Electronic Supplementary Material (ESI) for Dalton Transactions.

Dicationic Phosphonium Salts: Lewis Acid Catalysts for the Mukaiyama-Aldol Reaction

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Supporting Information

This PDF file includes:

1. Materials and Methods

Nuclear magnetic resonance spectroscopy (NMR)

NMR spectra were measured on a Bruker AVANCE 400 (^{1}H: 400 MHz, ^{11}B: 128 MHz, ^{13}C: 101 MHz, ^{31}P: 162 MHz, ^{19}F: 377 MHz) or Bruker DPX 300 (^{1}H: 300 MHz, ^{11}B: 96 MHz, ^{13}C: 75 MHz, ^{31}P: 121 MHz, ^{19}F: 282 MHz) at ambient temperature. ^{1}H and ^{13}C chemical shifts (δ) are given in ppm relative to TMS and absolute values of coupling constants (*J*) are provided in Hz. The solvent signals were used as references and the chemical shifts converted to the TMS scale. The corresponding solvent signals were used as a references: $CDCl_3$: δ (^{1}H): 7.26 ppm, δ (^{13}C): 77.16 ppm; CD_2Cl_2: δ (1H): 5.32 ppm, δ (13C): 53.84 ppm; CD_3CN: δ (^{1}H): 1.94 ppm, δ (^{13}C): 1.32 ppm, 118.26 ppm; d_6-DMSO: δ (^{13}C): 39.52 ppm The multiplicities in the ^{1}H-NMR spectra are assigned as follows: singlet (s), doublet (d), triplet (t), quartet (q), quintet (quin), sextet (sext), septet (sept), multiplet (m), broad (b s).

Infrared spectroscopy (IR)

IR spectra were recorded using ATR (attenuated total reflection) on a Nicolet FT-7199 spectrometer at room temperature. The characteristic absorption bands are given in cm^{-1}.

Mass spectrometry (MS)

Mass spectra were measured on a Finnigan MAT 8200 (EI, 70 eV) or Finnigan MAT 95 (ESI). High resolution masses were determined on a Bruker APEX III FT-MS (7 T magnet), a micro mass 70S-250 spectrometer (EI), an ABI/Sciex QStar Mass Spectrometer (DART), or on a JOEL AccuTOF-DART (DART). All masses are given in atomic units per elementary charge (*m/z*).

Flash column chromatography

Flash column chromatography was performed using silica gel 60 (Merck, 60 Å, 230-400 mesh 0.040-0.063 mm) and separations were conducted at slightly elevated pressure in a glass column.

Analytical gas chromatography GC-MS

Couplings were performed on an *Agilent Technology* GC 6890 Series and MSD 5973 (carrier gas: helium) with HP6890 Series Injector, employing an MN Optima®5 column (30 m × 0.25 mm × 0.25 mm). The mass spectra were recorded with an *Agilent Technology* 5973 Network MSD spectrometer. Quantitative evaluation of the integration was based on the substance peaks without considering response factors, unless stated otherwise.

2. Spectroscopic Data

2.1 Cyclopropenium-substituted phosphonium salts

2.1.1 NMR Spectra of Compound 10a

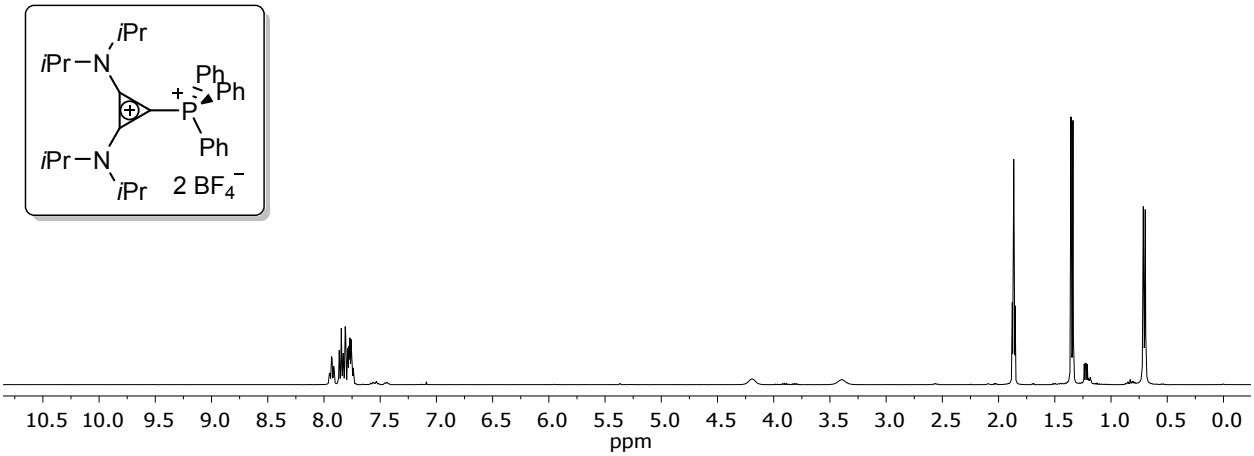


*Figure S1. ^{1}H NMR (CD_3CN) Spectrum of Compound **10a**.*

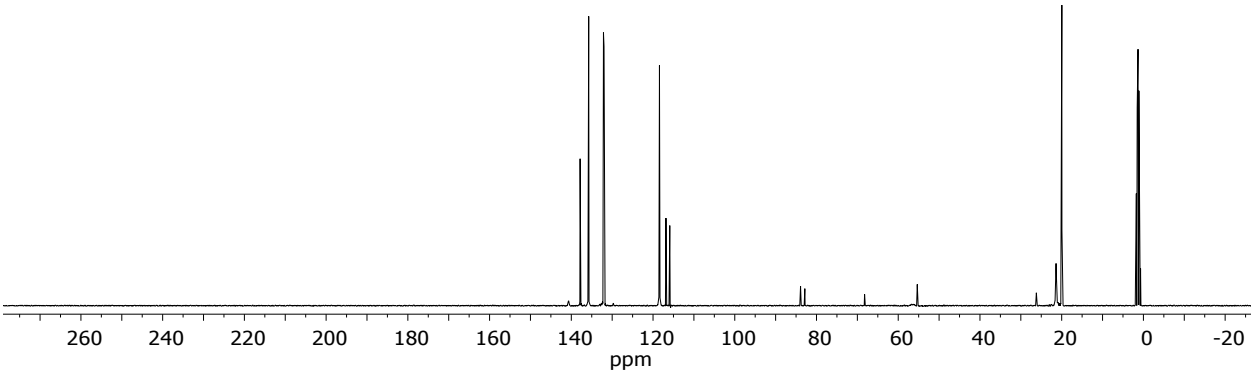


*Figure S2. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10a**.*

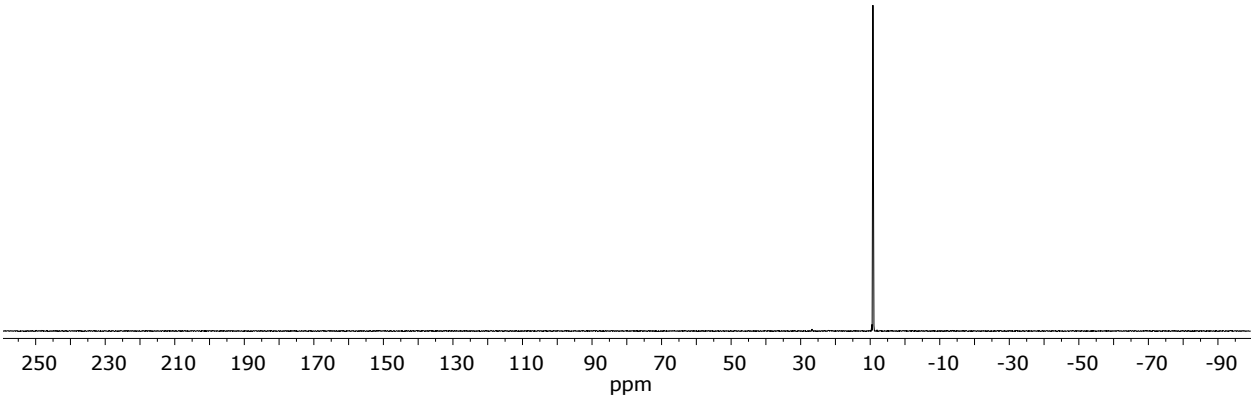


*Figure S3. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10a**.*

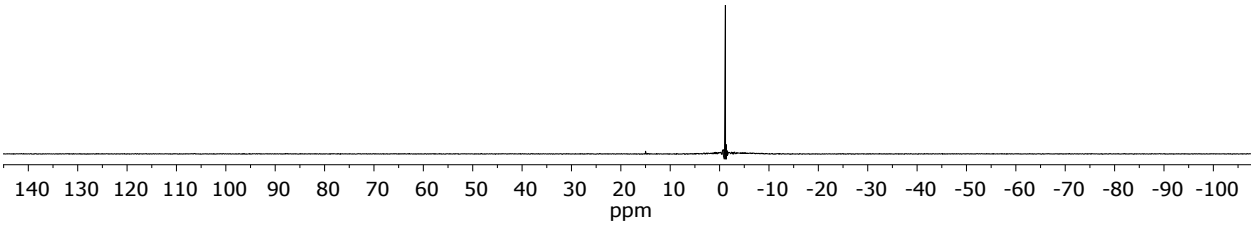


*Figure S4. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10a**.*

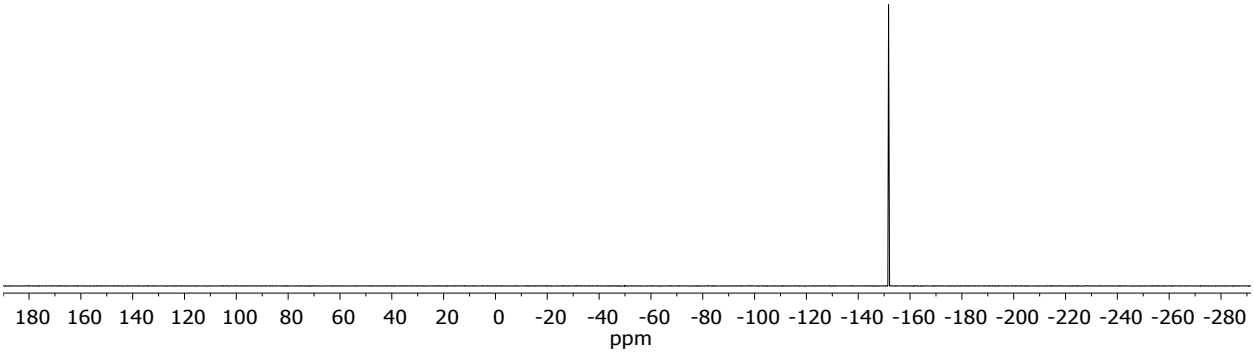
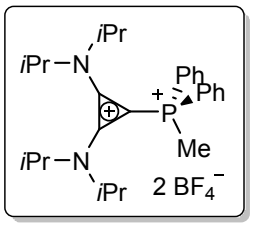


*Figure S5. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10a**.*

2.1.2 NMR Spectra of Compound 10b



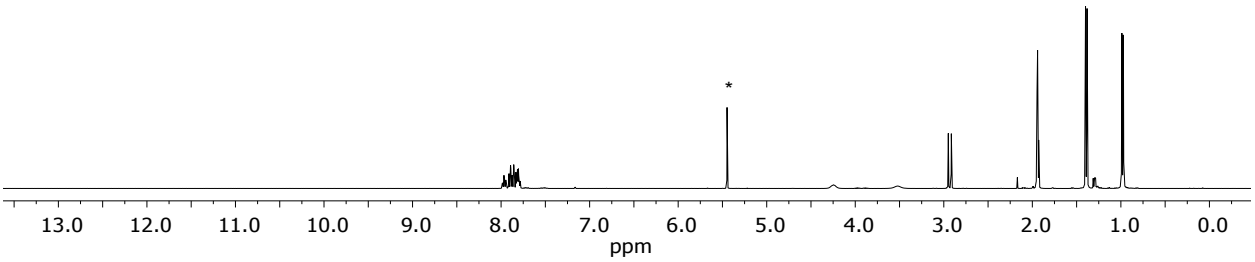


*Figure S6. ^{1}H NMR (CD_3CN) Spectrum of Compound **10b**. Asterisks denote solvent impurities.*

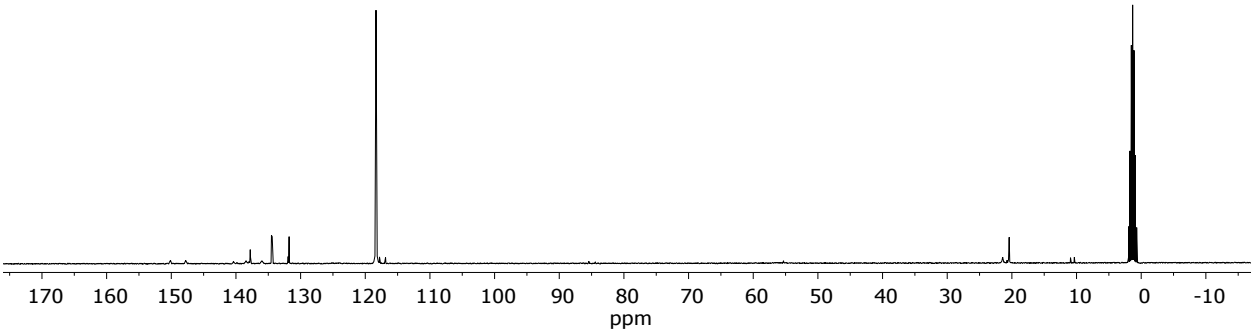


*Figure S7. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10b**.*

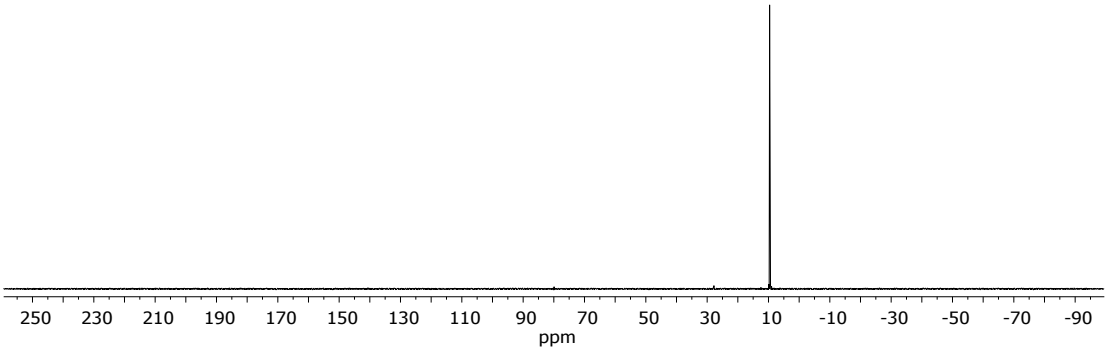


*Figure S8. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10b**.*

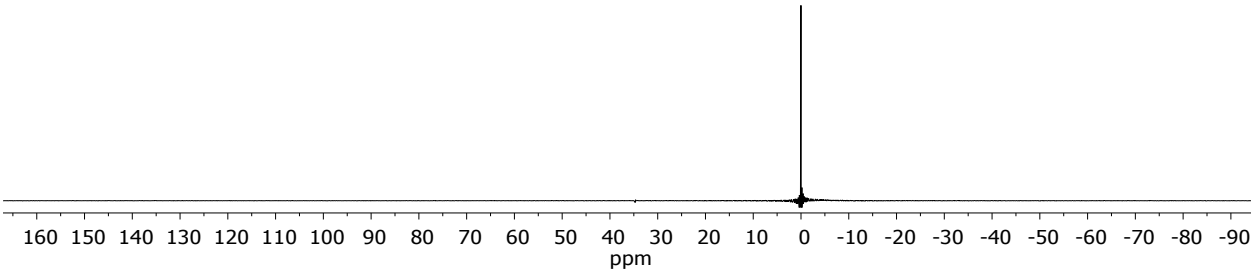


*Figure S9.$^{11}B\{^1H\}$ NMR (CD_3CN) Spectrum of Compound **10b**.*

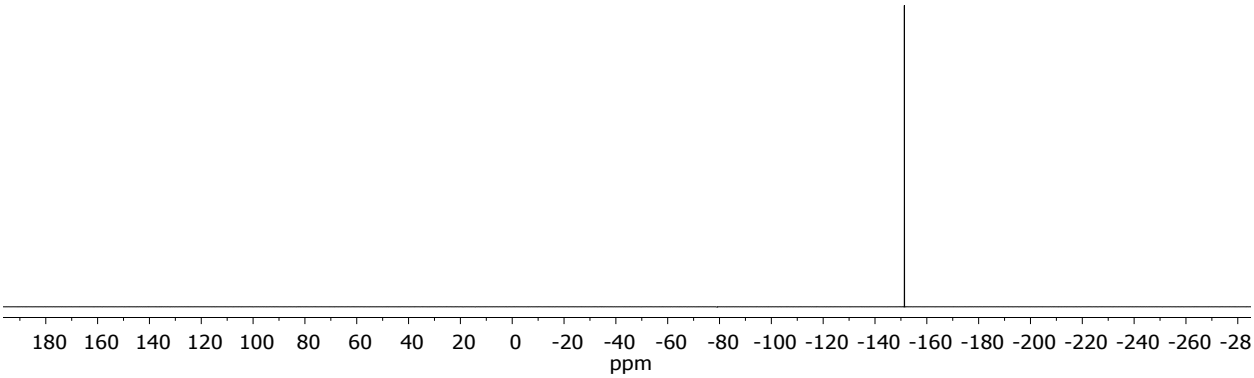


*Figure S10. $^{19}F\{^1H\}$ NMR (CD_3CN) Spectrum of Compound **10b**.*

2.1.3 NMR Spectra of Compound 10c

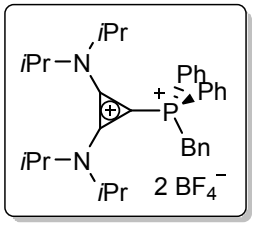


*Figure S11. ^1H NMR (CD_3CN) Spectrum of Compound **10c**.*

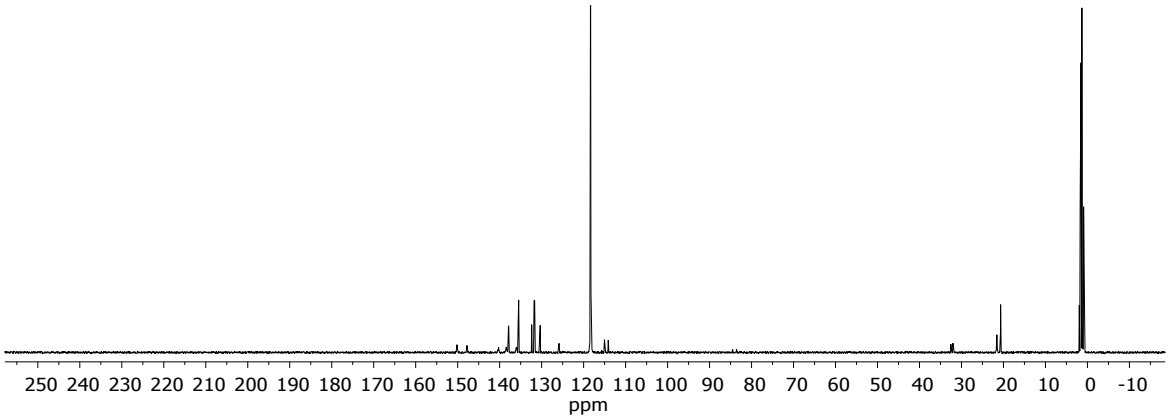


*Figure S12. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10c**.*

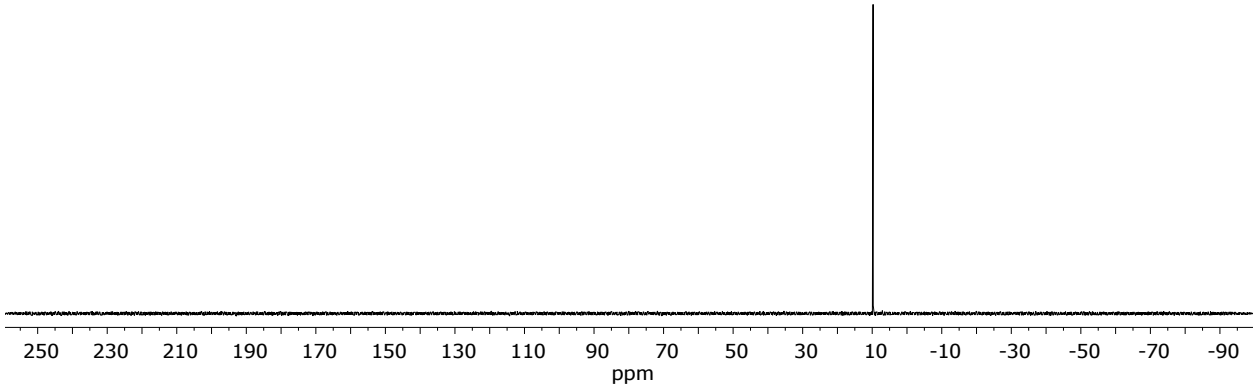


*Figure S13. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10c**.*

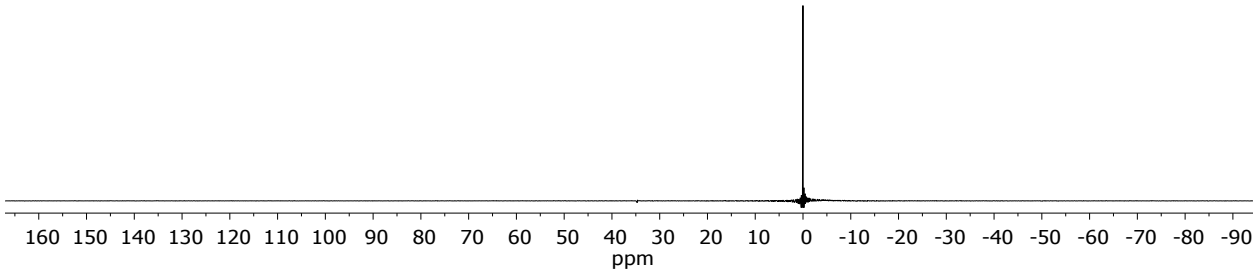


*Figure S14. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10c**.*

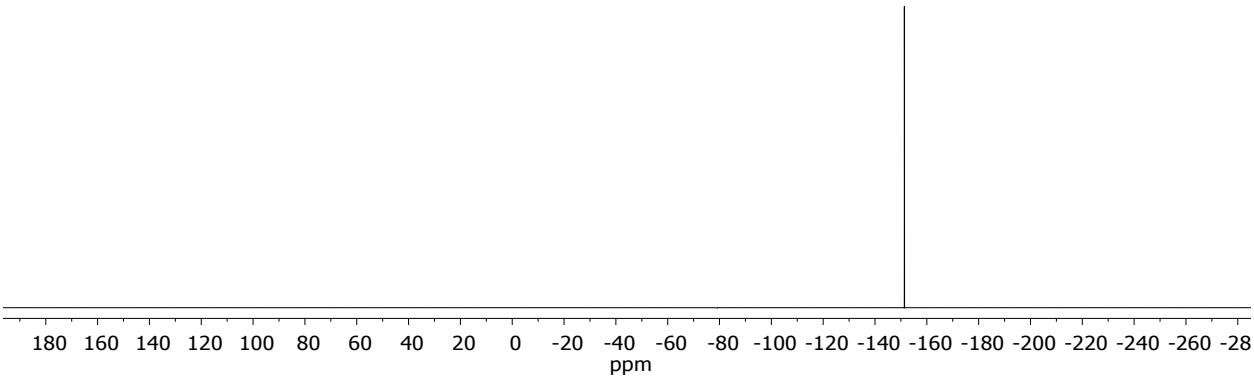


*Figure S15. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10c**.*

2.1.4 NMR Spectra of Compound 10d

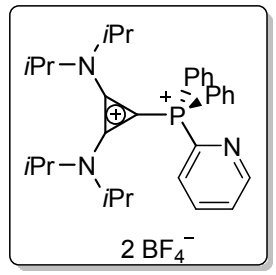


*Figure S16. ^{1}H NMR (CD_3CN) Spectrum of Compound **10d**. Asterisk denotes a solvent impurities.*

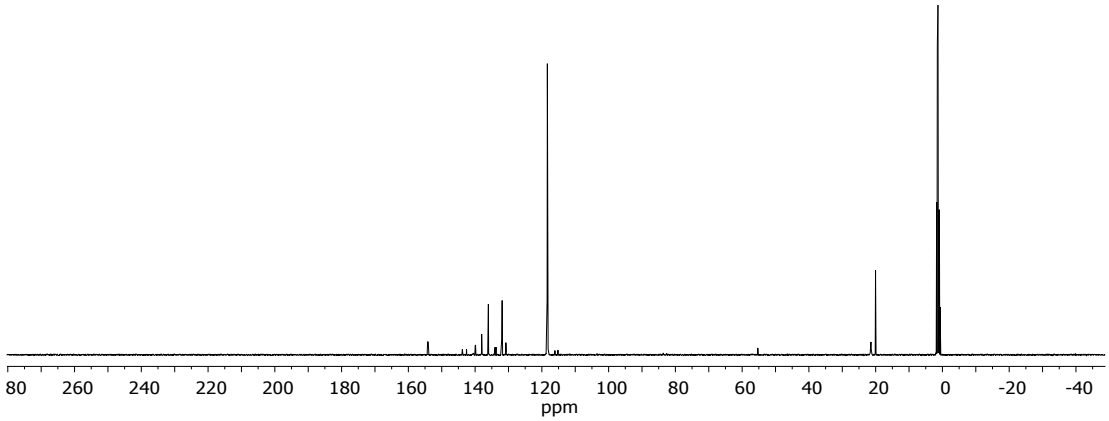


*Figure S17. $^{31}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10d**.*

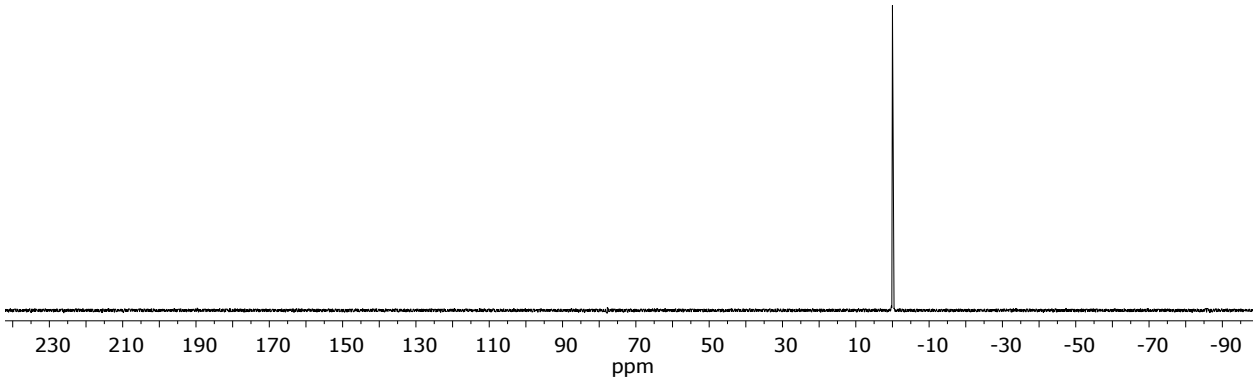


*Figure S18. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10d**.*

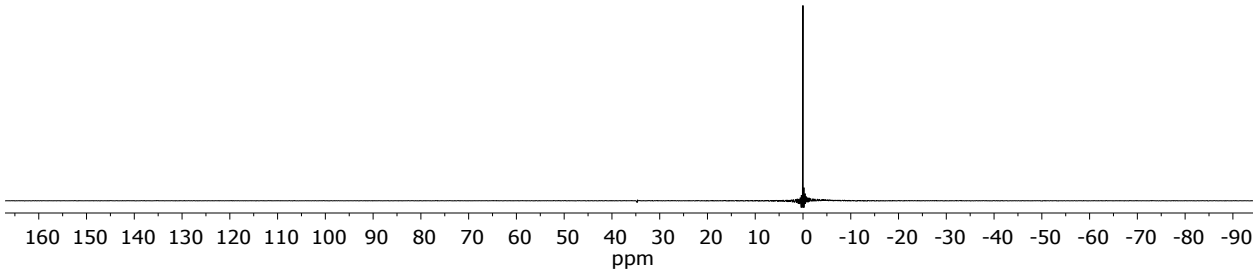


*Figure S19. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10d**.*

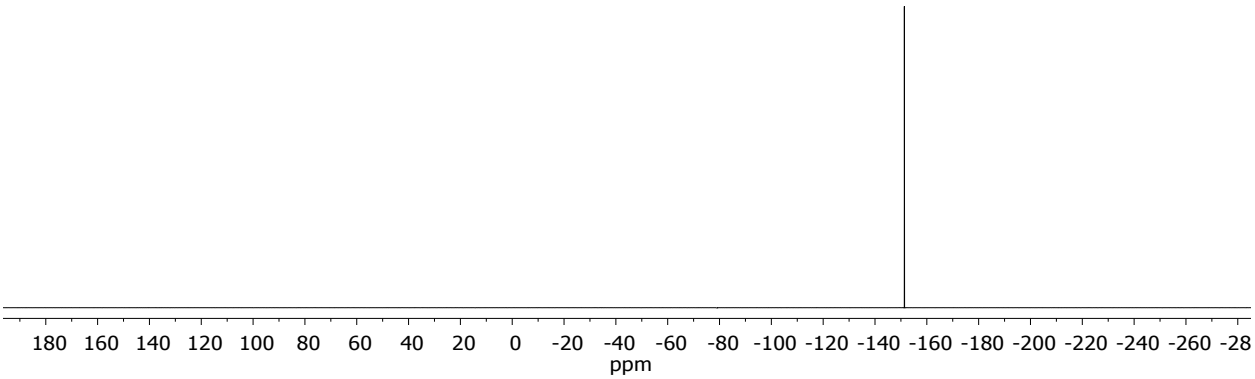
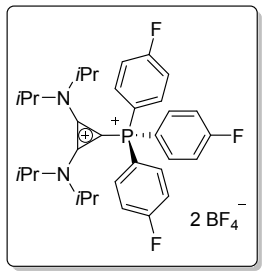


Figure S20. $^{19}F\{^{1}H\}$ *NMR (CD_3CN) Spectrum of Compound* ***10d****.*

2.1.5 NMR Spectra of Compound 10e



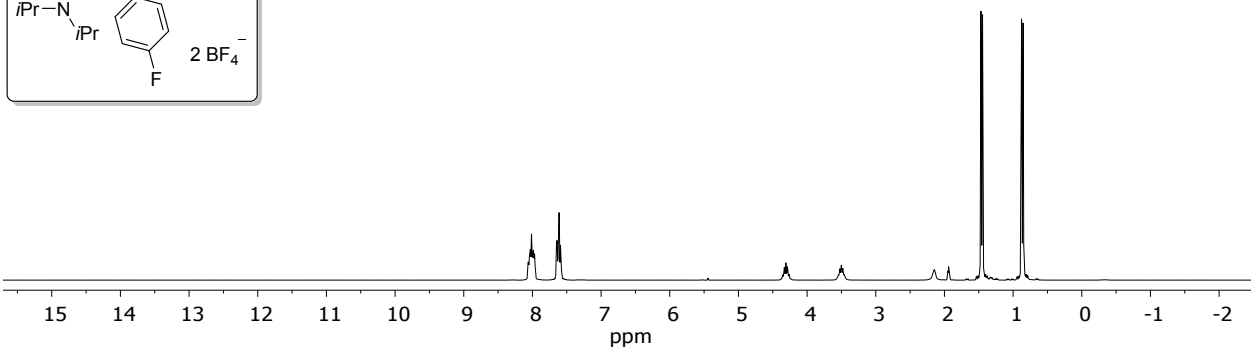


Figure S21. ^{1}H *NMR (CD_3CN) Spectrum of Compound* ***10e****.*

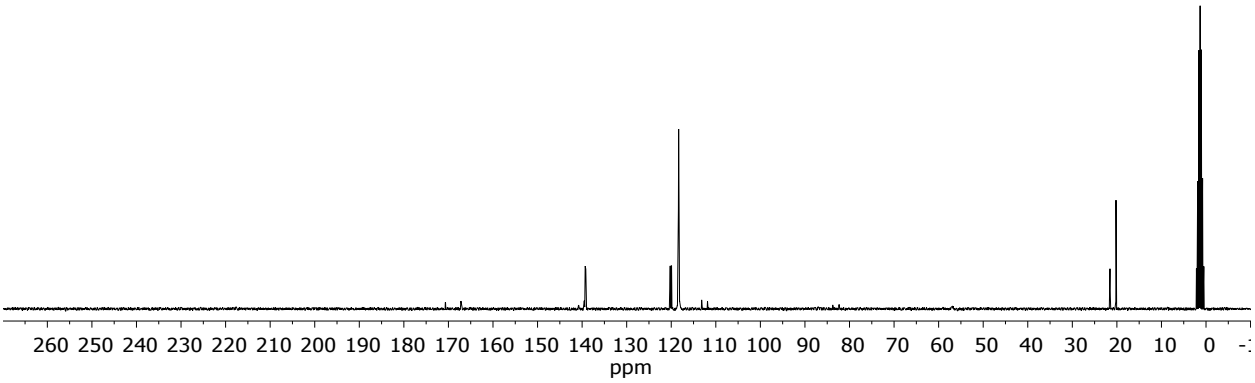


*Figure S22. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10e**.*

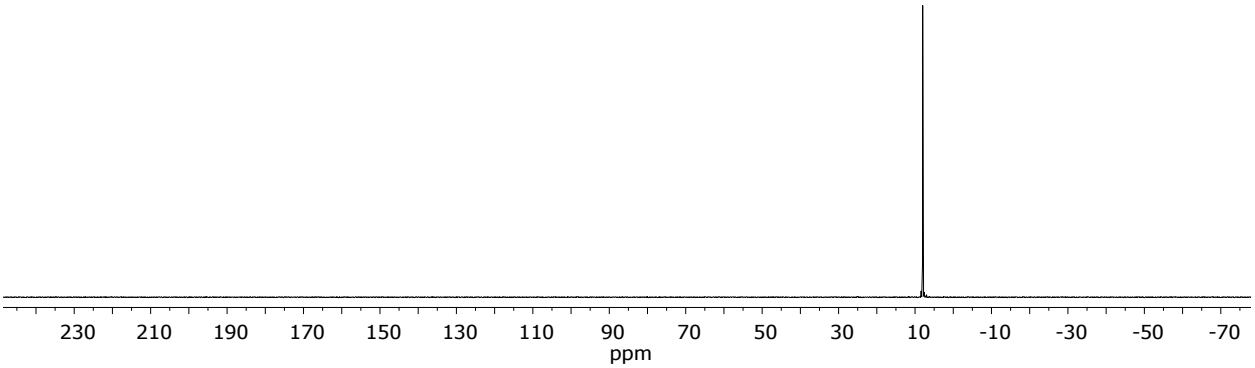


*Figure S23. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10e**.*

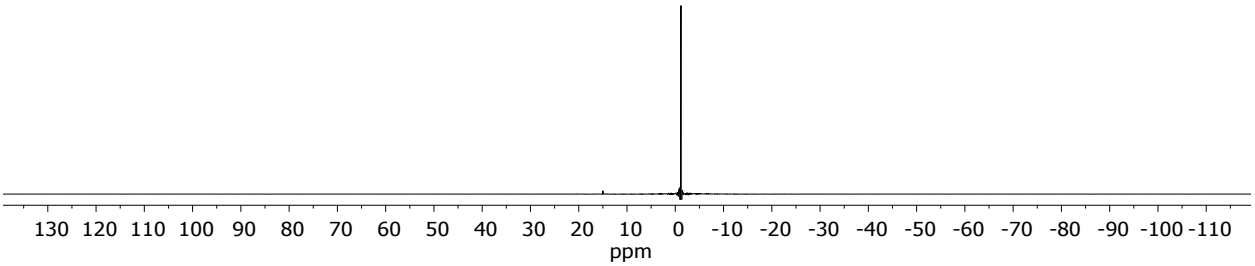


*Figure S24. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10e**.*

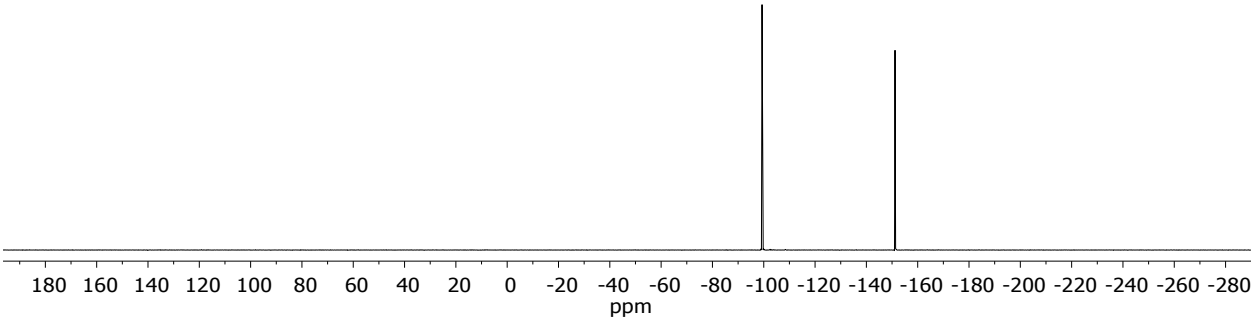
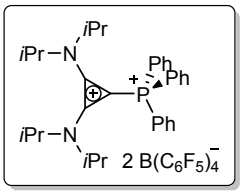


