Supporting Information

Organochalcogen Substituted Dimesityl Borane-Imidazole as Fluorogenic Fluoride and Cyanide Sensors in Aqueous Media

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Table S1: Crystallographic data and structure refinements for compounds

Compound	**6**	**7**	**8**
Empirical formula	$C_{34}H_{37}BN_2P$	$C_{28}H_{31}BN_2S$	$C_{28}H_{31}BN_2Se$
Formula weight	515.43	438.42	485.32
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/n$	*Pbca*	$P2_1/c$
a (Å)	15.112(2)	13.4720(6)	14.2614(11)
b (Å)	14.106(2)	16.3785(8)	14.9900(11)
c (Å)	15.546(2)	22.3897(10)	12.0328(9)
α, deg	90	90	90
β, deg	118.500(3)	90	112.336(2)
γ, deg	90	90	90
Volume/Å^3	2912.2(8)	4940.3(4)	2379.4(3)
Z	4	8	4
ρ_{calc} g/cm^3	1.176	1.179	1.355
μ, mm^{-1}	0.119	0.149	1.597
F(000)	1100.0	1872.0	1008.0
Temperature/K	100	100	100
Reflections collected	41305	56748	38401
Indep. reflns	7286	4229	5908
Data/restraints/parameters	7286/0/326	4229/0/296	5908/0/296
GOOF	1.043	1.028	1.027
R_1/wR_2 [$I>=2\sigma(I)$]	0.0572/0.1403	0.0367/0.0919	0.0311/0.0725
R_1/wR_2 [all data]	0.0922/0.1689	0.0457/0.1018	0.0417/0.0784

Table S1 Contd…

Compound	**11**	**11**-[F]	**7**-[CN]
Empirical formula	$C_{36}H_{39}BF_3N_2O_3PS$	$C_{35}H_{39}BFN_2P$	$C_{45}H_{67}BN_4S$
Formula weight	678.53	548.46	706.89
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/n$
a (Å)	12.4503(11)	12.8449(3)	11.7479(12)
b (Å)	10.8386(9)	15.6528(3)	24.278(3)
c (Å)	25.637(2)	15.9764(5)	16.0030(16)
α, deg	90	90	90
β, deg	90.125(3)	108.0330(10)	110.599(3)
γ, deg	90	90	90
Volume/Å^3	3459.6(5)	3054.40(13)	4272.4(8)
Z	4	4	4
ρ_{calc} g/cm^3	1.303	1.193	1.099
μ, mm^{-1}	0.194	0.119	0.110
F(000)	1424.0	1012.0	1544.0
Temperature/K	100	100	100
Reflections collected	45944	37420	67903
Indep. reflns	6798	5399	10571
Data/restraints/parameters	6798/0/432	5399/0/369	10571/0/471
GOOF	1.123	1.050	1.037
R_1/wR_2 [$I>=2\sigma(I)$]	0.0515/ 0.1015	0.0509/ 0.1311	0.0563/ 0.1369
R_1/wR_2 [all data]	0.0618/0.1058	0.0578/ 0.1368	0.0897/ 0.1587

Table S1 Contd…

Compound	**8**-[F]	**8**-[CN]	**9**-[F]
Empirical formula	$C_{44}H_{67}BFN_3Se$	$C_{45}H_{67}BN_4Se$	$C_{29}H_{34}BFN_2S$
Formula weight	746.77	753.80	472.45
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	P-1
a (Å)	13.5024(14)	11.6472(5)	8.2537(18)
b (Å)	20.021(2)	24.2300(12)	12.713(3)
c (Å)	15.4145(16	16.1687(8)	13.316(3)
α, deg	90	90	104.864(6)
β, deg	98.496(3)	110.482(2)	98.674(6)
γ, deg	90	90	106.478(6)
Volume/Å^3	4121.4(7)	4274.5(4)	1256.8(5)
Z	4	4	2
ρ_{calc}g/cm^3	1.204	1.171	1.248
μ, mm^{-1}	0.949	0.913	0.157
F(000)	1600.0	1616.0	504.0
Temperature/K	100	100	100
Reflections collected	64816	60245	13789
Indep. reflns	10239	10356	4381
Data/restraints/parameters	10239/0/462	10356/0/471	4381/0/297
GOOF	0.967	1.045	1.128
R_1/wR_2 [I>=2σ (I)]	0.0348/ 0.1110	0.0499/ 0.1083	0.1153/0.2958
R_1/wR_2 [all data]	0.0527/ 0.1306	0.0888/ 0.1223	0.1272/0.3023

Table S2: Selected bond parameters of compounds 7 and 8

Compound	**7**	**8**
Bond Distance (Å)	N1-C2 1.360(2), N1-C5 1.392(2), N1-C6 1.454(2), N3-C2 1.324(2), N3-C4 1.363(2), C5-C4 1.383(2), C5-B1 1.541(2), C2-S1 1.7512(17), C25-S1 1.7823(17), C7-B1 1.582(2) C16-B1 1.574(2),	N1-C2 1.356(2), N1-C5 1.396(2), N1-C6 1.464(2), N3-C2 1.330(2), N3-C4 1.361(2), C4-C5 1.389(2), C5-B1 1.534(2), Se1-C2 1.9053(17) Se1-C25 1.9300(18) , C7-B1 1.577(2), C16-B1 1.576(2),
Bond Angles (°)	C5-N1-C6 126.33(13), N3-C4-C5 112.52(15), C2-N1-C5 107.29(13), C2-N1-C6 126.17(14), C2-N3-C4 104.18(14), N1-C5-B1 127.90(14), C4-C5-N1 103.47(14), C4-C5-B1 128.14(15), N1-C2-S1 124.43(13), N3-C2-N1 112.49(15), N3-C2-S1 122.84(13), C5-B1-C16 116.17(14), C5-B1-C7 120.42(14), C16-B1-C7 123.41(15), C2-S1-C25 102.89(8)	C2-Se1-C25 93.18(7), C2-N1-C5 107.43(14), C2-N1-C6 125.61(15), C5-N1-C6 126.71(14), C2-N3-C4 104.05(14), N3-C4-C5 112.62(15), N1-C2-Se1 123.02(13), N3-C2-Se1 124.21(13), N3-C2-N1 112.63(15), N1-C5-B1 128.37(15), C4-C5-N1 103.25(14), C4-C5-B1 126.35(16), C5-B1-C16 117.24(15), C5-B1-C7 118.27(15), C16-B1-C7 124.46(15)

Selected bond parameters of compounds 6 and 11

Compound	**6**	**11**
Bond distance (Å)	C5 B1 1.537(3), C5 C4 1.389(3), P1 C2 1.829(2), N1 C5 1.389(2), N1 C2 1.362(3), N3 C4 1.360(3), N3 C2 1.336(3), C7 B1 1.571(3), C16 B1 1.580(3), P1 C31 1.833(2), P1 C25 1.827(2), N1 C6 1.457(3)	C5 B1 1.552(3), C5 C4 1.362(3), P1 C2 1.842(2) , N1 C5 1.395(3) , N1 C2 1.344(3) , N3 C4 1.364(3) , N3 C2 1.356(3) , C8 B1 1.579(3), C17 B1 1.573(3), P1 C26 1.828(2) , P1 C32 1.828(2), N3 C7 1.471(3) , N1 C6 1.467(3)
Bond angles (°)	C5 B1 C7 121.52(17), C5 B1 C16 115.04(17), C7 B1 C16 123.34(17), N1 C2 P1 122.63(15), N3 C2 P1 125.63(15), N3 C2 N1 111.71(17), N3 C4 C5 112.83(18), N1 C5 C4 103.05(17), N1 C5 B1 129.05(18),	C26 P1 C2 104.70(10), C32 P1 C2 99.05(10) , C32 P1 C26 103.17(10), C2 N3 C4 108.75(17) , C2 N3 C7 128.75(17) , C4 N3 C7 122.46(17) , C2 N1 C5 110.67(17) , C2 N1 C6 124.23(18) , C5 N1 C6 125.06(17), N3 C2 P1 132.87(16), N1 C2 P1 120.10(15), N1 C2 N3 106.66(17), N1 C5 B1 129.59(19), C4 C5 N1 104.46(18), C4 C5 B1 125.39(19),

C4 C5 B1 127.40(18)	C5 B1 C8 113.58(19), C5 B1 C17 121.54(19)	

Selected bond parameters of compound 7-[CN]**, 8**-[F] **and 8**-[CN]

Compound	**7**-[CN]	**8**-[F]	**8**-[CN]
Bond distance (Å)	S1-C2 1.751(2), S1-C25 1.791(2), C31-B1 1.634(3), C5-C4 1.379(2) C5-B1 1.623(3), N1-C5 1.389(2), N1-C2 1.362(2), N1-C6 1.451(2), N3-C4 1.372(2), N3-C2 1.326(2), C16-B1 1.654(3) , C7-B1 1.659(3) , C31-B1 1.634(3)	Se1-C2 1.8943(18), Se1-C25 1.9215(19), F1-B1 1.483(2), C5-C4 1.373(2), C5-B1 1.633(2) N1-C5 1.389(2), C8-C7 1.416(2), N1-C2 1.362(2), N1-C6 1.454(2), N3-C2 1.321(2), N3-C4 1.380(2), C8-C9 1.404(2), C7-B1 1.660(2), C16-B1 1.660(2),	Se1-C2 1.889(2), Se1-C26 1.932(3), C7-B1 1.626(4), C5-C4 1.375(3), C5-B1 1.625(4) N1-C5 1.385(3), N1-C2 1.360(3), N1-C6 1.459(3), N2-C2 1.317(3), N2-C4 1.372(3), N4-C7 1.150(3), C17-B1 1.657(4), C8-B1 1.659(4),
Bond Angle (°)	C2-S1-C25 101.78(10), C5-N1-C6 126.08(16), C2-N1-C5 108.41(15), C2-N1-C6 125.44(16), N3-C4-C5 112.86(16),	C2-Se1-C25 100.62(8), C5-N1-C6 126.80(14), C2-N1-C5 108.06(14), C5-C4-N3 112.89(15), C2-N1-C6 125.00(14),	C2-Se1-C26 98.93(12), C5-N1-C6 125.9(2), C2-N1-C5 108.5(2), C2-N1-C6 125.5(2), C2-N2-C4 104.2(2), N4-C7-B1 173.1(3), N1-C5-B1 128.1(2), C4-C5-N1 102.8(2), C4-C5-B1 129.1(2),

N1-C2-S1 123.08(15), C2-N3-C4 104.13(16), N3-C2-S1 125.22(15), N3-C2-N1 111.69(16), N1-C5-B1 128.09(15), C16 B1 C7 114.05(15), C4-C5-N1 102.88(15), C31-B1-C16 113.31(15), C4-C5-B1 129.02(16), C31-B1-C7 101.82(14), C5-B1-C16 104.16(14), C5-B1-C7 118.55(15), C5-B1-C31 104.89(15)

C2-N3-C4 103.66(14), C8-C7-B1 127.54(15), N1-C5-B1 125.42(14), C4-C5-N1 103.14(14), C4-C5-B1 130.87(15), N1-C2-Se1 123.32(13), N3-C2-Se1 124.01(13), N3-C2-N1 112.24(15), F1-B1-C16 111.87(13), F1-B1-C5 102.53(13), F1-B1-C7 103.23(12), C16-B1-C7 114.94(13), C5-B1-C16 104.65(13), C5-B1-C7 119.03(14)

C17-B1-C8 114.2(2), C7-B1-C17 113.2(2), C7-B1-C8 101.91(19), N1-C2-Se1 123.41(18), C5-B1-C17 103.94(19), N2-C2-Se1 124.85(19), C5-B1-C7 105.4(2), N2-C2-N1 111.7(2), C5-B1-C8 118.2(2), N2-C4-C5 112.8(2)

Selected bond parameters of compounds 9-[F] **and 11-**[F]

Compound	**9-**[F]	**11-**[F]
Bond distance (Å)	S1-C2 1.754(6),	C5-B1 1.644(5),
	S1-C26 1.792(7),	C4-C5 1.365(4)
	F1-B1 1.470(8),	P1-C2 1.818(3),
	N1-C2 1.356(7),	P1-C8 1.827(3),
	N1-C6 1.461(8),	P1-C14 1.817(4),
	N1-C5 1.383(8),	F1-B1 1.462(4),
	N3-C2 1.336(8),	N1-C2 1.357(4),
	N3-C4 1.381(8),	N1-C5 1.397(4),
	N3-C7 1.456(8),	N1-C6 1.465(4),
	C8-B1 1.648(9),	N3 -C2 1.348(4),
	C4-C5 1.372(9),	N3-C4 1.379(4),
	C5-B1 1.649(9),	N3-C7 1.472(4),
	C17-B1 1.658(10)	
Bond Angle (°)	C2-S1-C26 102.5(3),	C5-C4-N3 109.4(3),
	C2-N1-C6 123.4(5),	N1-C5-B1 127.5(3),
	C2-N1-C5 110.2(5),	C4-C5-N1 103.9(3),
	C5-N1-C6 126.3(5),	C4-C5-B1 128.6(3),
	C2-N3-C4 107.9(5),	N1-C2-P1 123.3(2),
	C2-N3-C7 126.9(5),	N3-C2-P1 130.6(2),
	C4-N3-C7 125.1(5),	N3-C2-N1 106.0(3),
	C9-C8-B1 126.6(5),	C2-N1-C5 111.4(3),
	C5-C4-N3 109.4(6),	C2-N1-C6 124.2(3),
	N1-C5-B1 126.6(5),	C5-N1-C6 124.3(3),
	C4-C5-N1 104.5(5),	C2-N3-C4 109.1(3),
	C4-C5-B1 128.4(6),	C2-N3-C7 127.2(3),
	N1-C2-S1 126.0(5),	
	N3-C2-S1 125.1(4),	
	N3-C2-N1 107.9(5),	

F1-B1-C8 102.5(5),

F1-B1-C17 111.0(5),

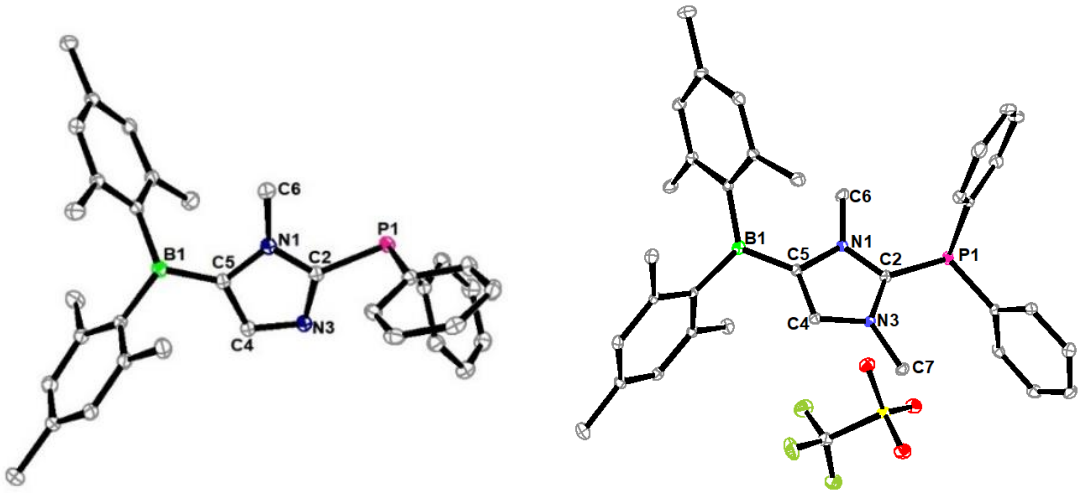
F1-B1-C5 104.5(5),

C8-B1-C17 119.7(5),

C8-B1-C5 117.0(5),

C5-B1-C17 101.3(5)

Crystal structures of **6**, **11**, and **8**-[CN]



(a) (b)

Figure S1: (a) Crystal structures of **6** and (b) **11.** Hydrogen atoms have been omitted for clarity (30 % ellipsoid probability)

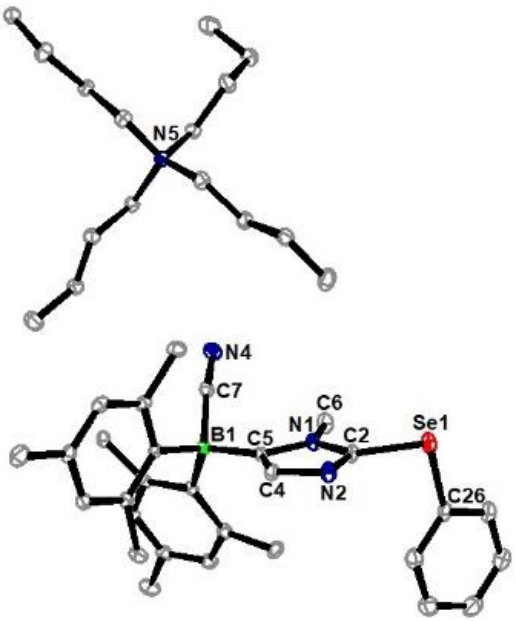


Figure S2: Crystal structure of **8**-[CN]. Hydrogen atoms have been omitted for clarity (30 % ellipsoid probability).

