Supporting Information for:

Müller versus Gutmann-Beckett for Assessing the Lewis Acidity of Boranes

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1. **General Details**:

All manipulations were performed under an inert atmosphere in a nitrogen filled MBraun Unilab glove box or using standard Schlenk techniques unless specified. Chloroform-d and benzene-d_6 for NMR spectroscopy were purchased from Cambridge Isotope Laboratories, Inc., dried by stirring for 5 days over CaH_2, distilled, and stored over 4 Å molecular sieves. All other solvents were purchased from commercial sources as anhydrous grade, dried further using a JC Meyer Solvent System with dual columns packed with solvent-appropriate drying agents, and stored over 3 or 4 Å molecular sieves. Boron tribromide, BCl_3 (1.0 M solution in hexanes), Et_2O•BF_3, BPh_3, $B(OMe)_3$, and FBN were purchased from commercial sources and used without further purification. Tris(pentafluorophenyl)borane was purified by drying with dimethylsilylchloride and $PhCF_3$ was used after distillation. Piers' borane, B*o*Cb_3, BrB^{Me}*o*Cb_2, BrB^{Ph}*o*Cb_2 and HB^{Me}*o*Cb_2 were prepared according to the literature procedure.[1-4] Multinuclear NMR spectra ($^{11}B\{^1H\}$, $^{19}F\{^1H\}$, and $^{31}P\{^1H\}$) were recorded on a Bruker Avance III HD 400 MHz instrument.

2. **Experimental Section**:

2.1. **FBN Probe method**:

A borane solution (0.06 mmol) in deuterated $CDCl_3$ or C_6D_6 (0.6 mL) was transferred to a vial with FBN (0.06 mmol). The mixture was stirred at 23 °C for 10 min. $PhCF_3$ was added as an internal standard (0.02 mmol) and the $^{19}F\{^1H\}$ NMR spectrum was recorded.

Entry	BR_3	δ FBN•BR_3 (ppm) $CDCl_3$	Δδ ^{19}F (ppm) $CDCl_3$	δ FBN•BR_3 (ppm) C_6D_6	Δδ ^{19}F (ppm) C_6D_6
1	BBr_3	–89.34	13.1	–92.64	11.3
2	BCl_3	–91.17	11.3	–93.63	10.3
3	$Et_2O•BF_3$	NR	--	NR	--
4	$PhBBr_2$	–92.79	9.6	–95.24	8.7
5	Ph_2BBr	–99.09	3.3	–100.23	3.7
6	BPh_3	NR	--	NR	--
7	$PhBCl_2$	–100.44	2.0	–103.92	3.0
8	$B(OMe)_3$	NR	--	NR	--
9	$HB(C_6F_5)_2$	–93.05	9.4	–94.66	9.3
10	$B(C_6F_5)_3$	–91.61	10.8	–93.15	10.8
11	$BrB^{Ph}oCb_2$	–88.74	13.7	–90.87	13.1
12	$BrB^{Me}oCb_2$	–87.74	14.7	–89.88	14.0
13	$HB^{Me}oCb_2$	–90.59	11.8	–91.65	12.3
14	B*o*Cb_3	–87.35	15.1	–89.29	14.6

Table S1. Shows the experimentally observed values of the ^{19}F FBN probe studies done using $CDCl_3$ and C_6D_6 as the solvents.

Δδ ^{19}F = δ FBN•BR_3 – δ FBN

δ FBN•BR_3 - $^{19}F\{^1H\}$ of the borane adduct with FBN in the corresponding deuterated solvent.

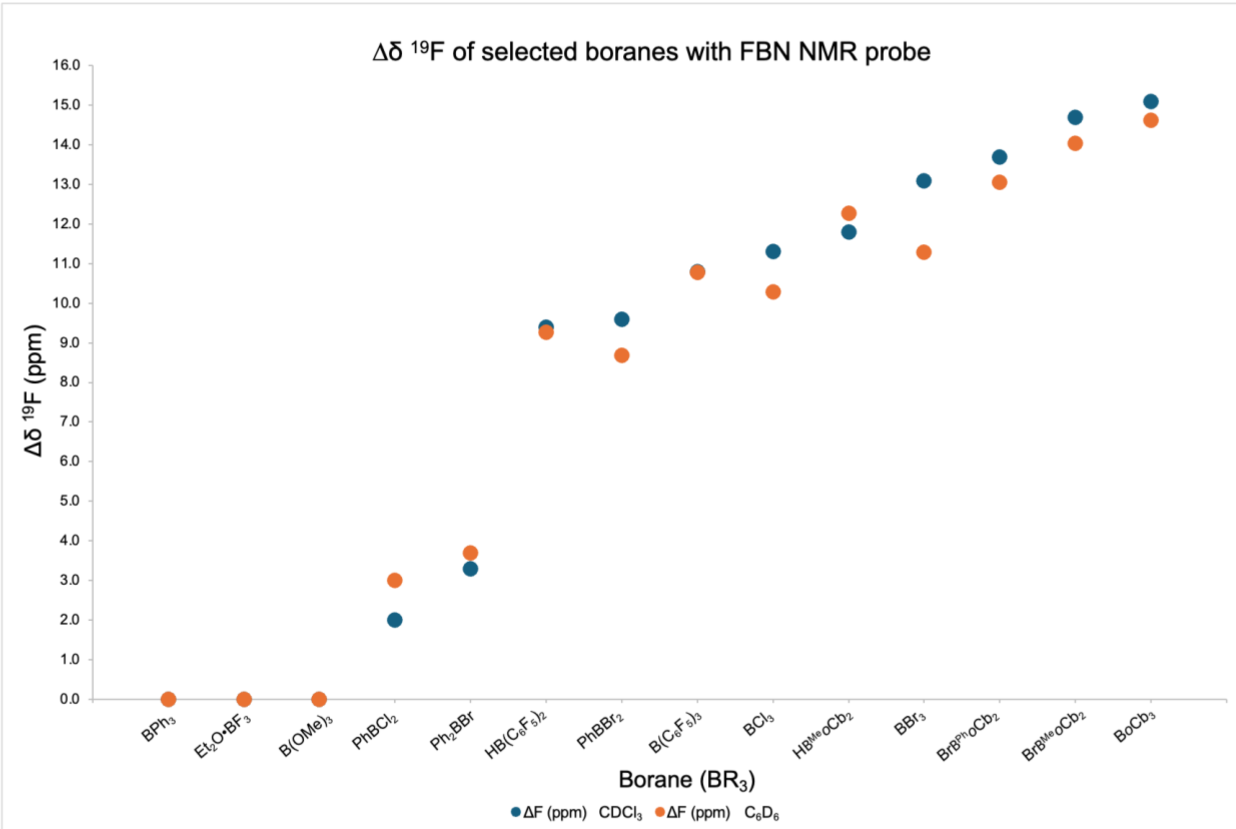
δ FBN - $^{19}F\{^1H\}$ shift of free FBN in the corresponding deuterated solvent.

δ FBN in $CDCl_3$ is -102.42 ppm and in C_6D_6 is -103.92 ppm.

Δδ ^{19}F - Change in $^{19}F\{^1H\}$ of the borane adduct with FBN and free FBN.

δ $PhCF_3$ in $CDCl_3$ is -62.74 ppm and in C_6D_6 is -62.46 ppm.

Figure S1: Plot showing the comparison of the Δδ ^{19}F values of the selected boranes in $CDCl_3$ and C_6D_6.



2.2. FBN Probe method with excess of Lewis acid:

A borane solution (0.18 mmol) in $CDCl_3$ (0.6 mL) was transferred to a vial with FBN (0.06 mmol). The mixture was stirred at 23 °C for 10 min. $PhCF_3$ was added as an internal standard (0.02 mmol) and the $^{19}F\{^1H\}$ and $^{11}B\{^1H\}$ NMR spectra were recorded.

Entry	BR_3	δ FBN•BR_3 (ppm) $CDCl_3$	Δδ ^{19}F (ppm) $CDCl_3$
1	BBr_3	–89.21	13.2
2	BCl_3	–90.23	12.1
3	Et_2O•BF_3	NR	--
4	$PhBBr_2$	–91.04	11.4
5	Ph_2BBr	–97.52	4.9
6	BPh_3	NR	--
7	$PhBCl_2$	–98.25	4.2
8	$B(OMe)_3$	NR	--
9	$HB(C_6F_5)_2$	–93.04	9.4
10	$B(C_6F_5)_3$	–91.59	10.8
11	$BrB^{Ph}\textit{o}Cb_2$	–88.74	13.7
12	$BrB^{Me}\textit{o}Cb_2$	–87.74	14.7
13	$HB^{Me}\textit{o}Cb_2$	–90.59	11.8
14	$B\textit{o}Cb_3$	–87.35	15.1

Table S2. $^{19}F\{^1H\}$ NMR FBN probe studies with excess of Lewis acid (3 equivalents) in $CDCl_3$ solvent.

δ FBN in $CDCl_3$ is -102.42 ppm.

δ $PhCF_3$ in $CDCl_3$ is -62.74 ppm.

Note: Multinuclear NMR studies show no indication of reactions with $CDCl_3$ and the Lewis acids.

2.3. Gutmann-Beckett studies:

A solution of $OPEt_3$ (0.06 mmol) in $CDCl_3$ (0.6 mL) was transferred to a vial containing the borane (0.06 mmol). The mixture was stirred at 23 °C for 5 min and the $^{31}P\{^1H\}$ NMR spectrum recorded.

Entry	BR_3	δ $Et_3PO•BR_3$ (ppm)	Δδ ^{31}P (ppm)
1	BBr_3	88.0	35.7
2	BCl_3	85.2	32.9
3	$Et_2O•BF_3$	78.5	26.2
4	$PhBBr_2$	86.6	34.3
5	Ph_2BBr	81.8	29.5
6	BPh_3	54.0	1.7
7	$PhBCl_2$	83.7	31.4
8	$B(OMe)_3$	52.3	NR
9	$HB(C_6F_5)_2$	80.9	28.6
10	$B(C_6F_5)_3$[5]	75.9	23.6
11	BrB^{Ph}*o*Cb_2	83.8	31.5
12	BrB^{Me}*o*Cb_2	86.2	33.9
13	HB^{Me}*o*Cb_2[2]	82.3	30.0
14	B*o*Cb_3[1]	79.8	27.5

Table S3. Gutmann Beckett studies done using $CDCl_3$ solvent.

^{31}P δ $OPEt_3$ in $CDCl_3$ appears at 52.3 ppm.

Δδ ^{31}P = δ $Et_3PO•BR_3$ – δ Et_3PO

δ $Et_3PO•BR_3$ - $^{31}P\{^1H\}$ of the borane adduct with $OPEt_3$ in $CDCl_3$.

δ Et_3PO - $^{31}P\{^1H\}$ shift of free $OPEt_3$ in $CDCl_3$.

Δδ ^{31}P - Change in $^{31}P\{^1H\}$ shift of the borane adducts with $OPEt_3$ and free $OPEt_3$.

2.4. Gutmann-Beckett studies with excess Lewis acid:

A solution of $OPEt_3$ (0.06 mmol) in $CDCl_3$ (0.6 mL) was transferred to a vial containing the borane (0.18 mmol). The mixture was stirred at 23 °C for 5 min and the $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ NMR spectra were recorded.

Entry	BR_3	δ $Et_3PO•BR_3$ (ppm)	Δδ ^{31}P (ppm)
1	BBr_3	88.2	35.9
2	BCl_3	85.2	32.9
3	$Et_2O•BF_3$	78.4	26.1
4	$PhBBr_2$	86.8	34.5
5	Ph_2BBr	81.8	29.5
6	BPh_3	57.1	4.8
7	$PhBCl_2$	83.7	31.4
8	$B(OMe)_3$	NR	NR
9	$HB(C_6F_5)_2$	80.9	28.6
10	$B(C_6F_5)_3$	75.9	23.6
11	$BrB^{Ph}\textit{o}Cb_2$	83.5	31.2
12	$BrB^{Me}\textit{o}Cb_2$	86.2	33.9
13	$HB^{Me}\textit{o}Cb_2$	82.5	30.2
14	$B\textit{o}Cb_3$	79.9	27.6

Table S4. $^{31}P\{^1H\}$ NMR Gutmann Beckett studies with excess Lewis acid in $CDCl_3$ solvent.

^{31}P δ $OPEt_3$ in $CDCl_3$ appears at 52.3 ppm.

Note: The strong Lewis acids $B\textit{o}Cb_3$, $HB^{Me}\textit{o}Cb_2$ and $B(C_6F_5)_3$, the triethylphosphine oxide adducts have all been structurally characterized by X-ray crystallography and reveal no deoxygenation reactivity.[1, 2, 6]

3. NMR Spectra:

Figure S2: $^{19}F\{^{1}H\}$ NMR spectrum of $PhCF_3$ in $CDCl_3$ (376 MHz)

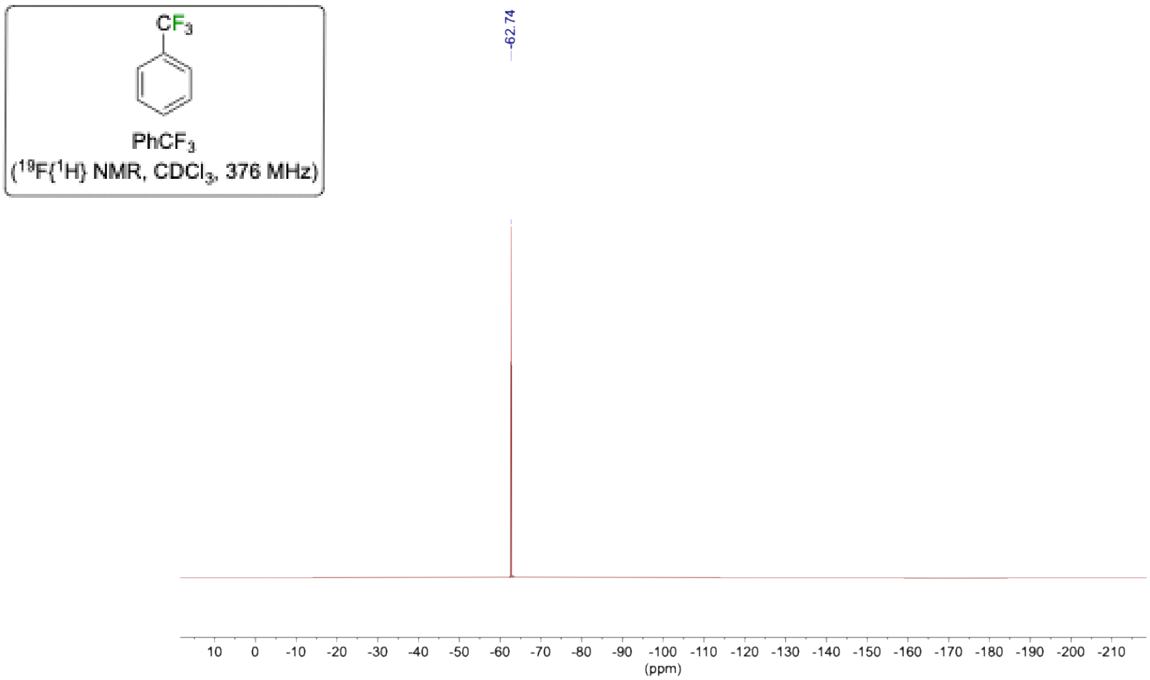


Figure S3: $^{19}F\{^{1}H\}$ NMR spectrum of $PhCF_3$ in C_6D_6 (376 MHz)

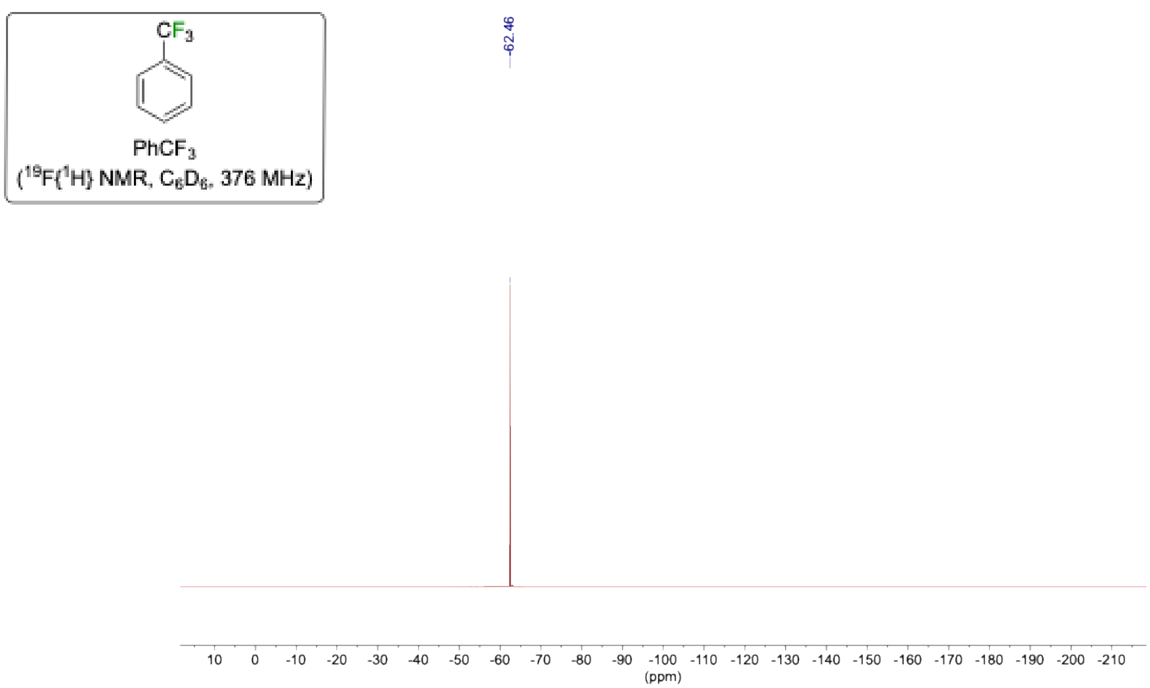


Figure S4: $^{19}F\{^1H\}$ NMR spectrum of FBN in $CDCl_3$ (376 MHz)

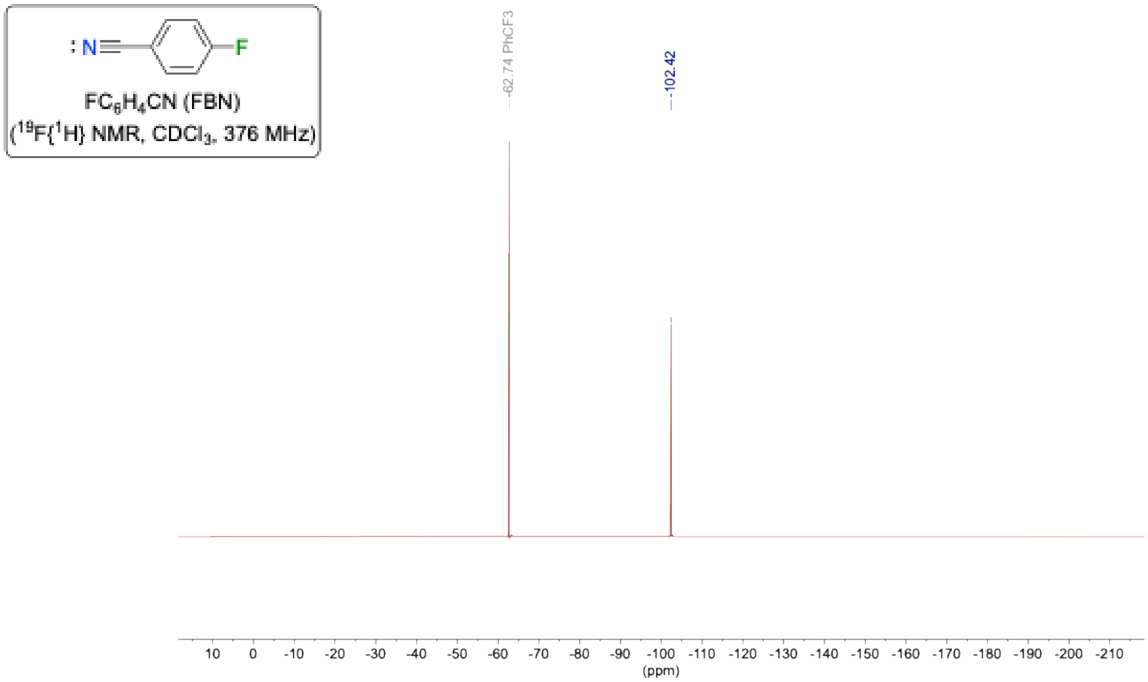


Figure S5: $^{19}F\{^1H\}$ NMR spectrum of FBN in C_6D_6 (376 MHz)

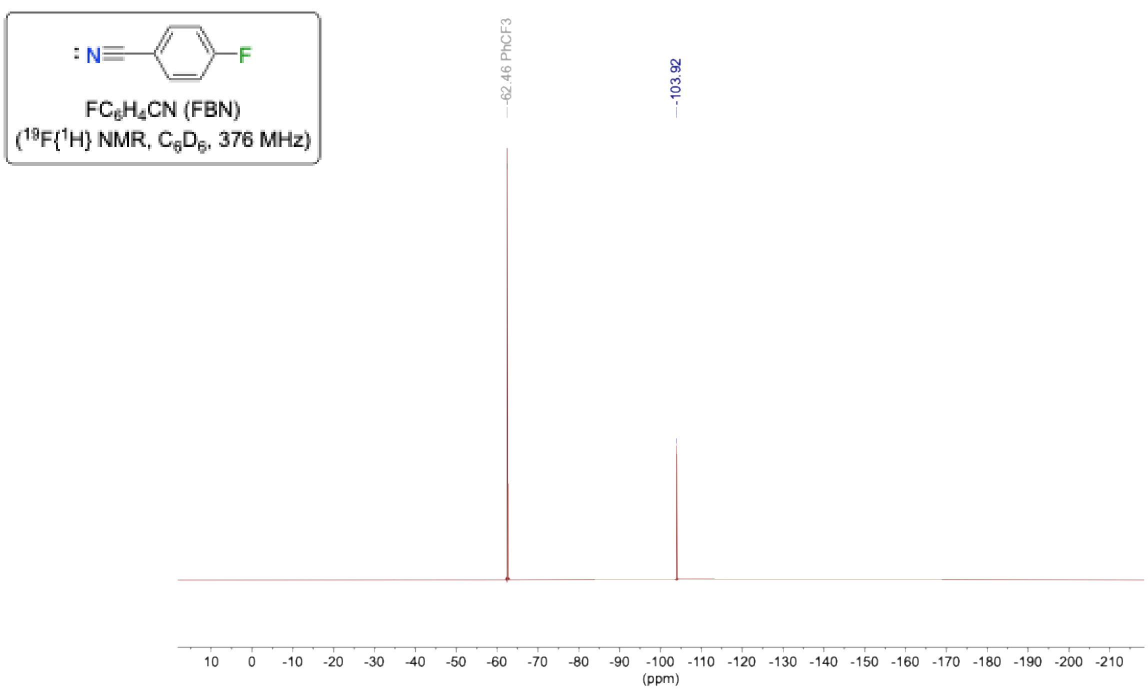


Figure S6: $^{19}F\{^1H\}$ NMR spectra of the FBN•BBr_3 adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of BBr_3.

