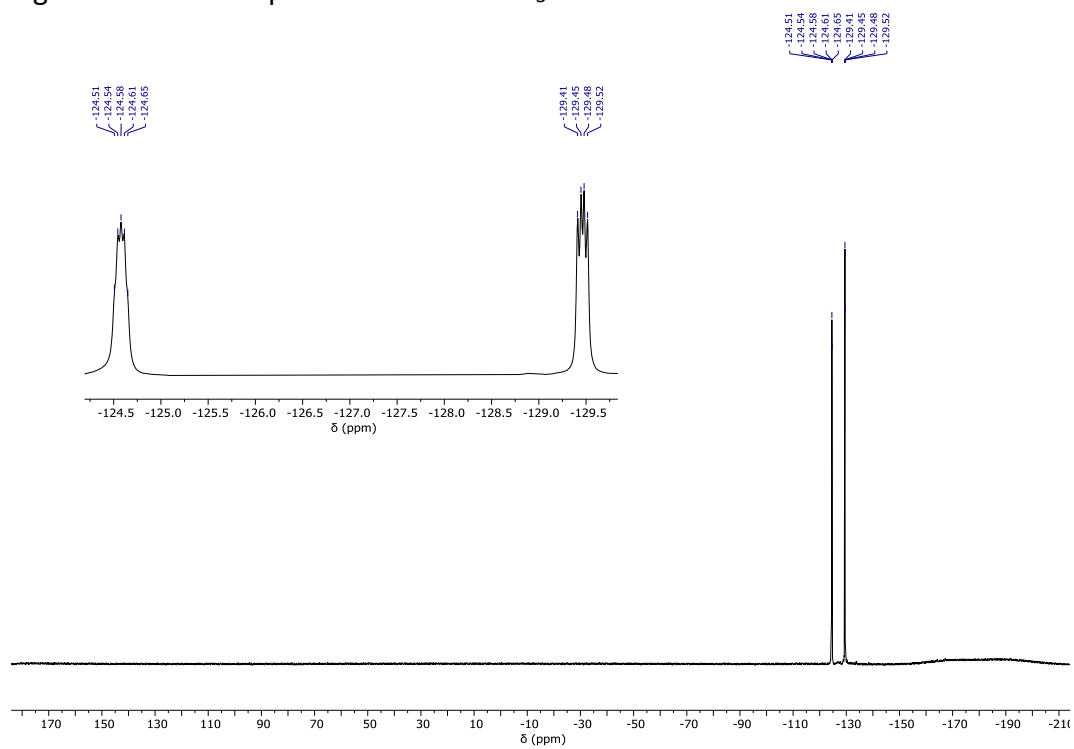
All synthetic manipulations were carried out under an atmosphere of dry, O₂-free N₂ employing an MBraun glove box and a Schlenk vacuum-line. Pentane, diethyl ether and toluene were purified with a Grubbs-type column system manufactured by Innovative Technology and dispensed into thick-walled glass Schlenk bombs equipped with Young-type Teflon valve stopcocks. Toluene-*d*₈ and C₆D₆ were each dried over CaH₂, vacuum-transferred into a Young bomb and stored over 4 Å molecular sieves. Dichloromethane, dichloromethane-*d*₂, acetonitrile and pyridine were each dried over CaH₂, vacuum-transferred into a Young bomb and stored over 4 Å molecular sieves. All solvents were thoroughly degassed after purification (three freeze-pump-thaw cycles). NMR spectra were recorded at 25 °C on a Bruker Avance 400 MHz spectrometer. Chemical shifts are given relative to SiMe₄ and referenced to the residual solvent signal (¹H, ¹³C) or relative to an external standard (¹¹B: 15% (Et₂O)BF₃; ¹⁹F: 15% (Et₂O)BF₃, ³¹P; 85% H₃PO₄). Chemical shifts (δ) are reported in ppm and coupling constants (*J*) as scalar values in Hz. Combustion analyses were performed in house employing a Perkin-Elmer CHN Analyzer.



Synthesis of B(C₆F₄P(SiMe₃)₂)₃ (**1**):

A solution of P(SiMe₃)₃ (1.47 g, 5.86 mmol) in 2 mL of toluene was added to a stirred solution of B(C₆F₅)₃ (1 g, 1.95 mmol) in dry toluene (18 mL) resulting in a bright yellow solution. After 4 days, all volatiles were removed *in vacuo*, and the resulting yellow solid was washed with cold pentane and dried (1.6 g, 1.6 mmol, 82 %).

¹H NMR (400 MHz, CDCl₃): δ 0.32 ppm (d, 54H, Si(CH₃)₃, ³J_{HP} = 6 Hz, ²J_{HSi} = 219 Hz). ³¹P{¹H} NMR (162 MHz, CDCl₃): δ -162.7 ppm (s). ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ 60.0 ppm (br). ¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ -125.0 ppm and -130.0 ppm (m, C₆F₄). Calcd. for C₃₆H₅₄BF₁₂P₃Si₆ (987.04): C 43.81%, H 5.51%. Found: C 43.62%, H 5.54%.

Figure S1. ^1H NMR spectrum of **1** in CDCl_3 Figure S2. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **1** in CDCl_3

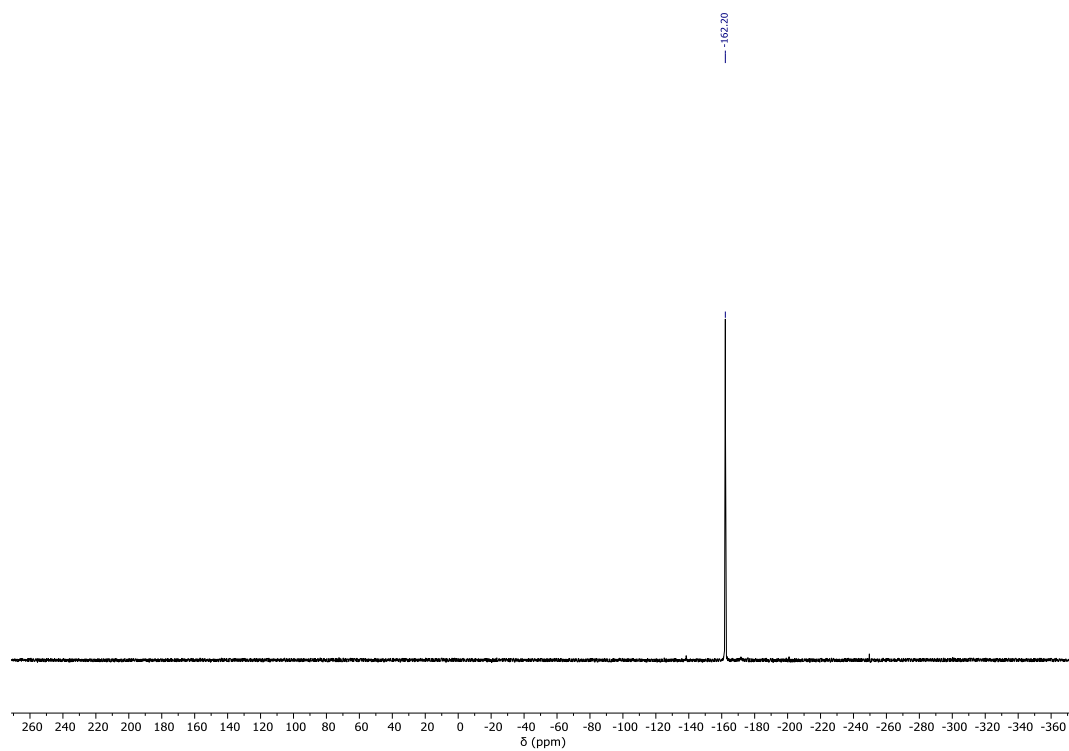


Figure S3. ^{31}P NMR spectrum of **1** in CDCl_3 .

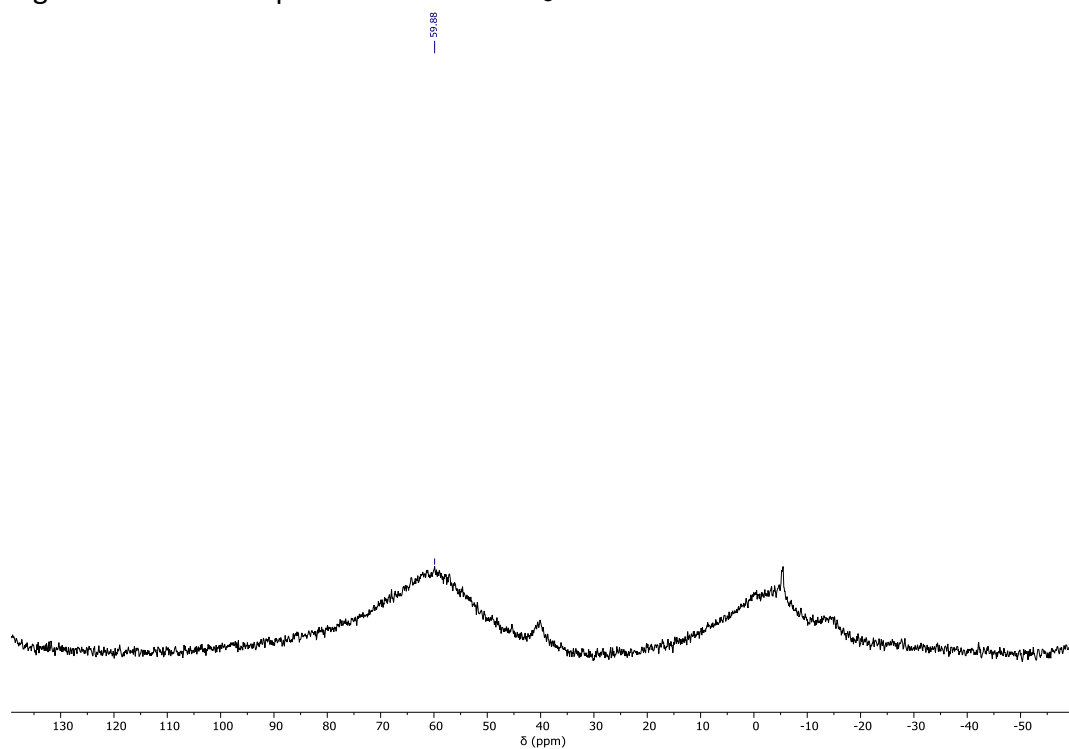
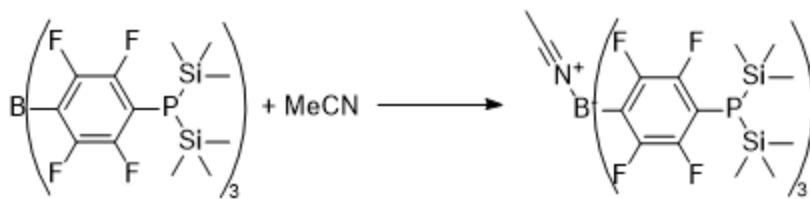


Figure S4. ^{11}B NMR spectrum of **1** in CDCl_3 .
(broad peak at 0 to -10 ppm is due to borosilicate glass).



Synthesis of (MeCN)B(C₆F₄P(SiMe₃)₂)₃ (**2**)

Compound **1** (0.050 g, 0.05 mmol) was dissolved in 2 mL of pentane. One drop (approximately 0.05 mL, 1.5 mmol), of acetonitrile was added to the yellow solution with strong stirring. The solution immediately turned colourless, and a fine white precipitate formed. After stirring for 5 minutes, this white powder was isolated by filtration and thoroughly washed with pentane. The isolated solid was then left in an open container for 2 h, to allow the remaining volatiles to evaporate. (47 mg, 0.046 mmol, 91%).

¹H NMR (400 MHz, CDCl₃): δ 2.66 (s, 3H, CH₃CN); 0.29 (d with ²⁹Si satellites, 54H, Si(CH₃)₃, ³J_{HP} = 6 Hz, ²J_{HSi} = 120 Hz). ¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ -126.9 (dt, P-C₆F₄, ³J_{PF} = 26 Hz, ³J_{FF} = 14 Hz); -135.0 (br s, B-C₆F₄). ³¹P{¹H} NMR (162 MHz, CDCl₃): δ -171.4 (t, ³J_{PF} = 14 Hz). ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -10.2 (br s, W_{1/2} ~ 628 Hz).