Table S3: Fluoride binding constants of $BMes_2$-containing organoborane compounds from the literature (compounds **(a)-(k)**) listed in chart 1

Compound	Solvent	Binding constant (M^{-1})
(a)	THF	$8.9(1.9) \times 10^4$
(b)	THF	5.0×10^7
(c)	DCM	6.3×10^4 -8.3×10^4
(d),(g)	$CHCl_3/H_2O$	10^8
(f)	MeOH	$\pm$420
(h)	$CH_3CN:H_2O$(1:1)	2.15×10^5
(i)	$DMSO:H_2O$(3:1)	$1.9 (3) \times 10^2$
(j)	THF	5×10^9
(k)	$THF:H_2O$ (4:1)	$1.4 (\pm 0.1) \times 10^4$

Table S4: Calculation of detection limit for 7 with CN in $CH_3CN:H_2O$(1:1) :

Blank reading for 7	**Normalized Intensity**
Reading 1	1.0
Reading 2	0.99513
Reading 3	0.99661
Reading 4	0.99764
Standard deviation(σ)	0.00177

The limit of detetction was calculated by formula

Detection limit= $-3\sigma/m$

Where, σ = standard deviation of blank readings and m is slope of fluorescence intensity vs. concentration of the TBACN obtained via linear regression

= -3 X 0.00177/-0.02262

= 0.234 mM

= 234μM

=(234 x 268.48)/1000

=62.8ppm

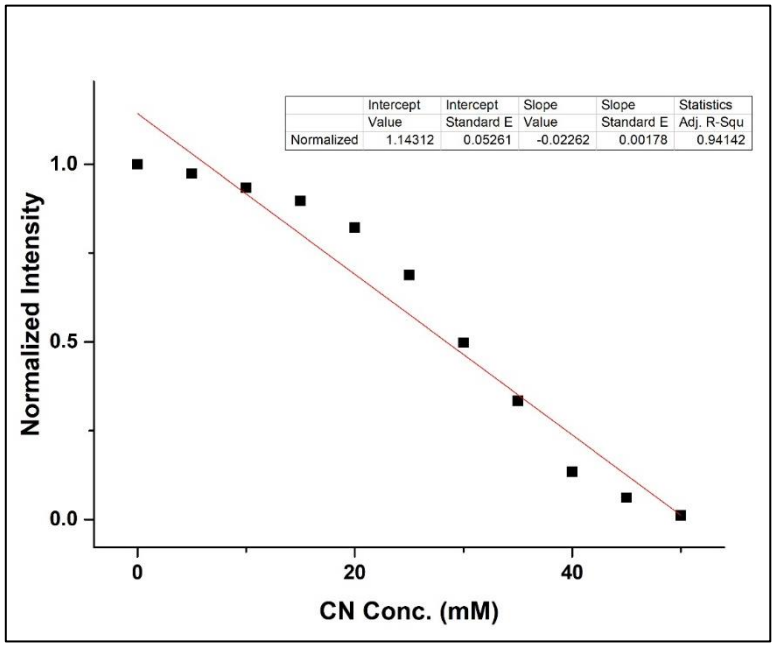


Figure S3: Linear Regression of fluorescence intensity of **7** with increasing concentration of CN^-

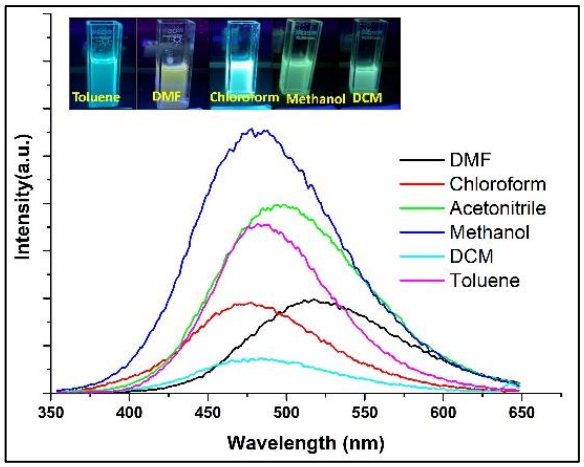


Figure S4: Absorbance and emission of compound **7** in various solvents (25 µM)

Table S5: Photophysical properties of compound **7** in various solvents

Solvent	λ_{max}[a] (nm)	λ_{em}(nm)	$\Delta\upsilon$[b] (cm^{-1})
DMF	332	520	10890
Chloroform	333	478	9110
Acetonitrile	330	515	10885
Methanol	331	478	9291
DCM	334	485	9322
Toluene	332	480	9287

λ_{max}[a] Longest absorption maxima wavelength (absorbance) λ_{em} (emission) [b] Stokes shift $\Delta\upsilon$ ($1/\lambda_{max} - 1/\lambda_{em}$)

Binding Constant Calculations:

Benesi-Henderson (BH) Method:

The slope was calculated by Linear fit in the graph between $1/A\text{-}A_0$ and 1/F via origin software.

The BH Equation for 1:1 complexation was used to calculate the K constant:

$$1/A\text{-}A_0 = 1/ K (A_{max}\text{-}A_0) \times [X^-] + 1/A_{max}\text{-}A_0 \text{ (For turn-on)}$$

$$\mathbf{1/A_0\text{-}A = 1/ K (A_0\text{-}A_{max}) \times [X^-] + 1/A_0\text{-}A_{max} \text{ (For turn-off,)}}$$

(All the compounds in here display turn-off fluorescence)

A = Absorbance, A_0 = Absorbance at initial host concentration (compounds **7**-**11**), A_{max} = Absorbance at maximum guest (X^-) concentration. (X= F or CN)

For compound 7:

Acetonitrile solution of **7** (2 mL, 2.5 x 10^{-5} M) in a cuvette was titrated against incremental addition (10 µL) of TBAX (X = F, CN) in acetonitrile. The changes observed in the absorption band at 330 nm were noted for the further calculations. The experimental absorbance data is given below. The fluoride binding constant of **7** was calculated using Bindfit online package and BH method.

For Compound 7-[F]**:**

Equivalence of fluoride ion	Fluoride concentration	Absorbance (A)
0.0	0	0.71511
0.1	3.73134E-6	0.67528
0.2	7.42574E-6	0.63308
0.3	1.10837E-5	0.58954
0.4	1.47059E-5	0.54658
0.5	1.82927E-5	0.50301
0.6	2.18447E-5	0.45616
0.7	2.53623E-5	0.41202
0.8	2.88462E-5	0.36026
0.9	3.22967E-5	0.30325
1.0	3.57143E-5	0.24497
1.1	3.90995E-5	0.187

For Compound 7-[CN]**:**

Equivalence of cyanide ion	Cyanide concentration	Absorbance (A)
0.0	0	0.618
0.1	2.48756E-6	0.548
0.2	4.9505E-6	0.492
0.3	7.38916E-6	0.418
0.4	9.80392E-6	0.347
0.5	1.21951E-5	0.3
0.6	1.45631E-5	0.218
0.7	1.69082E-5	0.138
0.8	1.92308E-5	0.101
0.9	2.15311E-5	0.039
1.0	2.38095E-5	0.009

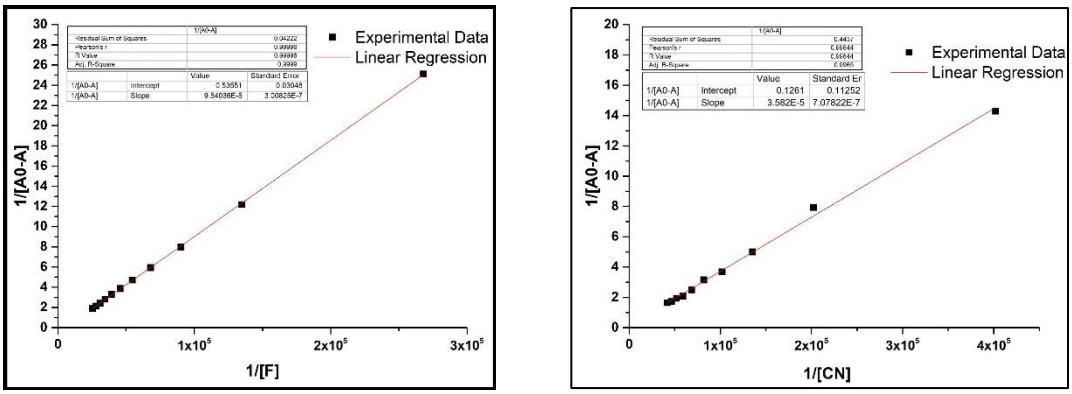
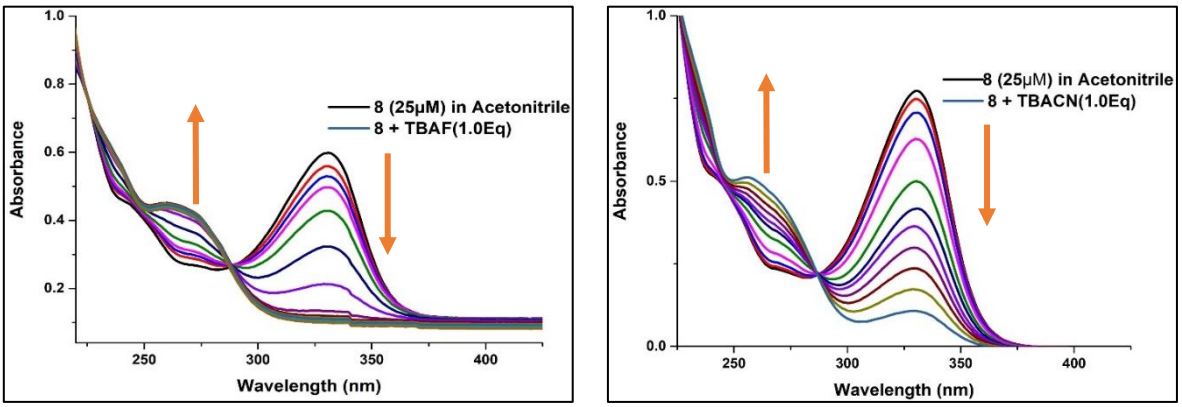


Figure S5: BH plot of **7** vs TBAF (left) and BH plot of **7** vs TBACN (right)

For compound 8:

Acetonitrile solution of **8** (2 mL, 2.5 x 10^{-5} M) in a cuvette was titrated against incremental addition (10 µL) of TBAX (X = F, CN) in acetonitrile. The changes observed in the absorption band at 330 nm were noted for the further calculations. The experimental absorbance data is given below. The fluoride binding constant of **8** was calculated using Bindfit online package and BH method.



(a) (b)

Figure S6: Change in absorption spectra upon addition of (a)TBAF and (b) TBACN in compound **8**.

For Compound 8-[F]**:**

Equivalence of fluoride ion	Fluoride concentration	Absorbance (A)
0.0	0	0.59754
0.1	3.73134E-6	0.55935
0.2	7.42574E-6	0.5292
0.3	1.10837E-5	0.49723
0.4	1.47059E-5	0.42805
0.5	1.82927E-5	0.32308
0.6	2.18447E-5	0.21255
0.7	2.53623E-5	0.13377
0.8	2.88462E-5	0.11933
0.9	3.22967E-5	0.1135
1.0	3.57143E-5	0.10979

For Compound 8-[CN]:

Equivalence of cyanide ion	Cyanide concentration	Absorbance (A)
0.0	0	0.77268
0.1	2.49169E-6	0.74812
0.2	4.96689E-6	0.70708
0.3	7.42574E-6	0.62664
0.4	9.86842E-6	0.49885
0.5	1.22951E-5	0.41649

0.6	1.47059E-5	0.36165
0.7	1.7101E-5	0.29727
0.8	1.94805E-5	0.23527
0.9	2.18447E-5	0.17123
1.0	2.41935E-5	0.10665

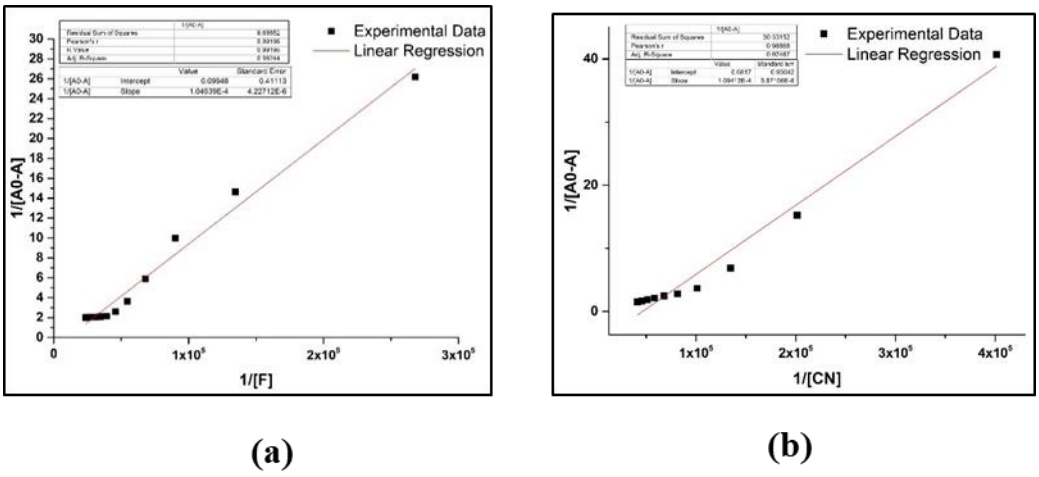
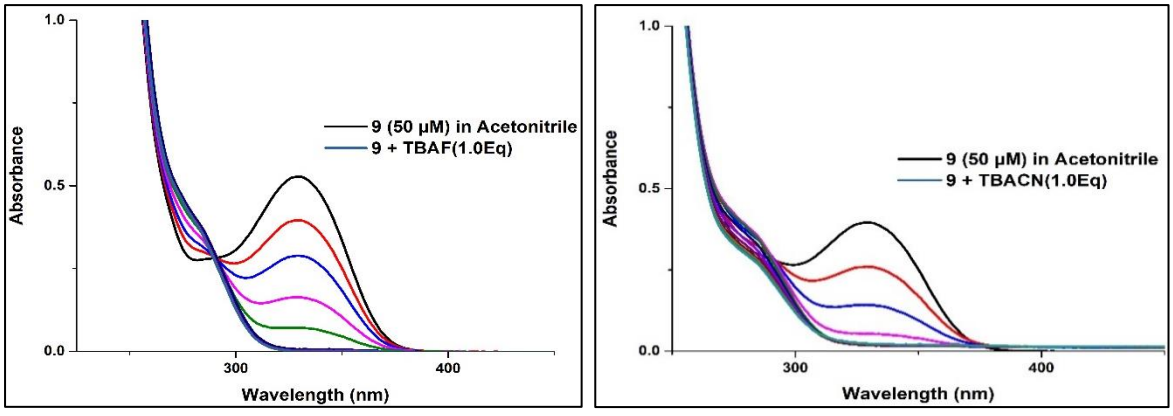


Figure S7: BH plot of **8** Vs TBAF (left) and BH plot of **8** Vs TBACN (right).