*Figure S25. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10e**.*

2.1.6 NMR Spectra of Compound 10a[$B(C_6F_5)_4$]



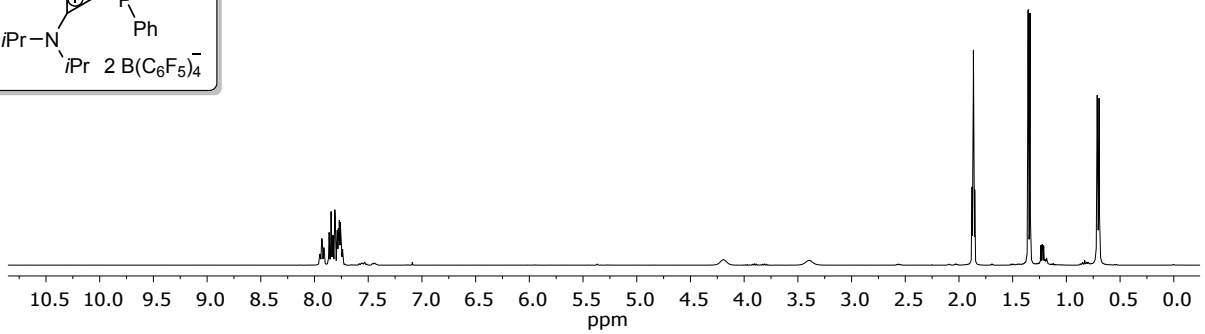


*Figure S26. ^{1}H NMR (CD_3CN) Spectrum of Compound **10a[$B(C_6F_5)_4$]**.*

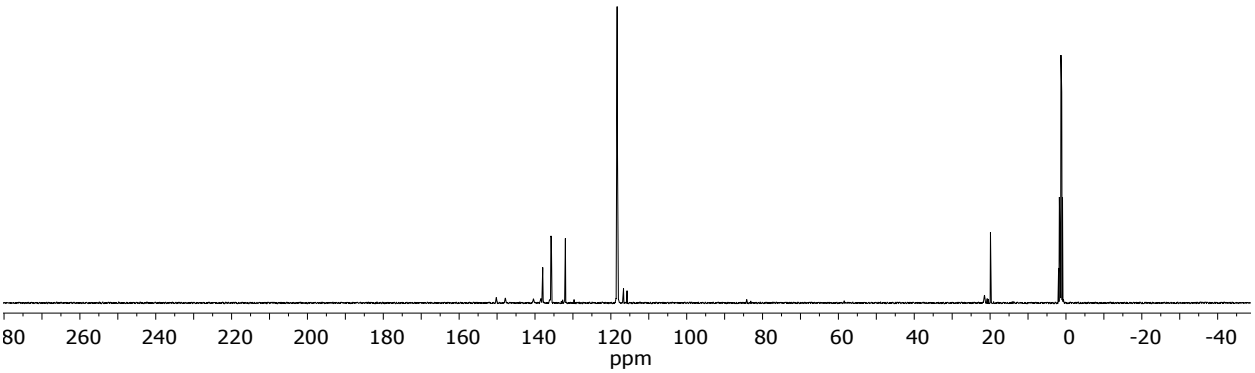


*Figure S27. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10a[$B(C_6F_5)_4$]**.*

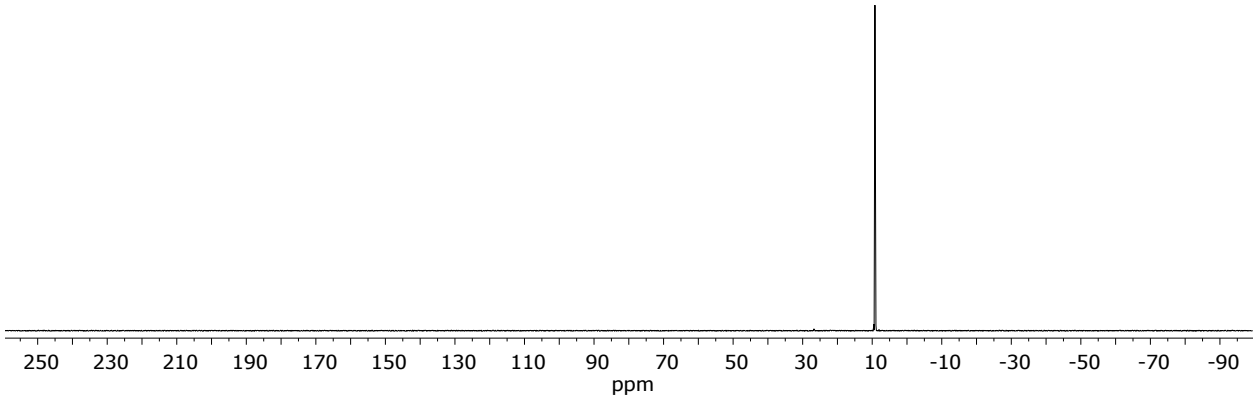


*Figure S28. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10a[B(C_6F_5)$_4$]**.*

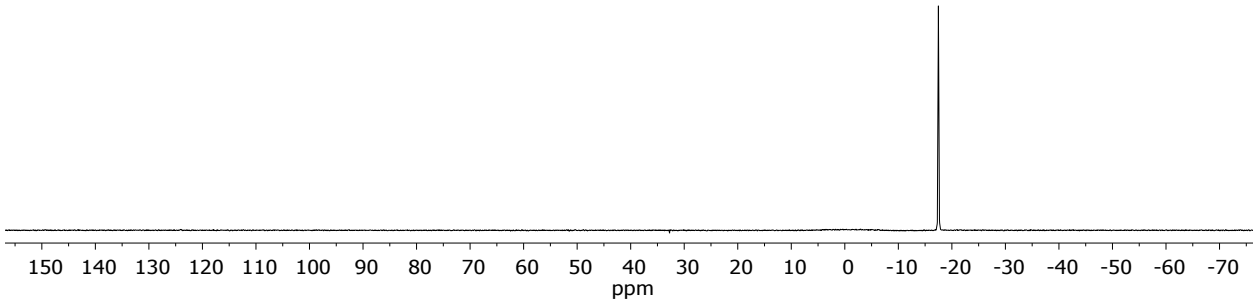


*Figure S29. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10a[B(C_6F_5)$_4$]**.*

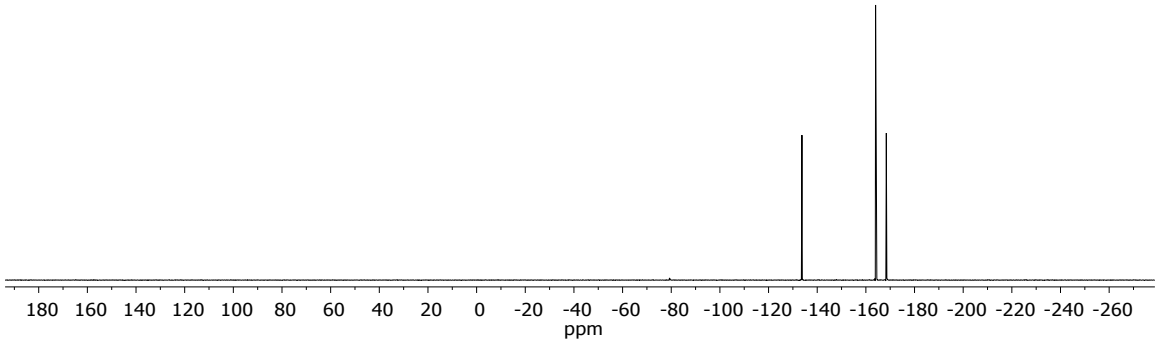
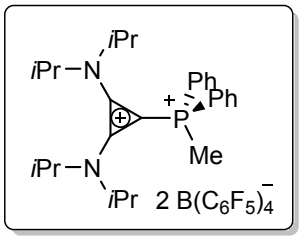


*Figure S30. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10a[B(C_6F_5)$_4$]**.*

2.1.7 NMR Spectra of Compound 10b[$B(C_6F_5)_4$]



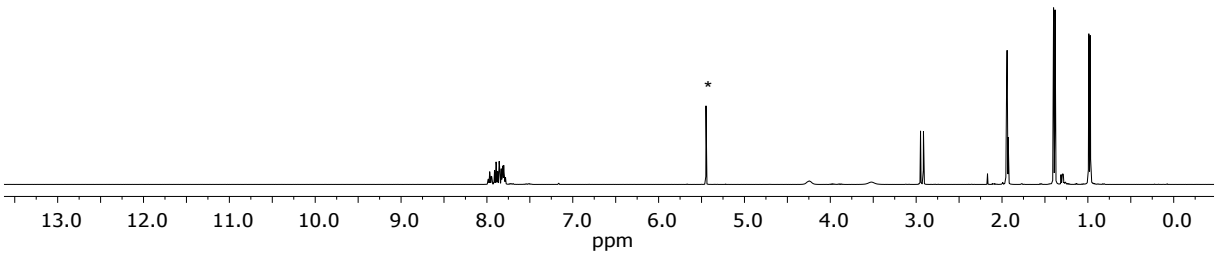


*Figure S31. ^{1}H NMR (CD_3CN) Spectrum of Compound **10b[$B(C_6F_5)_4$]**. Asterisk denotes a solvent impurity.*

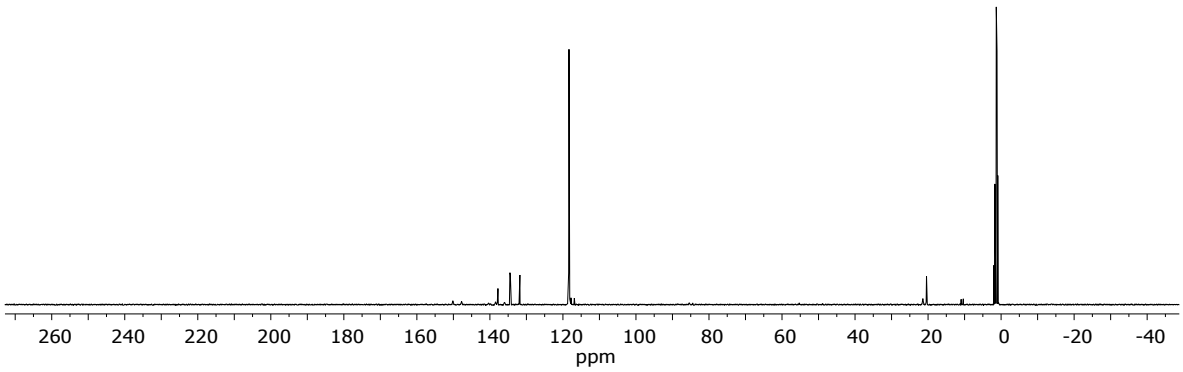


*Figure S32. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10b[$B(C_6F_5)_4$]**.*

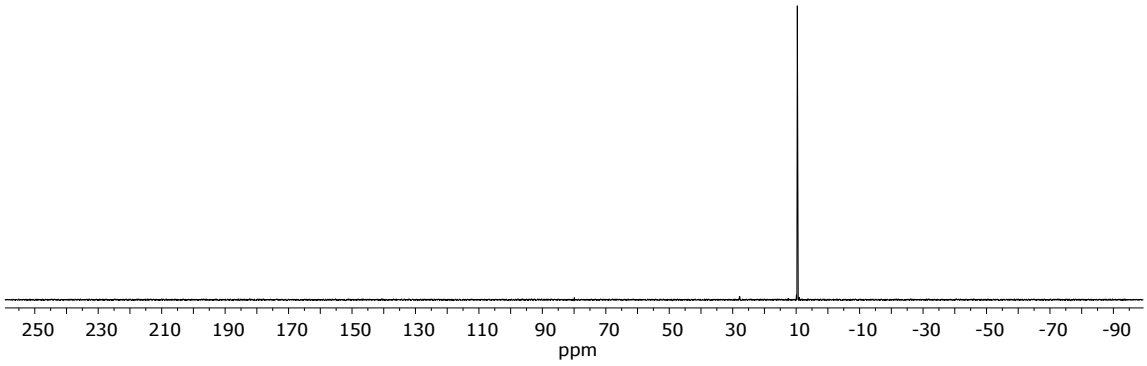


*Figure S33. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10b[$B(C_6F_5)_4$]**.*

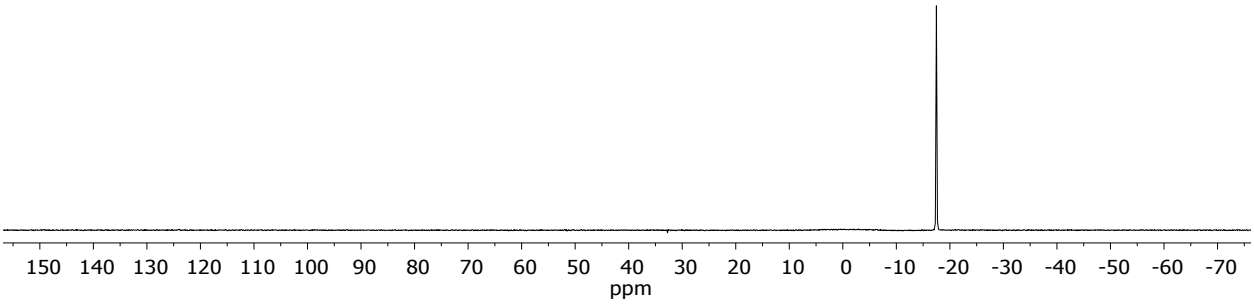


*Figure S34. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10b[B(C_6F_5)$_4$]**.*

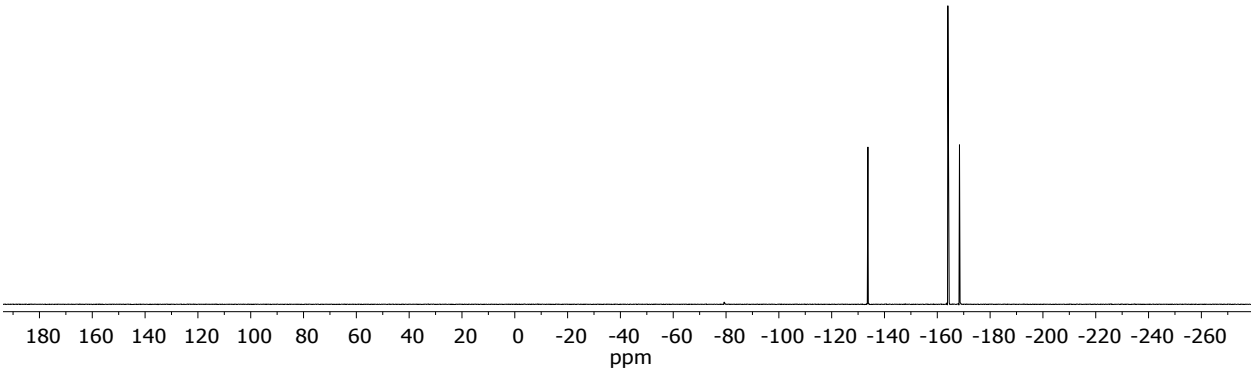


*Figure S35. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10b[B(C_6F_5)$_4$]**.*

2.1.8 NMR Spectra of Compound 10c[B(C_6F_5)$_4$]

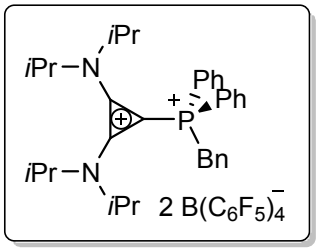


*Figure S36. ^{1}H NMR (CD_3CN) Spectrum of Compound **10c[B(C_6F_5)$_4$]**. Asterisk denotes a solvent impurities.*

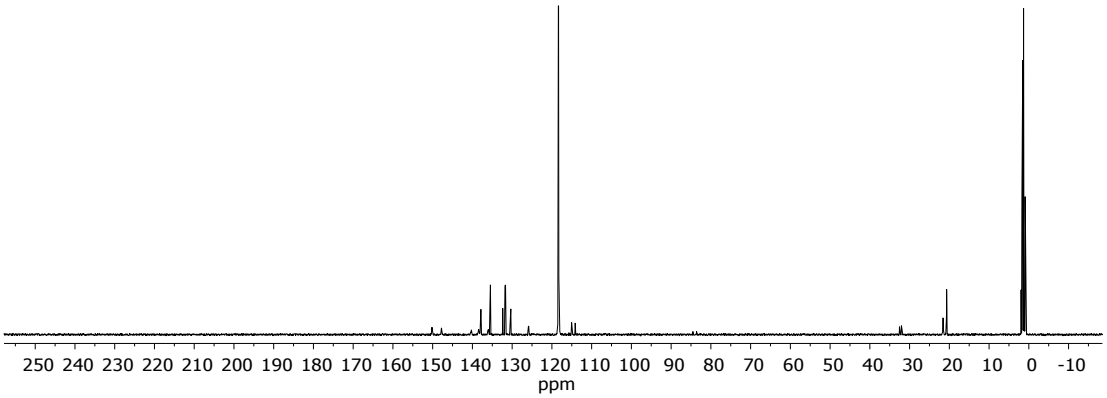


*Figure S37. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10c[B(C_6F_5)$_4$]**.*

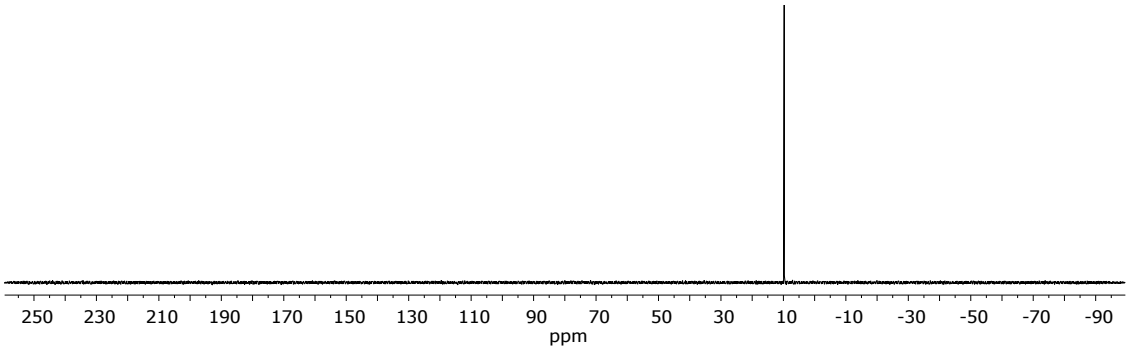


*Figure S38. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10c[B(C_6F_5)$_4$]**.*

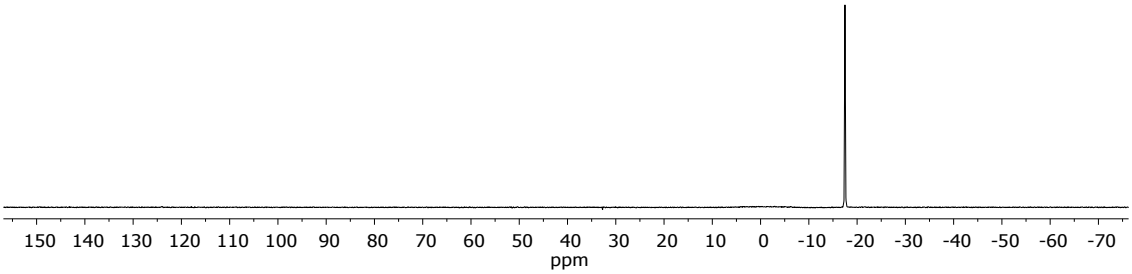


*Figure S39. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10c[B(C_6F_5)$_4$]**.*

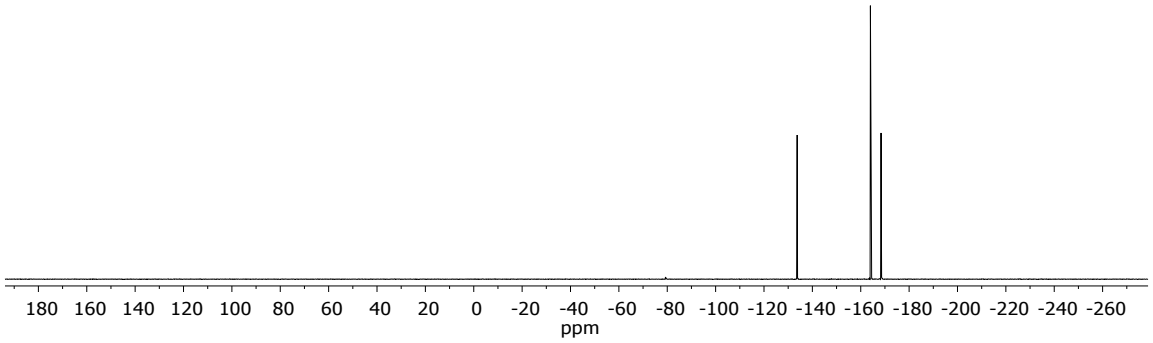


*Figure S40. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10c[B(C_6F_5)$_4$]**.*

2.1.9 NMR Spectra of Compound 10d[B(C_6F_5)$_4$]

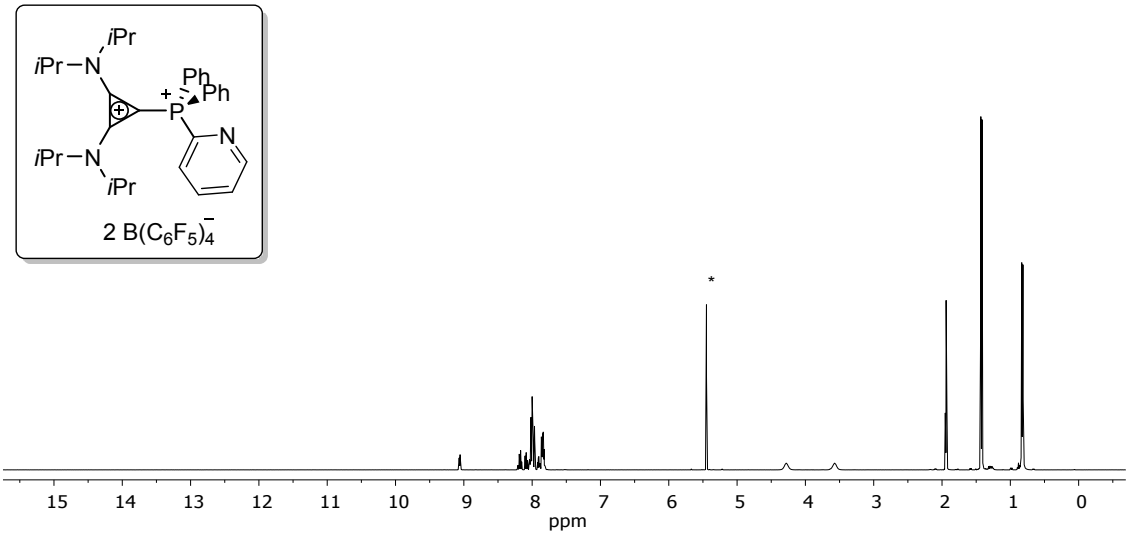


*Figure S41. ^{1}H NMR (CD_3CN) Spectrum of Compound **10d[B(C_6F_5)$_4$]**.*

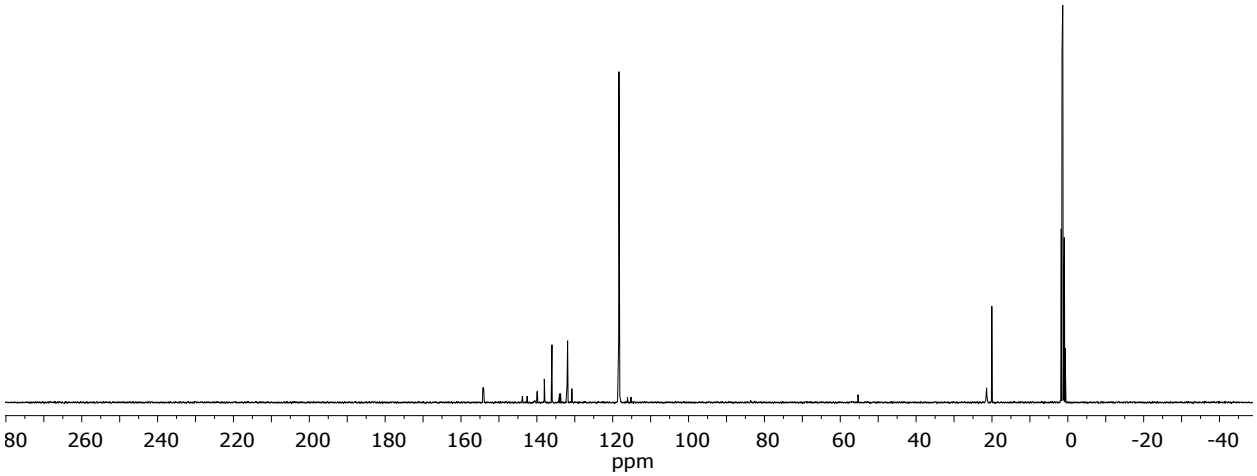


*Figure S42. $^{31}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10d[B(C_6F_5)$_4$]**.*

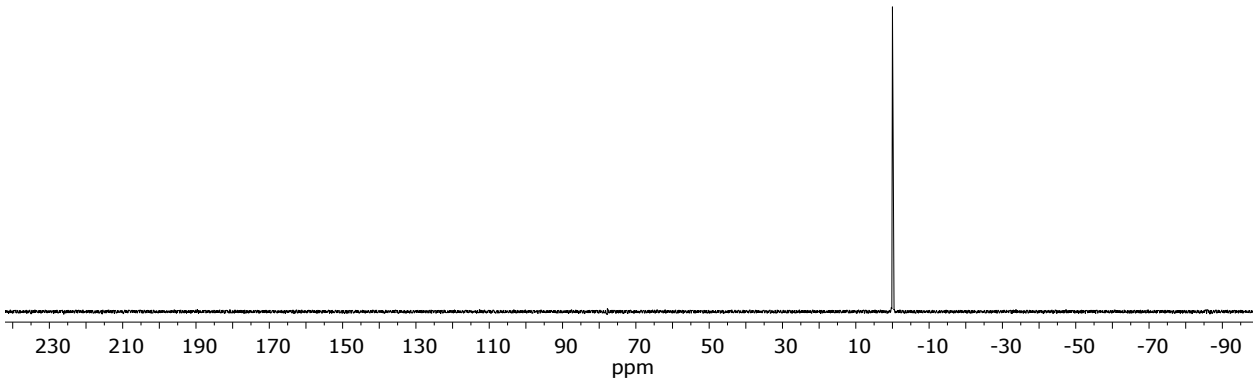


*Figure S43. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10d[B(C_6F_5)$_4$]**.*

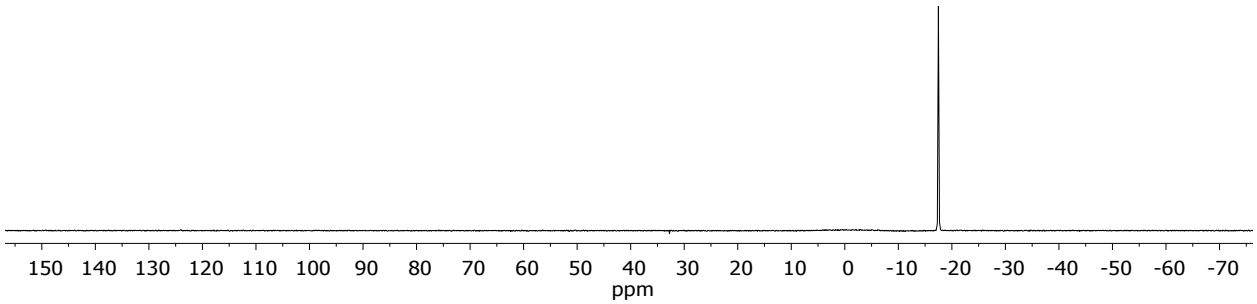


*Figure S44. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10d[B(C_6F_5)$_4$]**.*

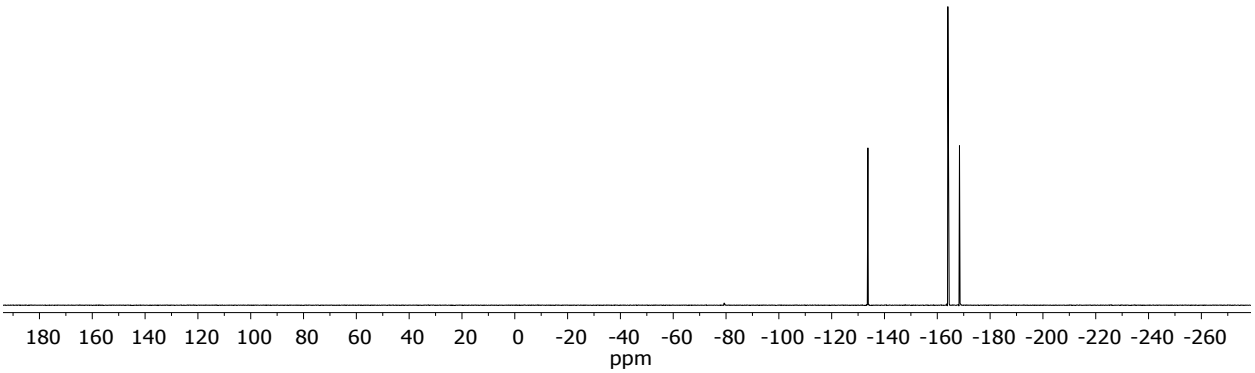


*Figure S45. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10d[$B(C_6F_5)_4$]**.*

