Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Blue Emissive Amidinate Based Tetra coordinate Boron Compounds:

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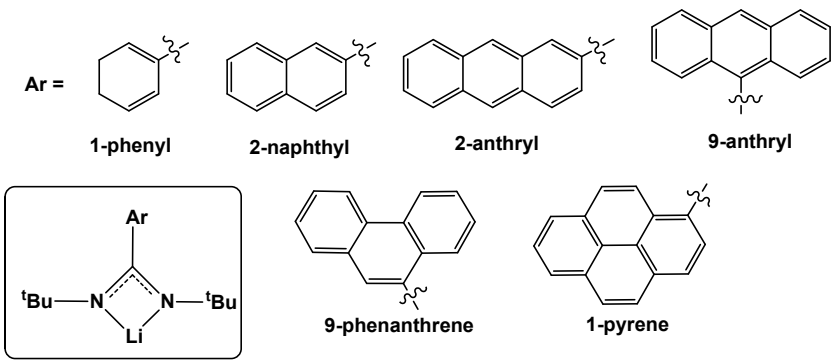
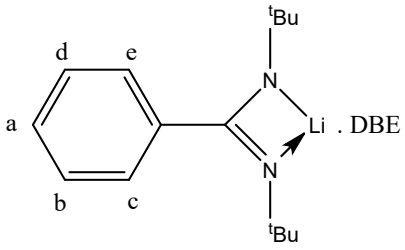
Contents

1. General synthetic procedure and Characterization:



Ar lithium salts (1-6Li) synthesis (Ar = 1-phenyl, 2-napthyl, 2-anthryl, 9-anthryl, 9-phenanthrene and 1-pyrene): A diethyl ether solution of bromo aryl (7.77 mmol) was taken in a 100ml Schleck flask and drop wise addition of n-BuLi (2.5 M in hexane, 7.77 mmol) was done at -78°C. After 4hr stirring the diethyl ether solution of carbodiimide (7.77 mmol) was added drop wise and stirred for additional 16 hr at room temperature. Diethyl ether was removed and after pentane wash (2*40 mL) powdery lithium salts were formed. The products used as such for further reactions. Yield: (57-93.9%).



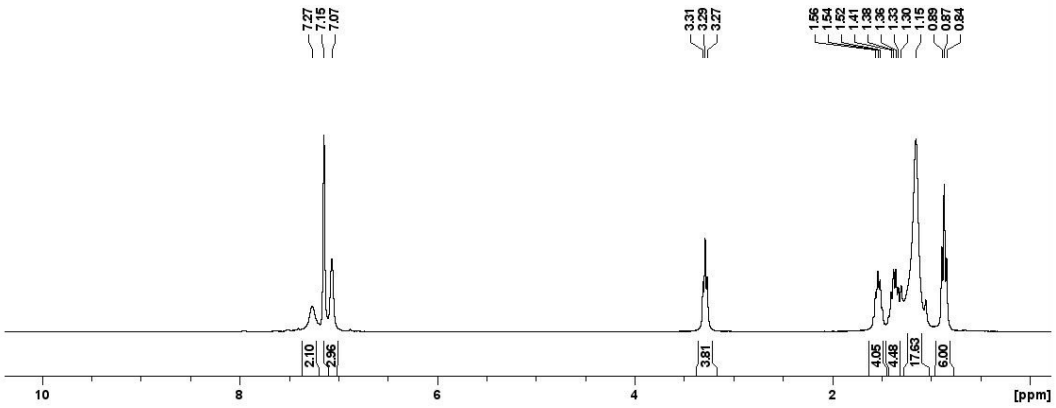


Figure S1:[1]H NMR spectrum ([C_6D_6, 300 MHz) of compound **1Li**

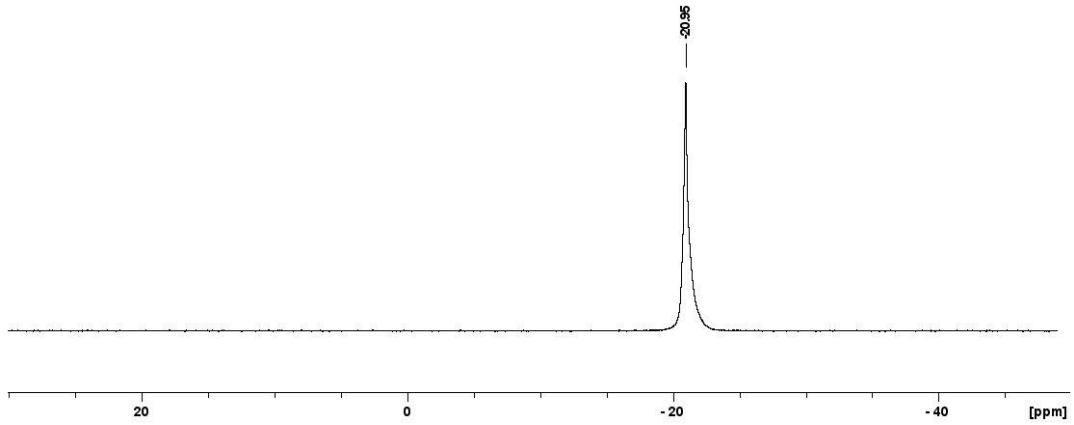
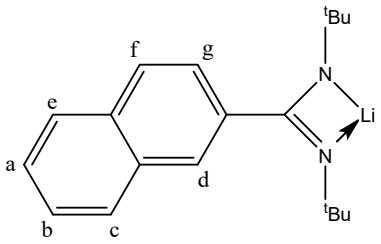