For compound 9:

Acetonitrile solution of **9** (2 mL, 5 x 10^{-5} M) in a cuvette was titrated against incremental addition (10 µL) of TBAX (X = F, CN) in acetonitrile. The changes observed in the absorption band at 330 nm were noted for further calculations. The experimental absorbance data is given below. The fluoride binding constant of **9** was calculated using Bindfit online package and BH method.



(a) (b)

Figure S8: The Change in absorption spectra upon addition of (a) TBAF and (b)TBACN in **9**.

For Compound 9-[F]**:**

Equivalence of fluoride ion	Fluoride concentration	Absorbance (A)
0.0	0	0.52306
0.1	4.97512E-6	0.39179
0.2	9.90099E-6	0.28593
0.3	1.47783E-5	0.16202
0.4	1.96078E-5	0.07133
0.5	2.43902E-5	0.00828
0.6	2.91262E-5	0.00296
0.7	3.38164E-5	0.00319
0.8	3.84615E-5	0.00221
0.9	4.30622E-5	0.00120
1.0	4.7619E-5	0.00118

For Compound 9-[CN]**:**

Equivalence of cyanide ion	Cyanide concentration	Absorbance (A)
0.0	0	0.39179
0.1	4.97512E-6	0.25801
0.2	9.90099E-6	0.14156
0.3	1.47783E-5	0.05364
0.4	1.96078E-5	0.02442
0.5	2.43902E-5	0.02341
0.6	2.91262E-5	0.02077
0.7	3.38164E-5	0.02073
0.8	3.84615E-5	0.01935
0.9	4.30622E-5	0.01911

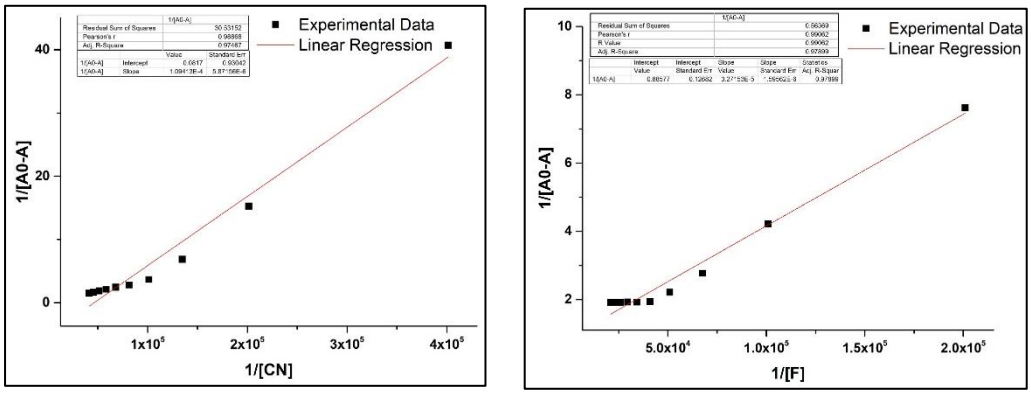
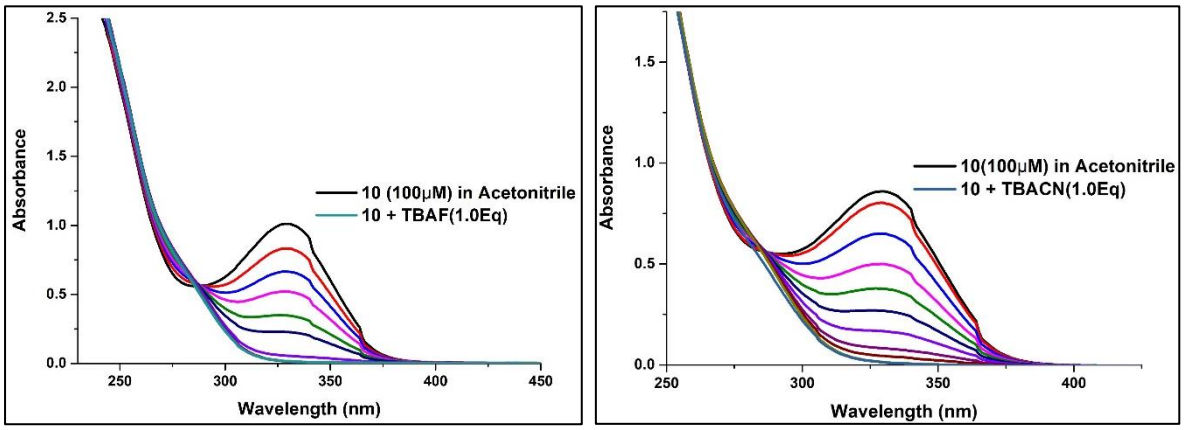


Figure S9: BH plot of **9** Vs TBAF (left) and BH plot of **9** Vs TBACN (right).

For compound 10:

Acetonitrile solution of **10** (2 mL, 1x 10^{-4} M) in a cuvette was titrated against incremental addition (10 µL) of TBAX (X = F, CN) in acetonitrile. The changes observed in the absorption band at 330 nm were noted for further calculations. The experimental absorbance data is given below. The fluoride binding constant of **10** was calculated using BH method.



(a) (b)

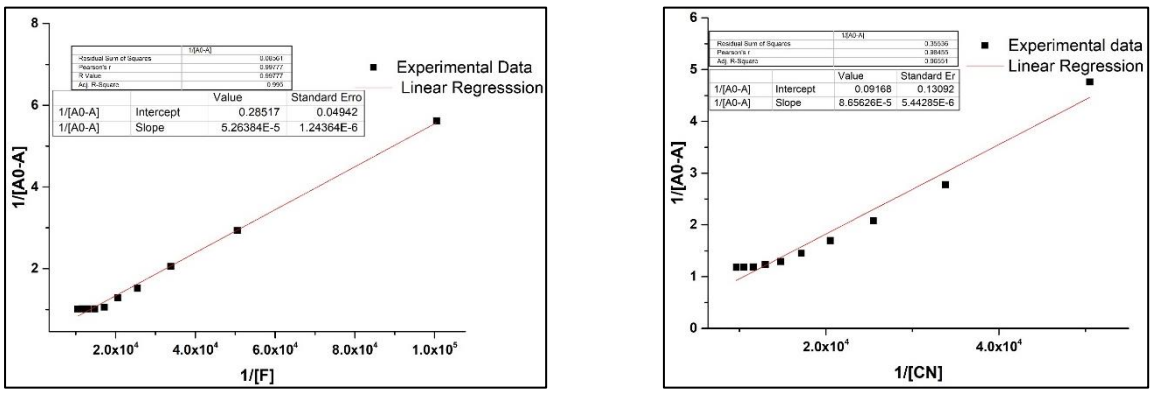
Figure S10: The change in absorption spectra upon addition of (a) TBAF and (b)TBACN in **10.**

For Compound 10-[F]**:**

Equivalence of Fluoride ion	Fluoride concentration	Absorbance (A)
0.0	0	0.998
0.1	9.95025E-6	0.82
0.2	1.9802E-5	0.657
0.3	2.95567E-5	0.512
0.4	3.92157E-5	0.34
0.5	4.87805E-5	0.222
0.6	5.82524E-5	0.052
0.7	6.76329E-5	0.014
0.8	7.69231E-5	0.013
0.9	8.61244E-5	0.012
1.0	9.52381E-5	0.011

For Compound 10-[CN]**:**

Equivalence of Cyanide ion	Cyanide concentration	Absorbance (A)
0.0	0	0.854
0.1	9.95025E-6	0.796
0.2	1.9802E-5	0.644
0.3	2.95567E-5	0.494
0.4	3.92157E-5	0.373
0.5	4.87805E-5	0.264
0.6	5.82524E-5	0.164
0.7	6.76329E-5	0.08
0.8	7.69231E-5	0.042
0.9	8.61244E-5	0.012
1	9.52381E-5	0.01

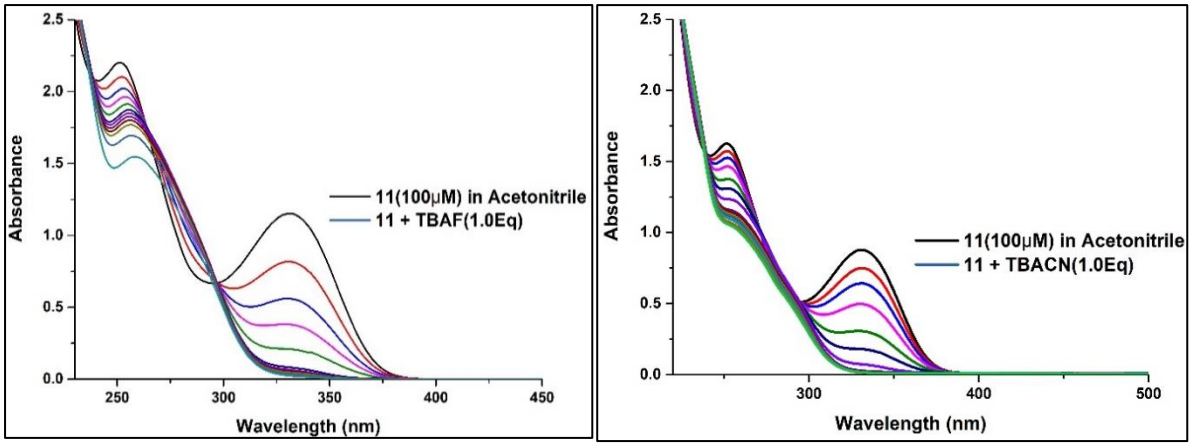


(a) (b)

Figure S11: (a) BH plot of **10** Vs TBAF and (b) BH plot of **10** Vs TBACN

For compound 11:

Acetonitrile solution of **11** (2 mL, 1x 10^{-4} M) in a cuvette was titrated against incremental addition (10 µL) of TBAX (X=F, CN)in Acetonitrile. The changes observed in the absorption band at 330 nm were noted for the further calculations. The experimental absorbance data is given below. The fluoride binding constant of **11** was calculated using BH method.



(a) (b)

Figure S12: The change in UV-Vis absorption spectra upon addition of (a)TBAF and (b) TBACN of **11**

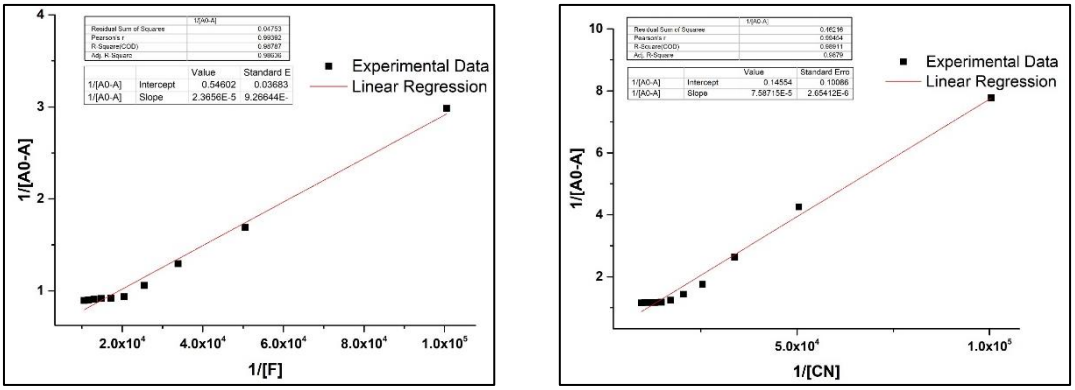
For Compound 11-[F]**:**

Equivalence of fluoride ion	Fluoride concentration	Absorbance (A)
0.0	0	1.15069
0.1	9.95025E-6	0.74896
0.2	1.9802E-5	0.64253
0.3	2.95567E-5	0.49724
0.4	3.92157E-5	0.30756
0.5	4.87805E-5	0.18208
0.6	5.82524E-5	0.0749
0.7	6.76329E-5	0.02899
0.8	7.69231E-5	0.01981
0.9	8.61244E-5	0.01935
1.0	9.52381E-5	0.01934

For Compound 11-[CN]**:**

Equivalence of Cyanide ion	Cyanide concentration	Absorbance (A)
0.0	0	0.87762
0.1	9.95025E-6	0.74896
0.2	1.9802E-5	0.64253
0.3	2.95567E-5	0.49724
0.4	3.92157E-5	0.30756

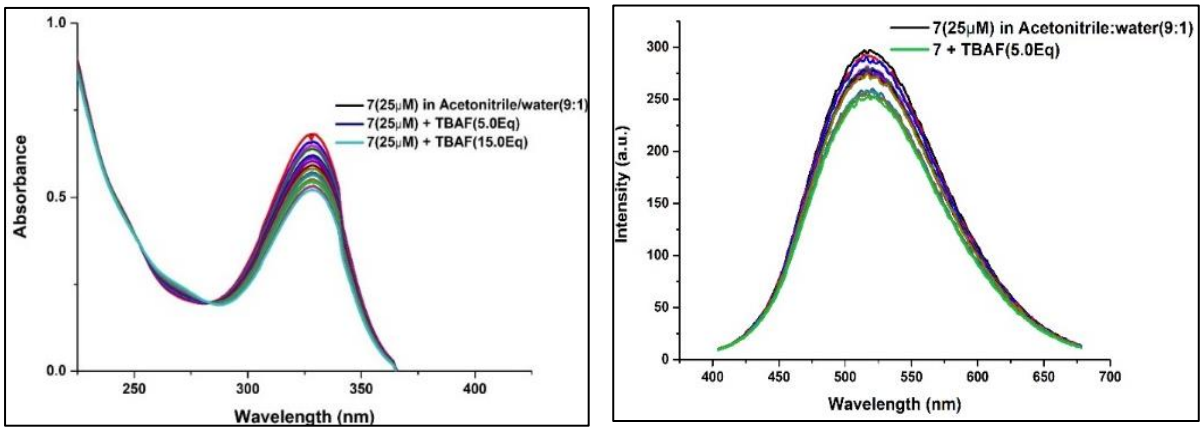
0.5	4.87805E-5	0.18208
0.6	5.82524E-5	0.0749
0.7	6.76329E-5	0.02899
0.8	7.69231E-5	0.01981
0.9	8.61244E-5	0.01935
1.0	9.52381E-5	0.01934



(a) (b)

Figure S13: (a) BH plot of **11** Vs TBAF(left) and (b) BH plot of **11** Vs TBACN(right).

Details of titration of 1, 7 and 8 with TBAF, and TBACN in aqueous media:



(a) (b)

Figure S14: (a) Absorbance and (b) emission spectra of titration of **7** in acteonitrile:water (9:1) (25 μM) upon incremental addition of TBAF.