2.1.10 NMR Spectra of Compound 10f

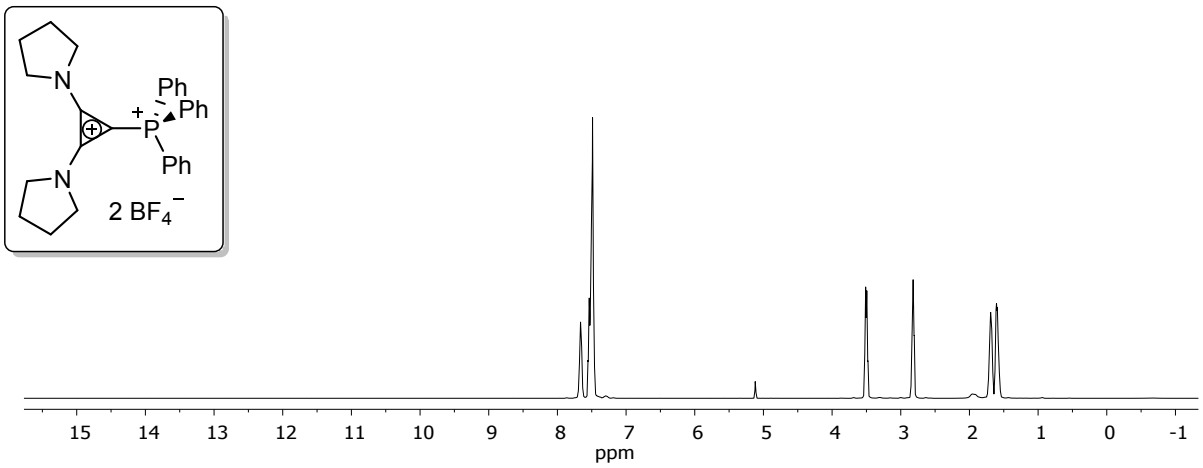


*Figure S46. ^{1}H NMR (CD_3CN) Spectrum of Compound **10f**.*

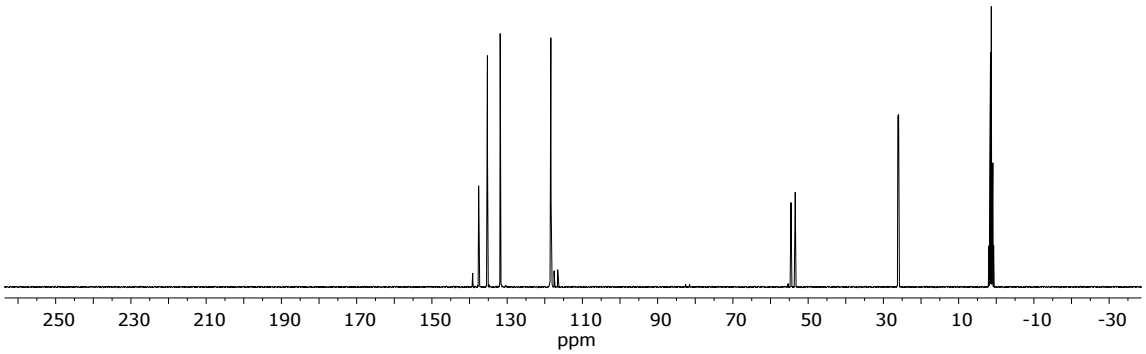


*Figure S47. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10f**.*

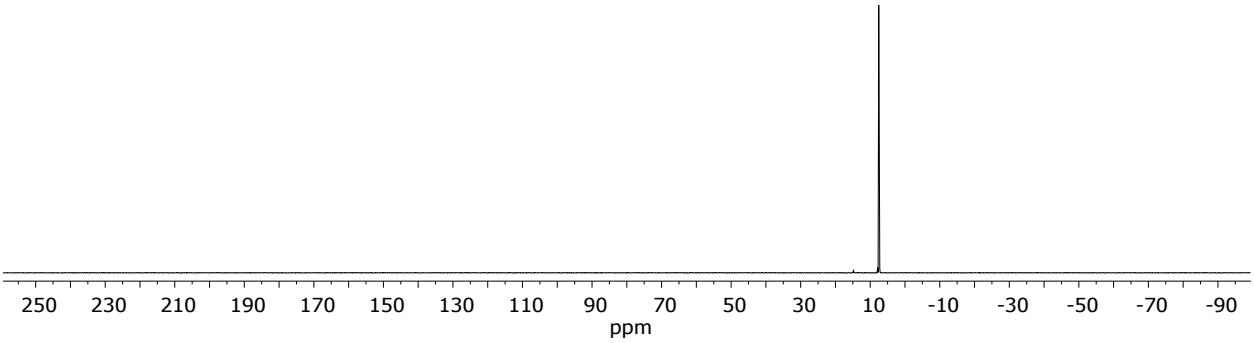


*Figure S48. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10f**.*

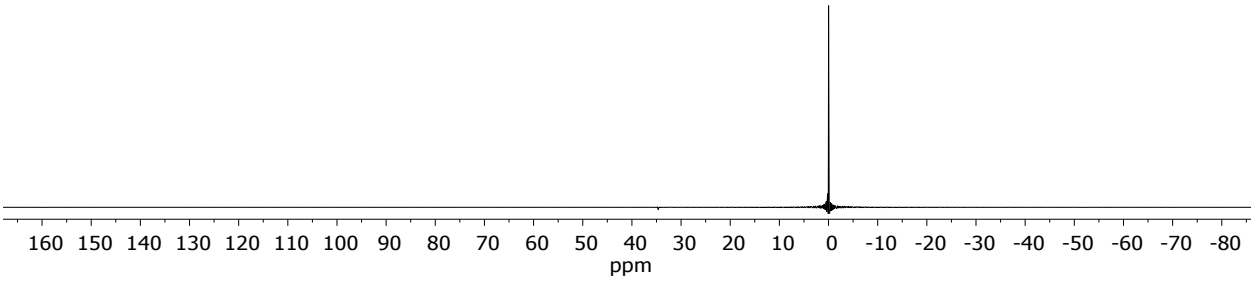


*Figure S49. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10f**.*

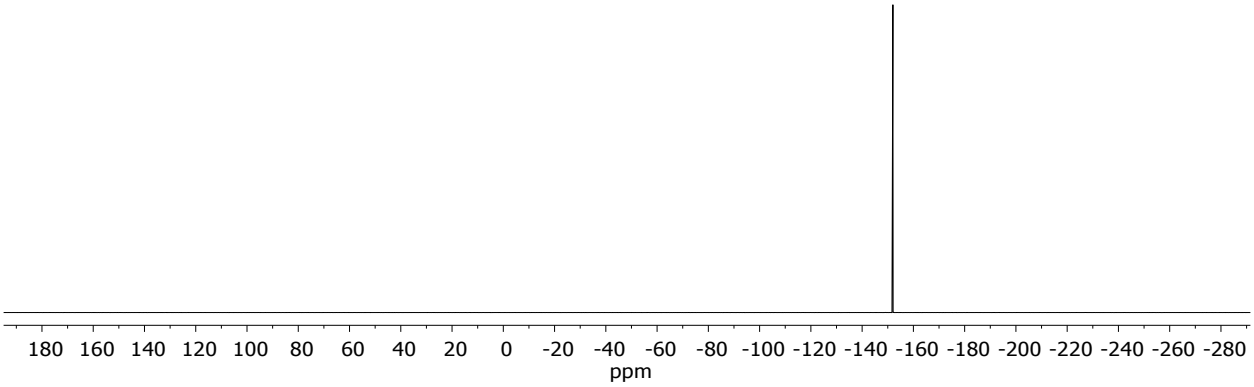


*Figure S50. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10f**.*

2.1.11 NMR Spectra of Compound 10f[$B(C_6F_5)_4$]

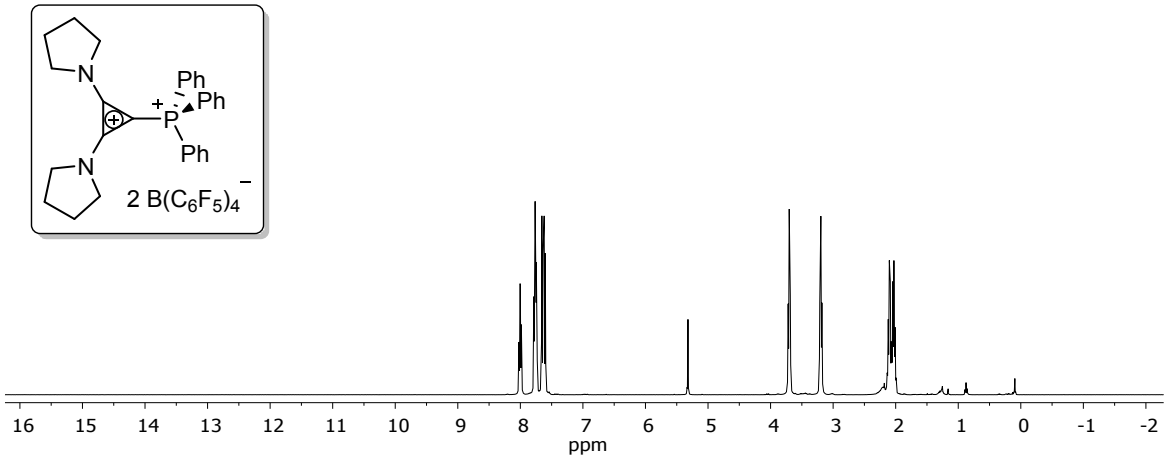


*Figure S51. ^{1}H NMR (CD_2Cl_2) Spectrum of Compound **10f[$B(C_6F_5)_4$]**.*

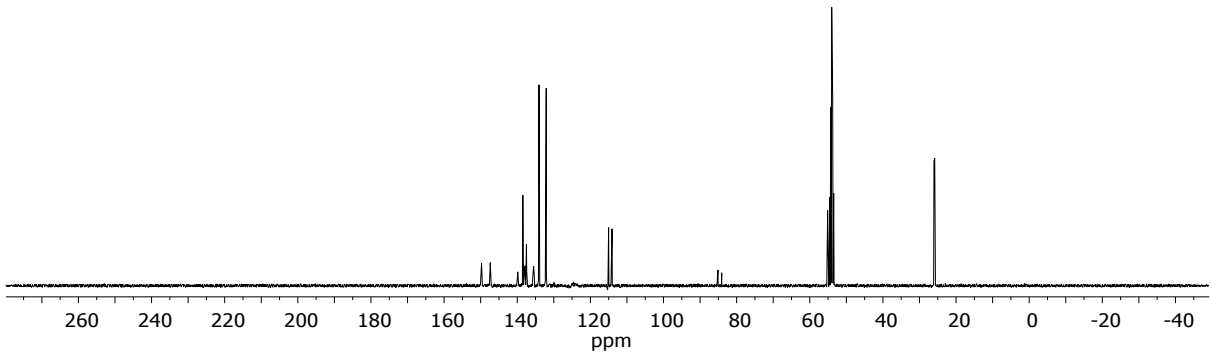


*Figure S52. $^{31}C\{^{1}H\}$ NMR (CD_2Cl_2) Spectrum of Compound **10f[$B(C_6F_5)_4$]**.*

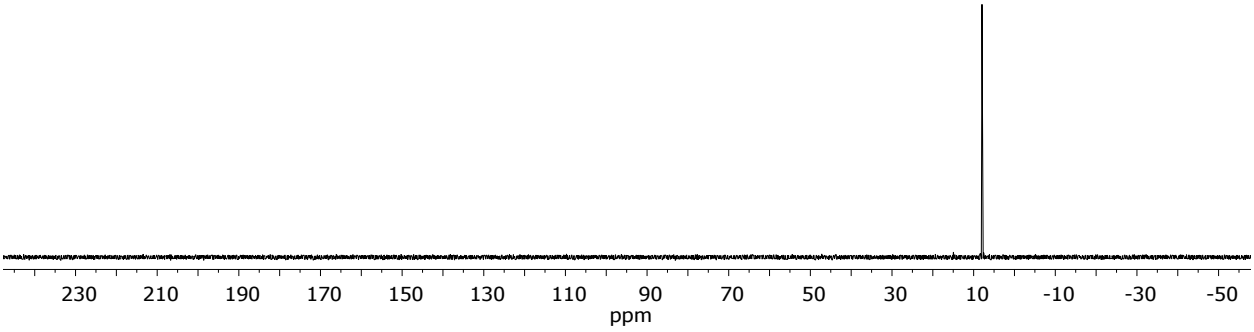


*Figure S53. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10f[$B(C_6F_5)_4$]**.*

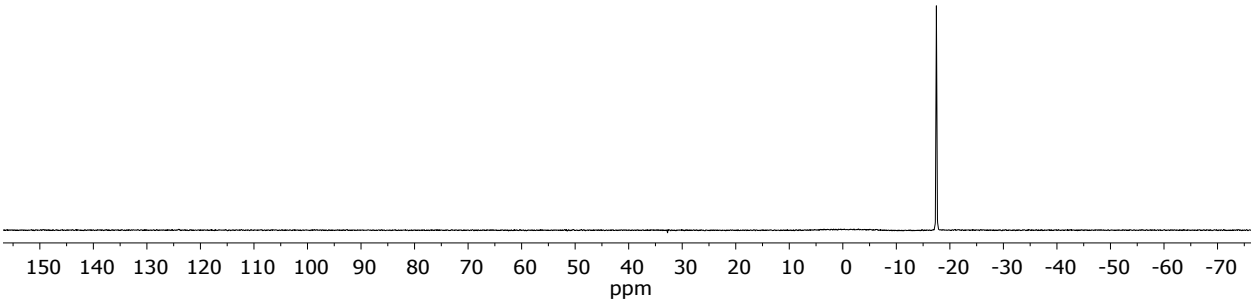


*Figure S54. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10f[B(C_6F_5)$_4$]**.*

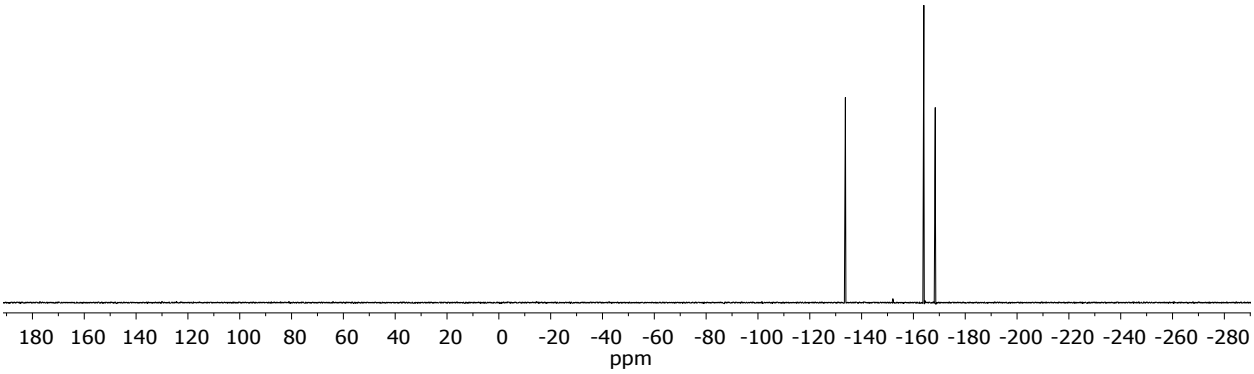


*Figure S55. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **10f[B(C_6F_5)$_4$]**.*

2.2 Pyridinium-substituted phosphonium salts

2.2.1 NMR Spectra of Compound 15(TfO)

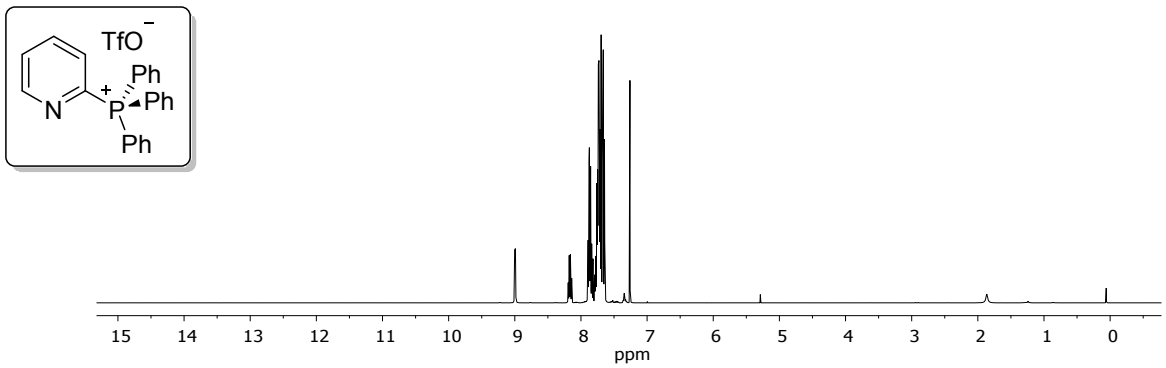


*Figure S56. ^{1}H NMR ($CDCl_3$) Spectrum of Compound **15(TfO)**.*

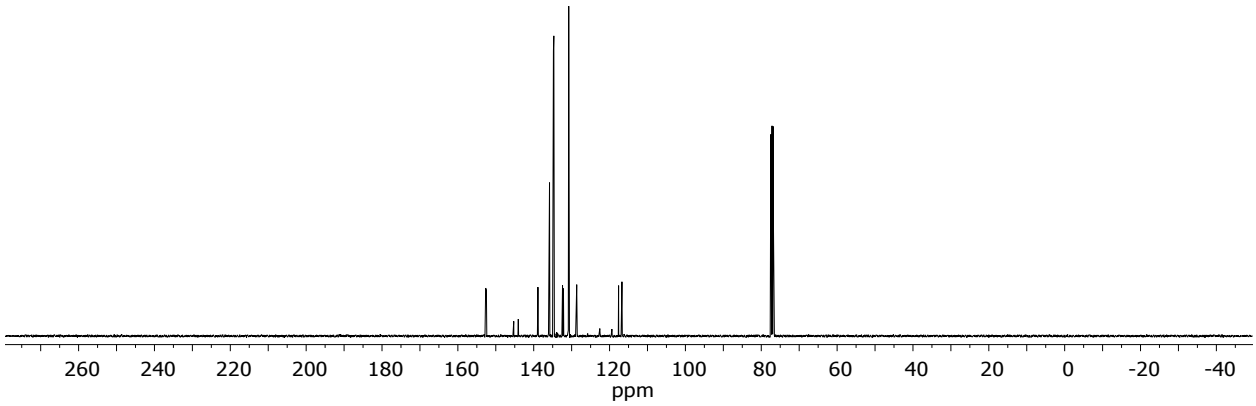


*Figure S57. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) Spectrum of Compound **15(TfO)**.*

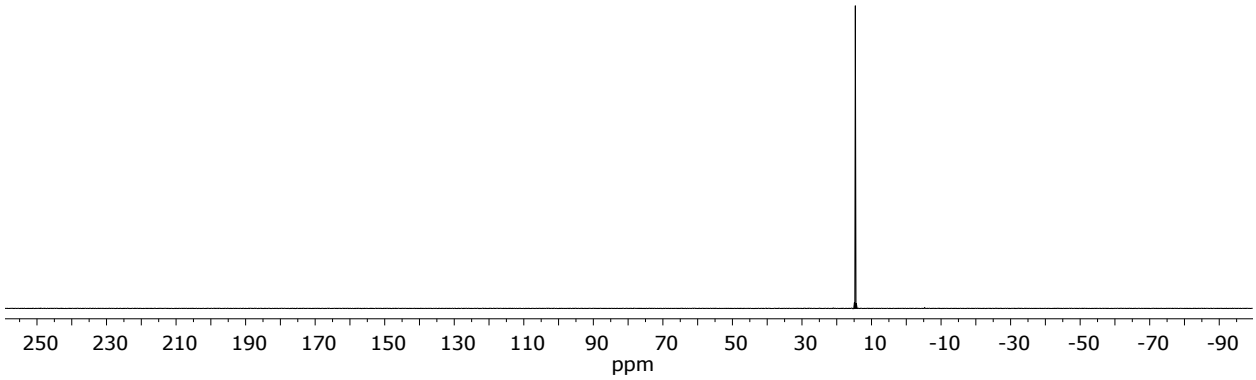


*Figure S58. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$) Spectrum of Compound **15(TfO)**.*

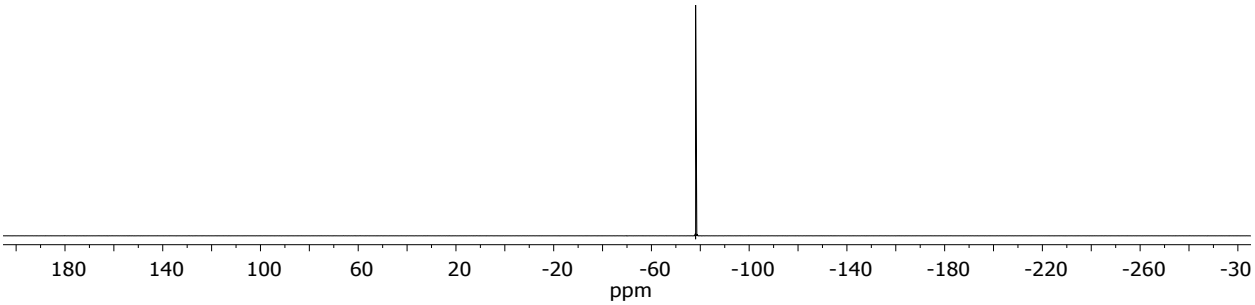
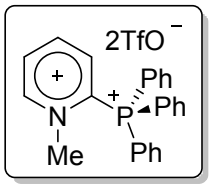


*Figure S59. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$) Spectrum of Compound **15(TfO)**.*

2.2.2 NMR Spectra of Compound 11a



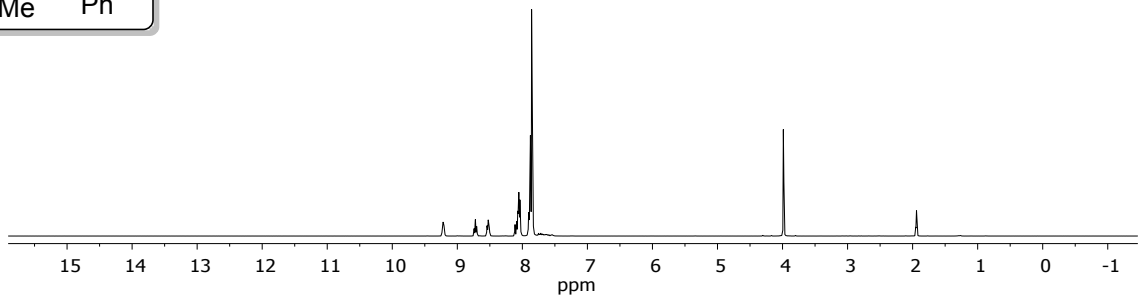


*Figure S60. ^{1}H NMR (CD_3CN) Spectrum of Compound **11a**.*

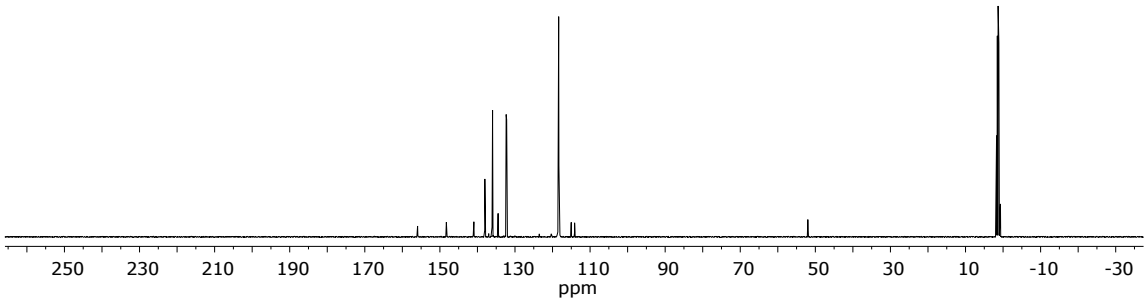


*Figure S61. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11a**.*

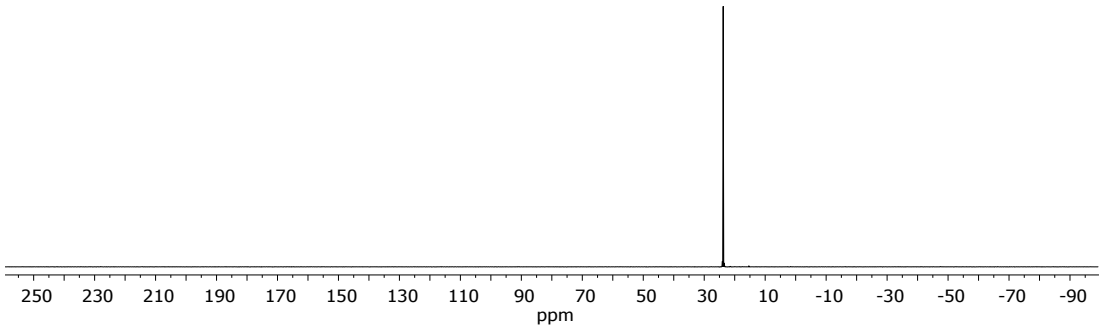


*Figure S62. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11a**.*

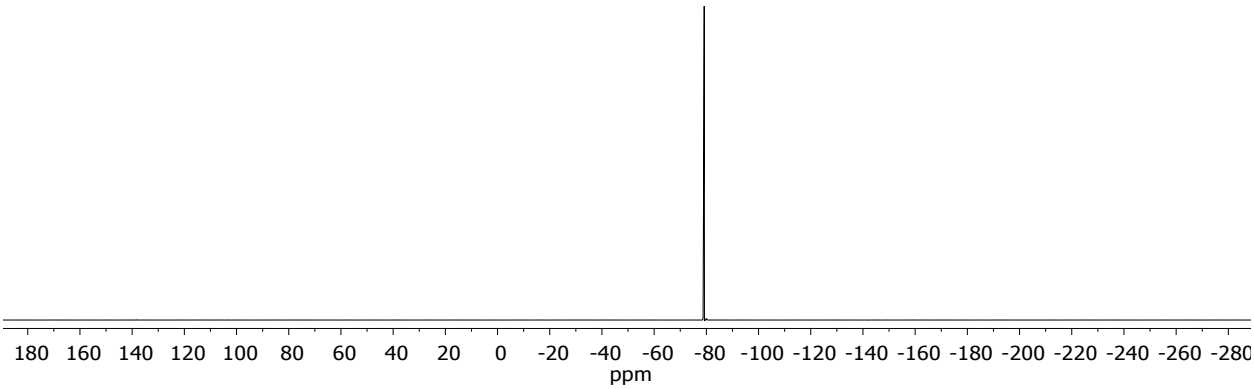


*Figure S63. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11a**.*

2.2.3 NMR Spectra of Compound 11a[$B(C_6F_5)_4$]

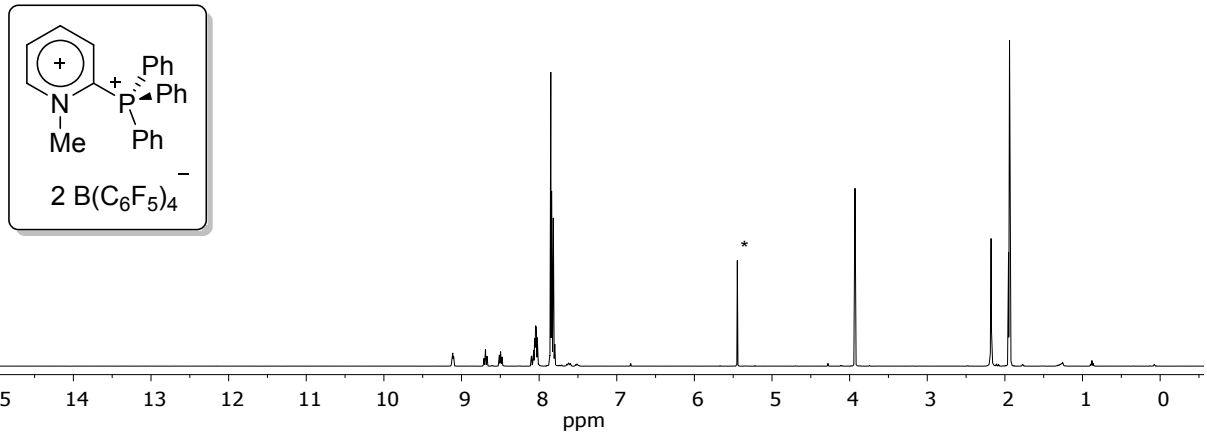


*Figure S64. ^{1}H NMR (CD_3CN) Spectrum of Compound **11a[$B(C_6F_5)_4$]**.*

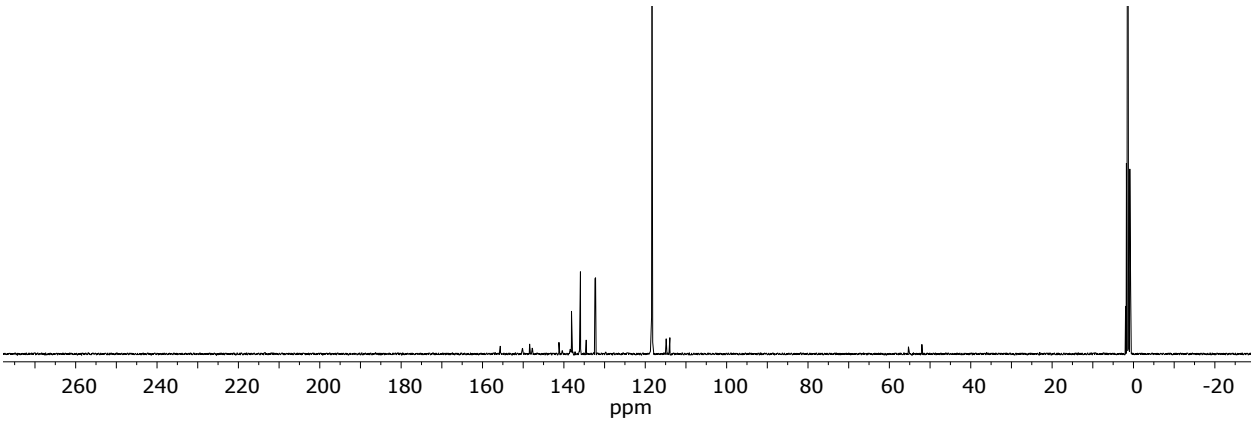


*Figure S65. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11a[B(C_6F_5)$_4$]**.*

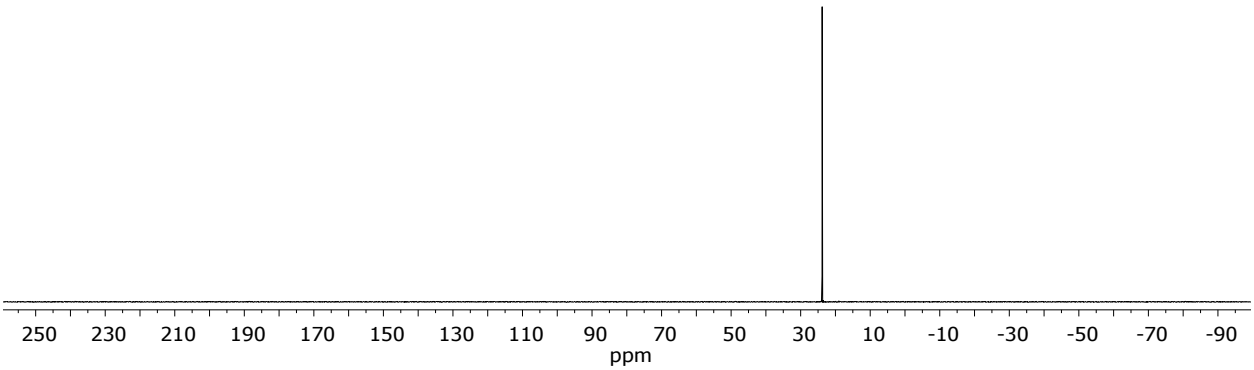


*Figure S66. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11a[B(C_6F_5)$_4$]**.*

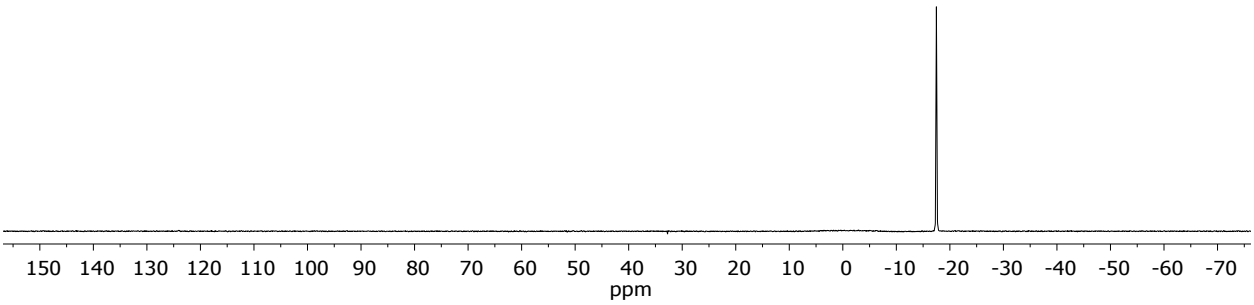


*Figure S67. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11a[B(C_6F_5)$_4$]**.*

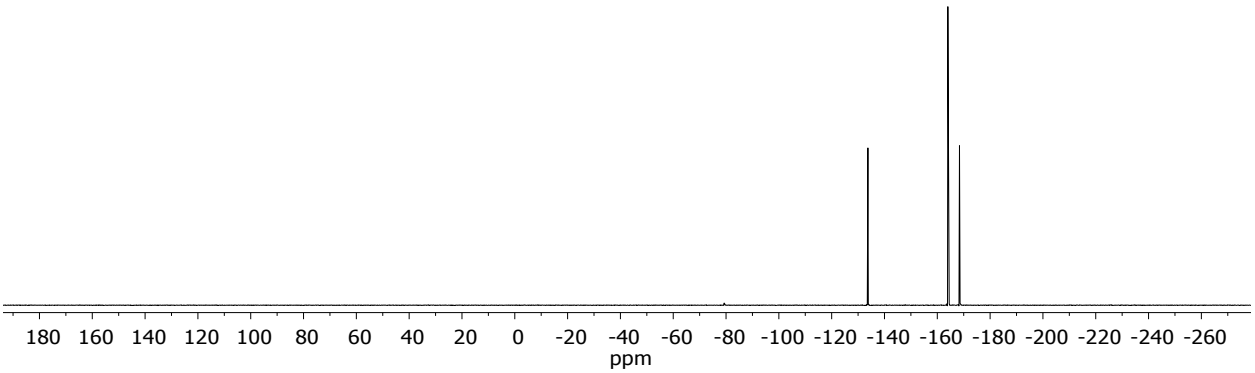


*Figure S68. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11a[B(C_6F_5)$_4$]**.*