Figure S2:^{7}Li NMR spectrum ([C_6D_6, 116.6 MHz) of compound **1Li**



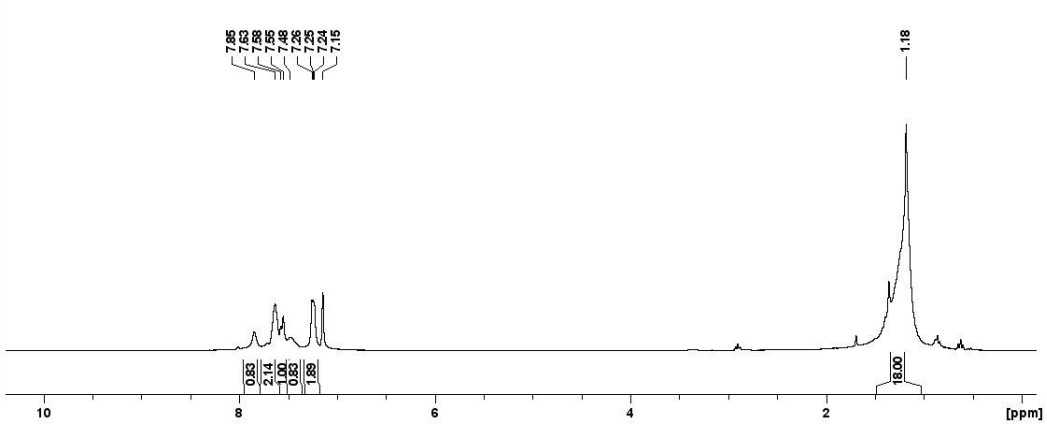


Figure S3:^{1}H NMR spectrum ([C_6D_6, 300 MHz) of compound **2Li**

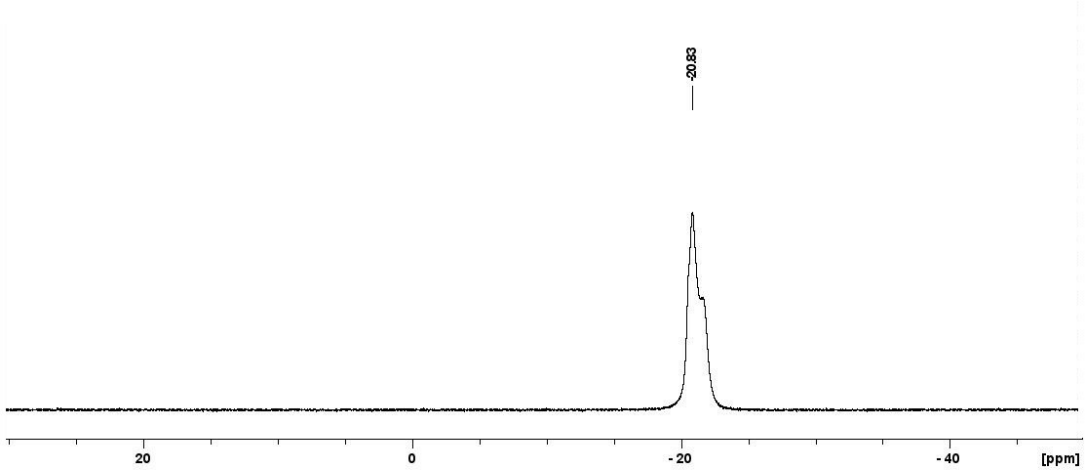


Figure S4:^{7}Li NMR spectrum ([C_6D_6, 116.6 MHz) of compound **2Li**

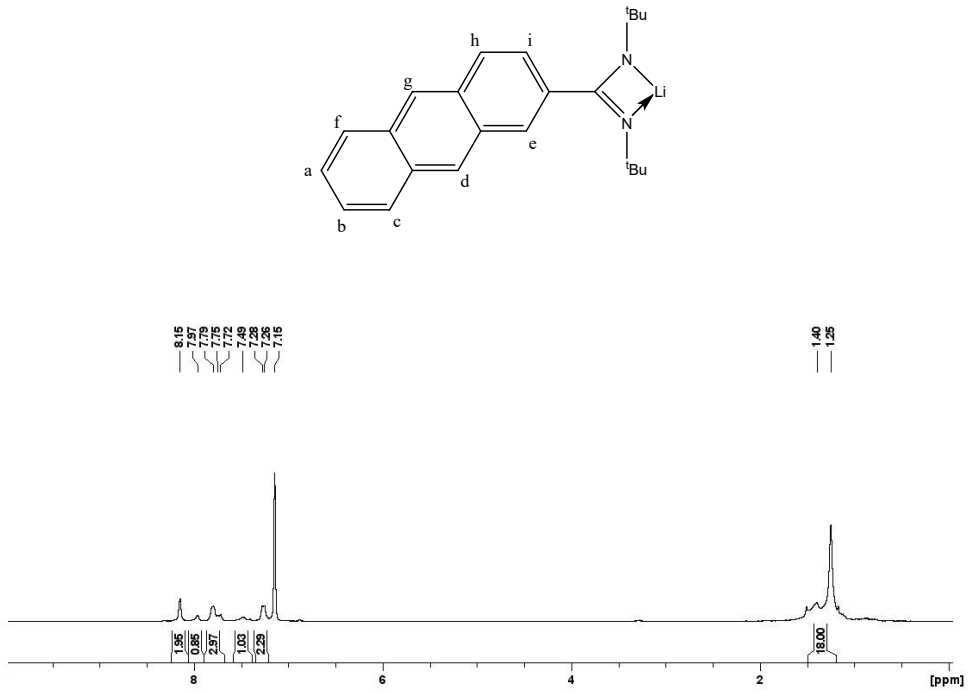


Figure S5:^{1}H NMR spectrum ([C_6D_6, 300 MHz) of compound **3Li**

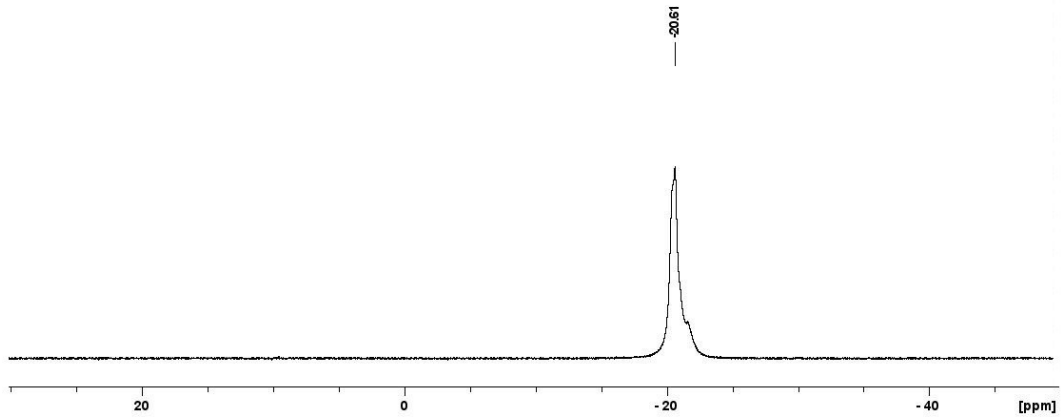


Figure S6:^{7}Li NMR spectrum ([C_6D_6, 116.6 MHz) of compound **3Li**

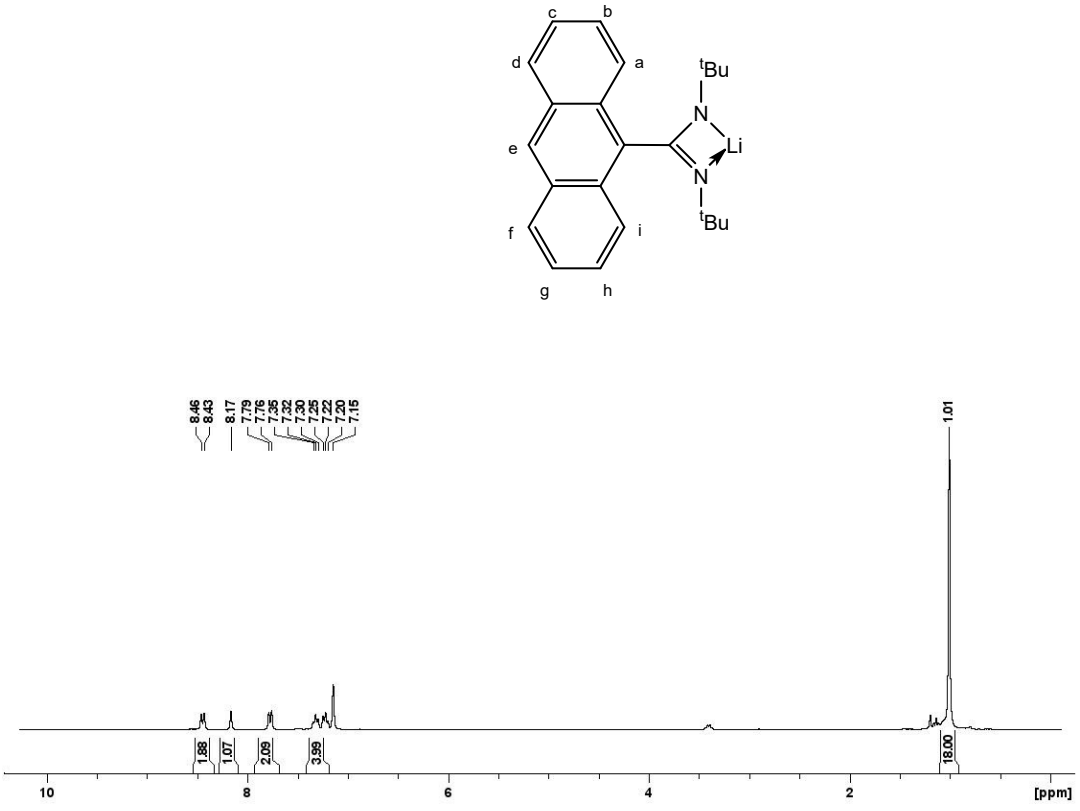


Figure S7:^{1}H NMR spectrum ([C_6D_6, 300 MHz) of compound **4Li**

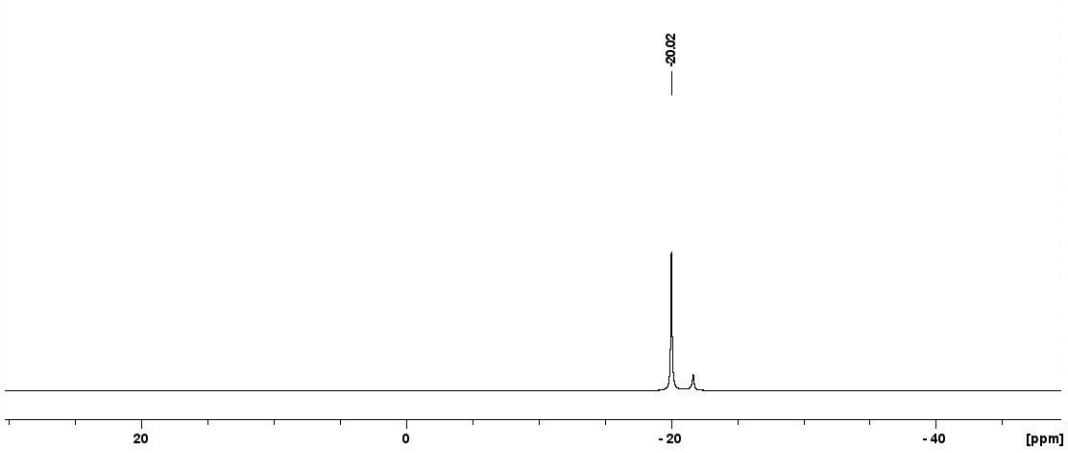


Figure S8:[7]Li NMR spectrum ([C_6D_6, 116.6 MHz) of compound **4Li**

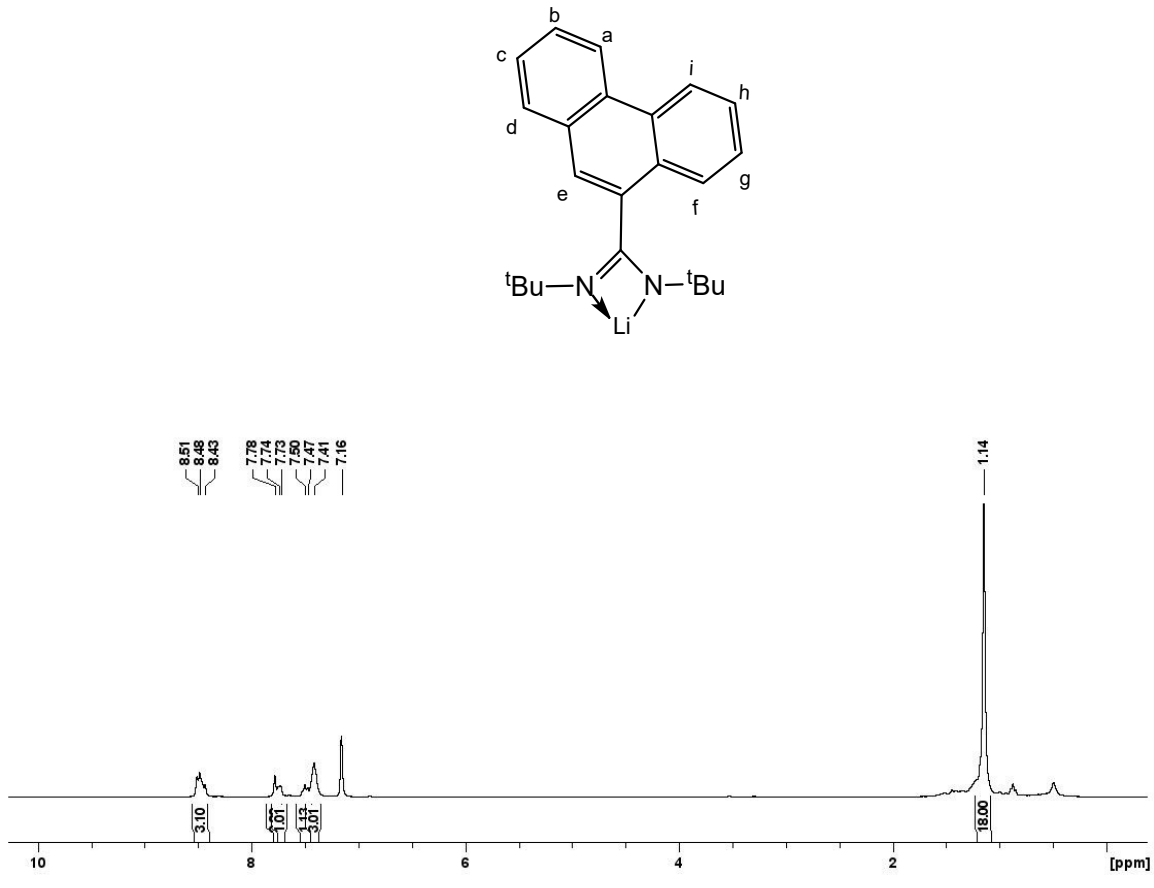


Figure S9:[1]H NMR spectrum ([C_6D_6, 300 MHz) of compound **5Li**

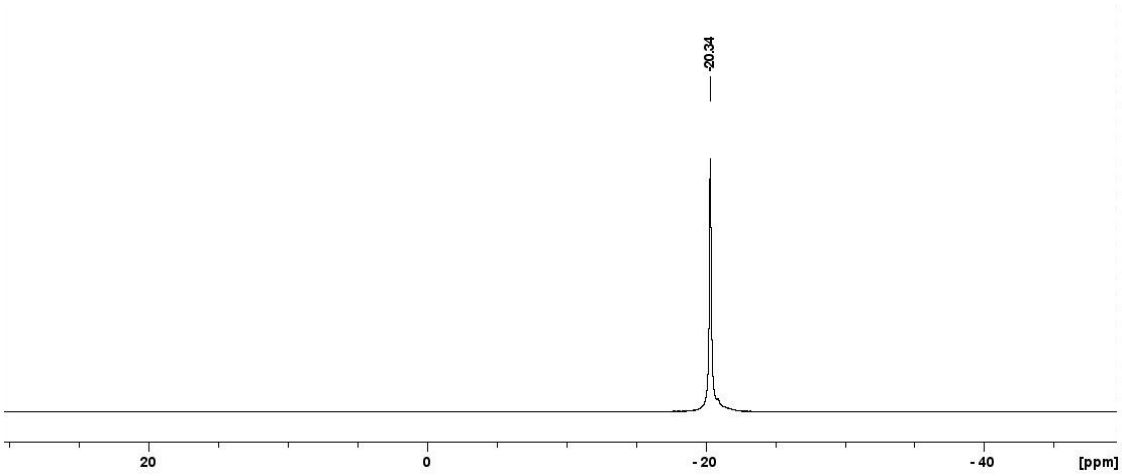


Figure S10:^{7}Li NMR spectrum ([C_6D_6, 116.6 MHz) of compound **5Li**

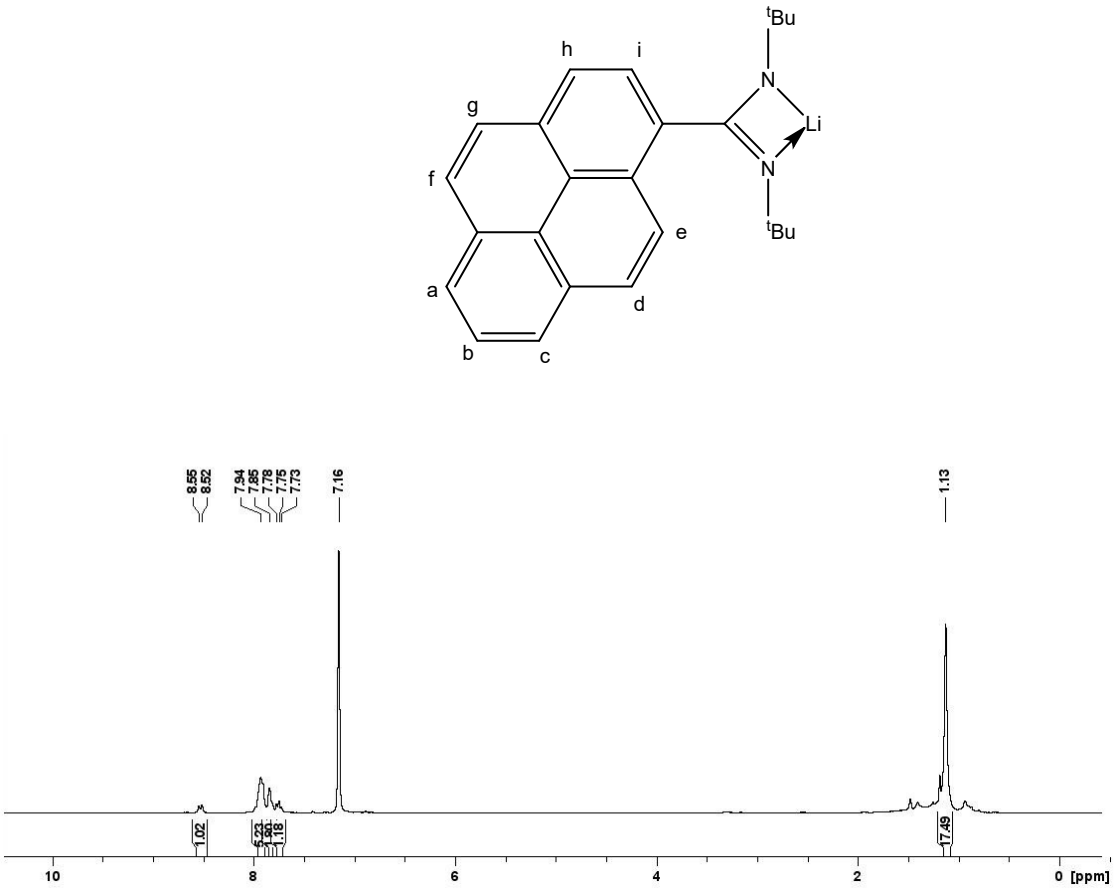


Figure S11:^{1}H NMR spectrum ([C_6D_6, 300 MHz) of compound **6Li**

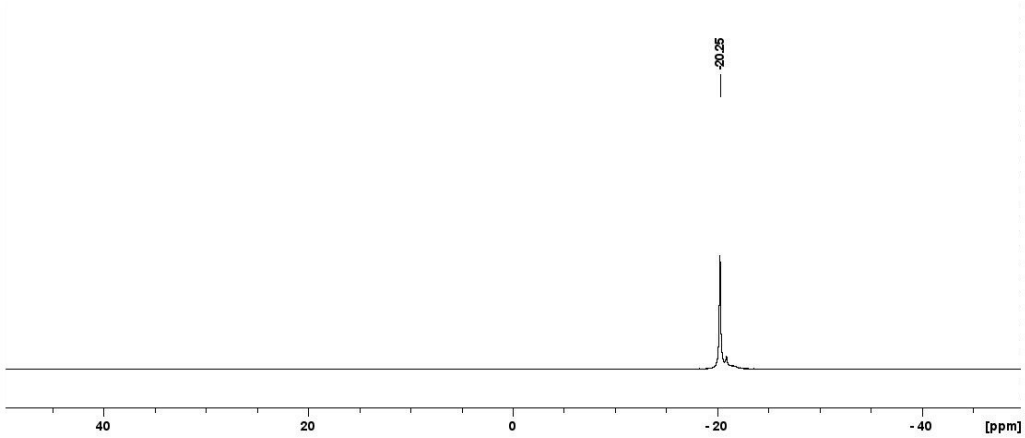
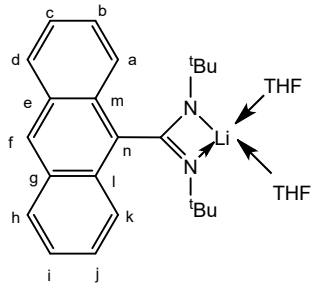


Figure S12:^{7}Li NMR spectrum ([C_6D_6, 116.6 MHz) of compound **6Li**

Compound 4-Li.2THF:



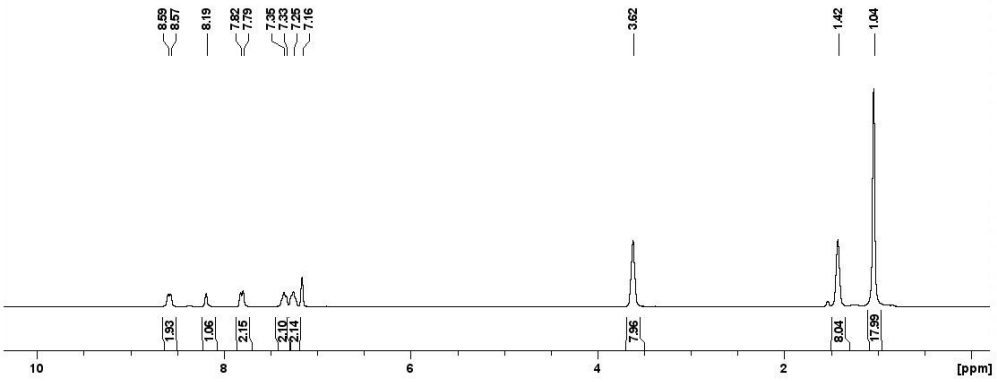


Figure S13:^{1}H NMR spectrum ([C_6D_6, 300 MHz) of compound **4-Li.2THF**

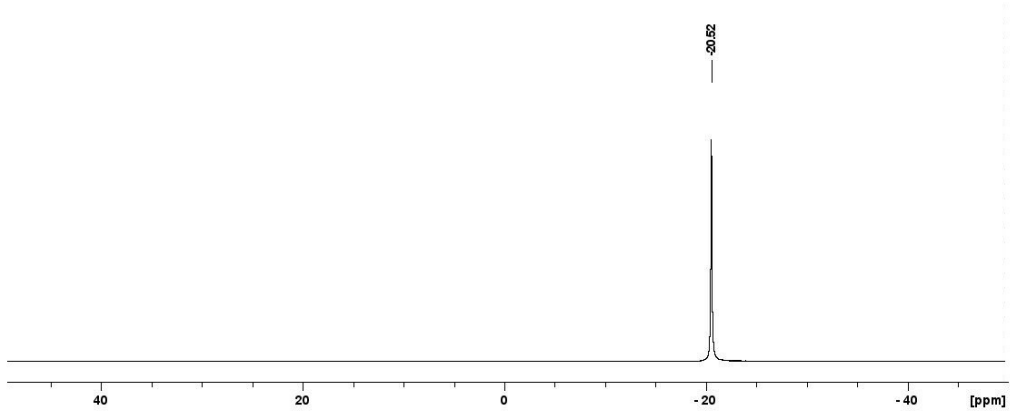


Figure S14:^{7}Li NMR spectrum ([C_6D_6, 116.6 MHz) of compound **4-Li.2THF**

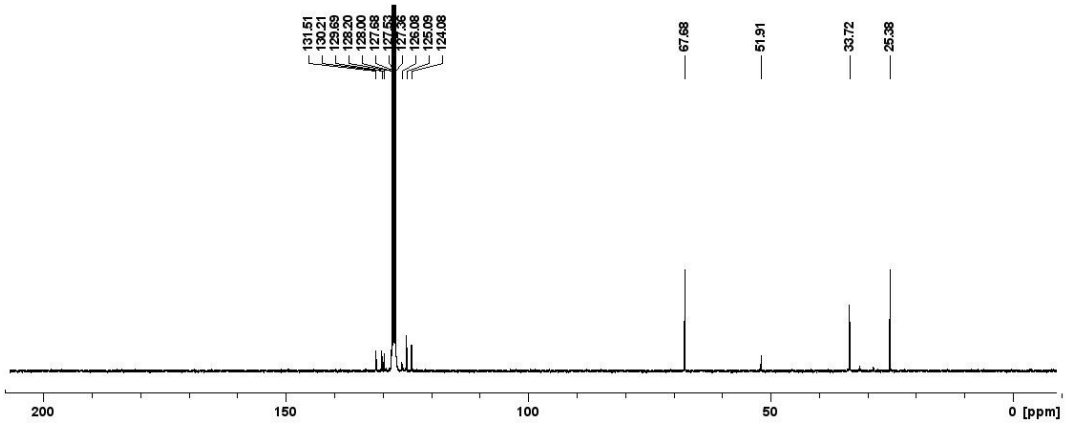
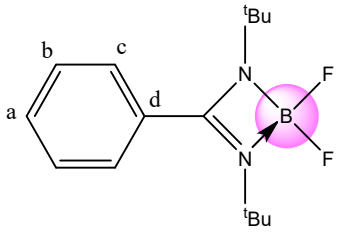


Figure S15:^{13}C NMR spectrum ([$CDCl_3$], 75 MHz) of compound **4-Li.2THF**.

Compound 1BF_2:



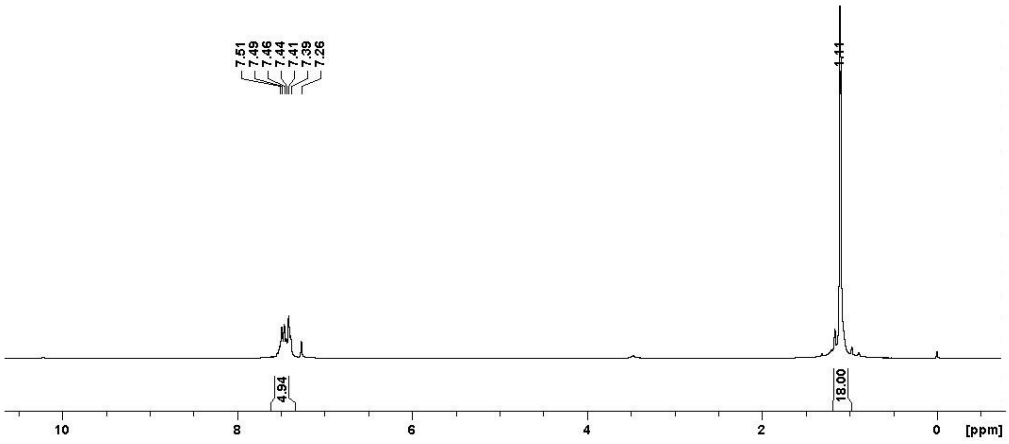


Figure S16:[1]H NMR spectrum ([$CDCl_3$, 300 MHz) of compound **1BF$_2$**.

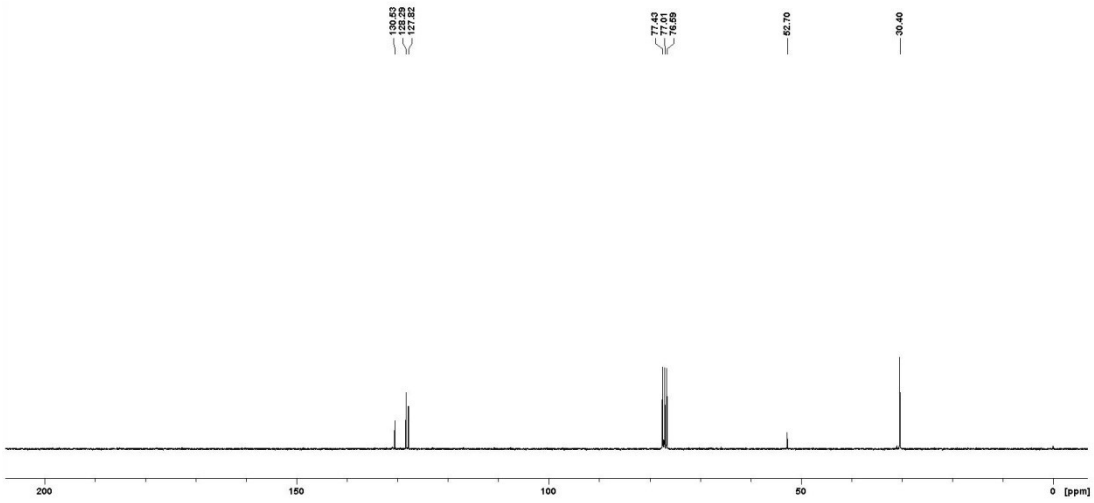


Figure S17:[13]C NMR spectrum ([$CDCl_3$], 75 MHz) of compound **1BF$_2$**.

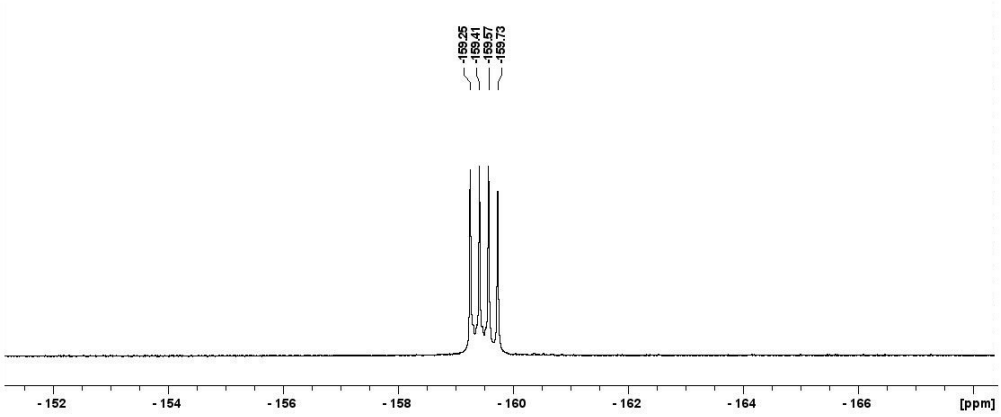


Figure S18:[19]F NMR spectrum ([$CDCl_3$], 282 MHz) of compound **1BF$_2$**.