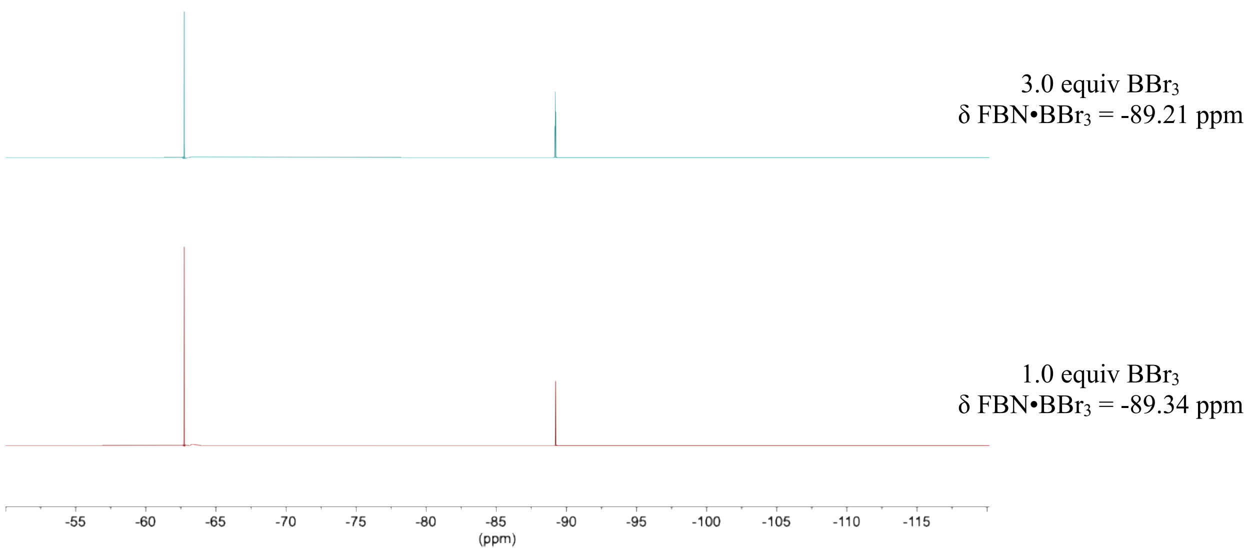


Figure S7: $^{19}F\{^1H\}$ NMR spectra of the FBN•BCl_3 adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of BCl_3.

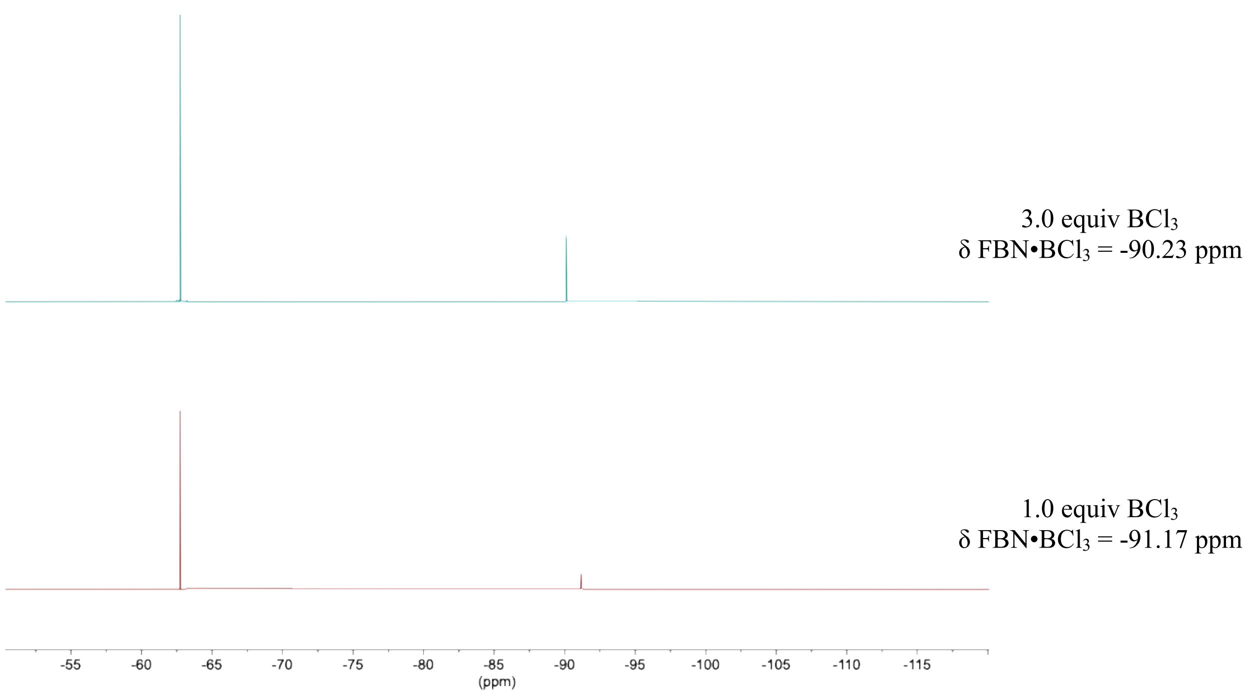


Figure S8: $^{19}F\{^1H\}$ NMR spectra of FBN with $Et_2O{\bullet}BF_3$ in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of $Et_2O{\bullet}BF_3$.

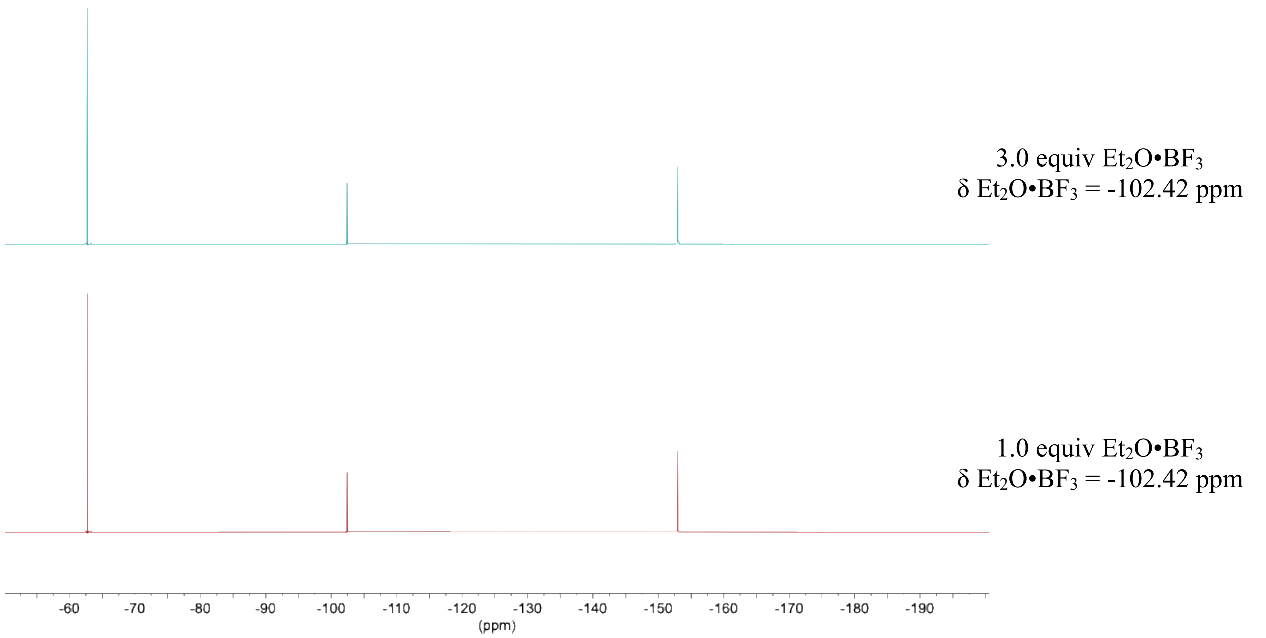


Figure S9: $^{19}F\{^1H\}$ NMR spectra of the $FBN{\bullet}BPhBr_2$ adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of $BPhBr_2$.

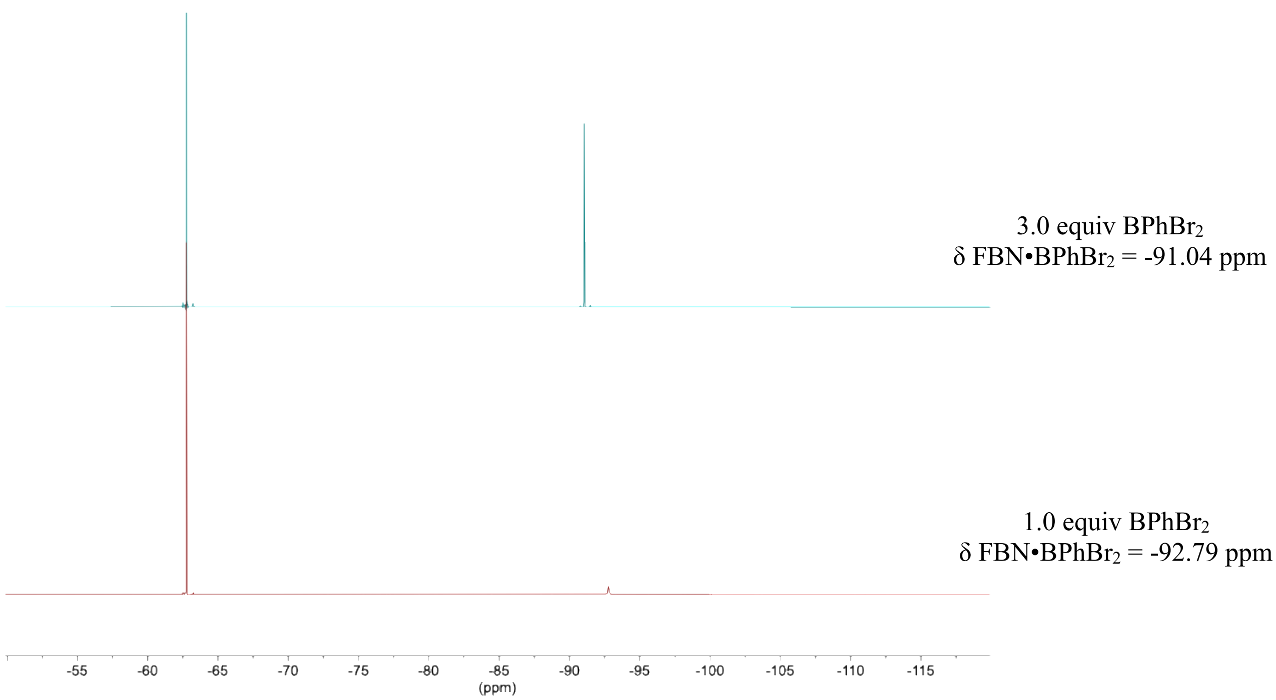


Figure S10: $^{19}F\{^{1}H\}$ NMR spectra of the FBN•BPh_2Br adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of BPh_2Br.

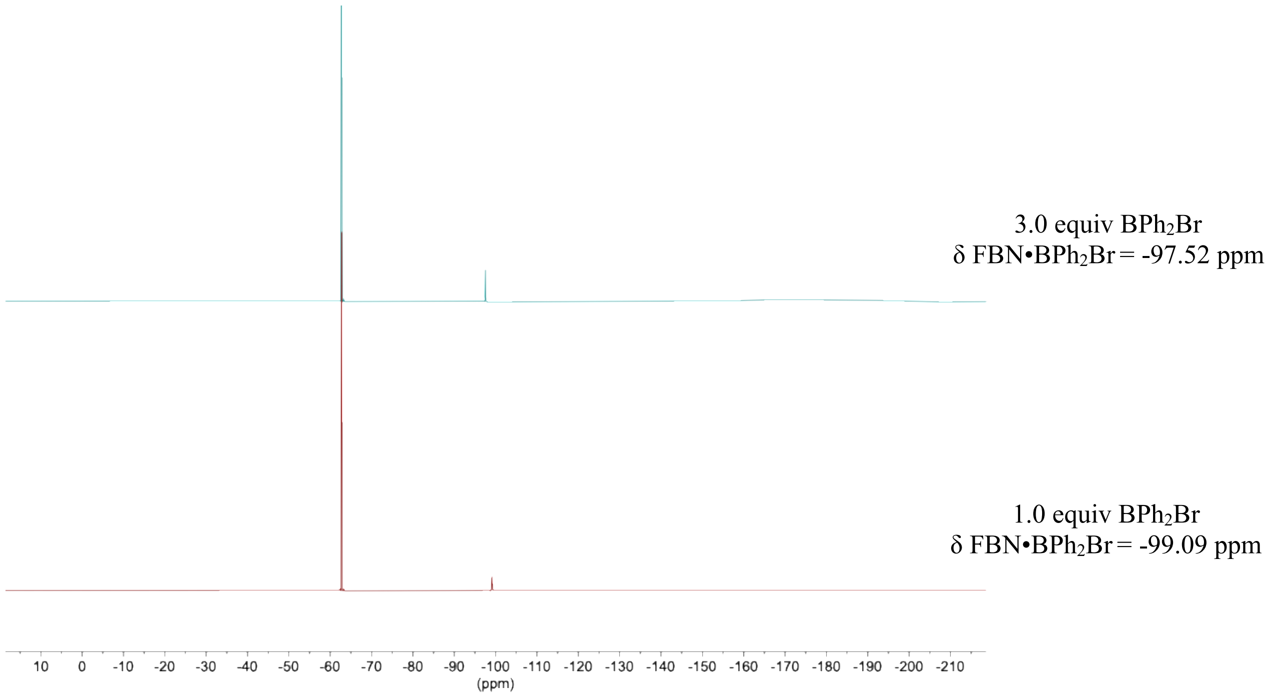


Figure S11: $^{19}F\{^{1}H\}$ NMR spectra of FBN with BPh_3 in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of BPh_3.

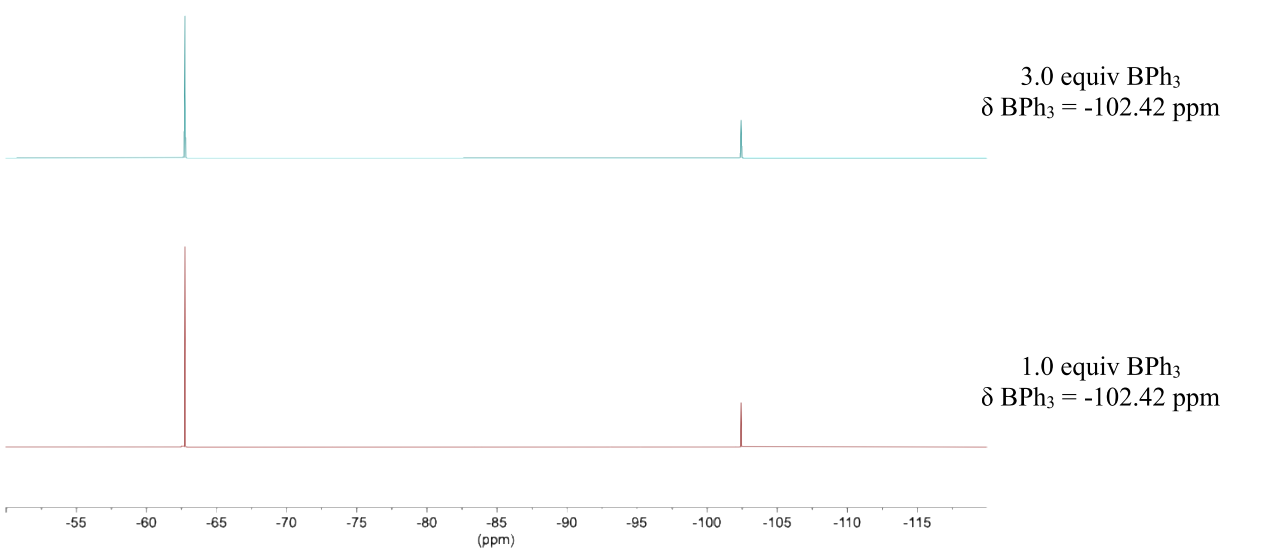


Figure S12: $^{19}F\{^{1}H\}$ NMR spectra of the FBN•$BPhCl_2$ adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of $BPhCl_2$.

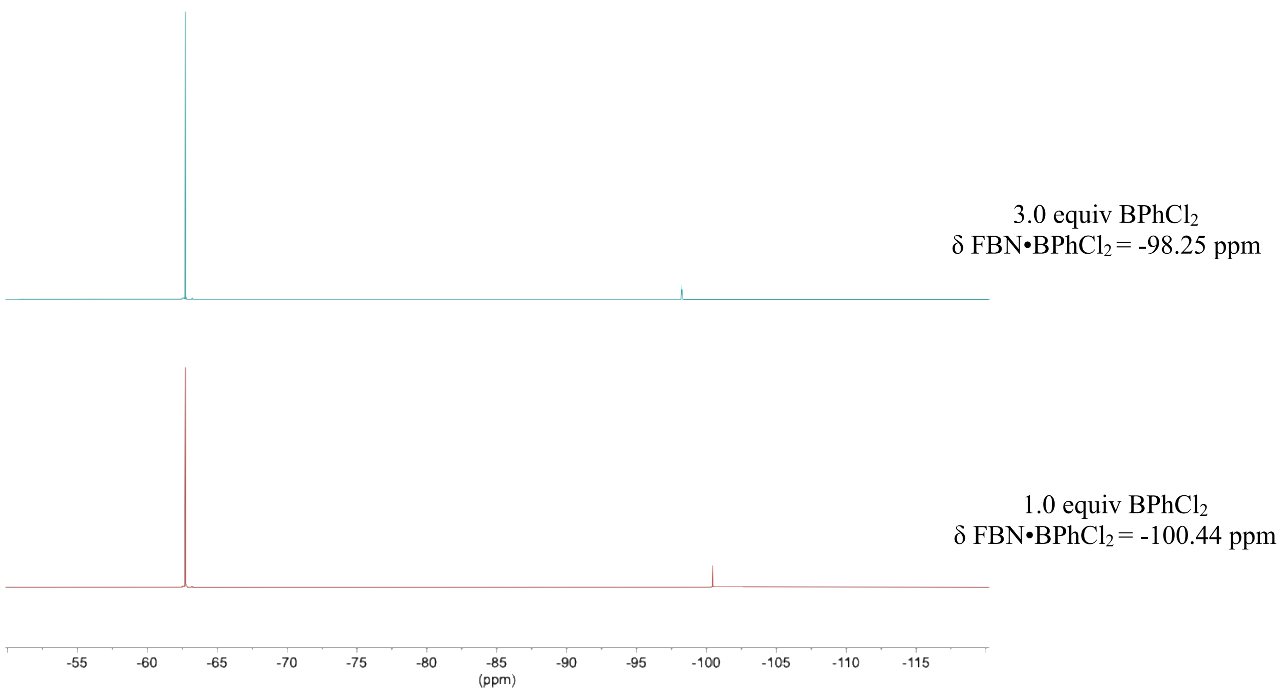


Figure S13: $^{19}F\{^{1}H\}$ NMR spectra of FBN with $B(OMe)_3$ in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of $B(OMe)_3$.