For Compound 7-[F] **in Acetonitrile:water (9:1)**

Equivalence of fluoride ion	Fluoride concentration	Absorbance(A)
0	0	0.68
1	2.48756E-5	0.665
2	4.9505E-5	0.657
3	7.38916E-5	0.648
4	9.80392E-5	0.639
5	1.21951E-4	0.619
6	1.45631E-4	0.612
7	1.69082E-4	0.603
8	1.92308E-4	0.591
9	2.15311E-4	0.581
10	2.38095E-4	0.571
11	2.60664E-4	0.564
12	2.83019E-4	0.551
13	3.05164E-4	0.544
14	3.27103E-4	0.53
15	3.48837E-4	0.52

For Compound 7-[CN] **in Acetonitrile: water (9:1):**

Equivalence of cyanide ion	Cyanide concentration	Absorbance(A)
0	0	0.648
0.1	2.48756E-6	0.643
0.2	4.9505E-6	0.636
0.3	7.38916E-6	0.63
0.4	9.80392E-6	0.62
0.5	1.21951E-5	0.606

0.6	1.45631E-5	0.591
0.7	1.69082E-5	0.577
0.8	1.92308E-5	0.556
0.9	2.15311E-5	0.535
1	2.38095E-5	0.508
1.2	2.83019E-5	0.469
1.4	3.27103E-5	0.435
1.6	3.7037E-5	0.405
1.8	4.12844E-5	0.367
2	4.54545E-5	0.329
2.2	4.95495E-5	0.288
2.4	5.35714E-5	0.252
2.6	5.75221E-5	0.217
2.8	6.14035E-5	0.184
3	6.52174E-5	0.145
3.2	6.89655E-5	0.112
3.4	7.26496E-5	0.085
3.6	7.62712E-5	0.064
3.8	7.98319E-5	0.05
4	8.33333E-5	0.038
4.2	8.67769E-5	0.028
4.4	9.01639E-5	0.021
4.6	9.34959E-5	0.015
4.8	9.67742E-5	0.012
5	1E-4	0.008

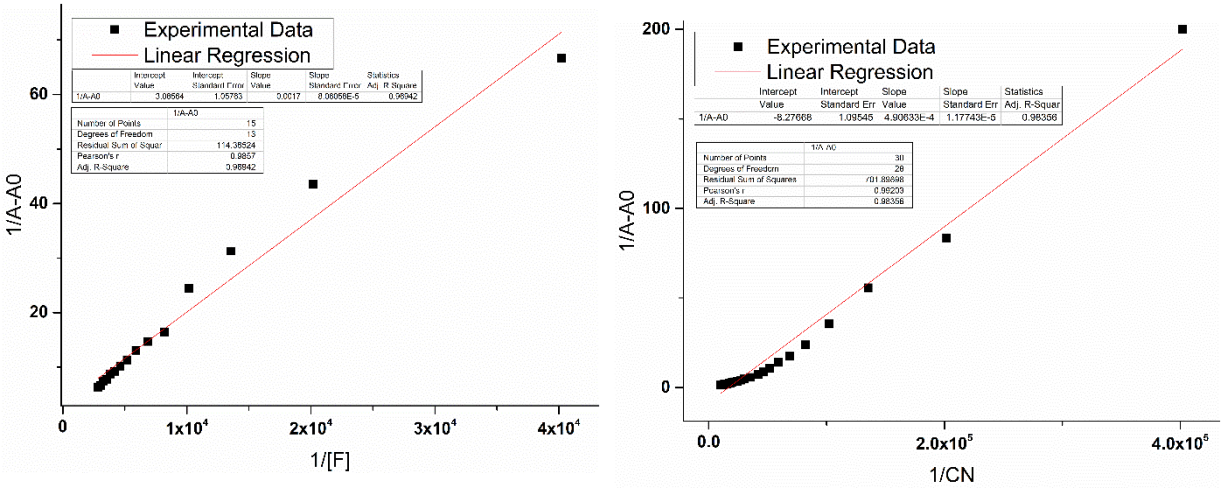
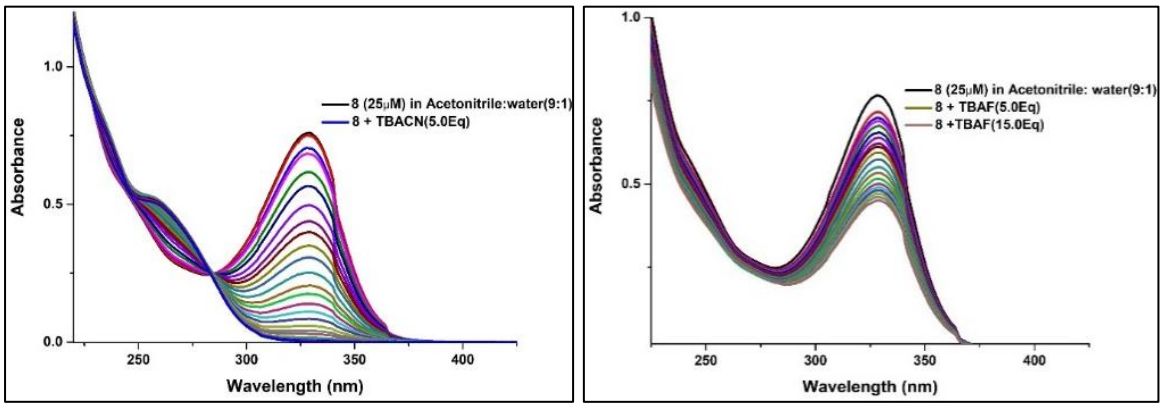


Figure S14(ii): BH plot of **7** Vs TBAF (left) and BH plot of **7** Vs TBACN (right) in CH_3CN:water (9:1).



(a) (b)

Figure S15(i): Absorbance spectra of titration of **8** in acteonitrile:water (9:1) (25 μM) upon incremental addition of (a) TBAF and (b) TBACN

For Compound 8-[F] **in Acetonitrile: water (9:1):**

Equivalence of Fluoride ion	Fluoride Concentration	Absorbance (A)
0	0	0.766
1	2.48756E-5	0.716
1.5	3.72208E-5	0.699
2	4.9505E-5	0.688
2.5	6.17284E-5	0.673
3	7.38916E-5	0.653
3.5	8.59951E-5	0.638
4	9.80392E-5	0.621
4.5	1.10024E-4	0.612
5	1.21951E-4	0.594
6	1.45631E-4	0.573
7	1.69082E-4	0.55

8	1.92308E-4	0.533
9	2.15311E-4	0.515
10	2.38095E-4	0.499
11	2.60664E-4	0.489
12	2.83019E-4	0.48
13	3.05164E-4	0.47
14	3.27103E-4	0.461
15	3.48837E-4	0.45

For Compound 8-[CN] **in Acetonitrile: water (9:1):**

Equivalence of cyanide ion	Cyanide concentration	Absorbance(A)
0	0	0.76
0.2	4.9505E-6	0.749
0.4	9.80392E-6	0.704
0.6	1.45631E-5	0.683
0.8	1.92308E-5	0.617
1	2.38095E-5	0.566
1.2	2.83019E-5	0.497
1.4	3.27103E-5	0.439
1.6	3.7037E-5	0.399
1.8	4.12844E-5	0.35
2	4.54545E-5	0.307
2.2	4.95495E-5	0.252
2.4	5.35714E-5	0.205
2.6	5.75221E-5	0.175
2.8	6.14035E-5	0.139
3	6.52174E-5	0.11
3.2	6.89655E-5	0.085
3.4	7.26496E-5	0.059
3.6	7.62712E-5	0.041
3.8	7.98319E-5	0.029
4	8.33333E-5	0.016
4.2	8.67769E-5	0.01
4.4	9.01639E-5	0.008
4.6	9.34959E-5	0.004
4.8	9.67742E-5	0.003
5	1E-4	0.002

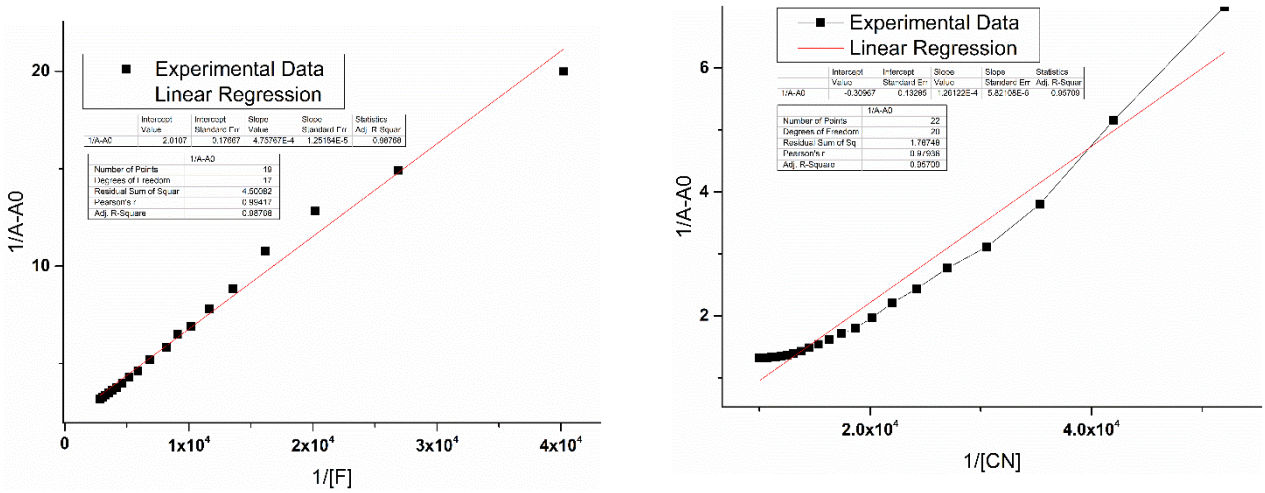
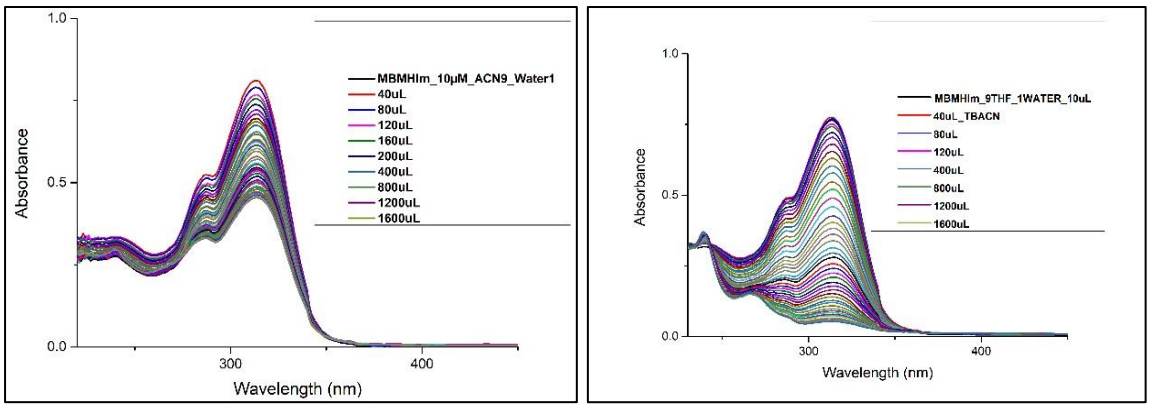


Figure S15(ii): BH plot of **8** Vs TBAF (left) and BH plot of **8** Vs TBACN (right) in acteonitrile:water (9:1).



(a) (b)

Figure S16 (i): The Change in absorption spectra upon addition of (a) TBAF and (b)TBACN in **1** in THF /water (9:1) (10 μM).

For Compound 1-[F] **in THF: water (9:1):**

Equivalence of Fluoride ion	Fluoride concentration	Absorbance
0	0	0.799
1	3.92157E-6	0.799
2	7.69231E-6	0.781
3	1.13208E-5	0.758
4	1.48148E-5	0.747
5	1.81818E-5	0.73
6	2.14286E-5	0.713
7	2.45614E-5	0.7
8	2.75862E-5	0.687
9	3.05085E-5	0.679
10	3.33333E-5	0.668
11	3.60656E-5	0.648

12	3.87097E-5	0.642
13	4.12698E-5	0.626
14	4.375E-5	0.622
15	4.61538E-5	0.617
16	4.84848E-5	0.609
17	5.07463E-5	0.598
18	5.29412E-5	0.589
19	5.50725E-5	0.574
20	5.71429E-5	0.567
21	5.91549E-5	0.554
22	6.11111E-5	0.55
23	6.30137E-5	0.542
24	6.48649E-5	0.537
25	6.66667E-5	0.535
26	6.84211E-5	0.531
27	7.01299E-5	0.524
28	7.17949E-5	0.514
29	7.34177E-5	0.504
30	7.5E-5	0.497
31	7.65432E-5	0.495
32	7.80488E-5	0.495
33	7.95181E-5	0.485
34	8.09524E-5	0.482
35	8.23529E-5	0.476
36	8.37209E-5	0.469
37	8.50575E-5	0.466
38	8.63636E-5	0.461
39	8.76404E-5	0.459
40	8.88889E-5	0.453
41	9.01099E-5	0.45
42	9.13043E-5	0.447

For Compound 1-[CN] in THF: water (9:1):

Equivalence of Cyanide ion	Cyanide concentration	Absorbance
0	0	0.756
1	3.92157E-6	0.766
2	7.69231E-6	0.761
3	1.13208E-5	0.743
4	1.48148E-5	0.734
5	1.81818E-5	0.713
6	2.14286E-5	0.697
7	2.45614E-5	0.674
8	2.75862E-5	0.648
9	3.05085E-5	0.625
10	3.33333E-5	0.598
11	3.60656E-5	0.574
12	3.87097E-5	0.542

13	4.12698E-5	0.517
14	4.375E-5	0.486
15	4.61538E-5	0.455
16	4.84848E-5	0.423
17	5.07463E-5	0.401
18	5.29412E-5	0.381
19	5.50725E-5	0.36
20	5.71429E-5	0.337
21	5.91549E-5	0.312
22	6.11111E-5	0.293
23	6.30137E-5	0.279
24	6.48649E-5	0.256
25	6.66667E-5	0.24
26	6.84211E-5	0.223
27	7.01299E-5	0.209
28	7.17949E-5	0.191
29	7.34177E-5	0.178
30	7.5E-5	0.165
31	7.65432E-5	0.15
32	7.80488E-5	0.139
33	7.95181E-5	0.126
34	8.09524E-5	0.119
35	8.23529E-5	0.107
36	8.37209E-5	0.097
37	8.50575E-5	0.09
38	8.63636E-5	0.084
39	8.76404E-5	0.078
40	8.88889E-5	0.073
41	9.01099E-5	0.064
42	9.13043E-5	0.059

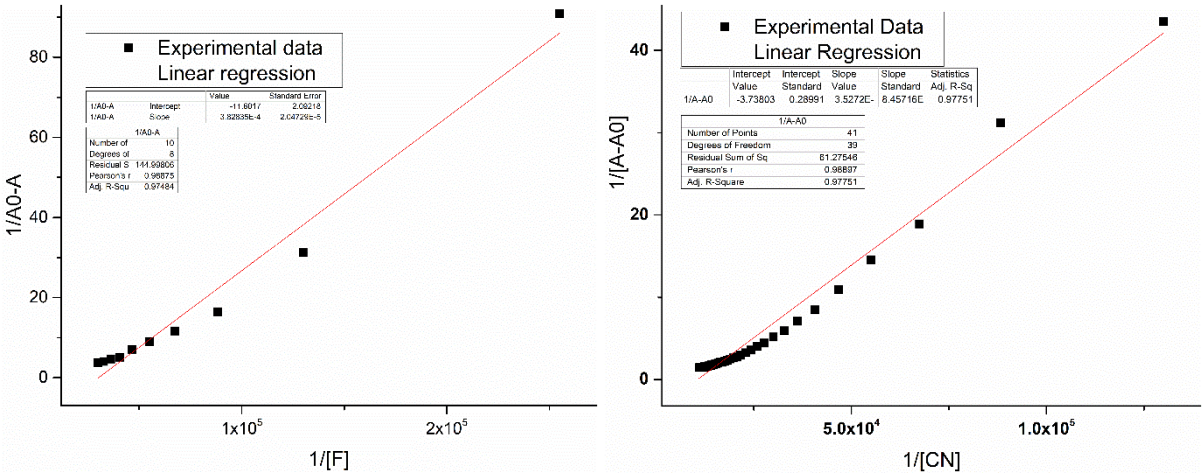


Figure S16(ii): BH plot of **1** Vs TBAF (left) and BH plot of **1** Vs TBACN (right) in THF:water (9:1).