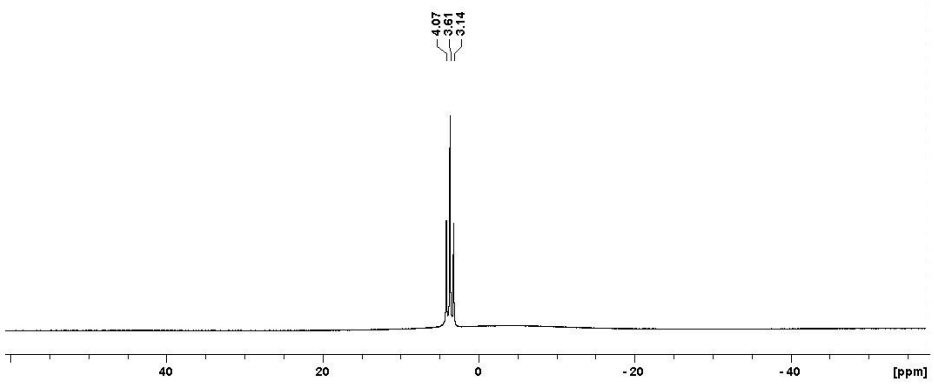
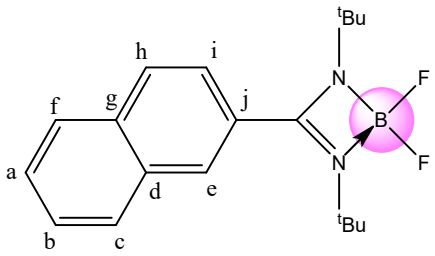


Figure S19:[11]B NMR spectrum ([$CDCl_3$], 96 MHz) of compound **1BF$_2$**.

Compound 2BF$_2$:



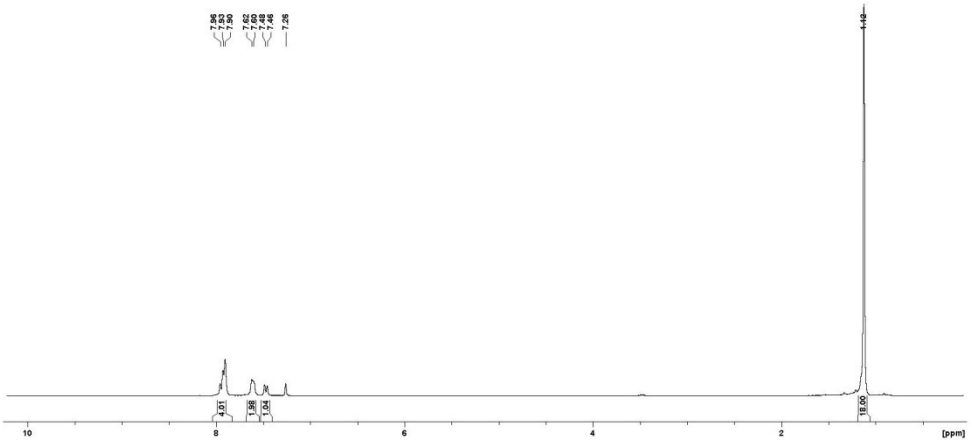


Figure S20:[1]H NMR spectrum ([$CDCl_3$, 300 MHz) of compound **2BF$_2$**.

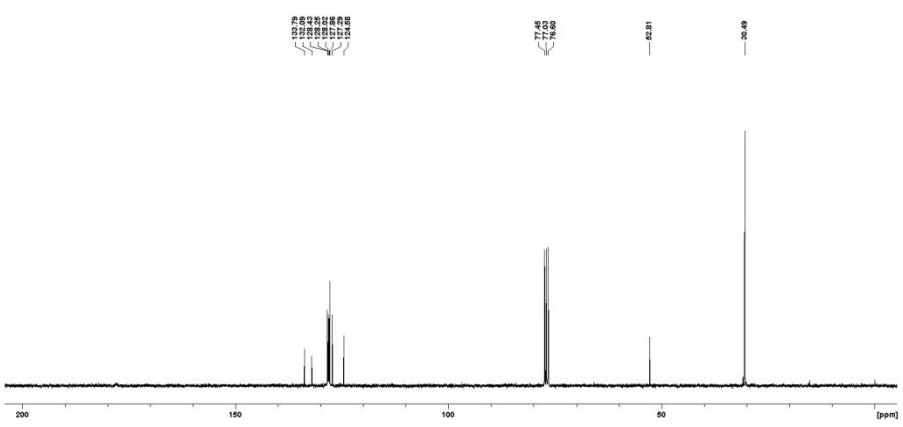


Figure S21:[13]C NMR spectrum ([$CDCl_3$], 75 MHz) of compound **$2BF_2$**.

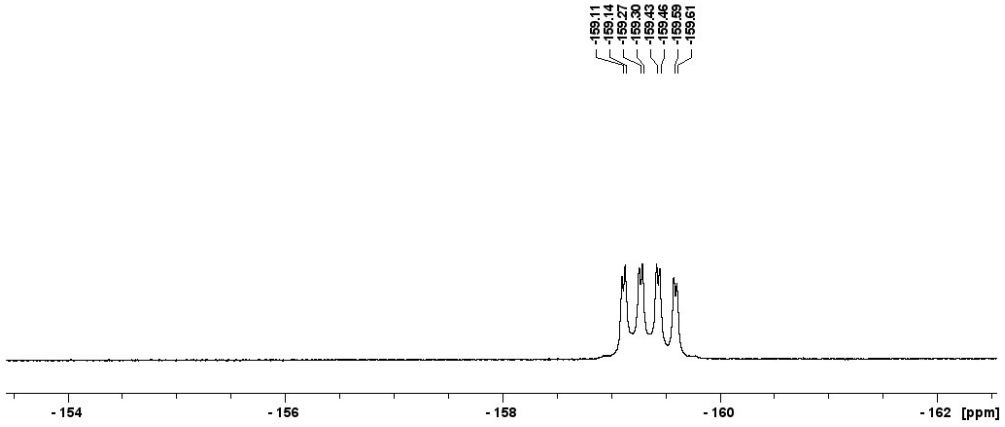


Figure S22:[19]F NMR spectrum ([$CDCl_3$], 282 MHz) of compound **$2BF_2$**.

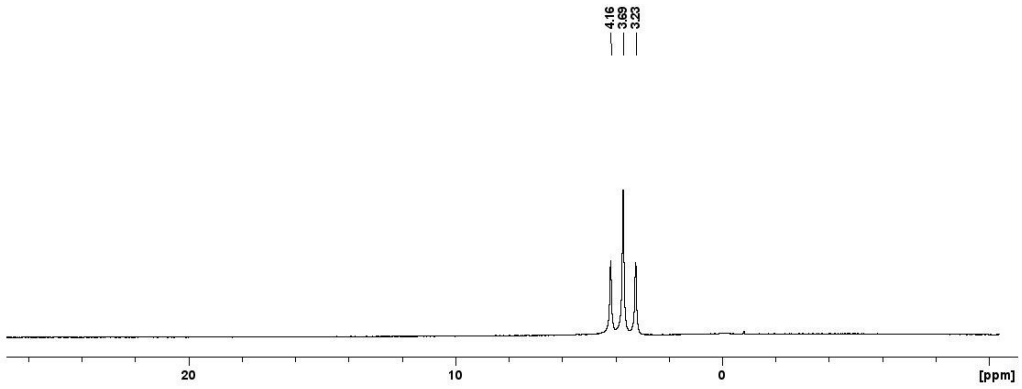
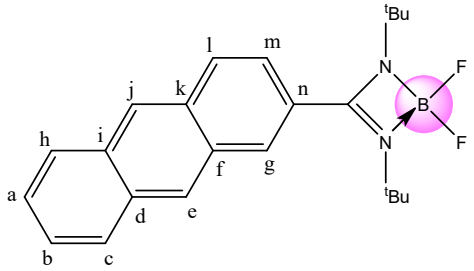


Figure S23:[11]B NMR spectrum ([$CDCl_3$], 96 MHz) of compound **$2BF_2$**.

Compound $3BF_2$:



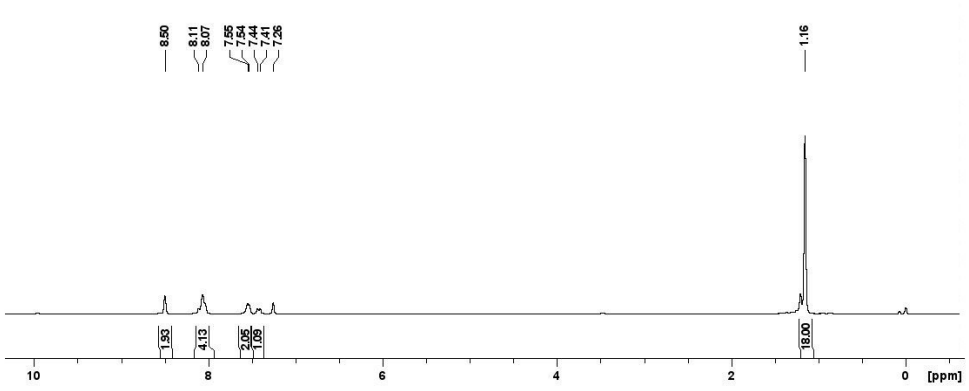


Figure S24:[1]H NMR spectrum ([$CDCl_3$, 300 MHz) of compound **$3BF_2$**.

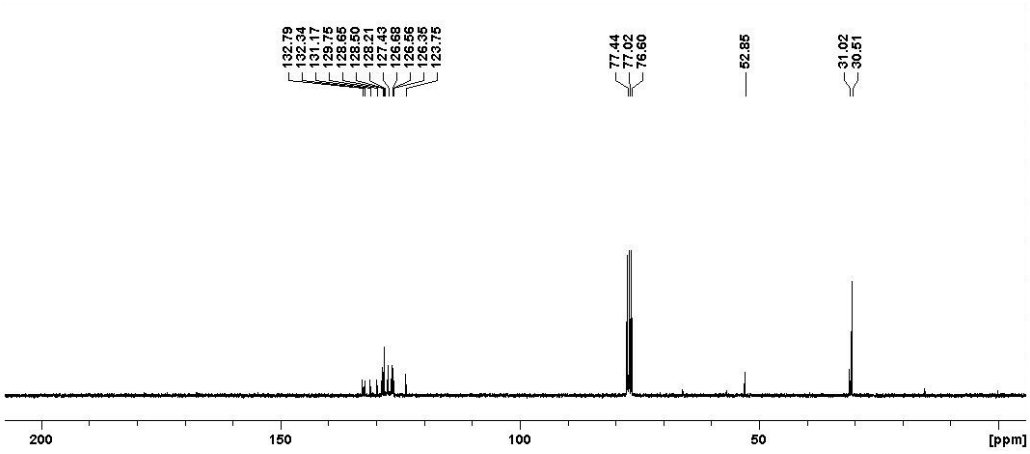


Figure S25:[13]C NMR spectrum ([$CDCl_3$], 75 MHz) of compound **$3BF_2$**.

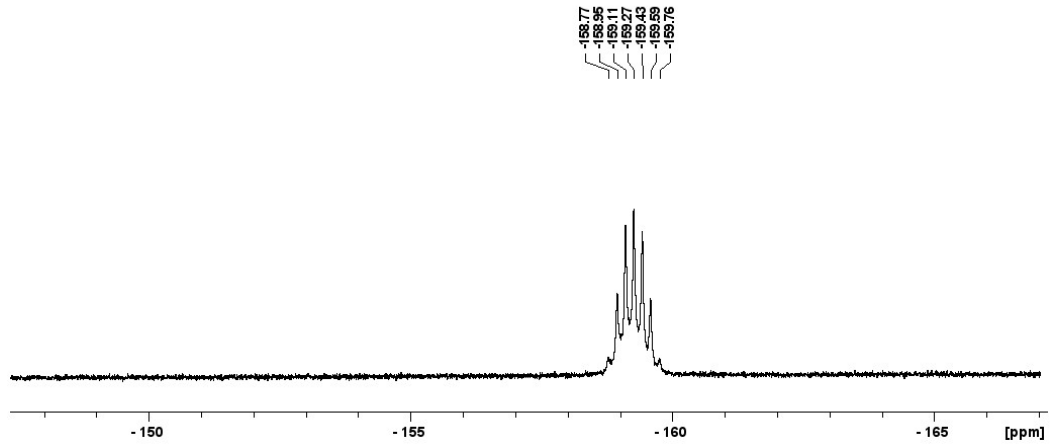


Figure S26:^{19}F NMR spectrum ([$CDCl_3$], 282 MHz) of compound **$3BF_2$**.

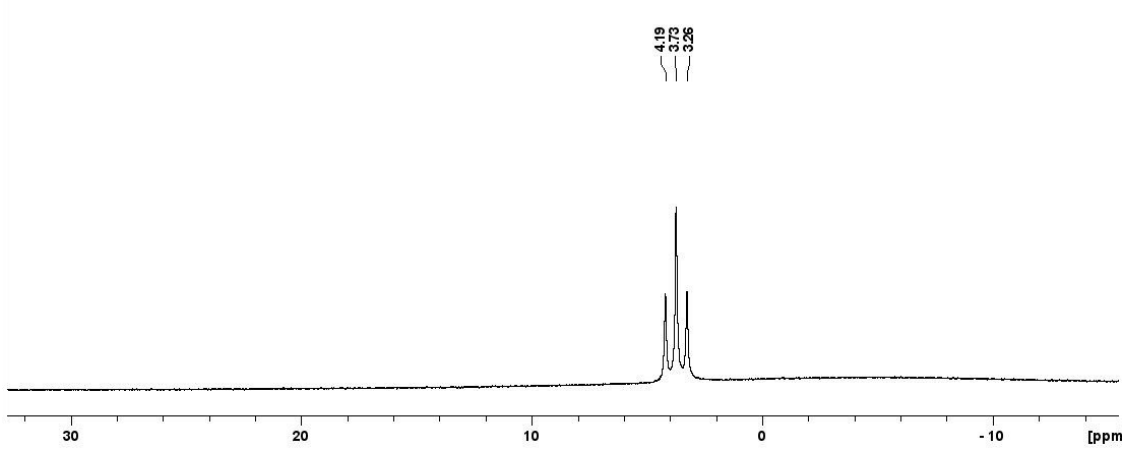
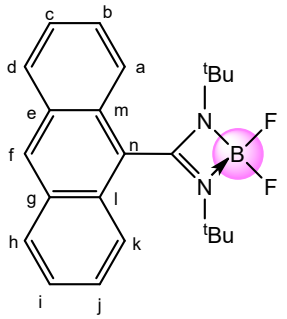


Figure S27:^{11}B NMR spectrum ([$CDCl_3$], 96 MHz) of compound **$3BF_2$**.

Compound $4BF_2$:



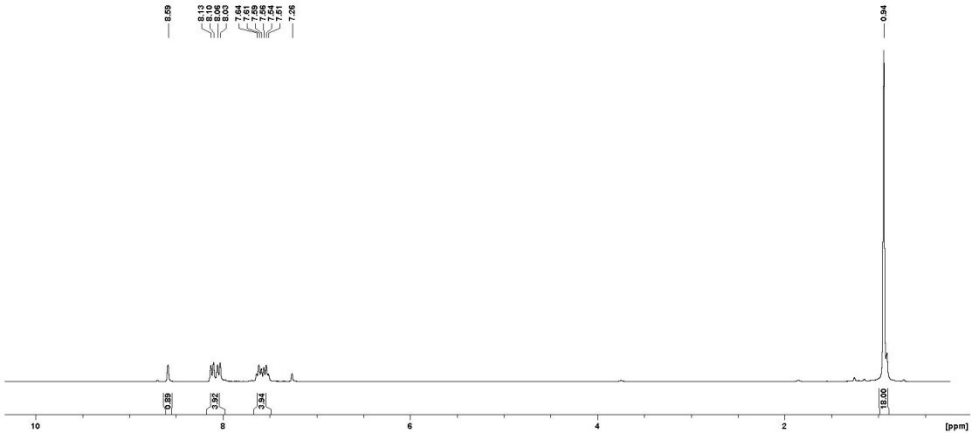


Figure S28:[1]H NMR spectrum ([$CDCl_3$, 300 MHz) of compound **4BF$_2$**.

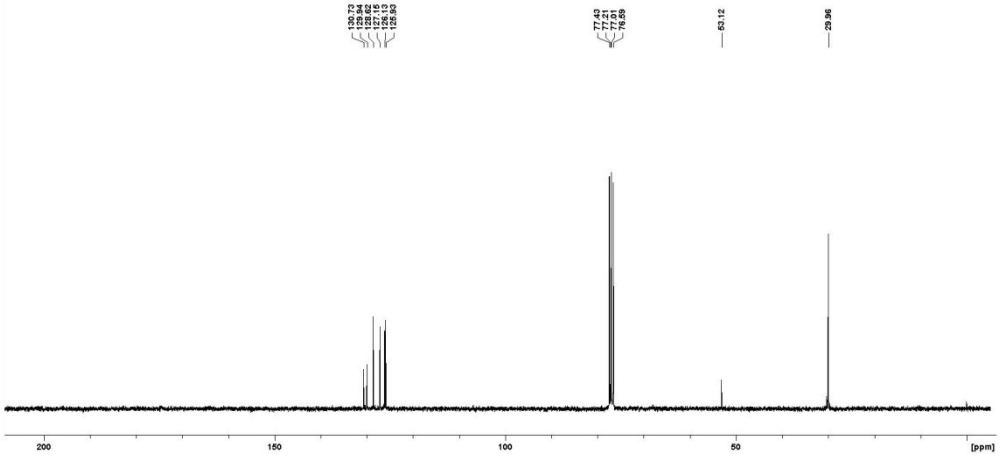


Figure S29:[13]C NMR spectrum ([$CDCl_3$], 75 MHz) of compound **4BF$_2$**.