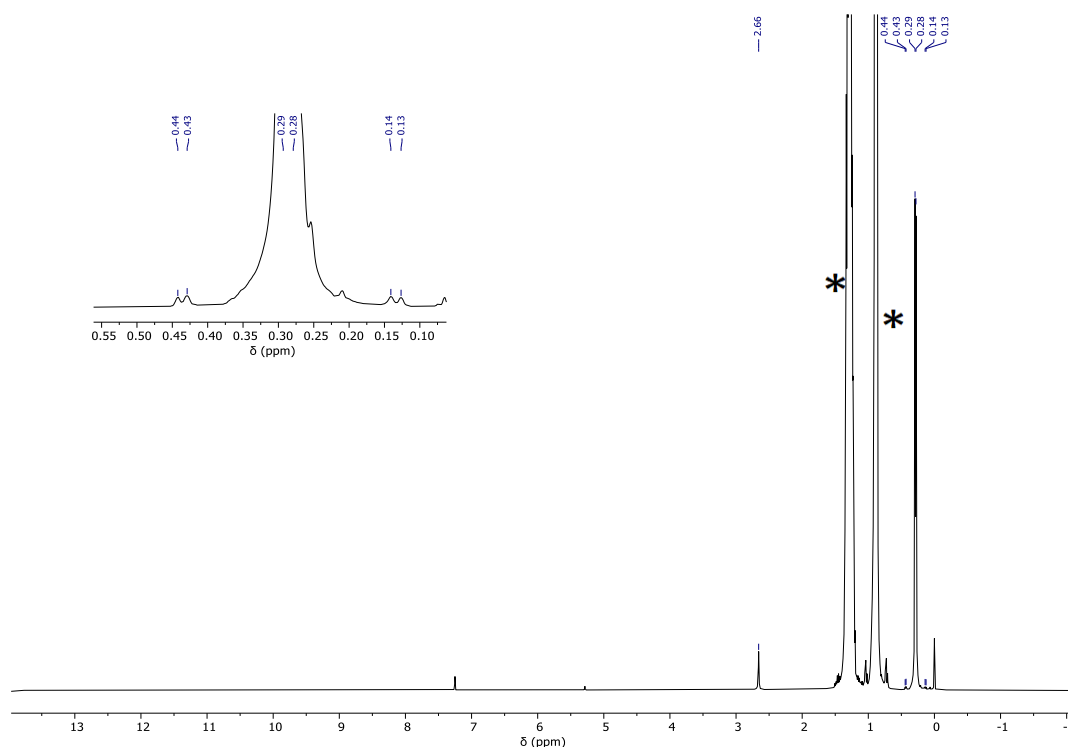
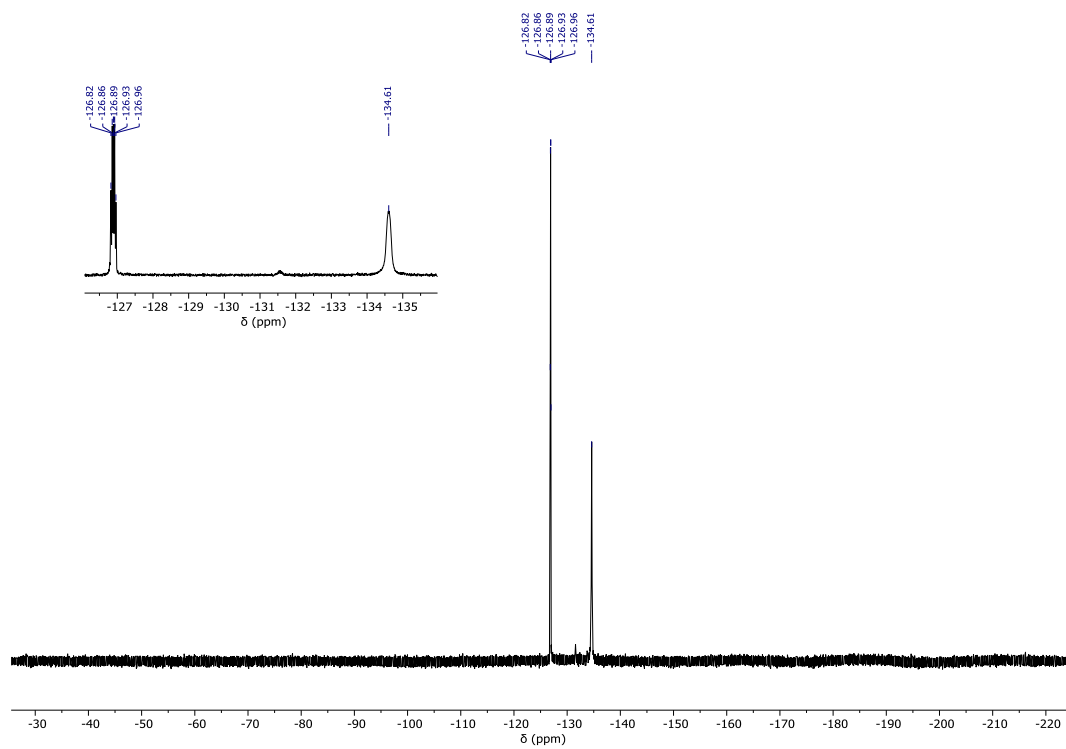
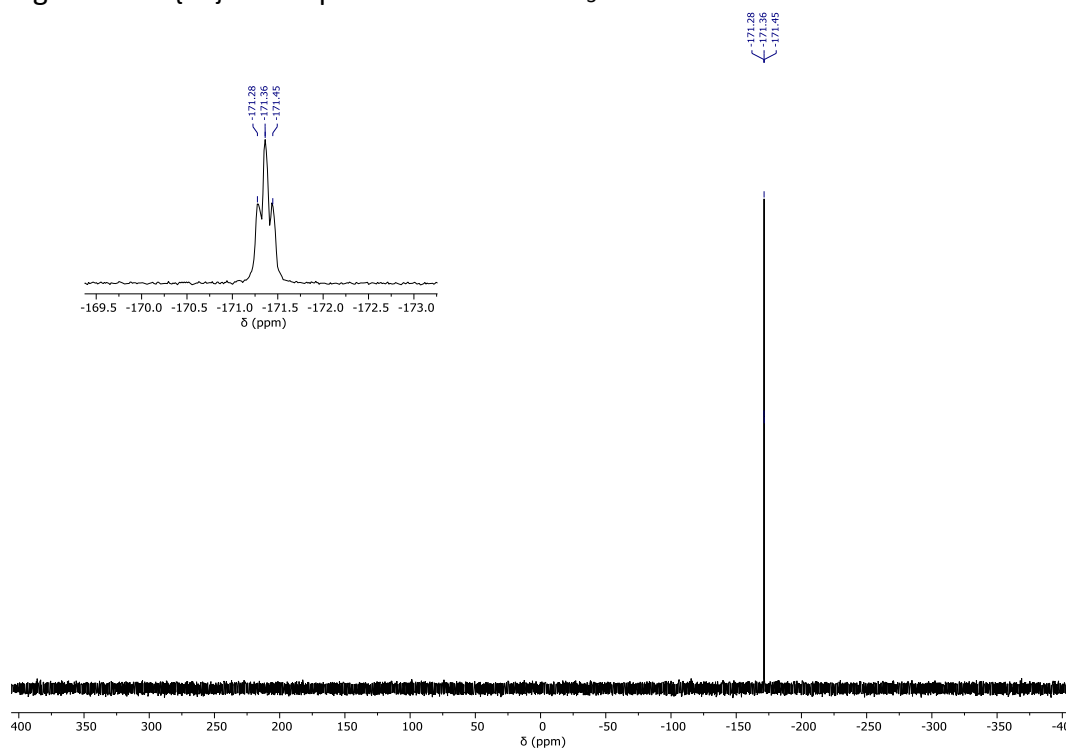
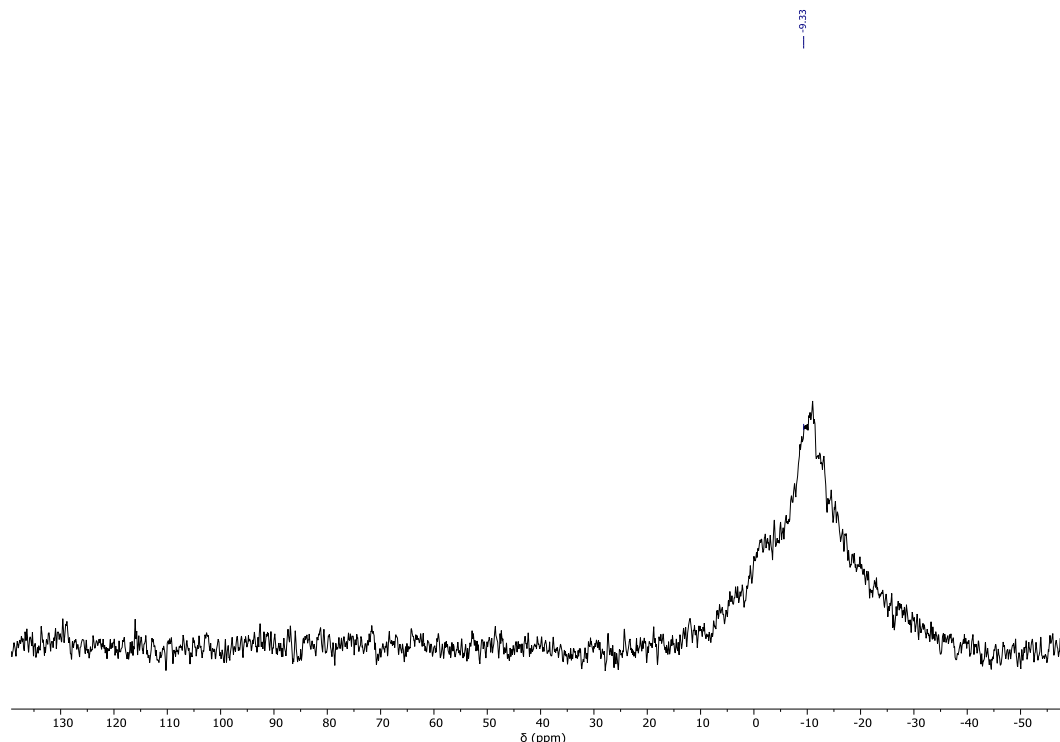
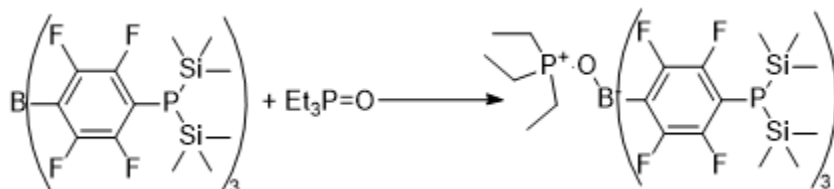


Figure S5 ¹H NMR Spectrum of **2** in CDCl₃

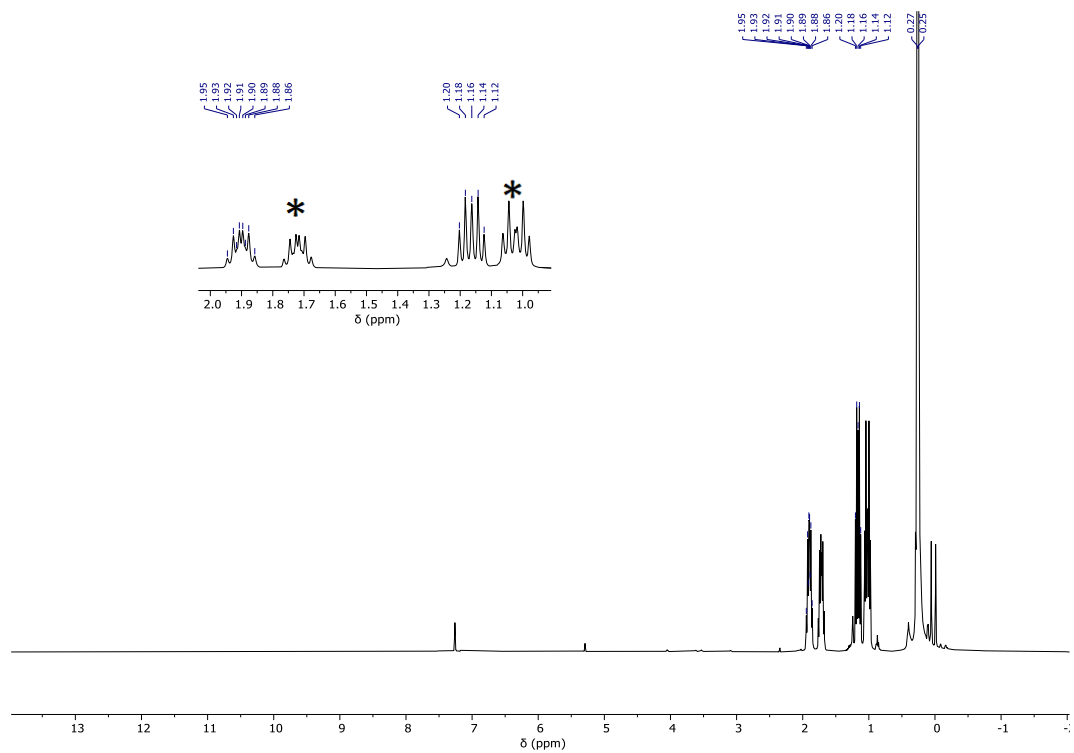
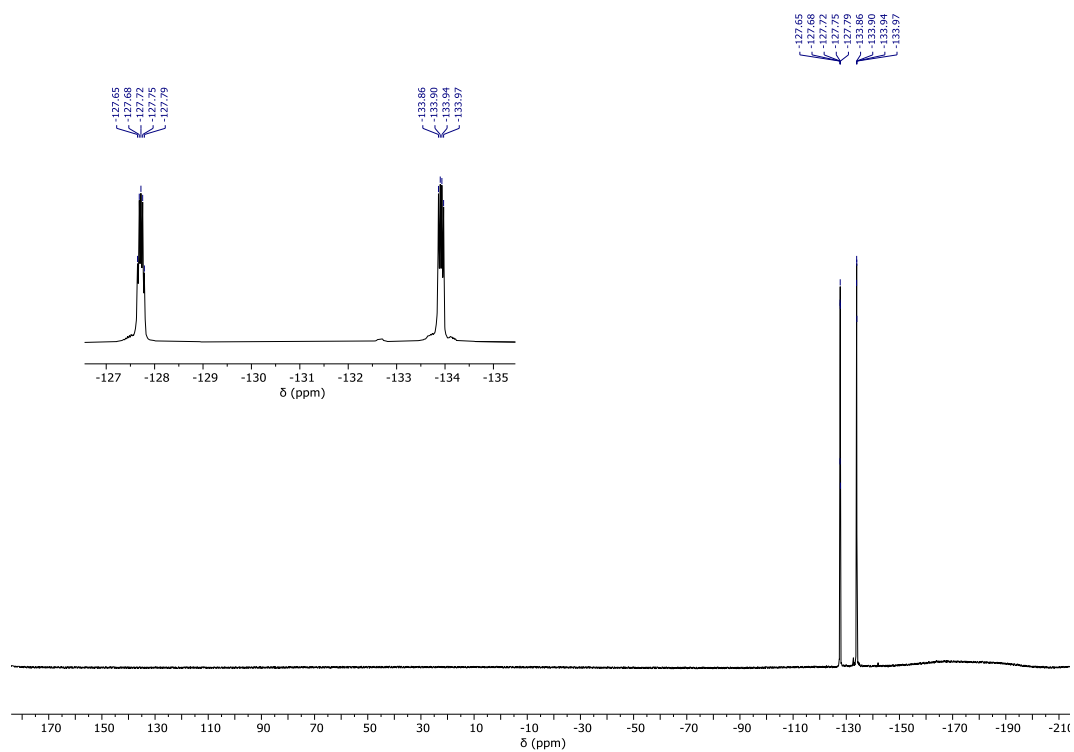
* Pentane

Figure S6 $^{19}\text{F}\{^1\text{H}\}$ NMR Spectrum of **2** in CDCl_3 Figure S7 $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of **2** in CDCl_3

Figure S8 ^{11}B NMR Spectrum of **2** in CDCl_3 **Synthesis of $(\text{Et}_3\text{PO})\text{B}(\text{C}_6\text{F}_4\text{P}(\text{SiMe}_3)_2)_3$ (**3**):**

Et_3PO (0.015 g, 0.11 mmol) and **1** (0.045g, 0.05 mmol) were each dissolved in 0.2 mL of CDCl_3 . These solutions were combined, and the bright yellow solution immediately turned colourless. NMR spectroscopy was taken of this reaction mixture without further purification, which showed quantitative conversion of **1** to **6**.

^1H NMR (400 MHz, CDCl_3): δ 1.18 (dq, 6H, PCH_2CH_3 , $^2J_{\text{HP}} = 12$ Hz, $^3J_{\text{HH}} = 7.7$ Hz); 0.45 (dt, 9H, PCH_2CH_3 , $^3J_{\text{HP}} = 19$ Hz, $^3J_{\text{HH}} = 8$ Hz); 0.25 (d, 54H, $^3J_{\text{HP}} = 5.5$ Hz). $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3): δ 73.6 (m, Et_3PO); -172.8 (t, PSiMe_3 , $^3J_{\text{PF}} = 13$ Hz). ^{19}F NMR (377 MHz, CDCl_3) δ -127.7 (dt, $^3J_{\text{FP}} = 27$, $^3J_{\text{FF}} = 14$ Hz), -133.9 (dd, $^3J_{\text{FP}} = 26$, $^3J_{\text{FF}} = 14$ Hz). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -2.4 (br, $W_{1/2} \sim 963$ Hz).

Figure S9. ^1H NMR Spectrum of **3** in C_6D_6 * Free Et_3PO Figure S10. ^{19}F NMR Spectrum of **3** in C_6D_6

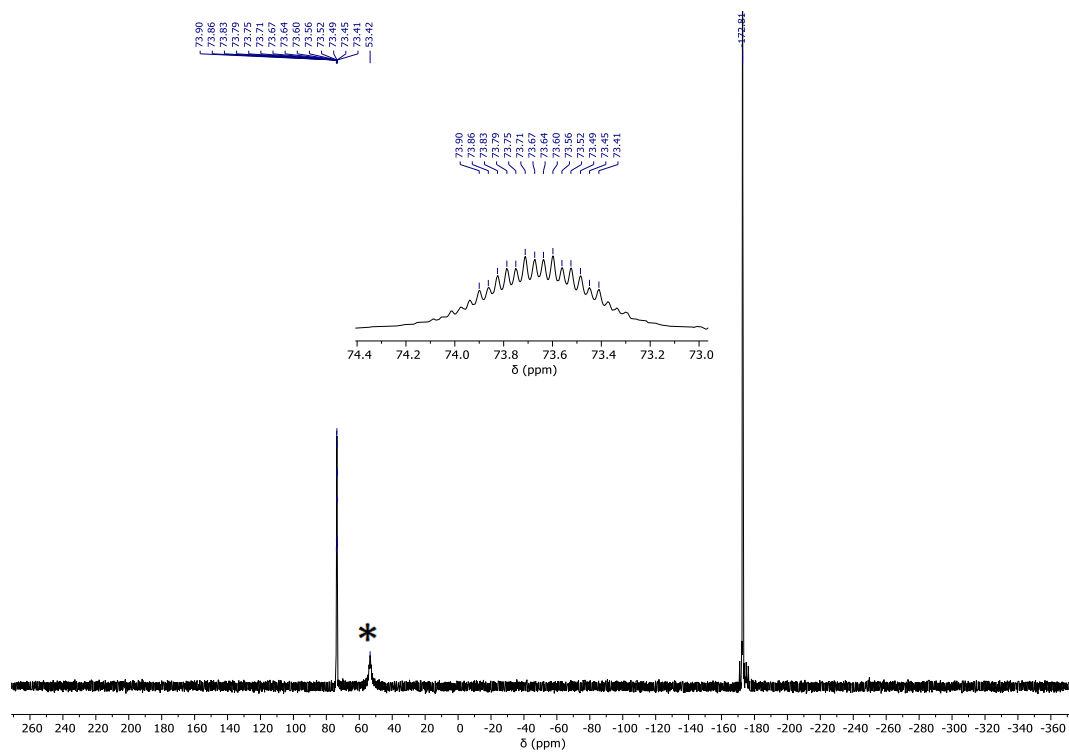


Figure S11. $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of **3** in C_6D_6