Table S6: Anion binding constant values for **7**-**11.** It is to be noted that except for **7** (CN^- binding), in all other cases the binding constants were calculated by assuming the reversibility between the substrate and anion binding (see the discussion in the main text).

Comp.	Solvent	Fluoride Binding Constant (M^{-1})		Cyanide Binding Constant (M^{-1})	
		BH Plot	Bindfit	BH Plot	Bindfit
1[10a]	THF	7.80×10^3	1.40×10^4	2.48×10^5	1.47×10^3
1	THF/Water (9/1)	1.49×10^4	3.02×10^6	2.51×10^4	2.72×10^6
4[10a]	Acetonitrile	1.54×10^4	5.21×10^3	1.270×10^4	4.844×10^4
7	Acetonitrile	1.98×10^4	3.91×10^4	-------	------
7	Acetonitrile/Water (9/1)	3.67×10^3	4.09×10^6	-------	------
8	Acetonitrile	2.2×10^4	5.66×10^3	1.37×10^4	9.60×10^4
8	Acetonitrile/Water (9/1)	6.65×10^3	1.4×10^6	1.04×10^4	3.30×10^6
9	Acetonitrile	1.47×10^4	1.07×10^4	5.85×10^4	1.01×10^4
10	Acetonitrile	1.92×10^4	3.33×10^4	6.91×10^3	4.95×10^4
11	Acetonitrile	2.82×10^4	3.24×10^4	1.53×10^4	4.33×10^4

NMR spectra of compounds:

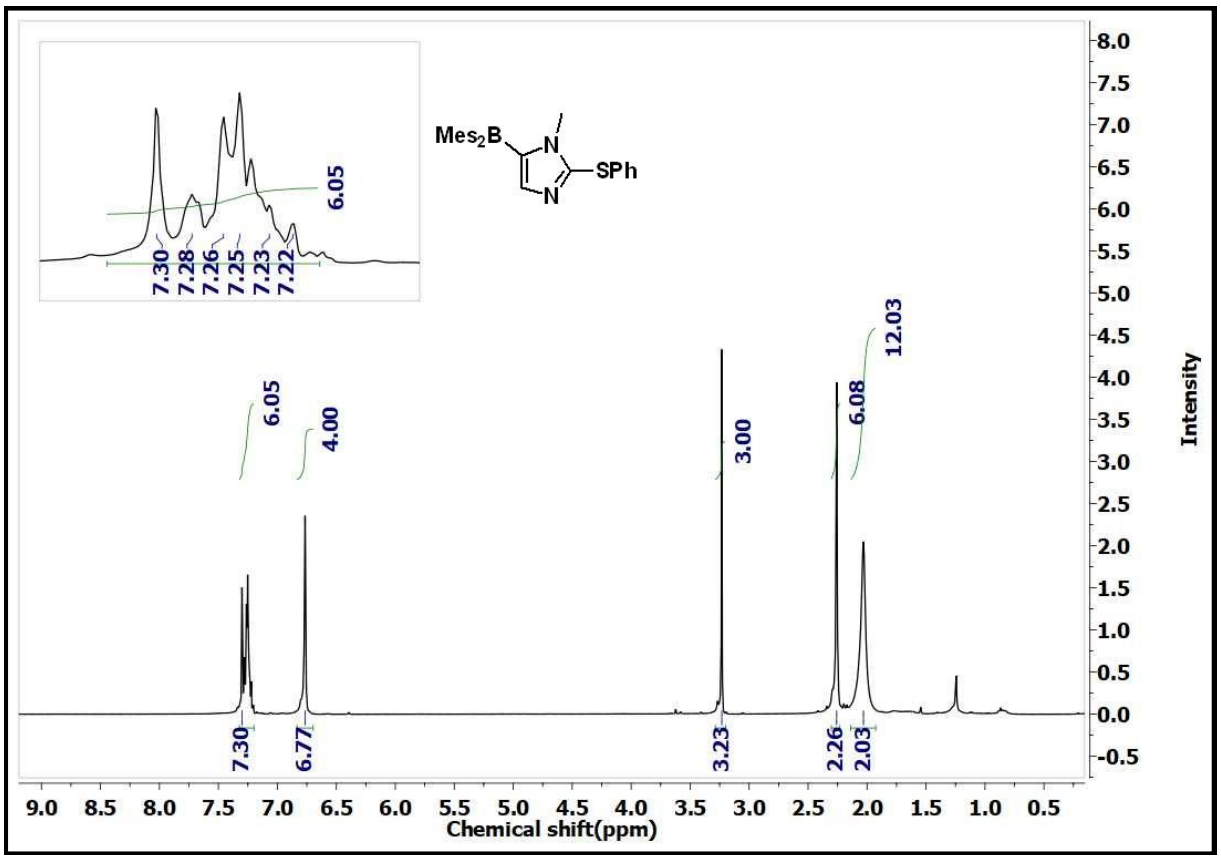


Figure S17: ^{1}H NMR of **7** ($CDCl_3$)

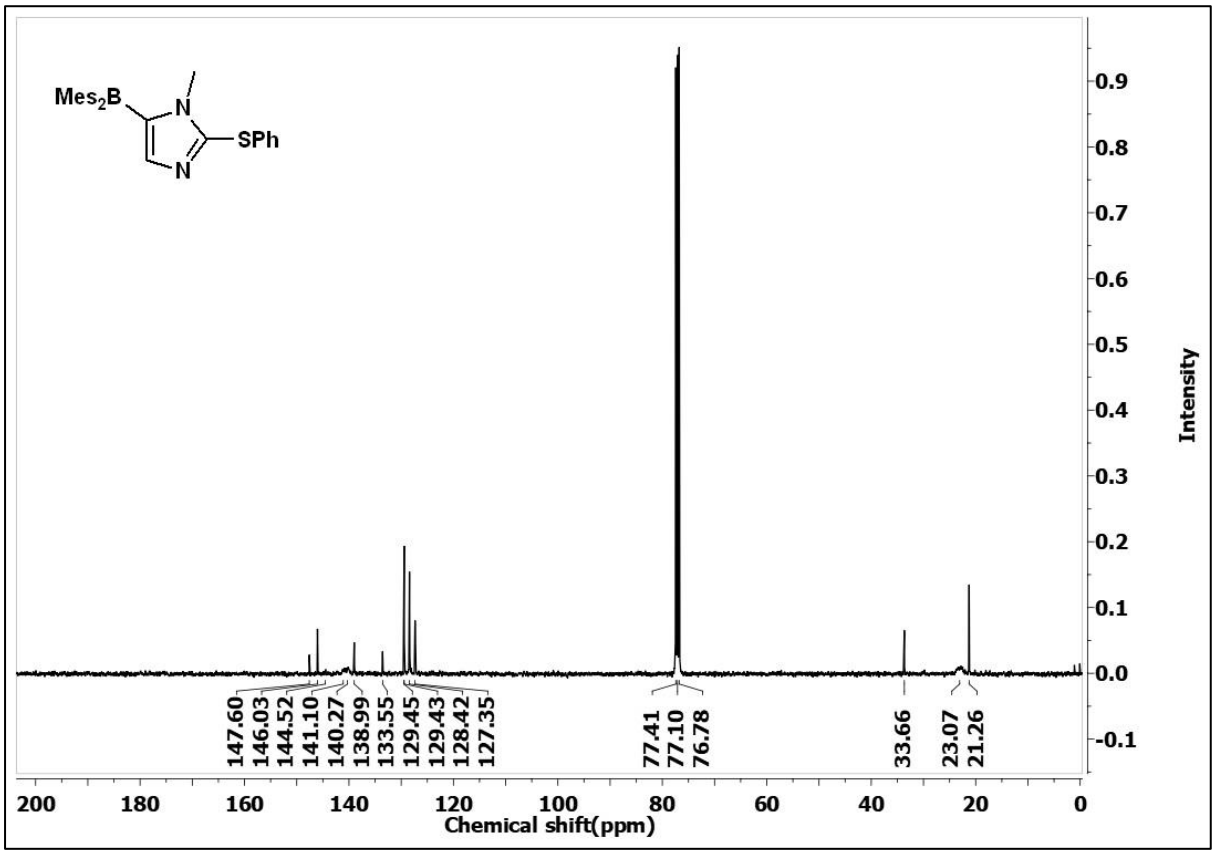


Figure S18: ^{13}C NMR of **7** ($CDCl_3$)

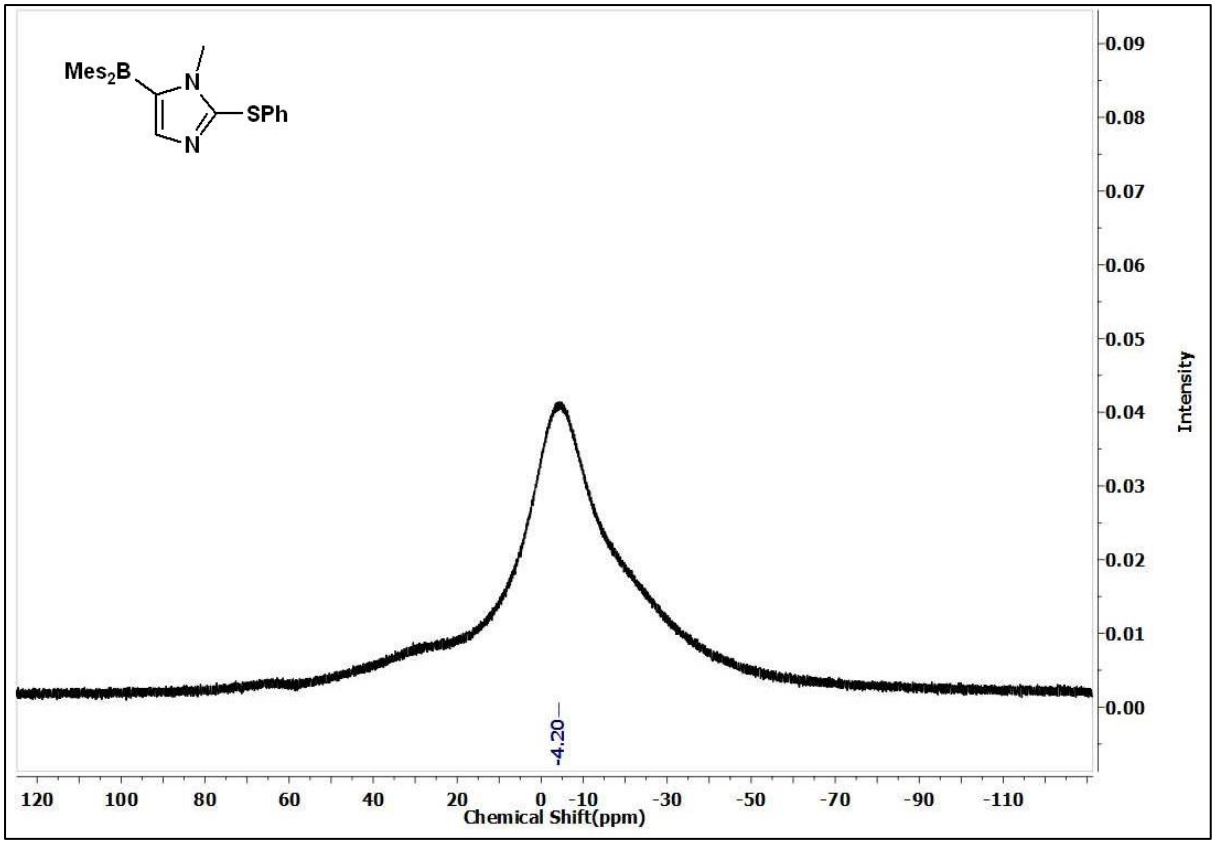


Figure S19: ^{11}B NMR of **7** ($CDCl_3$)

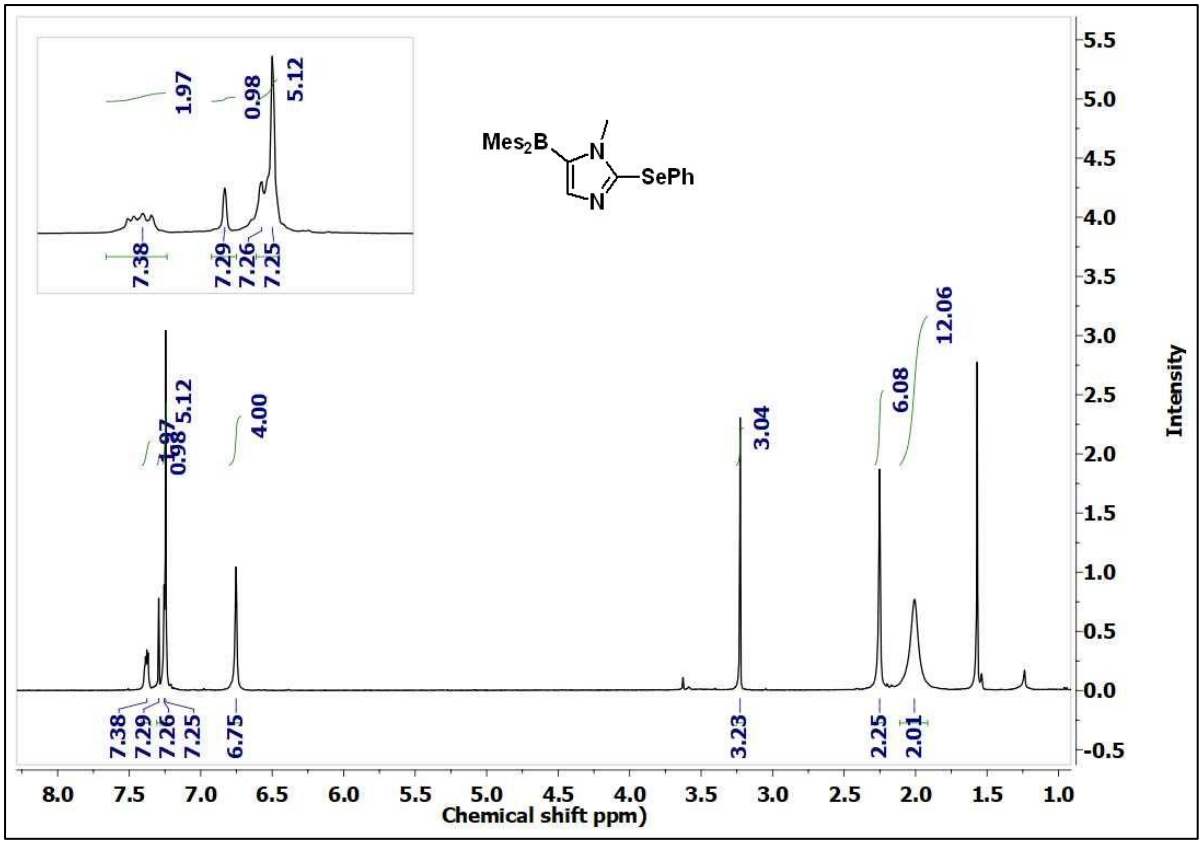


Figure S20: ^{1}H NMR of **8** ($CDCl_3$)