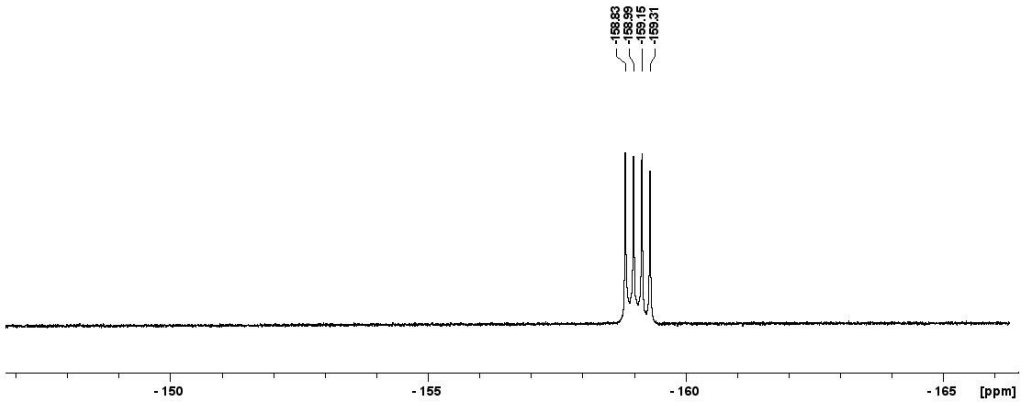


Figure S30:^{19}F NMR spectrum ([$CDCl_3$], 282 MHz) of compound **4BF$_2$**.

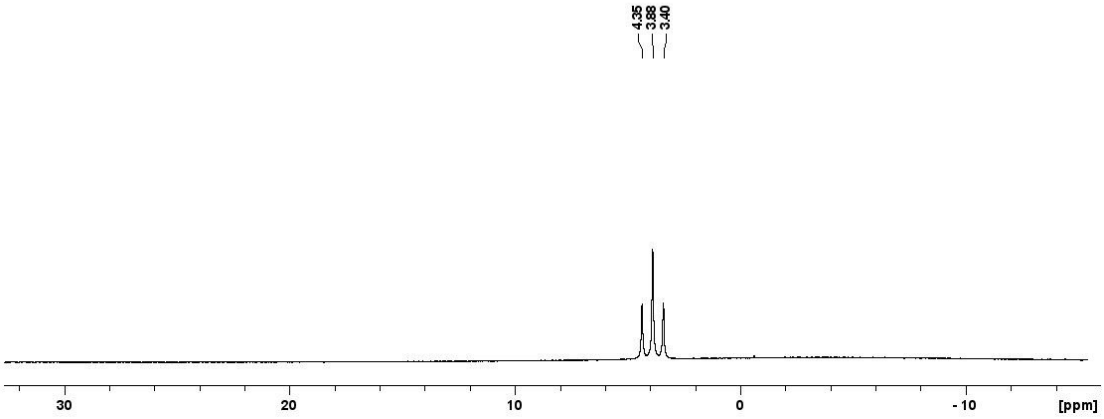
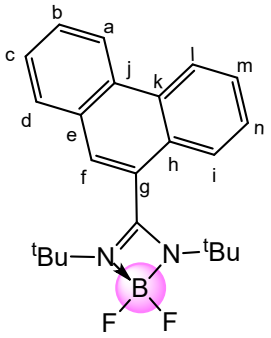


Figure S31:^{11}B NMR spectrum ([$CDCl_3$], 96 MHz) of compound **4BF$_2$**.

Compound 5BF$_2$:



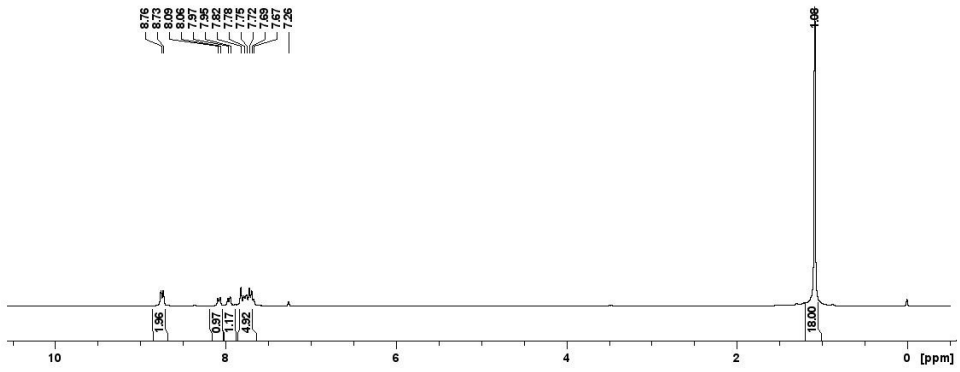


Figure S32:[1]H NMR spectrum ([$CDCl_3$, 300 MHz) of compound **5BF$_2$**.

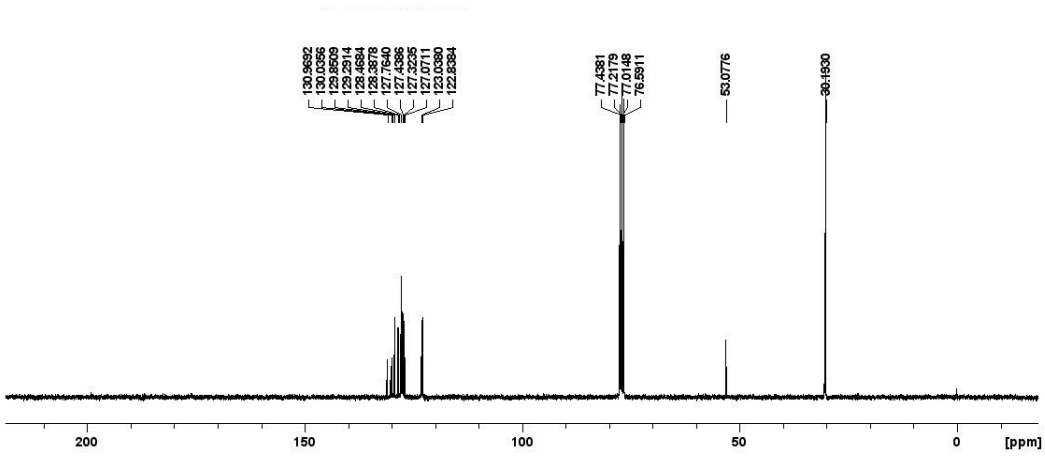


Figure S33:[13]C NMR spectrum ([$CDCl_3$], 75 MHz) of compound **5BF$_2$**.

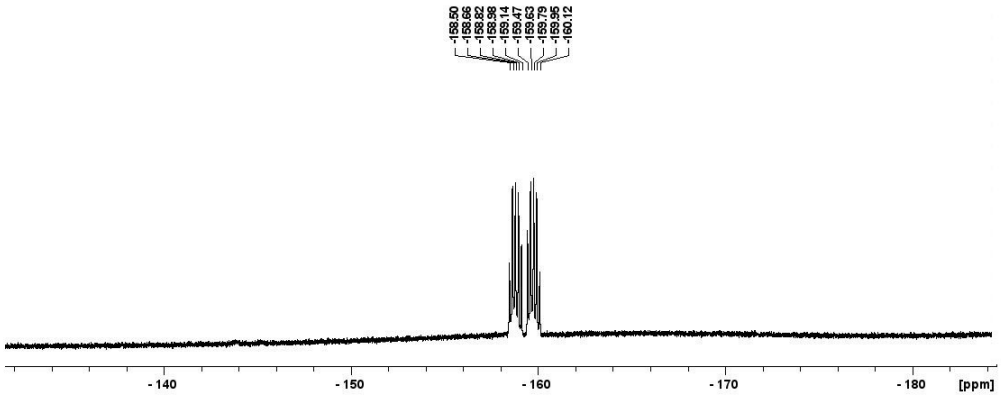


Figure S34:[19]F NMR spectrum ([$CDCl_3$], 282 MHz) of compound **5BF$_2$**.

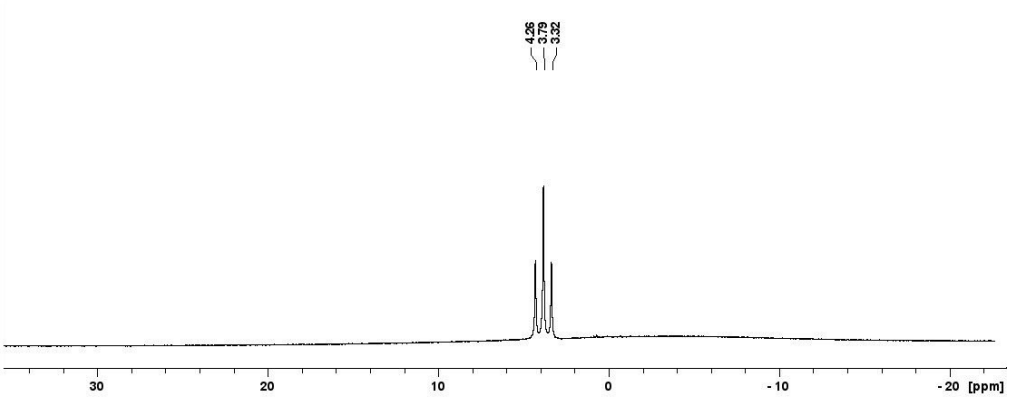
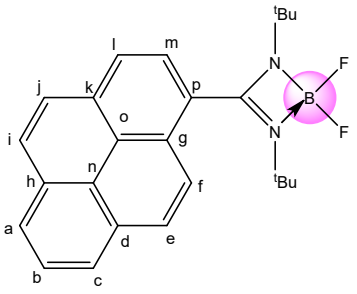


Figure S35:[11]B NMR spectrum ([$CDCl_3$], 96 MHz) of compound **5BF$_2$**.

Compound 6BF$_2$:



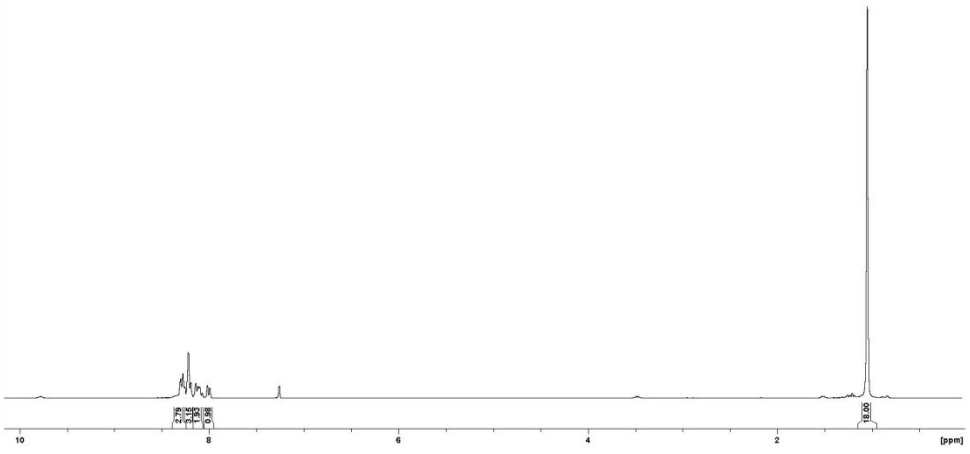


Figure S36:[1]H NMR spectrum ([$CDCl_3$, 300 MHz) of compound **6BF$_2$**.

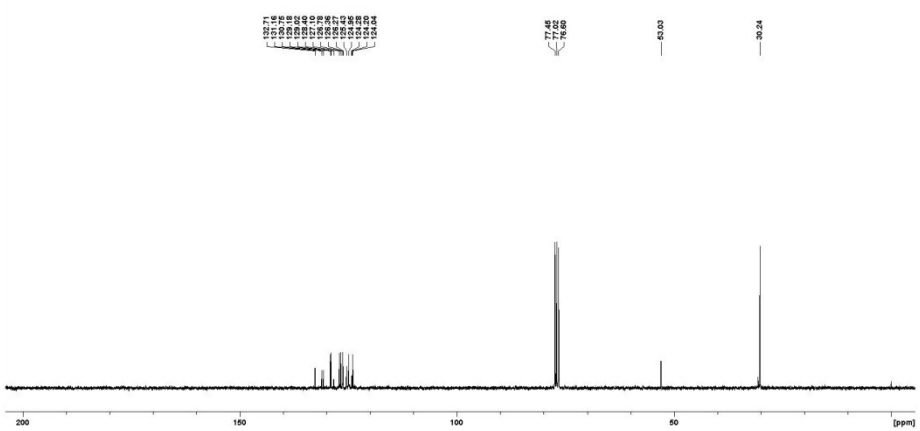


Figure S37:[13]C NMR spectrum ([$CDCl_3$], 75 MHz) of compound **$6BF_2$**.

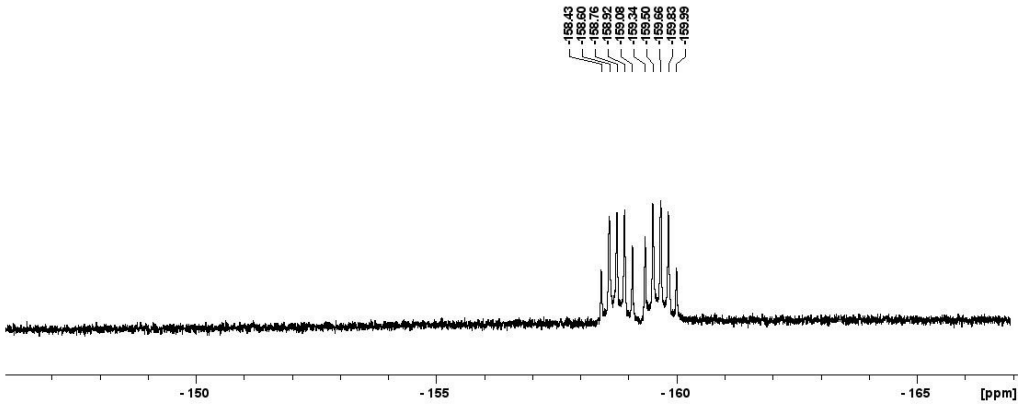


Figure S38:[19]F NMR spectrum ([$CDCl_3$], 282 MHz) of compound **$6BF_2$**.

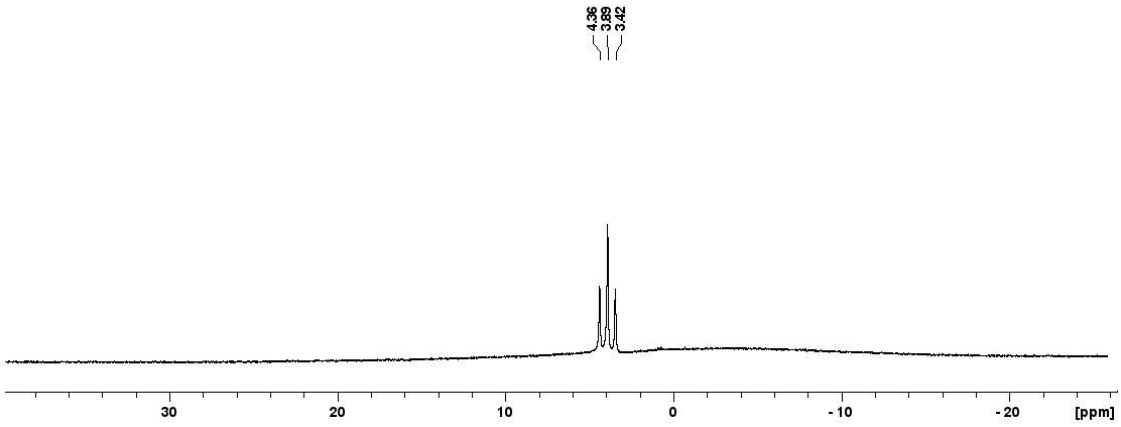


Figure S39:[11]B NMR spectrum ([$CDCl_3$], 96 MHz) of compound **6BF_2**.

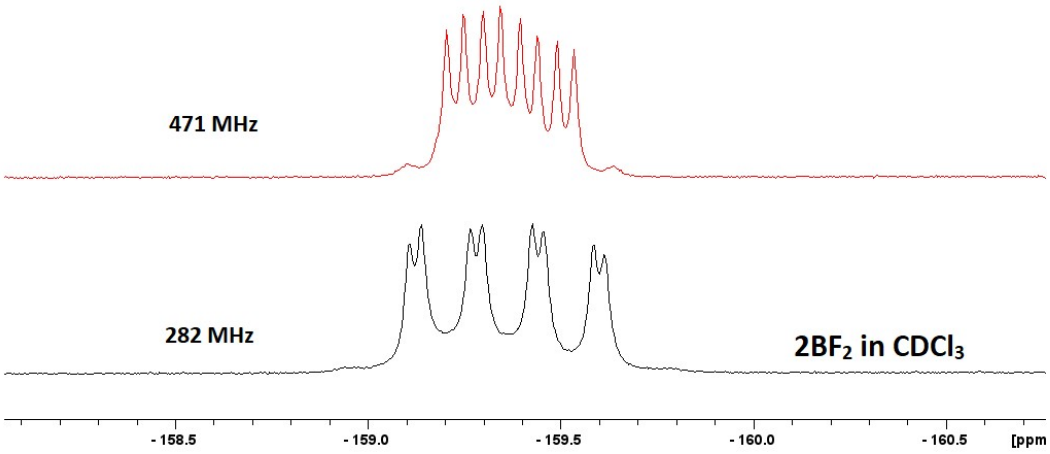


Figure S40: [19]F NMR spectra of **2BF_2** in $CDCl_3$ at 282 MHz and 471 MHz instrument.

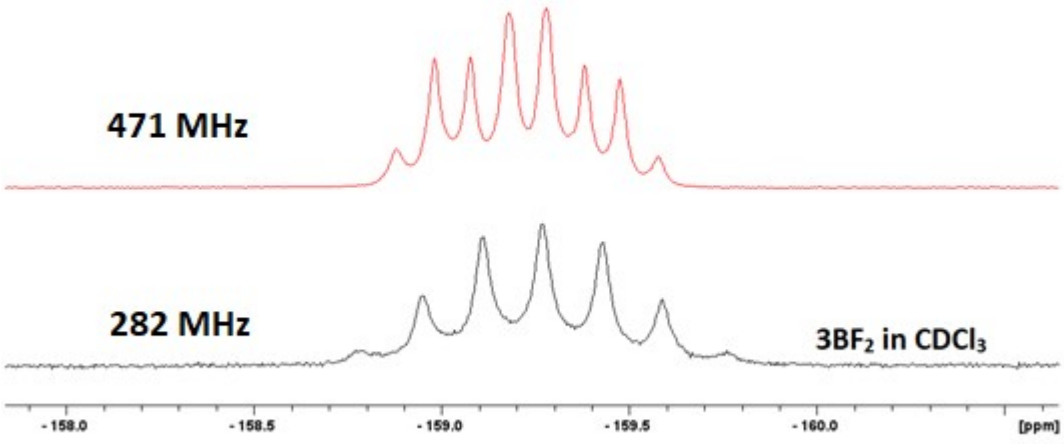


Figure S41: [19]F NMR spectra of **3BF_2** in $CDCl_3$ at 282 MHz and 471 MHz instrument.