* Free Et_3PO

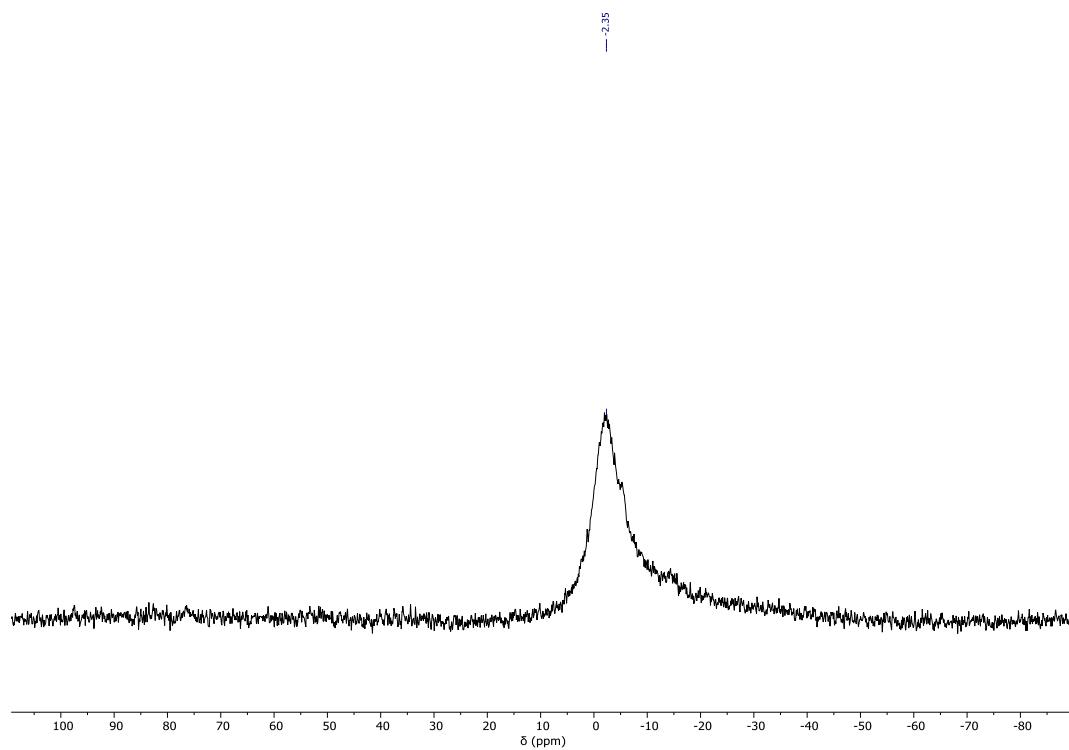
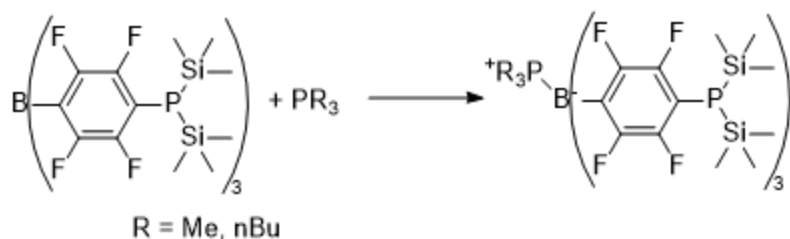


Figure S12. ^{11}B NMR Spectrum of **3** in C_6D_6



Synthesis of $(R_3P)B(C_6F_4P(SiMe_3)_2)_3$ (**R = Me 4, Bu 5**)

These compounds were prepared in a similar fashion and thus only one preparation is detailed. Compound **1** (0.012 g, 0.012 mmol) was dissolved in 3 mL of pentane. PMe_3 (0.05 g, 0.66 mmol) was added with strong stirring, and the yellow solution immediately turned colourless. This solution was put in the freezer for 2 days at $-10\text{ }^\circ\text{C}$, causing it to crystallize. The excess solvent was removed and the colourless crystals were washed with cold pentane and dried under vacuum (0.007g, 0.006 mmol, 54%).

4: ^1H NMR (400 MHz, CDCl_3): δ 1.37 (d, 9H, PMe_3 , $^3J_{\text{HP}} = 11$ Hz); 0.28 (d, 54H, $\text{Si}(\text{CH}_3)_3$, $^3J_{\text{HP}} = 6$ Hz). $^{19}\text{F}\{^1\text{H}\}$ NMR (377 MHz, CDCl_3) δ -126.8 (dt, 6F, $^3J_{\text{FF}} = 26$, 13 Hz), -130.0 (ddd, 6F, $^3J_{\text{FF}} = 26$, $^3J_{\text{PF}} = 13$, $^3J_{\text{HP}} = 6$ Hz). $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3) δ -6.4 (s, PMe_3); -171.5 (t, $^3J_{\text{PF}} = 13$ Hz). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3) δ -14.4 (s).

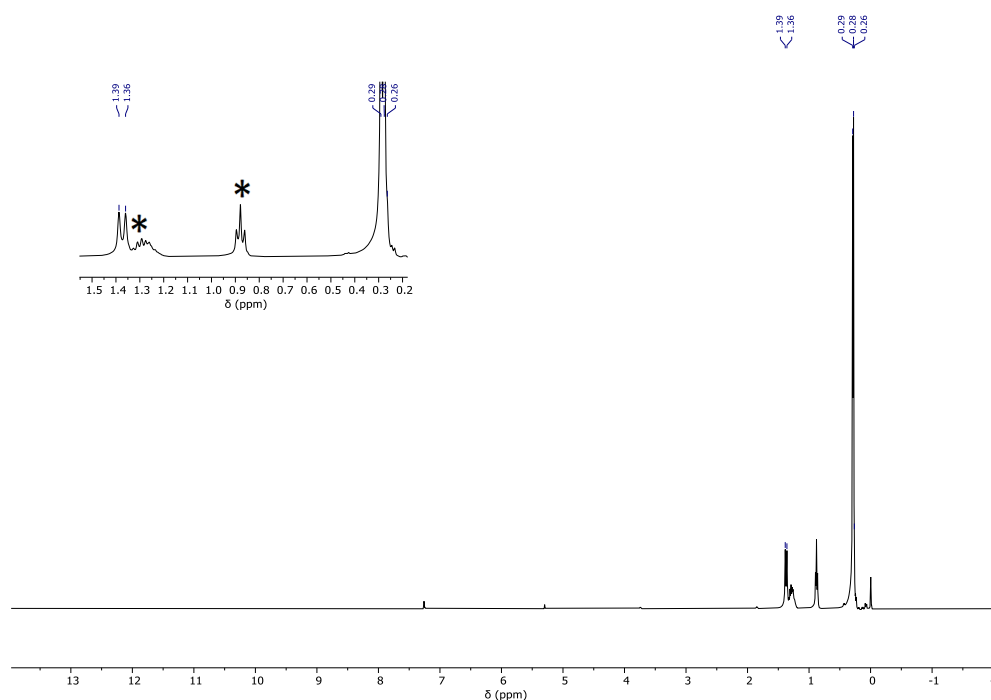
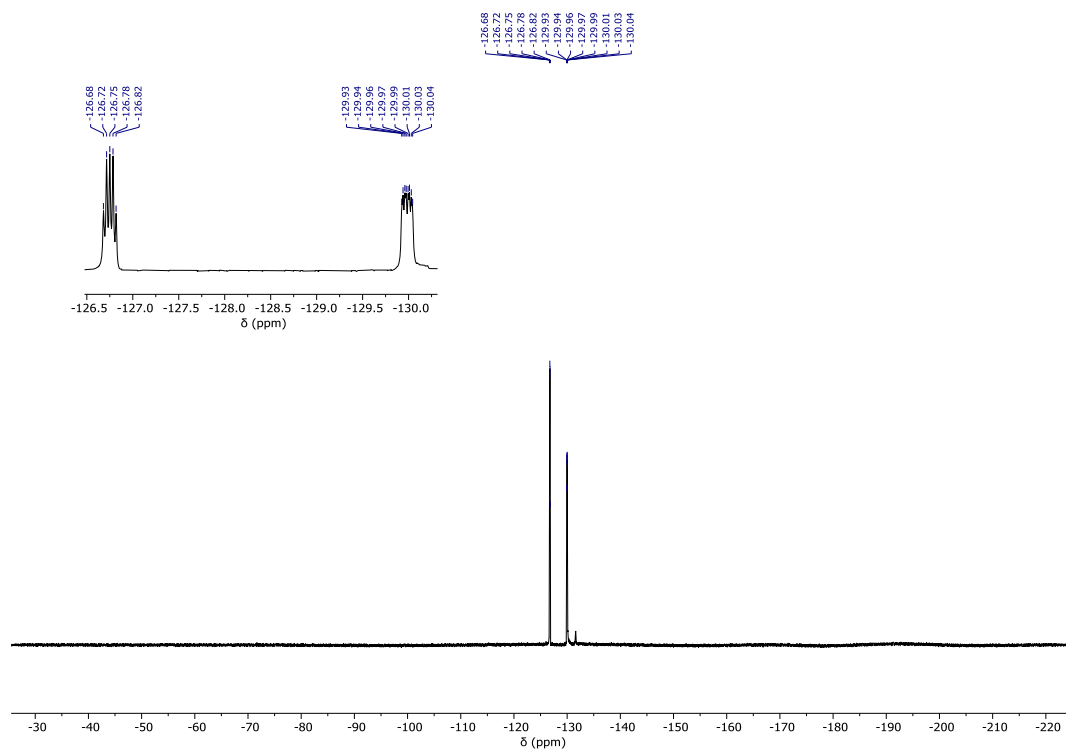
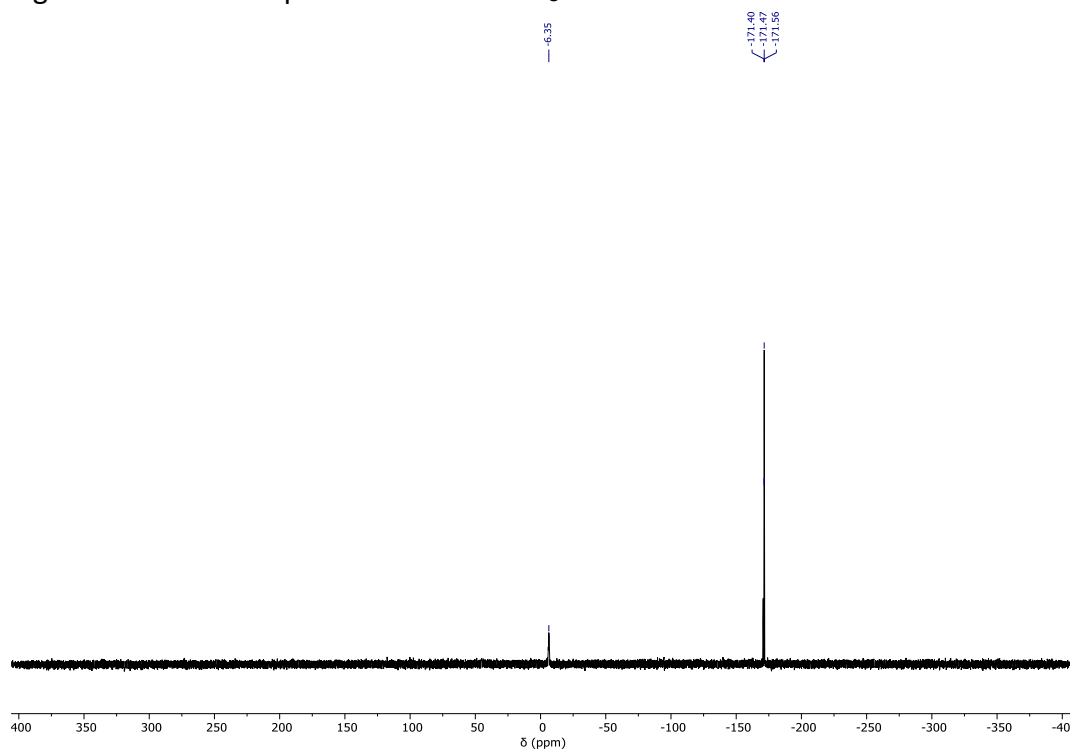


Figure S13 ^1H NMR Spectrum of **4** in CDCl_3

* pentane

Figure S14 ^{19}F NMR Spectrum of **4** in CDCl_3 Figure S15 $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of **4** in CDCl_3