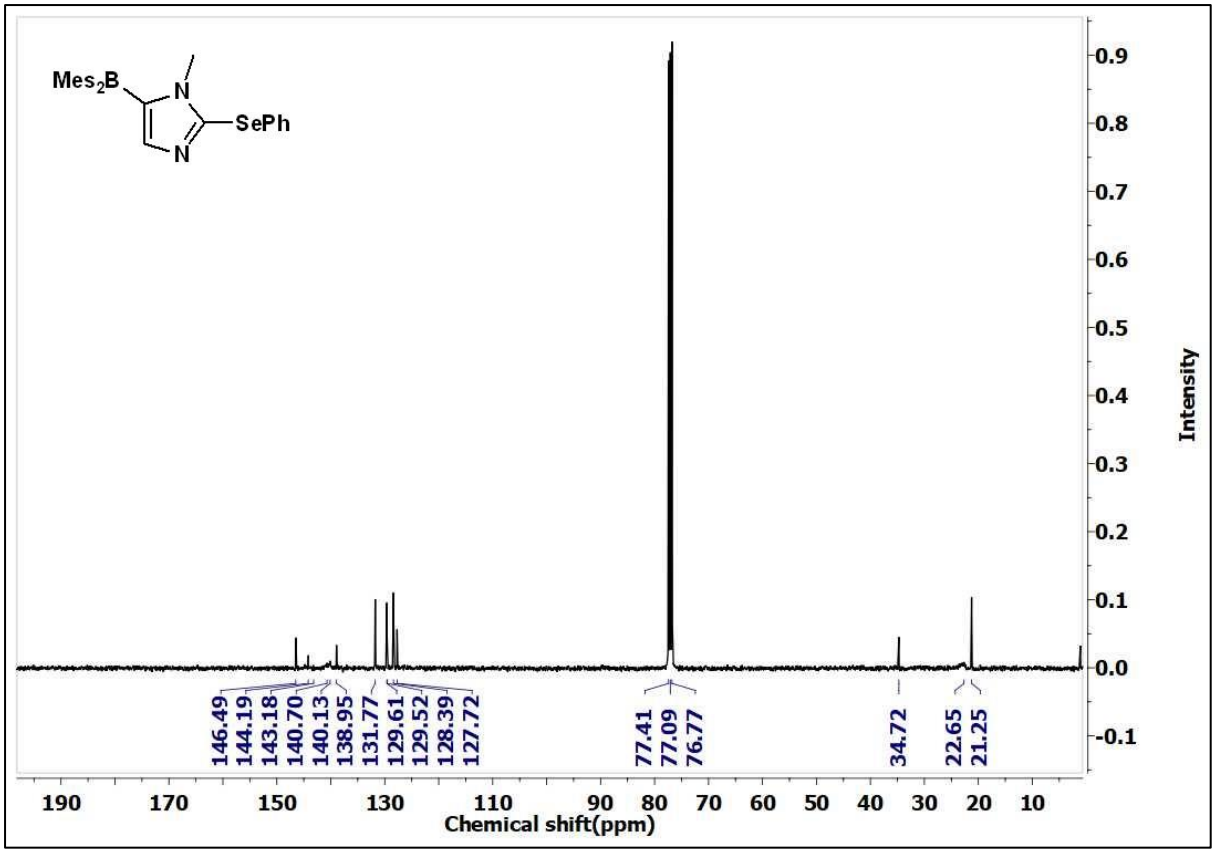


Figure S21: ^{13}C NMR of **8** ($CDCl_3$)

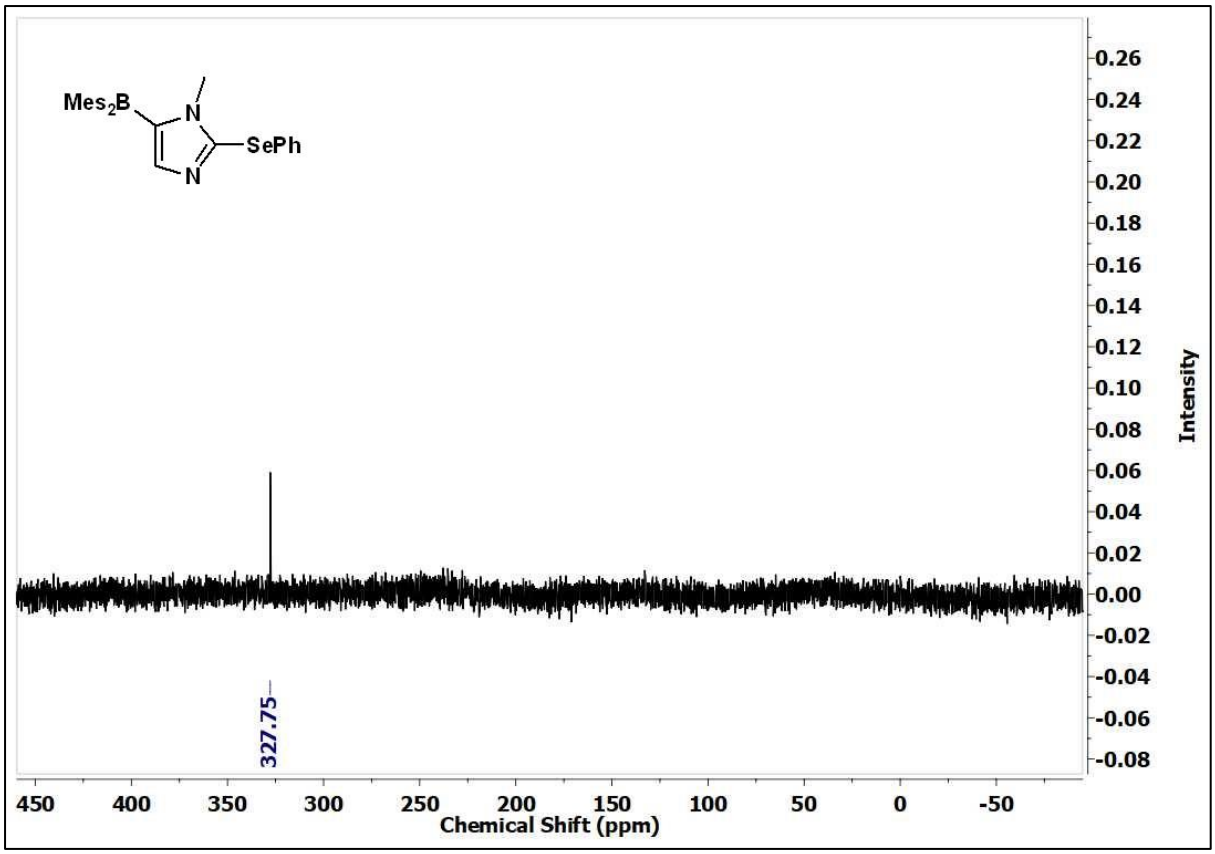


Figure S22: ^{77}Se NMR of **8** ($CDCl_3$)

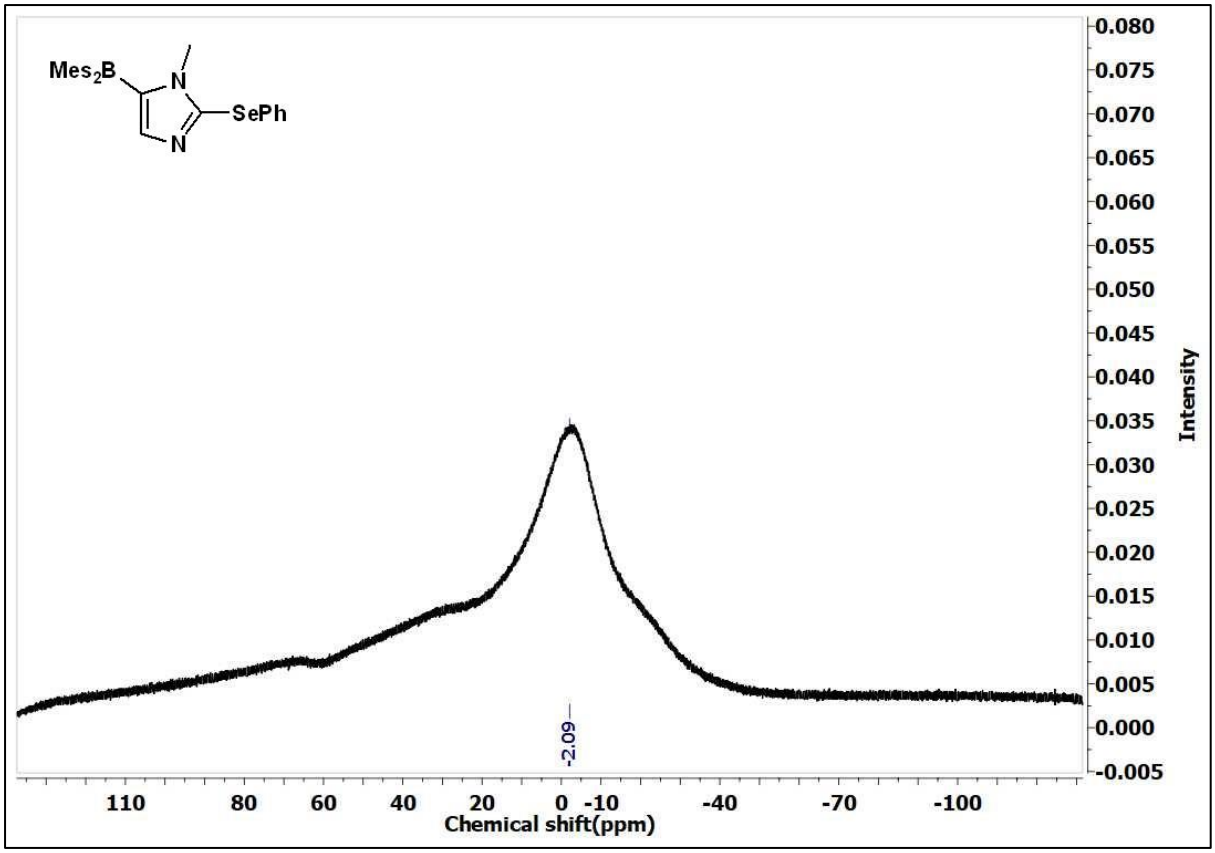


Figure S23: ^{11}B NMR of **8** ($CDCl_3$)

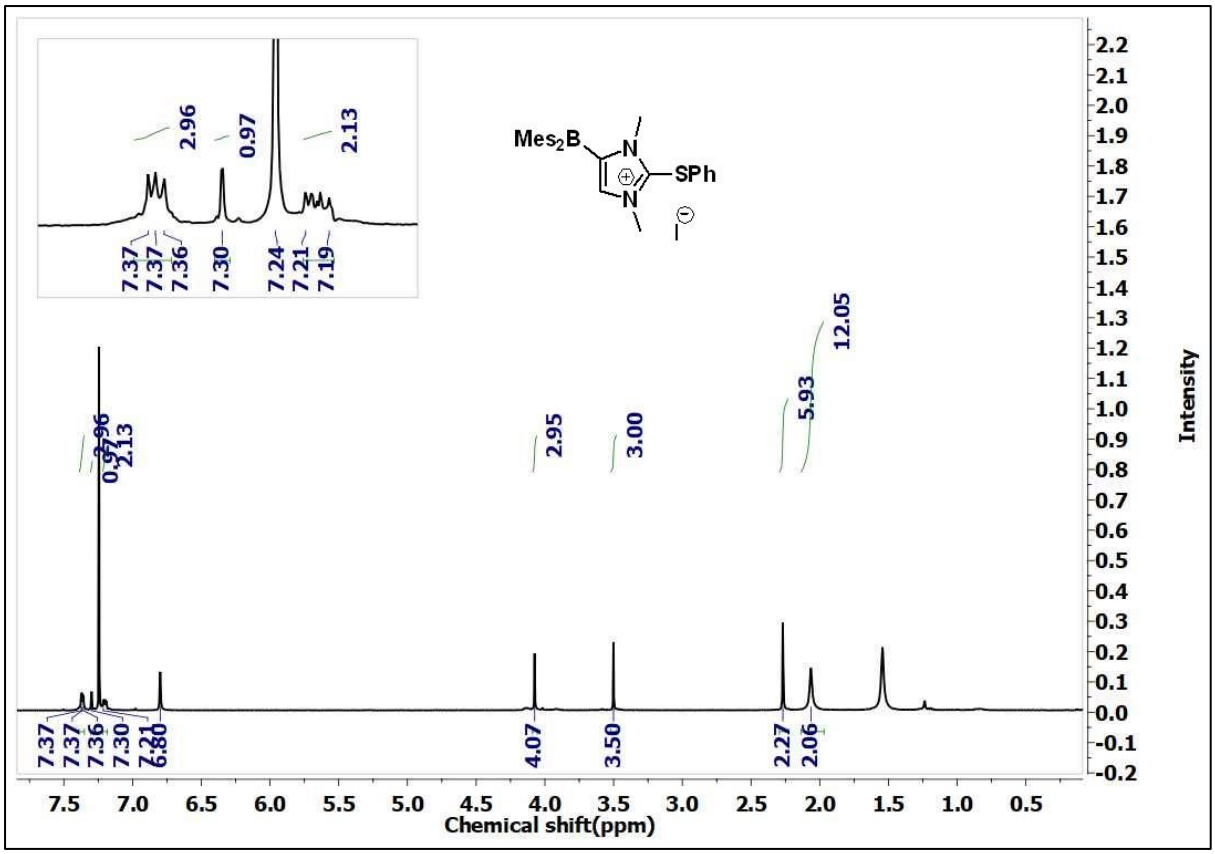


Figure S24: ^{1}H NMR of **9** ($CDCl_3$)

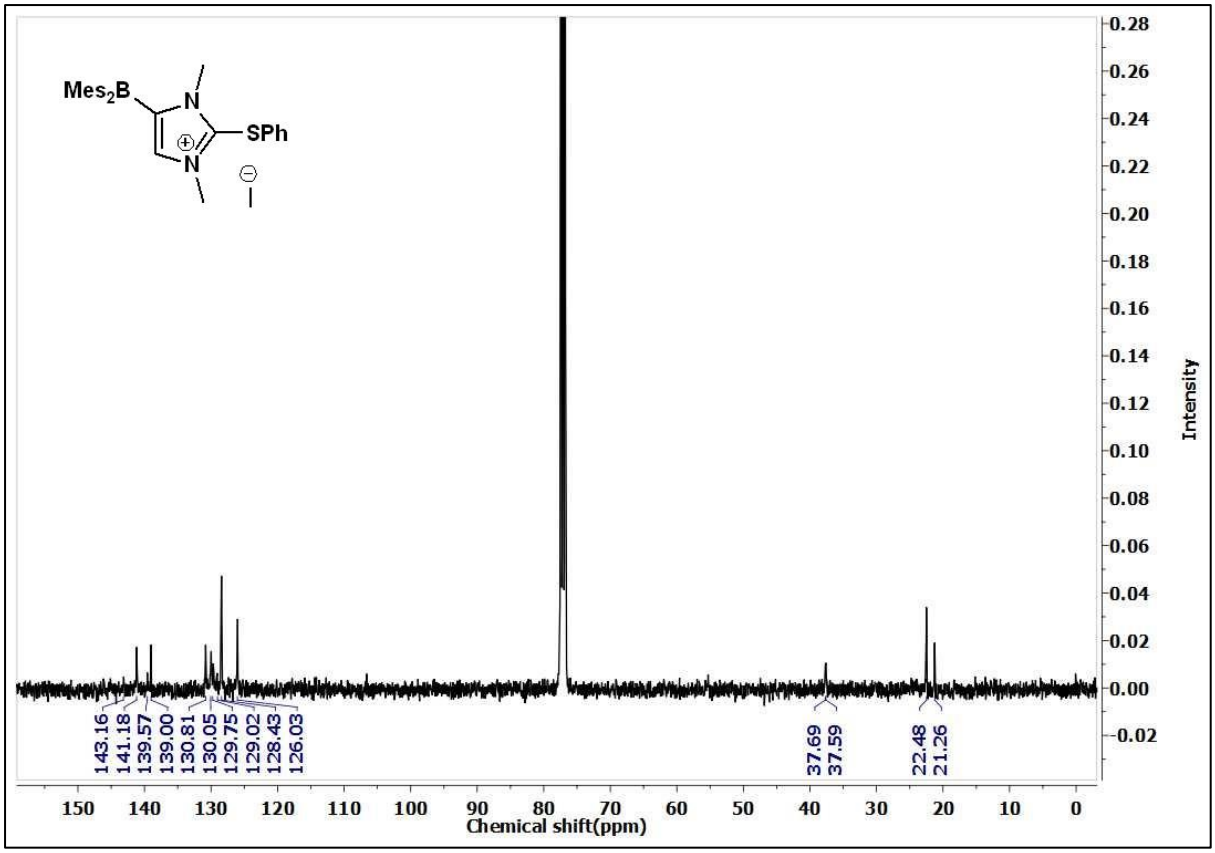


Figure S25: ^{13}C NMR of **9** ($CDCl_3$)