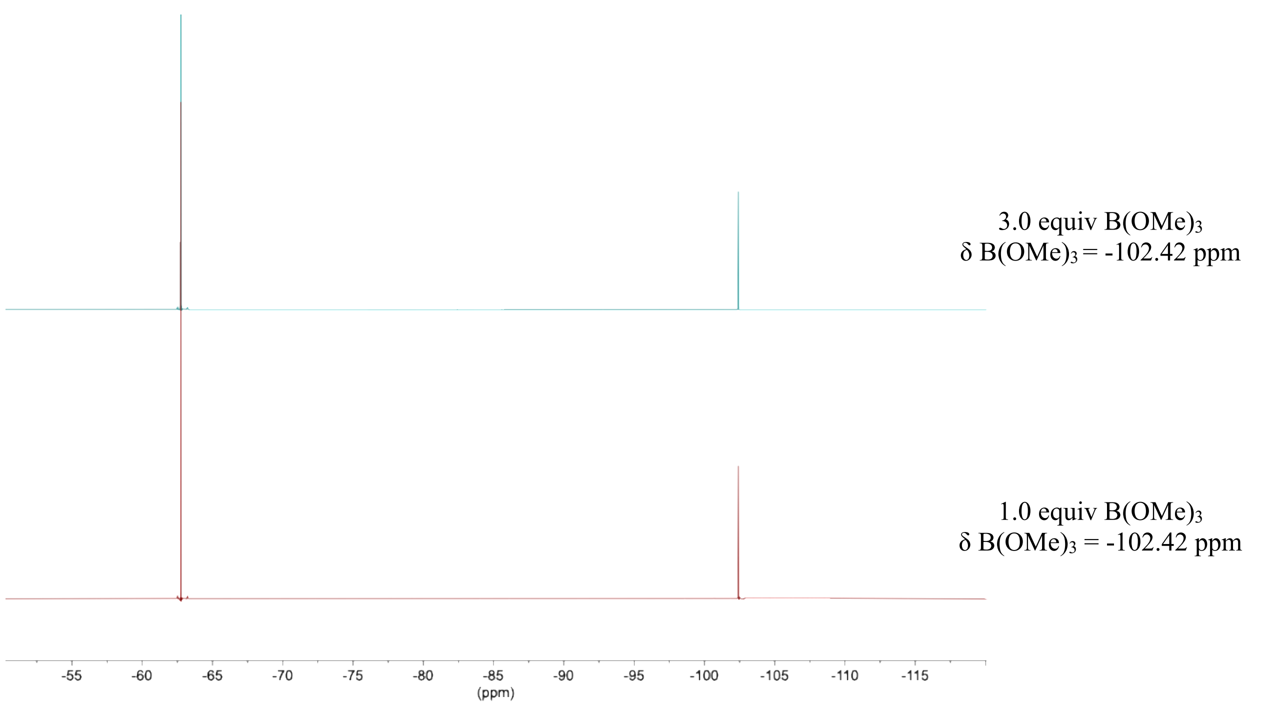


Figure S14: $^{19}F\{^{1}H\}$ NMR spectra of the FBN•$BH(C_6F_5)_2$ adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of $BH(C_6F_5)_2$.

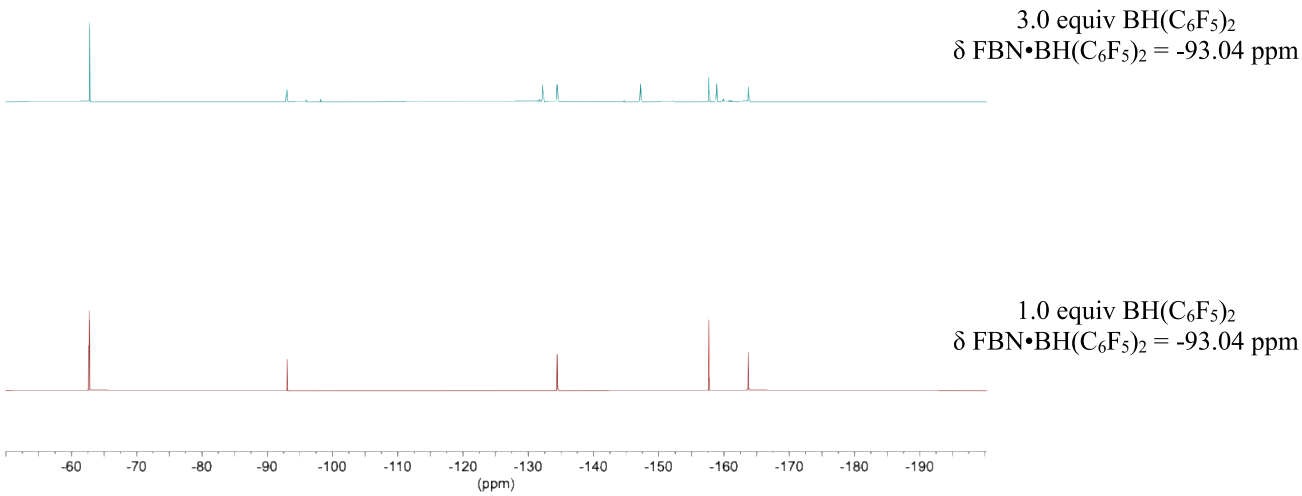


Figure S15: $^{19}F\{^{1}H\}$ NMR spectra of the FBN•$B(C_6F_5)_3$ adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of $B(C_6F_5)_3$.

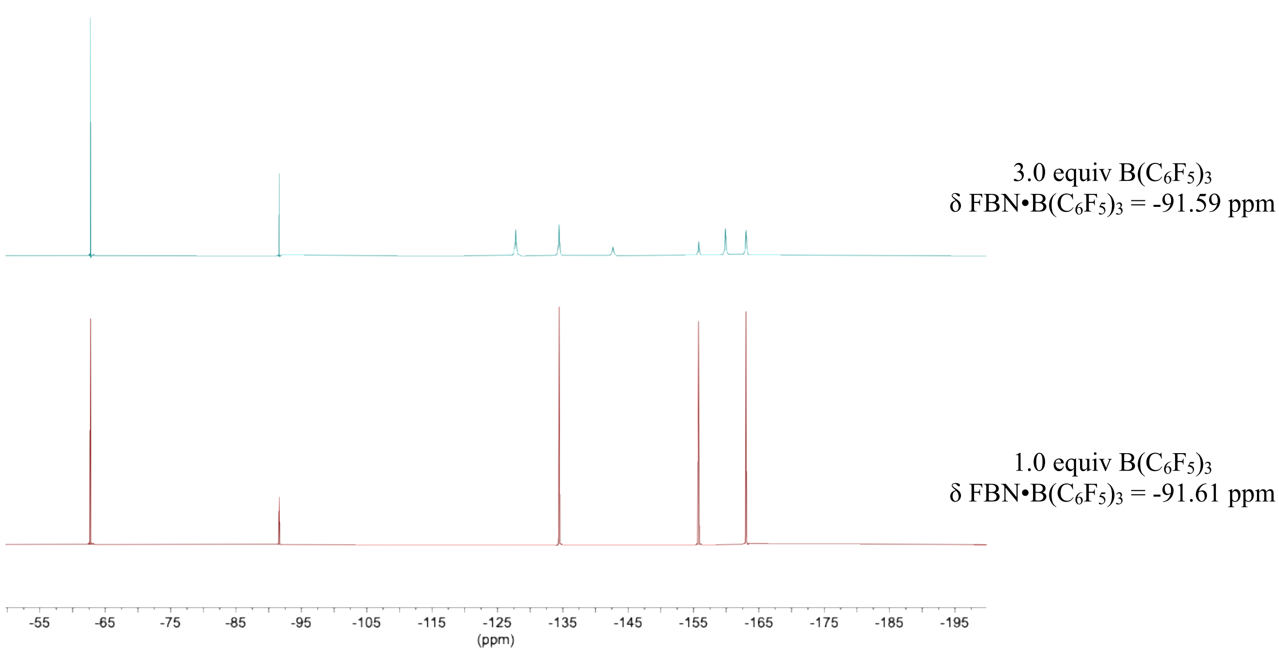


Figure S16: $^{19}F\{^{1}H\}$ NMR spectra of the FBN•BBr^{Ph}*o*Cb$_2$ adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of BBr^{Ph}*o*Cb$_2$.

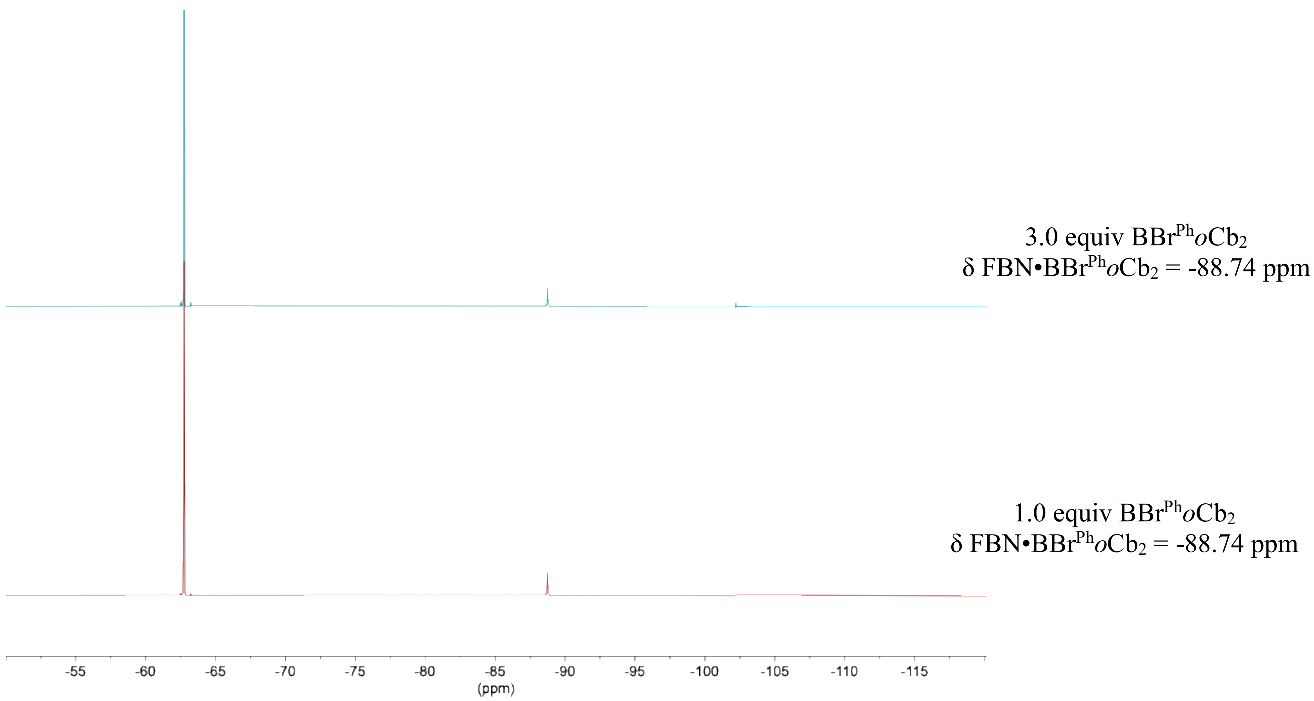


Figure S17: $^{19}F\{^{1}H\}$ NMR spectra of the FBN•BBr^{Me}*o*Cb$_2$ adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of BBr^{Me}*o*Cb$_2$.

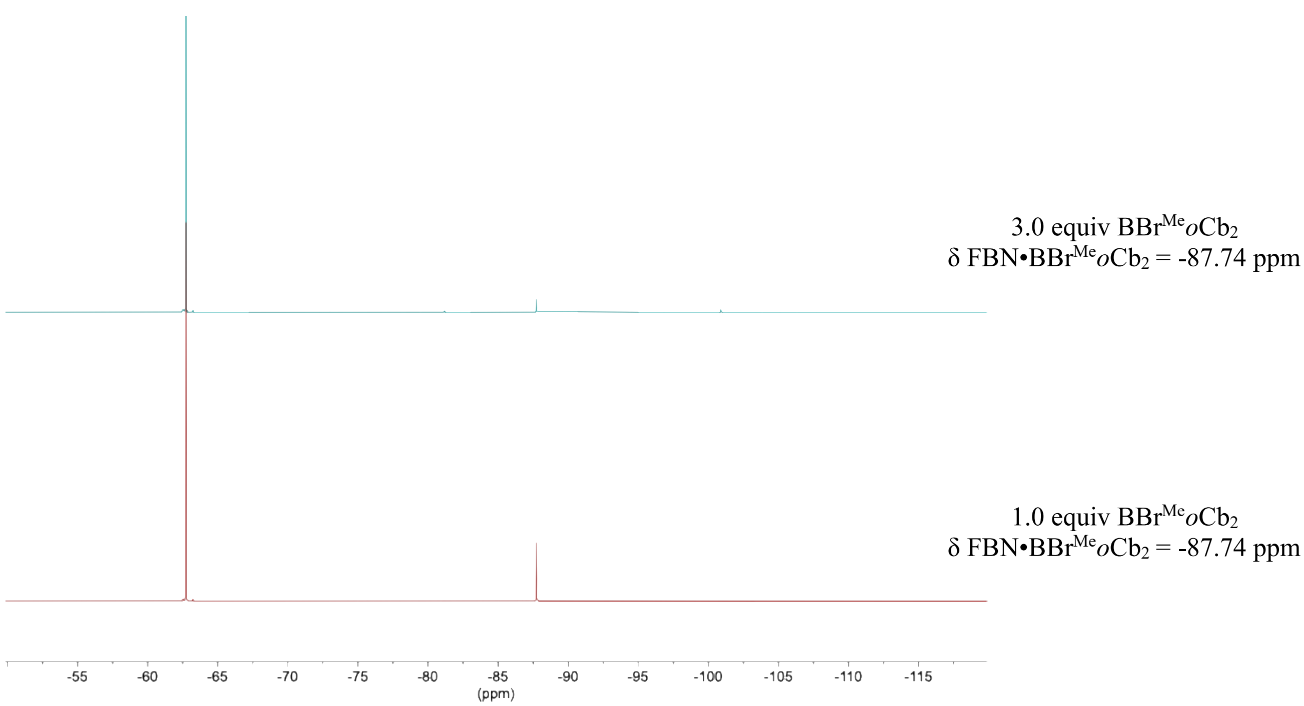


Figure S18: $^{19}F\{^{1}H\}$ NMR spectra of the FBN•BH^{Me}*o*Cb$_2$ adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of BH^{Me}*o*Cb$_2$.

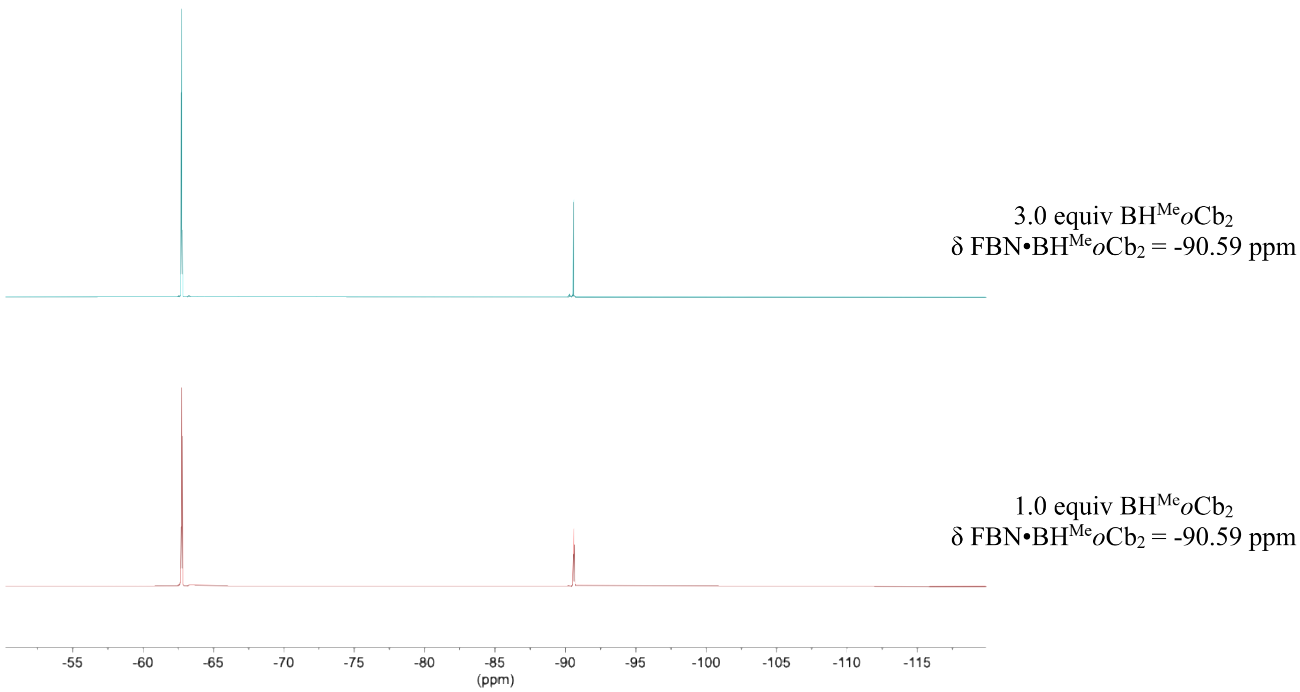


Figure S19: $^{19}F\{^{1}H\}$ NMR spectra of the FBN•B*o*Cb$_3$ adduct in $CDCl_3$ (376 MHz) with 1 and 3 equivalents of B*o*Cb$_3$.

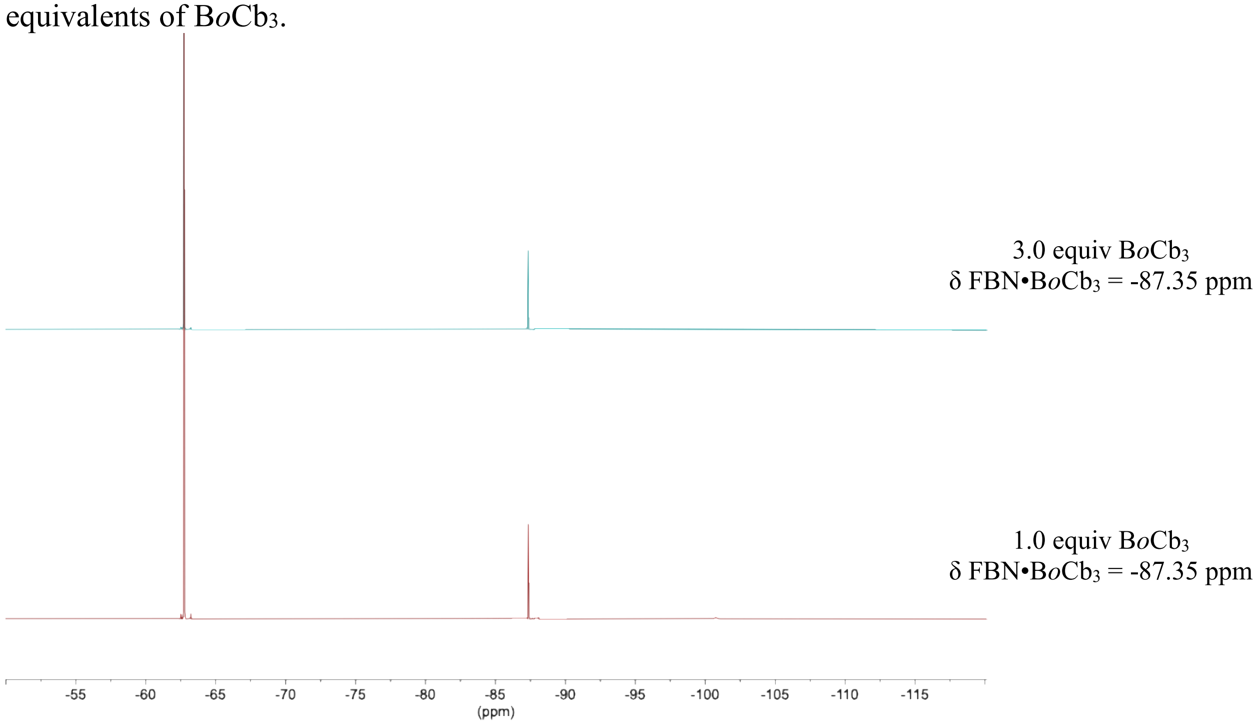


Figure S20: $^{31}P\{^{1}H\}$ NMR spectra of the $Et_3PO•BBr_3$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of BBr_3.

3.0 equiv BBr_3
δ $Et_3PO•BBr_3$ = 88.2 ppm

1.0 equiv BBr_3
δ $Et_3PO•BBr_3$ = 88.0 ppm

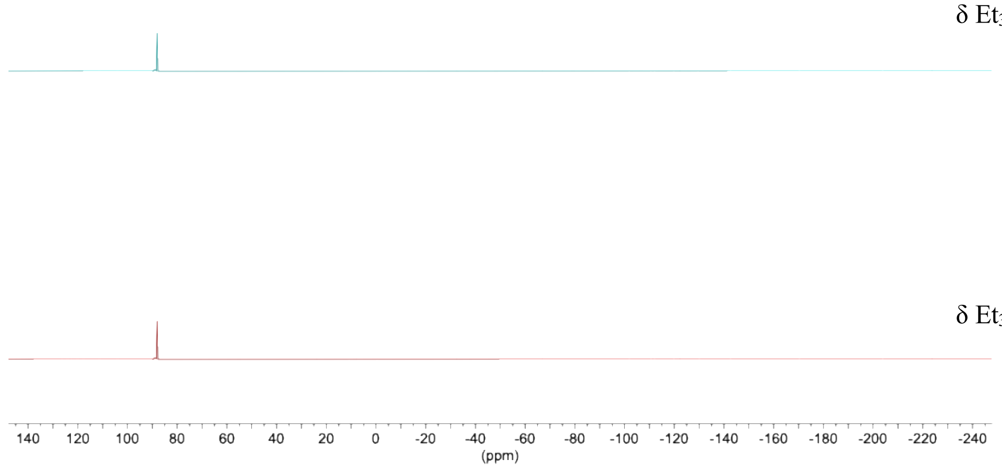


Figure S21: $^{31}P\{^{1}H\}$ NMR spectra of the $Et_3PO•BCl_3$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of BCl_3.