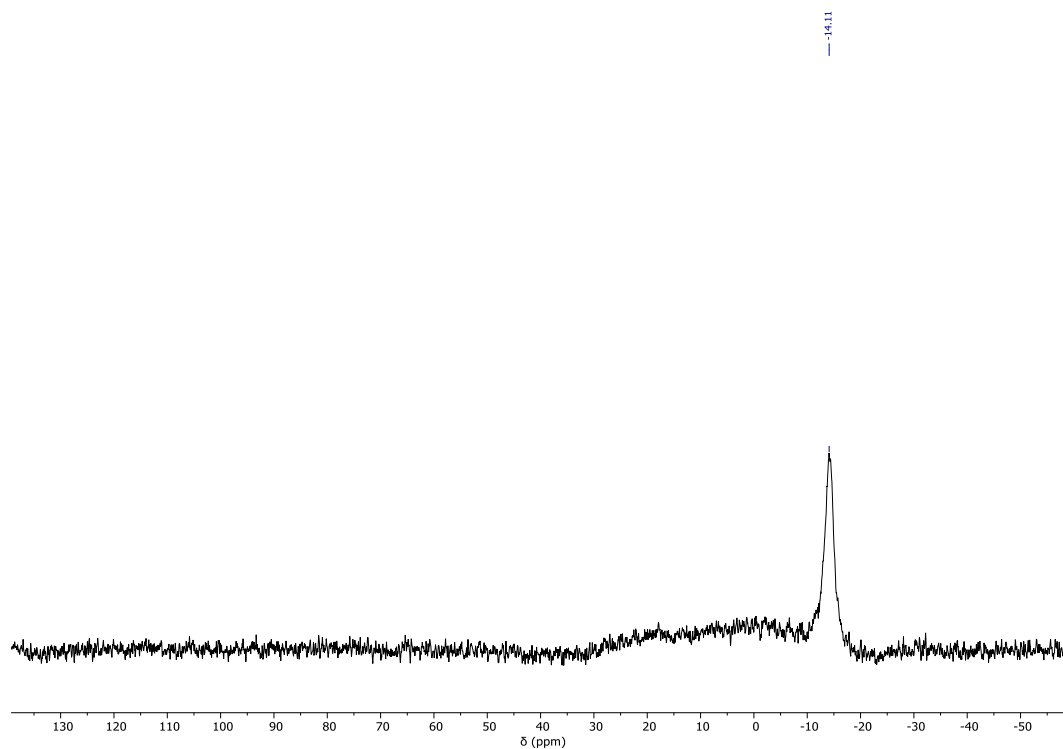
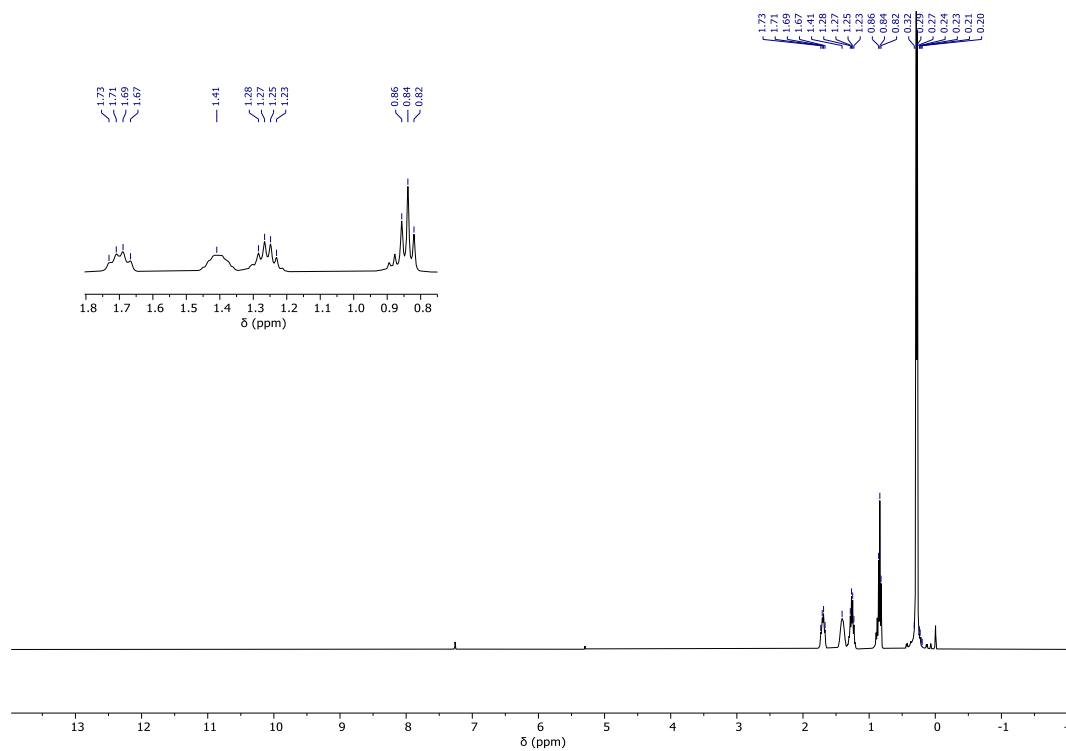
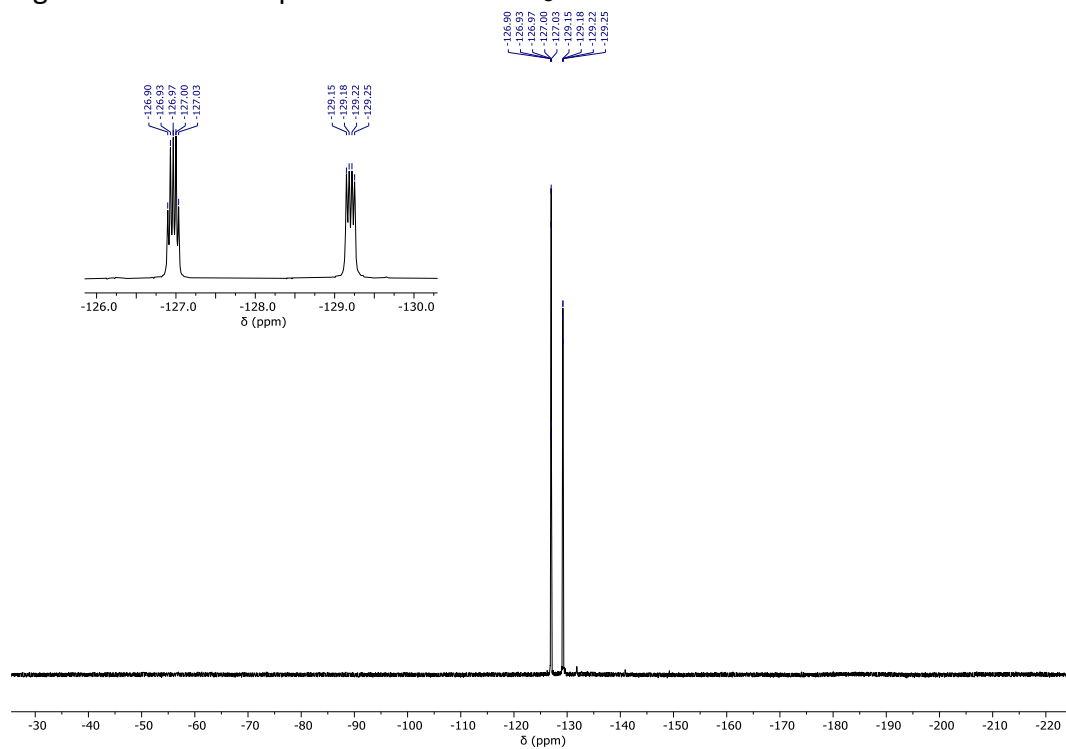
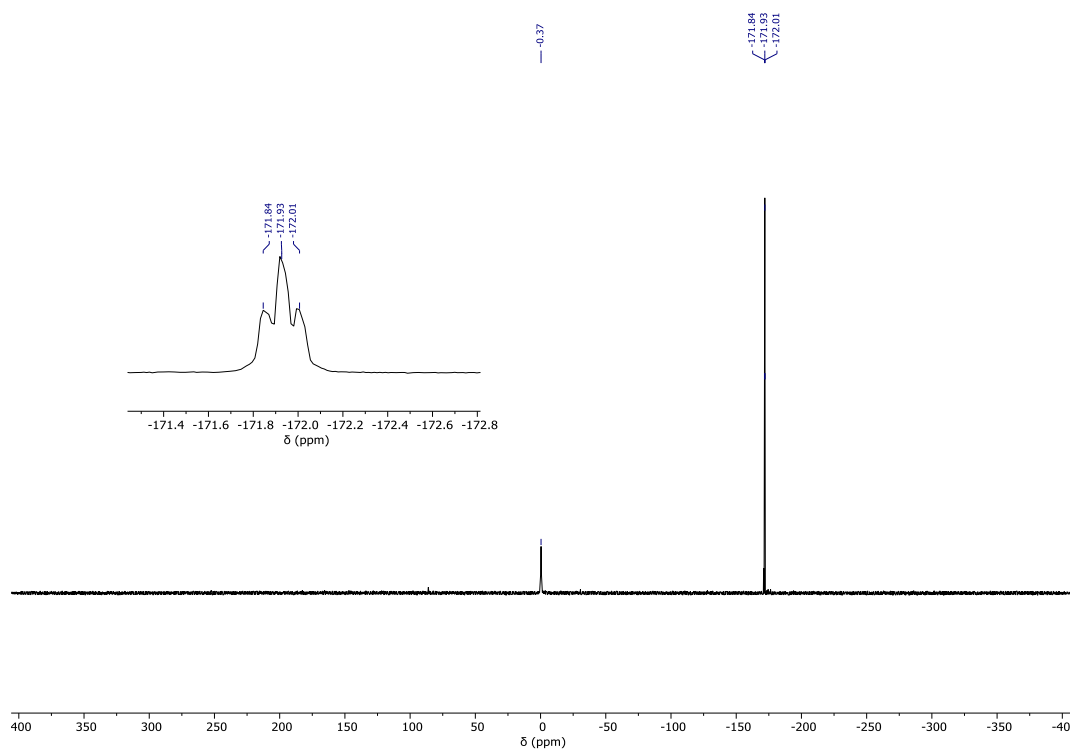
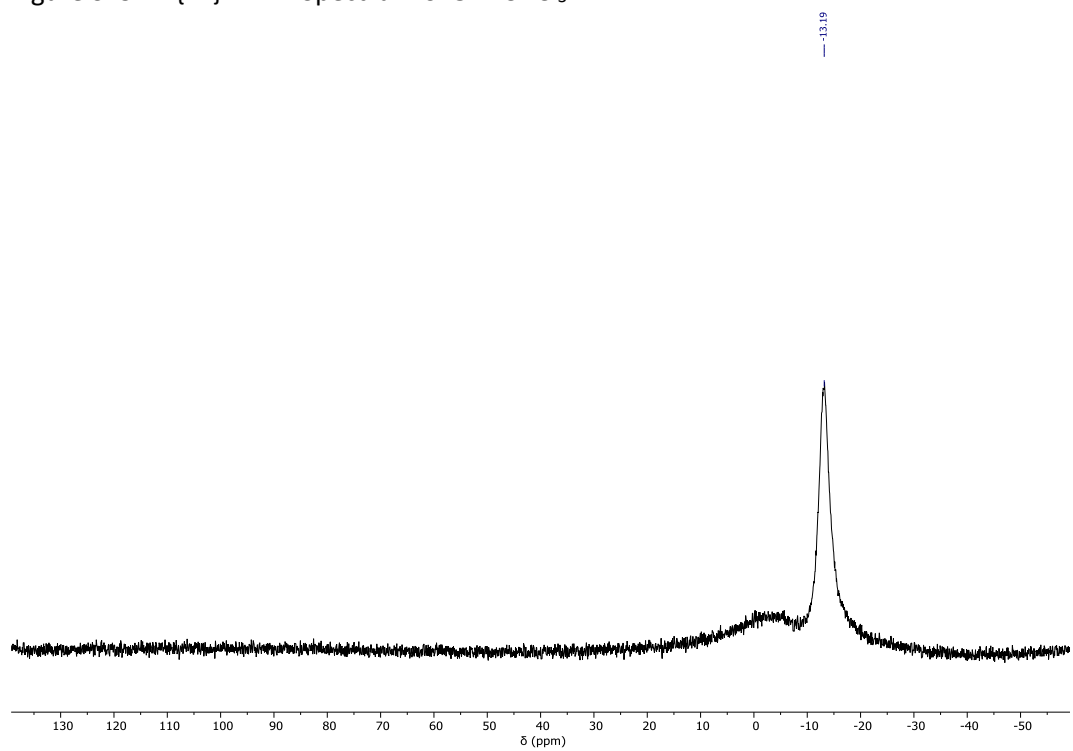
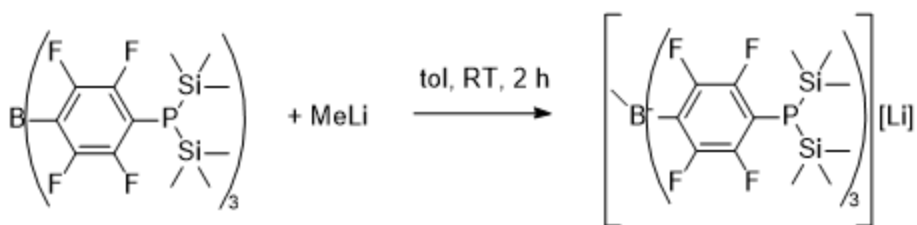


Figure S16 ^{11}B NMR Spectrum of **4** in CDCl_3

5: ^1H NMR (400 MHz, CDCl_3) δ 1.70 (m, 6H, C_4H_9), 1.47 – 1.34 (m, 6H, C_4H_9), 1.26 (q, 6H, $^3J_{\text{HH}} = 7$ Hz, C_4H_9), 0.84 (t, 9H, $^3J_{\text{HH}} = 7$ Hz, C_4H_9), 0.28 (d, 54H, $^3J_{\text{HP}} = 6$ Hz, $\text{P}(\text{Si}(\text{CH}_3)_3)_2$). $^{19}\text{F}\{^1\text{H}\}$ NMR (377 MHz, CDCl_3) δ -127.0 (dt, $^3J_{\text{FF}} = 26$ Hz, $^3J_{\text{FP}} = 13$ Hz), -129.2 (dd, $^3J_{\text{FF}} = 26$ Hz, $^3J_{\text{FP}} = 13$ Hz). ^{31}P NMR (162 MHz, CDCl_3) δ -0.4 (s, PnBu_3), -171.9 (t, $^3J_{\text{PF}} = 13$ Hz, $\text{P}(\text{Si}(\text{CH}_3)_3)_2$). ^{11}B NMR (128 MHz, CDCl_3) δ -13.2 (s).

Figure S17 ^1H NMR Spectrum of **5** in CDCl_3 Figure S18 ^{19}F NMR Spectrum of **5** in CDCl_3

Figure S19 $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of **5** in CDCl_3 Figure S20 ^{11}B NMR Spectrum of **5** in CDCl_3



Synthesis of [Li][MeB(C₆F₄P(SiMe₃)₂)₃] (**6**):

An aliquot of methyllithium (1.6 M in Et₂O, 0.2 mmol, 0.12 mL) was added to an empty vial equipped with a magnetic stir bar in the glovebox and immediately placed under vacuum until dry. The solid methyllithium was weighed, and a toluene solution (2 mL) of compound **1** (200 mg, 0.2 mmol) was added, causing the yellow solution to immediately turn colourless. After 2 h at room temperature, the solvent was removed *in vacuo*, the pale yellow solid was washed with cold pentane and dried under vacuum (107 mg, 0.11 mmol, 53%)

¹H NMR (400 MHz, Et₂O) δ 0.59 (s, 3H), 0.26 (d, *J* = 5.4 Hz, 54H). ³¹P NMR (162 MHz, Et₂O) δ -177.2 ¹⁹F{¹H} NMR (377 MHz, Et₂O) δ -130.7 (m), -131.5 (m). ¹¹B NMR (128 MHz, Et₂O) δ -14.0.

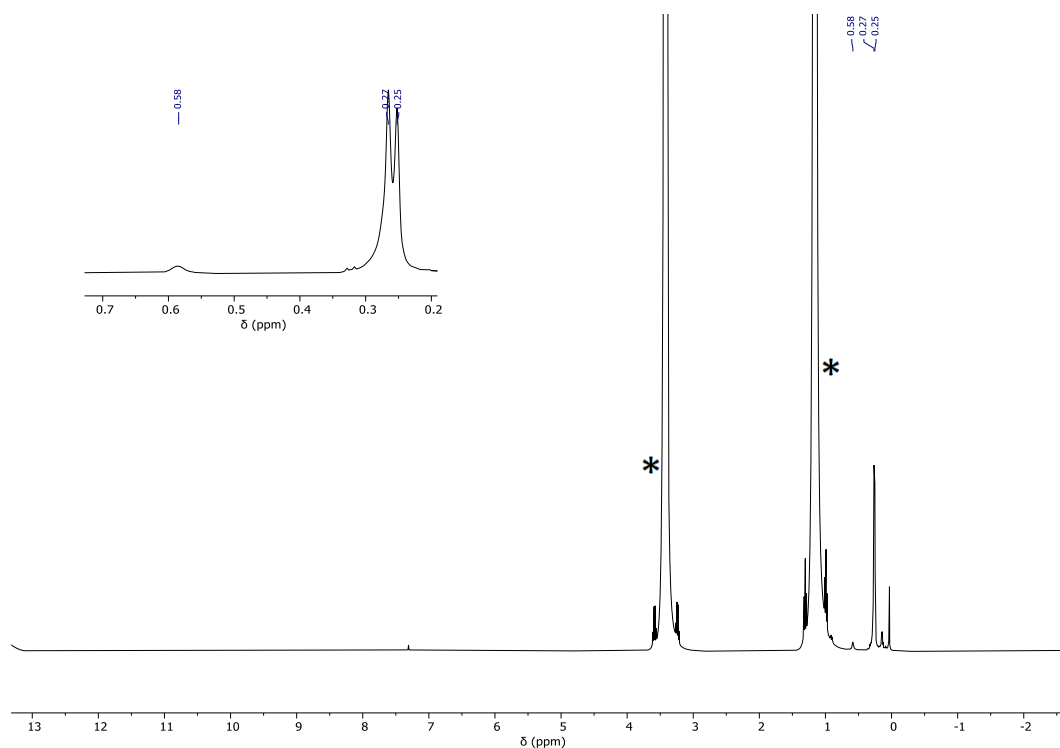
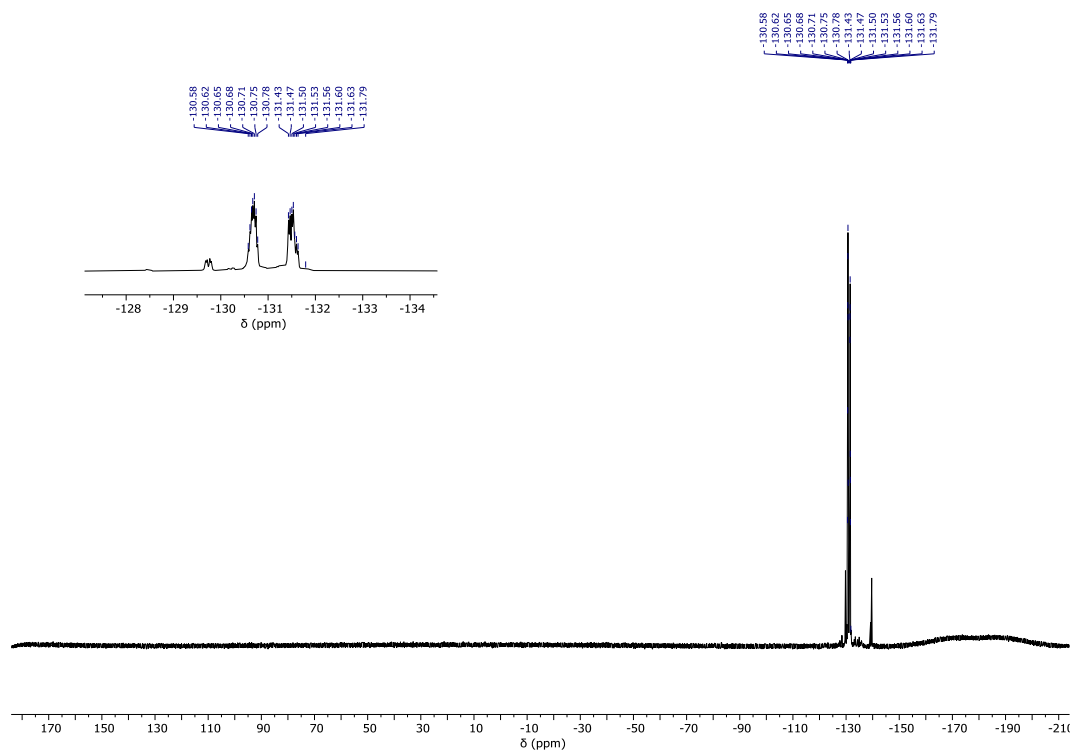
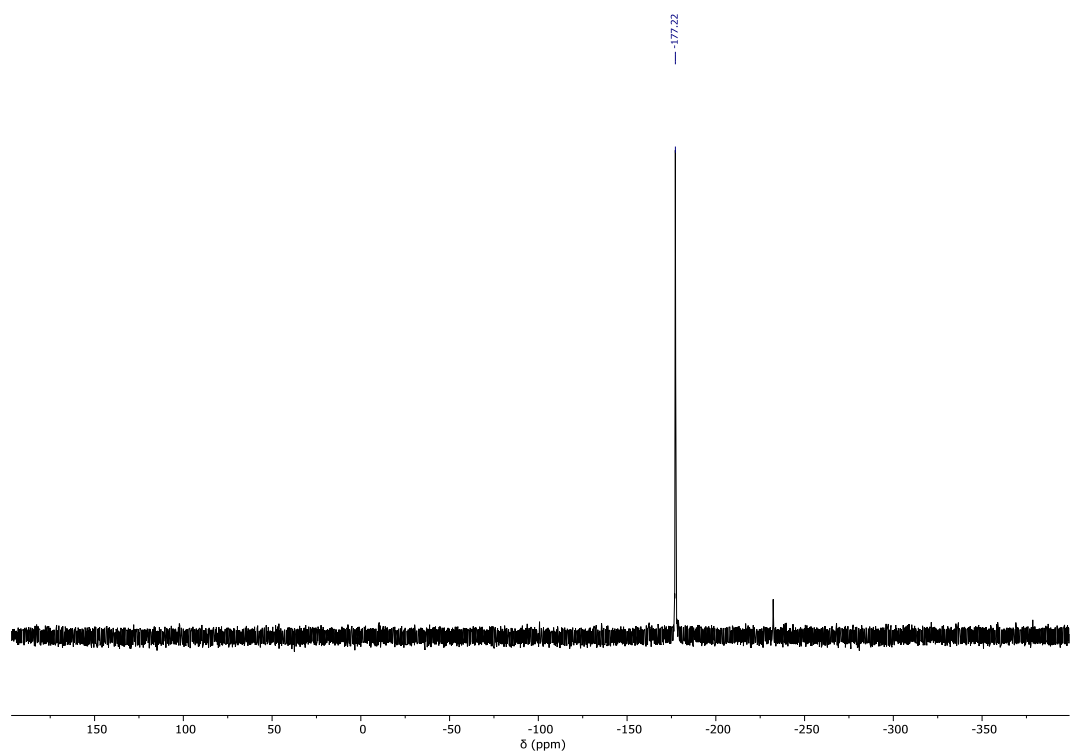
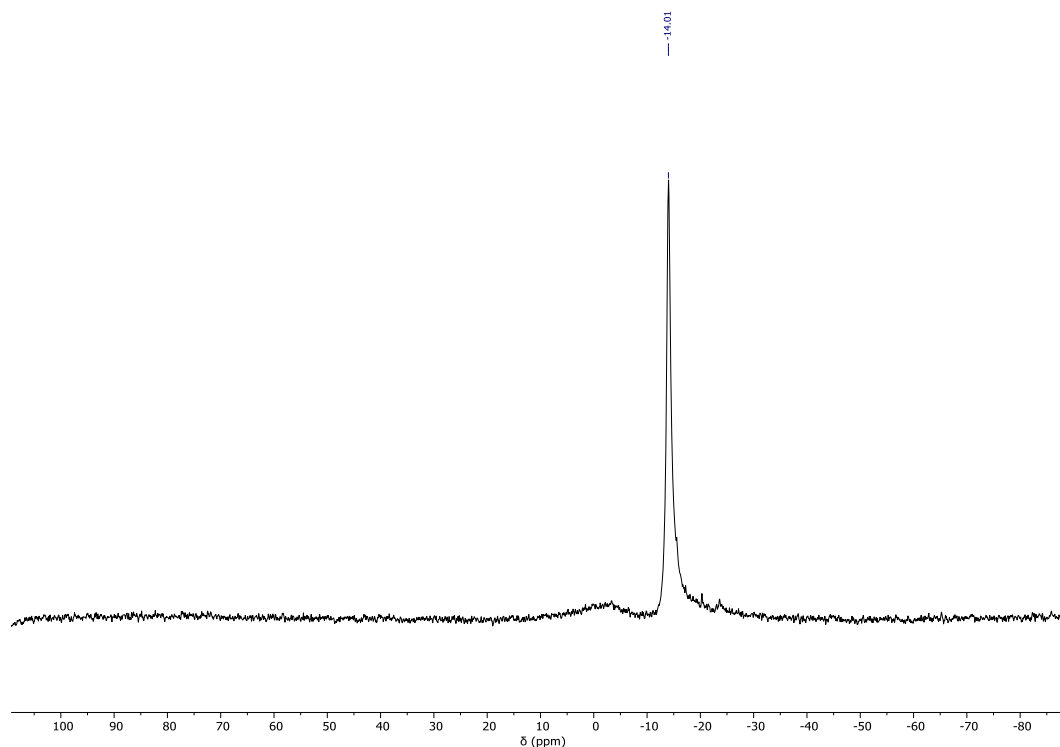
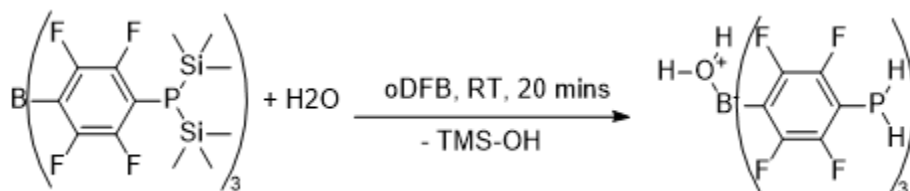