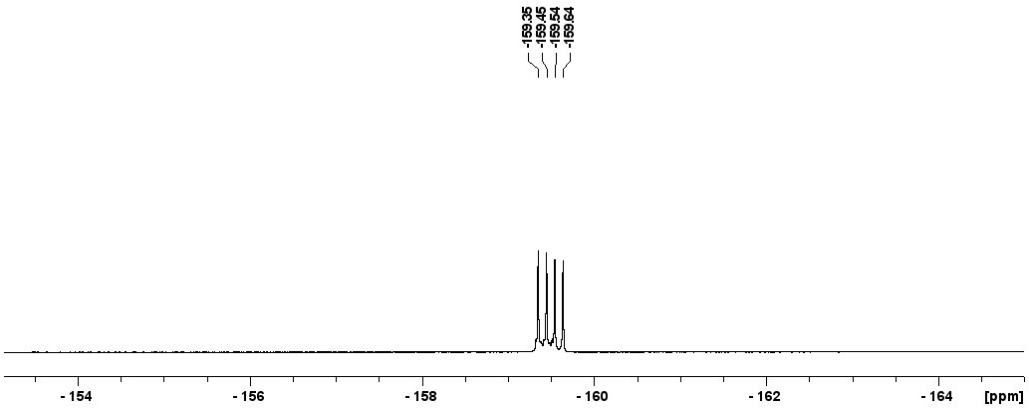


Figure S42:[19]F NMR spectrum ([$CDCl_3$], 470 MHz) of compound **1BF$_2$**.

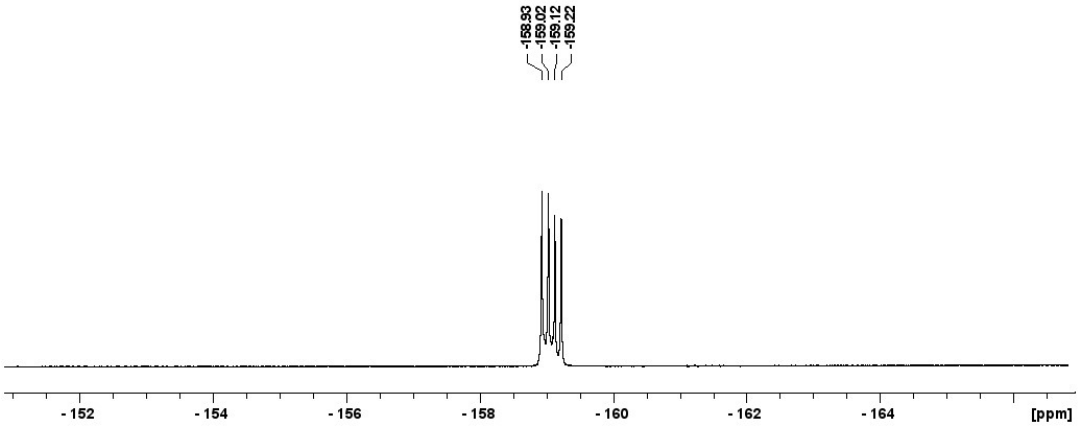


Figure S43:[19]F NMR spectrum ([$CDCl_3$], 470 MHz) of compound **4BF$_2$**.

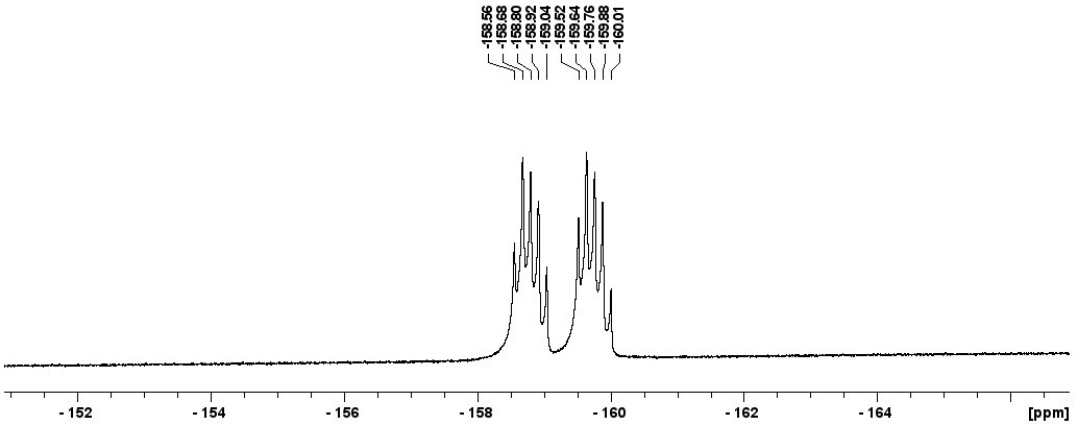


Figure S44:^{19}F NMR spectrum ([$CDCl_3$], 376 MHz) of compound **$5BF_2$**.

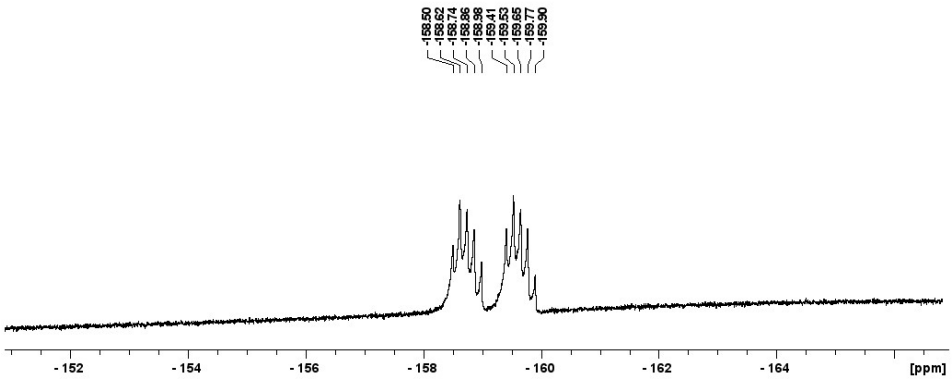


Figure S45:^{19}F NMR spectrum ([$CDCl_3$], 376 MHz) of compound **$6BF_2$**.

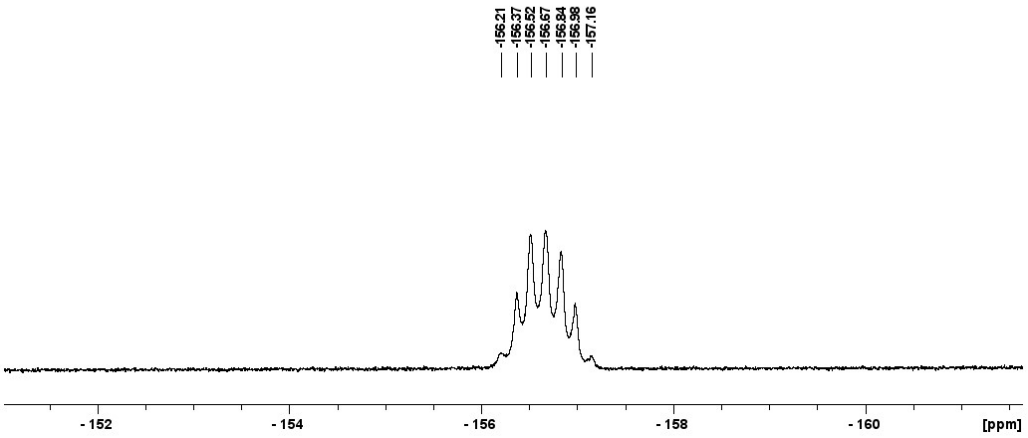


Figure S46:^{19}F NMR spectrum ([dmso-d6], 282 MHz) of compound **2BF$_2$**.

2. Variable temperature NMR and ^{1}H-^{19}F HOESY results:

2.2 Variable temperature NMR:

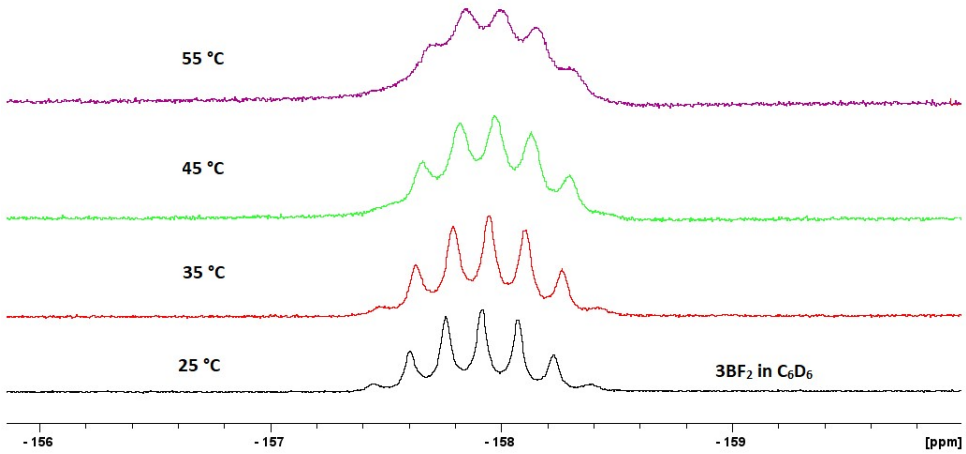


Figure S47: Variable temperature nmr spectra of **$3BF_2$** in C6D6.

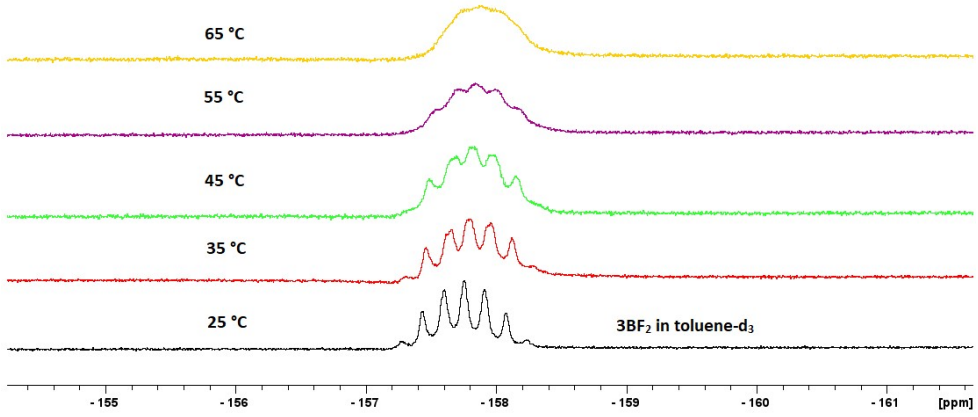


Figure S48: Variable temperature nmr spectra of **$3BF_2$** in toluene-d3.

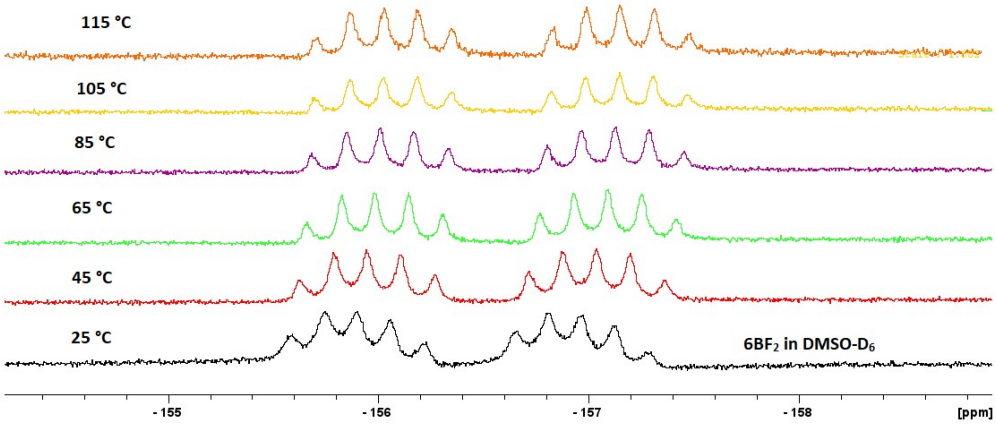


Figure S49: Variable temperature nmr spectra of **$6BF_2$** in dmso-d6.

2.2 $^{1}H–^{19}F$ HOESY spectra:

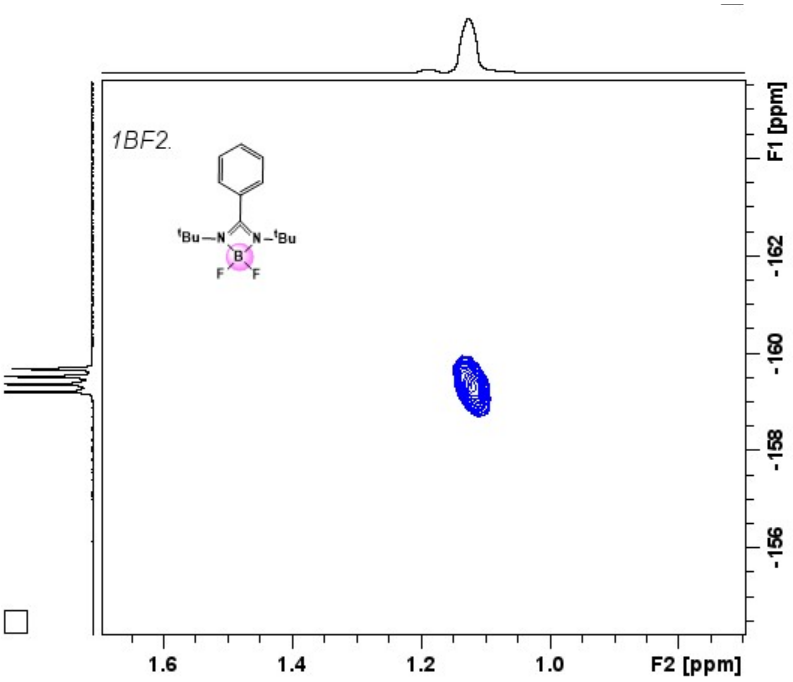


Figure S50: $^{1}H–^{19}F$ HOESY spectra of **$1BF_2$**.

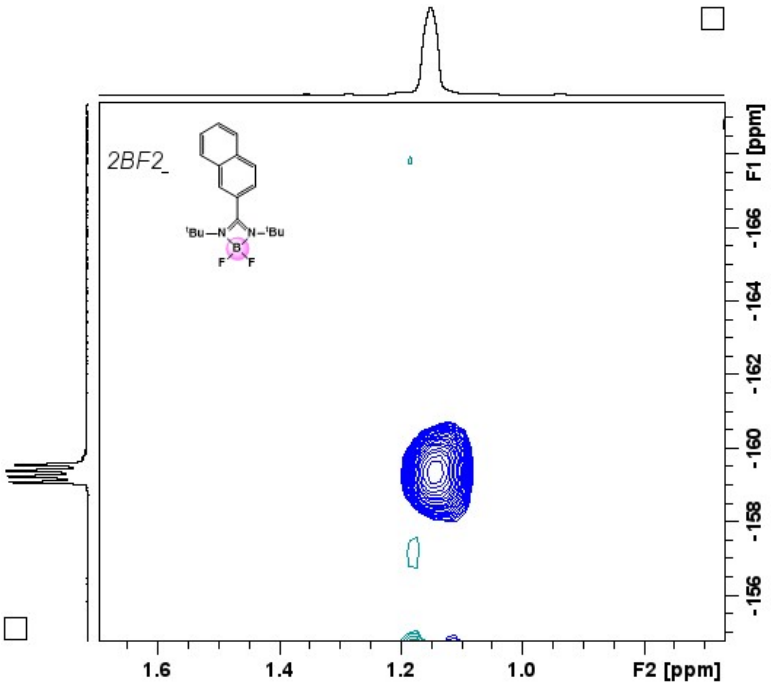


Figure S51: $^{1}H–^{19}F$ HOESY spectra of **$2BF_2$**.

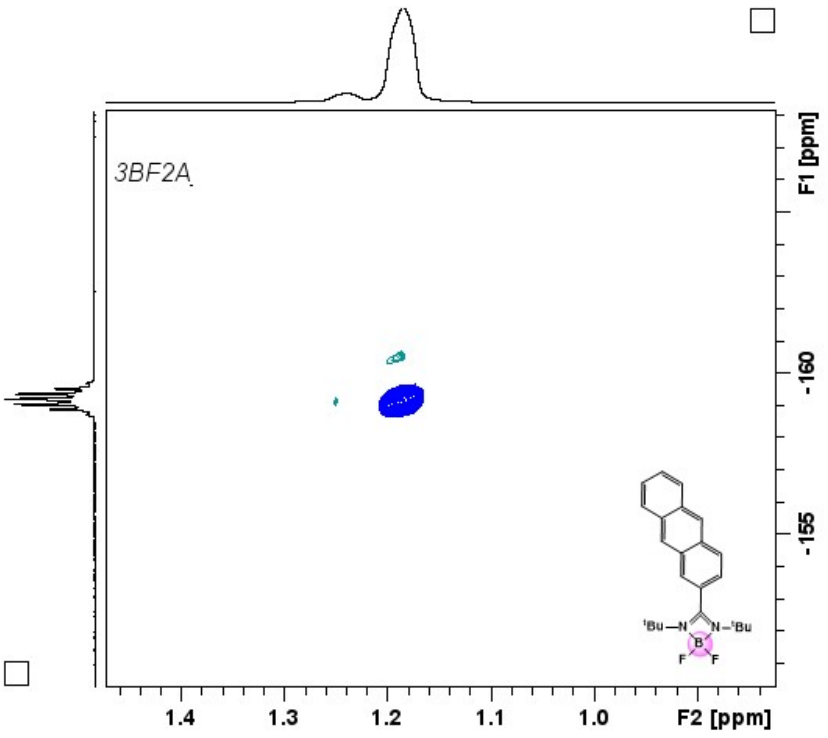


Figure S52: ^{1}H–^{19}F HOESY spectra of **3BF$_2$**.