2.2.4 NMR Spectra of Compound 17(I)

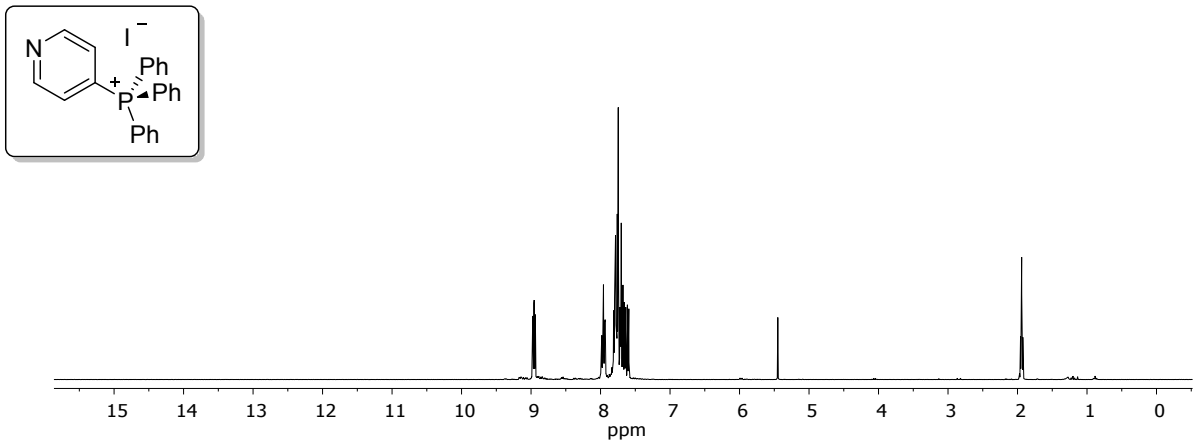


*Figure S69. ^{1}H NMR (CD_3CN) Spectrum of Compound **17(I)**.*

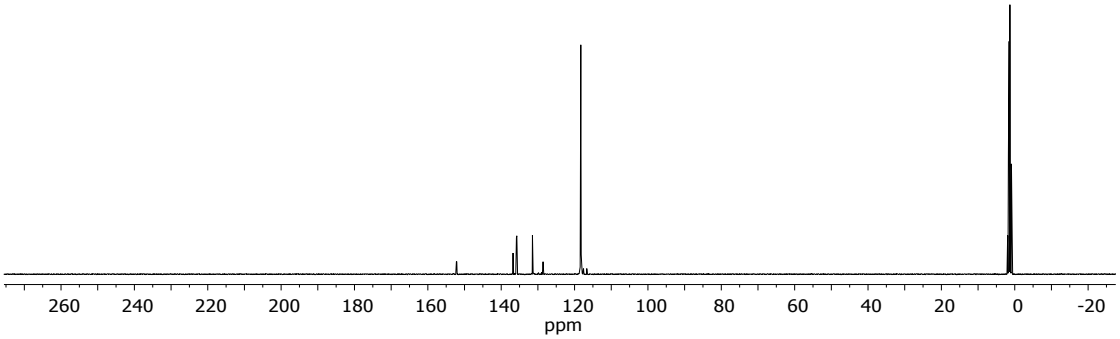


*Figure S70.$^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **17(I)**.*

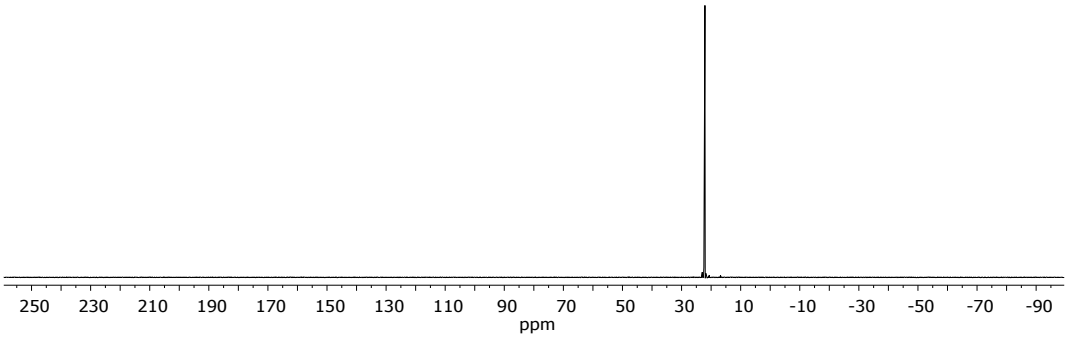


*Figure S71. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **17(I)**.*

2.2.5 NMR Spectra of Compound 11b

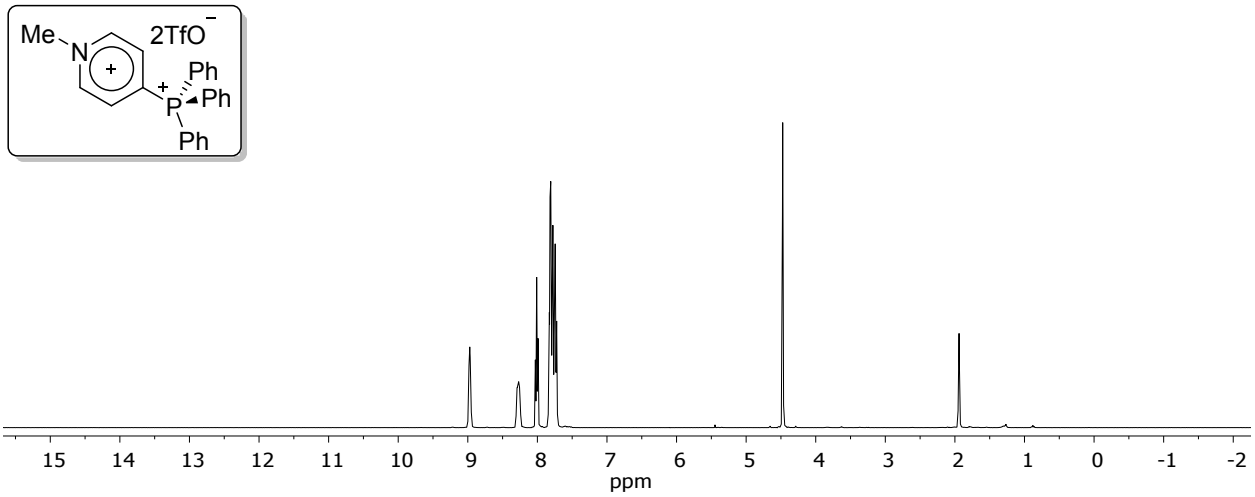


*Figure S72. ^{1}H NMR (CD_3CN) Spectrum of Compound **11b**.*

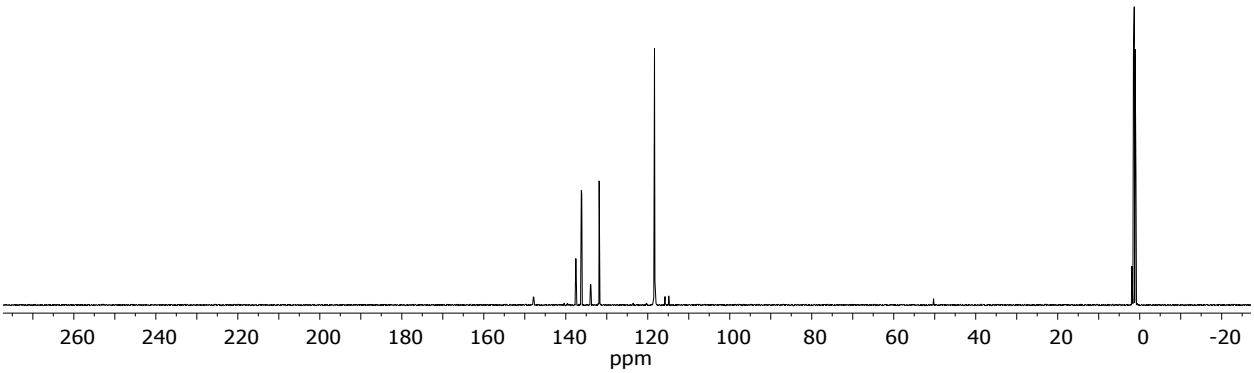


*Figure S73. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11b**.*

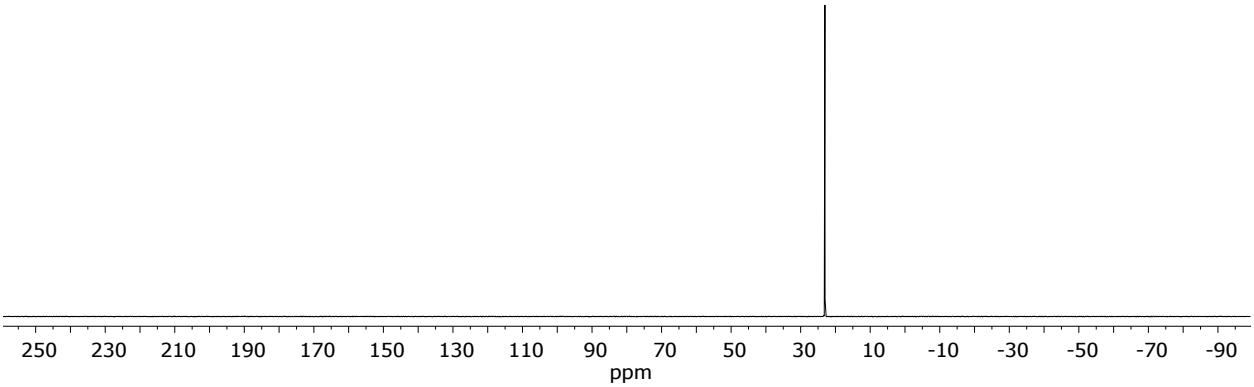


*Figure S74. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11b.***

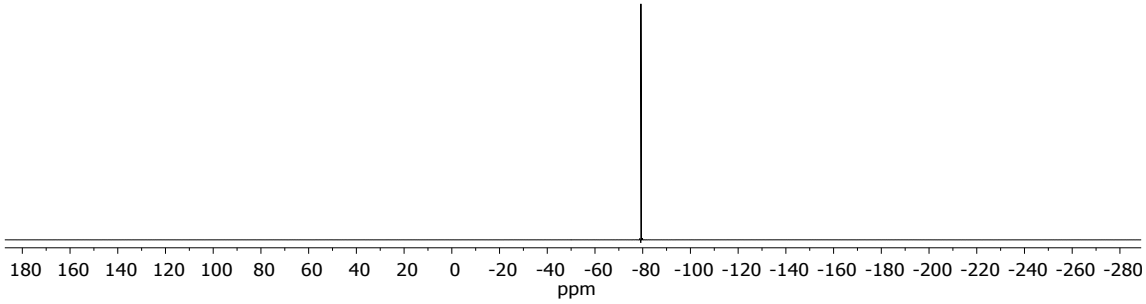


*Figure S75. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11b**.*

2.2.6 NMR Spectra of Compound 11b[$B(C_6F_5)_4$]

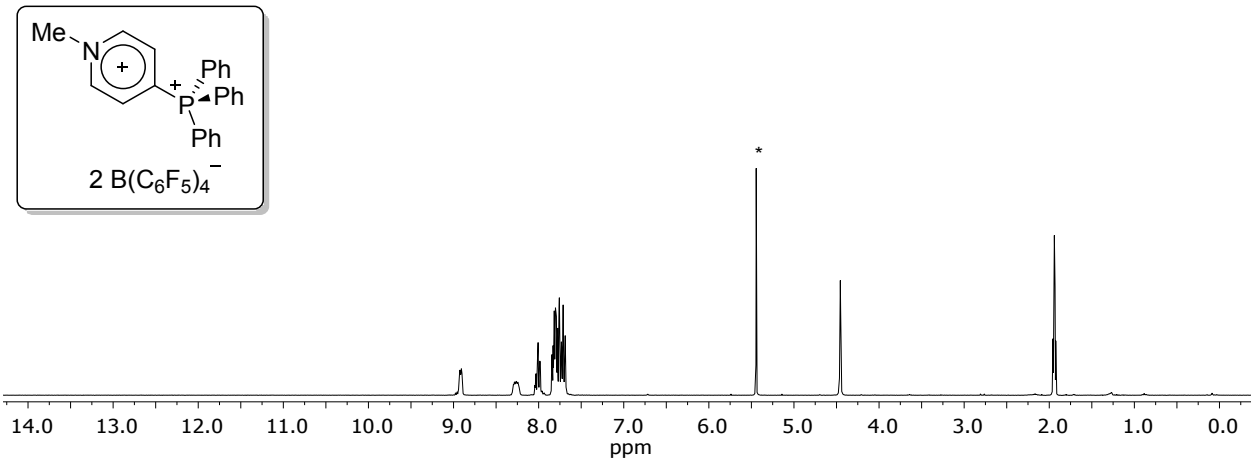


*Figure S76. ^{1}H NMR (CD_3CN) Spectrum of Compound **11b[$B(C_6F_5)_4$]**. Asterisk denotes a solvent impurities.*

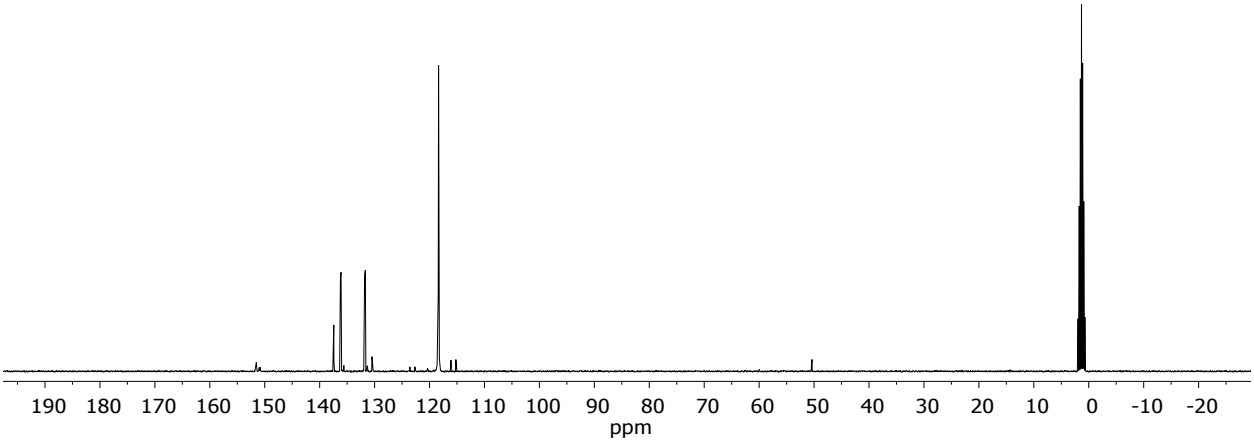


*Figure S77. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11b[$B(C_6F_5)_4$]**.*

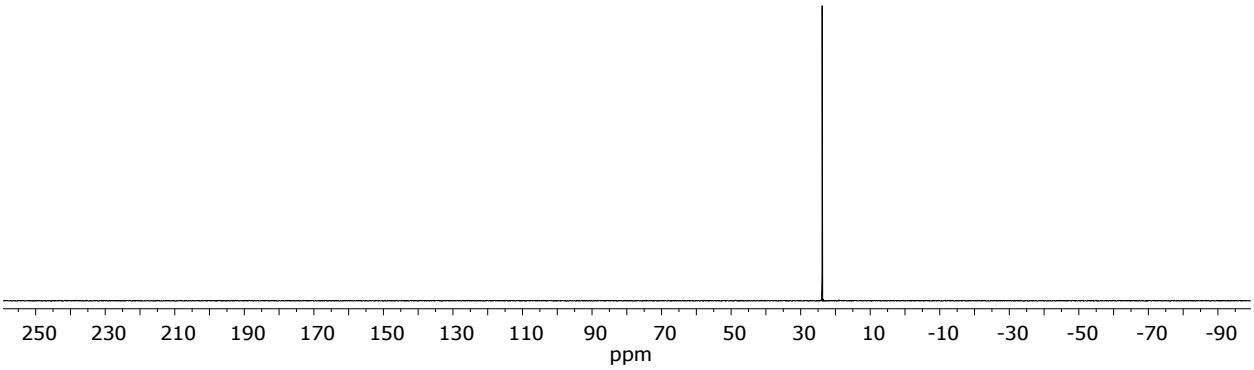


*Figure S78. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11b[$B(C_6F_5)_4$]**.*

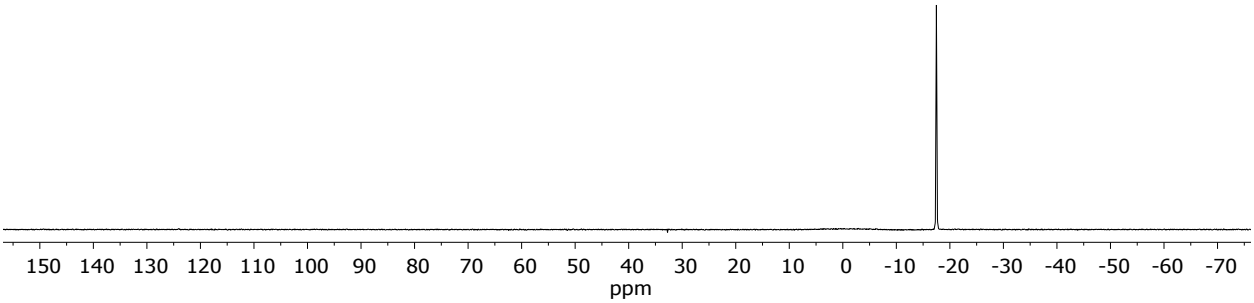


*Figure S79. $^{11}B\{^1H\}$ NMR (CD_3CN) Spectrum of Compound **11b[B(C_6F_5)$_4$].***

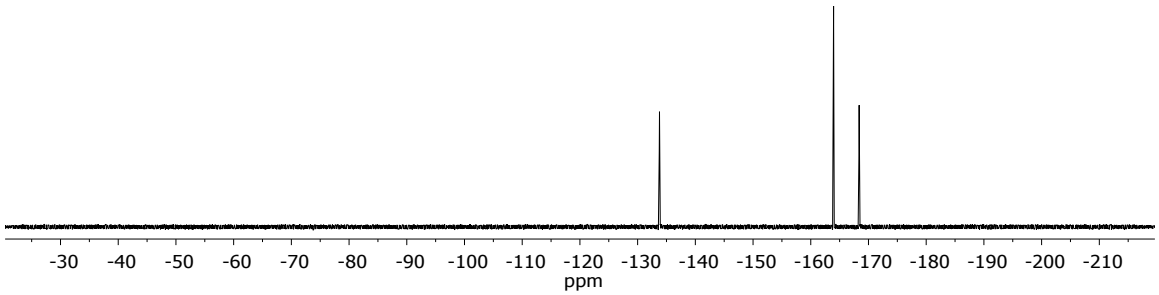
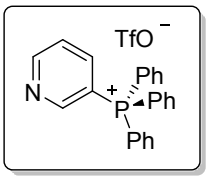


*Figure S80. $^{19}F\{^1H\}$ NMR (CD_3CN) Spectrum of Compound **11b[B(C_6F_5)$_4$]**.*

2.2.7 NMR Spectra of Compound 19(TfO)



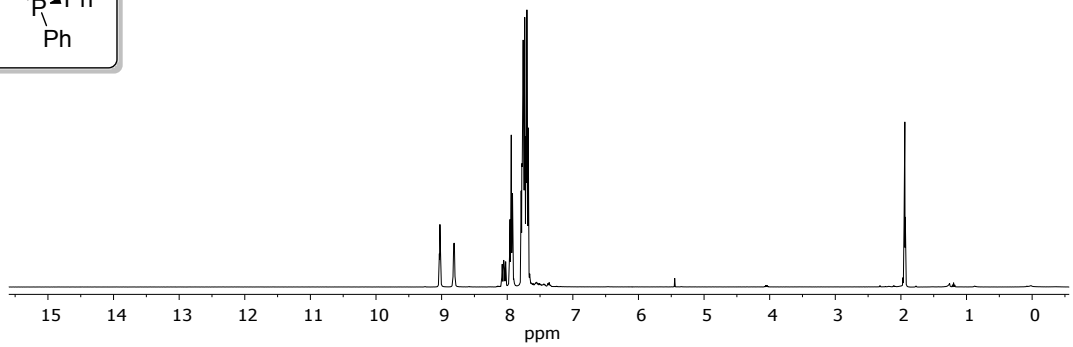


*Figure S81. ^1H NMR (CD_3CN) Spectrum of Compound **19(TfO)**.*

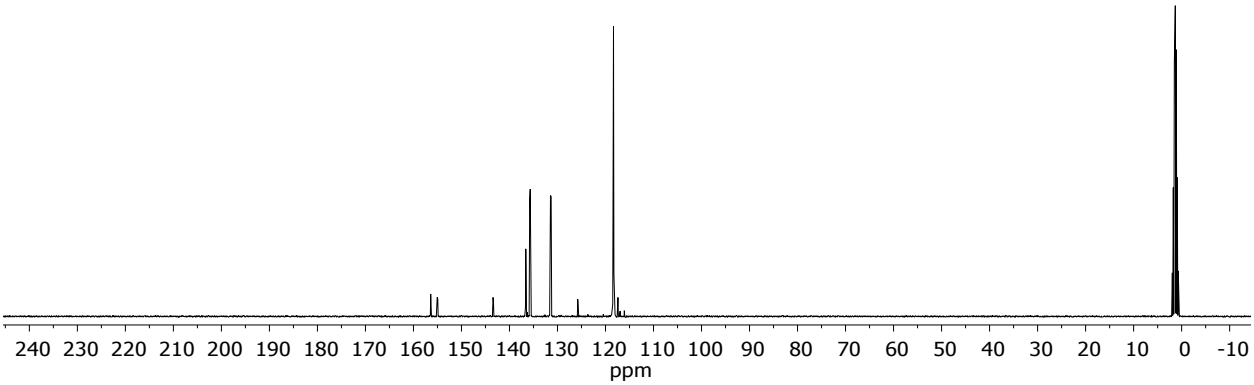


*Figure S82. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **19(TfO)**.*

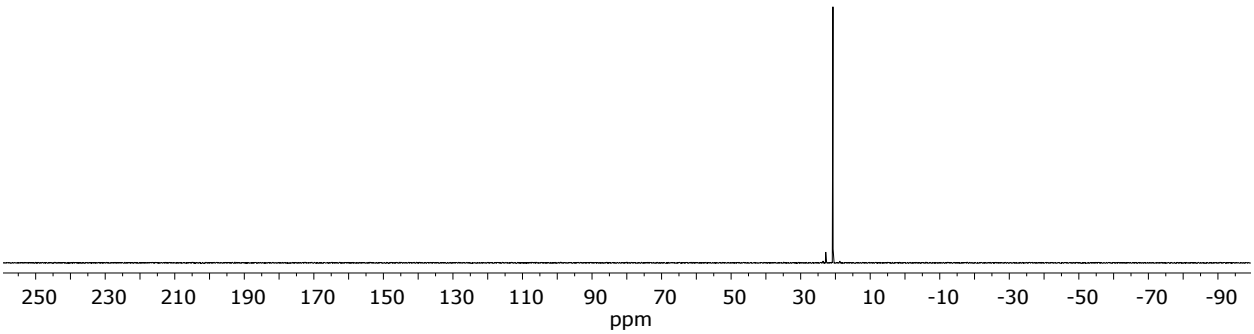


*Figure S83. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **19(TfO)**.*

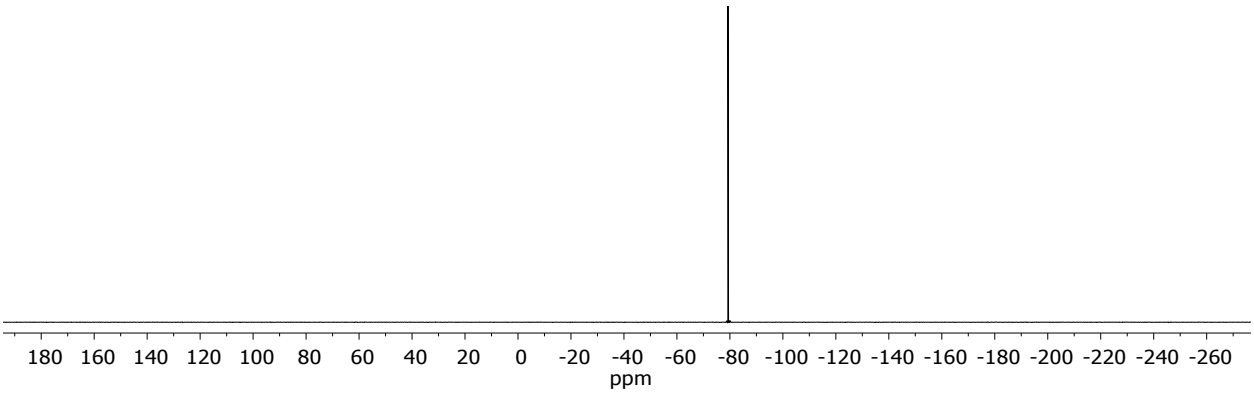
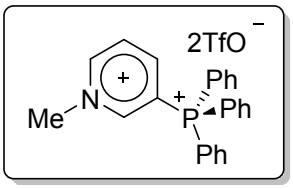


*Figure S84. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **19(TfO)**.*

2.2.8 NMR Spectra of Compound 11c



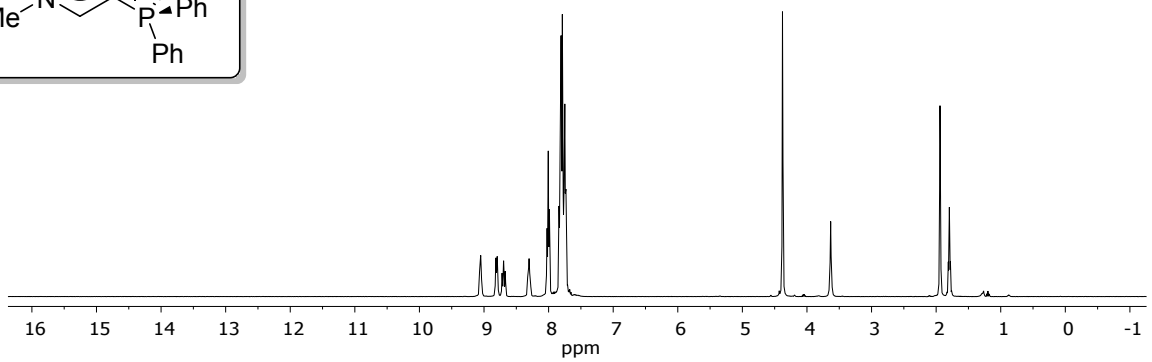


*Figure S85. ^{1}H NMR (CD_3CN) Spectrum of Compound **11c**.*

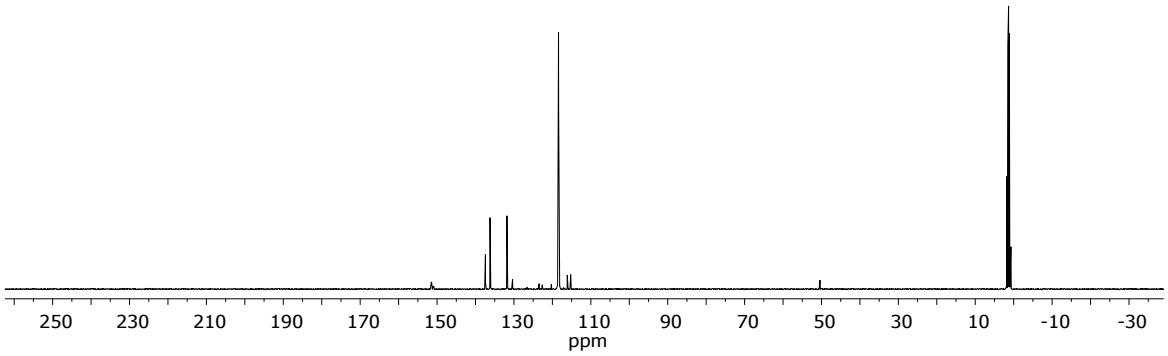


*Figure S86. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11c**.*

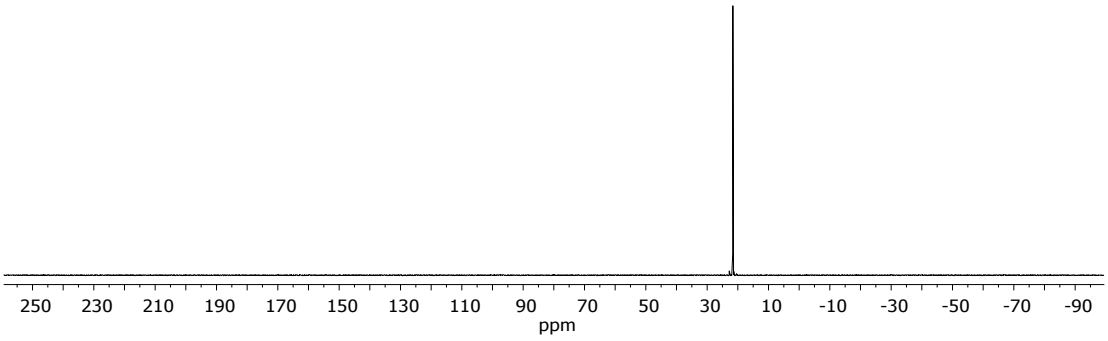


*Figure S87. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11c**.*

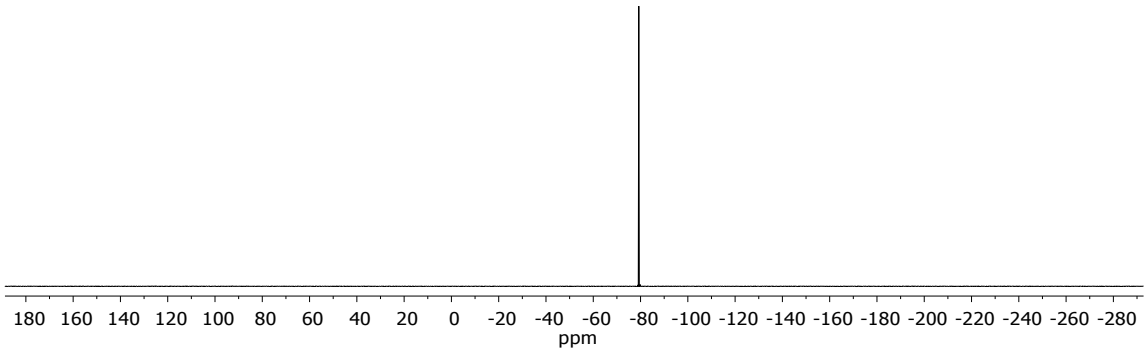


*Figure S88. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11c**.*

2.2.9 NMR Spectra of Compound 11c[$B(C_6F_5)_4$]

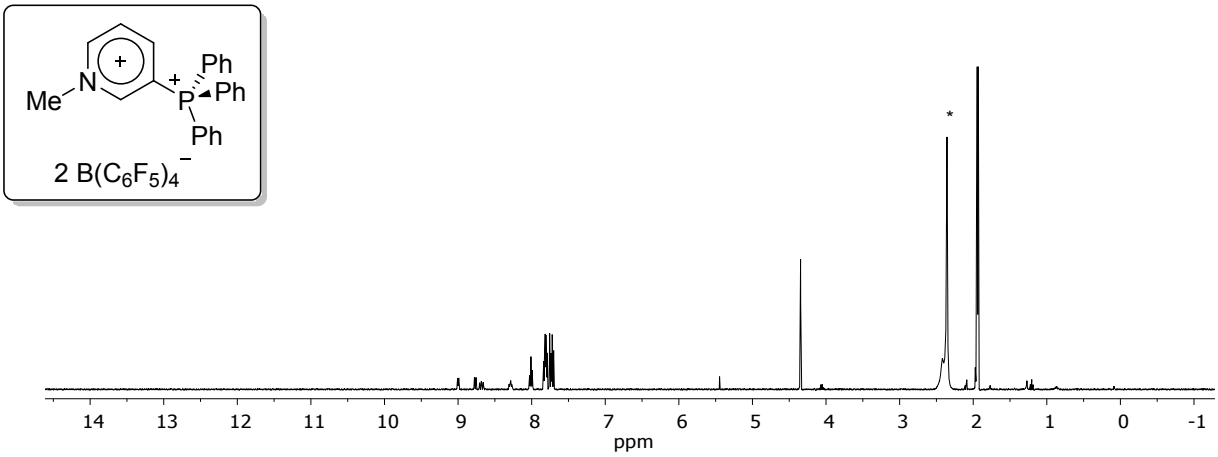


*Figure S89. ^{1}H NMR (CD_3CN) Spectrum of Compound **11c[$B(C_6F_5)_4$]**. Asterisk denotes a solvent impurity.*

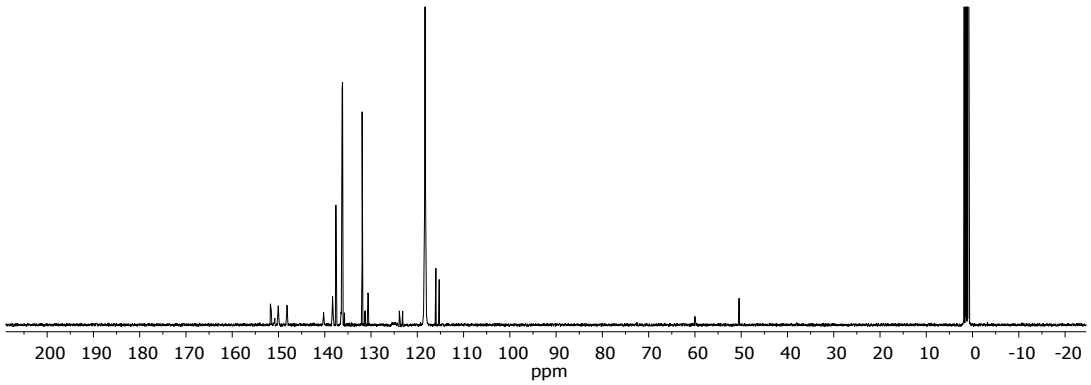


*Figure S90. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11c[$B(C_6F_5)_4$]**.*

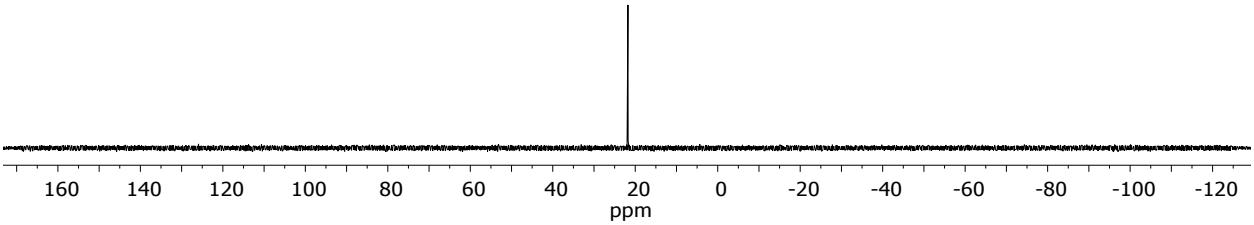


*Figure S91. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11c[B(C_6F_5)$_4$]**.*

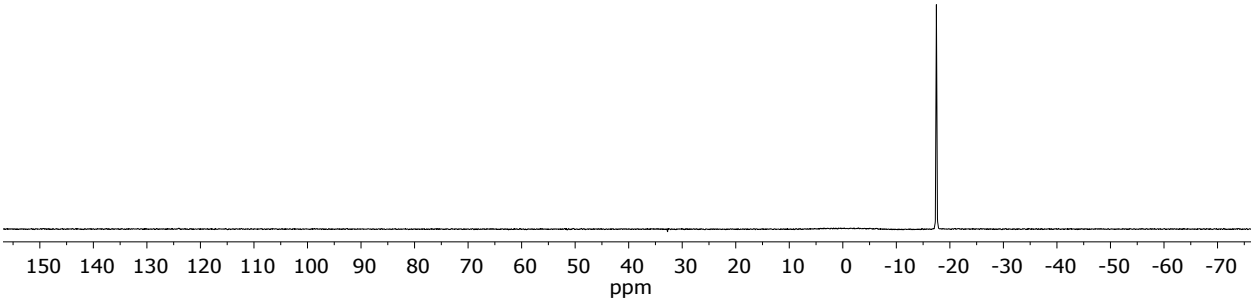


*Figure S92. $^{11}B\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11c[B(C_6F_5)$_4$]**.*

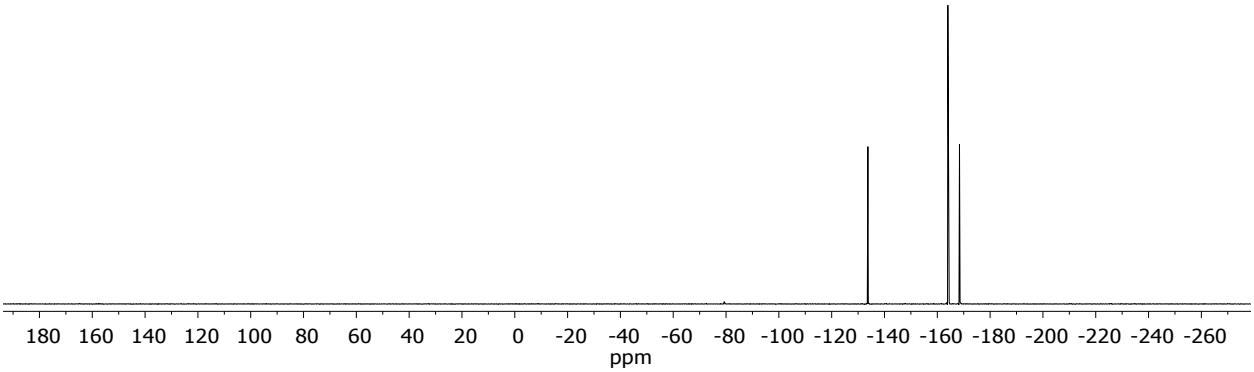


*Figure S93. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **11c[B(C_6F_5)$_4$]**.*

2.2.10 NMR Spectra of Compound 21

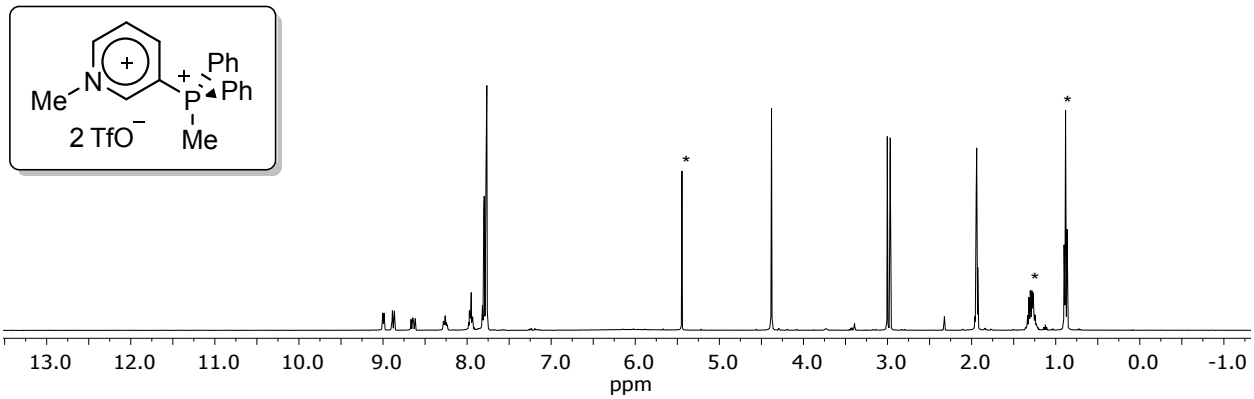


*Figure S94. ^{1}H NMR (CD_3CN) Spectrum of Compound **21.** Asterisks denote solvent impurities.*

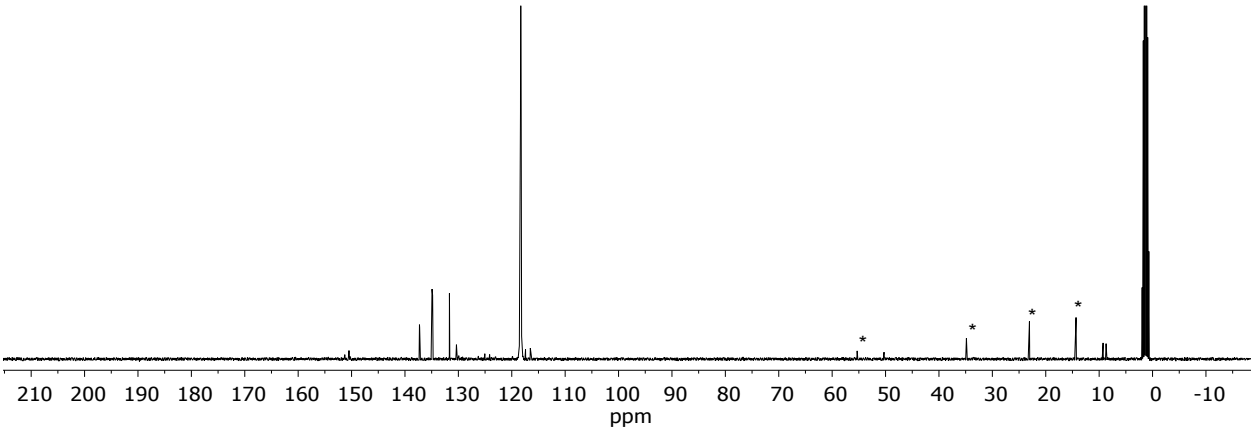


*Figure S95. $^{13}C\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **21.** Asterisks denote solvent impurities.*

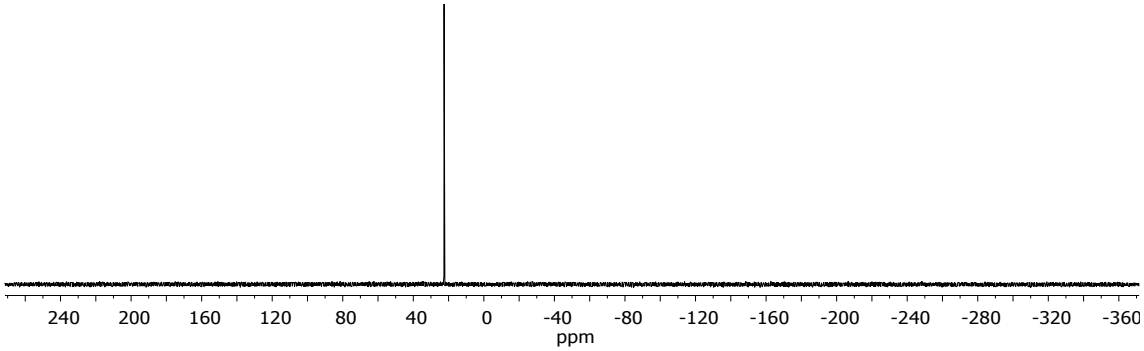


*Figure S96. $^{31}P\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **21.***