Figure S21. ¹H NMR spectrum of **6** in Et₂O

*Et₂O

Figure S22. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **6** in Et_2O Figure S23. ^{31}P NMR spectrum of **6** in Et_2O

Figure S24. ^{11}B NMR spectrum of **6** in Et_2O 

Synthesis of $(\text{H}_2\text{O})\text{B}(\text{C}_6\text{F}_4\text{PH}_2)_3$ (**7**):

BCF (0.2186 g, 0.427 mmol) and $\text{P}(\text{TMS})_3$ (0.3916 g, 1.56 mmol) were dissolved in oDFB and stirred for 4 days, forming a bright yellow solution of **1**. Under a nitrogen atmosphere, degassed distilled water (0.5 mL, 27.8 mmol) was added to the solution with strong stirring, immediately turning the bright yellow solution colourless. After 20 minutes of strong stirring, all volatiles were removed under vacuum, yielding a white powder. (0.195 g, 0.341 mmol, 79.8% yield).

After drying under vacuum, the white powder is no longer soluble in oDFB although it does dissolve effectively in coordinating solvents such as Et_2O , THF, and acetonitrile.

7. ^1H NMR (400 MHz, C_6D_6) δ 3.81 (dt, $^1J_{\text{HP}} = 209$, $^4J_{\text{HF}} = 4$ Hz). ^{19}F NMR (377 MHz, C_6D_6) δ -131.8 (ddd, $^3J_{\text{FF}} = 24$, 13 Hz, $^4J_{\text{FH}} = 4$ Hz), -134.8 (dd, $^3J_{\text{FF}} = 24$, 13 Hz). ^{31}P NMR (162 MHz, C_6D_6) δ -174.3 (t, $^1J_{\text{PH}} = 209$ Hz). ^{11}B NMR (128 MHz, C_6D_6): δ -1.2. HRMS [$\text{C}_{18}\text{H}_6\text{BO}_2\text{F}_{12}\text{P}_3$] $^+$ Calculated mass: 585.949. Measured mass: 585.949.

If D₂O is used instead of distilled water, compound **7_d** forms. This compound has no peaks in the ¹H NMR spectrum, and is identical to compound **7** in the ¹⁹F and ¹¹B NMR spectra. The ³¹P{¹H} NMR spectrum shows that the PD₂ species has formed instead of the PH₂.

7_d. ³¹P{¹H} NMR (162 MHz, C₆H₆) δ -178.9 (t, ¹J_{PD} = 32 Hz, PDH), -179.7 (p, ¹J_{PD} = 32 Hz, PD₂).

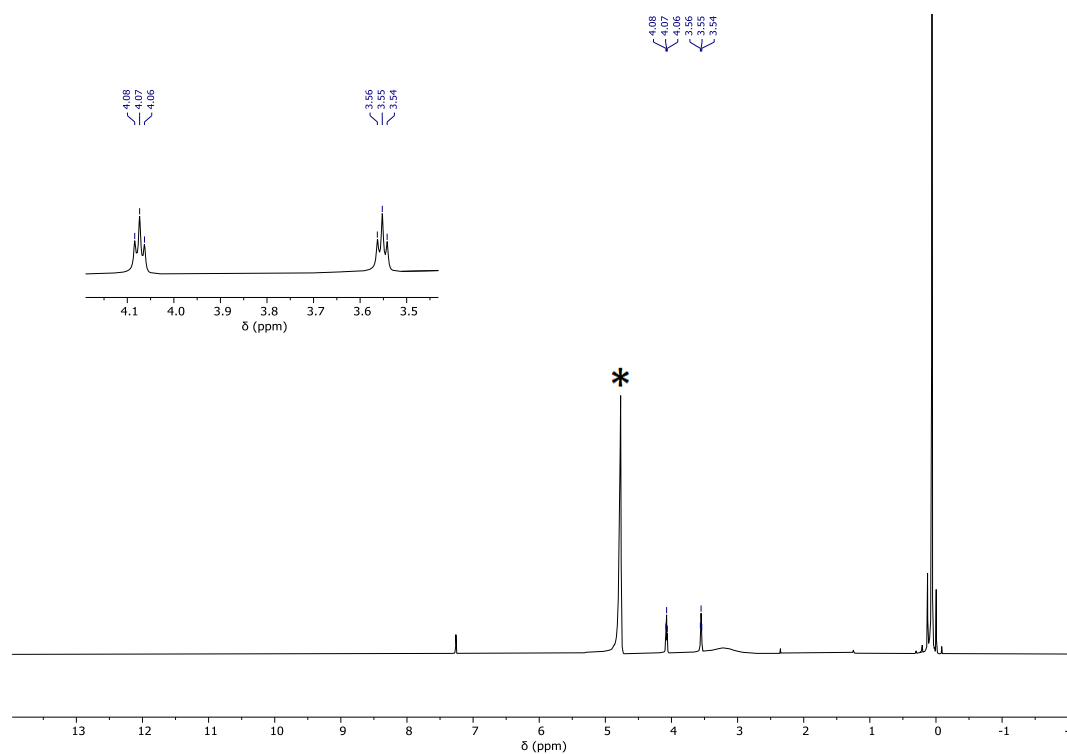
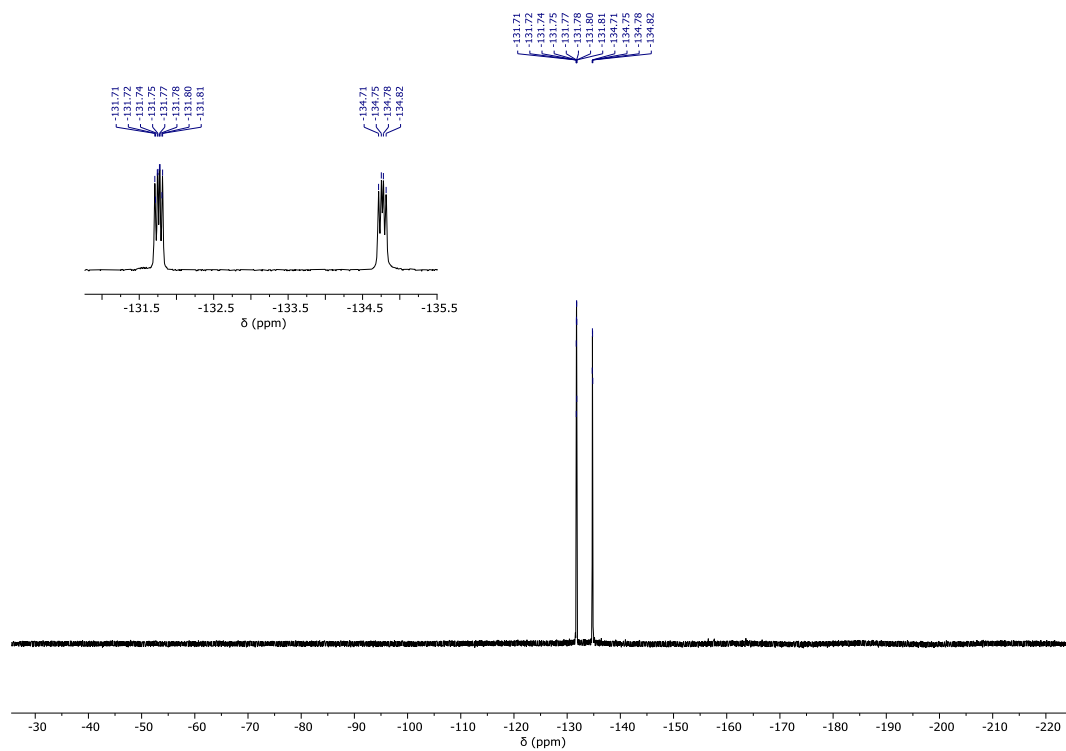
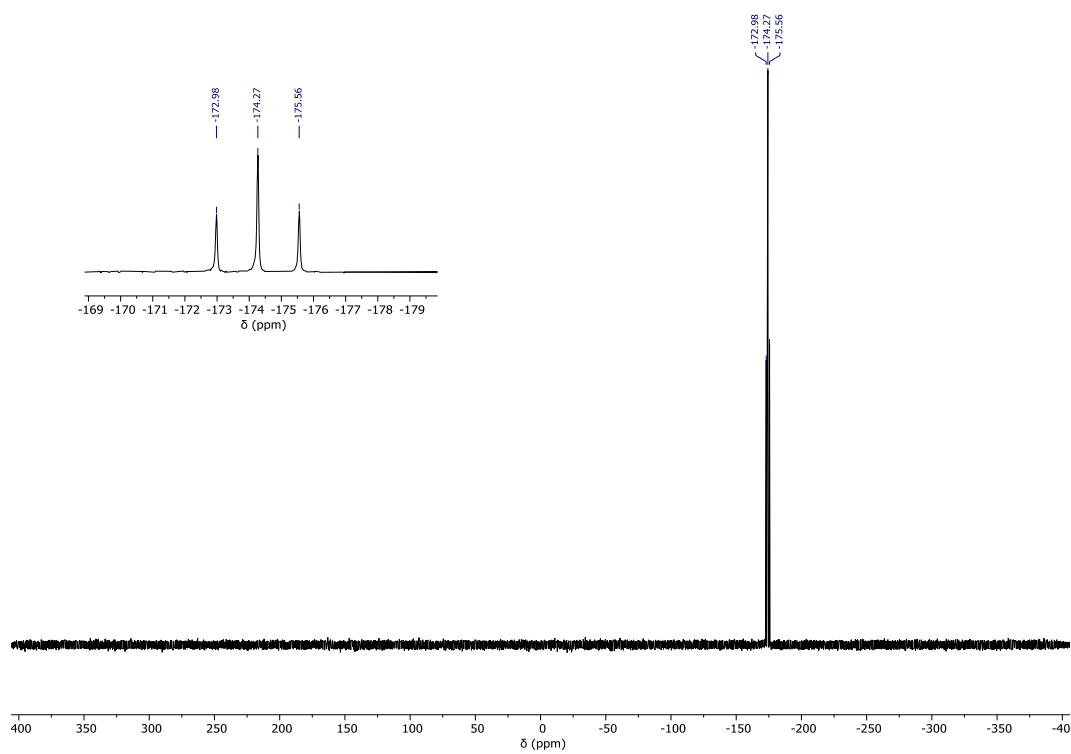
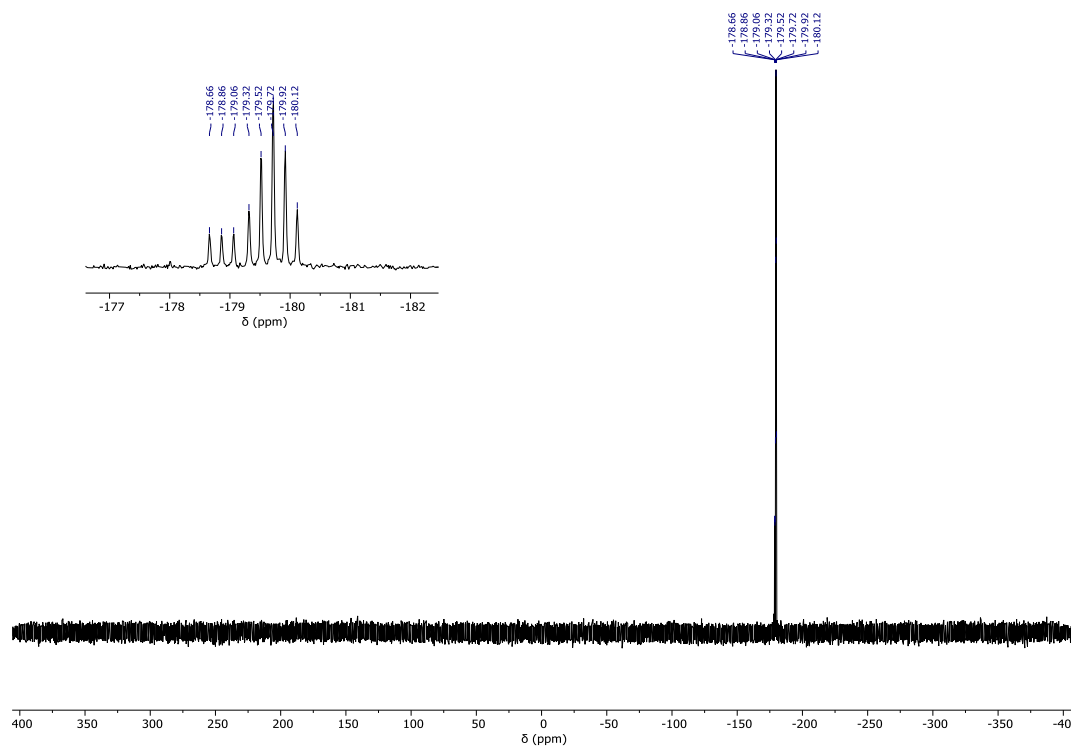
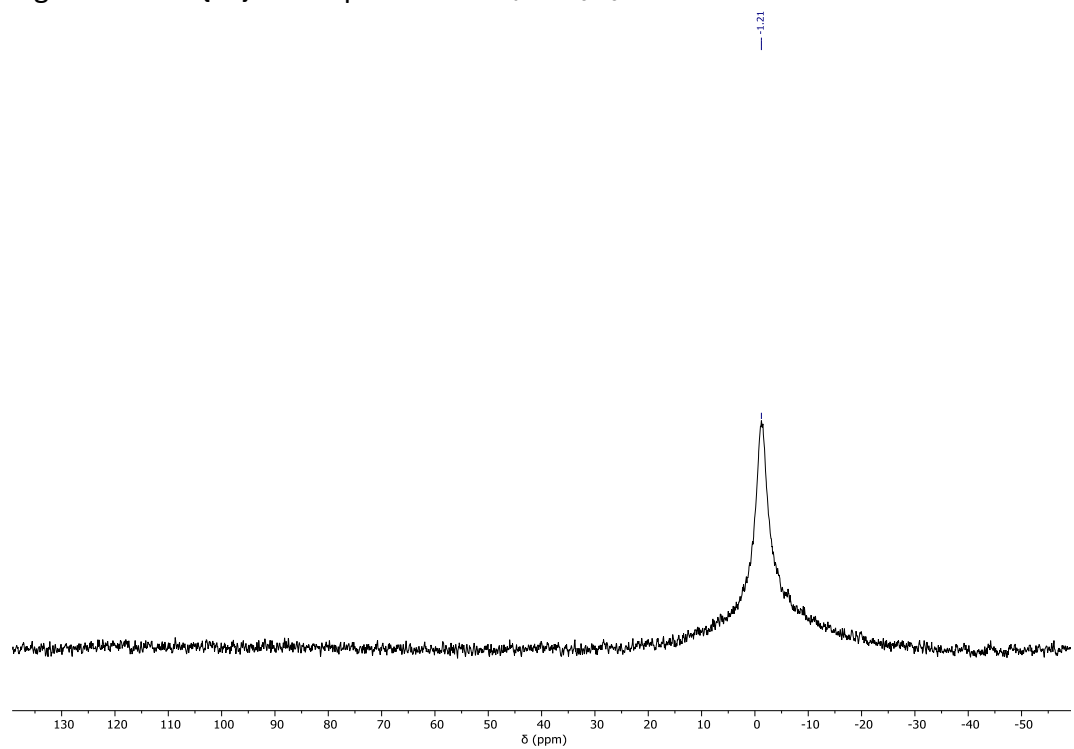
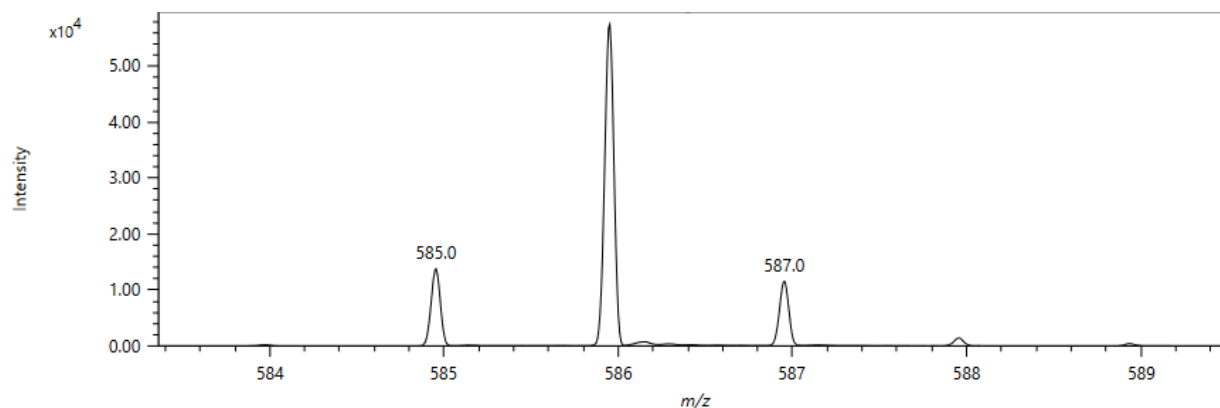