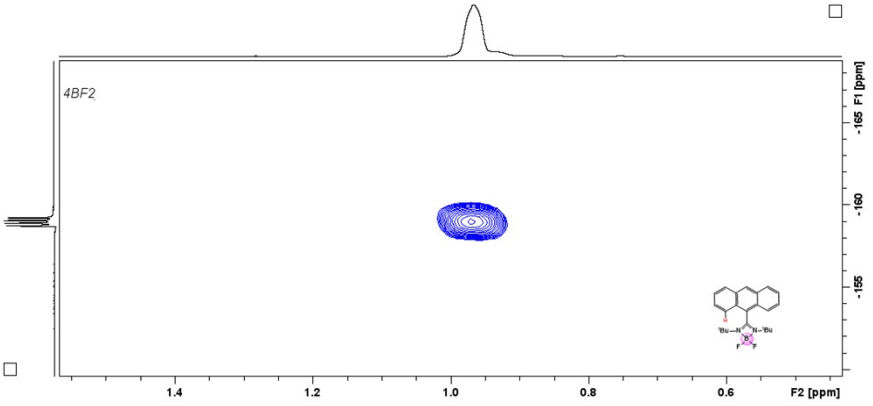


Figure S53: ^{1}H–^{19}F HOESY spectra of **4BF$_2$**.

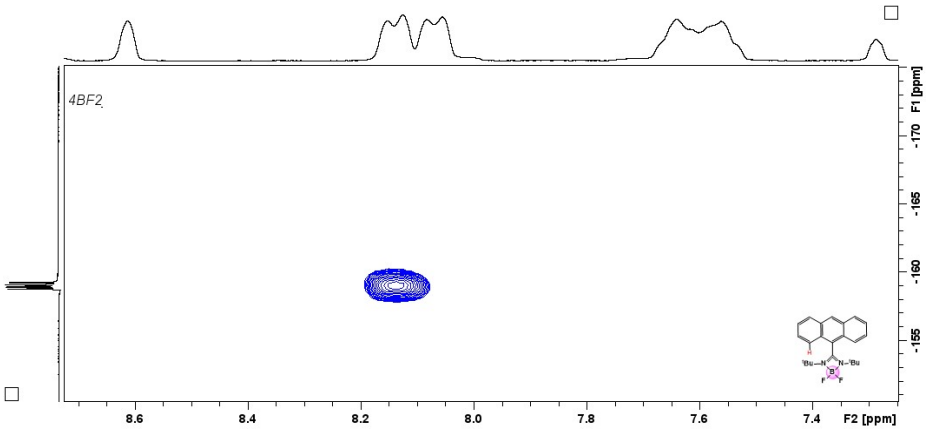


Figure S54: $^{1}H–^{19}F$ HOESY spectra of **$4BF_2$**.

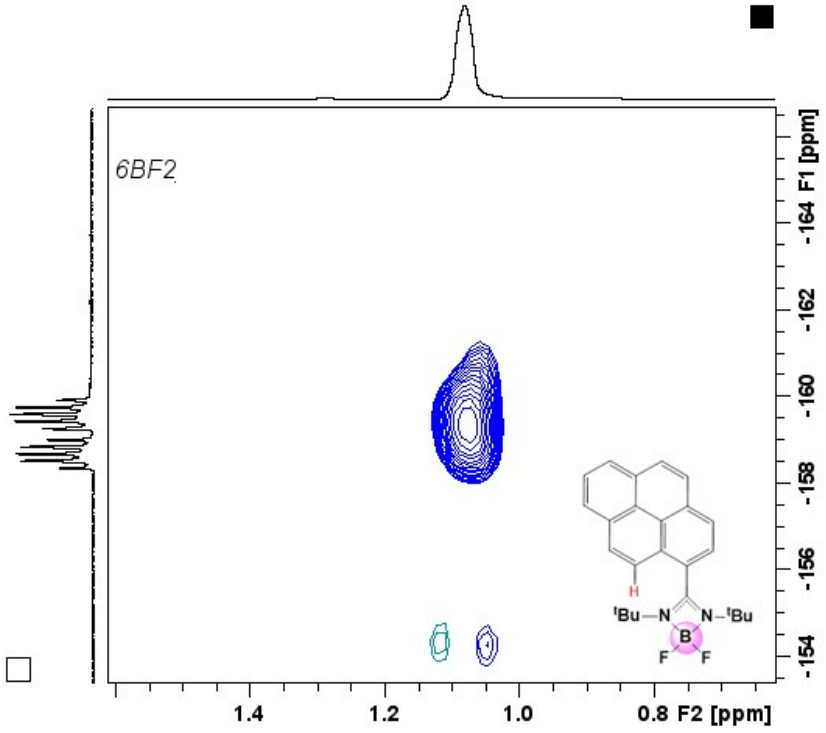


Figure S55: $^{1}H–^{19}F$ HOESY spectra of **$6BF_2$**.

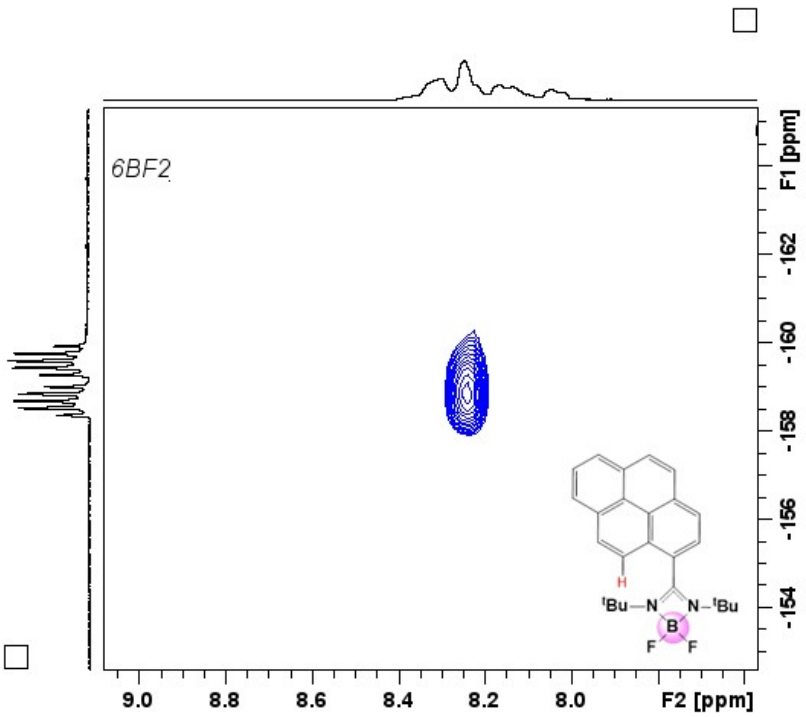


Figure S56: $^{1}H–^{19}F$HOESY spectra of **$6BF_2$**.

3. Crystallography data:

Table S1: Crystal data and structure refinement for **$1BF_2$**.

Identification code	**$1BF_2$**	
Empirical formula	C15 H23 B F2 N2	
Formula weight	280.16	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c n	
Unit cell dimensions	a = 10.9290(4) Å	□= 90°.
	b = 10.2818(4) Å	□= 90°.
	c = 13.9166(5) Å	□ = 90°.
Volume	1563.81(10) $Å^3$	
Z	4	
Density (calculated)	1.190 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	616	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	2.720 to 26.848°.	
Index ranges	-13<=h<=13, -9<=k<=13, -17<=l<=17	
Reflections collected	9858	
Independent reflections	1647 [R(int) = 0.0298]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.84727	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1647 / 0 / 93	
Goodness-of-fit on F^2	1.089	
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.1062	
R indices (all data)	R1 = 0.0466, wR2 = 0.1103	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.218 and -0.195 $e.Å^{-3}$	

Table S2: Crystal data and structure refinement for **$3BF_2$**.

Identification code	**$3BF_2$**
Empirical formula	C_{23} H_{27} B F_2 N_2
Formula weight	380.28
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 11.8480(9) Å □ = 90°.
	b = 9.1474(6) Å □ = 102.996(7)°.
	c = 20.2739(13) Å □ = 90°.
Volume	2141.0(3) $Å^3$
Z, Calculated density	4, 1.180 Mg/m^3
Absorption coefficient	0.080 mm^{-1}
F(000)	840
Crystal size	? x ? x ? mm^3
Theta range for data collection	2.841 to 28.911°.
Limiting indices	-15<=h<=12, -12<=k<=11, -25<=l<=27
Reflections collected / unique	23364 / 4887 [R(int) = 0.1958]
Completeness to theta = 25.242	98.3 %
Max. and min. transmission	1.00000 and 0.77081
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4887 / 0 / 259
Goodness-of-fit on F^2	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0978, wR2 = 0.2886
R indices (all data)	R1 = 0.1472, wR2 = 0.3254
Extinction coefficient	n/a
Largest diff. peak and hole	0.483 and -0.269 $e.Å^{-3}$

Table S3: Crystal data and structure refinement for **$4BF_2$**

Identification code	**$4BF_2$**
Empirical formula	C_{23} H_{27} B F_2 N_2
Formula weight	380.28
Temperature	106(2) K
Wavelength	0.71073 A

Crystal system, space group	Triclinic, P 1
Unit cell dimensions	a = 9.0546(12) Å □ = 93.097(4)°.
	b = 13.3307(17) Å □ = 99.783(4)°.
	c = 17.309(2) Å □ = 95.911(4)°.
Volume	2042.5(5) Å^3
Z, Calculated density	34, 1.571 Mg/m^3
Absorption coefficient	0.150 mm^{-1}
F(000)	952
Crystal size	0.397 x 0.216 x 0.170 mm
Theta range for data collection	2.297 to 33.670°.
Limiting indices	-14<=h<=14, -20<=k<=20, -26<=l<=26
Reflections collected / unique	118320 / 27416 [R(int) = 0.0405]
Completeness to theta = 25.242	99.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	27416 / 3 / 1009
Goodness-of-fit on F^2	1.636
Final R indices [I>2sigma(I)]	R1 = 0.1462, wR2 = 0.4158
R indices (all data)	R1 = 0.1818, wR2 = 0.4716
Absolute structure parameter	0.37(17)
Extinction coefficient	n/a
Largest diff. peak and hole	2.208 and -0.740 e. Å^{-3}

Table S4. Crystal data and structure refinement for **5BF2**.

Identification code	**5BF2**	
Empirical formula	C23 H27 B F2 N2	
Formula weight	56.84	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.9281(5) Å	a= 90°.
	b = 12.2645(4) Å	b= 95.120(4)°.
	c = 13.2506(4) Å	g = 90°.
Volume	2092.59(12) Å^3	
Z	30	
Density (calculated)	1.353 Mg/m^3	

Absorption coefficient	0.129 mm-1
F(000)	840
Crystal size	? x ? x ? mm3
Theta range for data collection	2.842 to 30.456°.
Index ranges	-18<=h<=18, -16<=k<=17, -18<=l<=15
Reflections collected	19461
Independent reflections	5648 [R(int) = 0.0301]
Completeness to theta = 25.242°	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5648 / 0 / 253
Goodness-of-fit on F2	0.965
Final R indices [I>2sigma(I)]	R1 = 0.0636, wR2 = 0.2325
R indices (all data)	R1 = 0.0957, wR2 = 0.2641
Extinction coefficient	n/a
Largest diff. peak and hole	0.474 and -0.295 e.$Å^{-3}$

Table S5. Crystal data and structure refinement for **4-Li.2THF**.

Identification code	**4-Li.2THF**
Empirical formula	C H Li N O
Formula weight	49.97
Temperature	108(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 15.8107(8) A alpha = 90 deg.
	b = 18.7330(8) A beta = 90 deg.
	c = 19.3851(9) A gamma = 90 deg.
Volume	5741.5(5) A^3
Z, Calculated density	87, 1.257 Mg/m^3
Absorption coefficient	0.101 mm^-1
F(000)	2175
Crystal size	0.347 x 0.307 x 0.299 mm
Theta range for data collection	2.415 to 31.453 deg.
Limiting indices	-22<=h<=22, -25<=k<=27, -19<=l<=28
Reflections collected / unique	51987 / 9292 [R(int) = 0.0490]
Completeness to theta = 25.242	99.6 %
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	9292 / 0 / 331
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0937, wR2 = 0.2569
R indices (all data)	R1 = 0.1143, wR2 = 0.2765
Extinction coefficient	n/a
Largest diff. peak and hole	1.601 and -1.157 e.A^-3

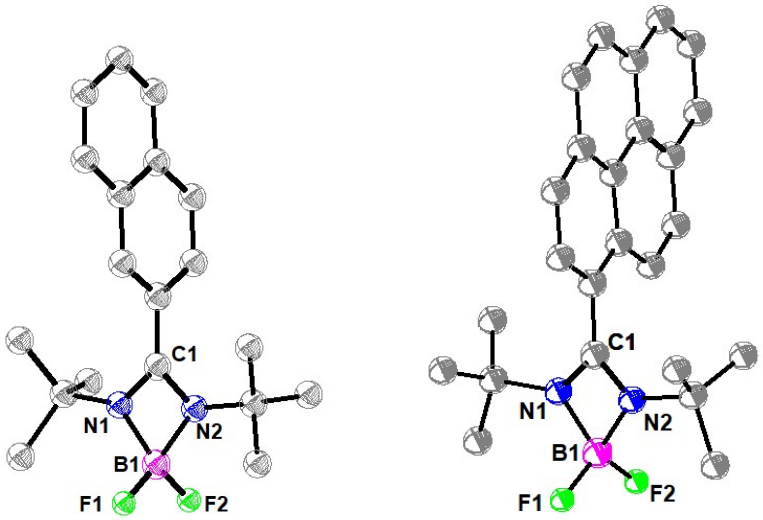
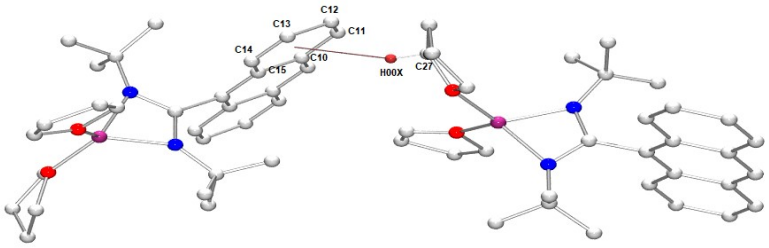
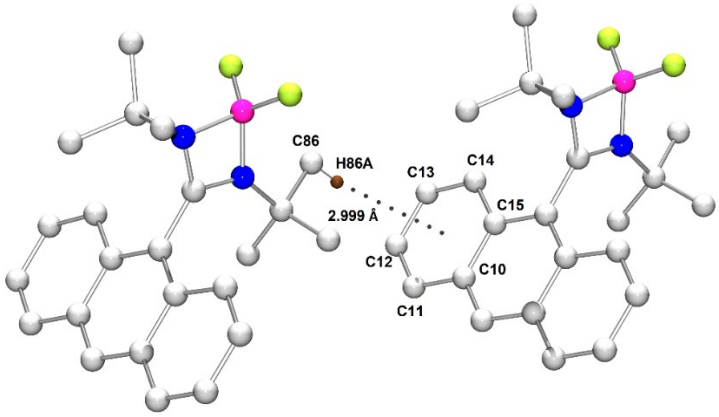


Figure S57: Solid-state structure diagram for compounds **2BF$_2$** (left) and **6BF$_2$** (right).

4-Li.2THF:



4-BF$_2$:



5-BF_2:

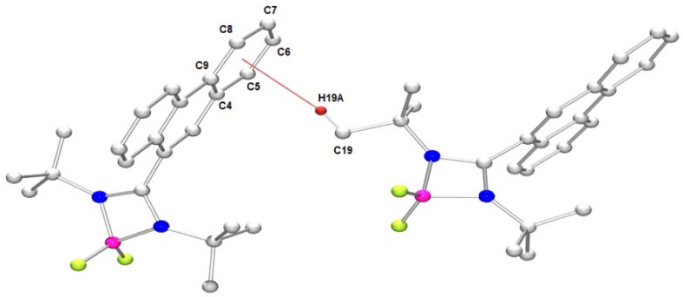


Fig. S58: Two-and 3- dimensional layer structures in the crystals of **4-Li.2THF** (top), **4-BF_2** and **5BF_2** (bottom) with a C–H···π interactions (black line) in the layer structures.

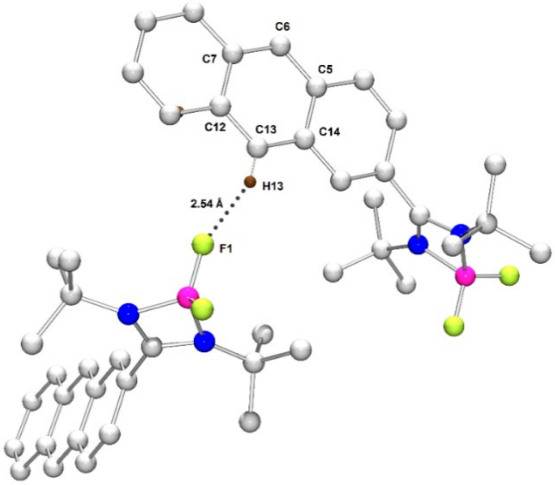


Fig. S59: Two-dimensional layer structure in the crystal of **3BF_2** with a C–H···F Hydrogen bonding interactions (black line) in the layer structures.