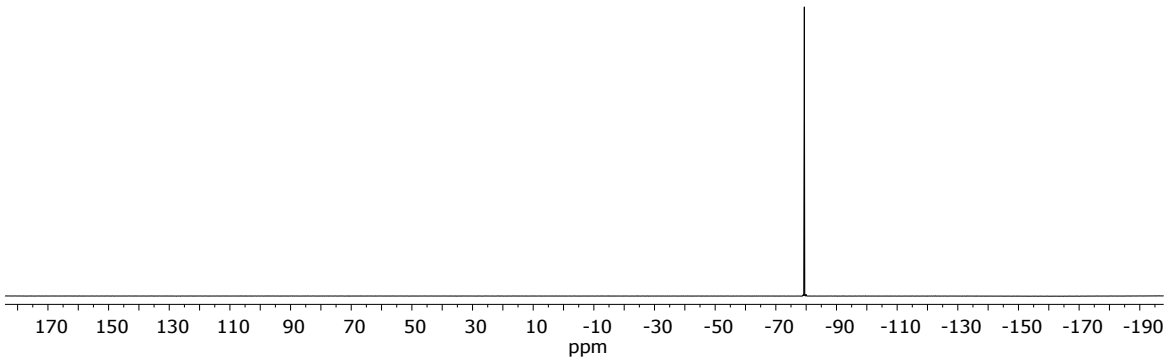
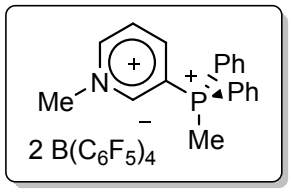


*Figure S97. $^{19}F\{^{1}H\}$ NMR (CD_3CN) Spectrum of Compound **21.***

2.2.11 NMR Spectra of Compound 21[$B(C_6F_5)_4$]



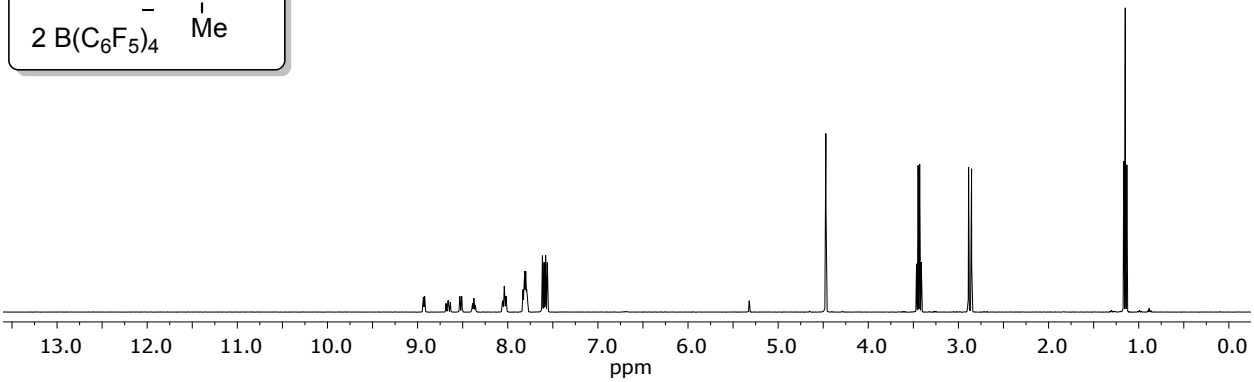


*Figure S98. ^{1}H NMR (CD_2Cl_2) Spectrum of Compound **21[$B(C_6F_5)_4$]**.*

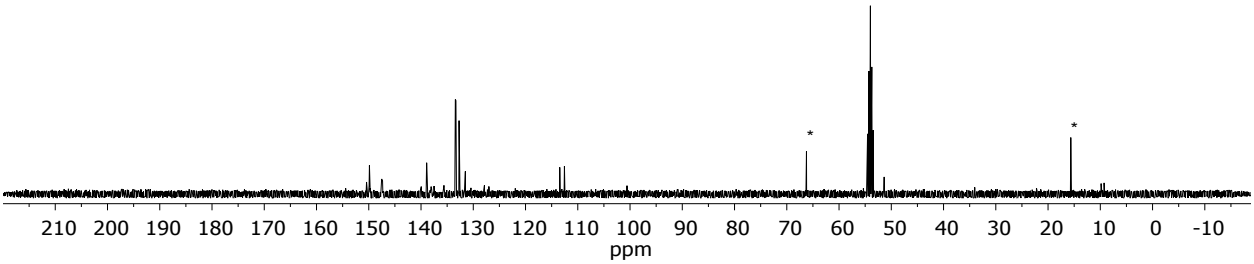


*Figure S99. $^{13}C\{^{1}H\}$ NMR (CD_2Cl_2) Spectrum of Compound **21[$B(C_6F_5)_4$]**.*

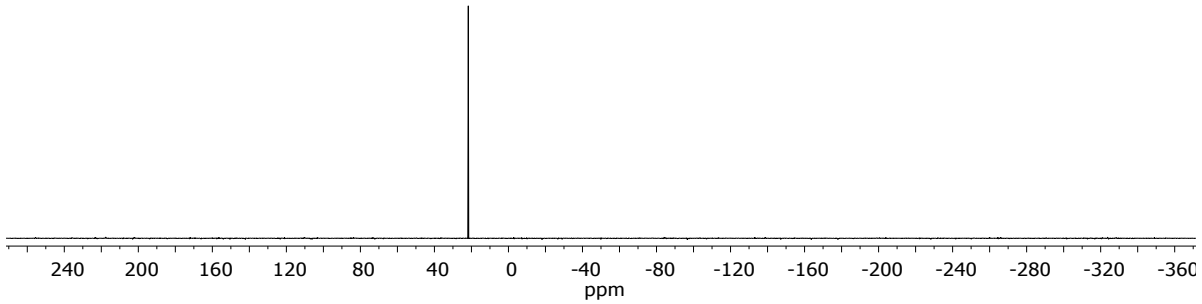


*Figure S100. $^{31}P\{^{1}H\}$ NMR (CD_2Cl_2) Spectrum of Compound **21[B(C_6F_5)$_4$]**.*

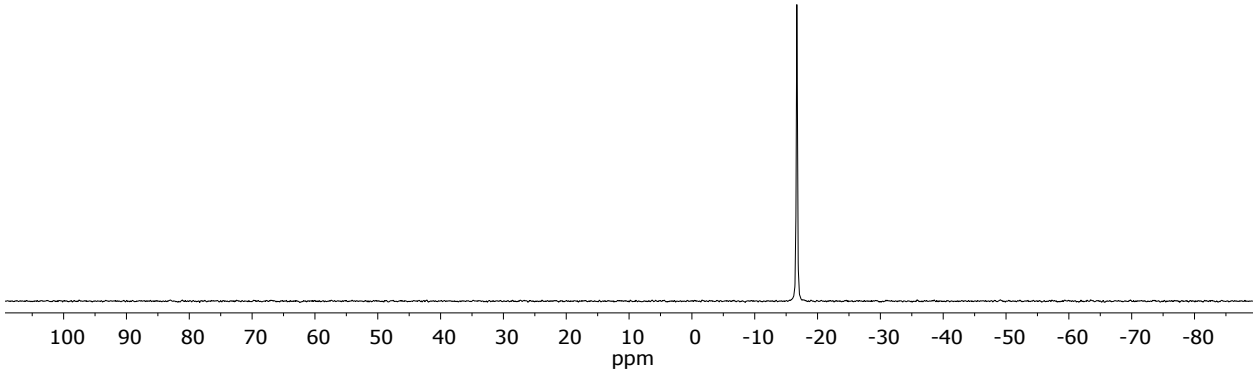


*Figure S101. $^{11}B\{^{1}H\}$ NMR (CD_2Cl_2) Spectrum of Compound **21[B(C_6F_5)$_4$]**.*

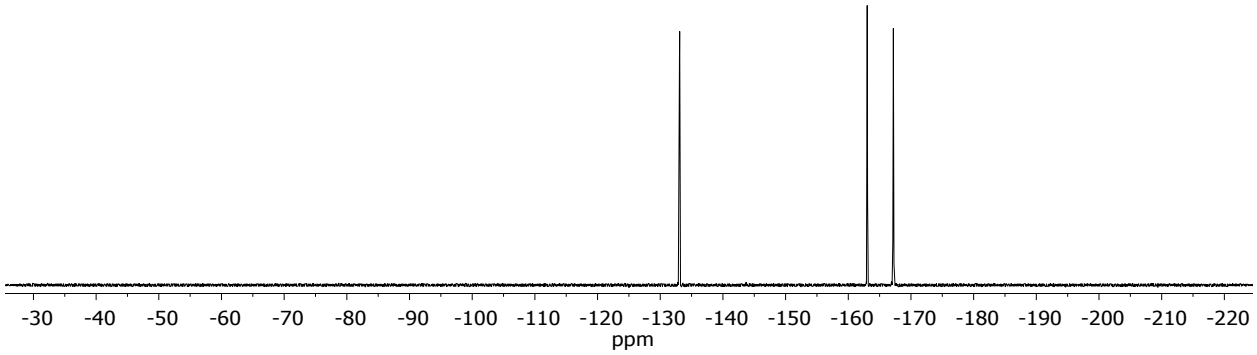


*Figure S102. $^{19}F\{^{1}H\}$ NMR (CD_2Cl_2) Spectrum of Compound **21[B(C_6F_5)$_4$]**.*

2.2.12 NMR Spectra of Compound 12[$B(C_6F_5)_4$]

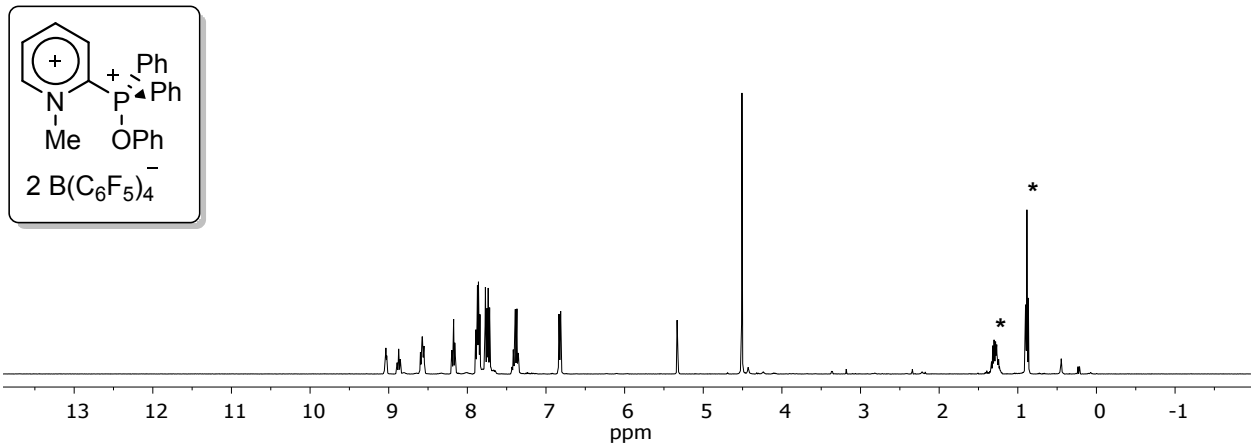


*Figure S103 ^{1}H NMR (CD_2Cl_2) Spectrum of Compound **12[$B(C_6F_5)_4$]**. Asterisks denote solvent impurities.*

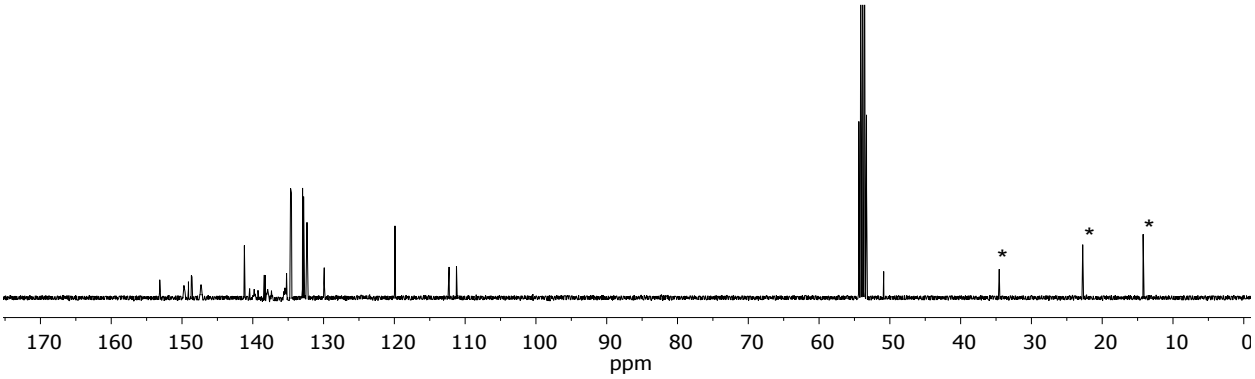


*Figure S104. $^{13}C\{^{1}H\}$NMR (CD_2Cl_2) Spectrum of Compound **12[$B(C_6F_5)_4$]**. Asterisks denote solvent impurities.*

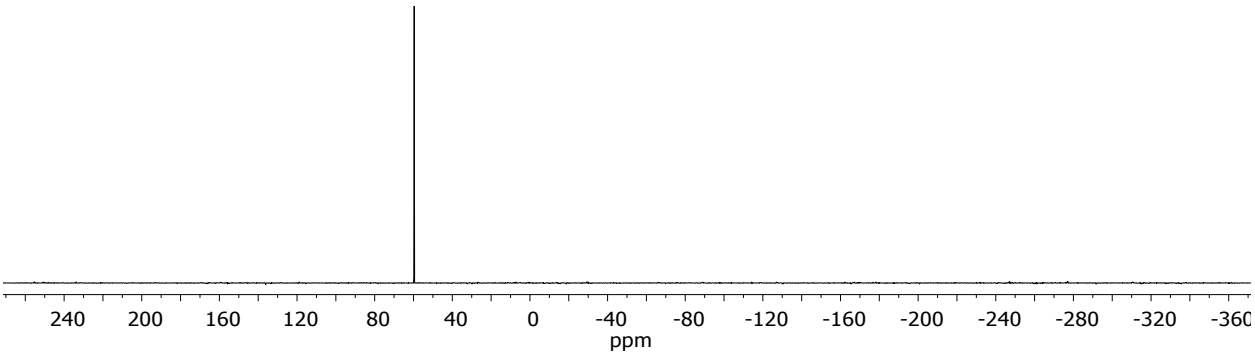


*Figure S105. $^{31}P\{^{1}H\}$NMR (CD_2Cl_2) Spectrum of Compound **12[$B(C_6F_5)_4$]**.*

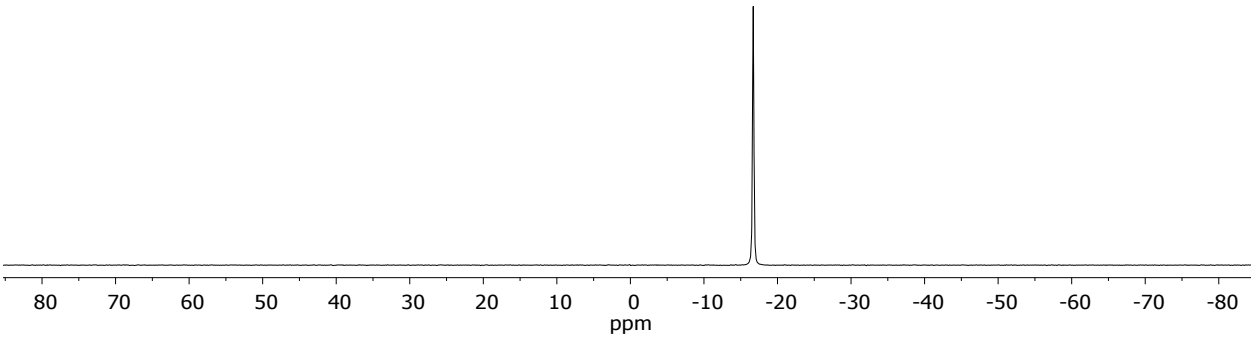


Figure S106. $^{11}B\{^1H\}$NMR (CD_2Cl_2) Spectrum of Compound ***12[B(C_6F_5)$_4$]}.***

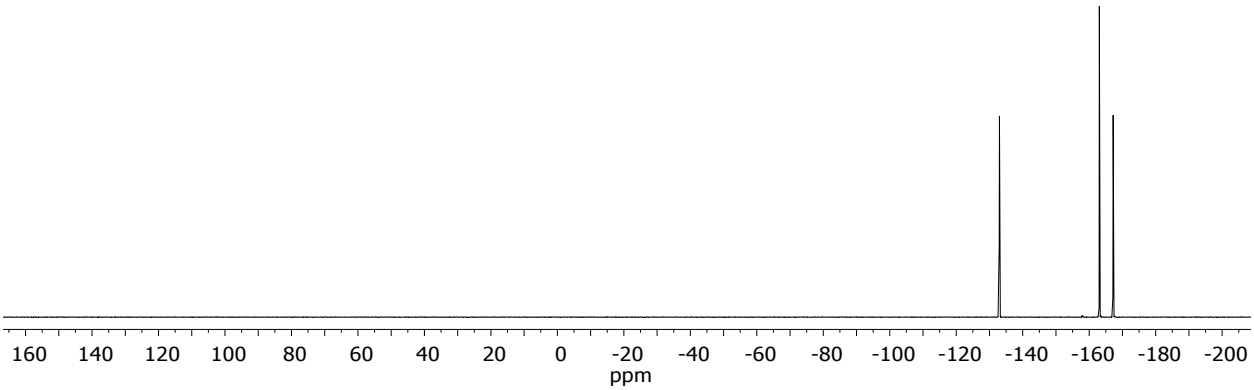


Figure S107. $^{19}F\{^1H\}$NMR (CD_2Cl_2) Spectrum of Compound ***12[B(C_6F_5)$_4$]}.***

2.3. Lewis Acid-catalyzed Mukaiyama-Aldol Condensation Reaction

General Method 1: The corresponding phosphonium salt (0.5-10 mol%) and 2-naphthaldehyde (1.0 equiv) were dissolved in Et_2O or CH_2Cl_2 and stirred for 5 to 10 min. Then, 1-methoxy-2-methyl-1-trimethylsiloxy-propene was added (1.2 equiv). The reaction progress was monitored by GC-MS and once full conversion was reached, the mixture was filtered through a silica plug and dried *in vacuo*. The product was isolated as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85 (m, 4H), 7.50 (m, 3H), 5.18 (s, 1H), 3.72 (s, 3H), 1.20 (s, 3H), 1.07 (s, 3H), 0.00 ppm (2, 9H). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** δ = 177.4, 138.6, 133.0, 132.8, 128.1, 127.7, 127.0, 126.7, 126.1, 125.9, 125.4, 79.4, 51.8, 49.4, 19.3, 0.1 ppm. **IR**: $\tilde{\nu}$ = 2976, 2953, 2845, 1733, 1693, 1599, 1510, 1463, 1436, 1366, 1248, 1192, 1167, 1133, 1083, 1017, 980, 876, 854, 840, 736, 679, 562, 478 cm^{-1}. **HRMS**: m/z 353.144270 (calcd. for $C_{19}H_{26}O_3Si_1$: 353.154342).

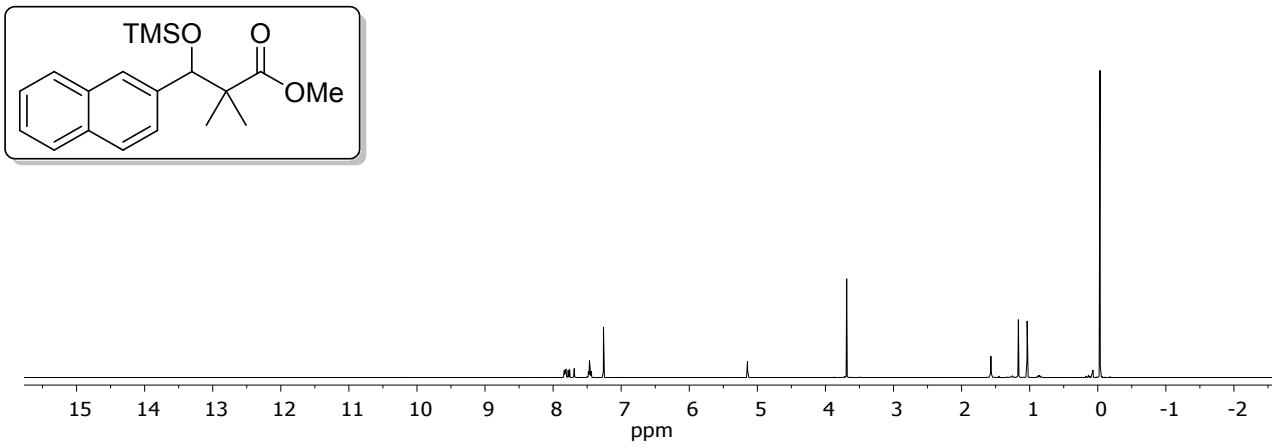


Figure S111. ^{1}H NMR ($CDCl_3$) spectrum of isolated product.

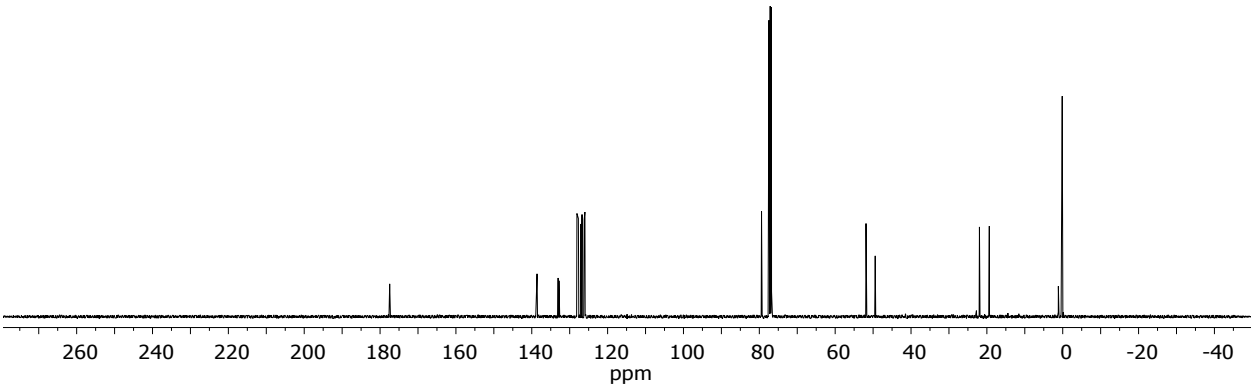


Figure S112. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectrum of isolated product.

General Method 2: The corresponding phosphonium salt (0.1 mol%) and 2-naphthaldehyde (1.0 equiv) were dissolved in CH_2Cl_2 and stirred for 5 min. Then, 1-methoxy-2-methyl-1-trimethylsiloxy-propene was added (1.2 equiv). After 5 min at ambient temperature, the solution was dried *in vacuo*. The remaining solid was dissolved in $CDCl_3$ and filtered through a Celite plug. Conversions were determined by ^{1}H NMR spectroscopy with a toluene internal standard.

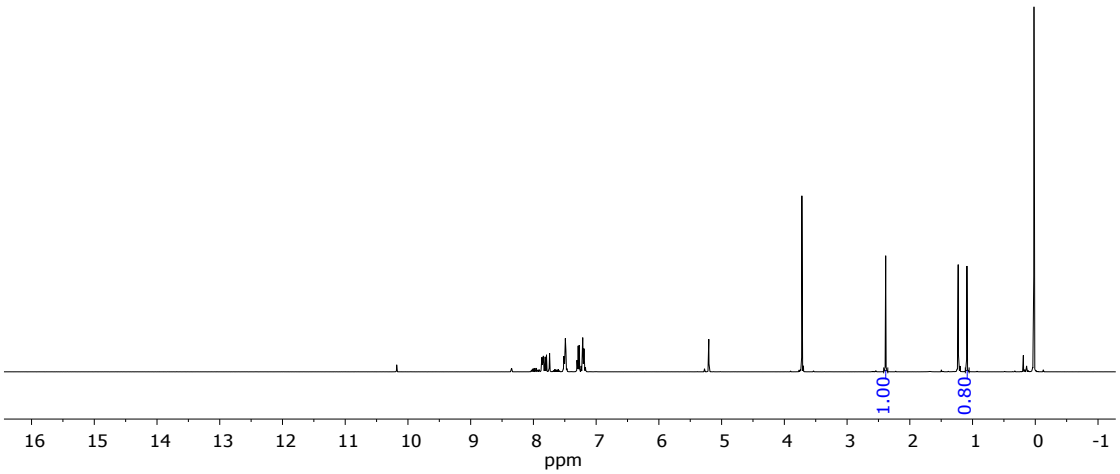


*Figure S113. ^{1}H NMR ($CDCl_3$) Spectrum of catalysis with compound **11a[B(C_6F_5)$_4$]** (1/3 trials shown here).*

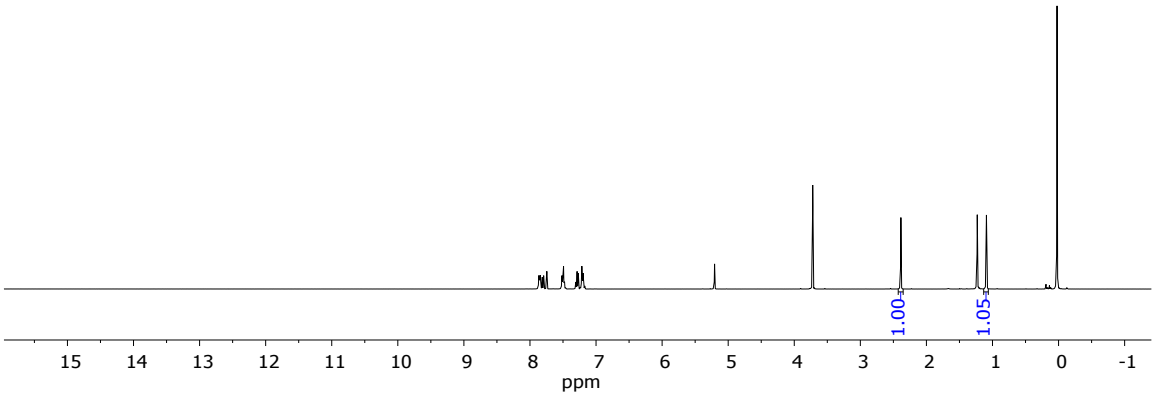


*Figure S114. ^{1}H NMR ($CDCl_3$) Spectrum of catalysis with compound **11c[B(C_6F_5)$_4$]** (1/3 trials shown here).*

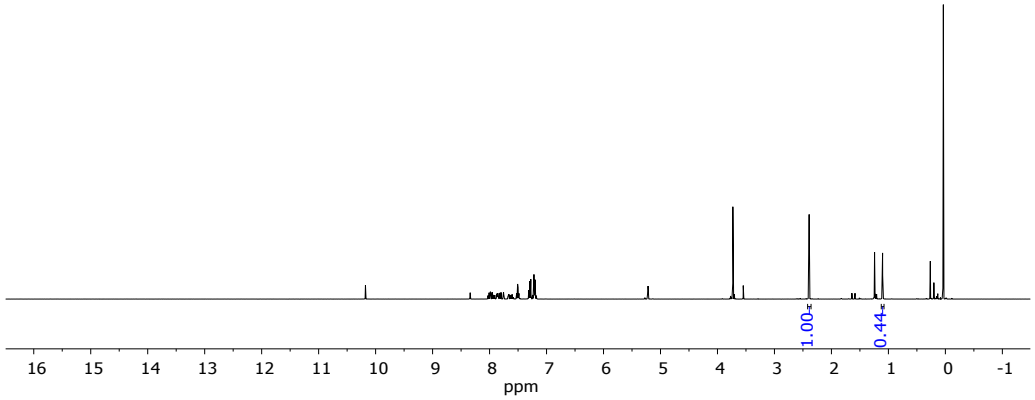


*Figure S115. ^{1}H NMR ($CDCl_3$) Spectrum of catalysis with compound **11b[B(C_6F_5)$_4$]** (1/3 trials shown here).*

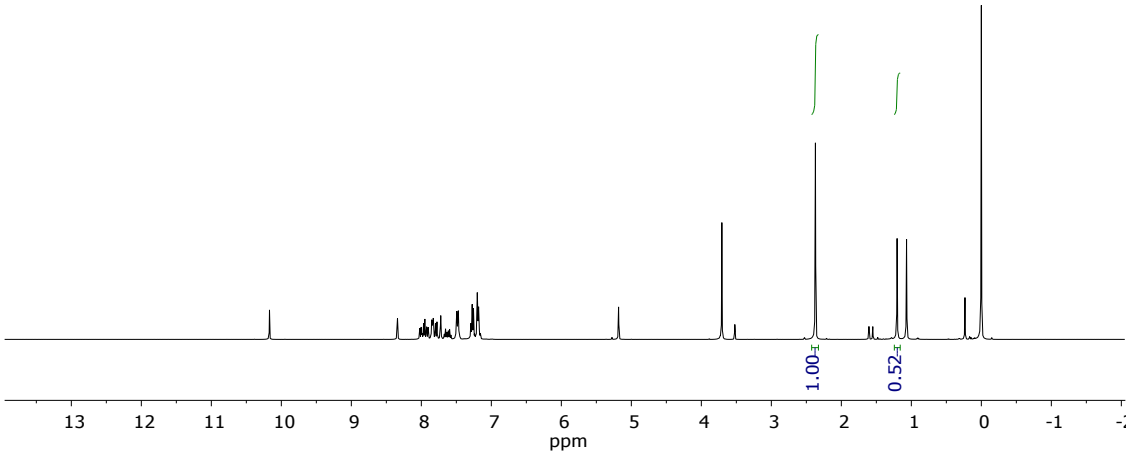


*Figure S116. ^{1}H NMR ($CDCl_3$) Spectrum of catalysis with compound **21[B(C_6F_5)$_4$]** (1/3 trials shown here).*

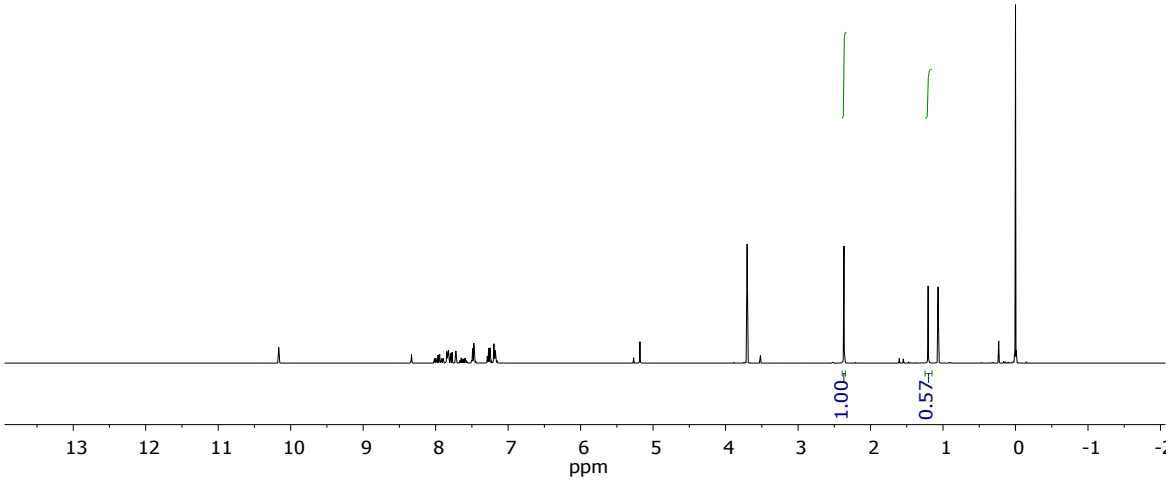


*Figure S117. ^{1}H NMR ($CDCl_3$) Spectrum of catalysis with compound **12[B(C_6F_5)$_4$]** (1/3 trials shown here).*

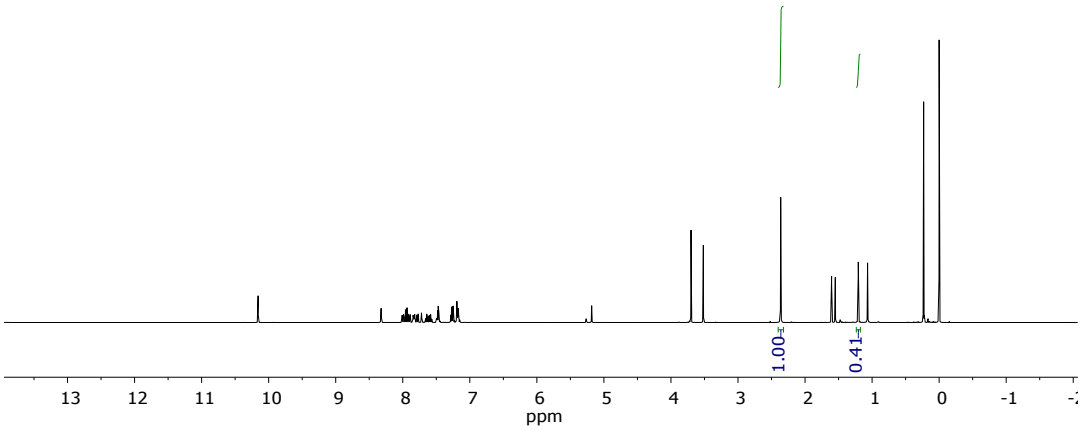
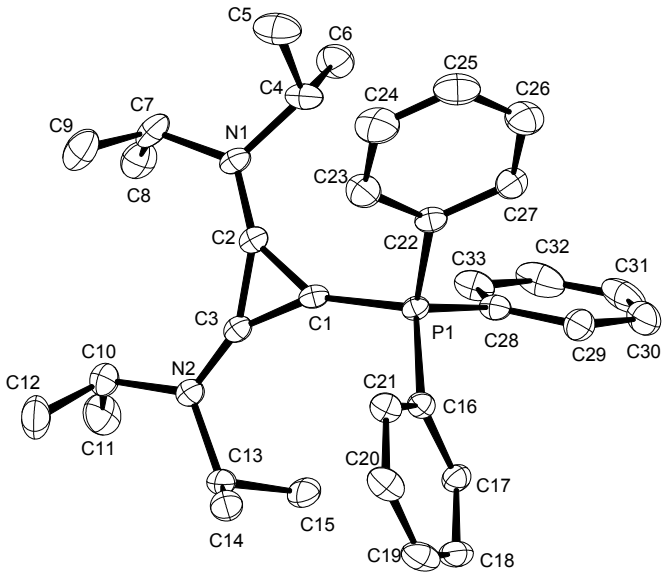


*Figure S118. ^{1}H NMR ($CDCl_3$) Spectrum of catalysis with **23[B(C_6F_5)$_4$]** (1/3 trials shown here).*

3. Crystallographic Details

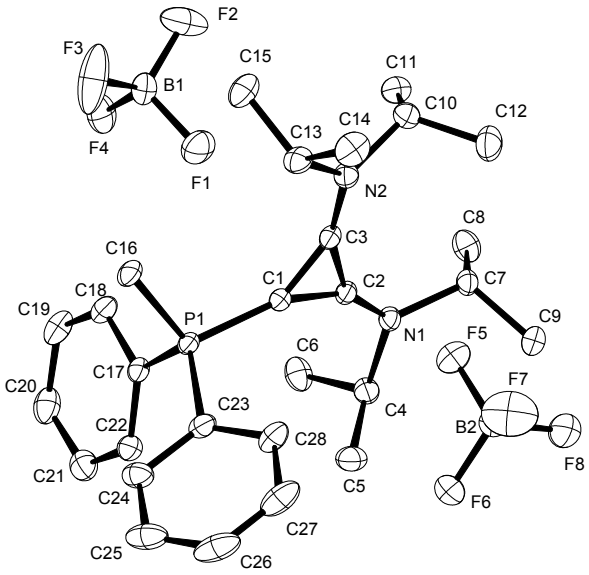
Compound 10a



Empirical formula	$C_{68}H_{90}B_4Cl_4F_{16}N_4P_2$	
Color	colourless	
Formula weight	1514.41 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$, (no. 14)	
Unit cell dimensions	a = 18.675(3) Å	α= 90°.
	b = 15.547(3) Å	β= 95.330(3)°
	c = 25.725(4) Å	γ = 90°.
Volume	7437(2) Å^3	
Z	4	
Density (calculated)	1.353 Mg · m^{-3}	
Absorption coefficient	0.285 mm^{-1}	
F(000)	3152 e	
Crystal size	0.20 x 0.09 x 0.08 mm^3	
□ range for data collection	1.292 to 30.498°.	
Index ranges	-26 ≤ h ≤ 26, -22≤ k ≤ 22, -36 ≤ l ≤ 36	
Reflections collected	208223	