Figure S25. ¹H NMR spectrum of **7** in C₆D₆

* DCM

Figure S26. ^{19}F NMR spectrum of **7** in C_6D_6 Figure S27. ^{31}P NMR spectrum of **7** in C_6D_6

Figure S28. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **7d** in C_6D_6 Figure S29. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **7** in C_6D_6

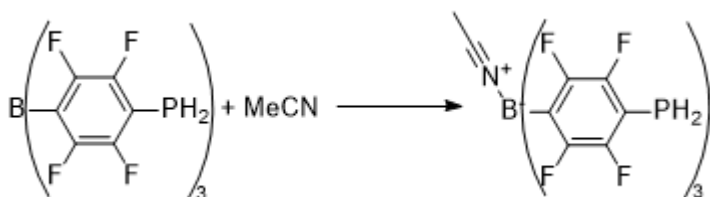


Elemental Composition

| Parameters | | Elements Set 1: | | | | | | | |
|------------|--------------|-----------------|-----|-----|----|----|---|----|---|
| Tolerance: | ±10.00 mDa | Symbol | C | H | O | N | B | F | P |
| Electron: | Odd | Min | 0 | 0 | 0 | 0 | 1 | 12 | 3 |
| Charge: | -1 | Max | 100 | 200 | 20 | 10 | 1 | 12 | 3 |
| DBE: | -1.5 - 100.0 | | | | | | | | |

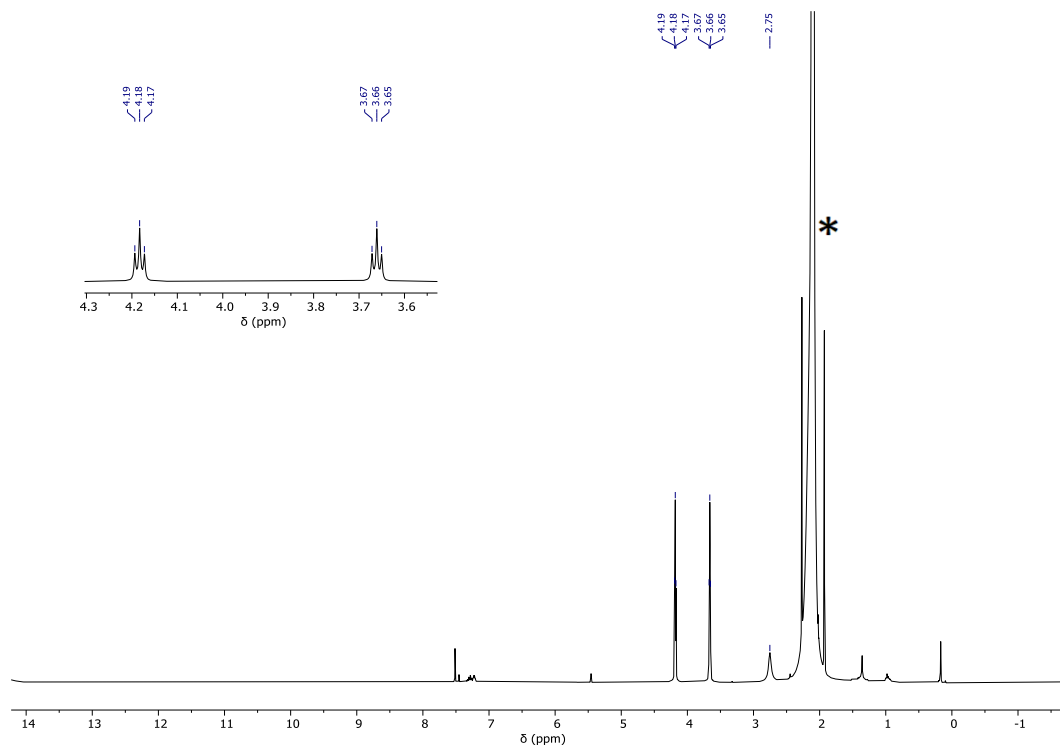
Results

| Mass | Intensity | Formula | Calculated Mass | Mass Difference [mDa] | Mass Difference [ppm] | DBE |
|-----------|-----------|-----------------------|-----------------|-----------------------|-----------------------|------|
| 585.94868 | 57440.71 | C18 H6 B O2 F12 P3 | 585.94876 | -0.07 | -0.12 | 12.0 |
| | | C2 H6 B N8 O7 F12 P3 | 585.94792 | 0.76 | 1.30 | 0.0 |
| | | C6 H10 B N2 O9 F12 P3 | 585.95061 | -1.92 | -3.28 | -1.0 |
| | | C14 H2 B N6 F12 P3 | 585.94607 | 2.61 | 4.46 | 13.0 |
| | | C7 H6 B N6 O5 F12 P3 | 585.95194 | -3.26 | -5.56 | 4.0 |
| | | C13 H6 B N2 O4 F12 P3 | 585.94473 | 3.95 | 6.74 | 8.0 |

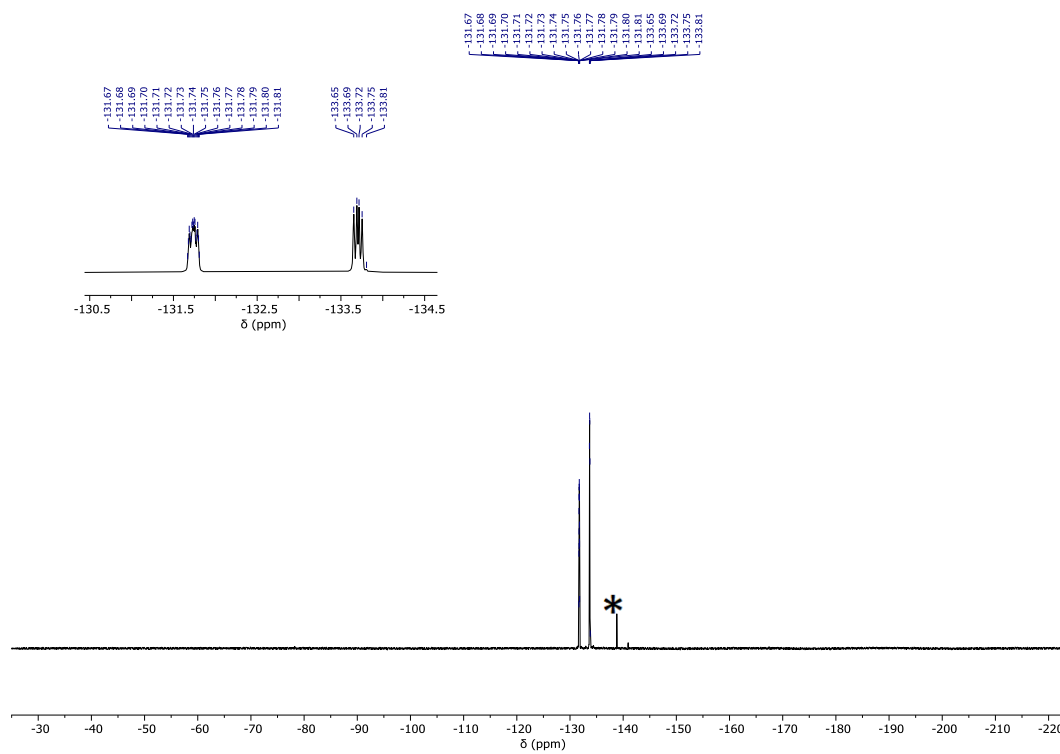
Figure S30. HRMS of **7**.**Synthesis of (MeCN)B(C₆F₄PH₂)₃ (**8**):**

Compound **7** (45 mg, 0.0787 mmol) was stirred in 1 mL of dry acetonitrile for 2 h at room temperature. The solvent was removed *in vacuo*, the solid was washed with 2 mL cold pentane and dried, yielding a white powder. (46 mg, 0.0773 mmol, 98 % yield)

¹H NMR (400 MHz, CDCl₃) δ 3.92 (dt, ¹J_{HP} = 209, ³J_{HF} = 4 Hz, 1H), 2.75 (br s, CH₃CN-B). ¹⁹F NMR (377 MHz, CDCl₃) δ -131.6 – -131.9 (m), -133.7 (dd, ³J_{FF} = 24, 14 Hz). ³¹P NMR (162 MHz, CDCl₃) δ -175.1 (t, ¹J_{PH} = 209 Hz). ¹¹B NMR (128 MHz, CDCl₃) δ -10.8.