3.0 equiv BCl_3
δ $Et_3PO•BCl_3$ = 85.2 ppm

1.0 equiv BCl_3
δ $Et_3PO•BCl_3$ = 85.2 ppm

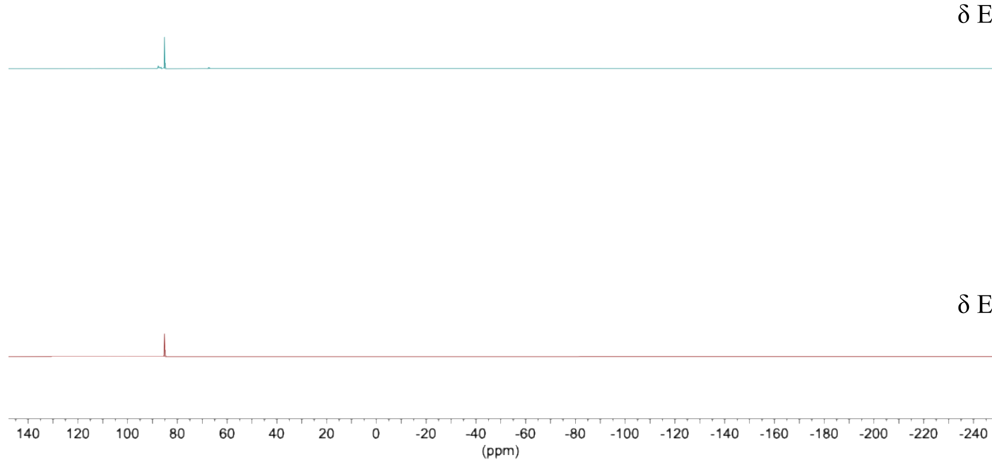


Figure S22: $^{31}P\{^{1}H\}$ NMR spectra of Et_3PO with $Et_2O•BF_3$ in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $Et_2O•BF_3$.

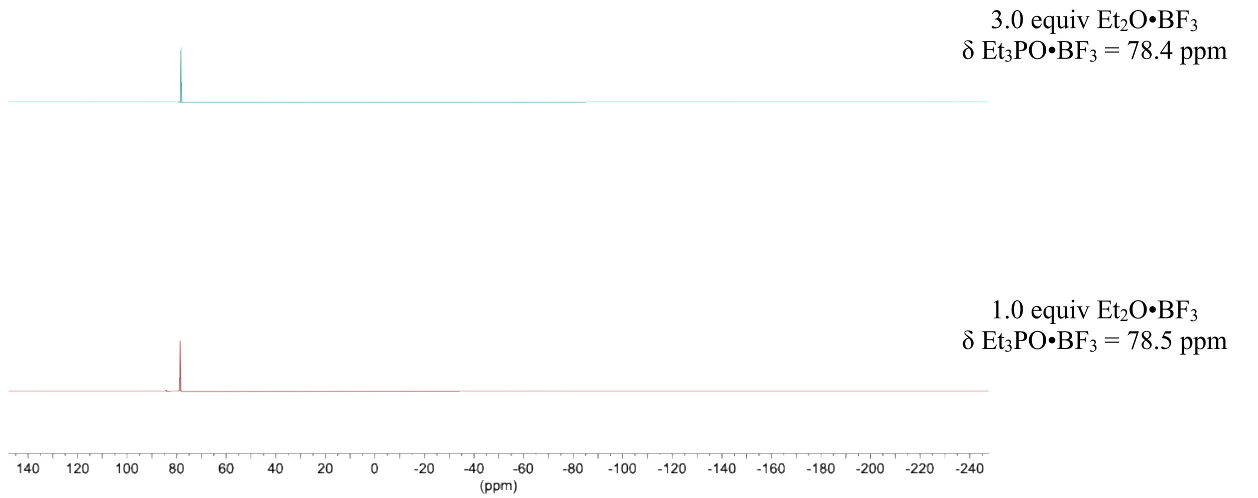


Figure S23: $^{31}P\{^{1}H\}$ NMR spectra of the $Et_3PO•BPhBr_2$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $BPhBr_2$.

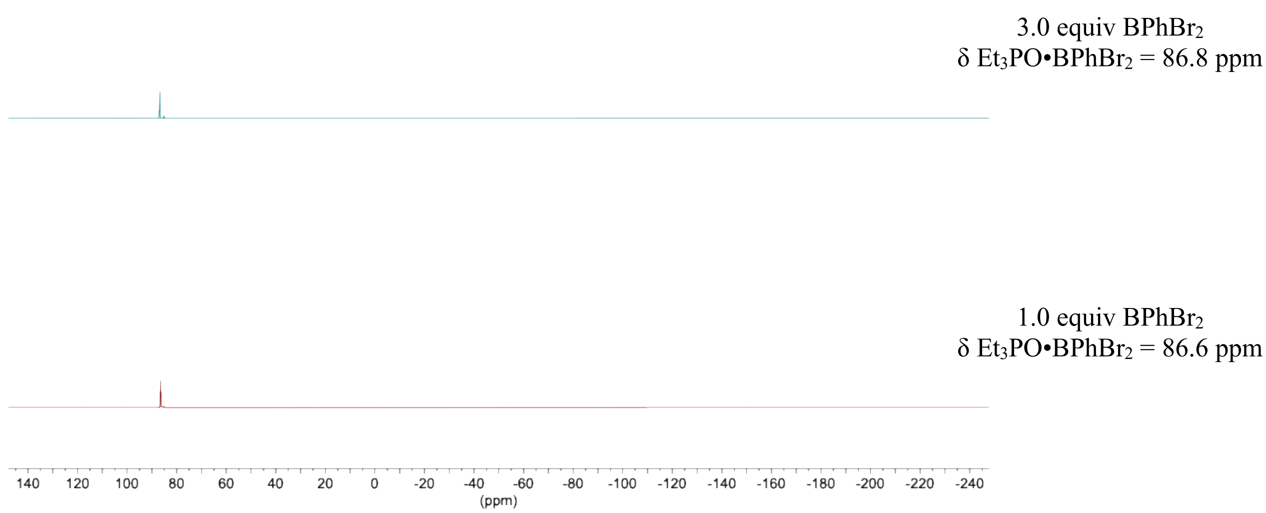


Figure S24: $^{31}P\{^{1}H\}$ NMR spectra of the $Et_3PO{\bullet}BPh_2Br$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of BPh_2Br.

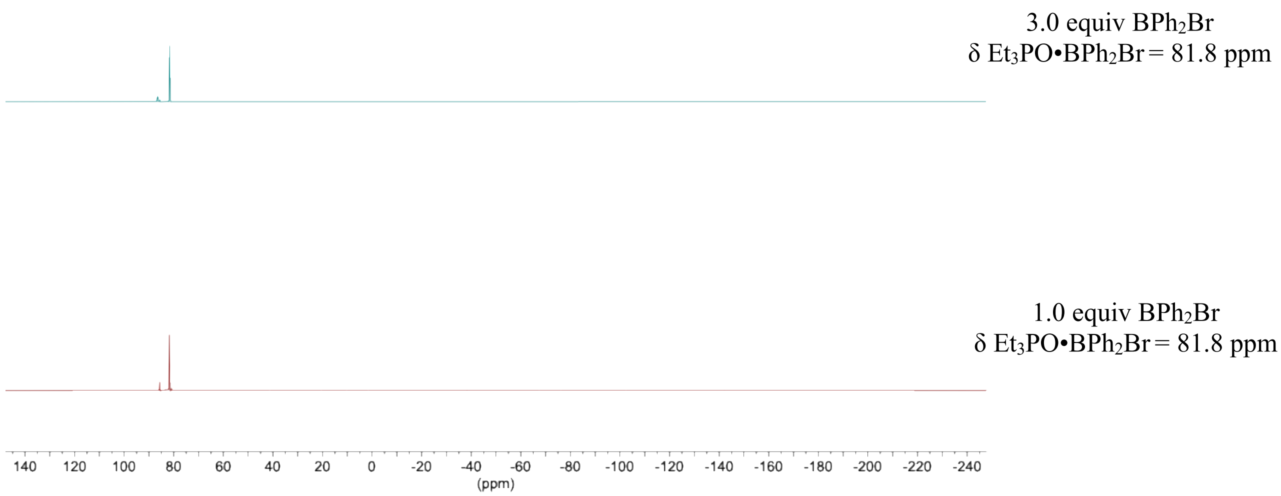


Figure S25: $^{31}P\{^{1}H\}$ NMR spectra of the $Et_3PO{\bullet}BPh_3$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of BPh_3.

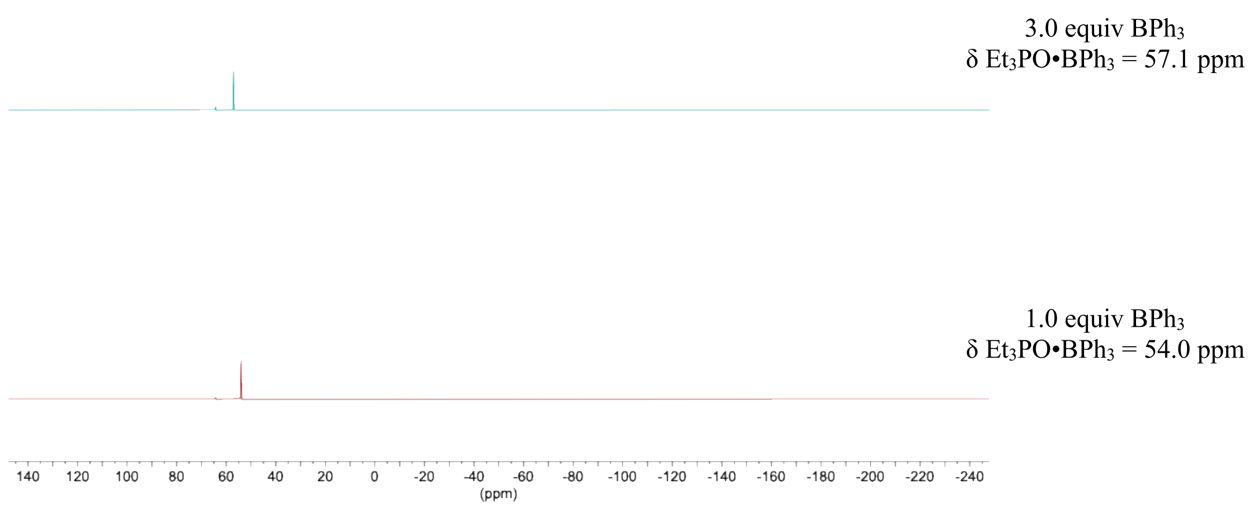


Figure S26: $^{31}P\{^1H\}$ NMR spectra of the $Et_3PO•BPhCl_2$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $BPhCl_2$.

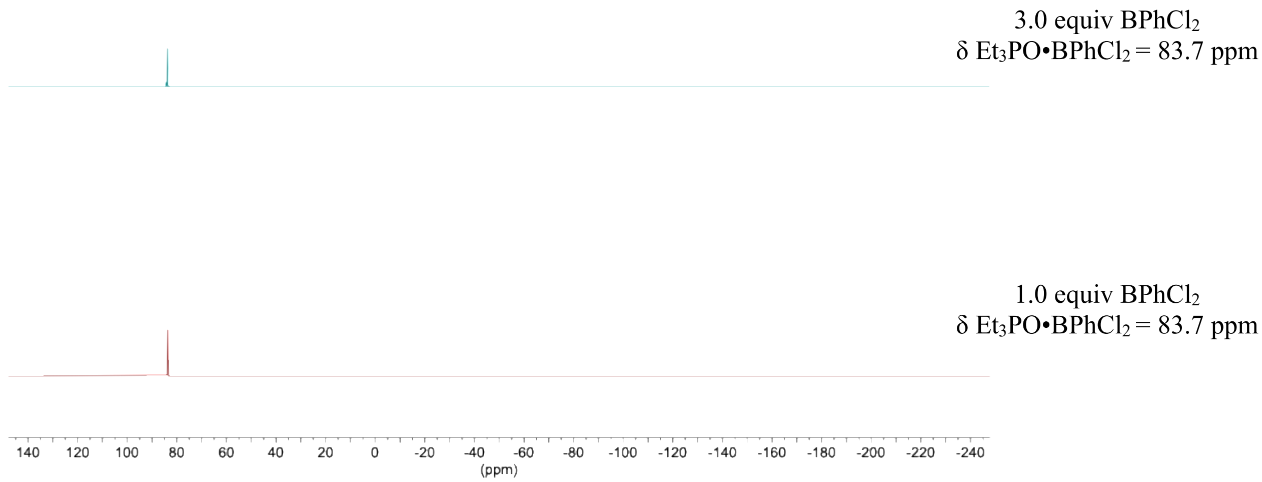


Figure S27: $^{31}P\{^1H\}$ NMR spectra of Et_3PO with $B(OMe)_3$ in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $B(OMe)_3$.

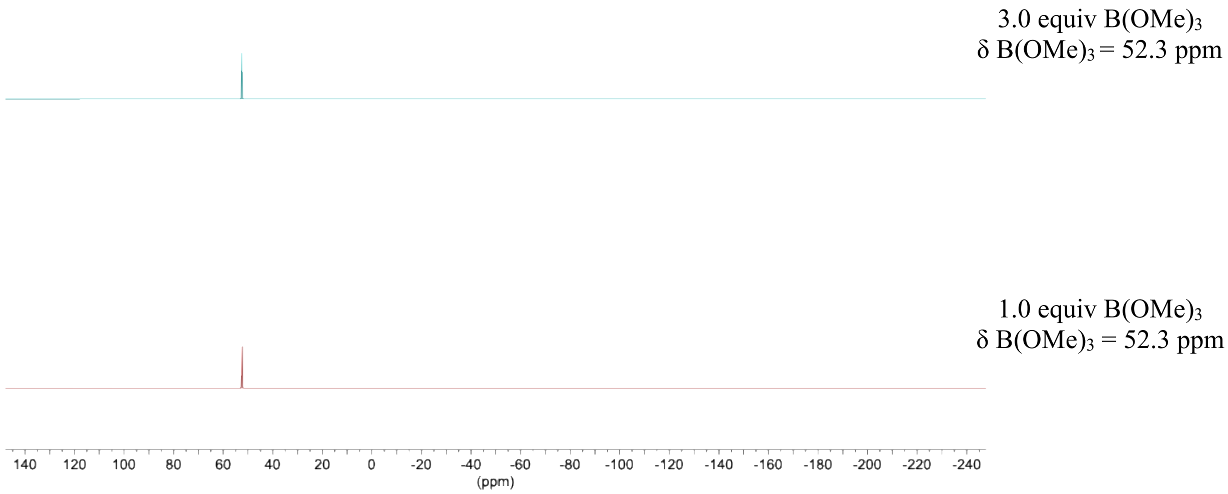


Figure S28: $^{31}P\{^{1}H\}$ NMR spectra of the $Et_3PO{\bullet}BH(C_6F_5)_2$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $BH(C_6F_5)_2$.

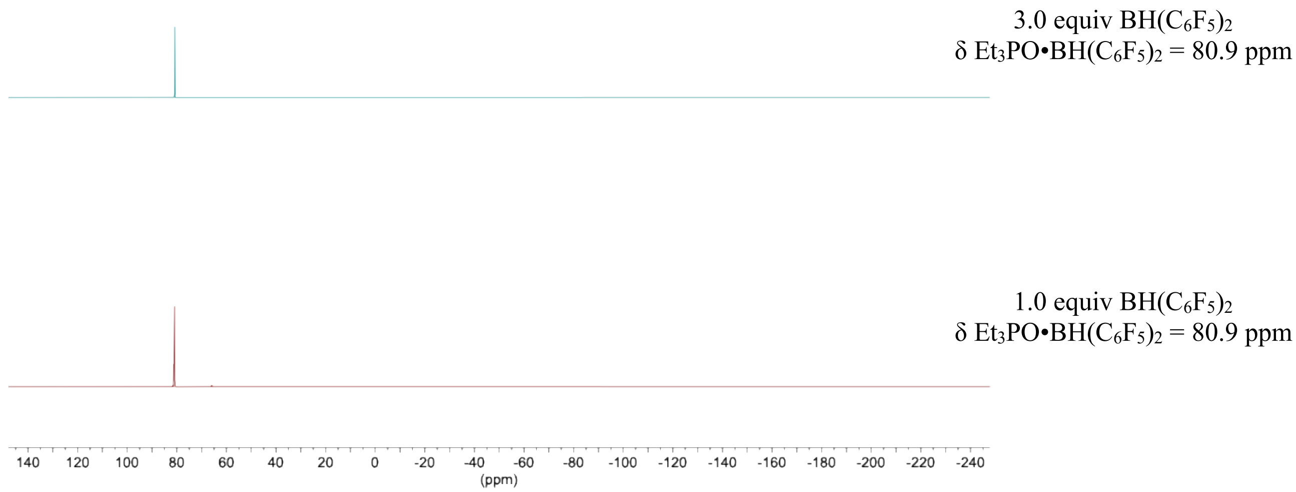


Figure S29: $^{31}P\{^{1}H\}$ NMR spectra of the $Et_3PO{\bullet}B(C_6F_5)_3$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $B(C_6F_5)_3$.

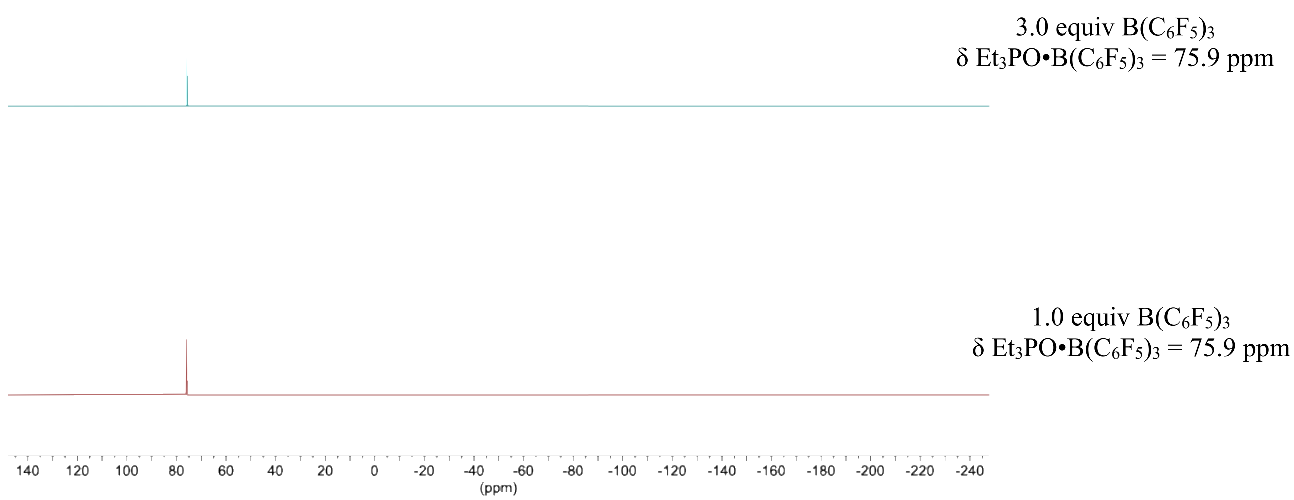


Figure S30: $^{31}P\{^{1}H\}$ NMR spectra of the Et_3PO•$BBr^{Ph}oCb_2$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $BBr^{Ph}oCb_2$.

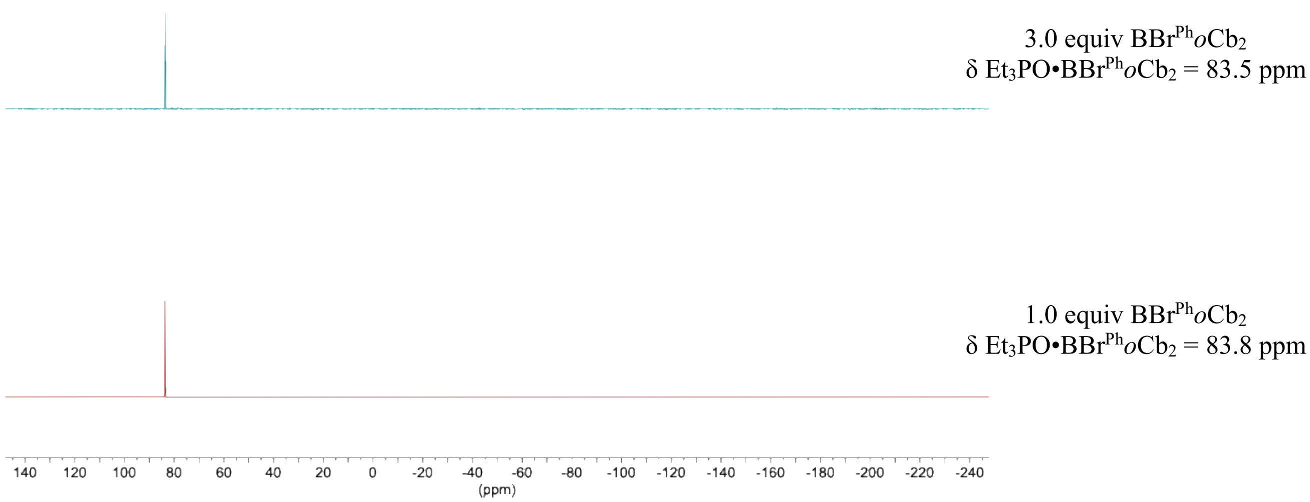


Figure S31: $^{31}P\{^{1}H\}$ NMR spectra of the Et_3PO•$BBr^{Me}oCb_2$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $BBr^{Me}oCb_2$.