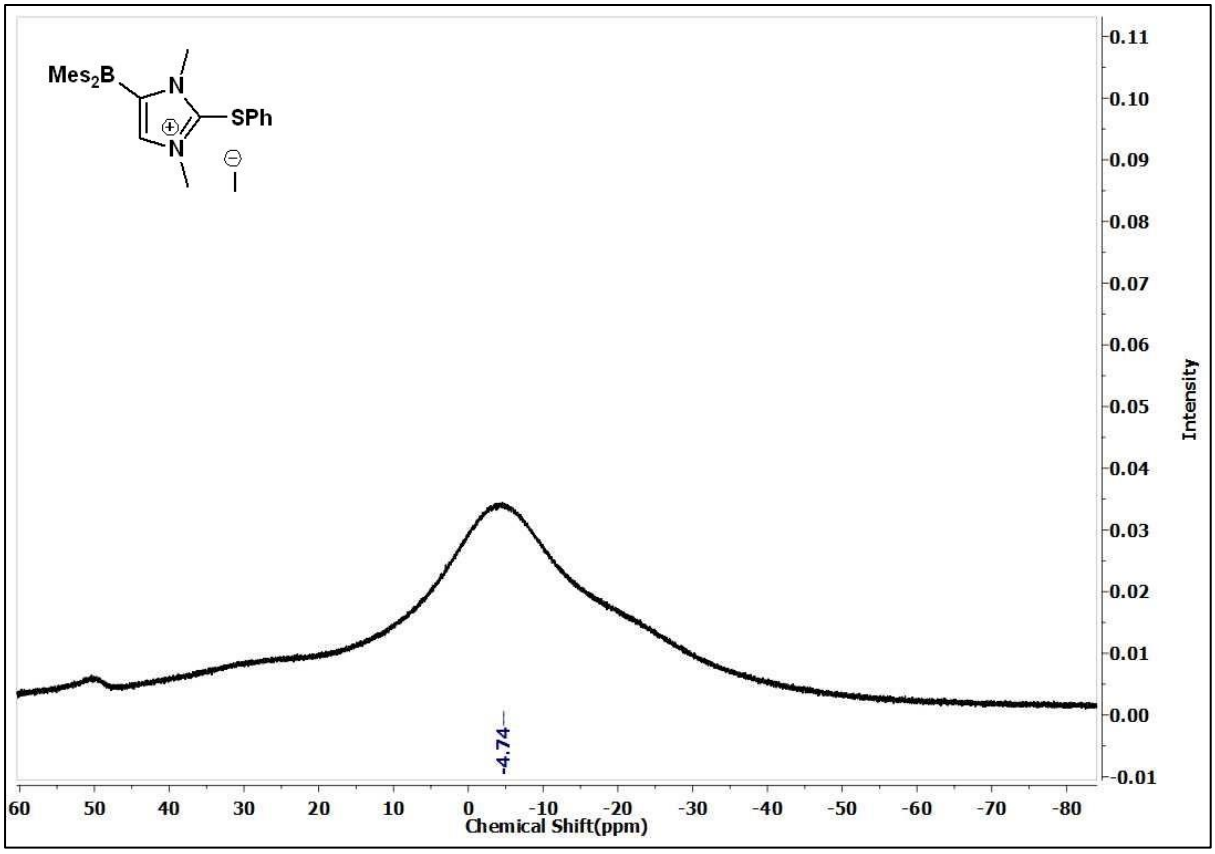


Figure S26: ^{11}B NMR of **9** ($CDCl_3$)

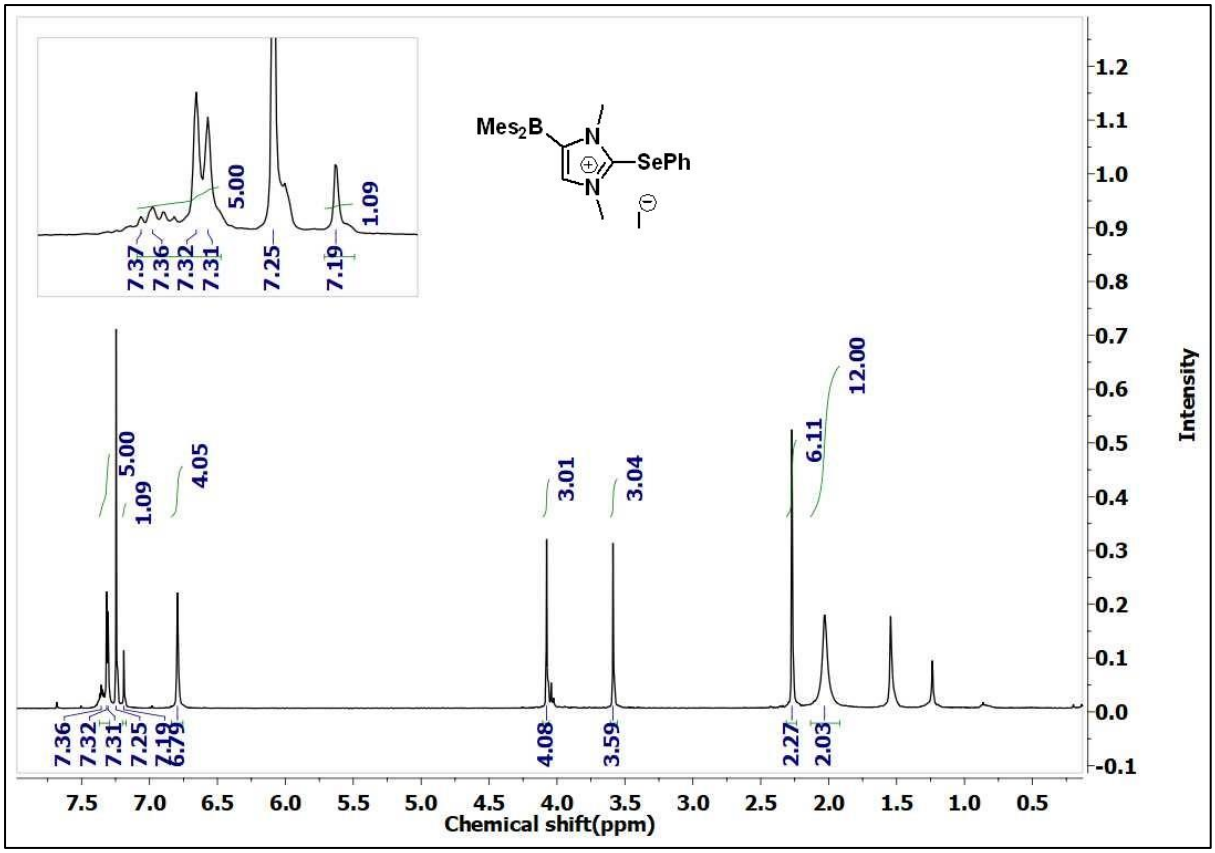
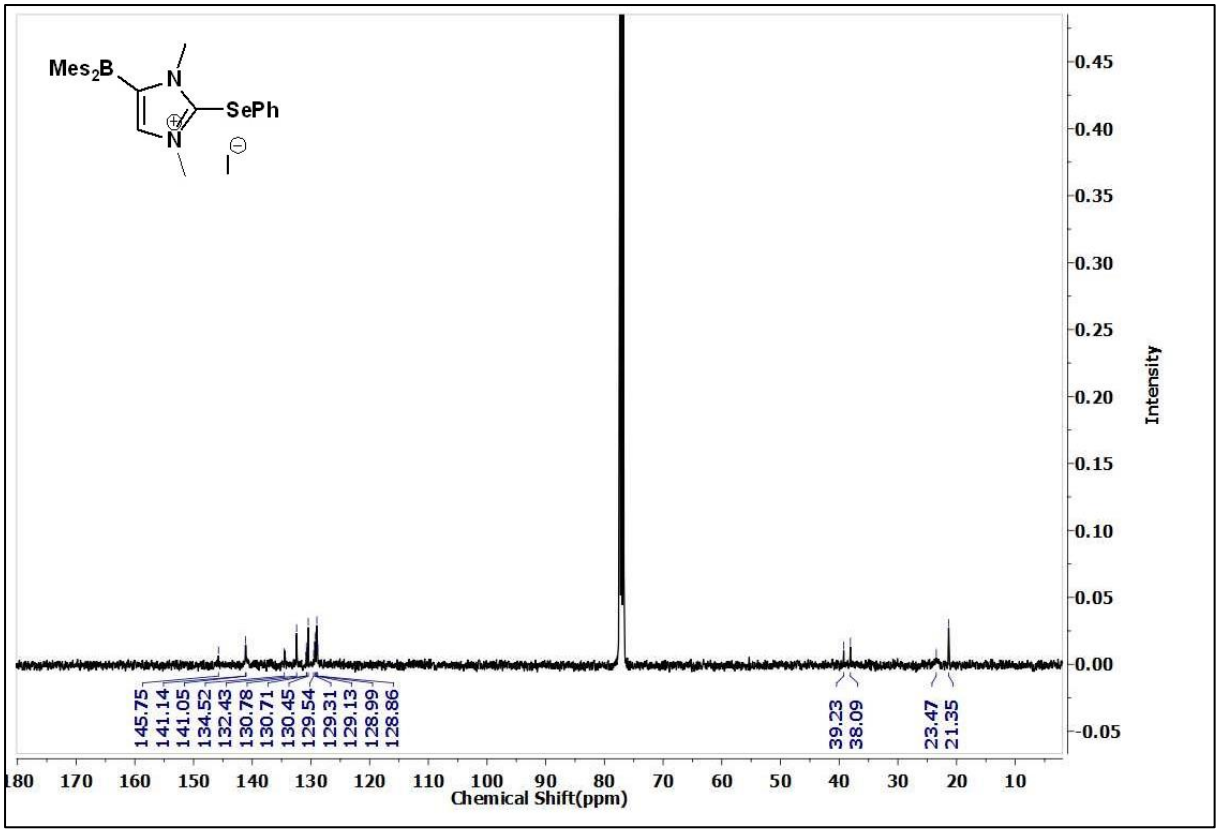


Figure S27: ^{1}H NMR of **10** ($CDCl_3$)



FigureS28: ^{13}C NMR of **10** ($CDCl_3$)

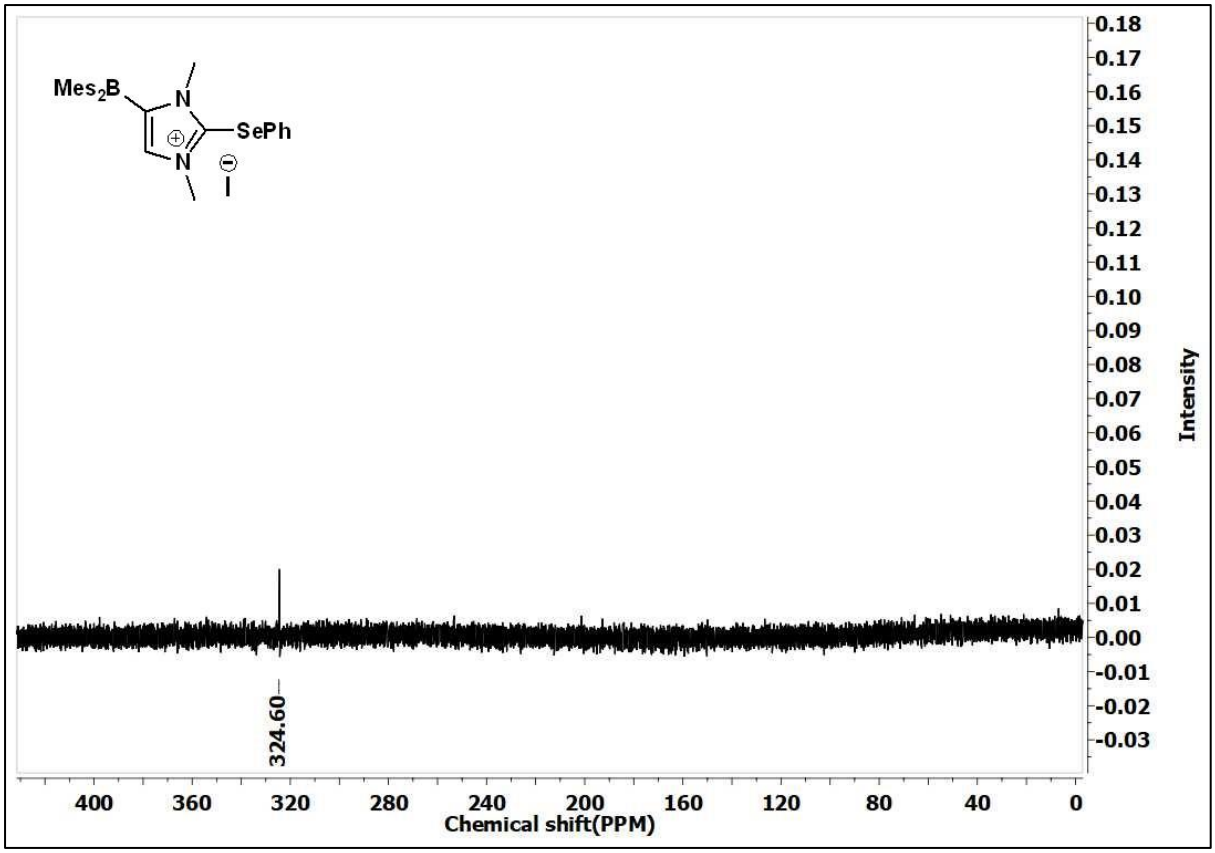


Figure S29: ^{77}Se NMR of **10** ($CDCl_3$)