Independent reflections	22623 [R_{int} = 0.0748]	
Reflections with I>2□(I)	15874	
Completeness to □ = 25.242°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.99 and 0.97	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	22623 / 4 / 982	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2□(I)]	R_1 = 0.0727	wR^2 = 0.1778
R indices (all data)	R_1 = 0.1068	wR^2 = 0.2013
Largest diff. peak and hole	1.6 and -1.2 e · $Å^{-3}$	

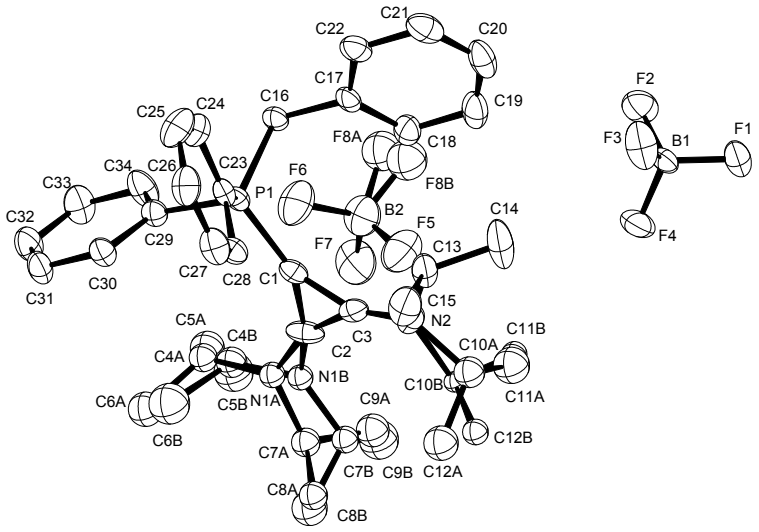
Compound 10b



Empirical formula	$C_{28}H_{41}B_2F_8N_2P$	
Color	yellow	
Formula weight	610.22 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$, (no. 14)	
Unit cell dimensions	a = 12.0346(11) Å	α= 90°

	b = 14.9554(13) Å	β= 96.277(4)°
	c = 17.2268(5) Å	γ = 90°
Volume	3081.9(4) $Å^3$	
Z	4	
Density (calculated)	1.315 $Mg \cdot m^{-3}$	
Absorption coefficient	0.159 mm^{-1}	
F(000)	1280 e	
Crystal size	0.27 x 0.26 x 0.14 mm^3	
□ range for data collection	2.724 to 33.728°.	
Index ranges	-18 ≤ h ≤ 18, -23≤ k ≤ 23, -23 ≤ l ≤ 26	
Reflections collected	49604	
Independent reflections	12221 [R_{int} = 0.0321]	
Reflections with I>2□(I)	10677	
Completeness to □ = 25.242°	99.2 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.98 and 0.96	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12221 / 0 / 379	
Goodness-of-fit on F^2	1.113	
Final R indices [I>2□(I)]	R_1 = 0.0600	wR^2 = 0.1609
R indices (all data)	R_1 = 0.0681	wR^2 = 0.1666
Largest diff. peak and hole	1.0 and -0.8 e $\cdot Å^{-3}$	

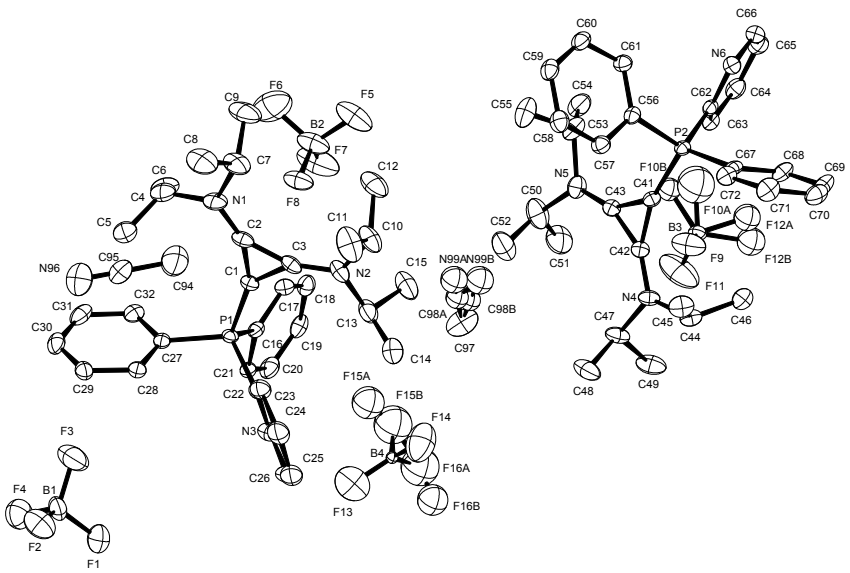
Compound 10c



Empirical formula	$C_{34}H_{45}B_2F_8N_2P$	
Color	colorless	
Formula weight	686.31 g · mol^{-1}	
Temperature	100 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	*Cc*, (no. 9)	
Unit cell dimensions	a = 14.2328(7) Å	α= 90°
	b = 14.8040(7) Å	β= 92.5451(18)°
	c = 16.3008(8) Å	γ = 90°
Volume	3431.2(3) Å^3	
Z	4	
Density (calculated)	1.329 Mg · m^{-3}	
Absorption coefficient	1.327 mm^{-1}	
F(000)	1440 e	
Crystal size	0.33 x 0.20 x 0.15 mm^3	
□ range for data collection	4.311 to 67.690°.	
Index ranges	-16 ≤ h ≤ 17, -17≤ k ≤ 17, -19 ≤ l ≤ 17	
Reflections collected	39935	
Independent reflections	5328 [R_{int} = 0.0478]	
Reflections with I>2□(I)	5225	
Completeness to □ = 67.679°	96.6 %	

Absorption correction	Gaussian	
Max. and min. transmission	0.84 and 0.62	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5328 / 2 / 427	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2□(I)]	R_1 = 0.0768	wR^2 = 0.2006
R indices (all data)	R_1 = 0.0774	wR^2 = 0.2017
Absolute structure parameter	0.01(4)	
Largest diff. peak and hole	0.7 and -0.7 e · Å^{-3}	

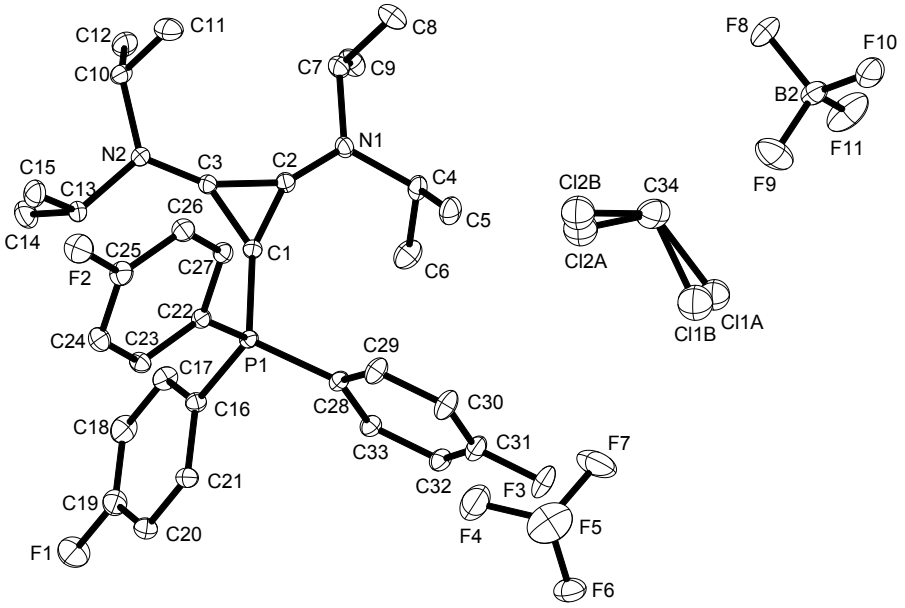
Compound 10d



Empirical formula	$C_{34}H_{45}B_2F_8N_4P$	
Color	colorless	
Formula weight	714.33 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*1, (no. 2)	
Unit cell dimensions	a = 10.7253(19) Å	α= 113.338(3)°
	b = 18.314(3) Å	β= 90.980(3)°
	c = 20.167(4) Å	γ = 93.392(3)°

Volume	3627.2(11) $Å^3$	
Z	4	
Density (calculated)	1.308 $Mg \cdot m^{-3}$	
Absorption coefficient	0.147 mm^{-1}	
F(000)	1496 e	
Crystal size	0.36 x 0.25 x 0.05 mm^3	
□ range for data collection	1.904 to 26.915°.	
Index ranges	-13 ≤ h ≤ 13, -23≤ k ≤ 23, -25 ≤l ≤ 25	
Reflections collected	63233	
Independent reflections	15574 [R_{int} = 0.0628]	
Reflections with I>2□(I)	11213	
Completeness to □ = 25.242°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.99 and 0.94	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15574 / 0 / 890	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2□(I)]	R_1 = 0.0829	wR^2 = 0.2185
R indices (all data)	R_1 = 0.1138	wR^2 = 0.2454
Largest diff. peak and hole	1.6 and -0.8 e $\cdot Å^{-3}$	

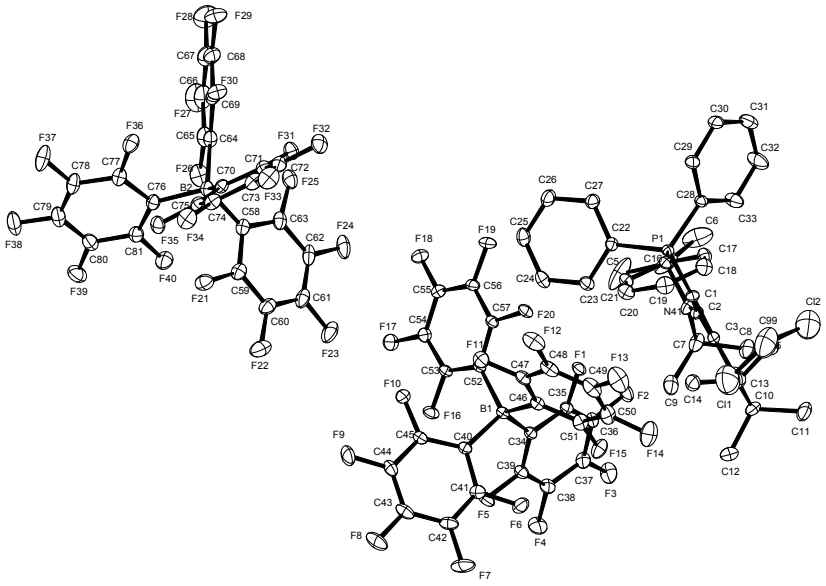
Compound 10e



Empirical formula	$C_{33}\ H_{40}\ F_3\ N_2\ P,\ C\ H_2\ Cl_2,\ 2\ (B\ F_4)$	
Color	yellow	
Formula weight	811.18 g·mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1$, (no. 4)	
Unit cell dimensions	a = 10.6966(4) Å	α= 90°
	b = 10.6522(9) Å	β= 93.699(4)°
	c = 16.6805(9) Å	γ = 90°
Volume	1896.7(2) Å^3	
Z	2	
Density (calculated)	1.420 Mg·m^{-3}	
Absorption coefficient	0.295 mm^{-1}	
F(000)	836 e	
Crystal size	0.29 x 0.17 x 0.13 mm^3	
□ range for data collection	2.701 to 36.027°.	
Index ranges	-17 ≤ h ≤ 16, -17≤ k ≤ 17, -27≤ l ≤ 27	
Reflections collected	48825	
Independent reflections	17618 [R_{int} = 0.0192]	

Reflections with I > 2□(I)	16837	
Completeness to □ = 27.500°	98.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.98277 and 0.97101	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17618 / 1 / 476	
Goodness-of-fit on F^2	1.038	
Final R indices [I > 2□(I)]	R_1 = 0.0370	wR^2 = 0.0972
R indices (all data)	R_1 = 0.0396	wR^2 = 0.0998
Absolute structure parameter	0.017(8)	
Extinction coefficient	0	
Largest diff. peak and hole	1.181 and -1.043 e·Å^{-3}	

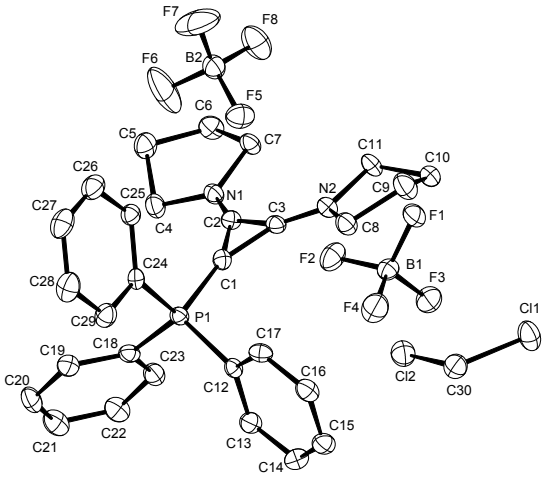
Compound 10a[$B(C_6F_5)_4$]



Empirical formula	$C_{82}H_{45}B_2Cl_2F_{40}N_2P$	
Color	colorless	
Formula weight	1941.69 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*1, (no. 2)	
Unit cell dimensions	a = 13.695(2) Å	α= 74.793(3)°

	b = 14.092(3) Å	β= 79.927(3)°
	c = 23.634(4) Å	γ = 74.645(3)°
Volume	4217.0(13) $Å^3$	
Z	2	
Density (calculated)	1.529 $Mg \cdot m^{-3}$	
Absorption coefficient	0.230 mm^{-1}	
F(000)	1940 e	
Crystal size	0.32 x 0.28 x 0.16 mm^3	
□ range for data collection	0.899 to 35.050°.	
Index ranges	-22 ≤ h ≤ 22, -22≤ k ≤ 22, -38 ≤ l ≤ 36	
Reflections collected	157159	
Independent reflections	37011 [R_{int} = 0.0327]	
Reflections with I>2□(I)	27017	
Completeness to □ = 25.242°	99.7 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.97 and 0.95	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	37011 / 0 / 1170	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2□(I)]	R_1 = 0.0596	wR^2 = 0.1884
R indices (all data)	R_1 = 0.0796	wR^2 = 0.2032
Largest diff. peak and hole	1.5 and -2.1 e · $Å^{-3}$	

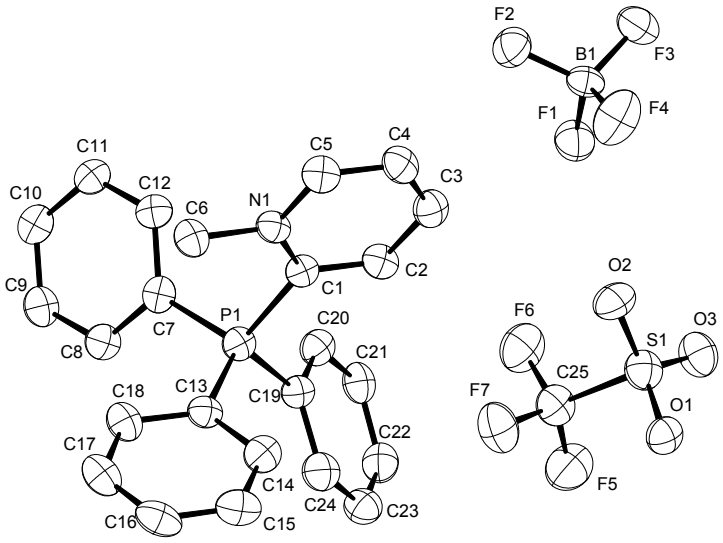
Compound 10f



Empirical formula	$C_{30}H_{33}B_2Cl_2F_8N_2P$	
Color	yellow	
Formula weight	697.07 g · mol^{-1}	
Temperature	100 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$, (no. 14)	
Unit cell dimensions	a = 18.9664(7) Å	α= 90°
	b = 8.8053(4) Å	β= 107.093(2)°
	c = 19.8740(8) Å	γ = 90°
Volume	3172.4(2) Å^3	
Z	4	
Density (calculated)	1.459 Mg · m^{-3}	
Absorption coefficient	2.962 mm^{-1}	
F(000)	1432 e	
Crystal size	0.25 x 0.14 x 0.06 mm^3	
□ range for data collection	2.437 to 67.892°.	
Index ranges	-22 ≤ h ≤ 22, -10≤ k ≤ 10, -23 ≤ l ≤ 23	
Reflections collected	73064	
Independent reflections	5697 [R_{int} = 0.0474]	
Reflections with I>2□(I)	5138	
Completeness to □ = 67.679°	99.3 %	

Absorption correction	Gaussian	
Max. and min. transmission	0.92 and 0.72	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5697 / 0 / 406	
Goodness-of-fit on F^2	1.529	
Final R indices [I>2□(I)]	R_1 = 0.0812	wR^2 = 0.2351
R indices (all data)	R_1 = 0.0863	wR^2 = 0.2396
Largest diff. peak and hole	2.9 and -0.9 e · Å^{-3}	

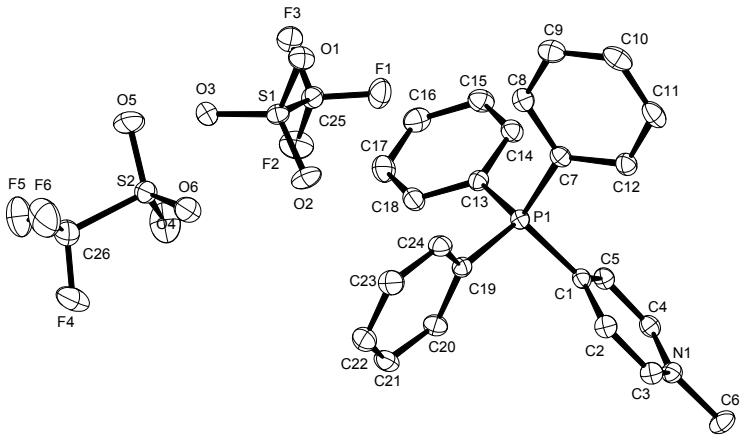
Compound 11a'



Empirical formula	$C_{25}H_{22}BF_7NO_3PS$	
Color	colorless	
Formula weight	591.27 g · mol^{-1}	
Temperature	100 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$, (no. 14)	
Unit cell dimensions	a = 13.937(4) Å	α = 90°
	b = 10.516(3) Å	β = 104.909(7)°
	c = 18.021(5) Å	γ = 90°

Volume	2552.5(13) $Å^3$	
Z	4	
Density (calculated)	1.539 $Mg \cdot m^{-3}$	
Absorption coefficient	2.464 mm^{-1}	
F(000)	1208 e	
Crystal size	0.22 x 0.03 x 0.02 mm^3	
□ range for data collection	3.281 to 58.923°.	
Index ranges	-14 ≤ h ≤ 14, -11≤ k ≤ 11, -19 ≤ l ≤ 19	
Reflections collected	31276	
Independent reflections	3490 [R_{int} = 0.1417]	
Reflections with I>2□(I)	2429	
Completeness to □ = 67.679°	75.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.96 and 0.72	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3490 / 0 / 354	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2□(I)]	R_1 = 0.0669	wR^2 = 0.1614
R indices (all data)	R_1 = 0.1040	wR^2 = 0.1832
Extinction coefficient	0.0036(4)	
Largest diff. peak and hole	0.5 and -0.5 e · $Å^{-3}$	

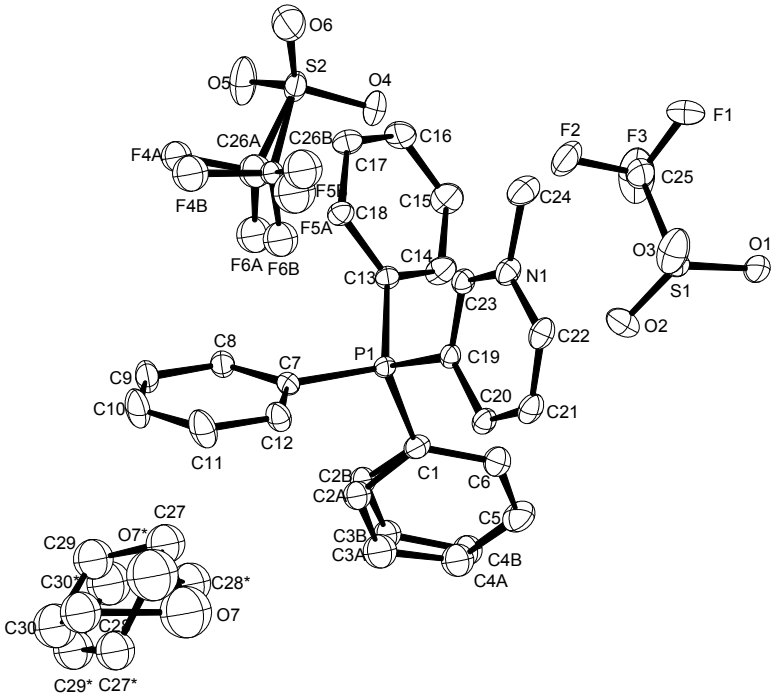
Compound 11b



Empirical formula	$C_{26}H_{22}F_6NO_6PS_2$	
Color	colorless	
Formula weight	653.53 g · mol^{-1}	
Temperature	100 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$, (no. 14)	
Unit cell dimensions	a = 9.4391(3) Å	α= 90°
	b = 10.3400(4) Å	β= 94.4003(10)°
	c = 28.9765(10) Å	γ = 90°
Volume	2819.78(17) $Å^3$	
Z	4	
Density (calculated)	1.539 Mg · m^{-3}	
Absorption coefficient	3.001 mm^{-1}	
F(000)	1336 e	
Crystal size	0.27 x 0.12 x 0.10 mm^3	
□ range for data collection	3.059 to 67.808°.	
Index ranges	-11 □ h □ 11, -11□ k □ 12, -34 □ l □ 34	
Reflections collected	65121	
Independent reflections	5075 [R_{int} = 0.0414]	
Reflections with I>2□(I)	4714	

Completeness to □ = 67.679°	99.4 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.85 and 0.62	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5075 / 0 / 380	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2□(I)]	R_1 = 0.0379	wR^2 = 0.0977
R indices (all data)	R_1 = 0.0405	wR^2 = 0.1001
Largest diff. peak and hole	0.3 and -0.6 e · $Å^{-3}$	

Compound 11c



Empirical formula	$C_{56}H_{52}F_{12}N_2O_{13}P_2S_4$
Color	colourless
Formula weight	1379.17 g·mol^{-1}
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*C*2/*c*, (no. 15)

Unit cell dimensions	a = 26.974(4) Å	α= 90°
	b = 14.0542(18) Å	β= 108.586(3)°
	c = 17.075(2) Å	γ = 90°
Volume	6135.7(14) $Å^3$	
Z	4	
Density (calculated)	1.493 $Mg·m^{-3}$	
Absorption coefficient	0.307 mm^{-1}	
F(000)	2832 e	
Crystal size	0.22 x 0.18 x 0.05 mm^3	
□ range for data collection	1.593 to 37.313°.	
Index ranges	-39 ≤ h ≤ 39, -20≤ k ≤ 23, -27 ≤ l ≤ 25	
Reflections collected	136310	
Independent reflections	13021 [R_{int} = 0.0423]	
Reflections with I>2□(I)	8913	
Completeness to □ = 25.242°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.98565 and 0.94315	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13021 / 0 / 394	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2□(I)]	R_1 = 0.0657	wR^2 = 0.1715
R indices (all data)	R_1 = 0.1111	wR^2 = 0.2005
Largest diff. peak and hole	1.317 and -1.222 $e·Å^{-3}$	

4. Computational Details

Table S1. FIA and ω values for cations of compounds under investigation

Compound	FIA (kJ mol^{-1})	ω (eV)
10a[B(C$_6$F$_5$)$_4$]	809	3.97
10b[B(C$_6$F$_5$)$_4$]	831	4.07
10c[B(C$_6$F$_5$)$_4$]	825	4.02
10d[B(C$_6$F$_5$)$_4$]	810	3.98
10e[B(C$_6$F$_5$)$_4$]	832	4.19
10f[B(C$_6$F$_5$)$_4$]	814	4.13
11a[B(C$_6$F$_5$)$_4$]	834	5.99
11c[B(C$_6$F$_5$)$_4$]	829	5.71
11b[B(C$_6$F$_5$)$_4$]	837	6.15
21[B(C$_6$F$_5$)$_4$]	859	5.93
12[B(C$_6$F$_5$)$_4$]	920	6.12
23[B(C$_6$F$_5$)$_4$]	889	6.29
[(C$_6$F$_5$)$_3$PF]$^+$ [a]	777	5.04
B(C$_6$F$_5$)$_3$	452	1.41

[a] Values from [J. H. W. LaFortune, T. C. Johnstone, M. Pérez, D. Winkelhaus, V. Podgorny and D. W. Stephan, *Dalton Trans.*, **2016**, *45*, 18156-18162.]

Table S2. Cartesian coordinates (Å) of the cation of **10a[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.825172	4.762394	12.812446
2	7	0	1.214233	8.358579	12.561304
3	7	0	4.400487	7.965080	10.621231
4	6	0	2.902160	6.430028	12.133370
5	6	0	2.243675	7.668657	12.139574
6	6	0	3.464405	7.485705	11.398564
7	6	0	0.197930	7.677480	13.448085
8	1	0	0.568480	6.647675	13.555181
9	6	0	0.159467	8.323804	14.834698
10	1	0	1.150306	8.331941	15.308651
11	1	0	-0.519985	7.746672	15.477157
12	1	0	-0.226791	9.352659	14.801214
13	6	0	-1.178534	7.635284	12.778635
14	1	0	-1.626236	8.634238	12.679191
15	1	0	-1.858354	7.040657	13.404768
16	1	0	-1.139314	7.167639	11.785370
17	6	0	0.964975	9.806152	12.220820
18	1	0	0.025942	10.026788	12.745618
19	6	0	2.037483	10.720475	12.818089
20	1	0	2.097461	10.600847	13.908355
21	1	0	1.779464	11.767927	12.608824
22	1	0	3.036373	10.535942	12.400223
23	6	0	0.700560	9.997548	10.725528
24	1	0	1.565048	9.731607	10.102074
25	1	0	0.463012	11.052440	10.530048
26	1	0	-0.156063	9.394478	10.394801
27	6	0	4.387256	9.404238	10.176138
28	1	0	3.483064	9.823669	10.632724
29	6	0	4.254690	9.512284	8.654925
30	1	0	5.142957	9.134226	8.128820
31	1	0	4.148725	10.571897	8.383101
32	1	0	3.370955	8.976545	8.280717
33	6	0	5.600725	10.157594	10.727007
34	1	0	5.665622	10.083736	11.821774
35	1	0	5.509695	11.220660	10.463396
36	1	0	6.546014	9.799478	10.294999
37	6	0	5.539127	7.107421	10.126933
38	1	0	6.131782	7.799717	9.514736
39	6	0	5.026189	5.993151	9.215148
40	1	0	4.383524	5.286095	9.757073
41	1	0	5.879126	5.425947	8.817790
42	1	0	4.462706	6.398719	8.364148
43	6	0	6.420038	6.626669	11.279461
44	1	0	6.777760	7.468121	11.888392
45	1	0	7.299744	6.111740	10.869277
46	1	0	5.895916	5.913985	11.930260
47	6	0	4.355145	3.827076	12.596805
48	6	0	5.315420	3.769884	13.625591
49	1	0	5.155742	4.291281	14.569938
50	6	0	6.474505	3.012349	13.447544
51	1	0	7.212278	2.960905	14.249526
52	6	0	6.678697	2.307496	12.256764
53	1	0	7.580975	1.707369	12.127710
54	6	0	5.719143	2.351531	11.238796
55	1	0	5.868401	1.783737	10.319145
56	6	0	4.556359	3.104781	11.403125
57	1	0	3.799328	3.106381	10.617565
58	6	0	1.498730	3.870941	11.973105
59	6	0	1.339913	2.496751	12.251262
60	1	0	2.017262	1.982763	12.936102
61	6	0	0.317988	1.780683	11.627208
62	1	0	0.195417	0.718379	11.843496
63	6	0	-0.536102	2.417966	10.719580
64	1	0	-1.327616	1.850152	10.227927
65	6	0	-0.369060	3.775624	10.430577
66	1	0	-1.024377	4.266190	9.709394
67	6	0	0.643788	4.506250	11.056097
68	1	0	0.777488	5.560835	10.811044
69	6	0	2.490209	4.993752	14.576194
70	6	0	1.534683	4.200645	15.236239
71	1	0	0.924099	3.486508	14.682484
72	6	0	1.359694	4.334397	16.616121
73	1	0	0.618009	3.717515	17.125743
74	6	0	2.130991	5.248738	17.339914
75	1	0	1.994335	5.343283	18.418374
76	6	0	3.075676	6.046250	16.683512
77	1	0	3.675292	6.762721	17.247282
78	6	0	3.256624	5.926345	15.304852
79	1	0	3.995094	6.556033	14.803244

Table S3. Cartesian coordinates (Å) of the fluoride adduct of the cation of **10a[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.335387	7.969406	12.081117
2	7	0	3.331290	7.636041	9.819292
3	6	0	2.171500	6.182236	11.666136
4	6	0	1.383545	7.327317	11.592599
5	6	0	2.520190	7.182486	10.758792
6	6	0	-0.451367	7.314250	13.176197
7	1	0	0.059317	6.358725	13.353126
8	6	0	-0.388756	8.125871	14.473125
9	1	0	0.649722	8.303197	14.784618
10	1	0	-0.890167	7.564510	15.273970
11	1	0	-0.902935	9.094854	14.383301
12	6	0	-1.886283	7.016563	12.731601
13	1	0	-2.468904	7.934327	12.560192
14	1	0	-2.399914	6.451479	13.522302
15	1	0	-1.905811	6.411411	11.814438
16	6	0	-0.109021	9.317520	11.614744
17	1	0	-0.994556	9.525019	12.231984
18	6	0	0.923492	10.403403	11.934786
19	1	0	1.134139	10.437776	13.012342
20	1	0	0.536986	11.386672	11.630866
21	1	0	1.876109	10.242833	11.411991
22	6	0	-0.577688	9.293269	10.156001
23	1	0	0.228726	9.023782	9.460196
24	1	0	-0.948449	10.287029	9.867137
25	1	0	-1.395428	8.572308	10.018967
26	6	0	3.091508	8.957364	9.165998
27	1	0	2.183606	9.345254	9.644320
28	6	0	2.808391	8.804228	7.667481
29	1	0	3.686927	8.438674	7.116094
30	1	0	2.544613	9.784128	7.244715
31	1	0	1.971574	8.115817	7.482410
32	6	0	4.234407	9.937443	9.451927
33	1	0	4.402476	10.056707	10.531469
34	1	0	3.984699	10.922470	9.032350
35	1	0	5.178398	9.616065	8.988407
36	6	0	4.521582	6.839843	9.368128
37	1	0	4.984540	7.475294	8.599775
38	6	0	4.086337	5.536364	8.695563
39	1	0	3.568736	4.870926	9.398784
40	1	0	4.969563	4.998777	8.323096
41	1	0	3.418795	5.730168	7.844279
42	6	0	5.538409	6.649344	10.495053
43	1	0	5.877370	7.618077	10.888133
44	1	0	6.416011	6.113480	10.106512
45	1	0	5.128082	6.068011	11.330533
46	6	0	4.059799	3.578556	12.286503
47	6	0	5.146169	3.524216	13.181044
48	1	0	5.151555	4.146281	14.073237
49	6	0	6.224921	2.673110	12.935764
50	1	0	7.045449	2.626586	13.654013
51	6	0	6.261434	1.894531	11.775004
52	1	0	7.111781	1.238442	11.580478
53	6	0	5.201899	1.960116	10.867738
54	1	0	5.219194	1.359085	9.956810
55	6	0	4.100865	2.779853	11.130467
56	1	0	3.267874	2.781782	10.428403
57	6	0	1.342952	3.552148	11.764693
58	6	0	1.225333	2.211009	12.186512
59	1	0	1.836871	1.846797	13.015581
60	6	0	0.340772	1.330417	11.565212
61	1	0	0.269179	0.298579	11.914388
62	6	0	-0.450078	1.766542	10.494363
63	1	0	-1.140348	1.077535	10.004478
64	6	0	-0.343734	3.086132	10.056257
65	1	0	-0.948378	3.436206	9.217214
66	6	0	0.545040	3.967568	10.689406
67	1	0	0.611990	4.991921	10.316793
68	6	0	1.835245	4.535944	14.351202
69	6	0	0.500846	4.119989	14.523713
70	1	0	-0.113769	3.869820	13.660174
71	6	0	-0.058149	4.013558	15.800206
72	1	0	-1.096304	3.693276	15.906401
73	6	0	0.710638	4.295981	16.931456
74	1	0	0.279085	4.195881	17.929064
75	6	0	2.036122	4.709913	16.775363
76	1	0	2.646799	4.937628	17.650912
77	6	0	2.589914	4.845773	15.500748
78	1	0	3.609751	5.207909	15.399575
79	15	0	2.597416	4.661927	12.658560
80	9	0	3.748815	5.836538	13.313456

Table S4. Cartesian coordinates (Å) of the cation of **10b[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	4.502950	3.060453	9.133609
2	7	0	1.877308	5.340350	6.921232
3	7	0	0.485356	2.926893	9.424868
4	6	0	2.866868	3.597137	8.615568
5	6	0	2.035880	4.410696	7.826267
6	6	0	1.476572	3.491728	8.784196
7	6	0	3.050627	5.986354	6.224418
8	1	0	2.584347	6.782906	5.629901
9	6	0	4.002025	6.647710	7.219999
10	1	0	3.474883	7.358450	7.871102
11	1	0	4.770241	7.205776	6.667144
12	1	0	4.524406	5.912733	7.847876
13	6	0	3.728481	5.010351	5.262483
14	1	0	4.200665	4.173346	5.794221
15	1	0	4.514492	5.539631	4.705941
16	1	0	3.015342	4.604619	4.532769
17	6	0	0.504514	5.832378	6.536500
18	1	0	-0.182487	5.215827	7.127455
19	6	0	0.219222	5.583151	5.053442
20	1	0	0.856287	6.191243	4.395697
21	1	0	-0.821465	5.866420	4.842596
22	1	0	0.342467	4.525094	4.782927
23	6	0	0.315229	7.295686	6.944832
24	1	0	0.509397	7.451486	8.015498
25	1	0	-0.724857	7.588313	6.743136
26	1	0	0.956911	7.977717	6.369221
27	6	0	-0.973985	3.179985	9.133249
28	1	0	-1.485751	2.484092	9.811538
29	6	0	-1.342590	2.765814	7.706890
30	1	0	-0.822862	3.356704	6.940801
31	1	0	-2.422090	2.905348	7.556716
32	1	0	-1.113890	1.705796	7.531293
33	6	0	-1.395454	4.594508	9.538735
34	1	0	-1.212662	4.772071	10.607051
35	1	0	-2.472331	4.718157	9.358553
36	1	0	-0.871533	5.374877	8.970927
37	6	0	0.800337	1.932817	10.515228
38	1	0	1.895482	1.952213	10.586591
39	6	0	0.230382	2.385192	11.862241
40	1	0	0.571727	3.393622	12.133358
41	1	0	0.573234	1.690540	12.641944
42	1	0	-0.868289	2.366173	11.879139
43	6	0	0.354903	0.522424	10.120223
44	1	0	-0.739363	0.439055	10.055886
45	1	0	0.684145	-0.188944	10.890677
46	1	0	0.784867	0.208783	9.158522
47	6	0	4.372717	1.352455	9.741972
48	1	0	5.394867	0.989867	9.922214
49	1	0	3.894841	0.702249	8.997807
50	1	0	3.818282	1.320600	10.687612
51	6	0	5.662485	3.038208	7.755928
52	6	0	5.549065	2.025024	6.781446
53	1	0	4.747312	1.284977	6.825023
54	6	0	6.477106	1.960692	5.742898
55	1	0	6.395042	1.173120	4.992463
56	6	0	7.516622	2.896592	5.671442
57	1	0	8.246605	2.835674	4.862590
58	6	0	7.628512	3.902505	6.636297
59	1	0	8.444006	4.625300	6.583446
60	6	0	6.704554	3.980237	7.681251
61	1	0	6.806304	4.756141	8.441356
62	6	0	5.072197	4.113786	10.478916
63	6	0	6.275861	3.776363	11.132959
64	1	0	6.870656	2.918012	10.813403
65	6	0	6.718621	4.556314	12.201267
66	1	0	7.648858	4.296143	12.708341
67	6	0	5.973309	5.665001	12.620790
68	1	0	6.325547	6.269504	13.458113
69	6	0	4.780822	5.999475	11.972391
70	1	0	4.202485	6.864064	12.301170
71	6	0	4.325585	5.227094	10.901835
72	1	0	3.393103	5.492232	10.401412