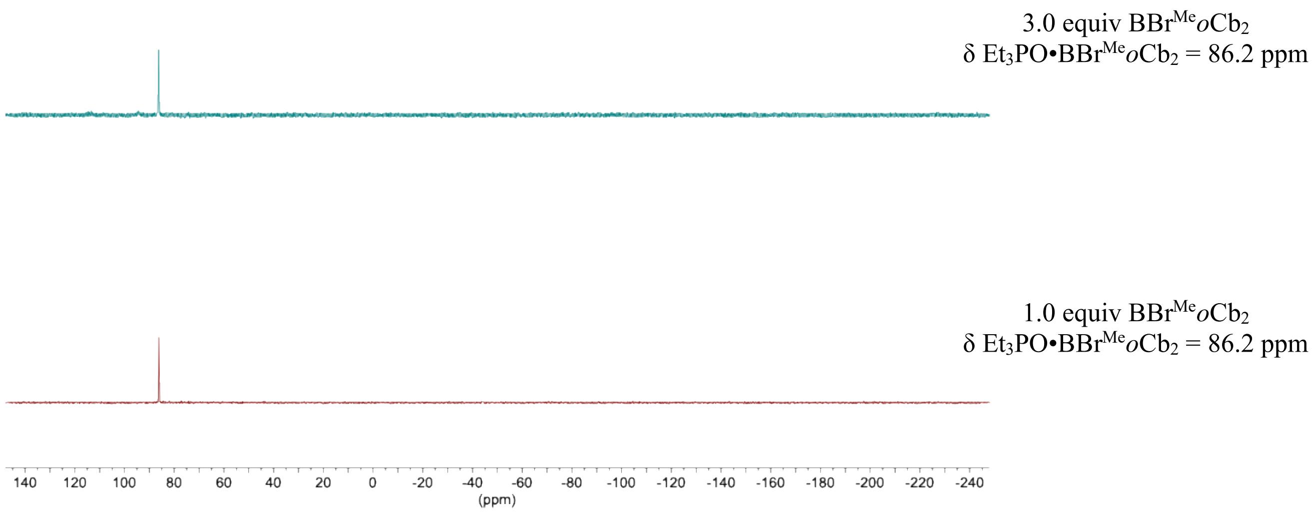


Figure S32: $^{31}P\{^{1}H\}$ NMR spectra of the Et_3PO•$BH^{Me}o$$Cb_2$ adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of $BH^{Me}o$$Cb_2$.

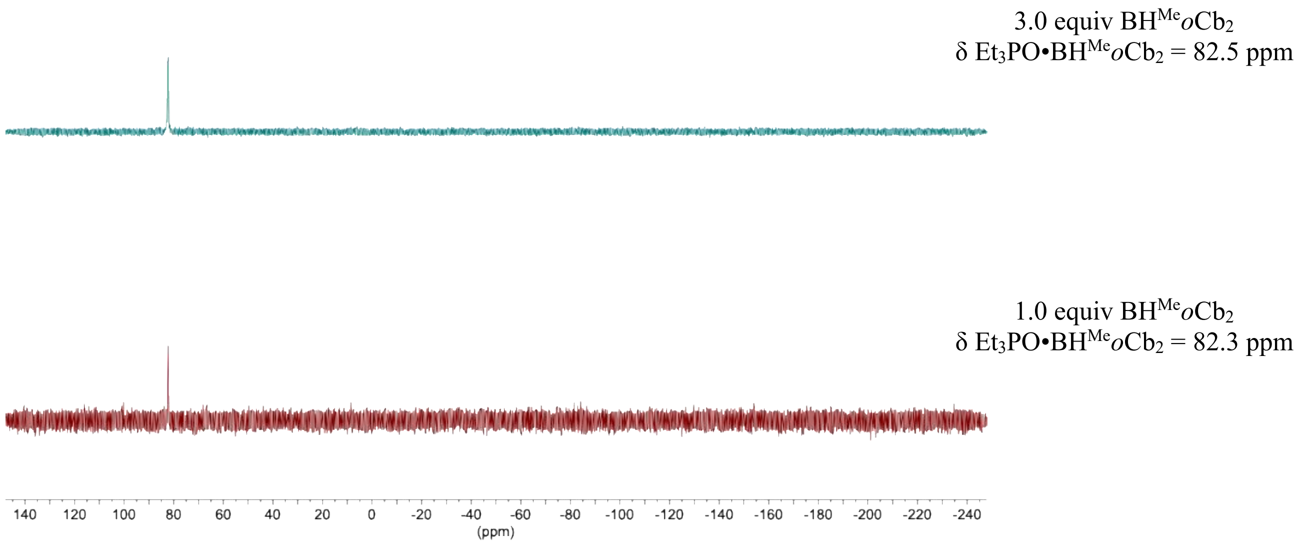


Figure S33: $^{31}P\{^{1}H\}$ NMR spectra of the Et_3PO•B*o*Cb_3 adduct in $CDCl_3$ (162 MHz) with 1 and 3 equivalents of B*o*Cb_3.

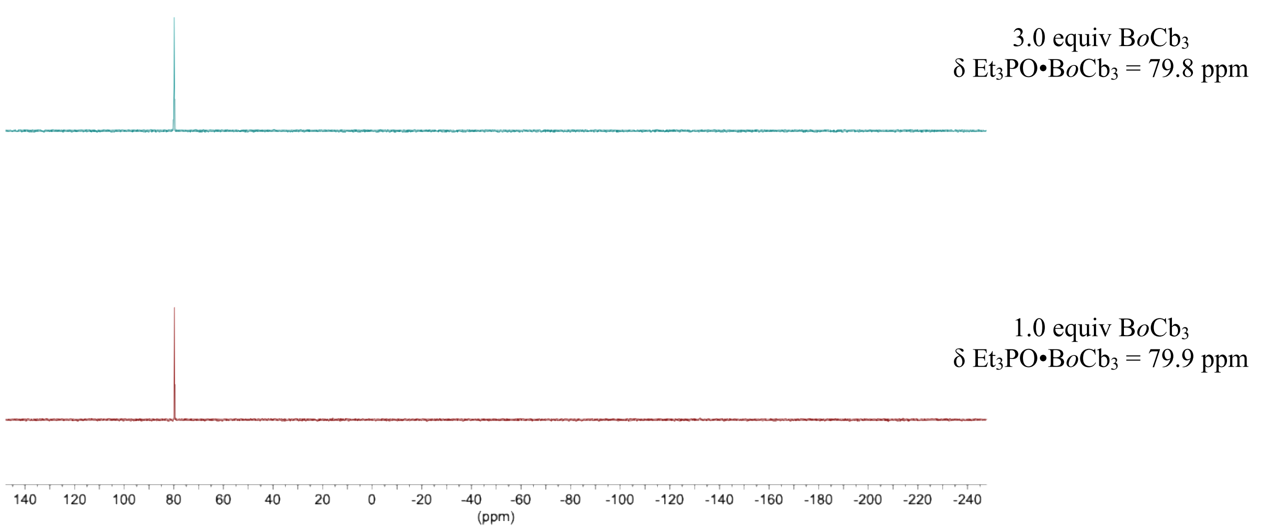


Figure S34: $^{11}B\{^{1}H\}$ NMR spectrum of the FBN•BBr_3 adduct in $CDCl_3$ (128 MHz) with 3 equivalents of BBr_3.

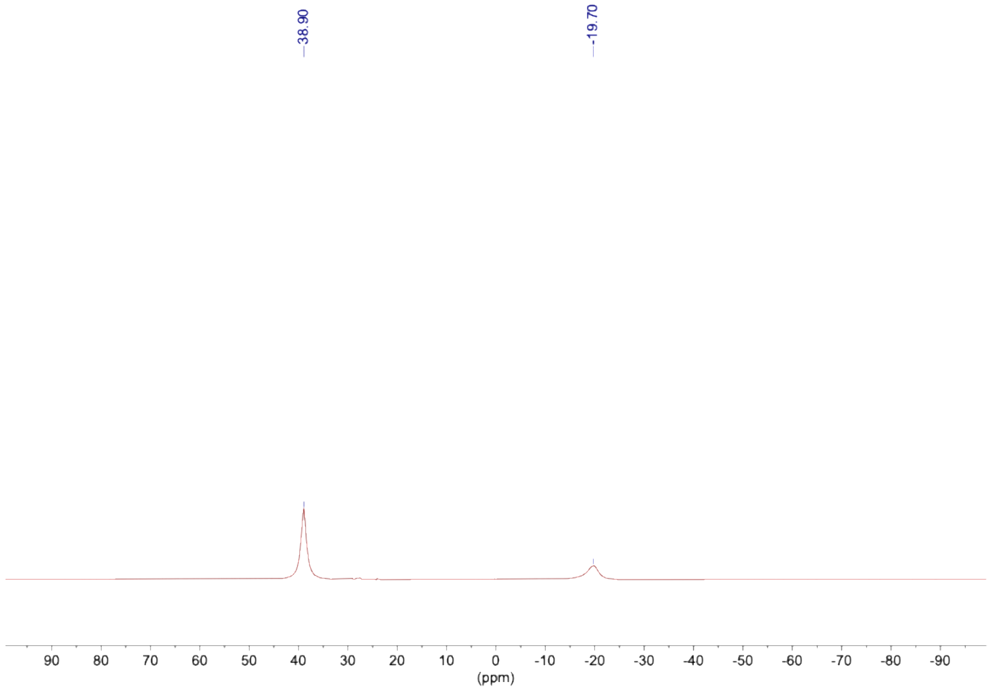


Figure S35: $^{11}B\{^{1}H\}$ NMR spectrum of the FBN•BCl_3 adduct in $CDCl_3$ (128 MHz) with 3 equivalents of BCl_3.

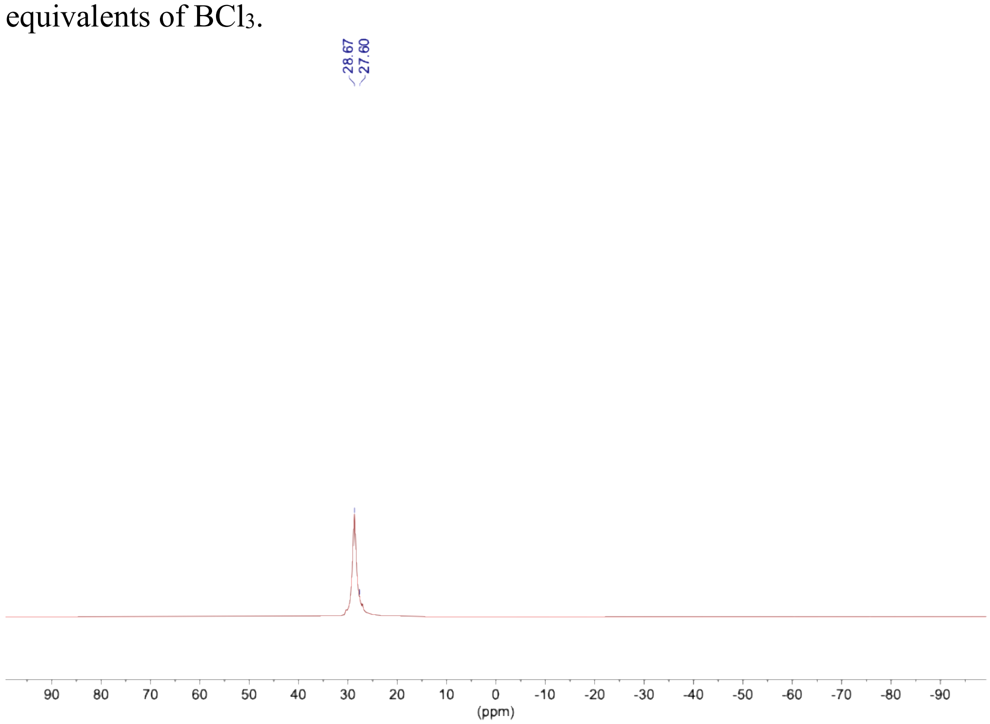


Figure S36: $^{11}B\{^1H\}$ NMR spectrum of the FBN•$BPhBr_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents of $BPhBr_2$.

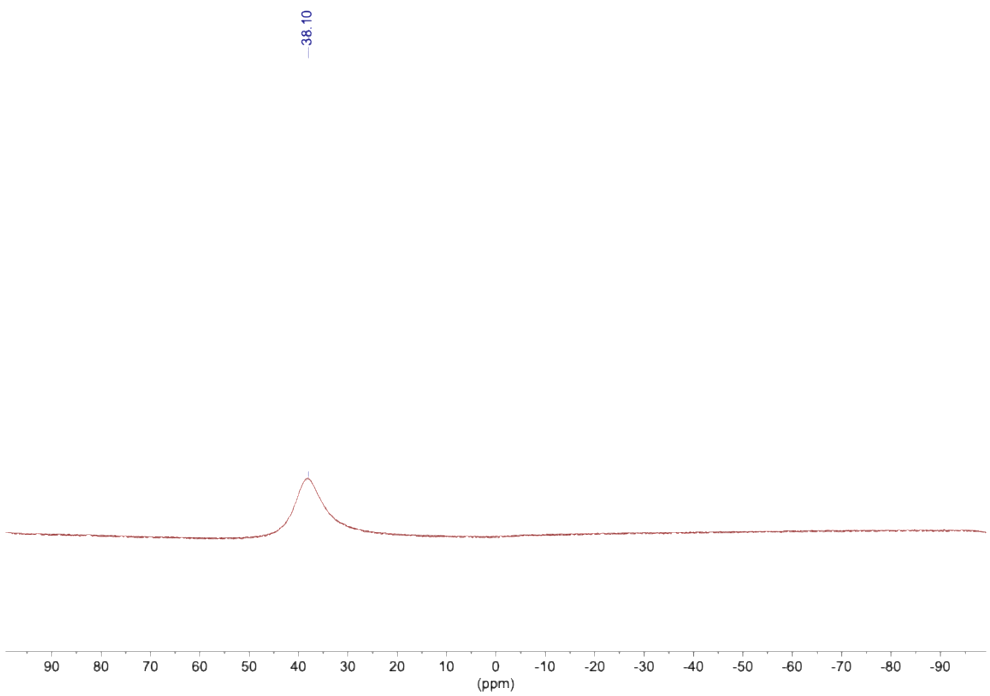


Figure S37: $^{11}B\{^1H\}$ NMR spectrum of the FBN•BPh_2Br adduct in $CDCl_3$ (128 MHz) with 3 equivalents of BPh_2Br.

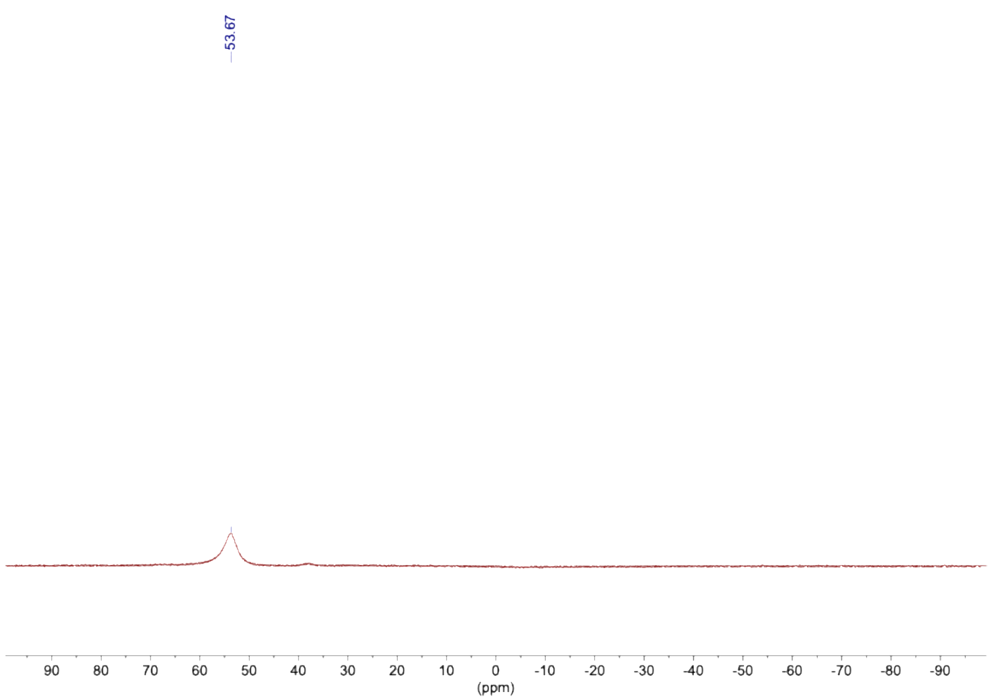


Figure S38: $^{11}B\{^{1}H\}$ NMR spectrum of the FBN•$BPhCl_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $BPhCl_2$.

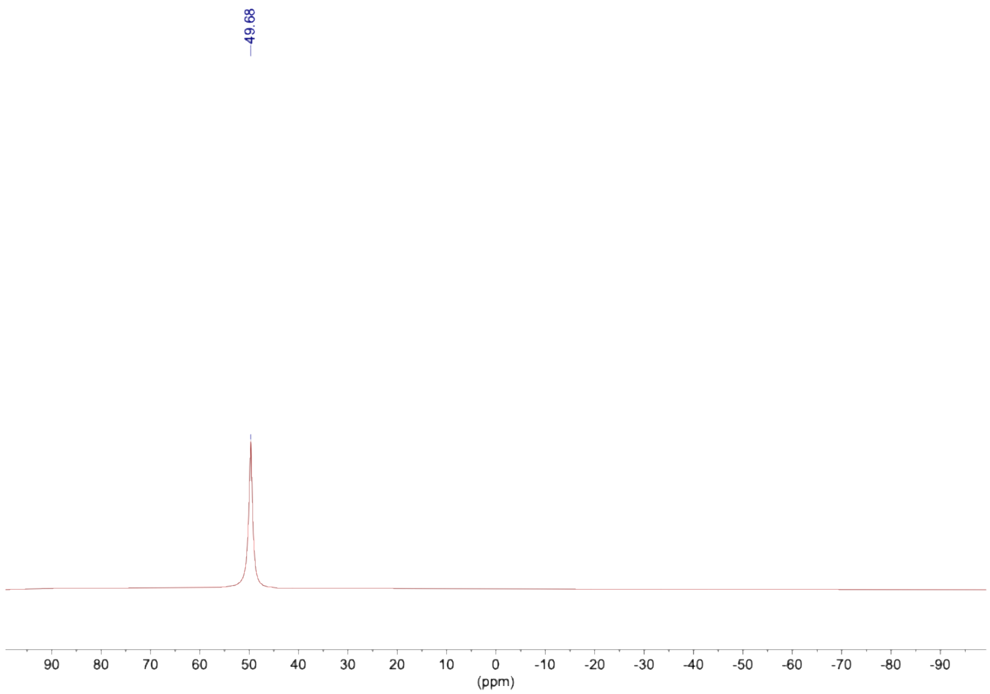


Figure S39: $^{11}B\{^{1}H\}$ NMR spectrum of the FBN•$BH(C_6F_5)_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $BH(C_6F_5)_2$.

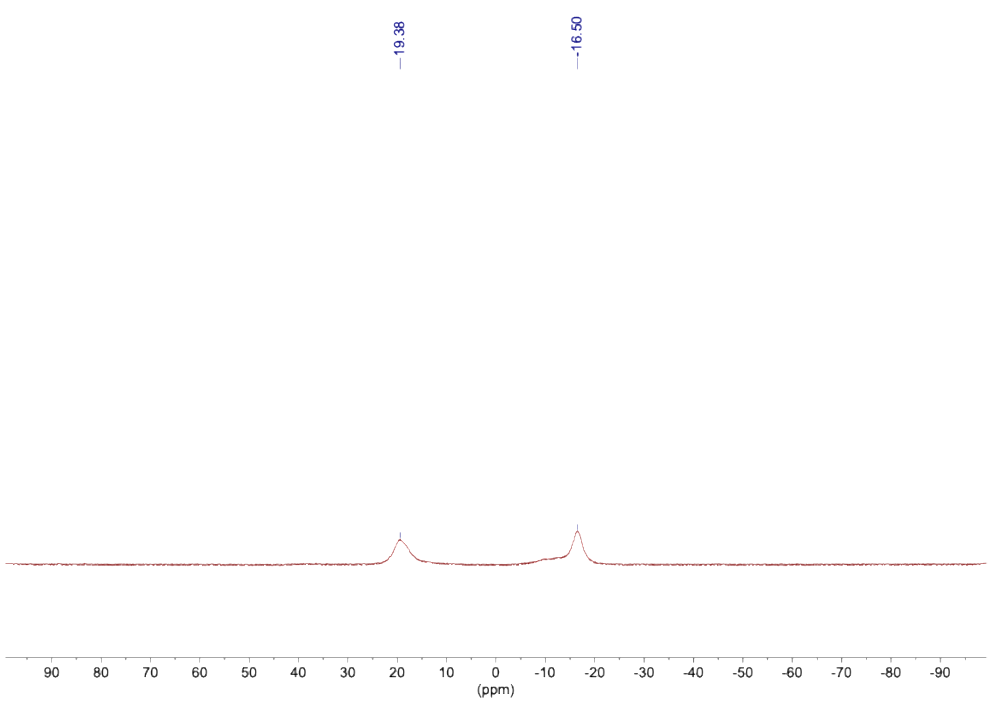


Figure S40: $^{11}B\{^1H\}$ NMR spectrum of the FBN•$B(C_6F_5)_3$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $B(C_6F_5)_3$.