Table S6: Summary of photophysical properties of **1BF2-6BF2** in different solvents

Compounds	Solvent	λ_{abs}[a] /nm (ε x 10^3/M^{-1} cm^{-1})	λ_{ems}[b] (nm)	ϕ_F[c] (%)	τ[d] (ns)
1BF2	Toluene	-	297	<0.1	
	THF	263(6.4)	335, 349	<0.1	
	CH_2Cl_2	262(3.6)	333, 353, 367	<0.1	0.1
	CH_3CN	265(2.1)	365, 385	<0.1	
2BF2	Toluene	286(0.7), 321(0.1)	354, 370	1.64	
	THF	278(3.6), 322(0.3)	334, 352	0.98	
	CH_2Cl_2	279(4.8), 321(0.7)	356, 374, 414	1.07	0.6
	CH_3CN	279(3.5), 321(0.7)	370, 420	0.64	
3BF2	Toluene	329(3.2), 346(5.3), 364(7.0), 384(5.9)	448, 472	18.9	
	THF	329(2.7), 345(4.3), 362(5.7), 382(4.7)	455, 477	18.0	
	CH_2Cl_2	328(2.5), 346(3.9), 363(5.0), 384(4.2)	455, 485	48.1	11.8
	CH_3CN	328(2.6), 344(4.0), 360(5.0), 381(4.1)	456, 504	39.4	
4-BF2	Toluene	334(2.3), 351(4.5), 368(6.4), 389(5.5)	404, 418, 440, 466	8.7	
	THF	334(3.2), 350(6.0), 368(8.7), 388(7.5)	402, 418, 442, 470	10.9	
	CH_2Cl_2	335(3.0), 350(5.5), 368(7.7), 389(6.5)	420, 440, 470	17.5	3.5
	CH_3CN	332(2.4), 349(4.4), 367(6.1), 387(5.0)	417, 440, 469	12.2	
5BF2	Toluene	291(8.0), 303(8.1)	360, 372	<0.1	
	THF	290(19.1), 302(8.3)	332, 350	<0.1	
	CH_2Cl_2	291(9.3), 302(8.9)	400, 422	<0.1	0.6
	CH_3CN	290(9.4), 301(9.3)	370, 388	<0.1	
6BF2	Toluene	330(11.0), 346(14.6)	380, 430, 468	4.9	
	THF	265(13.9),277(17.0), 329(14.7), 345(19.8)	404, 446, 470	12.0	
	CH_2Cl_2	267(12.4),277(15.7), 329(12.0), 345(16.4)	450, 472	22.7	2.7
	CH_3CN	268(8.0), 276(10.8), 327(8.0), 343(11.3)	446, 470	8.1	

[a]Absorption maximum (concentration = 10^{-4} M), [b]Excited at λ_{max}, [c]Absolute fluorescence quantum yield using integrating sphere. [d]Fluorescence life-time.

Table S7: Reduction potentials and HOMO-LUMO gap derived from experiments and DFT studies.

Electrochemical		Experimental			DFT		
Compounds	($E^{1/2}_{red}$), V[a]	HOMO-LUMO gap[b]	LUMO[c] eV	HOMO[d] eV	HOMO eV	LUMO eV	HOMO-LUMO gap (eV)
$1BF_2$	-2.13	4.46	-2.46	-6.92	-6.133	-1.08	5.05
$2BF_2$	-2.02	3.91	-2.61	-6.52	-6.104	-1.629	4.47
$3BF_2$	-2.58	3.12	-2.01	-5.13	-5.674	-2.158	3.51
$4BF_2$	-2.29	3.12	-2.37	-5.49	-5.649	-2.146	3.50
$5BF_2$	-2.17	3.91	-2.56	-6.47	-6.087	-1.515	4.44
$6BF_2$	-2.80	3.47	-1.88	-5.35	-5.731	-1.991	3.74

[a]Reduction potential values ($E^{1/2}_{red}$) V of compounds **$1BF_2$-$6BF_2$** (vs. Ferrocene/Ferrocenium) with 0.1 M Bu_4NPF_6 in THF as the supporting electrolyte (scan rate 100 mV/s). [b]Absorption onset of the longest wavelength of UV band. [c]Calculated from E_{pc} of the reduction wave with reference to Fc/Fc^+. [d]Calculated from HOMO-LUMO gap and LUMO.

4. Computational studies

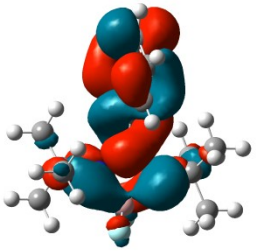
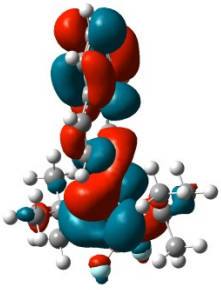
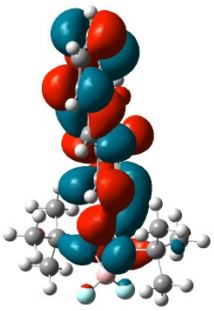
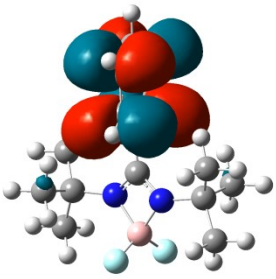
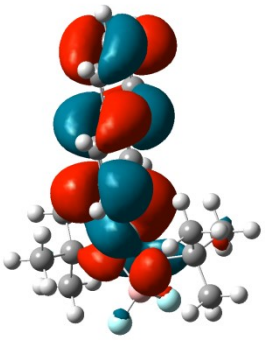
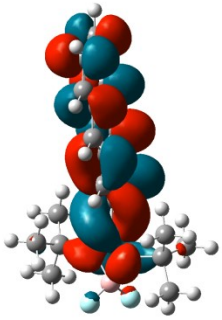
Table S8: Calculated electronic transitions for compound **$1BF_2$-$6BF_2$** from TD-DFT (B3LYP) calculations

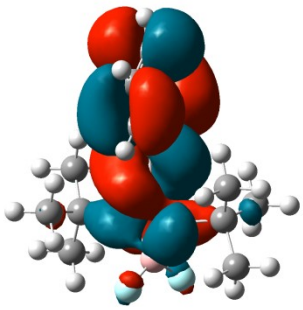
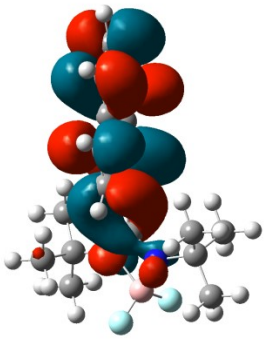
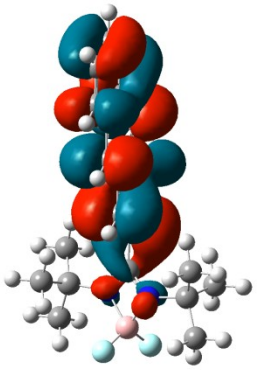
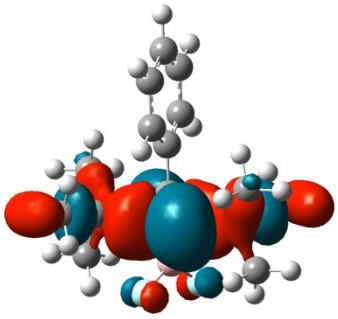
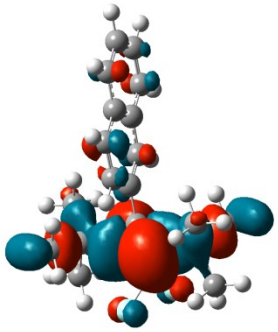
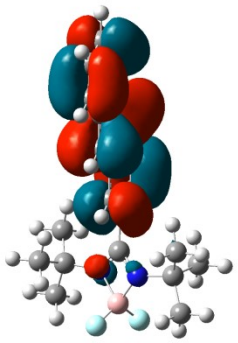
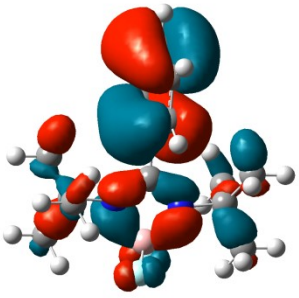
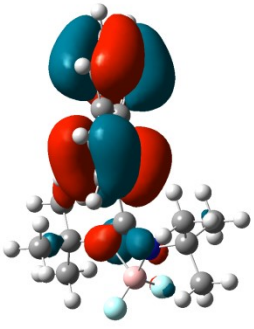
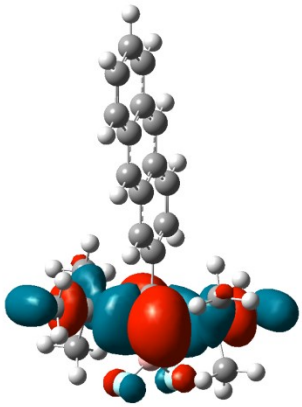
Compound	Transition	MO contributions	Energy gap eV (nm)	Oscillator strength/f
$1BF_2$	$S_0 \rightarrow S_1$	HOMO→LUMO HOMO→LUMO+2	4.38 (282)	0.0413
	$S_0 \rightarrow S_2$	HOMO→LUMO+1	4.79 (258)	0.0022
	$S_0 \rightarrow S_3$	HOMO-2→LUMO HOMO-1→LUMO+1	5.28 (234)	0.0012
$2BF_2$	$S_0 \rightarrow S_1$	HOMO→LUMO	3.85 (321)	0.0122
	$S_0 \rightarrow S_2$	HOMO-2→LUMO HOMO-2→LUMO+1	4.27 (290)	0.0323

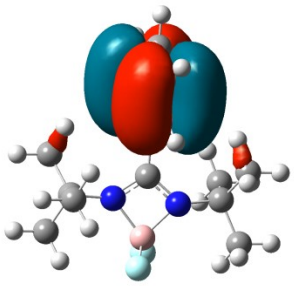
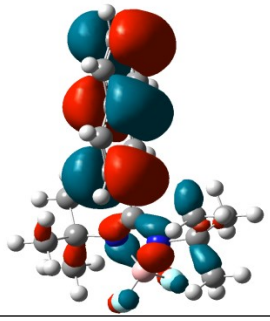
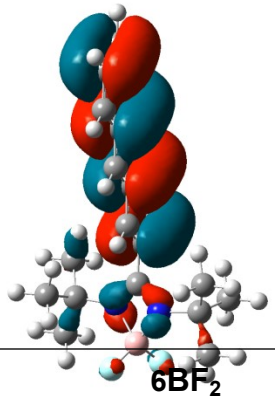
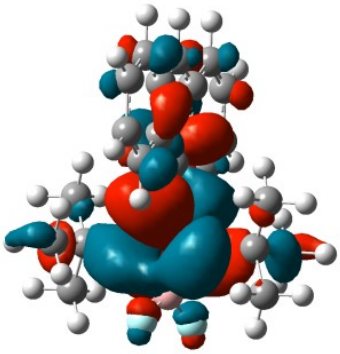
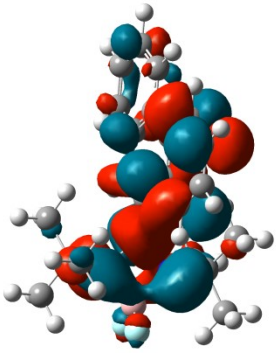
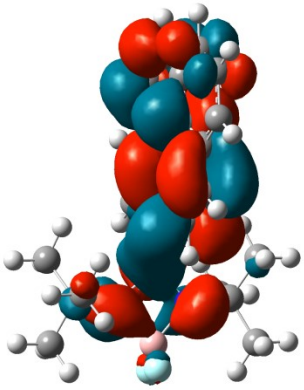
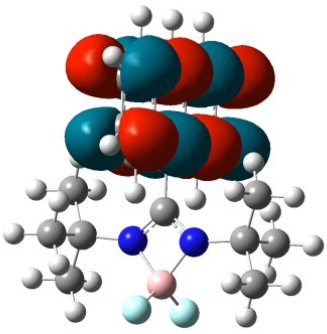
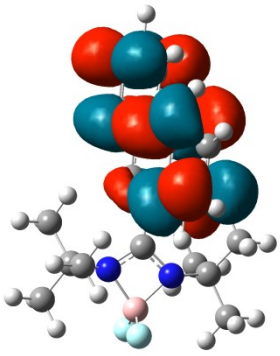
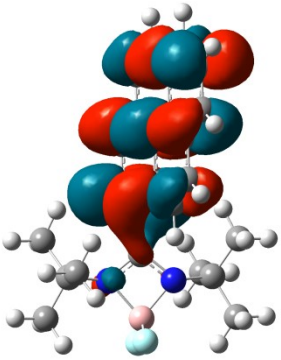
		HOMO-1→LUMO HOMO-1→LUMO+1		
	$S_0 \rightarrow S_3$	HOMO-2→LUMO HOMO-1→LUMO HOMO-1→LUMO+1 HOMO→LUMO+1	4.39 (281)	0.0113
$3BF_2$	$S_0 \rightarrow S_1$	HOMO-2→LUMO+1 HOMO→LUMO	3.18 (389)	0.0466
	$S_0 \rightarrow S_2$	HOMO-1→LUMO	3.40 (363)	0.0060
	$S_0 \rightarrow S_3$	HOMO-2→LUMO HOMO→LUMO+1	3.79 (326)	0.0004
$4BF_2$	$S_0 \rightarrow S_1$	HOMO-2→LUMO+1 HOMO→LUMO	3.17 (390)	0.0942
	$S_0 \rightarrow S_2$	HOMO-1→LUMO	3.21 (386)	0.0013
	$S_0 \rightarrow S_3$	HOMO-2→LUMO HOMO→LUMO+1	3.87 (320)	0.0035
$5BF_2$	$S_0 \rightarrow S_1$	HOMO-1→LUMO HOMO→LUMO	3.79 (326)	0.0100
	$S_0 \rightarrow S_2$	HOMO-2→LUMO HOMO-1→LUMO+1 HOMO→LUMO+1	3.95 (313)	0.0003
	$S_0 \rightarrow S_3$	HOMO-2→LUMO+1 HOMO-1→LUMO	4.15 (298)	0.1001

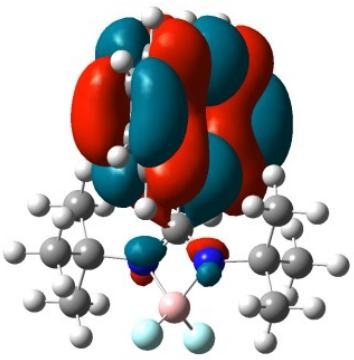
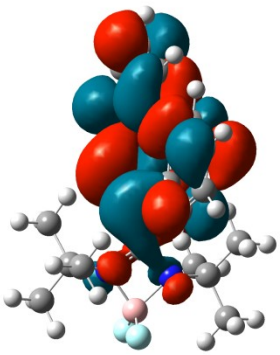
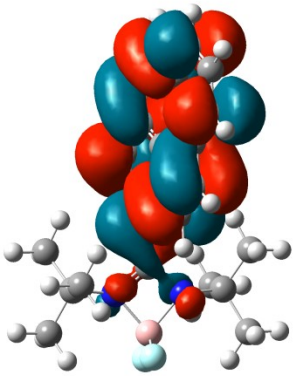
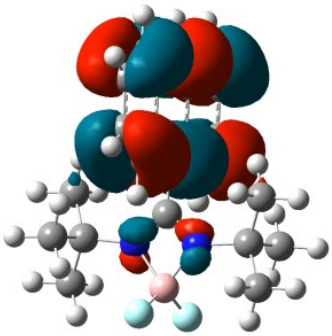
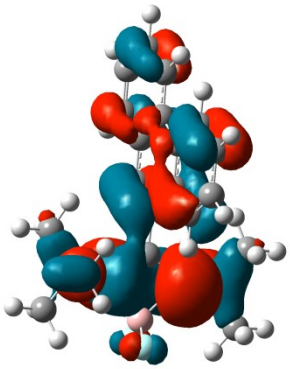
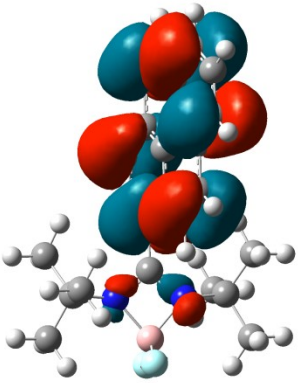
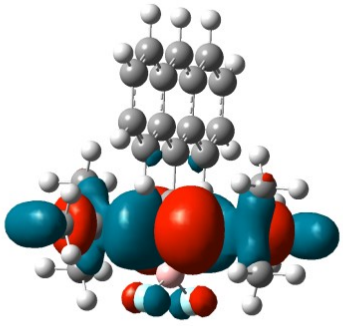
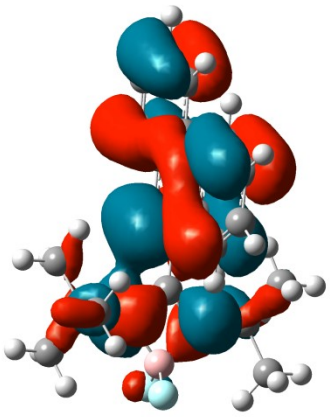
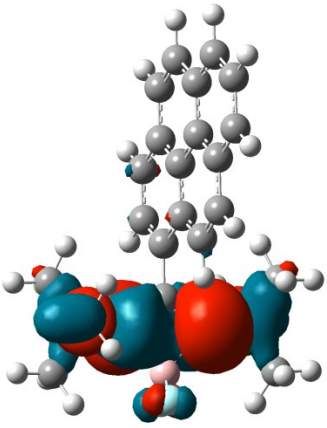
		HOMO→LUMO		
6BF$_2$	$S_0 \rightarrow S_1$	HOMO-1→LUMO HOMO→LUMO	3.49 (355)	0.0126
	$S_0 \rightarrow S_2$	HOMO-2→LUMO+1 HOMO-1→LUMO HOMO→LUMO	3.58 (345)	0.3303
	$S_0 \rightarrow S_3$	HOMO-2→LUMO HOMO→LUMO+1	3.74 (331)	0.0048

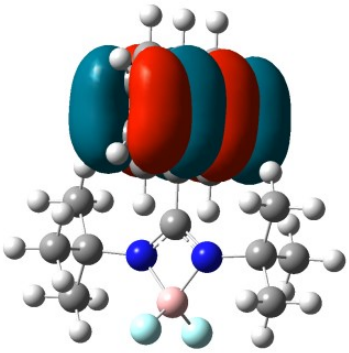
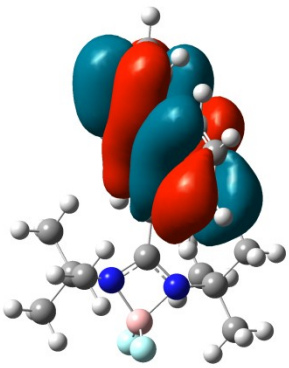
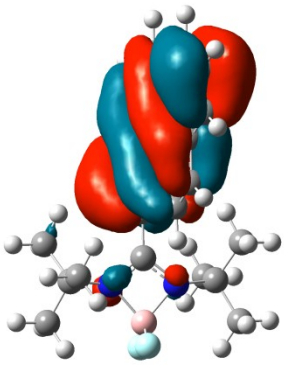
Table S9: Computed orbitals for compounds**1-6BF$_2$**

Compound	**1BF$_2$**	**2BF$_2$**	**3BF$_2$**
LUMO+2	 -0.031 eV(78)	 -0.134 eV(91)	 -0.380 eV(104)
LUMO+1	 -0.641 eV(77)		