Table S5. Cartesian coordinates (Å) of the fluoride adduct of the cation of **10b[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.069451	3.987574	6.912696
2	7	0	0.649201	2.160471	10.189437
3	6	0	2.644485	2.988258	8.750733
4	6	0	1.548689	3.397424	7.992277
5	6	0	1.365465	2.690731	9.211348
6	6	0	1.979618	4.634581	5.905931
7	1	0	1.288875	5.003613	5.134644
8	6	0	2.717210	5.835871	6.500653
9	1	0	2.010940	6.576621	6.901083
10	1	0	3.308880	6.324553	5.713229
11	1	0	3.401682	5.536389	7.305643
12	6	0	2.909570	3.613664	5.249161
13	1	0	3.649778	3.219268	5.958128
14	1	0	3.468655	4.099814	4.437311
15	1	0	2.345861	2.773528	4.819879
16	6	0	-0.399635	4.028182	6.645159
17	1	0	-0.853899	3.515847	7.502477
18	6	0	-0.761479	3.244147	5.378959
19	1	0	-0.347480	3.709766	4.472875
20	1	0	-1.854425	3.222485	5.262677
21	1	0	-0.402606	2.206446	5.430796
22	6	0	-0.928689	5.466202	6.617788
23	1	0	-0.679588	6.006507	7.541973
24	1	0	-2.023231	5.448853	6.515948
25	1	0	-0.532516	6.036713	5.765200
26	6	0	-0.844874	2.116271	10.195901
27	1	0	-1.085961	1.609539	11.141119
28	6	0	-1.393418	1.238104	9.066186
29	1	0	-1.140858	1.629549	8.071151
30	1	0	-2.489132	1.182399	9.134813
31	1	0	-0.996173	0.216094	9.135640
32	6	0	-1.459788	3.517648	10.267889
33	1	0	-1.100024	4.059333	11.153285
34	1	0	-2.554171	3.440509	10.336984
35	1	0	-1.224259	4.124526	9.382864
36	6	0	1.374176	1.561579	11.359253
37	1	0	2.437769	1.752770	11.157915
38	6	0	1.014513	2.277344	12.664617
39	1	0	1.196931	3.358239	12.592053
40	1	0	1.642160	1.882689	13.475757
41	1	0	-0.033761	2.114779	12.955464
42	6	0	1.154683	0.047637	11.436682
43	1	0	0.107162	-0.206474	11.657245
44	1	0	1.767408	-0.369290	12.248489
45	1	0	1.443621	-0.450913	10.500641
46	6	0	4.308293	0.976258	8.894570
47	1	0	5.272806	0.454646	8.934737
48	1	0	3.818702	0.712516	7.945783
49	1	0	3.679122	0.593243	9.710047
50	6	0	5.801236	3.094459	7.822703
51	6	0	6.043594	2.148508	6.809807
52	1	0	5.409487	1.270404	6.699948
53	6	0	7.099836	2.319913	5.911235
54	1	0	7.261629	1.581821	5.123691
55	6	0	7.950236	3.421292	6.029470
56	1	0	8.784312	3.547339	5.336829
57	6	0	7.728197	4.360625	7.041100
58	1	0	8.390566	5.221898	7.144820
59	6	0	6.655462	4.211129	7.921544
60	1	0	6.480717	4.960030	8.691792
61	6	0	5.015230	2.850262	10.832444
62	6	0	5.960917	1.902450	11.262869
63	1	0	6.371071	1.170739	10.566858
64	6	0	6.418019	1.906952	12.582812
65	1	0	7.171233	1.181115	12.894081
66	6	0	5.915430	2.836263	13.498030
67	1	0	6.269021	2.834073	14.530605
68	6	0	4.969458	3.776736	13.080962
69	1	0	4.582930	4.514822	13.786285
70	6	0	4.533117	3.797458	11.753789
71	1	0	3.834325	4.564939	11.424148
72	15	0	4.464443	2.858482	9.074238
73	9	0	4.294297	4.607948	9.168003

Table S6. Cartesian coordinates (Å) of the cation of **10c[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	7.528835	4.549486	4.905225
2	7	0	7.763631	4.364526	8.876318
3	7	0	4.420331	3.413111	7.211002
4	6	0	6.795489	4.152028	6.492612
5	6	0	6.935649	4.131717	7.886124
6	6	0	5.676021	3.781485	7.255064
7	6	0	9.091187	5.007222	8.539503
8	1	0	9.046359	5.188518	7.456902
9	6	0	9.227547	6.357051	9.250328
10	1	0	9.309367	6.250552	10.341218
11	1	0	8.383957	7.024873	9.026835
12	1	0	10.149464	6.847214	8.906970
13	6	0	10.265231	4.066081	8.815676
14	1	0	11.191112	4.545819	8.469314
15	1	0	10.157587	3.112167	8.281827
16	1	0	10.392323	3.859948	9.887737
17	6	0	7.578114	3.954326	10.317102
18	1	0	8.498688	4.320090	10.790140
19	6	0	7.571617	2.428765	10.449755
20	1	0	7.463549	2.153458	11.508223
21	1	0	8.511038	1.992889	10.084054
22	1	0	6.743447	1.966270	9.896886
23	6	0	6.416535	4.663228	11.009717
24	1	0	5.439300	4.297409	10.676835
25	1	0	6.459942	5.750527	10.857771
26	1	0	6.482137	4.474384	12.090495
27	6	0	3.492246	3.286784	8.394720
28	1	0	2.558123	2.942124	7.932651
29	6	0	3.216906	4.657804	9.017318
30	1	0	4.130323	5.131699	9.398952
31	1	0	2.518840	4.544507	9.858479
32	1	0	2.759617	5.338655	8.287368
33	6	0	3.921727	2.201803	9.378758
34	1	0	4.105451	1.246865	8.867224
35	1	0	3.113426	2.040815	10.105958
36	1	0	4.817714	2.476592	9.945607
37	6	0	3.798335	3.161175	5.854485
38	1	0	4.604361	3.359959	5.135400
39	6	0	2.646609	4.125448	5.569118
40	1	0	1.783123	3.954336	6.227596
41	1	0	2.300773	3.959489	4.539225
42	1	0	2.960891	5.174004	5.653803
43	6	0	3.383616	1.692210	5.729798
44	1	0	4.216454	1.008688	5.946069
45	1	0	3.045631	1.503961	4.701222
46	1	0	2.545629	1.440260	6.395281
47	6	0	7.140295	6.305870	4.493346
48	1	0	7.743034	6.889109	5.207113
49	1	0	7.582013	6.475641	3.497704
50	6	0	5.698267	6.758270	4.547845
51	6	0	5.213207	7.388795	5.705768
52	1	0	5.862882	7.502676	6.577705
53	6	0	3.925989	7.932147	5.731634
54	1	0	3.572645	8.448461	6.625790
55	6	0	3.108229	7.849846	4.599768
56	1	0	2.112373	8.295517	4.610552
57	6	0	3.580584	7.217175	3.445592
58	1	0	2.954556	7.167825	2.553273
59	6	0	4.867291	6.673084	3.418827
60	1	0	5.235022	6.215236	2.498310
61	6	0	6.916348	3.388851	3.669598
62	6	0	6.914041	3.768921	2.313908
63	1	0	7.176007	4.783701	2.011485
64	6	0	6.591256	2.831062	1.331937
65	1	0	6.586004	3.130026	0.282801
66	6	0	6.286732	1.513608	1.689943
67	1	0	6.041479	0.783074	0.917458
68	6	0	6.305422	1.128123	3.034451
69	1	0	6.078673	0.097707	3.312148
70	6	0	6.619770	2.059461	4.025777
71	1	0	6.639675	1.746400	5.071712
72	6	0	9.331811	4.376248	4.983849
73	6	0	9.880078	3.081073	5.076183
74	1	0	9.232237	2.204873	5.141848
75	6	0	11.263622	2.907896	5.051945
76	1	0	11.682997	1.902742	5.116313
77	6	0	12.108820	4.016637	4.924295
78	1	0	13.190405	3.875956	4.890536
79	6	0	11.569238	5.302288	4.825300
80	1	0	12.225616	6.166495	4.712663
81	6	0	10.184787	5.489433	4.854956
82	1	0	9.791565	6.501762	4.762052

Table S7. Cartesian coordinates (Å) of the fluoride adduct of the cation of **10c[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	7.383841	5.728548	8.731834
2	7	0	4.080325	4.330854	7.268794
3	6	0	6.434883	4.974417	6.450718
4	6	0	6.548838	5.279723	7.802453
5	6	0	5.327900	4.772401	7.268073
6	6	0	8.728406	6.215472	8.274350
7	1	0	8.692566	6.150478	7.178847
8	6	0	8.941471	7.682907	8.660734
9	1	0	9.010322	7.819331	9.750167
10	1	0	8.132090	8.322485	8.281445
11	1	0	9.888222	8.039122	8.230319
12	6	0	9.864878	5.308858	8.755244
13	1	0	10.809280	5.649068	8.307594
14	1	0	9.704041	4.266456	8.448218
15	1	0	9.990541	5.342734	9.847594
16	6	0	7.167134	5.626077	10.207157
17	1	0	8.085153	6.058516	10.629402
18	6	0	7.101332	4.164522	10.663192
19	1	0	6.961876	4.116714	11.752811
20	1	0	8.029998	3.632593	10.416015
21	1	0	6.268786	3.625157	10.192688
22	6	0	6.005649	6.490573	10.699657
23	1	0	5.034850	6.118570	10.351411
24	1	0	6.118013	7.531536	10.366014
25	1	0	5.984589	6.485899	11.798827
26	6	0	3.092977	4.489396	8.379592
27	1	0	2.186560	4.016004	7.977662
28	6	0	2.765225	5.965412	8.627424
29	1	0	3.651940	6.532233	8.941948
30	1	0	2.008827	6.053759	9.420499
31	1	0	2.370106	6.437987	7.718396
32	6	0	3.467571	3.715554	9.644765
33	1	0	3.721520	2.671776	9.413607
34	1	0	2.610417	3.711551	10.333337
35	1	0	4.310463	4.171289	10.177169
36	6	0	3.580358	3.705433	5.997389
37	1	0	4.420250	3.798610	5.296875
38	6	0	2.389271	4.464173	5.407270
39	1	0	1.487352	4.381045	6.031675
40	1	0	2.142609	4.030977	4.427540
41	1	0	2.622540	5.527057	5.256008
42	6	0	3.294861	2.214990	6.206281
43	1	0	4.181360	1.686311	6.582926
44	1	0	3.007223	1.760222	5.247358
45	1	0	2.460990	2.048421	6.904801
46	6	0	7.105232	6.659229	4.507830
47	1	0	7.629181	7.163891	5.334904
48	1	0	7.631465	6.920621	3.579584
49	6	0	5.688984	7.180845	4.450939
50	6	0	5.157640	7.903434	5.534955
51	1	0	5.776368	8.071010	6.420798
52	6	0	3.873828	8.454451	5.482309
53	1	0	3.496714	9.032807	6.328294
54	6	0	3.088114	8.292722	4.337738
55	1	0	2.091796	8.735286	4.286035
56	6	0	3.602161	7.580323	3.249524
57	1	0	3.006151	7.464071	2.342260
58	6	0	4.886327	7.032096	3.304114
59	1	0	5.278312	6.502087	2.434900
60	6	0	6.738623	4.240201	3.126912
61	6	0	7.363826	4.816240	2.006093
62	1	0	8.155618	5.556709	2.126859
63	6	0	7.014509	4.417913	0.713559
64	1	0	7.529403	4.857943	-0.142222
65	6	0	6.014636	3.461237	0.518608
66	1	0	5.733190	3.159843	-0.491825
67	6	0	5.393558	2.878078	1.625401
68	1	0	4.627104	2.114053	1.482830
69	6	0	5.767498	3.247630	2.920400
70	1	0	5.320366	2.737599	3.771114
71	6	0	9.152108	4.677325	4.927472
72	6	0	9.776876	3.434367	5.154815
73	1	0	9.168856	2.547522	5.315719
74	6	0	11.169669	3.329614	5.162193
75	1	0	11.632208	2.355838	5.333231
76	6	0	11.966525	4.456026	4.943851
77	1	0	13.054613	4.369206	4.945184
78	6	0	11.360448	5.693545	4.716115
79	1	0	11.971076	6.580107	4.535801
80	6	0	9.967213	5.805359	4.705891
81	1	0	9.533901	6.784523	4.512612
82	15	0	7.309460	4.766887	4.814038
83	9	0	7.120732	3.098146	5.300512

Table S8. Cartesian coordinates (Å) of the cation of **10d[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.219409	-4.253009	14.170461
2	7	0	1.757480	-4.719119	12.926967
3	7	0	0.910183	-2.808196	16.048681
4	7	0	-4.024470	-5.213743	15.865125
5	6	0	-0.428404	-4.090472	14.232748
6	6	0	0.892957	-4.253084	13.790132
7	6	0	0.600924	-3.512371	14.989705
8	6	0	1.322283	-5.523110	11.726112
9	1	0	2.265633	-5.742136	11.208762
10	6	0	0.451254	-4.690273	10.786544
11	1	0	0.961490	-3.767516	10.478582
12	1	0	-0.513318	-4.429005	11.243256
13	1	0	0.235749	-5.274357	9.881128
14	6	0	0.695669	-6.850966	12.150775
15	1	0	-0.252937	-6.702932	12.685022
16	1	0	1.376339	-7.431056	12.788437
17	1	0	0.476953	-7.451024	11.256642
18	6	0	3.235058	-4.474029	13.089955
19	1	0	3.314973	-3.883257	14.010300
20	6	0	3.785740	-3.639360	11.930743
21	1	0	3.239705	-2.693089	11.810287
22	1	0	3.760944	-4.182645	10.975594
23	1	0	4.838445	-3.398764	12.135325
24	6	0	3.992832	-5.788243	13.293646
25	1	0	3.971477	-6.426743	12.399209
26	1	0	3.597641	-6.362454	14.143481
27	1	0	5.048031	-5.560763	13.500098
28	6	0	2.318668	-2.430047	16.432357
29	1	0	2.180978	-1.854020	17.357134
30	6	0	3.154856	-3.662225	16.786567
31	1	0	3.284976	-4.344720	15.935837
32	1	0	2.697685	-4.227421	17.610111
33	1	0	4.154622	-3.343852	17.112677
34	6	0	2.948638	-1.487480	15.403831
35	1	0	2.350622	-0.573725	15.285558
36	1	0	3.060569	-1.951449	14.414402
37	1	0	3.949825	-1.191272	15.746331
38	6	0	-0.203356	-2.333358	16.954181
39	1	0	-1.123024	-2.723035	16.493004
40	6	0	-0.066505	-2.936146	18.354584
41	1	0	0.818997	-2.559354	18.885888
42	1	0	-0.018629	-4.033359	18.325780
43	1	0	-0.943991	-2.649997	18.951092
44	6	0	-0.283227	-0.805346	16.973460
45	1	0	-0.408871	-0.390968	15.964088
46	1	0	0.602801	-0.349260	17.437692
47	1	0	-1.152553	-0.502487	17.573650
48	6	0	-2.869730	-2.566141	14.175586
49	6	0	-2.106690	-1.529425	13.601863
50	1	0	-1.101442	-1.720275	13.221062
51	6	0	-2.646279	-0.245164	13.505973
52	1	0	-2.059023	0.555445	13.053461
53	6	0	-3.935255	0.011610	13.984662
54	1	0	-4.353099	1.016868	13.909143
55	6	0	-4.692383	-1.018630	14.552275
56	1	0	-5.700144	-0.819200	14.919790
57	6	0	-4.174270	-2.311910	14.642897
58	1	0	-4.769807	-3.120511	15.066996
59	6	0	-2.698133	-5.216510	15.660649
60	6	0	-1.785283	-5.938279	16.435540
61	1	0	-0.716695	-5.926391	16.217594
62	6	0	-2.295411	-6.699587	17.495006
63	1	0	-1.625269	-7.289012	18.123018
64	6	0	-3.669916	-6.697573	17.727936
65	1	0	-4.103516	-7.279903	18.542025
66	6	0	-4.497966	-5.938216	16.889106
67	1	0	-5.580563	-5.915740	17.036765
68	6	0	-2.832606	-5.144193	12.731032
69	6	0	-2.953151	-6.546855	12.768310
70	1	0	-2.665447	-7.109401	13.658293
71	6	0	-3.476597	-7.221160	11.665093
72	1	0	-3.582677	-8.306538	11.695743
73	6	0	-3.884991	-6.505948	10.533178
74	1	0	-4.306858	-7.037644	9.678633
75	6	0	-3.774459	-5.111710	10.500031
76	1	0	-4.110672	-4.554888	9.624210
77	6	0	-3.253225	-4.423608	11.596873
78	1	0	-3.196451	-3.334173	11.577219

Table S9. Cartesian coordinates (Å) of the fluoride adduct of the cation of **10d[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.826422	-5.156241	13.868389
2	7	0	0.578581	-3.373711	16.950081
3	7	0	-4.095527	-5.350312	16.262137
4	6	0	-0.500990	-4.489163	14.864708
5	6	0	0.858890	-4.671643	14.622433
6	6	0	0.410463	-4.018034	15.808598
7	6	0	1.548489	-5.807392	12.539020
8	1	0	2.505166	-6.287121	12.287147
9	6	0	1.223541	-4.773103	11.457039
10	1	0	2.020875	-4.023809	11.361623
11	1	0	0.275924	-4.261921	11.669960
12	1	0	1.125672	-5.284071	10.488031
13	6	0	0.492222	-6.906362	12.648414
14	1	0	-0.511896	-6.495855	12.815595
15	1	0	0.731637	-7.619014	13.450586
16	1	0	0.456778	-7.463299	11.701561
17	6	0	3.247883	-5.113213	14.330125
18	1	0	3.217536	-4.546841	15.269178
19	6	0	4.147497	-4.352715	13.351190
20	1	0	3.771008	-3.338147	13.159984
21	1	0	4.247167	-4.874179	12.388508
22	1	0	5.155792	-4.267595	13.780865
23	6	0	3.774826	-6.518741	14.641474
24	1	0	3.852888	-7.141214	13.738342
25	1	0	3.131932	-7.039487	15.365414
26	1	0	4.783655	-6.443526	15.072033
27	6	0	1.917718	-3.065370	17.541291
28	1	0	1.674632	-2.498238	18.450457
29	6	0	2.650926	-4.333183	17.991152
30	1	0	2.881239	-5.005382	17.153488
31	1	0	2.051268	-4.895582	18.719963
32	1	0	3.601879	-4.061694	18.471430
33	6	0	2.740928	-2.137331	16.642748
34	1	0	2.195575	-1.205793	16.438355
35	1	0	2.993485	-2.598648	15.678122
36	1	0	3.684020	-1.876173	17.143526
37	6	0	-0.636869	-2.899565	17.699660
38	1	0	-1.488504	-3.202161	17.074294
39	6	0	-0.757241	-3.596982	19.057540
40	1	0	0.065060	-3.324397	19.736025
41	1	0	-0.779454	-4.689441	18.948059
42	1	0	-1.693894	-3.285504	19.540922
43	6	0	-0.654069	-1.373961	17.828896
44	1	0	-0.580013	-0.884461	16.849107
45	1	0	0.153399	-1.000730	18.476272
46	1	0	-1.604813	-1.065409	18.285739
47	6	0	-3.096092	-2.889432	14.611305
48	6	0	-2.316769	-1.720879	14.514058
49	1	0	-1.253667	-1.790934	14.281235
50	6	0	-2.903862	-0.463858	14.667326
51	1	0	-2.287989	0.434005	14.587046
52	6	0	-4.279462	-0.354323	14.891862
53	1	0	-4.741024	0.629389	14.995658
54	6	0	-5.062275	-1.508612	14.960256
55	1	0	-6.140452	-1.431113	15.111740
56	6	0	-4.480387	-2.773301	14.826998
57	1	0	-5.097735	-3.666031	14.887124
58	6	0	-2.791327	-5.442602	15.940575
59	6	0	-1.927975	-6.286352	16.660155
60	1	0	-0.879773	-6.392101	16.377007
61	6	0	-2.426946	-7.031787	17.734664
62	1	0	-1.772034	-7.705896	18.291052
63	6	0	-3.772555	-6.907694	18.073559
64	1	0	-4.205845	-7.469108	18.902509
65	6	0	-4.564990	-6.049316	17.304133
66	1	0	-5.629842	-5.926812	17.525001
67	6	0	-3.169323	-5.697423	13.226543
68	6	0	-3.294572	-7.061089	13.538097
69	1	0	-2.852476	-7.465165	14.448648
70	6	0	-3.988773	-7.920861	12.681888
71	1	0	-4.063498	-8.981662	12.927498
72	6	0	-4.597733	-7.421278	11.528756
73	1	0	-5.155691	-8.089639	10.870439
74	6	0	-4.490417	-6.061304	11.220263
75	1	0	-4.967258	-5.663431	10.322645
76	6	0	-3.763768	-5.205229	12.048762
77	1	0	-3.660116	-4.154129	11.783027
78	15	0	-2.275372	-4.509898	14.329394
79	9	0	-1.541429	-3.843857	12.869619

Table S10. Cartesian coordinates (Å) of the cation of **10e[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.426061	4.650033	12.442648
2	6	0	0.201807	5.133540	11.952250
3	6	0	0.653229	5.472256	13.277066
4	6	0	-0.544392	4.474104	9.701240
5	1	0	-1.450804	4.746382	9.145086
6	6	0	0.661013	4.973619	8.905815
7	1	0	0.611298	6.058928	8.743496
8	1	0	0.668575	4.487804	7.920215
9	1	0	1.611377	4.732561	9.400747
10	6	0	-0.572384	2.963559	9.932798
11	1	0	0.283062	2.625606	10.533828
12	1	0	-0.523681	2.445111	8.965263
13	1	0	-1.497517	2.652486	10.436530
14	6	0	-1.932187	6.065386	11.166470
15	1	0	-1.841057	6.496088	12.170410
16	6	0	-1.946521	7.210264	10.149934
17	1	0	-1.039151	7.827283	10.213660
18	1	0	-2.811133	7.856401	10.356599
19	1	0	-2.054599	6.850691	9.116740
20	6	0	-3.200252	5.209313	11.119967
21	1	0	-3.373382	4.770499	10.127187
22	1	0	-4.066449	5.848306	11.342072
23	1	0	-3.177775	4.399664	11.862950
24	6	0	-0.629619	6.904201	14.862883
25	1	0	-0.375264	7.191537	15.891825
26	6	0	-0.697562	8.194052	14.041154
27	1	0	0.231539	8.772278	14.135615
28	1	0	-1.521365	8.819252	14.412540
29	1	0	-0.876159	8.010918	12.972827
30	6	0	-1.929647	6.099349	14.929477
31	1	0	-2.234957	5.700536	13.952758
32	1	0	-2.740428	6.746885	15.290945
33	1	0	-1.837912	5.256781	15.628283
34	6	0	1.633757	5.836307	15.468315
35	1	0	2.359101	5.179763	14.966296
36	6	0	1.102173	5.117866	16.711618
37	1	0	0.403179	5.740484	17.287997
38	1	0	1.946651	4.886660	17.375904
39	1	0	0.602676	4.172196	16.460010
40	6	0	2.329593	7.157037	15.804595
41	1	0	2.717600	7.654125	14.905336
42	1	0	3.177377	6.952308	16.473247
43	1	0	1.664779	7.853596	16.335143
44	6	0	2.856421	2.267603	13.343564
45	6	0	1.750117	2.029454	14.180337
46	1	0	0.921205	2.737548	14.217497
47	6	0	1.687226	0.872254	14.953481
48	1	0	0.834619	0.660376	15.599281
49	6	0	2.744441	-0.038374	14.884810
50	6	0	3.853424	0.167197	14.058085
51	1	0	4.650332	-0.576610	14.025682
52	6	0	3.903679	1.320910	13.281748
53	1	0	4.756708	1.473349	12.617760
54	6	0	4.225777	4.904739	12.996295
55	6	0	5.215126	4.454200	13.891698
56	1	0	5.202243	3.430176	14.266701
57	6	0	6.221573	5.317853	14.319902
58	1	0	6.996072	4.989239	15.013806
59	6	0	6.230798	6.629544	13.840780
60	6	0	5.257527	7.107608	12.957547
61	1	0	5.301559	8.141369	12.612817
62	6	0	4.251725	6.240009	12.539345
63	1	0	3.485766	6.610338	11.854167
64	6	0	3.438778	3.270445	10.667749
65	6	0	4.305011	4.066734	9.889919
66	1	0	4.715221	4.995832	10.286615
67	6	0	4.672512	3.661815	8.609770
68	1	0	5.350466	4.256344	7.996546
69	6	0	4.171738	2.453180	8.118497
70	6	0	3.322323	1.636098	8.871128
71	1	0	2.974369	0.689563	8.456032
72	6	0	2.957989	2.048964	10.148737
73	1	0	2.316643	1.403482	10.750379
74	9	0	2.688990	-1.147315	15.625344
75	9	0	7.195186	7.460052	14.245459
76	9	0	4.527273	2.057264	6.894409
77	7	0	-0.695270	5.219111	11.004821
78	7	0	0.538121	6.043837	14.449122
79	15	0	2.991463	3.758896	12.343130

Table S11. Cartesian coordinates (Å) of the fluoride adduct of the cation of **10e[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.207864	4.002284	13.078488
2	6	0	-0.132190	4.232879	12.768118
3	6	0	0.427961	4.737009	13.968005
4	6	0	-0.977491	3.395359	10.615450
5	1	0	-1.973349	3.459685	10.155324
6	6	0	0.006711	4.136229	9.708067
7	1	0	-0.313096	5.174471	9.543139
8	1	0	0.053808	3.634582	8.731197
9	1	0	1.021649	4.151649	10.126266
10	6	0	-0.649506	1.913761	10.812084
11	1	0	0.310534	1.775051	11.326742
12	1	0	-0.577737	1.417823	9.833934
13	1	0	-1.430634	1.406434	11.395344
14	6	0	-2.495815	4.652127	12.252475
15	1	0	-2.379734	5.113943	13.240691
16	6	0	-2.903966	5.747444	11.261104
17	1	0	-2.147266	6.542475	11.203207
18	1	0	-3.851465	6.199408	11.587485
19	1	0	-3.066333	5.349157	10.248945
20	6	0	-3.546617	3.542596	12.368267
21	1	0	-3.727750	3.041671	11.406085
22	1	0	-4.502643	3.978431	12.691581
23	1	0	-3.251013	2.782663	13.105384
24	6	0	-0.821657	6.077703	15.646979
25	1	0	-0.476237	6.527022	16.588738
26	6	0	-1.293151	7.227244	14.750107
27	1	0	-0.499123	7.975365	14.621630
28	1	0	-2.159923	7.725219	15.207582
29	1	0	-1.593955	6.883488	13.751201
30	6	0	-1.910086	5.062018	16.008294
31	1	0	-2.266436	4.500198	15.133725
32	1	0	-2.774835	5.581091	16.445327
33	1	0	-1.540093	4.336834	16.746195
34	6	0	1.678313	5.553191	15.880195
35	1	0	2.424352	4.998072	15.296263
36	6	0	1.566687	4.901238	17.261286
37	1	0	0.846876	5.420586	17.911300
38	1	0	2.544118	4.947351	17.761833
39	1	0	1.271837	3.845103	17.186544
40	6	0	2.128063	7.015615	15.947863
41	1	0	2.240899	7.445137	14.943105
42	1	0	3.102748	7.070329	16.452700
43	1	0	1.428342	7.639211	16.524170
44	6	0	2.838806	1.791485	13.341260
45	6	0	1.698350	1.267492	13.966383
46	1	0	0.787921	1.864228	14.042988
47	6	0	1.678309	-0.024025	14.509820
48	1	0	0.788310	-0.427677	14.993857
49	6	0	2.828995	-0.798628	14.420931
50	6	0	3.990148	-0.322317	13.809064
51	1	0	4.875536	-0.957107	13.757173
52	6	0	3.982368	0.965140	13.277357
53	1	0	4.894063	1.333033	12.800826
54	6	0	4.342136	4.102895	13.672922
55	6	0	4.573929	3.526170	14.936655
56	1	0	3.920182	2.738990	15.310301
57	6	0	5.636500	3.941905	15.740481
58	1	0	5.813560	3.501134	16.722048
59	6	0	6.493992	4.926581	15.255655
60	6	0	6.302367	5.520741	14.009535
61	1	0	6.992347	6.291020	13.663528
62	6	0	5.216063	5.118895	13.234145
63	1	0	5.047176	5.609389	12.278627
64	6	0	3.353488	2.978209	10.872864
65	6	0	4.027810	3.843454	9.984801
66	1	0	4.267623	4.858524	10.290458
67	6	0	4.384561	3.428497	8.703477
68	1	0	4.921785	4.089111	8.022302
69	6	0	4.030782	2.144815	8.291435
70	6	0	3.341655	1.268894	9.126204
71	1	0	3.075540	0.273422	8.769523
72	6	0	3.021364	1.688187	10.417638
73	1	0	2.503995	0.989396	11.072314
74	9	0	2.825943	-2.044927	14.939461
75	9	0	7.534916	5.320154	16.016118
76	9	0	4.359998	1.742200	7.048321
77	7	0	-1.146718	4.096287	11.931359
78	7	0	0.401851	5.411419	15.104416
79	15	0	2.945991	3.531125	12.594873
80	9	0	2.842247	5.184096	11.969822

Table S12. Cartesian coordinates (Å) of the cation of **10f[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.715220	8.393816	5.806748
2	6	0	2.383976	9.280433	6.838240
3	6	0	3.370062	8.268792	7.037665
4	6	0	0.665709	11.016834	6.478569
5	1	0	0.067733	10.301348	5.898156
6	1	0	1.186926	11.690373	5.781102
7	6	0	-0.125258	11.789631	7.537333
8	1	0	-0.922342	11.157417	7.956361
9	1	0	-0.594306	12.688439	7.118642
10	6	0	0.932755	12.111203	8.607507
11	1	0	1.554478	12.962489	8.292940
12	1	0	0.493861	12.359169	9.581593
13	6	0	1.779019	10.834331	8.678534
14	1	0	2.829091	11.016792	8.941873
15	1	0	1.353558	10.098127	9.377575
16	6	0	5.093492	6.535875	7.408599
17	1	0	5.878402	6.901467	6.728611
18	1	0	4.482772	5.794101	6.877955
19	6	0	5.669348	6.040613	8.738494
20	1	0	4.979122	5.325634	9.210539
21	1	0	6.633219	5.535681	8.600210
22	6	0	5.782308	7.322598	9.582172
23	1	0	6.670798	7.902337	9.290810
24	1	0	5.851239	7.120964	10.658096
25	6	0	4.506233	8.096658	9.233534
26	1	0	3.654082	7.782368	9.855656
27	1	0	4.618272	9.186724	9.298027
28	6	0	3.914178	6.970103	3.537755
29	6	0	4.909188	7.564664	2.740226
30	1	0	4.826939	8.607465	2.431156
31	6	0	5.999482	6.800937	2.317248
32	1	0	6.765605	7.257436	1.688929
33	6	0	6.099305	5.454691	2.682011
34	1	0	6.947494	4.860159	2.338470
35	6	0	5.105820	4.860421	3.470313
36	1	0	5.175394	3.804331	3.735752
37	6	0	4.010664	5.610389	3.899368
38	1	0	3.221407	5.131917	4.483077
39	6	0	2.315345	9.470730	3.181017
40	6	0	1.329132	9.597992	2.186297
41	1	0	0.627788	8.785584	1.991055
42	6	0	1.245613	10.780189	1.446573
43	1	0	0.480193	10.879297	0.675535
44	6	0	2.136680	11.829233	1.691925
45	1	0	2.068805	12.748351	1.107631
46	6	0	3.115970	11.705800	2.685504
47	1	0	3.811500	12.525019	2.874559
48	6	0	3.209240	10.531665	3.433458
49	1	0	3.978668	10.443098	4.204066
50	6	0	1.001386	6.905074	3.961899
51	6	0	0.013623	6.919684	4.963157
52	1	0	0.152095	7.502989	5.875055
53	6	0	-1.148690	6.164490	4.798887
54	1	0	-1.911303	6.166769	5.578969
55	6	0	-1.331974	5.402347	3.640142
56	1	0	-2.241514	4.812407	3.516259
57	6	0	-0.349772	5.385163	2.643561
58	1	0	-0.490737	4.784357	1.743915
59	6	0	0.820940	6.129448	2.798456
60	1	0	1.588511	6.099482	2.022814
61	7	0	1.688512	10.283944	7.287926
62	7	0	4.238862	7.693441	7.815820
63	15	0	2.484180	7.920519	4.088271

Table S13. Cartesian coordinates (Å) of the fluoride adduct of the cation of **10f[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.917787	7.935970	5.947961
2	6	0	1.296584	8.605711	6.996222
3	6	0	2.415208	7.784616	7.237237
4	6	0	-0.599869	10.114904	6.523237
5	1	0	-1.065036	9.372308	5.861207
6	1	0	-0.080820	10.862221	5.902416
7	6	0	-1.580190	10.764151	7.506344
8	1	0	-2.367118	10.047756	7.786970
9	1	0	-2.067639	11.647750	7.075789
10	6	0	-0.700980	11.099341	8.725354
11	1	0	-0.120340	12.015369	8.538855
12	1	0	-1.280770	11.249537	9.644647
13	6	0	0.239330	9.892207	8.831991
14	1	0	1.221325	10.142058	9.257432
15	1	0	-0.207826	9.079677	9.427731
16	6	0	4.429722	6.405383	7.561823
17	1	0	5.171999	7.040298	7.054374
18	1	0	4.057959	5.664770	6.841134
19	6	0	4.974681	5.796694	8.858003
20	1	0	4.420532	4.880041	9.111692
21	1	0	6.036703	5.534891	8.772658
22	6	0	4.711353	6.891273	9.908642
23	1	0	5.472465	7.682551	9.834704
24	1	0	4.719318	6.511040	10.937821
25	6	0	3.336106	7.445696	9.514073
26	1	0	2.517123	6.869561	9.974634
27	1	0	3.206844	8.507332	9.767230
28	6	0	3.337160	6.330204	3.604827
29	6	0	4.509926	6.585059	2.873086
30	1	0	4.791041	7.607520	2.625899
31	6	0	5.321993	5.528514	2.456014
32	1	0	6.215103	5.737512	1.864427
33	6	0	5.002343	4.212396	2.804230
34	1	0	5.646463	3.390281	2.487119
35	6	0	3.853117	3.953646	3.555478
36	1	0	3.595775	2.929543	3.831981
37	6	0	3.011518	5.003563	3.934664
38	1	0	2.093274	4.782007	4.480573
39	6	0	1.856792	9.165759	3.060143
40	6	0	0.524140	9.503235	2.759612
41	1	0	-0.296289	8.896777	3.141377
42	6	0	0.232077	10.611407	1.959827
43	1	0	-0.808907	10.861240	1.746623
44	6	0	1.265060	11.382244	1.421674
45	1	0	1.036841	12.236867	0.782137
46	6	0	2.592920	11.053381	1.708730
47	1	0	3.407689	11.650557	1.295468
48	6	0	2.889260	9.968584	2.535769
49	1	0	3.925035	9.755063	2.788361
50	6	0	0.634077	6.761266	3.815429
51	6	0	-0.302217	6.400229	4.795254
52	1	0	-0.146525	6.679112	5.839802
53	6	0	-1.446843	5.656972	4.471763
54	1	0	-2.156338	5.384766	5.255877
55	6	0	-1.674210	5.262505	3.153569
56	1	0	-2.563459	4.683765	2.897725
57	6	0	-0.748248	5.608483	2.161385
58	1	0	-0.912775	5.299769	1.127309
59	6	0	0.390107	6.343464	2.491454
60	1	0	1.102477	6.597125	1.702112
61	7	0	0.385822	9.452105	7.420380
62	7	0	3.306288	7.258700	8.040655
63	15	0	2.240154	7.716271	4.148112
64	9	0	3.723481	8.553577	4.645081