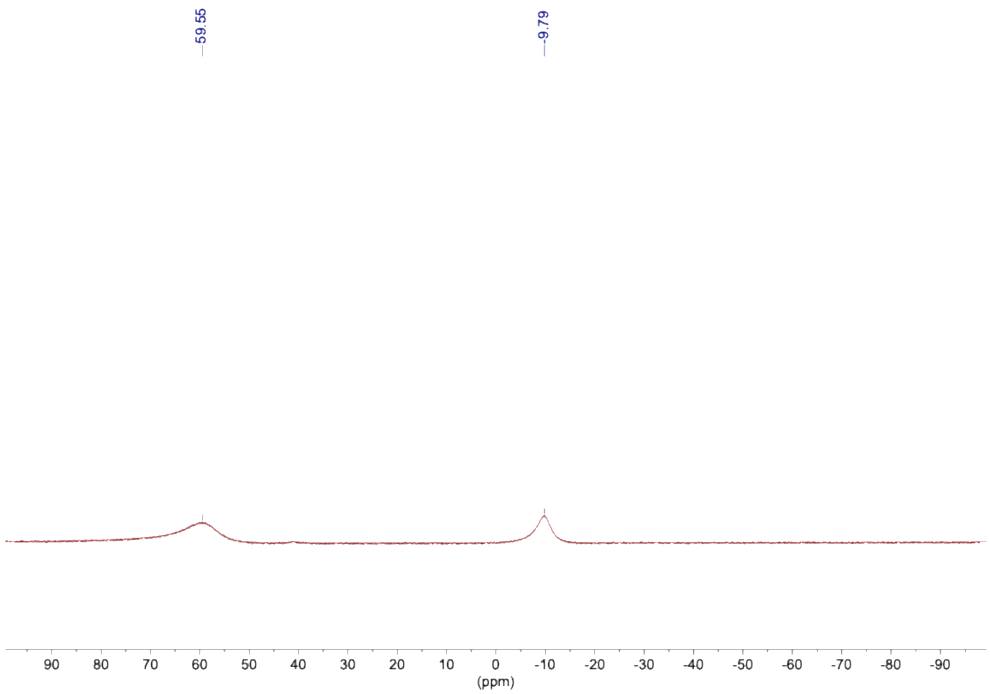


Figure S41: $^{11}B\{^1H\}$ NMR spectrum of the FBN•$BBr^{Ph}o Cb_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $BBr^{Ph}o Cb_2$.

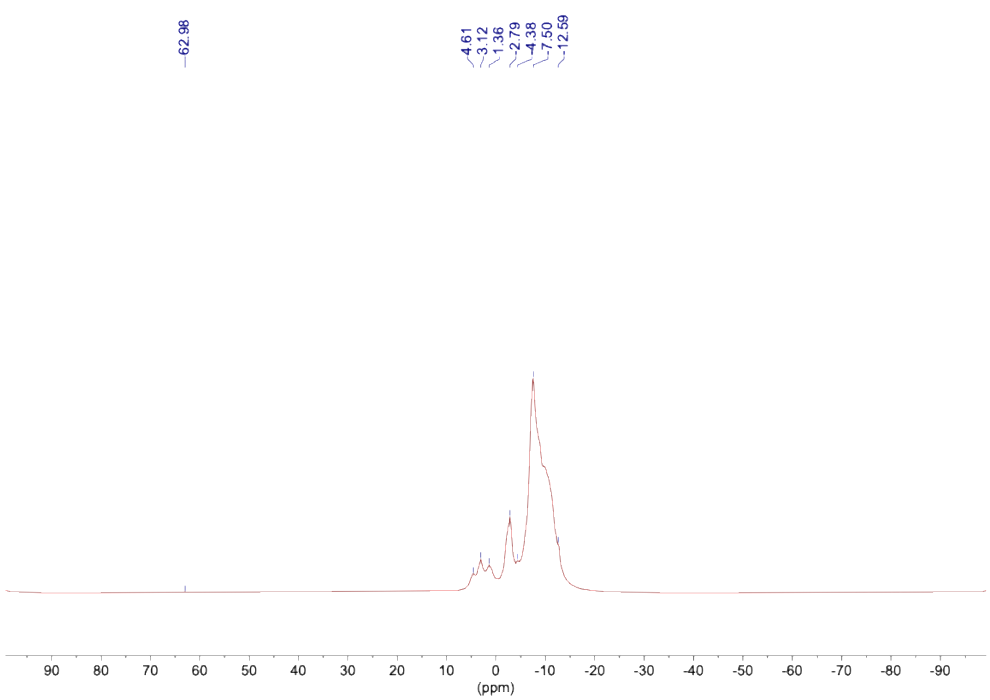


Figure S42: $^{11}B\{^{1}H\}$ NMR spectrum of the FBN•BBr^{Me}*o*Cb$_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents BBr^{Me}*o*Cb$_2$.

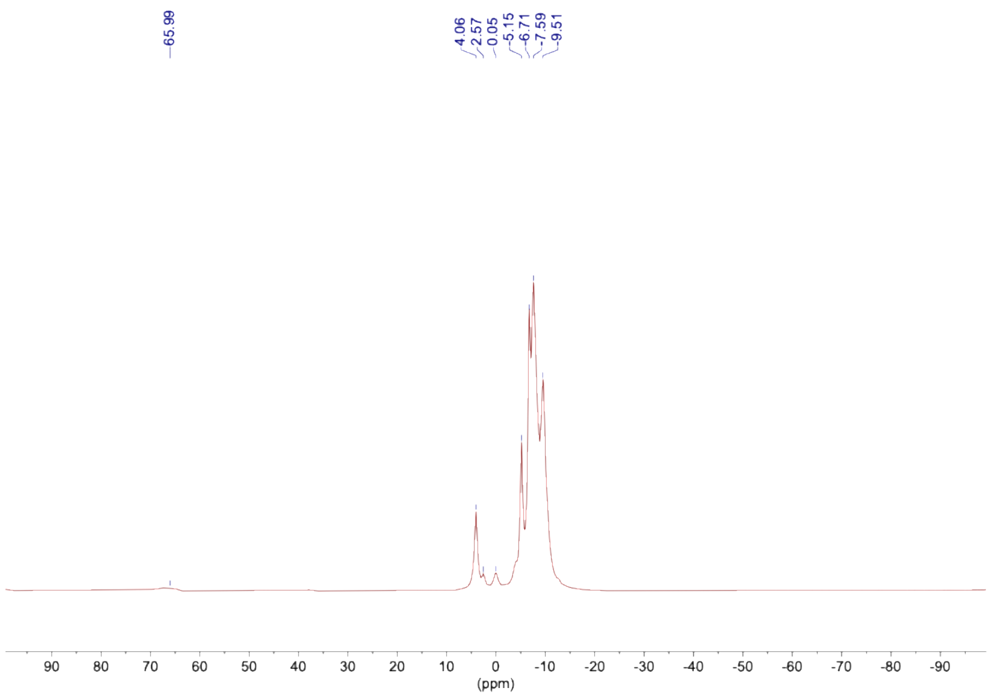


Figure S43: $^{11}B\{^{1}H\}$ NMR spectrum of the FBN•BH^{Me}*o*Cb$_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents BH^{Me}*o*Cb$_2$.

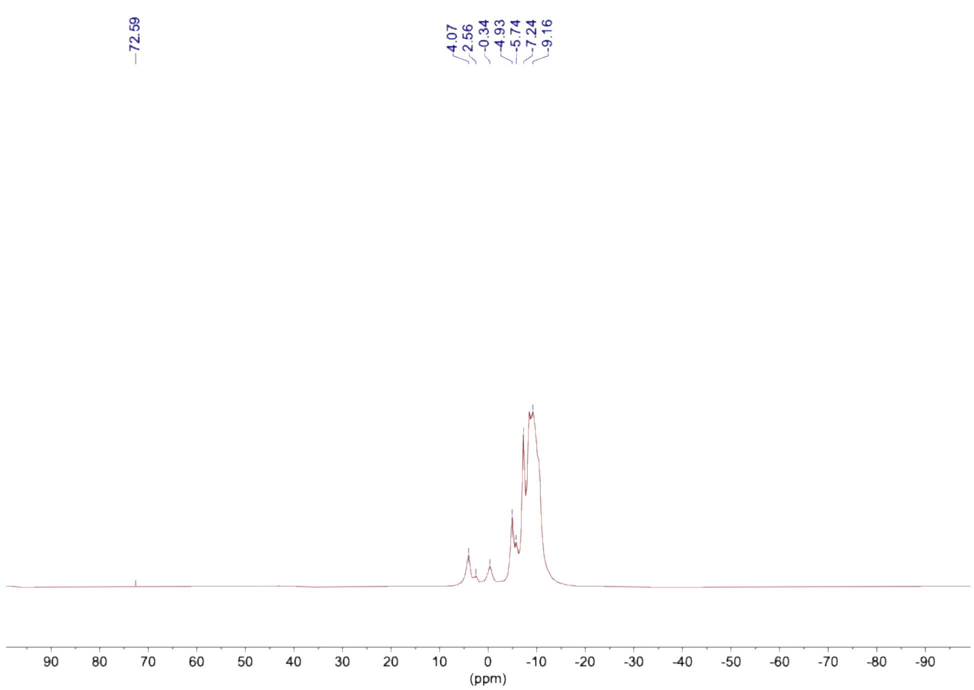


Figure S44: $^{11}B\{^{1}H\}$ NMR spectrum of the FBN•B*o*Cb_3 adduct in $CDCl_3$ (128 MHz) with 3 equivalents B*o*Cb_3.

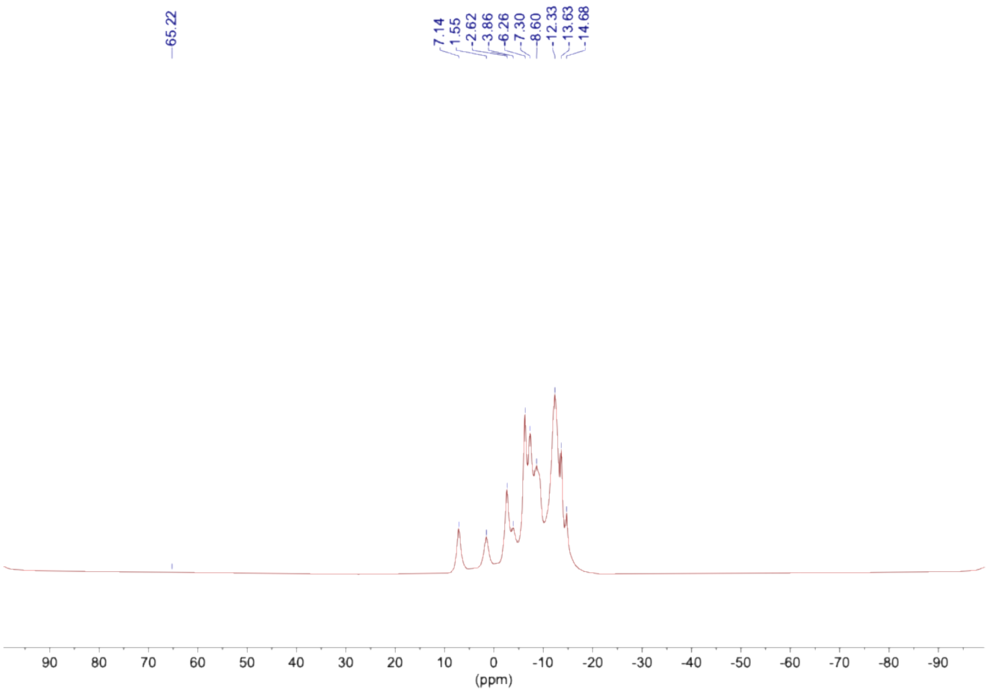


Figure S45: $^{11}B\{^{1}H\}$ NMR spectrum of the Et_3PO•BBr_3 adduct in $CDCl_3$ (128 MHz) with 3 equivalents of BBr_3.

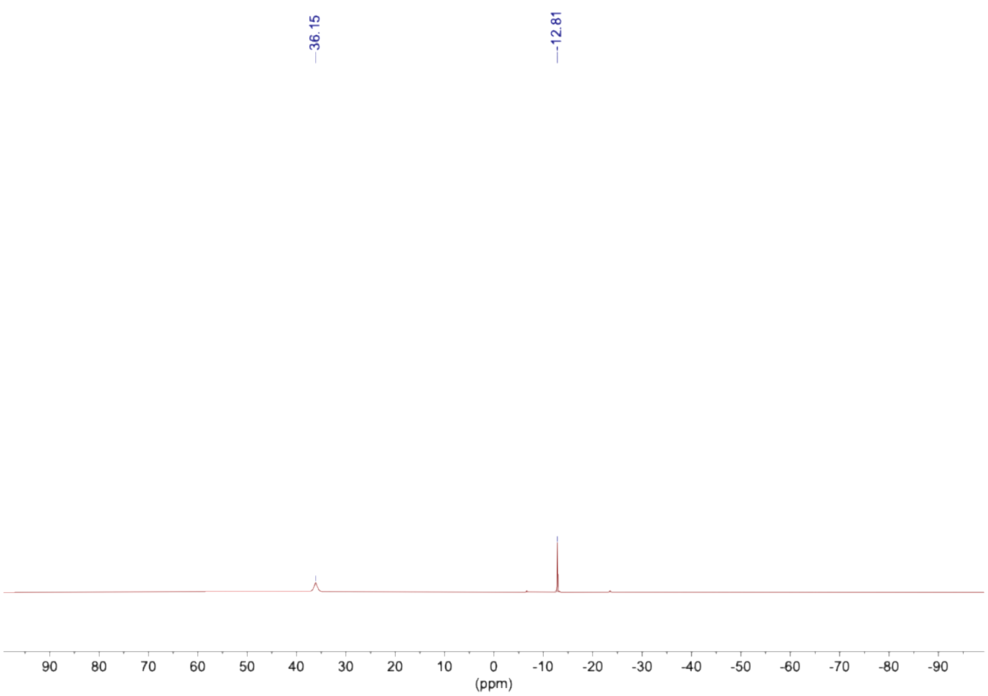


Figure S46: $^{11}B\{^{1}H\}$ NMR spectrum of the $Et_3PO{\bullet}BCl_3$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents of BCl_3.

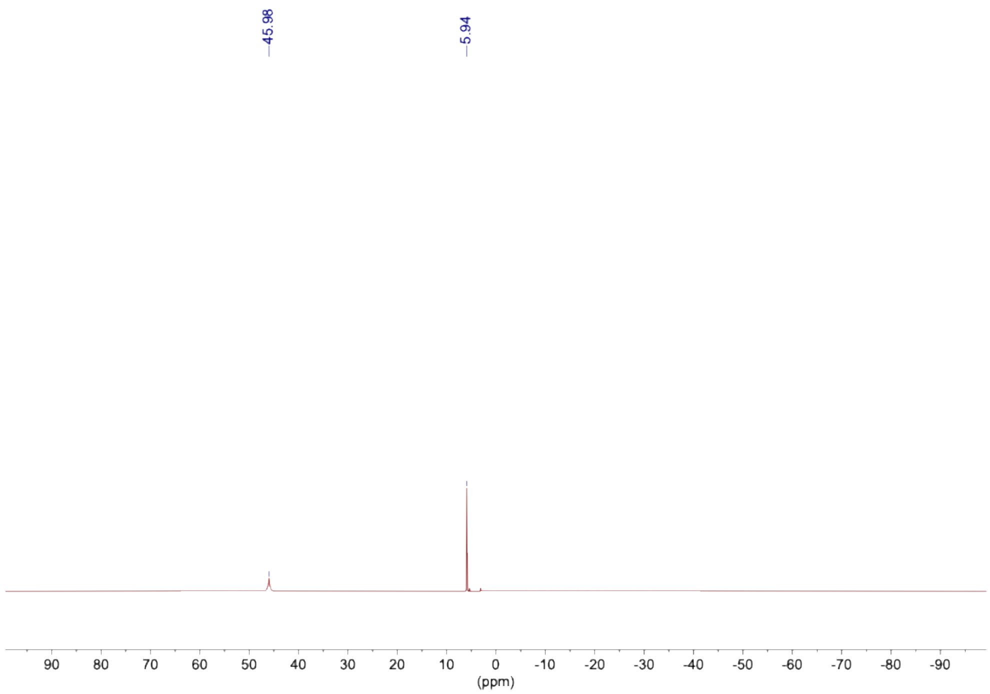


Figure S47: $^{11}B\{^{1}H\}$ NMR spectrum of Et_3PO with $Et_2O{\bullet}BF_3$ in $CDCl_3$ (128 MHz) with 3 equivalents of $Et_2O{\bullet}BF_3$.

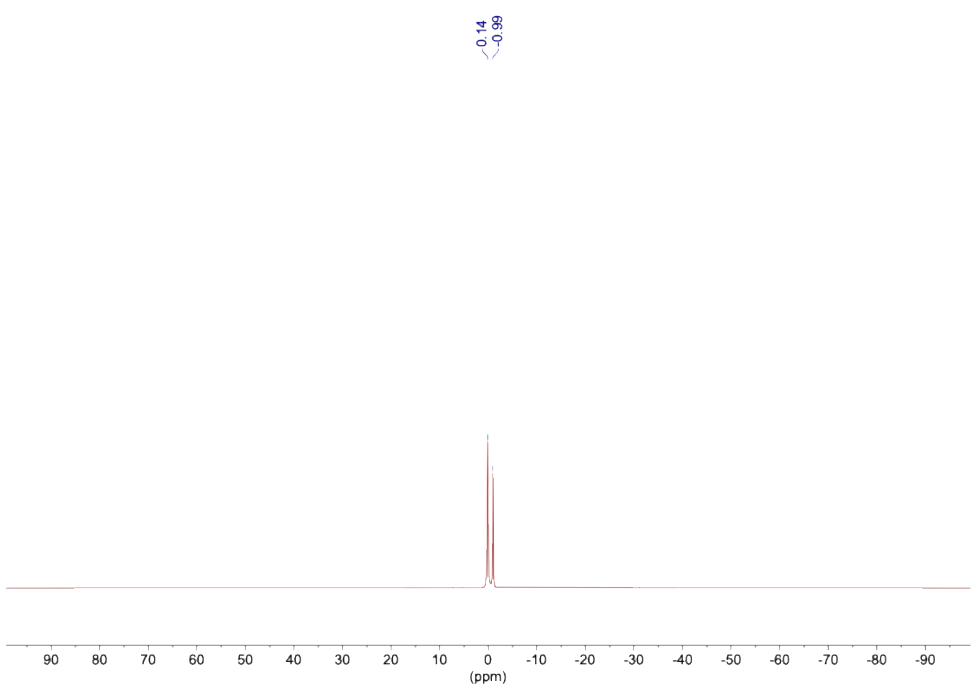


Figure S48: $^{11}B\{^{1}H\}$ NMR spectrum of the Et_3PO•$BPhBr_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents of $BPhBr_2$.

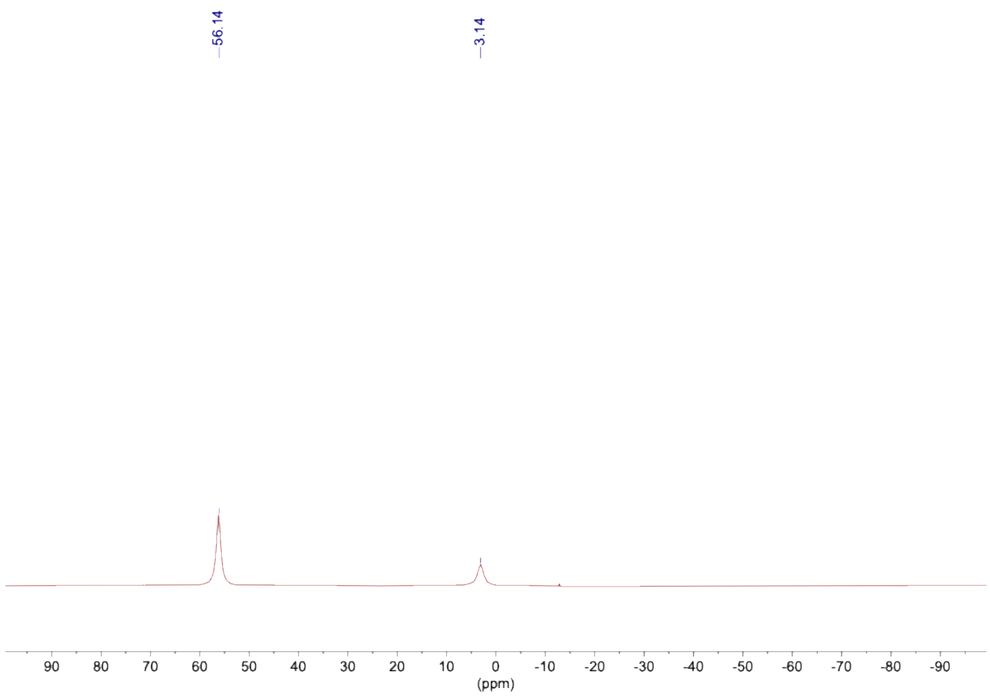


Figure S49: $^{11}B\{^{1}H\}$ NMR spectrum of the Et_3PO•BPh_2Br adduct in $CDCl_3$ (128 MHz) with 3 equivalents of BPh_2Br.