		-0.953 eV(90)	-0.992 eV(103)
LUMO	 -1.080 eV(76)	 -1.629 eV(89)	 -2.158 eV(102)
HOMO	 -6.133 eV(75)	 -6.104 eV(88)	 -5.674 eV(101)
HOMO-1	 -7.218 eV(74)	 -6.331 eV(87)	 -6.115 eV(100)

HOMO-2	 -7.384 eV(73)		
Compound	**$4BF_2$**	**$5BF_2$**	**$6BF_2$**
LUMO+2	 -0.437 eV(104)	 -0.489 eV(104)	 -0.549 eV(110)
LUMO+1	 -0.724 eV(103)	 -1.237 eV(103)	 -1.079 eV(109)

LUMO	 -2.146 eV(102)	 -1.600 eV(102)	 -1.991 eV(108)
HOMO	 -5.649 eV(101)	 -6.048 eV(101)	 -5.731 eV(107)
HOMO-1	 -6.028 eV(100)	 -6.227 eV(100)	 -6.079 eV(106)

HOMO-2	 -6.889 eV(99)	 -6.431 eV(99)	 -6.631 eV(105)

Compound $1BF_2$

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

---

1 9 0 2.814379 0.305490 -1.106761
2 7 0 0.846662 1.019607 0.249890
3 6 0 0.012392 -0.000005 -0.000009
4 6 0 -1.473061 -0.000113 -0.000006
5 6 0 0.723900 2.471013 -0.010685
6 6 0 -2.178504 0.192451 1.196090
7 1 0 -1.631389 0.345757 2.120713
8 6 0 -0.419234 3.099995 0.803656
9 1 0 -0.404087 4.187221 0.675233
10 1 0 -1.399352 2.740441 0.483094
11 1 0 -0.300889 2.882465 1.869699
12 6 0 2.062899 3.088614 0.431345
13 1 0 2.044525 4.172585 0.283687
14 1 0 2.250577 2.885277 1.489825
15 1 0 2.889756 2.672752 -0.149309
16 6 0 -3.572906 0.183754 1.194652
17 1 0 -4.112775 0.324740 2.126043
18 6 0 -4.271668 -0.000303 0.000004
19 1 0 -5.357511 -0.000378 0.000007
20 6 0 0.509481 2.714564 -1.518843
21 1 0 0.508264 3.787558 -1.738635

22 1 0 1.309039 2.241097 -2.094308
23 1 0 -0.449997 2.302990 -1.849110
24 5 0 2.061189 0.000161 -0.000006
25 9 0 2.814423 -0.305055 1.106750
26 7 0 0.846829 -1.019487 -0.249894
27 6 0 0.724322 -2.470915 0.010690
28 6 0 -2.178486 -0.192769 -1.196098
29 1 0 -1.631356 -0.345997 -2.120726
30 6 0 -0.418718 -3.100115 -0.803615
31 1 0 -0.403379 -4.187335 -0.675163
32 1 0 -1.398893 -2.740726 -0.483046
33 1 0 -0.300429 -2.882594 -1.869667
34 6 0 2.063420 -3.088274 -0.431374
35 1 0 2.045245 -4.172249 -0.283712
36 1 0 2.251034 -2.884906 -1.489858
37 1 0 2.890216 -2.672262 0.149259
38 6 0 -3.572888 -0.184264 -1.194650
39 1 0 -4.112745 -0.325323 -2.126038
40 6 0 0.509991 -2.714500 1.518856
41 1 0 0.508970 -3.787494 1.738652
42 1 0 1.309482 -2.240889 2.094296
43 1 0 -0.449550 -2.303094 1.849149

Compound $2BF_2$

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
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1 9 0 -3.497909 -0.175308 -1.412580
2 9 0 -3.795735 0.378285 0.795675
3 7 0 -1.628647 1.050919 -0.243122
4 6 0 -0.875032 -0.006008 0.093169
5 6 0 0.592249 -0.064992 0.312458
6 6 0 2.869544 0.079978 -0.547783
7 6 0 1.464708 0.146337 -0.737875
8 1 0 1.075484 0.363359 -1.728323
9 7 0 -1.772541 -0.998422 0.189980
10 6 0 3.380538 -0.194111 0.762718
11 6 0 3.784945 0.281815 -1.615853
12 1 0 3.394243 0.489086 -2.608388
13 6 0 2.459946 -0.398178 1.825920
14 1 0 2.845558 -0.602691 2.820963
15 6 0 -1.490717 2.490495 0.072734
16 6 0 5.647394 -0.053582 -0.102985
17 1 0 6.720738 -0.102291 0.054071
18 6 0 -1.661648 -2.446589 -0.094205

19 6 0 4.786714 -0.253803 0.952368
20 1 0 5.172637 -0.461452 1.946757
21 6 0 1.103502 -0.345205 1.610879
22 1 0 0.408647 -0.511514 2.427252
23 6 0 5.142177 0.216627 -1.398729
24 1 0 5.832945 0.372592 -2.221796
25 5 0 -2.901363 0.072252 -0.200687
26 6 0 -0.266020 3.108082 -0.624296
27 1 0 -0.302491 2.924101 -1.702588
28 1 0 -0.260828 4.191284 -0.464313
29 1 0 0.673331 2.709011 -0.235932
30 6 0 -2.769562 3.159243 -0.463037
31 1 0 -2.868740 2.993708 -1.539946
32 1 0 -3.653560 2.747836 0.029442
33 1 0 -2.735849 4.237224 -0.278885
34 6 0 -1.209888 -2.661686 -1.553499
35 1 0 -0.196231 -2.279014 -1.711320
36 1 0 -1.208259 -3.728428 -1.801702
37 1 0 -1.888547 -2.145459 -2.237395
38 6 0 -1.400901 2.687493 1.599652
39 1 0 -1.390161 3.753803 1.849562
40 1 0 -2.261058 2.224159 2.090338
41 1 0 -0.485579 2.240146 2.000953
42 6 0 -0.692918 -3.141243 0.877523
43 1 0 -0.986577 -2.955525 1.915342
44 1 0 -0.715182 -4.222452 0.706570
45 1 0 0.337335 -2.804552 0.743179
46 6 0 -3.076451 -3.020548 0.101389
47 1 0 -3.428490 -2.839394 1.121288
48 1 0 -3.780391 -2.554036 -0.591780
49 1 0 -3.072518 -4.099788 -0.079051

Compound $3BF_2$

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

---

1 9 0 -4.792862 0.416747 0.546517
2 9 0 -4.302900 -0.057422 -1.646138
3 7 0 -2.749526 -0.982294 0.073172
4 7 0 -2.526443 1.079317 -0.259967
5 6 0 -0.389594 -0.109468 0.452870
6 6 0 2.346093 -0.336750 1.166159
7 6 0 4.323366 0.187795 -0.805754
8 6 0 -1.827767 -0.007336 0.101118

9 6 0 1.965585 0.042975 -0.174405
10 6 0 0.577443 0.154111 -0.488612
11 1 0 0.289689 0.448449 -1.493542
12 6 0 4.704495 -0.193122 0.535412
13 6 0 2.963937 0.295138 -1.123751
14 1 0 2.676240 0.581232 -2.132613
15 6 0 3.704656 -0.443855 1.484204
16 1 0 3.991560 -0.729947 2.493325
17 6 0 -2.639279 -2.418445 -0.269155
18 6 0 5.352621 0.441984 -1.765125
19 1 0 5.063578 0.728485 -2.772715
20 6 0 -0.008585 -0.492386 1.780234
21 1 0 -0.784887 -0.696148 2.509974
22 6 0 6.674208 0.327188 -1.425040
23 1 0 7.446143 0.522816 -2.163208
24 6 0 1.312480 -0.591631 2.121000
25 1 0 1.595912 -0.872446 3.131618
26 6 0 6.095493 -0.301184 0.847007
27 1 0 6.380473 -0.588034 1.855640
28 6 0 -2.398838 2.499148 0.141404
29 6 0 7.050273 -0.049391 -0.102170
30 1 0 8.103410 -0.135208 0.148146
31 5 0 -3.815975 0.128681 -0.375359
32 6 0 -2.048813 -2.575339 -1.685286
33 1 0 -2.644798 -2.009313 -2.405845
34 1 0 -2.045120 -3.628680 -1.985227
35 1 0 -1.016722 -2.211806 -1.721691
36 6 0 -4.077687 -2.966250 -0.241737
37 1 0 -4.526012 -2.823672 0.746070
38 1 0 -4.077049 -4.035954 -0.471940
39 1 0 -4.699570 -2.451678 -0.977927
40 6 0 -1.787072 -3.181942 0.758323
41 1 0 -0.741713 -2.865853 0.744189
42 1 0 -1.814449 -4.253099 0.533128
43 1 0 -2.179962 -3.037602 1.769559
44 6 0 -1.096243 3.124557 -0.386589
45 1 0 -0.210894 2.689042 0.081074
46 1 0 -1.093511 4.198489 -0.173515
47 1 0 -1.017368 2.993490 -1.470347
48 6 0 -2.472504 2.617387 1.677315
49 1 0 -3.388776 2.149186 2.046295
50 1 0 -2.469760 3.669202 1.982715
51 1 0 -1.614407 2.128676 2.150754
52 6 0 -3.600320 3.221491 -0.494707
53 1 0 -3.584475 3.109840 -1.582991
54 1 0 -3.567961 4.288472 -0.254594

55 1 0 -4.539740 2.807509 -0.121676

Compound $4BF_2$

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

---

1 9 0 3.566865 1.065509 0.416203
2 9 0 3.565020 -1.071792 -0.419285
3 6 0 -1.425362 -1.225494 -0.120448
4 6 0 0.758449 -0.001524 0.000668
5 6 0 -3.547712 0.001672 0.000380
6 1 0 -4.635201 0.002650 0.000864
7 6 0 -2.869616 -1.214480 -0.128094
8 7 0 1.596966 -0.359099 0.984825
9 6 0 -3.568859 2.455779 0.264061
10 1 0 -4.655328 2.434166 0.269495
11 6 0 -3.572550 -2.452410 -0.263734
12 1 0 -4.658999 -2.429308 -0.268862
13 6 0 1.490035 0.342676 -2.457633
14 6 0 -0.730871 -0.000414 0.000211
15 6 0 -1.423490 1.225964 0.120738
16 6 0 -0.756913 2.487573 0.243592
17 1 0 0.327023 2.514814 0.222277
18 6 0 -2.898294 -3.637013 -0.384146
19 1 0 -3.443425 -4.570334 -0.487312
20 6 0 -1.474199 -3.651337 -0.372109
21 1 0 -0.949225 -4.597444 -0.463949
22 6 0 -1.468849 3.651794 0.371814
23 1 0 -0.942404 4.597165 0.463091
24 7 0 1.597239 0.355193 -0.984250
25 6 0 -0.760611 -2.488278 -0.243604
26 1 0 0.323368 -2.517074 -0.222681
27 6 0 -2.867618 1.216942 0.128510
28 6 0 -2.892856 3.639538 0.384072
29 1 0 -3.436615 4.573664 0.487163
30 5 0 2.810656 -0.002413 -0.001724
31 6 0 1.490495 -0.342536 2.458298
32 6 0 1.512470 -1.113374 -2.970265
33 1 0 1.540337 -1.131064 -4.065146
34 1 0 2.393580 -1.634771 -2.588756
35 1 0 0.619767 -1.657477 -2.646774
36 6 0 2.737458 1.087754 -2.968325
37 1 0 2.732081 1.126832 -4.061857
38 1 0 2.762241 2.111403 -2.583363
39 1 0 3.650576 0.579399 -2.647094

40 6 0 0.225444 1.061998 -2.952794
41 1 0 0.250828 1.124793 -4.045307
42 1 0 -0.685967 0.529304 -2.672016
43 1 0 0.166896 2.078805 -2.554616
44 6 0 0.223963 -1.057126 2.955357
45 1 0 -0.686232 -0.525065 2.669354
46 1 0 0.165135 -2.076264 2.563402
47 1 0 0.246904 -1.113111 4.048374
48 6 0 2.735766 -1.090118 2.970474
49 1 0 2.740799 -1.108395 4.064560
50 1 0 2.746931 -2.121180 2.605004
51 1 0 3.650444 -0.596697 2.631059
52 6 0 1.517688 1.114625 2.967302
53 1 0 0.622062 1.658076 2.650852
54 1 0 1.555523 1.134813 4.061812
55 1 0 2.395416 1.634984 2.576821

Compound $5BF_2$

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

---

1 9 0 -3.859926 0.152592 -1.444560
2 9 0 -3.962646 0.055343 0.846475
3 6 0 -1.109247 0.065246 -0.176169
4 7 0 -1.956428 -0.971864 -0.287306
5 6 0 -1.830359 2.449848 0.502486
6 7 0 -1.932724 1.119985 -0.134510
7 5 0 -3.157957 0.089745 -0.265932
8 6 0 -1.818713 -2.270640 -0.982728
9 6 0 -1.819128 2.293378 2.037301
10 1 0 -1.844224 3.275446 2.521677
11 1 0 -2.690518 1.720353 2.363893
12 1 0 -0.915406 1.775012 2.372539
13 6 0 -3.095651 3.213309 0.069727
14 1 0 -3.091662 4.220750 0.496750
15 1 0 -3.143960 3.296775 -1.019911
16 1 0 -3.994928 2.695855 0.413804
17 6 0 -0.584447 3.218407 0.032916
18 1 0 -0.610495 4.234151 0.440529
19 1 0 0.341515 2.747583 0.369291
20 1 0 -0.559116 3.291364 -1.058728
21 6 0 -0.661388 -3.103540 -0.408451
22 1 0 0.309631 -2.637189 -0.590321
23 1 0 -0.777784 -3.246473 0.669489
24 1 0 -0.651113 -4.089537 -0.884232

25 6 0 -3.148179 -3.011013 -0.750869
26 1 0 -3.120082 -3.994275 -1.230114
27 1 0 -3.331740 -3.150482 0.318572
28 1 0 -3.983073 -2.444743 -1.171510
29 6 0 -1.613699 -2.034819 -2.493911
30 1 0 -0.656304 -1.539801 -2.685999
31 1 0 -1.612980 -2.988094 -3.033260
32 1 0 -2.416792 -1.408705 -2.890093
33 6 0 0.378251 0.048270 -0.134088
34 6 0 1.069363 0.480085 -1.229743
35 6 0 1.082097 -0.405796 1.047212
36 6 0 2.499864 0.486146 -1.267893
37 1 0 0.528228 0.831743 -2.103445
38 6 0 2.510358 -0.396934 1.053296
39 6 0 0.384391 -0.842425 2.199606
40 6 0 3.184245 0.926206 -2.425141
41 6 0 3.236691 0.049327 -0.129154
42 6 0 3.170621 -0.828389 2.227895
43 1 0 -0.700013 -0.860040 2.183969
44 6 0 1.062841 -1.256112 3.328965
45 6 0 4.563305 0.938666 -2.470741
46 1 0 2.601773 1.255391 -3.281415
47 6 0 4.648687 0.073446 -0.208862
48 6 0 2.468449 -1.247883 3.341660
49 1 0 4.253622 -0.831437 2.265507
50 1 0 0.510593 -1.587288 4.202967
51 6 0 5.297805 0.506970 -1.350436
52 1 0 5.079670 1.278038 -3.363348
53 1 0 5.245806 -0.253364 0.634437
54 1 0 3.006171 -1.571761 4.227623
55 1 0 6.383244 0.513220 -1.380808

Compound $6BF_2$

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---
1 9 0 -4.663003 0.364764 0.263338
2 9 0 -3.841836 0.021364 -1.852365
3 6 0 -1.652995 -0.036259 0.236286
4 7 0 -2.304763 1.072866 -0.153123
5 6 0 -2.418717 -2.433560 -0.326078
6 7 0 -2.554369 -1.002732 0.019188
7 5 0 -3.554484 0.135188 -0.513778
8 6 0 -2.247119 2.463398 0.350433
9 6 0 -1.749081 -2.578089 -1.708308

10 1 0 -1.739630 -3.627999 -2.020296
11 1 0 -2.297606 -1.997184 -2.454070
12 1 0 -0.713676 -2.224506 -1.682987
13 6 0 -3.856255 -2.981788 -0.387829
14 1 0 -3.842341 -4.049349 -0.627170
15 1 0 -4.363948 -2.846361 0.571678
16 1 0 -4.433788 -2.462378 -1.156849
17 6 0 -1.623321 -3.204644 0.740090
18 1 0 -1.640858 -4.273653 0.504586
19 1 0 -0.578692 -2.889340 0.782636
20 1 0 -2.067111 -3.067941 1.731076
21 6 0 -0.845973 3.074454 0.187034
22 1 0 -0.105808 2.576931 0.817619
23 1 0 -0.510016 3.014587 -0.852031
24 1 0 -0.873940 4.130054 0.476080
25 6 0 -3.254900 3.256382 -0.500666
26 1 0 -3.269884 4.304797 -0.187761
27 1 0 -2.984309 3.213591 -1.559880
28 1 0 -4.261326 2.846069 -0.386472
29 6 0 -2.676683 2.498201 1.832216
30 1 0 -1.957186 1.961463 2.459348
31 1 0 -2.729426 3.531489 2.191730
32 1 0 -3.658900 2.034789 1.952666
33 6 0 -0.277457 -0.158296 0.786530
34 6 0 0.859494 0.011339 -0.038521
35 6 0 -0.123303 -0.452455 2.147508
36 6 0 2.157997 -0.123854 0.545380
37 6 0 0.767017 0.300559 -1.445721
38 6 0 1.138651 -0.568441 2.717392
39 1 0 -1.008534 -0.588379 2.760596
40 6 0 3.325071 0.030252 -0.263041
41 6 0 2.295471 -0.411156 1.938246
42 6 0 1.883207 0.442020 -2.212599
43 1 0 -0.215220 0.415958 -1.890758
44 1 0 1.235960 -0.787939 3.776714
45 6 0 3.200278 0.314092 -1.656169
46 6 0 4.623081 -0.099372 0.318864
47 6 0 3.613882 -0.533926 2.495878
48 1 0 1.789649 0.660114 -3.272980
49 6 0 4.361350 0.460243 -2.432003
50 6 0 5.755486 0.056057 -0.496482
51 6 0 4.724283 -0.385159 1.723251
52 1 0 3.705708 -0.751276 3.556442
53 6 0 5.623492 0.332279 -1.855966
54 1 0 4.264825 0.676186 -3.492446
55 1 0 6.742819 -0.042093 -0.053566

56 1 0 5.714506 -0.482146 2.160154
57 1 0 6.510900 0.448831 -2.470735