Figure S31. ^1H NMR spectrum of **8** in $\text{CDCl}_3/\text{MeCN}$

* Free MeCN

Figure S32. ^{19}F NMR spectrum of **8** in $\text{CDCl}_3/\text{MeCN}$

* oDFB

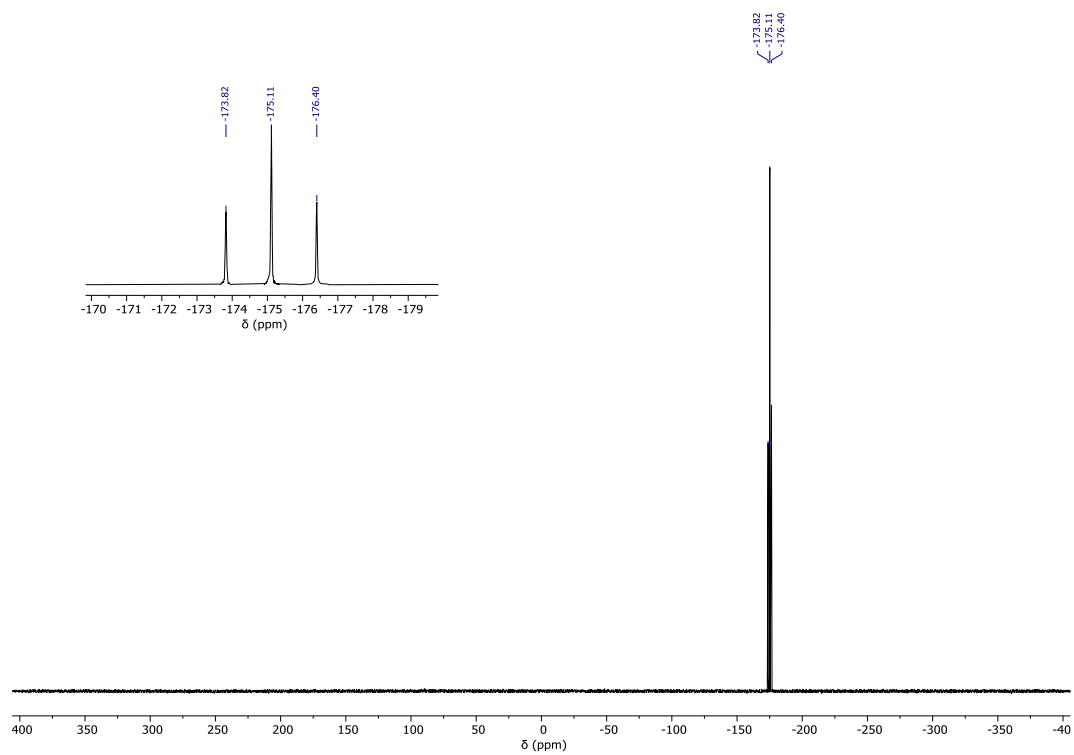


Figure S33. ^{31}P NMR spectrum of **8** in $\text{CDCl}_3/\text{MeCN}$

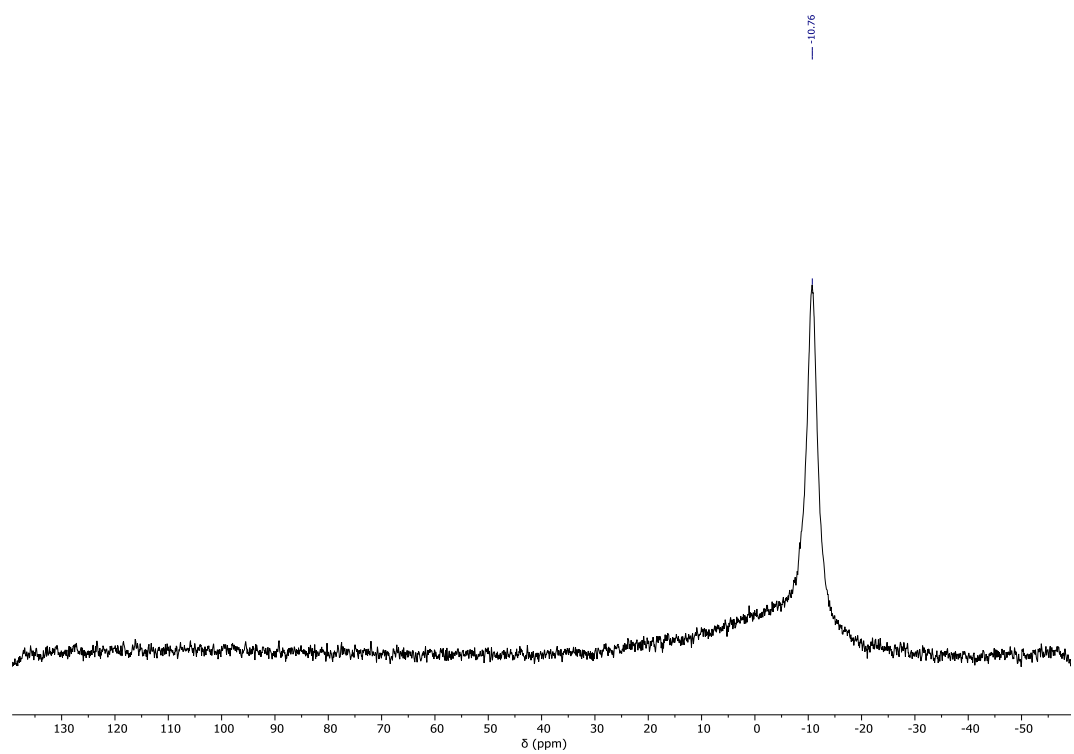
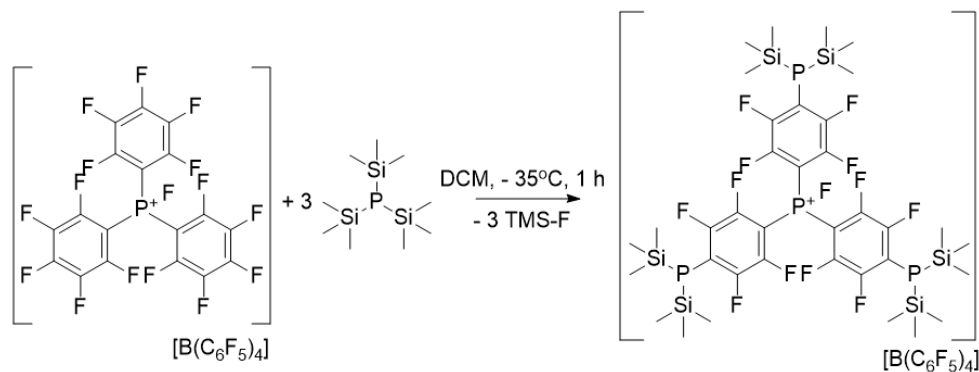


Figure S34. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **8** in $\text{CDCl}_3/\text{MeCN}$



Synthesis of $[\text{PF}(\text{C}_6\text{F}_4\text{P}(\text{SiMe}_3)_2)_3][\text{B}(\text{C}_6\text{F}_5)_4]$ (**9**):

$[\text{PF}(\text{C}_6\text{F}_5)_3][\text{B}(\text{C}_6\text{F}_5)_4]$ (80 mg, 0.065 mmol) and $\text{P}(\text{TMS})_3$ (47.5 mg, 0.190 mmol) were dissolved in DCM and the solutions were cooled to -35°C . They were then combined with strong stirring and allowed to warm to room temperature. All volatiles were removed under vacuum, and the product was washed with pentane, yielding a bright orange powder (95 mg, 0.056 mmol, 88%).

^1H NMR (400 MHz, CDCl_3) δ 0.38 (d, 54H, $\text{Si}(\text{CH}_3)_3$, $^3J_{\text{HP}} = 6$ Hz). ^{19}F NMR (377 MHz, CDCl_3) δ -115.9 (d, PF, $^1J_{\text{FP}} = 1050$ Hz), -116.5 (s, C_6F_4), -129.1 (s, C_6F_4), -133.1 (s, ortho- BC_6F_5), -163.9 (t, $^3J_{\text{FF}} = 20$ Hz, para- BC_6F_5), -167.7 (s, meta- BC_6F_5). $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3) δ 62.6 (d, PF, $^1J_{\text{PF}} = 1040$ Hz), -139.4 (s, $\text{P}(\text{SiMe}_3)_2$). ^{11}B NMR (128 MHz, CDCl_3) δ -16.7 (s, $\text{B}(\text{C}_6\text{F}_5)_4$). Calcd. for $\text{C}_{60}\text{H}_{54}\text{BF}_{33}\text{P}_4\text{Si}_6$ (1704.14): C 42.26%, H 3.19%. Found: C 42.29%, H 2.96%.

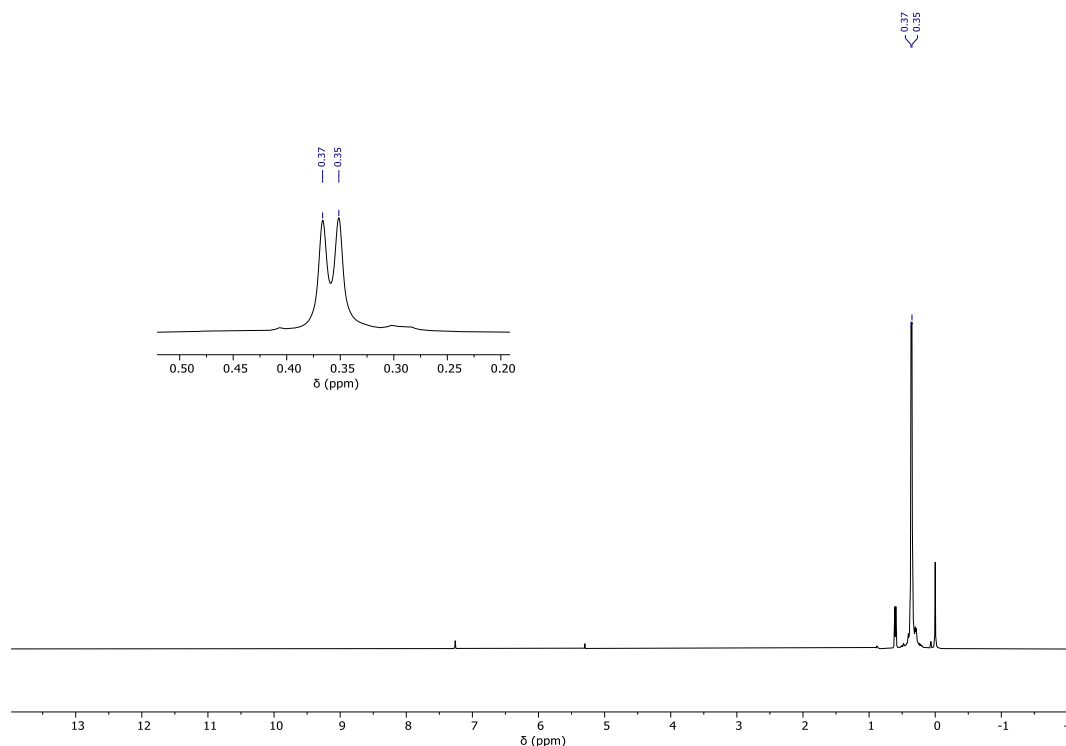
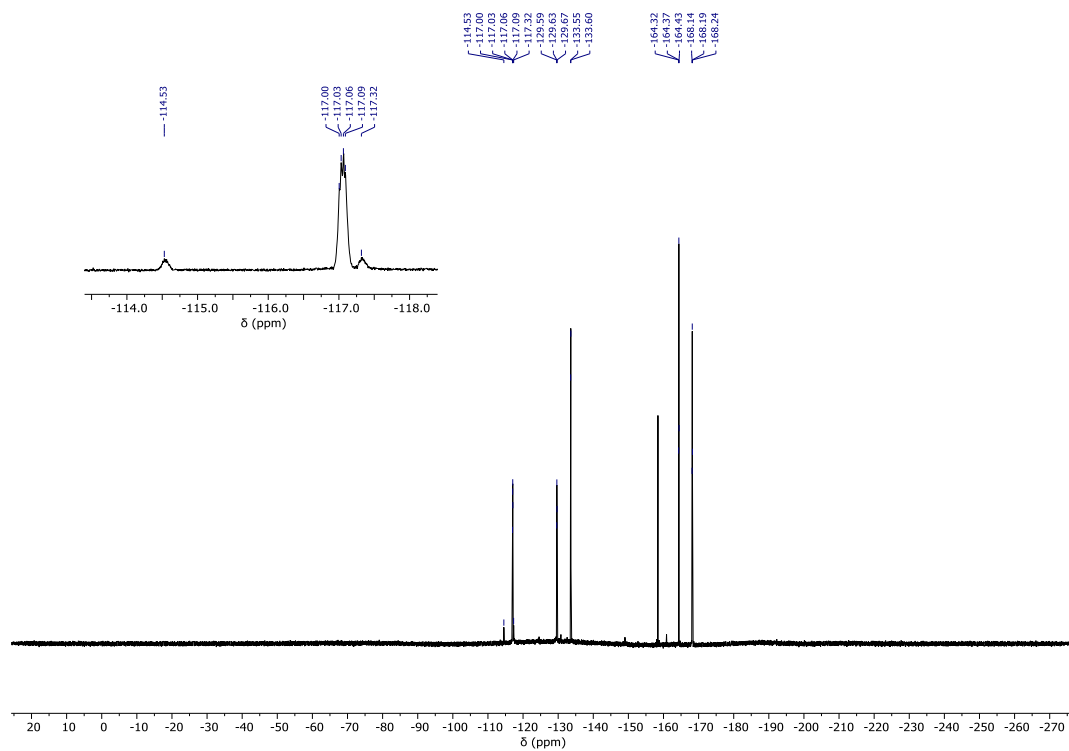
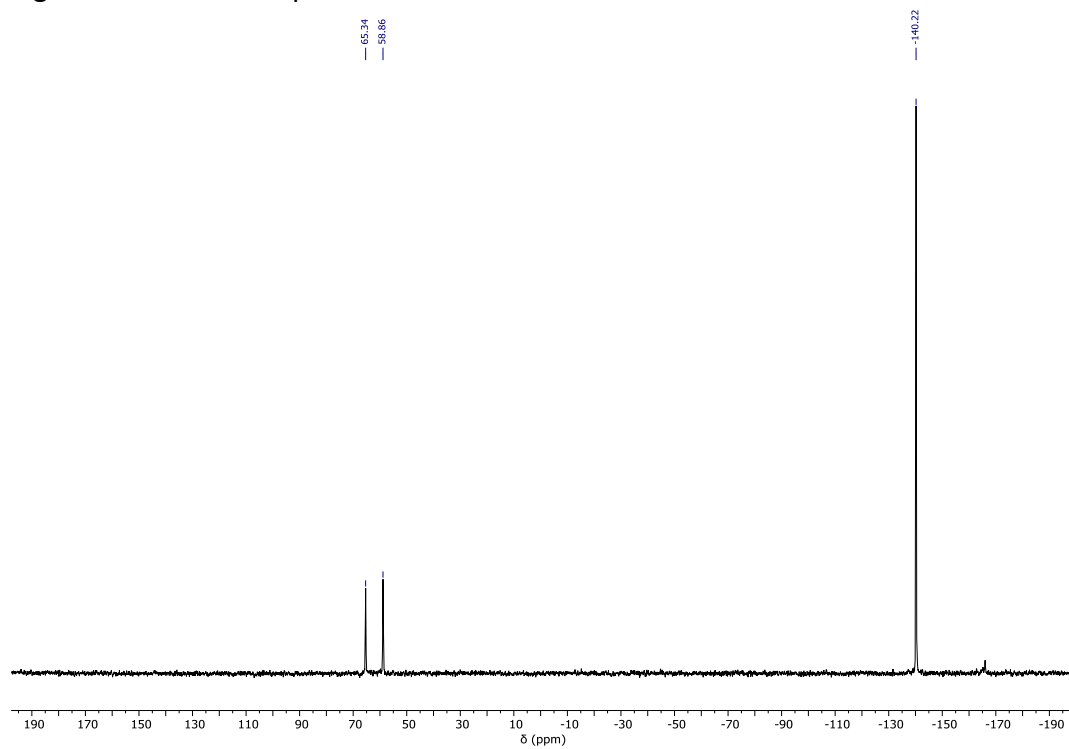


Figure S35. ^1H NMR Spectrum of **9** in CDCl_3 .

Figure S36. ^{19}F NMR Spectrum of **9** in CDCl_3 .Figure S37. ^{31}P NMR Spectrum of **9** in CDCl_3 .

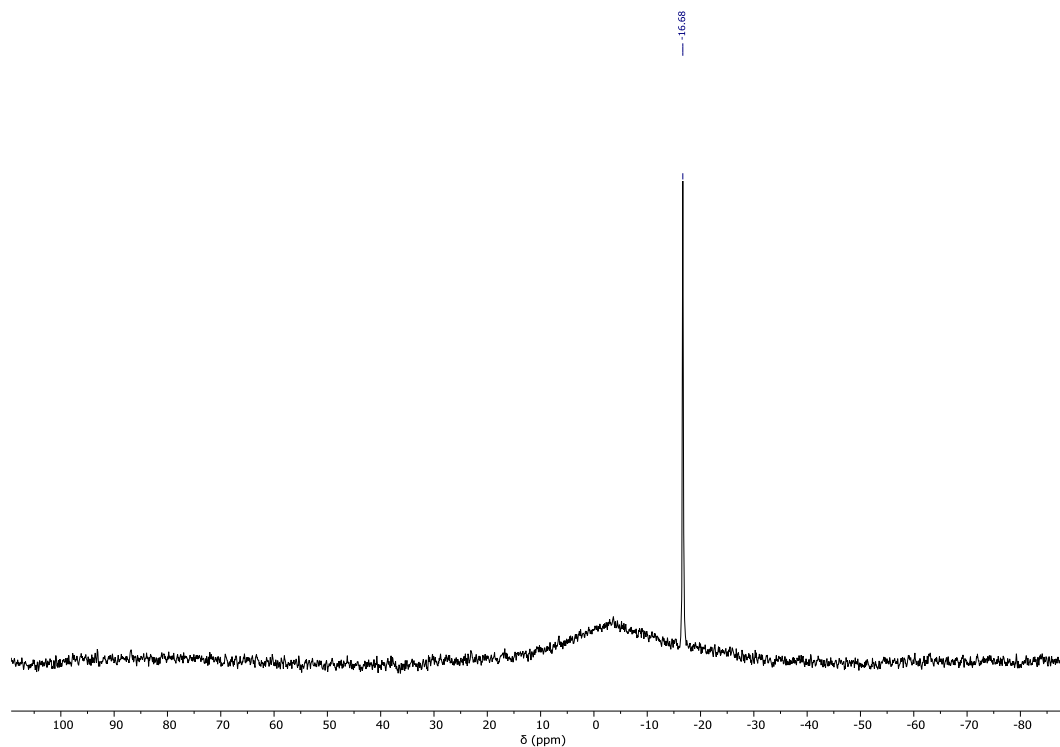
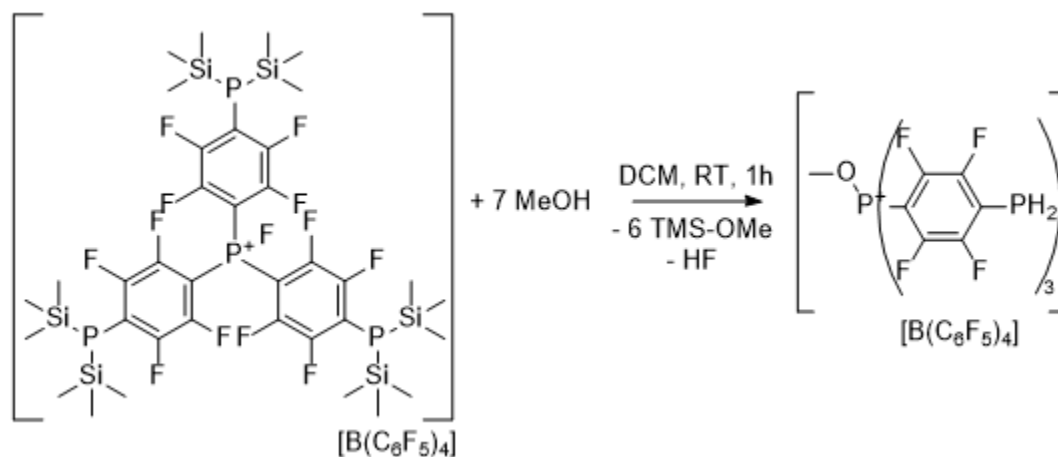


Figure S38. ^{11}B NMR Spectrum of **9** in CDCl_3 .