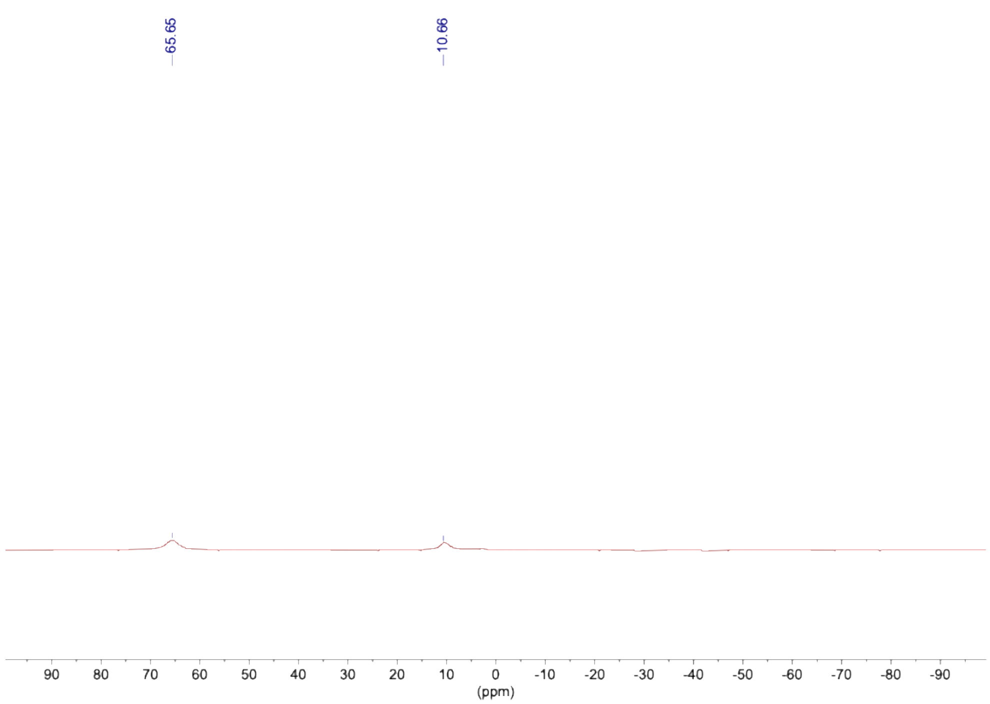


Figure S50: $^{11}B\{^1H\}$ NMR spectrum of the $Et_3PO{\bullet}BPh_3$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents of BPh_3.

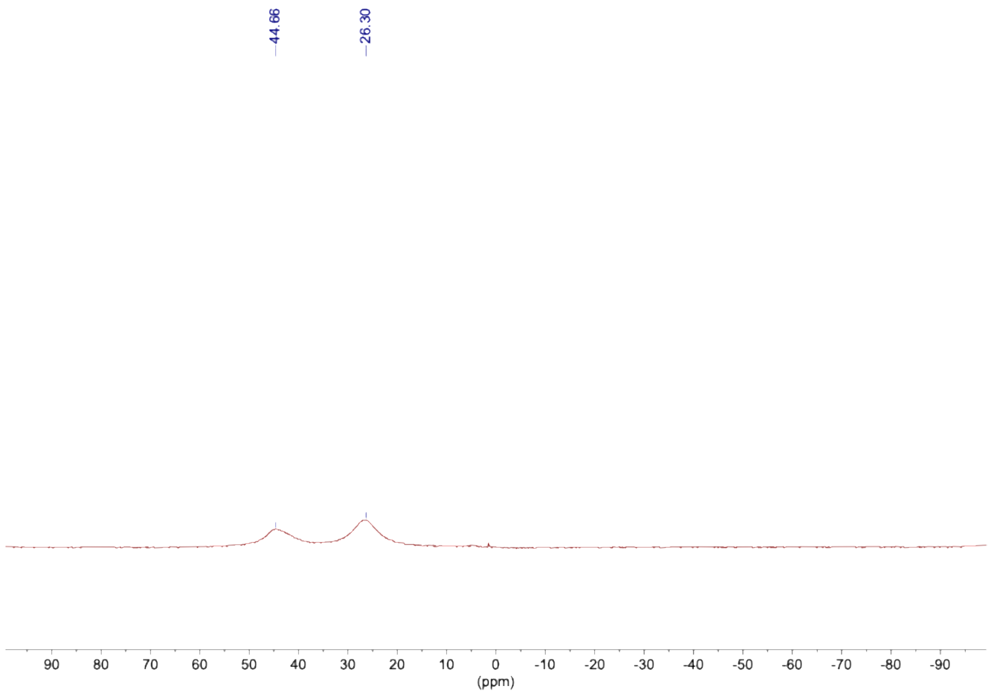


Figure S51: $^{11}B\{^1H\}$ NMR spectrum of the $Et_3PO{\bullet}BPhCl_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents of $BPhCl_2$.

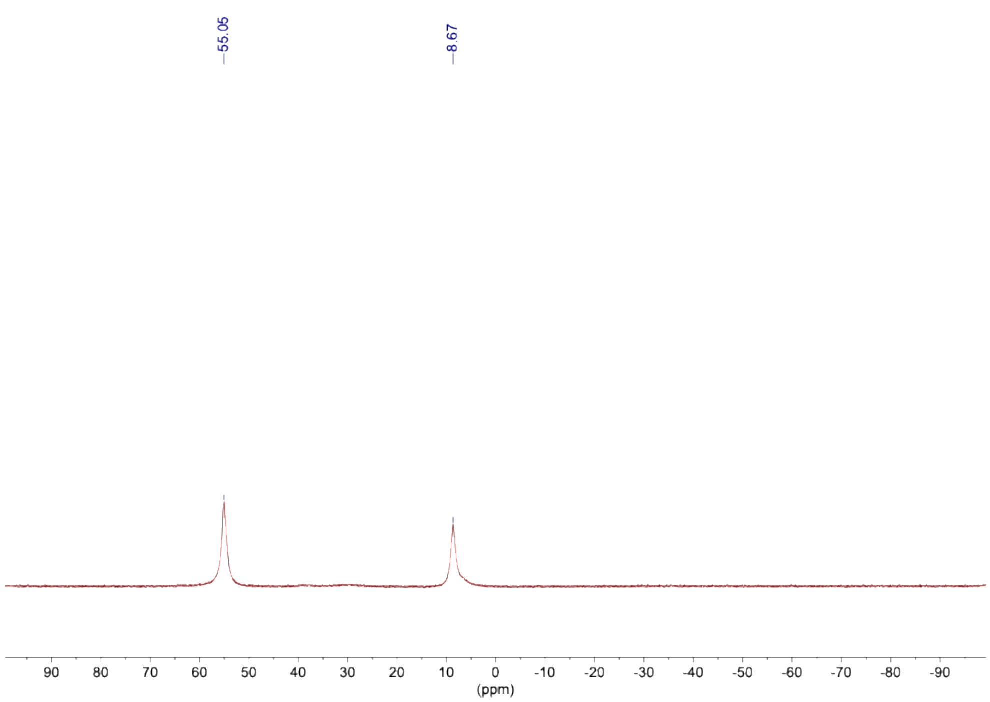


Figure S52: $^{11}B\{^{1}H\}$ NMR spectrum of the $Et_3PO{\bullet}BH(C_6F_5)_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $BH(C_6F_5)_2$.

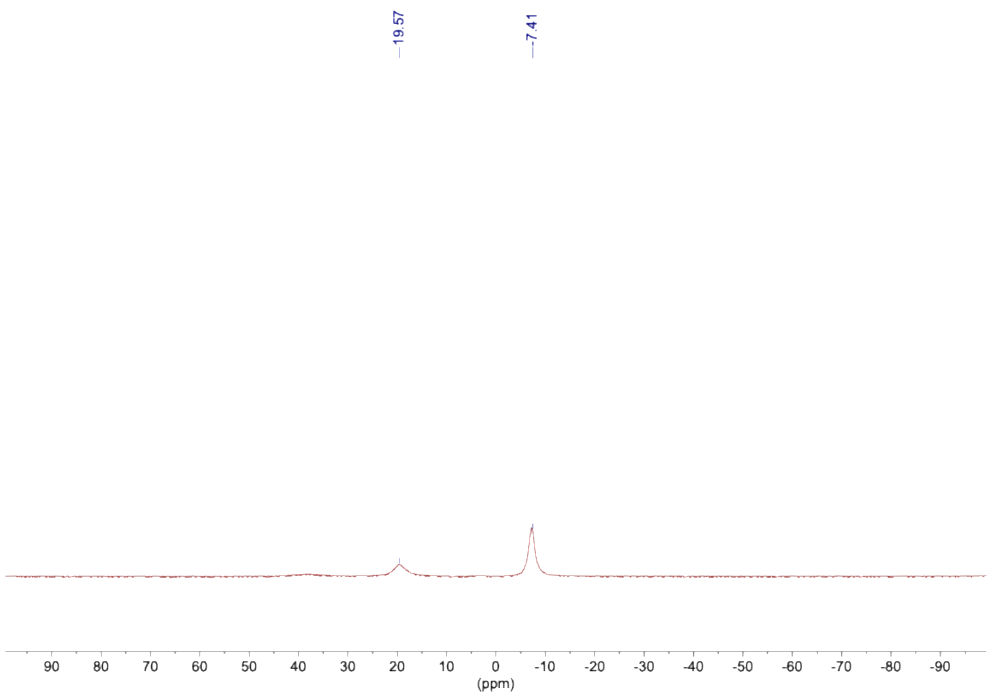


Figure S53: $^{11}B\{^{1}H\}$ NMR spectrum of the $Et_3PO{\bullet}B(C_6F_5)_3$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $B(C_6F_5)_3$.

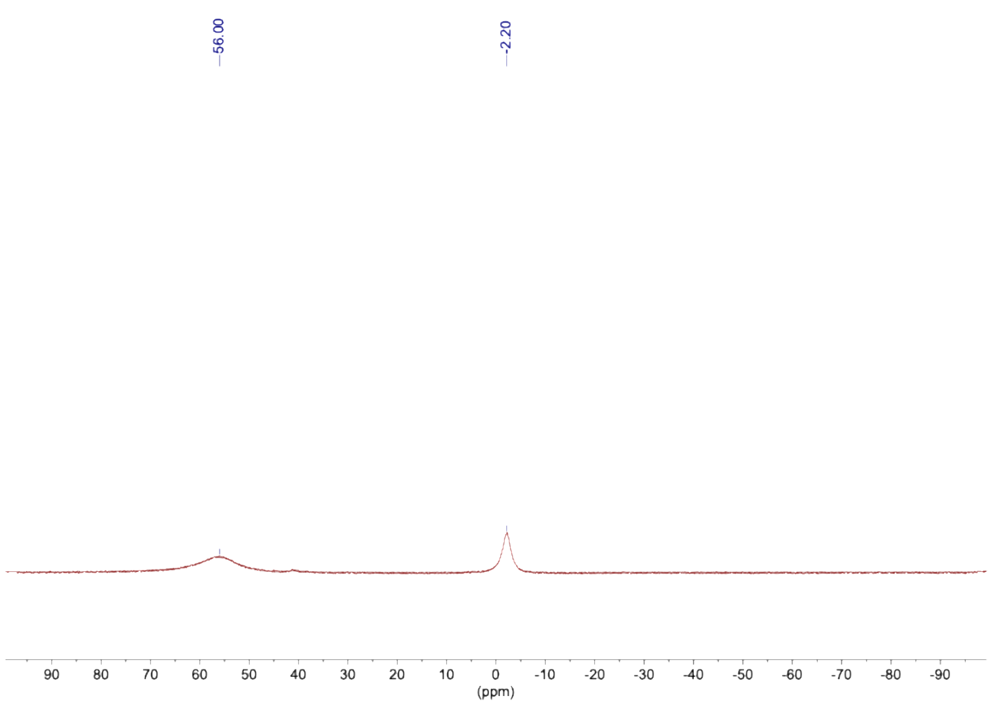


Figure S54: $^{11}B\{^{1}H\}$ NMR spectrum of the $Et_3PO•BBr^{Ph}oCb_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $BBr^{Ph}oCb_2$.

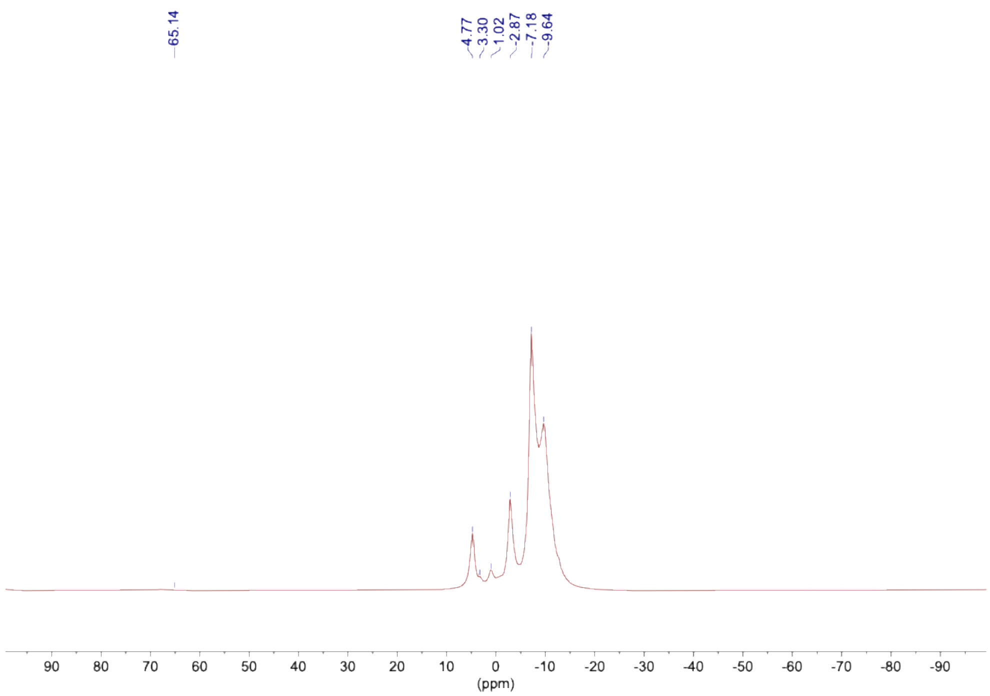


Figure S55: $^{11}B\{^{1}H\}$ NMR spectrum of the $Et_3PO•BBr^{Me}oCb_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $BBr^{Me}oCb_2$.

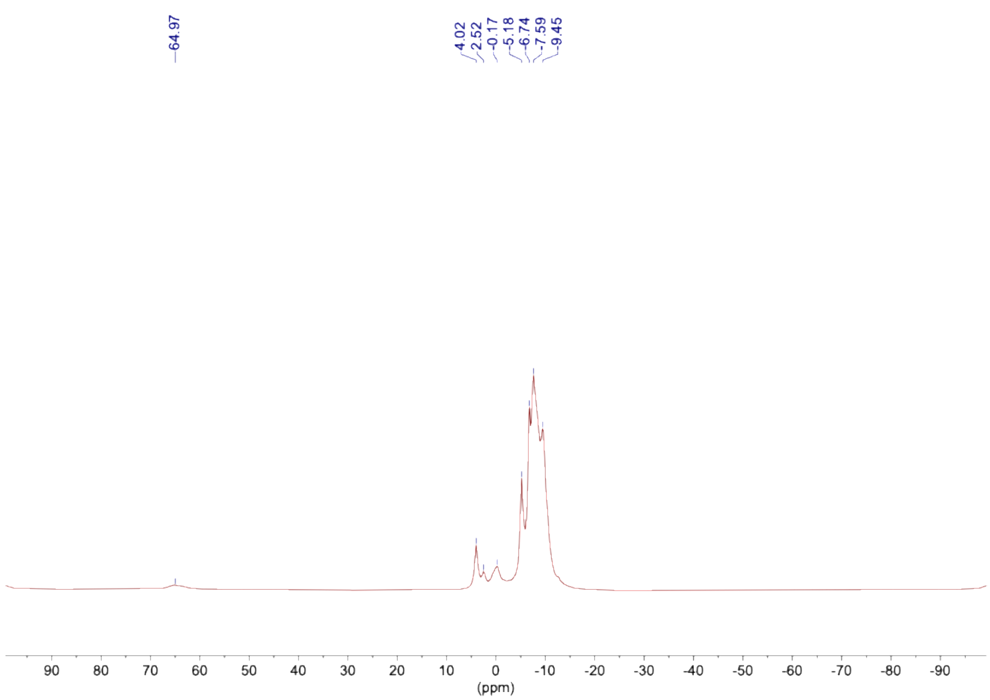


Figure S56: ${}^{11}B\{{}^{1}H\}$ NMR spectrum of the $Et_3PO{\bullet}BH^{Me}\textit{o}Cb_2$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $BH^{Me}\textit{o}Cb_2$.

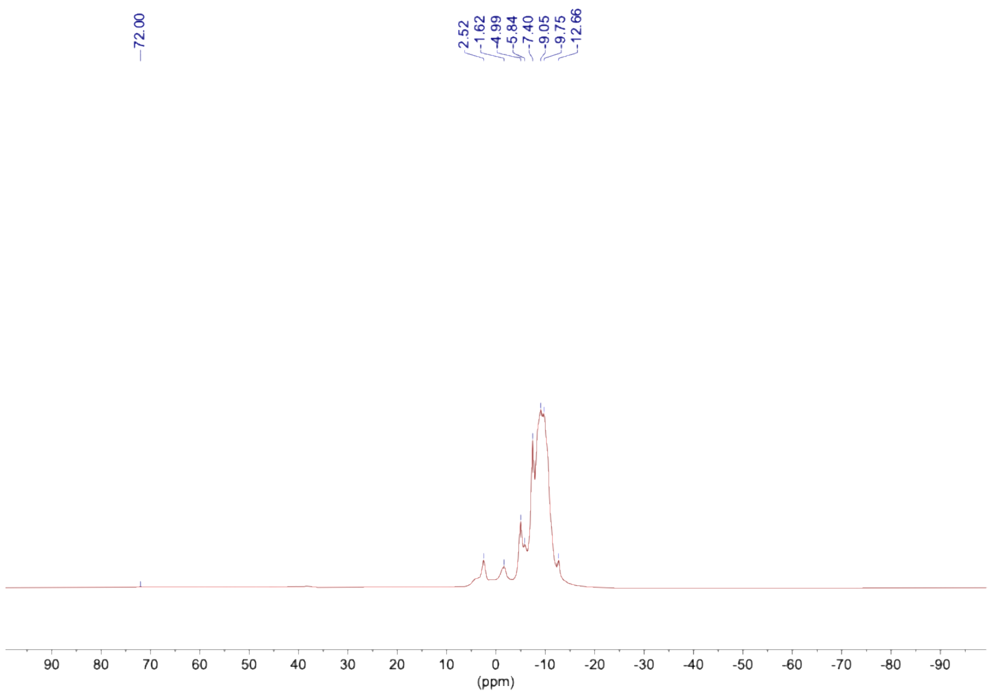
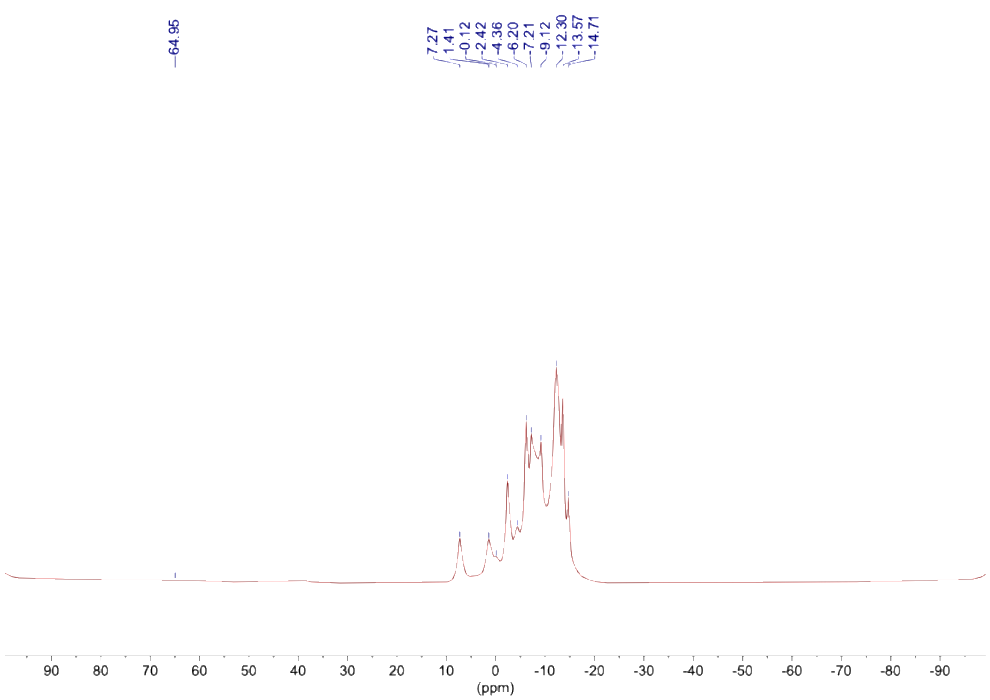


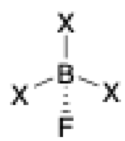
Figure S57: ${}^{11}B\{{}^{1}H\}$ NMR spectrum of the $Et_3PO{\bullet}B\textit{o}Cb_3$ adduct in $CDCl_3$ (128 MHz) with 3 equivalents $B\textit{o}Cb_3$.



4. Theoretical Calculations:

Calculations were performed using Gaussian 16.[7] Coordinates (gas phase calculations) and enthalpy/free energies are given for BPV86/SVP geometry optimizations and single point vibrational frequency calculations. Enthalpies are given for fluoride and each Lewis acid. The values for $HB^{Me}oCb_2$, $BrB^{Me}oCb_2$, $HB(C_6F_5)_2$, $B(C_6F_5)_3$ and $BoCb_3$, have been reported and were used.[1, 2] Fluoride and hydride affinities were calculated using Krossing's method, which uses an isodesmic comparison to the fluoride and hydride affinity of $[(CH_3)_3–Si]^+$.[8]

Percent buried volume values (% V_{Bur}) were obtained using the SambVca 2.1 routine for all Lewis acids below, using their Cartesian coordinates for their optimized geometries obtained using BPV86/SVP method.[9, 10] The values were obtained using the start orientation (below) looking down the z axis (B-F bond) and with the xy plane defined as the B-X3 plane of the molecule.