Table S14. Cartesian coordinates (Å) of the cation of **11a[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.105271	-0.304490	-0.623735
2	6	0	3.091418	0.634336	-0.327367
3	1	0	2.797796	1.559702	0.168407
4	6	0	4.432664	0.404926	-0.657660
5	1	0	5.193128	1.148712	-0.413712
6	6	0	4.774042	-0.782248	-1.299783
7	1	0	5.801473	-1.013489	-1.582054
8	6	0	3.771447	-1.698638	-1.586527
9	1	0	3.975363	-2.644541	-2.087921
10	6	0	1.485531	-2.512489	-1.652928
11	1	0	0.992993	-2.208462	-2.584916
12	1	0	0.742053	-2.643935	-0.860373
13	1	0	2.021054	-3.455447	-1.802228
14	6	0	0.279116	1.794343	0.391246
15	6	0	-0.157885	2.836326	-0.450324
16	1	0	-0.491673	2.632560	-1.467976
17	6	0	-0.193078	4.143938	0.038077
18	1	0	-0.542421	4.950218	-0.608409
19	6	0	0.203785	4.416856	1.351247
20	1	0	0.168602	5.440620	1.727525
21	6	0	0.629557	3.380468	2.192110
22	1	0	0.920543	3.593111	3.221868
23	6	0	0.664876	2.068023	1.722580
24	1	0	0.969333	1.261862	2.393303
25	6	0	-0.168738	-0.992998	1.170191
26	6	0	-1.453649	-0.792152	1.720076
27	1	0	-2.113010	-0.011247	1.335710
28	6	0	-1.876651	-1.585516	2.786753
29	1	0	-2.870460	-1.431447	3.209726
30	6	0	-1.027561	-2.562785	3.319326
31	1	0	-1.363171	-3.175699	4.157370
32	6	0	0.255392	-2.744598	2.793410
33	1	0	0.924513	-3.490578	3.224514
34	6	0	0.689901	-1.963081	1.720854
35	1	0	1.705030	-2.100123	1.344050
36	7	0	2.472844	-1.470990	-1.258416
37	15	0	0.326916	0.088679	-0.182761
38	6	0	-0.626236	-0.128384	-1.698984
39	6	0	-1.835942	-0.846745	-1.691164
40	6	0	-0.157273	0.461581	-2.893194
41	6	0	-2.576083	-0.959773	-2.870527
42	1	0	-2.197971	-1.321521	-0.778567
43	6	0	-0.905696	0.335749	-4.064372
44	1	0	0.783091	1.017975	-2.916471
45	6	0	-2.115247	-0.370138	-4.052106
46	1	0	-3.516239	-1.513217	-2.864234
47	1	0	-0.545547	0.792355	-4.987557
48	1	0	-2.698558	-0.463032	-4.969642

Table S15. Cartesian coordinates (Å) of the fluoride adduct of the cation of **11a[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.308882	0.322843	-0.328695
2	6	0	3.063806	0.805618	0.747061
3	1	0	2.532917	1.208449	1.606826
4	6	0	4.455375	0.794844	0.734682
5	1	0	5.014764	1.153756	1.599759
6	6	0	5.116838	0.342679	-0.408534
7	1	0	6.203071	0.343048	-0.490908
8	6	0	4.356644	-0.119147	-1.463534
9	1	0	4.802832	-0.488761	-2.385559
10	6	0	2.342436	-0.821827	-2.577123
11	1	0	1.332164	-0.440850	-2.724310
12	1	0	2.284277	-1.898365	-2.380335
13	1	0	2.954223	-0.622186	-3.464045
14	6	0	0.402548	2.132608	0.383819
15	6	0	0.357896	3.162202	-0.575746
16	1	0	0.235645	2.934325	-1.631932
17	6	0	0.426925	4.510784	-0.211720
18	1	0	0.372400	5.278393	-0.986045
19	6	0	0.549223	4.874769	1.130243
20	1	0	0.594917	5.926890	1.416267
21	6	0	0.600966	3.873571	2.102997
22	1	0	0.685009	4.137033	3.159181
23	6	0	0.531839	2.527246	1.733610
24	1	0	0.555663	1.777099	2.525582
25	6	0	-0.276524	-0.362545	1.480013
26	6	0	-1.445586	0.215659	2.006673
27	1	0	-1.921743	1.057424	1.501320
28	6	0	-2.010817	-0.292216	3.178609
29	1	0	-2.932366	0.146375	3.564946
30	6	0	-1.393408	-1.347339	3.857609
31	1	0	-1.829386	-1.731339	4.781451
32	6	0	-0.221346	-1.912350	3.347500
33	1	0	0.261372	-2.739984	3.869871
34	6	0	0.325524	-1.438909	2.152259
35	1	0	1.207301	-1.923042	1.734366
36	7	0	2.993725	-0.161663	-1.414418
37	6	0	-0.804331	0.341868	-1.497837
38	6	0	-2.022915	-0.332733	-1.301931
39	6	0	-0.575166	0.977462	-2.731783
40	6	0	-2.999583	-0.333223	-2.300272
41	1	0	-2.211425	-0.868819	-0.371611
42	6	0	-1.550024	0.957022	-3.733990
43	1	0	0.366880	1.486283	-2.941500
44	6	0	-2.769290	0.312076	-3.517747
45	1	0	-3.942119	-0.854477	-2.124470
46	1	0	-1.350443	1.451682	-4.686155
47	1	0	-3.531840	0.303852	-4.297973
48	15	0	0.405358	0.271168	-0.106324
49	9	0	0.694455	-1.425168	-0.556421

Table S16. Cartesian coordinates (Å) of the cation of **11b[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.110764	-0.223027	-0.612117
2	6	0	3.171479	0.577091	-0.151372
3	1	0	3.009224	1.448332	0.485365
4	6	0	4.469155	0.266192	-0.519045
5	1	0	5.335349	0.845794	-0.197722
6	6	0	0.238077	1.837682	0.372749
7	6	0	-0.306773	2.825171	-0.465093
8	1	0	-0.697279	2.568083	-1.453806
9	6	0	-0.377131	4.142888	-0.004253
10	1	0	-0.813502	4.912720	-0.643119
11	6	0	0.095508	4.468968	1.272488
12	1	0	0.031305	5.498698	1.626590
13	6	0	0.633871	3.478734	2.107193
14	1	0	0.979173	3.732254	3.110034
15	6	0	0.708706	2.159497	1.664253
16	1	0	1.089962	1.383345	2.332962
17	6	0	-0.107357	-0.957832	1.209904
18	6	0	-1.204216	-0.539059	1.985950
19	1	0	-1.694299	0.418934	1.790206
20	6	0	-1.671128	-1.354744	3.021822
21	1	0	-2.525477	-1.028533	3.619145
22	6	0	-1.044283	-2.573415	3.295181
23	1	0	-1.406855	-3.199849	4.111295
24	6	0	0.049699	-2.987798	2.531068
25	1	0	0.539802	-3.936142	2.751189
26	6	0	0.523486	-2.187553	1.487501
27	1	0	1.378071	-2.534246	0.912591
28	15	0	0.351017	0.131106	-0.163500
29	6	0	-0.585220	-0.180744	-1.673069
30	6	0	-1.750208	-0.965849	-1.656686
31	6	0	-0.143853	0.418160	-2.874321
32	6	0	-2.474175	-1.142776	-2.839450
33	1	0	-2.091703	-1.437177	-0.736039
34	6	0	-0.877912	0.231748	-4.046373
35	1	0	0.759525	1.034114	-2.898618
36	6	0	-2.042599	-0.547005	-4.026400
37	1	0	-3.378961	-1.751094	-2.829648
38	1	0	-0.545191	0.696630	-4.975560
39	1	0	-2.615392	-0.690062	-4.944088
40	6	0	2.422722	-1.315615	-1.456392
41	1	0	1.651094	-1.960269	-1.878685
42	6	0	3.736092	-1.572694	-1.781174
43	1	0	4.041927	-2.401258	-2.422471
44	6	0	6.156769	-1.075656	-1.694323
45	1	0	6.422716	-0.432687	-2.543870
46	1	0	6.808131	-0.858453	-0.823583
47	1	0	6.242833	-2.142058	-1.976001
48	7	0	4.741140	-0.789582	-1.312221

Table S17. Cartesian coordinates (Å) of the fluoride adduct of the cation of **11b[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.239595	0.500325	-0.258102
2	6	0	3.073797	0.227487	0.839887
3	1	0	2.658266	0.052700	1.832964
4	6	0	4.443482	0.151107	0.669672
5	1	0	5.127723	-0.066497	1.488903
6	6	0	0.157252	2.294912	0.295026
7	6	0	-1.160089	2.766498	0.468644
8	1	0	-2.001887	2.075950	0.372601
9	6	0	-1.415471	4.105262	0.763605
10	1	0	-2.444915	4.443951	0.894560
11	6	0	-0.356020	5.012628	0.890621
12	1	0	-0.555281	6.060690	1.120563
13	6	0	0.954463	4.566868	0.721271
14	1	0	1.788259	5.264979	0.817940
15	6	0	1.205462	3.219014	0.426852
16	1	0	2.244460	2.907112	0.303775
17	6	0	-0.277445	-0.178411	1.510957
18	6	0	-0.203049	0.611539	2.674051
19	1	0	0.218336	1.615699	2.634070
20	6	0	-0.675804	0.124192	3.895835
21	1	0	-0.594961	0.745738	4.789288
22	6	0	-1.265112	-1.139759	3.967726
23	1	0	-1.652216	-1.511484	4.918135
24	6	0	-1.354212	-1.927844	2.816112
25	1	0	-1.810568	-2.918105	2.863141
26	6	0	-0.845791	-1.464397	1.602264
27	1	0	-0.875614	-2.109941	0.727760
28	6	0	-0.598208	0.468514	-1.652293
29	6	0	-1.341213	-0.660326	-2.044484
30	6	0	-0.600326	1.606708	-2.479183
31	6	0	-2.091535	-0.636233	-3.220462
32	1	0	-1.329281	-1.560786	-1.434001
33	6	0	-1.316165	1.607255	-3.680038
34	1	0	-0.053690	2.503509	-2.185627
35	6	0	-2.073595	0.492397	-4.046225
36	1	0	-2.682862	-1.510208	-3.498890
37	1	0	-1.294459	2.491608	-4.319277
38	1	0	-2.650310	0.502379	-4.972803
39	6	0	2.853911	0.706337	-1.507817
40	1	0	2.260847	0.914592	-2.399098
41	6	0	4.226191	0.620186	-1.628557
42	1	0	4.746932	0.762354	-2.575345
43	6	0	6.476898	0.267076	-0.721071
44	1	0	6.869877	1.260179	-0.974154
45	1	0	6.927948	-0.077844	0.214479
46	1	0	6.713365	-0.442841	-1.522913
47	7	0	5.009315	0.343621	-0.550522
48	15	0	0.385456	0.456095	-0.091159
49	9	0	0.831187	-1.250767	-0.497345

Table S18. Cartesian coordinates (Å) of the cation of **11c[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.124852	-0.224093	-0.553485
2	6	0	3.182623	0.550664	-0.054596
3	1	0	2.981177	1.408354	0.590429
4	6	0	4.499342	0.230872	-0.400789
5	1	0	5.340501	0.817387	-0.030512
6	6	0	4.742129	-0.847573	-1.235516
7	1	0	5.743310	-1.147703	-1.546094
8	6	0	0.245061	1.860860	0.384166
9	6	0	-0.248927	2.848332	-0.489552
10	1	0	-0.604736	2.584740	-1.486115
11	6	0	-0.310856	4.176392	-0.062549
12	1	0	-0.704763	4.939942	-0.734786
13	6	0	0.115678	4.523771	1.223243
14	1	0	0.058652	5.562575	1.552553
15	6	0	0.599988	3.542060	2.096836
16	1	0	0.914711	3.811985	3.106032
17	6	0	0.664622	2.210231	1.687132
18	1	0	1.010614	1.446834	2.387492
19	6	0	-0.130941	-0.941365	1.217919
20	6	0	-1.267632	-0.579217	1.971113
21	1	0	-1.794250	0.355931	1.771927
22	6	0	-1.717530	-1.423753	2.986837
23	1	0	-2.596717	-1.143765	3.568975
24	6	0	-1.040977	-2.617561	3.261852
25	1	0	-1.392806	-3.269396	4.063093
26	6	0	0.088776	-2.975565	2.518529
27	1	0	0.619084	-3.902755	2.740051
28	6	0	0.545461	-2.144150	1.494932
29	1	0	1.433718	-2.434892	0.931884
30	15	0	0.354420	0.141417	-0.136322
31	6	0	-0.578824	-0.187774	-1.642577
32	6	0	-1.763731	-0.944810	-1.576701
33	6	0	-0.150650	0.355051	-2.874123
34	6	0	-2.515397	-1.150094	-2.736341
35	1	0	-2.097305	-1.373176	-0.630485
36	6	0	-0.911606	0.140858	-4.023375
37	1	0	0.763621	0.949850	-2.940253
38	6	0	-2.093355	-0.608336	-3.954151
39	1	0	-3.433863	-1.736529	-2.685286
40	1	0	-0.586175	0.564688	-4.974680
41	1	0	-2.686404	-0.769885	-4.855803
42	6	0	2.428431	-1.294398	-1.396741
43	1	0	1.662827	-1.928685	-1.843594
44	7	0	3.711629	-1.590953	-1.720106
45	6	0	4.014799	-2.735267	-2.622210
46	1	0	4.539872	-2.360908	-3.509832
47	1	0	4.648061	-3.453927	-2.087072
48	1	0	3.078080	-3.215771	-2.920203

Table S19. Cartesian coordinates (Å) of the fluoride adduct of the cation of **11c[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.256831	0.454873	-0.310845
2	6	0	3.160597	1.169898	0.482463
3	1	0	2.799682	1.751604	1.331361
4	6	0	4.531465	1.148564	0.190103
5	1	0	5.248831	1.678621	0.816223
6	6	0	4.982549	0.460141	-0.917825
7	1	0	6.029150	0.415858	-1.216738
8	6	0	0.306360	2.179603	0.556154
9	6	0	-0.009317	3.224162	-0.331229
10	1	0	-0.300051	3.003833	-1.358118
11	6	0	0.002237	4.561457	0.083366
12	1	0	-0.264325	5.346282	-0.627302
13	6	0	0.336127	4.891020	1.397852
14	1	0	0.339404	5.933116	1.722080
15	6	0	0.646735	3.869573	2.301046
16	1	0	0.889577	4.108578	3.338418
17	6	0	0.627518	2.535541	1.884963
18	1	0	0.835470	1.757951	2.624313
19	6	0	-0.336816	-0.327480	1.564988
20	6	0	-1.498658	0.269727	2.086095
21	1	0	-1.933681	1.145493	1.602239
22	6	0	-2.107820	-0.260545	3.226067
23	1	0	-3.025228	0.192308	3.605846
24	6	0	-1.537040	-1.354479	3.883386
25	1	0	-2.005153	-1.755058	4.784250
26	6	0	-0.368977	-1.936125	3.382033
27	1	0	0.078845	-2.792000	3.889942
28	6	0	0.217859	-1.443108	2.214611
29	1	0	1.094723	-1.936793	1.798915
30	6	0	-0.651705	0.440006	-1.484968
31	6	0	-1.944582	-0.103797	-1.439402
32	6	0	-0.174568	0.981610	-2.690314
33	6	0	-2.752150	-0.086738	-2.579388
34	1	0	-2.319789	-0.554786	-0.519453
35	6	0	-0.983922	0.983861	-3.831203
36	1	0	0.825040	1.418720	-2.750856
37	6	0	-2.275276	0.453802	-3.776913
38	1	0	-3.757520	-0.508500	-2.530741
39	1	0	-0.603268	1.408387	-4.762073
40	1	0	-2.907309	0.459669	-4.666326
41	6	0	2.777630	-0.244174	-1.404575
42	1	0	2.147188	-0.852173	-2.048638
43	7	0	4.098638	-0.214058	-1.703745
44	6	0	4.607840	-0.948052	-2.886371
45	1	0	5.091439	-0.241259	-3.572058
46	1	0	5.331308	-1.704862	-2.558577
47	1	0	3.768839	-1.436772	-3.390425
48	15	0	0.395325	0.347441	0.017581
49	9	0	0.688112	-1.367524	-0.450834

Table S20. Cartesian coordinates (Å) of the cation of **21[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.024905	-0.176556	-0.727608
2	6	0	3.061889	0.767612	-0.755820
3	1	0	2.887279	1.786854	-0.404509
4	6	0	4.323890	0.394669	-1.231135
5	1	0	5.149848	1.105751	-1.263493
6	6	0	0.346200	1.931213	0.512213
7	6	0	0.323281	3.032207	-0.372411
8	1	0	0.288054	2.892712	-1.454756
9	6	0	0.325123	4.327798	0.144057
10	1	0	0.296537	5.179645	-0.536960
11	6	0	0.347407	4.533239	1.529351
12	1	0	0.339364	5.549748	1.926139
13	6	0	0.366471	3.443368	2.405809
14	1	0	0.369979	3.606178	3.484448
15	6	0	0.365348	2.139978	1.905867
16	1	0	0.355533	1.295626	2.596563
17	6	0	-0.147925	-0.973657	1.078761
18	6	0	-1.480307	-1.431634	1.123290
19	1	0	-2.222728	-1.088293	0.401371
20	6	0	-1.862464	-2.339988	2.111832
21	1	0	-2.892892	-2.696566	2.145155
22	6	0	-0.930968	-2.788354	3.054429
23	1	0	-1.237299	-3.497235	3.825401
24	6	0	0.391890	-2.331057	3.015313
25	1	0	1.114550	-2.679027	3.754875
26	6	0	0.789911	-1.424671	2.032399
27	1	0	1.822561	-1.068614	2.018100
28	15	0	0.322749	0.258901	-0.135520
29	6	0	2.294097	-1.472771	-1.171391
30	1	0	1.551573	-2.271098	-1.163272
31	6	0	-0.748250	0.170621	-1.596051
32	1	0	-0.792047	-0.857988	-1.979144
33	1	0	-1.759080	0.503728	-1.322112
34	1	0	-0.363235	0.834432	-2.381717
35	6	0	4.531442	-0.903371	-1.667303
36	1	0	5.489151	-1.257706	-2.049759
37	7	0	3.521654	-1.814829	-1.631380
38	6	0	3.787374	-3.198652	-2.113137
39	1	0	4.023213	-3.163328	-3.184437
40	1	0	4.635629	-3.613837	-1.555191
41	1	0	2.897912	-3.814169	-1.947985

Table S21. Cartesian coordinates (Å) of the fluoride adduct of the cation of **21[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.761879	-0.249384	-1.341604
2	6	0	2.802581	0.658128	-1.606263
3	1	0	2.728176	1.688635	-1.254061
4	6	0	3.937480	0.235924	-2.298161
5	1	0	4.756324	0.921404	-2.515972
6	6	0	-0.107295	2.043720	-0.048608
7	6	0	-0.361102	2.970254	-1.076521
8	1	0	-0.336377	2.669567	-2.123500
9	6	0	-0.643805	4.305009	-0.772531
10	1	0	-0.820074	5.015743	-1.581739
11	6	0	-0.714645	4.722037	0.558524
12	1	0	-0.952368	5.760743	0.794539
13	6	0	-0.479454	3.804039	1.587110
14	1	0	-0.535944	4.122123	2.629529
15	6	0	-0.157626	2.479516	1.290064
16	1	0	0.055086	1.779415	2.096574
17	6	0	-0.679292	-1.027638	0.533002
18	6	0	-2.074375	-1.148353	0.387787
19	1	0	-2.627192	-0.475007	-0.266351
20	6	0	-2.781264	-2.115256	1.105356
21	1	0	-3.865612	-2.177566	0.999646
22	6	0	-2.104500	-2.997906	1.951849
23	1	0	-2.657963	-3.758906	2.504752
24	6	0	-0.718691	-2.892567	2.096677
25	1	0	-0.184624	-3.568814	2.766671
26	6	0	-0.009984	-1.904153	1.408815
27	1	0	1.060732	-1.794118	1.571618
28	6	0	1.917208	-1.558912	-1.778547
29	1	0	1.168178	-2.332956	-1.609325
30	6	0	-0.793082	0.151598	-1.993040
31	1	0	-0.892488	-0.901368	-2.296041
32	1	0	-1.800444	0.572299	-1.880459
33	1	0	-0.300531	0.687735	-2.817202
34	6	0	4.045004	-1.088912	-2.695878
35	1	0	4.911596	-1.487260	-3.221025
36	7	0	3.044573	-1.962252	-2.427380
37	6	0	3.151767	-3.370338	-2.876019
38	1	0	2.582210	-3.500986	-3.805515
39	1	0	4.204964	-3.612618	-3.050120
40	1	0	2.749233	-4.027663	-2.097329
41	15	0	0.231738	0.271494	-0.399209
42	9	0	1.442140	0.314528	0.900199

Table S22. Cartesian coordinates (Å) of the cation of **12[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.007734	-0.301247	-0.621687
2	6	0	3.035015	0.578952	-0.289645
3	1	0	2.802970	1.442827	0.333015
4	6	0	4.341708	0.372302	-0.750456
5	1	0	5.137038	1.068060	-0.477989
6	6	0	4.599913	-0.726907	-1.563331
7	1	0	5.594310	-0.932311	-1.960681
8	6	0	3.557580	-1.593437	-1.869728
9	1	0	3.701290	-2.475519	-2.493360
10	6	0	1.266606	-2.397059	-1.796264
11	1	0	0.647893	-1.986222	-2.602094
12	1	0	0.644883	-2.639067	-0.927895
13	1	0	1.780358	-3.301428	-2.136380
14	6	0	0.262161	1.791632	0.498874
15	6	0	0.306981	2.798317	-0.493559
16	1	0	0.343745	2.536121	-1.552990
17	6	0	0.292349	4.137236	-0.110545
18	1	0	0.319044	4.918758	-0.871313
19	6	0	0.236519	4.478851	1.248600
20	1	0	0.220483	5.530159	1.541341
21	6	0	0.198079	3.483938	2.231442
22	1	0	0.150837	3.756503	3.286645
23	6	0	0.212812	2.136813	1.866216
24	1	0	0.178004	1.362969	2.634059
25	6	0	-0.111656	-1.018774	1.342617
26	6	0	-1.409653	-0.936830	1.898092
27	1	0	-2.139857	-0.221114	1.516458
28	6	0	-1.758856	-1.786703	2.947063
29	1	0	-2.760548	-1.728578	3.375207
30	6	0	-0.829149	-2.703734	3.452027
31	1	0	-1.108947	-3.360954	4.277074
32	6	0	0.460174	-2.777471	2.912095
33	1	0	1.185311	-3.483886	3.318494
34	6	0	0.824608	-1.940923	1.857473
35	1	0	1.840707	-1.994295	1.461454
36	7	0	2.297471	-1.395789	-1.405758
37	15	0	0.297405	0.082355	0.002073
38	8	0	-0.543777	-0.138945	-1.341158
39	6	0	-1.992950	-0.184338	-1.409683
40	6	0	-2.696348	1.001904	-1.588206
41	6	0	-2.605785	-1.433714	-1.389079
42	6	0	-4.085892	0.924556	-1.742484
43	1	0	-2.182396	1.961688	-1.628159
44	6	0	-3.995141	-1.489136	-1.546937
45	1	0	-2.023582	-2.346825	-1.263253
46	6	0	-4.732947	-0.314370	-1.720877
47	1	0	-4.657745	1.841252	-1.892601
48	1	0	-4.496076	-2.458187	-1.542076
49	1	0	-5.814730	-0.365602	-1.849600

Table S23. Cartesian coordinates (Å) of the fluoride adduct of the cation of **12[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.759434	-0.359554	-1.176841
2	6	0	2.715327	0.658578	-1.283120
3	1	0	2.572584	1.561729	-0.691753
4	6	0	3.821827	0.523670	-2.114483
5	1	0	4.551527	1.330931	-2.192405
6	6	0	3.993892	-0.664531	-2.831749
7	1	0	4.848827	-0.826179	-3.487144
8	6	0	3.055628	-1.664511	-2.683204
9	1	0	3.132840	-2.624136	-3.192022
10	6	0	1.007948	-2.643435	-1.842109
11	1	0	0.255738	-2.503749	-2.627003
12	1	0	0.515702	-2.686744	-0.866484
13	1	0	1.568716	-3.569690	-2.009066
14	6	0	-0.012055	1.752730	0.194192
15	6	0	-0.098147	2.630992	-0.899153
16	1	0	-0.016415	2.246566	-1.917022
17	6	0	-0.281672	3.999336	-0.684072
18	1	0	-0.331776	4.679296	-1.536252
19	6	0	-0.411696	4.492582	0.617800
20	1	0	-0.569286	5.559725	0.783530
21	6	0	-0.334479	3.619946	1.708137
22	1	0	-0.434388	4.002699	2.725089
23	6	0	-0.114858	2.256572	1.503143
24	1	0	-0.022710	1.586031	2.358160
25	6	0	-0.702263	-1.162818	1.003372
26	6	0	-2.069214	-0.909906	1.213170
27	1	0	-2.556087	-0.050180	0.753434
28	6	0	-2.812681	-1.748030	2.049441
29	1	0	-3.867445	-1.529946	2.223866
30	6	0	-2.213412	-2.854688	2.655042
31	1	0	-2.801275	-3.510797	3.299132
32	6	0	-0.853216	-3.108508	2.451094
33	1	0	-0.373347	-3.957636	2.940675
34	6	0	-0.094019	-2.257267	1.646392
35	1	0	0.979481	-2.426370	1.552352
36	7	0	1.962484	-1.509607	-1.880542
37	8	0	-0.612899	-0.233703	-1.518604
38	6	0	-1.979686	-0.331283	-1.786239
39	6	0	-2.753156	0.815946	-2.001810
40	6	0	-2.555475	-1.600610	-1.929566
41	6	0	-4.100368	0.685150	-2.353383
42	1	0	-2.307014	1.803825	-1.897338
43	6	0	-3.901884	-1.719832	-2.284207
44	1	0	-1.957623	-2.493975	-1.747829
45	6	0	-4.680054	-0.578458	-2.496223
46	1	0	-4.696944	1.583319	-2.523305
47	1	0	-4.342190	-2.712576	-2.393336
48	1	0	-5.730106	-0.673041	-2.776041
49	15	0	0.279600	-0.028096	-0.045254
50	9	0	1.504082	-0.045155	1.156796

Table S24. Cartesian coordinates (Å) of **23[B(C_6F_5)$_4$]**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.012548	-0.287082	-0.727239
2	6	0	3.040827	0.634135	-0.535971
3	1	0	2.807169	1.586289	-0.059903
4	6	0	4.351037	0.351481	-0.943817
5	1	0	5.144719	1.083986	-0.786549
6	6	0	4.618924	-0.874005	-1.547220
7	1	0	5.619148	-1.147309	-1.884685
8	6	0	3.577607	-1.776849	-1.717128
9	1	0	3.724172	-2.753622	-2.178274
10	6	0	1.275383	-2.531255	-1.575849
11	1	0	0.763609	-2.307635	-2.520856
12	1	0	0.566303	-2.560045	-0.741295
13	1	0	1.768618	-3.505318	-1.655167
14	6	0	0.367829	1.861439	0.453760
15	6	0	0.365148	2.930741	-0.469816
16	1	0	0.342362	2.753450	-1.546917
17	6	0	0.381777	4.242623	0.001102
18	1	0	0.370861	5.070725	-0.709067
19	6	0	0.399686	4.495671	1.379230
20	1	0	0.404452	5.525457	1.740366
21	6	0	0.400850	3.437281	2.293644
22	1	0	0.403435	3.637805	3.365933
23	6	0	0.384709	2.116983	1.840051
24	1	0	0.364058	1.297241	2.559459
25	6	0	-0.176478	-0.995475	1.140827
26	6	0	-1.526216	-1.387895	1.257343
27	1	0	-2.283304	-1.035776	0.554872
28	6	0	-1.904818	-2.238117	2.297569
29	1	0	-2.948363	-2.542399	2.390223
30	6	0	-0.953075	-2.695809	3.215721
31	1	0	-1.256962	-3.361496	4.025241
32	6	0	0.386634	-2.304097	3.102755
33	1	0	1.125047	-2.660491	3.822445
34	6	0	0.782054	-1.453270	2.070275
35	1	0	1.828587	-1.148053	1.997562
36	7	0	2.310215	-1.494903	-1.318260
37	15	0	0.293061	0.170356	-0.138665
38	6	0	-0.842095	0.101965	-1.554112
39	1	0	-0.416490	0.646785	-2.407641
40	1	0	-1.063655	-0.930470	-1.848205
41	1	0	-1.775811	0.601530	-1.257579

Table S25. Cartesian coordinates (Å) of **22.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.609707	-0.384753	-1.550357
2	6	0	2.264791	0.662139	-2.209395
3	1	0	1.872465	1.672755	-2.095682
4	6	0	3.404128	0.430179	-2.974491
5	1	0	3.911112	1.259396	-3.470410
6	6	0	3.886245	-0.876072	-3.101401
7	1	0	4.769792	-1.110842	-3.693549
8	6	0	3.216191	-1.892850	-2.451130
9	1	0	3.531242	-2.933570	-2.506871
10	6	0	1.473246	-2.796745	-1.004209
11	1	0	0.494320	-3.000326	-1.455944
12	1	0	1.350712	-2.543459	0.053997
13	1	0	2.117393	-3.674231	-1.115254
14	6	0	0.105849	1.781515	0.093593
15	6	0	-1.004578	2.608358	-0.162948
16	1	0	-1.870652	2.230938	-0.705206
17	6	0	-1.027406	3.925435	0.299283
18	1	0	-1.904276	4.546560	0.109592
19	6	0	0.066514	4.444952	0.996981
20	1	0	0.050727	5.478106	1.348239
21	6	0	1.176380	3.634137	1.249569
22	1	0	2.031103	4.030360	1.800476
23	6	0	1.194052	2.306284	0.816682
24	1	0	2.046643	1.671472	1.050269
25	6	0	-1.115937	-1.078096	0.348780
26	6	0	-2.033555	-1.864963	-0.370405
27	1	0	-2.037746	-1.871264	-1.460049
28	6	0	-2.962474	-2.663593	0.302662
29	1	0	-3.656761	-3.280863	-0.269973
30	6	0	-3.011350	-2.659597	1.698635
31	1	0	-3.746369	-3.273201	2.222286
32	6	0	-2.116756	-1.864381	2.421697
33	1	0	-2.153873	-1.849129	3.512271
34	6	0	-1.163126	-1.092422	1.757044
35	1	0	-0.456151	-0.495197	2.330726
36	7	0	2.111158	-1.647909	-1.690853
37	6	0	-0.895484	0.296185	-2.081336
38	1	0	-0.473648	1.131806	-2.656382
39	1	0	-0.840398	-0.600206	-2.717328
40	1	0	-1.956231	0.503252	-1.891184
41	15	0	0.091386	0.040347	-0.486452
42	9	0	1.269653	-0.406099	0.774049

Table S26. Cartesian coordinates (Å) of $B(C_6F_5)_3$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.094953	2.489641	-0.656690
2	6	0	0.515293	1.487129	-1.433171
3	6	0	1.611722	1.905108	-2.210128
4	6	0	2.069444	3.221994	-2.234028
5	6	0	1.436055	4.179230	-1.434702
6	6	0	0.349688	3.810999	-0.634289
7	5	0	0.006554	0.001806	-1.434001
8	9	0	2.248187	1.026002	-3.012134
9	9	0	3.103895	3.580476	-3.009614
10	9	0	-0.248120	4.728704	0.140651
11	9	0	-1.135786	2.185124	0.146397
12	6	0	-1.534094	-0.299791	-1.440231
13	6	0	-2.443158	0.451045	-2.209290
14	6	0	-3.812186	0.188026	-2.241266
15	6	0	-4.326049	-0.850980	-1.458539
16	6	0	-3.465811	-1.618242	-0.666235
17	6	0	-2.099458	-1.340984	-0.680003
18	9	0	-1.999981	1.452779	-2.997326
19	9	0	-1.318258	-2.101370	0.115191
20	9	0	-3.963347	-2.605858	0.093382
21	9	0	-4.637892	0.914306	-3.009819
22	6	0	1.037863	-1.181754	-1.430635
23	6	0	0.844706	-2.347137	-2.196280
24	6	0	1.752099	-3.405460	-2.214062
25	6	0	2.901219	-3.332630	-1.419856
26	6	0	3.133662	-2.200729	-0.631809
27	6	0	2.215542	-1.151582	-0.660104
28	9	0	-0.238813	-2.463587	-2.992212
29	9	0	1.537974	-4.487284	-2.978070
30	9	0	4.230462	-2.139114	0.138400
31	9	0	2.480872	-0.091899	0.131896
32	9	0	3.775507	-4.343456	-1.413798
33	9	0	-5.637113	-1.110209	-1.467543
34	9	0	1.868432	5.443945	-1.435570

Table S27. Cartesian coordinates (Å) of $[FB(C_6F_5)_3]^-$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.125172	2.589072	-0.607718
2	6	0	0.550241	1.713780	-1.617001
3	6	0	1.450908	2.276476	-2.525841
4	6	0	1.931976	3.586852	-2.438268
5	6	0	1.495770	4.408471	-1.400931
6	6	0	0.579141	3.904818	-0.478797
7	9	0	1.907043	1.563351	-3.590586
8	9	0	2.810983	4.071141	-3.348529
9	9	0	0.133179	4.703928	0.520273
10	9	0	-0.799139	2.198028	0.302263
11	6	0	-1.558038	0.001975	-2.151554
12	6	0	-2.280662	0.972430	-2.850875
13	6	0	-3.631257	0.843013	-3.192817
14	6	0	-4.319975	-0.314903	-2.838493
15	6	0	-3.641069	-1.324700	-2.157038
16	6	0	-2.291911	-1.150834	-1.837734
17	9	0	-1.689441	2.125606	-3.264131
18	9	0	-1.698016	-2.196815	-1.214112
19	9	0	-4.298208	-2.462371	-1.826627
20	9	0	-4.278929	1.825155	-3.864822
21	6	0	1.057013	-0.867034	-2.453887
22	6	0	0.808433	-1.487096	-3.681125
23	6	0	1.690533	-2.382622	-4.295192
24	6	0	2.901965	-2.684220	-3.676389
25	6	0	3.210119	-2.076730	-2.459674
26	6	0	2.297159	-1.188723	-1.884341
27	9	0	-0.332302	-1.231653	-4.376376
28	9	0	1.387206	-2.957752	-5.483889
29	9	0	4.394720	-2.348474	-1.861092
30	9	0	2.693558	-0.611718	-0.724043
31	9	0	3.770117	-3.546936	-4.251617
32	9	0	-5.625843	-0.461476	-3.157757
33	9	0	1.947171	5.678906	-1.295800
34	5	0	0.016489	0.133319	-1.617410
35	9	0	0.025449	-0.313482	-0.257156

Table S28. Cartesian coordinates (Å) of CF_2O.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.392343	-0.881189	0.000024
2	8	0	1.574231	-0.881188	-0.000009
3	9	0	-0.396439	0.193561	-0.000006
4	9	0	-0.396439	-1.955938	0.000039

Table S29. Cartesian coordinates (Å) of CF_3O^-.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.922255	-0.027060	-0.141732
2	9	0	-0.535423	0.520074	1.151943
3	9	0	-0.535528	-1.420909	0.031214
4	9	0	-2.365460	-0.126958	0.031190
5	8	0	-0.515657	0.548010	-1.137934