Synthesis of $[\text{CH}_3\text{OP}(\text{C}_6\text{F}_4\text{PH}_2)_3][\text{B}(\text{C}_6\text{F}_5)_4]$ (**10**)



Product **9** (15 mg, 0.009 mmol) was dissolved in DCM to form a bright orange solution. To this solution was added one drop of dry, degassed methanol (approx 0.05 mL, approx. 1.2 mmol) with strong stirring, causing the solution to instantly turn colourless. After 10 minutes, all volatiles were removed under vacuum, yielding a pale yellow solid (10 mg, 0.008 mmol, 90%).

$^1\text{H}\{^{19}\text{F}\}$ NMR (400 MHz, CDCl_3) δ 6.25 (s, 3H, O- CH_3), 3.82 (d, 6H, PH_2 , $^3J_{\text{HP}} = 214.9$ Hz). ^{19}F NMR (377 MHz, CDCl_3) δ -124.9 (s, 6F, C_6F_4), -132.8 (s, 8F, $\text{B}(\text{C}_6\text{F}_5)_4$), -134.5 (s, 6F, C_6F_4), -163.0 (t, 4F, $\text{B}(\text{C}_6\text{F}_5)_4$, $^3J_{\text{FF}} = 21$ Hz), -166.9 (t, 8F, $\text{B}(\text{C}_6\text{F}_5)_4$, $^3J_{\text{FF}} = 20$ Hz). ^{31}P NMR (162 MHz, CDCl_3) δ 36.7 (s, P-OMe), -164.4 (t, $^1J_{\text{PH}} = 220$ Hz, PH_2). ^{19}F NMR (377 MHz, CDCl_3) δ -120.8, -127.8, -132.8, -163.3 (t, $J = 20$ Hz), -167.2. ^{31}P NMR (162 MHz, CDCl_3) δ 6.2 (s, 1P, P-O CH_3), -168.1 (t, 3P, PH_2 , $^1J_{\text{PH}} = 215$ Hz). ^{11}B NMR (128 MHz, CDCl_3) δ -16.7 (s, $\text{B}(\text{C}_6\text{F}_5)_4$). HRMS: formula, calc observed. HRMS: $[\text{C}_{18}\text{H}_7\text{OF}_{12}\text{P}_4]^+$ Calculated mass: 590.925. Measured mass: 590.925.

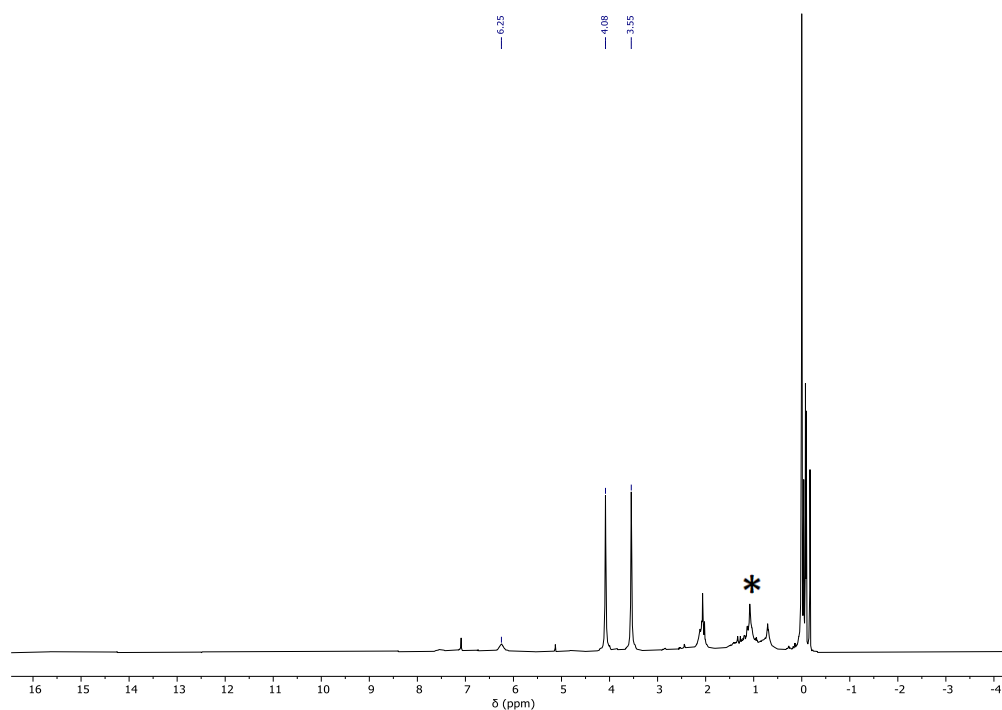
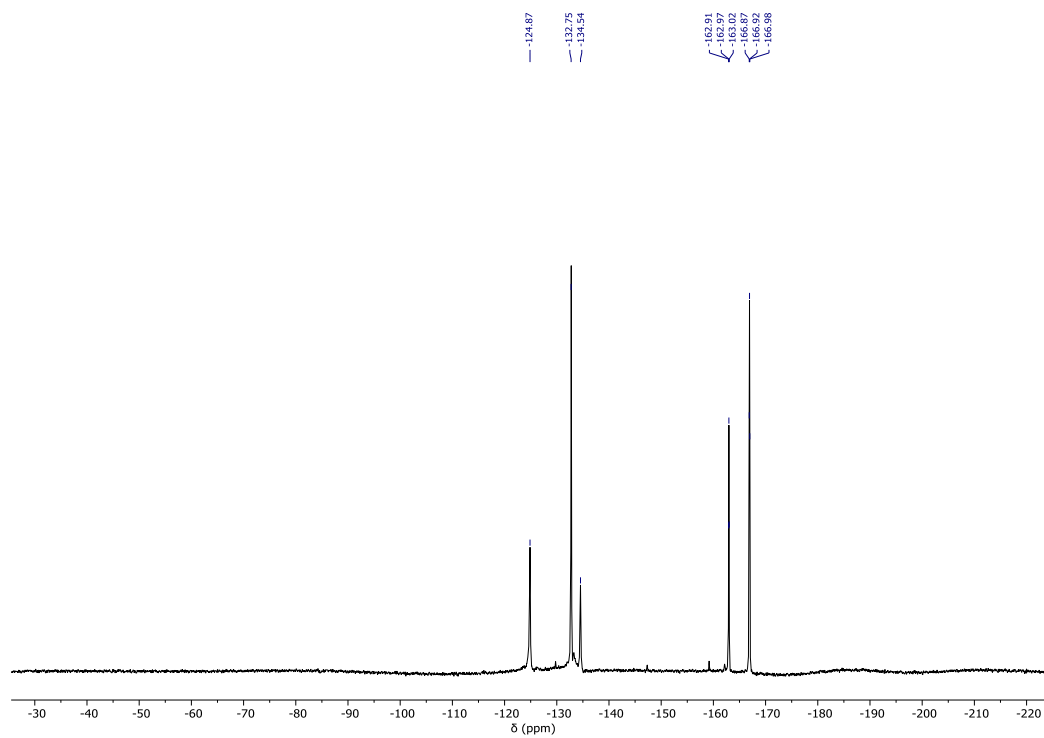
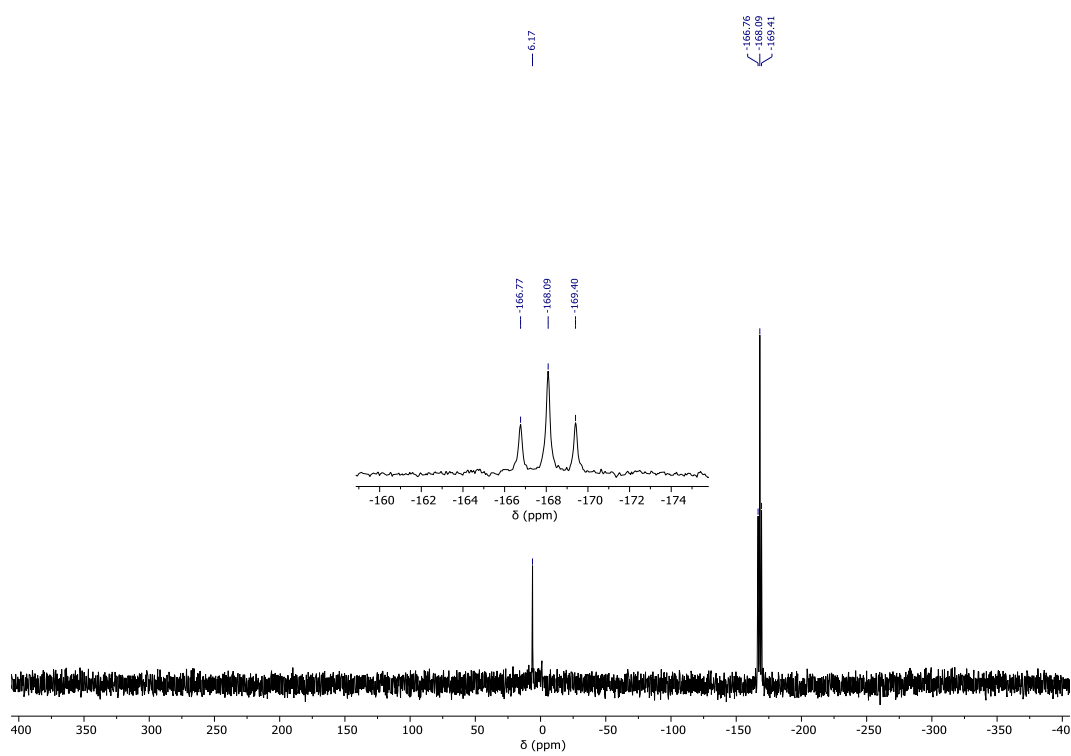
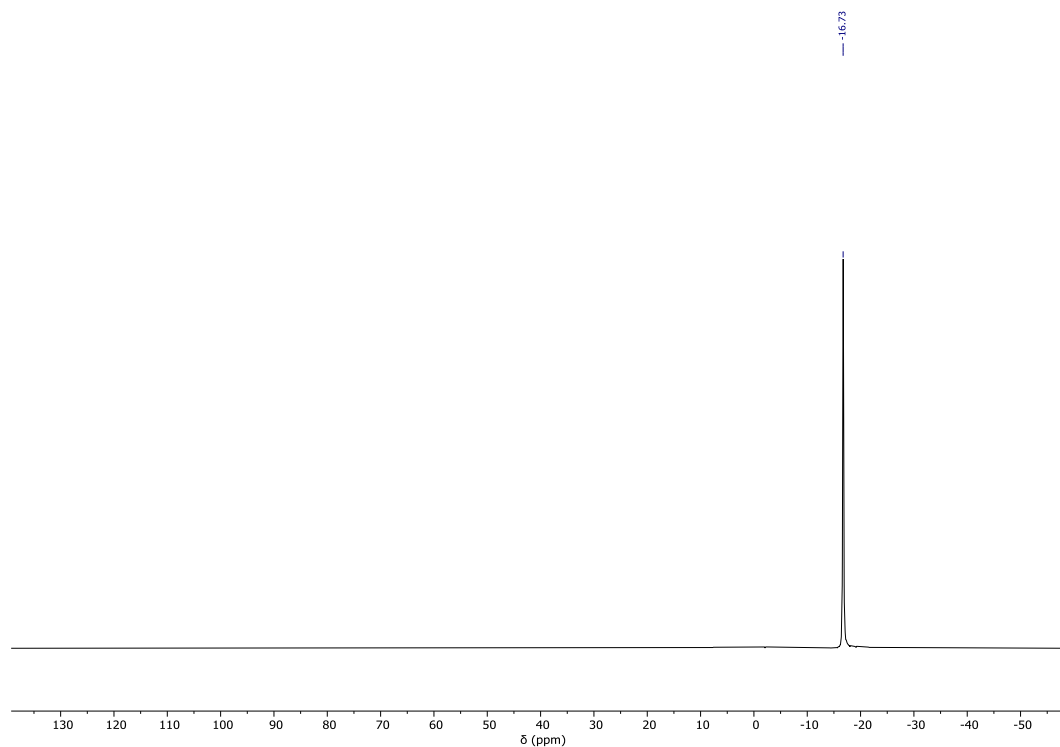
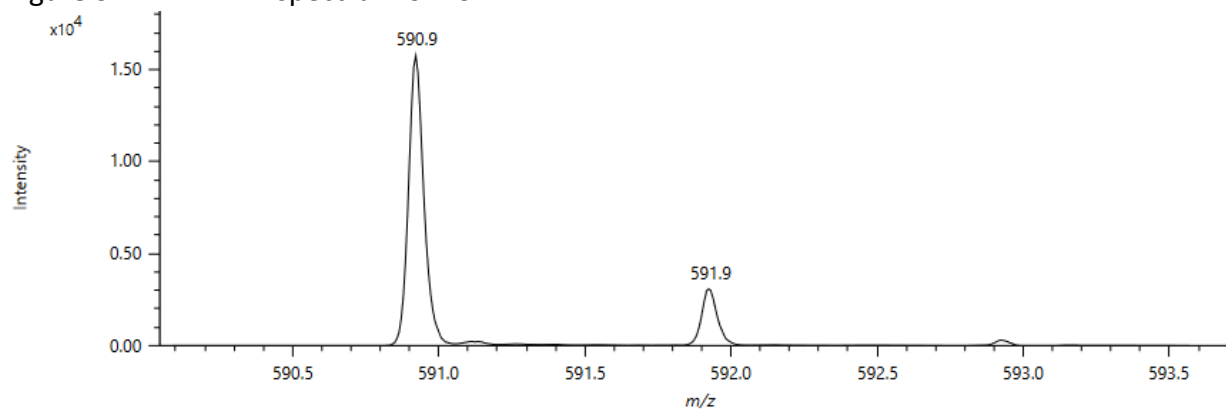


Figure S39. $^1\text{H}\{^{19}\text{F}\}$ NMR spectrum of **10** in C_6D_6
*pentane

Figure S40. ^{19}F NMR spectrum of **10**.Figure S41. ^{31}P NMR spectrum of **10**.

Figure S42. ^{11}B NMR spectrum of **10**.

Elemental Composition

Parameters

Tolerance: ± 10.00 ppm
 Electron: Odd/Even
 Charge: +1
 DBE: -1.5 - 100.0

Elements Set 1:

| Symbol | C | H | O | N | F | P |
|--------|-----|-----|----|----|----|---|
| Min | 0 | 0 | 0 | 0 | 12 | 0 |
| Max | 100 | 200 | 20 | 10 | 12 | 4 |

Results

| Mass | Intensity | Formula | Calculated Mass | Mass Difference [mDa] | Mass Difference [ppm] | DBE |
|-----------|-----------|---------------------|-----------------|-----------------------|-----------------------|------|
| 590.92509 | 15761.52 | C2 H2 N7 O13 F12 P | 590.92511 | -0.02 | -0.04 | 0.0 |
| | | C18 H7 O F12 P4 | 590.92503 | 0.06 | 0.10 | 11.5 |
| | | C8 H6 N4 O7 F12 P3 | 590.92522 | -0.14 | -0.23 | 3.5 |
| | | C12 H3 N3 O7 F12 P2 | 590.92491 | 0.17 | 0.29 | 8.0 |
| | | C4 H9 N5 O7 F12 P4 | 590.92553 | -0.45 | -0.76 | -1.0 |
| | | C16 N2 O7 F12 P | 590.92460 | 0.48 | 0.82 | 12.5 |

Figure S43. HRMS of **10**.