X - Substituted groups

BBr_3
Enthalpy: -7747.325412 Hartree

B	0.000000	0.000000	0.000000
Br	-0.000000	1.915714	0.000000
Br	1.659057	-0.957857	0.000000
Br	1.659057	-0.957857	0.000000

$F•BBr_3^–$
Enthalpy: -7847.243280 Hartree

B	0.000014	0.000125	0.515729
Br	-1.093788	1.616102	-0.186018
Br	1.947301	0.138473	-0.186242
Br	-0.853747	-1.754645	-0.185967
F	0.000900	0.000204	1.884366

BCl_3
Enthalpy: -1405.262034 Hartree

B	0.000000	0.000000	0.000000
Cl	0.000000	1.756188	0.000000

Cl -1.520903 -0.878094 0.000000
Cl 1.520903 -0.878094 0.000000

F•BCl$_3^-$
Enthalpy: -1505.165955 Hartree

B -0.000037 0.000029 0.315128
F 0.000179 -0.000067 1.693552
Cl -0.791950 1.602831 -0.329704
Cl -0.992226 -1.487189 -0.329739
Cl 1.784092 -0.115614 -0.329827

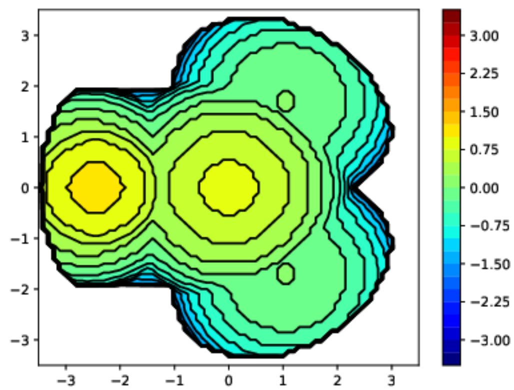
PhBBr$_2$
Enthalpy: -5404.571547 Hartree

C -3.932520 -0.000067 -0.000013
C -3.228539 -1.217602 -0.000239
C -1.827627 -1.215874 -0.000256
C -1.090618 -0.000042 0.000008
C -1.827650 1.215781 0.000295
C -3.228560 1.217482 0.000231
H -5.033769 -0.000076 -0.000040
H -3.777063 -2.172008 -0.000440
H -1.281803 -2.171860 -0.000408
H -1.281838 2.171778 0.000462
H -3.777104 2.171877 0.000415
B 0.463245 0.000014 -0.000005
Br 1.480769 -1.645369 0.000095
Br 1.480615 1.645430 -0.000099

F•BPhBr$_2^-$
Enthalpy: -5504.478274 Hartree

C -3.898773 -0.000063 -0.379047
C -2.947420 -0.000189 -1.418033
C -1.575941 -0.000175 -1.121101
C -1.102431 -0.000031 0.212817
C -3.454904 0.000075 0.953535
H -4.977367 -0.000074 -0.609555
H -3.282918 -0.000301 -2.469216
H -0.838352 -0.000281 -1.939933
H -1.733518 0.000193 2.285609
H -4.188369 0.000170 1.778266
B 0.462442 0.000008 0.599295
Br 0 1.382521 -1.708013 -0.237694
Br 1.382404 1.708054 -0.237809

F 0.696798 0.000065 1.964726

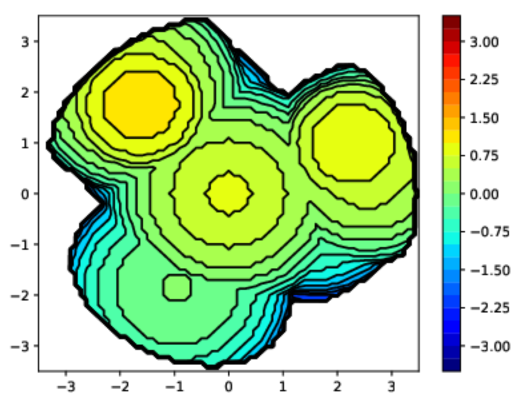


Ph_2BBr
Enthalpy: -3061.808864 Hartree

C	-3.897514	-1.666223	0.130088
C	-3.799177	-0.394220	-0.464649
C	-2.564780	0.269584	-0.501270
C	-1.386954	-0.325310	0.026847
C	-1.514363	-1.613023	0.617960
C	-2.753398	-2.270829	0.679752
H	-4.868988	-2.183917	0.169580
H	-4.693322	0.084081	-0.894197
H	-2.501068	1.272959	-0.951000
H	-0.628614	-2.096980	1.058321
H	-2.827234	-3.259835	1.158509
B	0.000012	0.395499	0.000410
Br	0.000047	2.354107	-0.000056
C	1.386966	-0.325342	-0.026435
C	1.514158	-1.613006	-0.617715
C	2.564949	0.269446	0.501435
C	2.753145	-2.270858	-0.679898
H	0.628259	-2.096877	-1.057867
C	3.799306	-0.394417	0.464437
H	2.501398	1.272783	0.951272
C	3.897429	-1.666356	-0.130465
H	2.826834	-3.259811	-1.158788
H	4.693580	0.083786	0.893828
H	4.868869	-2.184093	-0.170269

$F{\bullet}BPh_2Br^-$
Enthalpy: -3161.705532 Hartree

C	-3.837765	-1.665921	-0.375284
C	-3.199929	-0.860146	-1.335828
C	-2.009017	-0.184489	-1.016362
C	-1.403922	-0.291844	0.259074
C	-2.072854	-1.103809	1.208210
C	-3.268209	-1.779852	0.905011
H	-4.775001	-2.193405	-0.620170
H	-3.642428	-0.748757	-2.340681
H	-1.541221	0.479897	-1.761875
H	-1.639502	-1.193966	2.217909
H	-3.762260	-2.398935	1.673802
B	0.009282	0.397046	0.680727
Br	0.123828	2.339940	-0.291226
C	1.332003	-0.414855	0.187015
C	1.509235	-0.899748	-1.131289
C	2.372502	-0.688903	1.106633
C	2.660200	-1.606443	-1.516971
H	0.720660	-0.712997	-1.878840
C	3.531569	-1.394178	0.734734
H	2.256900	-0.329656	2.142104
C	3.683033	-1.858288	-0.583160
H	2.762919	-1.967006	-2.554913
H	4.323936	-1.585090	1.479277
H	4.588598	-2.412780	-0.881598
F	0.060659	0.630049	2.073728



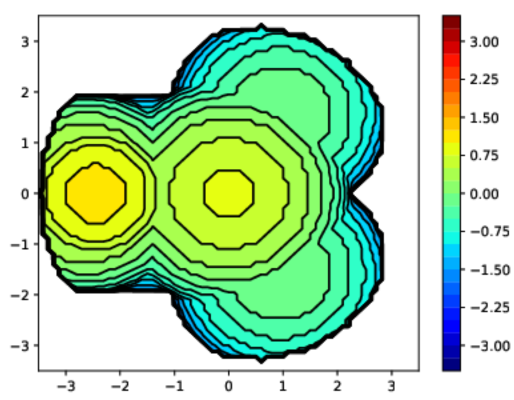
$PhBCl_2$
Enthalpy: -1176.538961 Hartree

C	0.000000228	-0.000000002	-0.000000080
C	0.000000249	-0.000000307	0.000000063
C	0.000000761	-0.000000000	0.000000056
C	-0.000000426	-0.000000002	-0.000000102

C	0.000000248	0.000000309	0.000000138
H	-0.000000298	-0.000000000	0.000000006
H	-0.000000129	0.000000119	-0.000000009
H	0.000000162	-0.000000130	-0.000000008
H	0.000000162	0.000000130	0.000000019
H	-0.000000130	-0.000000119	-0.000000040
B	-0.000000865	0.000000000	-0.000000026
Cl	0.000000231	0.000000264	0.000000007
Cl	0.000000231	-0.000000264	0.000000009

F•BPhCl$_2^–$
Enthalpy: -1276.435622 Hartree

C	-3.341047	-0.231161	0.002270
C	-2.474799	-1.342036	0.012246
C	-1.083602	-1.153715	0.010313
C	-0.504292	0.137671	-0.001524
C	-1.394936	1.235375	-0.011401
C	-2.792053	1.062027	-0.009597
H	-4.434742	-0.375346	0.003736
H	-2.893287	-2.363435	0.021572
H	-0.413357	-2.028811	0.018085
H	-0.967137	2.251300	-0.020757
H	-3.458348	1.942316	-0.017526
B	1.097598	0.383214	-0.003906
Cl	1.863748	-0.432361	1.565138
Cl	1.864113	-0.464240	-1.555745
F	1.427737	1.739019	-0.017678



BrB^{Ph}*o*Cb$_2$
Enthalpy: -3722.743 Hartree

B	-0.000000	0.000000	0.669511

B	1.441331 0.990239 -1.677033
H	1.164540 0.008031 -2.298261
B	0.262347 2.221390 -1.154355
H	-0.894452 2.080547 -1.444784
B	0.730891 2.745890 0.482877
H	-0.097195 2.954578 1.331559
B	2.193803 1.841257 0.937368
H	2.382854 1.440357 2.047827
B	3.510710 2.297696 -0.162965
H	4.641331 2.166400 0.230916
B	2.337509 3.521347 0.381535
H	2.654108 4.382006 1.166213
B	1.135885 3.759304 -0.928623
H	0.569191 4.810660 -1.106275
B	1.574755 2.659282 -2.279833
H	1.343468 2.894430 -3.440853
B	3.038776 1.768102 -1.797415
H	3.848154 1.290634 -2.549705
B	2.852225 3.483173 -1.332680
H	3.568378 4.327716 -1.814165
B	-1.441330 -0.990240 -1.677033
H	-1.164539 -0.008031 -2.298261
B	-0.262346 -2.221390 -1.154355
H	0.894453 -2.080547 -1.444783
B	-0.730890 -2.745889 0.482877
H	0.097196 -2.954577 1.331560
B	-2.193803 -1.841257 0.937368
H	-2.382854 -1.440357 2.047827
B	-3.510709 -2.297697 -0.162965
H	-4.641330 -2.166401 0.230915
B	-3.038776 -1.768103 -1.797415
H	-3.848153 -1.290635 -2.549705
B	-1.574754 -2.659283 -2.279832
H	-1.343467 -2.894431 -3.440852
B	-1.135884 -3.759305 -0.928622
H	-0.569190 -4.810661 -1.106273
B	-2.337509 -3.521347 0.381536
H	-2.654107 -4.382006 1.166214
B	-2.852224 -3.483174 -1.332680
H	-3.568376 -4.327718 -1.814165
Br	-0.000001 0.000001 2.591857
C	0.939085 1.112440 -0.030105
C	2.620448 0.847185 -0.409958
C	-0.939084 -1.112440 -0.030104
C	-2.620447 -0.847185 -0.409959
C	3.247369 -0.508390 -0.174540

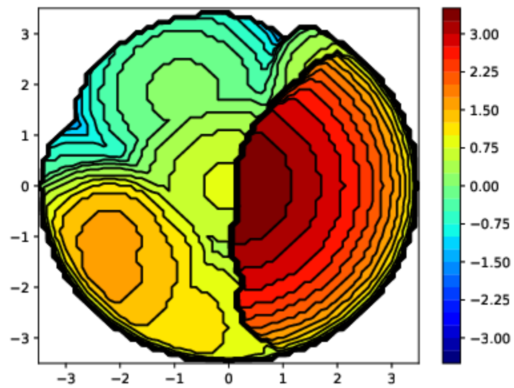
C 3.591908 -0.948537 1.122171
H 3.386935 -0.308577 1.989923
C 4.208461 -2.194901 1.312499
H 4.467813 -2.519706 2.331414
C 4.499413 -3.017820 0.213120
H 4.984781 -3.993871 0.364274
C 4.169944 -2.584538 -1.081466
H 4.395844 -3.218065 -1.952259
C 3.547227 -1.343165 -1.274775
H 3.298066 -1.015989 -2.293134
C -3.247369 0.508389 -0.174541
C -3.547227 1.343165 -1.274776
H -3.298065 1.015988 -2.293135
C -4.169944 2.584537 -1.081467
H -4.395844 3.218065 -1.952260
C -4.499414 3.017819 0.213119
H -4.984783 3.993870 0.364272
C -4.208463 2.194900 1.312498
H -4.467815 2.519706 2.331413
C -3.591909 0.948536 1.122170
H -3.386937 0.308576 1.989922

F•BBr^{Ph}*o*Cb$_2^-$
Enthalpy: -3822.692 Hartree

B 1.568056 0.754640 -1.695838
H 1.324818 -0.279976 -2.247065
B 0.352096 2.007215 -1.349127
H -0.784335 1.837224 -1.691560
B 0.748638 2.708073 0.221298
H -0.098774 3.028354 1.008065
B 2.194084 1.853426 0.811502
H 2.356673 1.558268 1.963370
B 3.551865 2.262021 -0.286216
H 4.677643 2.210993 0.145993
B 2.341001 3.494036 0.101430
H 2.619668 4.441073 0.802136
B 1.191482 3.581996 -1.268672
H 0.614213 4.602526 -1.572637
B 1.685535 2.359914 -2.480556
H 1.485595 2.475176 -3.668965
B 3.152632 1.566792 -1.877203
H 3.997034 1.031767 -2.553068
B 2.918009 3.309765 -1.587081
H 3.637368 4.121388 -2.127255
B -1.415276 -1.157456 -1.642761

H	-1.053109 -0.230540 -2.304060
B	-0.346115 -2.443777 -1.050030
H	0.824671 -2.402305 -1.321067
B	-0.896968 -2.890964 0.572632
H	-0.127669 -3.168278 1.452451
B	-2.294657 -1.873153 0.957564
H	-2.502960 -1.440067 2.053128
B	-3.609191 -2.283442 -0.178795
H	-4.746738 -2.067438 0.162295
B	-3.055784 -1.837187 -1.806629
H	-3.814220 -1.324847 -2.592551
B	-1.641414 -2.832088 -2.212166
H	-1.389849 -3.115111 -3.362073
B	-1.327540 -3.918472 -0.824561
H	-0.832710 -5.015939 -0.959008
B	-2.543714 -3.559989 0.436714
H	-2.948496 -4.378960 1.231272
B	-3.005395 -3.540961 -1.293191
H	-3.769145 -4.348089 -1.776337
Br	-0.687789 0.675153 2.472441
C	0.962021 1.028125 -0.092779
C	2.718048 0.779523 -0.425512
C	-0.958508 -1.245599 0.024436
C	-2.604834 -0.904706 -0.427414
C	3.467908 -0.484674 -0.066231
C	4.127563 -0.603152 1.175343
H	4.022665 0.196694 1.920084
C	4.901009 -1.733780 1.470943
H	5.400368 -1.807211 2.449620
C	5.033241 -2.769668 0.531009
H	5.636490 -3.660604 0.765945
C	4.387007 -2.658227 -0.709862
H	4.479214 -3.460899 -1.457757
C	3.614092 -1.525142 -1.006817
H	3.118576 -1.447041 -1.983398
C	-3.232584 0.465178 -0.274876
C	-3.367021 1.313614 -1.394989
H	-2.960752 0.999261 -2.365346
C	-4.023921 2.548679 -1.287357
H	-4.109620 3.195225 -2.174211
C	-4.563149 2.957532 -0.057331
H	-5.074975 3.928837 0.029439
C	-4.442742 2.117185 1.060779
H	-4.858389 2.424746 2.032728
C	-3.784653 0.882857 0.954433
H	-3.692564 0.235389 1.834751

F 1.170744 -1.061231 1.254508
B 0 0.173524 -0.205463 0.778969



BBr^{Me}*o*Cb$_2$
Enthalpy: -3339.639166 Hartree

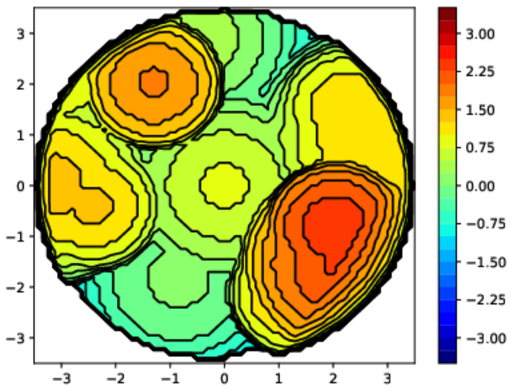
C	1.409438	-0.172749	-0.167800
C	2.683299	0.456612	0.790475
C	2.467324	1.686067	1.662867
H	1.486581	1.666241	2.173062
H	2.544264	2.618784	1.077082
H	3.249927	1.696062	2.443988
C	-1.483324	-0.070866	-0.180173
C	-1.816929	0.547749	2.493683
H	-0.934217	-0.024404	2.835010
H	-2.572844	0.519202	3.300038
H	-1.531779	1.604752	2.335056
C	-2.416207	-0.058698	1.232548
B	1.560195	-1.897982	-0.246757
H	0.567915	-2.557700	-0.320558
B	-1.856397	-1.470096	-1.121533
H	-0.980089	-1.947494	-1.788004
B	-3.571992	-1.317023	-1.571510
H	-3.964223	-1.770667	-2.619099
B	-4.188863	0.228173	-0.903764
H	-5.024791	0.907576	-1.447830
B	-0.010010	0.586475	-0.248320
B	3.658210	-0.818401	1.391990
H	4.119124	-0.666140	2.495379
B	4.199843	0.202949	0.039083
H	5.032724	1.057717	0.209375
B	1.889875	-1.013077	1.261880
H	1.166855	-0.966713	2.222428

B	-3.090580	-2.365829	-0.193574
H	-3.134481	-3.571281	-0.218872
B	3.100150	-2.228767	-1.061118
H	3.220109	-3.210020	-1.753461
B	4.410179	-1.569896	-0.043627
H	5.512245	-2.058212	0.022110
B	2.071546	-0.861876	-1.603792
H	1.414472	-0.778835	-2.610671
B	2.979692	-2.323603	0.727518
H	3.015242	-3.356237	1.350721
B	-3.407596	-1.457121	1.309956
H	-3.601055	-1.926445	2.403368
B	-1.759668	-1.557198	0.658183
H	-0.867282	-2.031201	1.298927
B	3.849581	-0.655226	-1.484333
H	4.517652	-0.477414	-2.473322
B	-4.084812	0.130084	0.871798
H	-4.739537	0.755589	1.667799
B	2.776198	0.631970	-0.925988
H	2.612504	1.722704	-1.393539
B	-4.539481	-1.319960	-0.068043
H	-5.656156	-1.773076	0.004402
B	-2.856732	1.014801	-0.046568
H	-2.656662	2.183490	0.124787
B	-2.523811	0.130044	-1.552381
H	-2.084944	0.740535	-2.493842
B	0.034263	2.484922	-0.565127

F•BBr^{Me}*o*Cb$_2^-$
Enthalpy: -3439.597154 Hartree

C	1.481715	0.178649	-0.022024
C	2.836466	-0.355894	0.895018
C	2.702578	-1.519419	1.871078
H	2.106090	-2.338547	1.430742
H	2.216966	-1.202588	2.809602
H	3.717145	-1.899072	2.095829
C	-1.457984	0.242268	0.068813
C	-2.935041	-2.063662	0.785972
H	-2.925700	-2.731714	-0.092531
H	-3.848834	-2.252890	1.380951
H	-2.052182	-2.299027	1.405369
C	-2.936884	-0.599082	0.366889
B	2.060749	0.688453	-1.564272
H	1.344089	0.519591	-2.518042
B	-1.749572	1.434109	-1.127503

H	-0.862671	1.694627	-1.894920
B	-2.943676	2.579548	-0.447032
H	-2.917616	3.752334	-0.748166
B	-3.347090	2.023602	1.206037
H	-3.608485	2.773891	2.119711
B	-0.000999	-0.599401	0.320836
B	4.297594	-0.214495	0.004901
H	5.136516	-1.061705	0.203395
B	3.880196	0.948409	1.278551
H	4.437753	0.912292	2.350631
B	2.787408	-0.723377	-0.779169
H	2.613884	-1.861036	-1.106381
B	-3.467861	1.307455	-1.594561
H	-3.827013	1.534172	-2.728234
B	3.149287	2.087103	-1.267972
H	3.231377	2.989968	-2.071100
B	4.528436	1.523909	-0.286599
H	5.642643	1.994745	-0.360956
B	1.673156	1.874005	-0.306078
H	0.703874	2.565509	-0.387491
B	3.839663	0.470273	-1.566983
H	4.434269	0.170101	-2.578132
B	-4.188542	-0.013662	-0.645498
H	-4.998388	-0.819319	-1.040784
B	-2.517665	-0.157298	-1.246930
H	-2.191756	-1.018192	-2.014882
B	3.172308	2.381545	0.503558
H	3.273696	3.481685	0.998426
B	-4.117505	0.434557	1.067828
H	-4.876328	-0.068680	1.862672
B	2.108555	1.163359	1.259331
H	1.466947	1.262063	2.271020
B	-4.460819	1.683359	-0.153962
H	-5.562271	2.182271	-0.234696
H	-1.989214	0.145585	2.575237
B	-1.680954	1.869967	0.599400
H	-0.754195	2.446642	1.096102
F	0.011343	-0.973152	1.676194
Br	-0.036355	-2.398382	-0.787881



F^-
Enthalpy: -99.687657 Hartree

F	0.000000	0.000000	0.000000

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