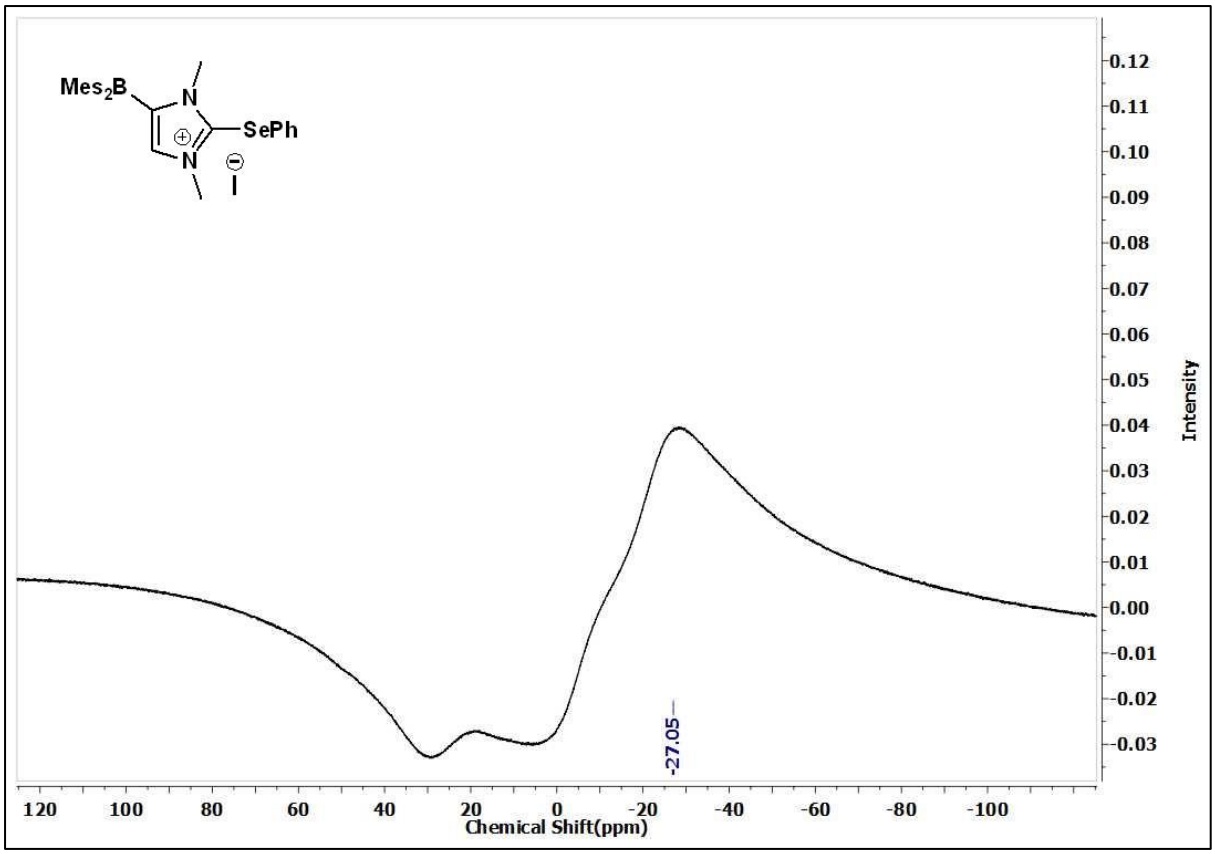


Figure S30: ^{11}B NMR of **10** ($CDCl_3$)

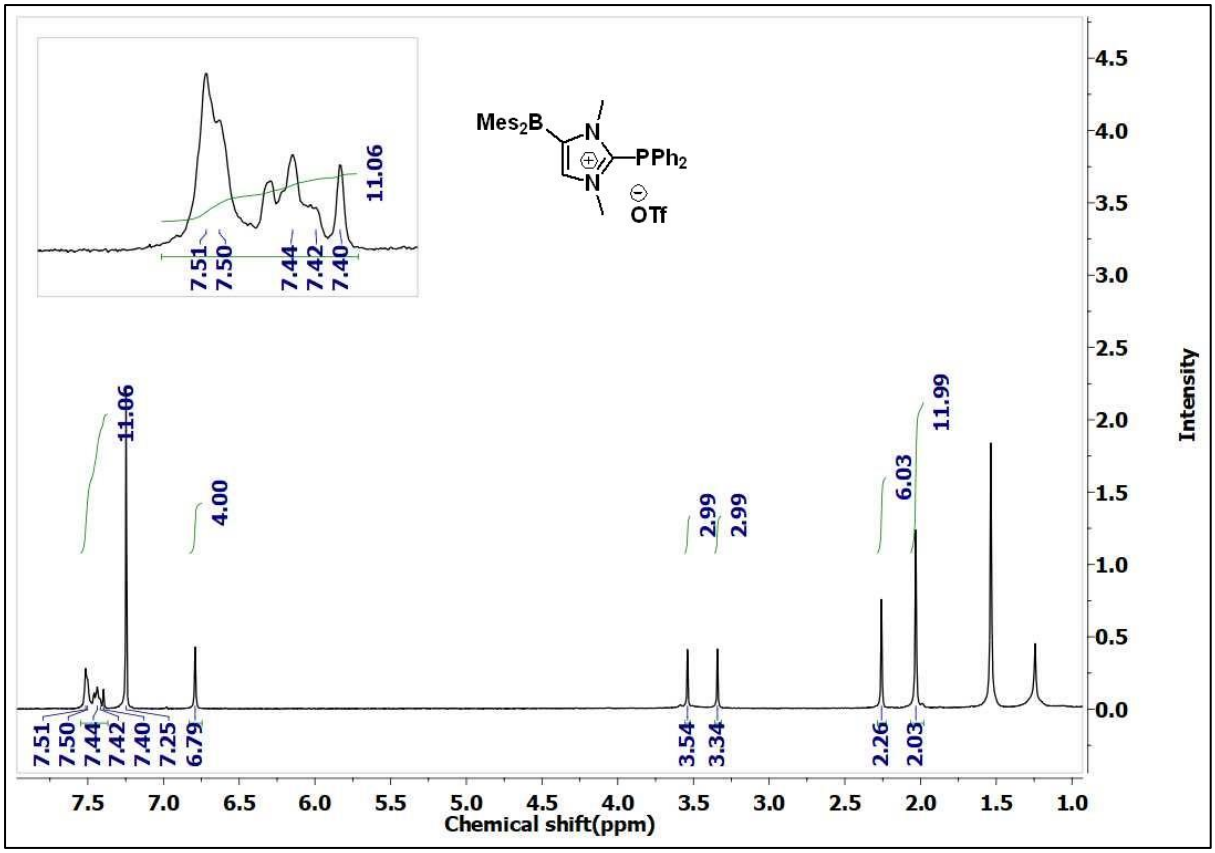


Figure S31: ^{1}H NMR of **11** ($CDCl_3$)

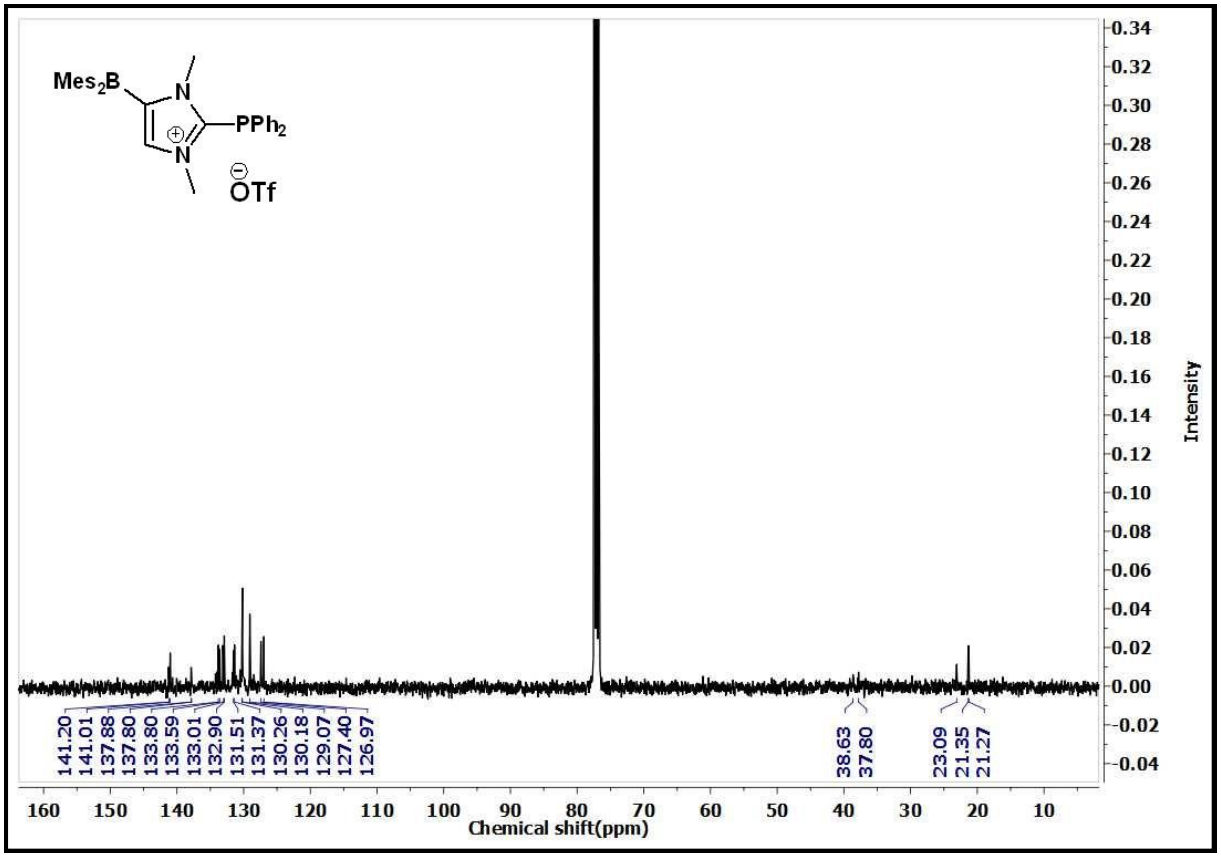


Figure S32: ^{13}C NMR of **11** ($CDCl_3$)

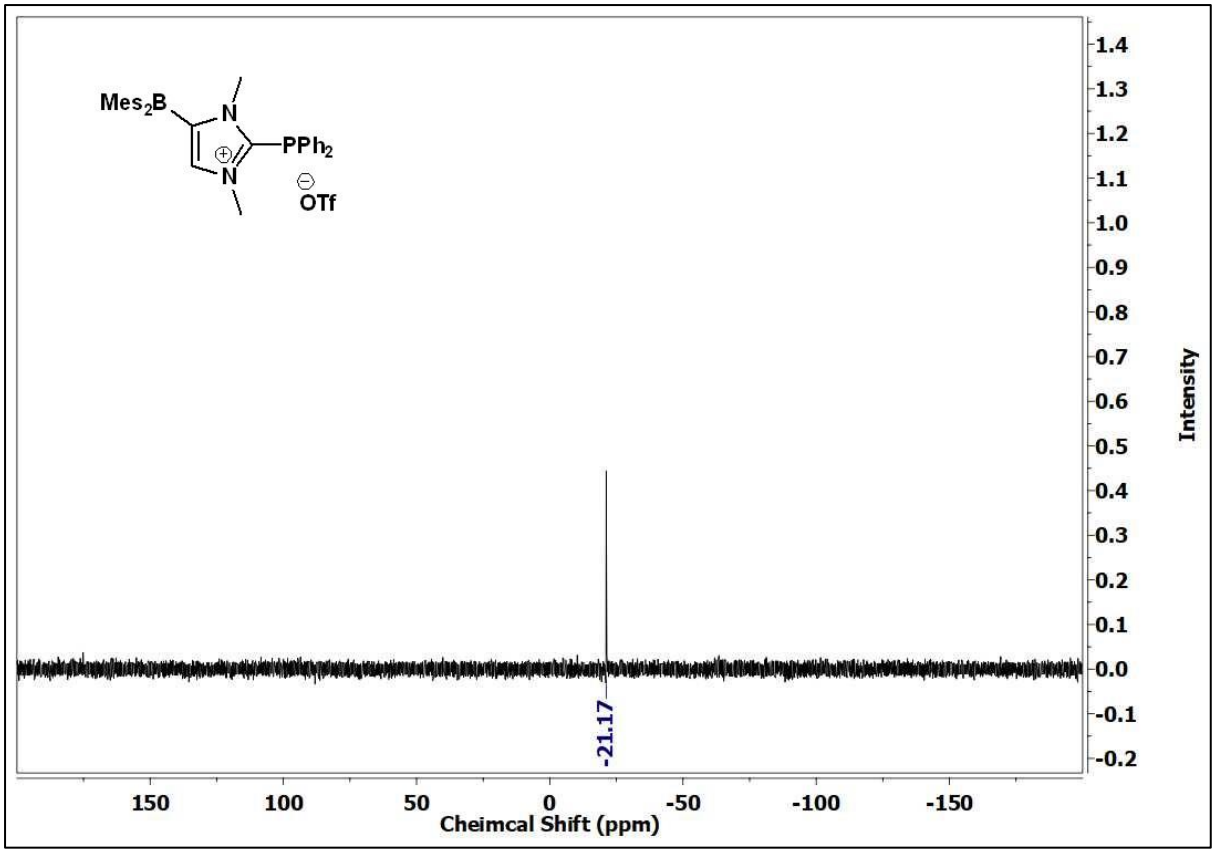


Figure S33: ^{31}P NMR of **11** ($CDCl_3$)

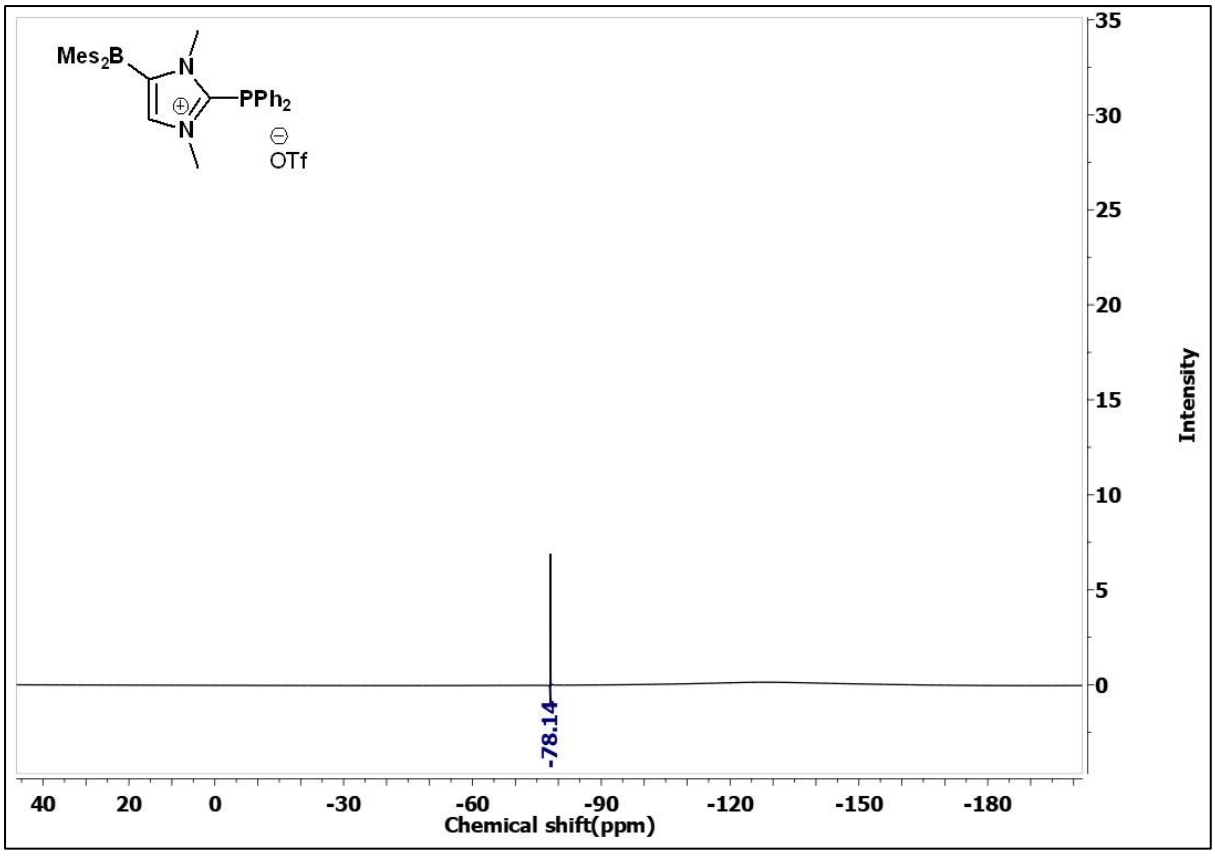


Figure S34: ^{19}F NMR of **11**($CDCl_3$)

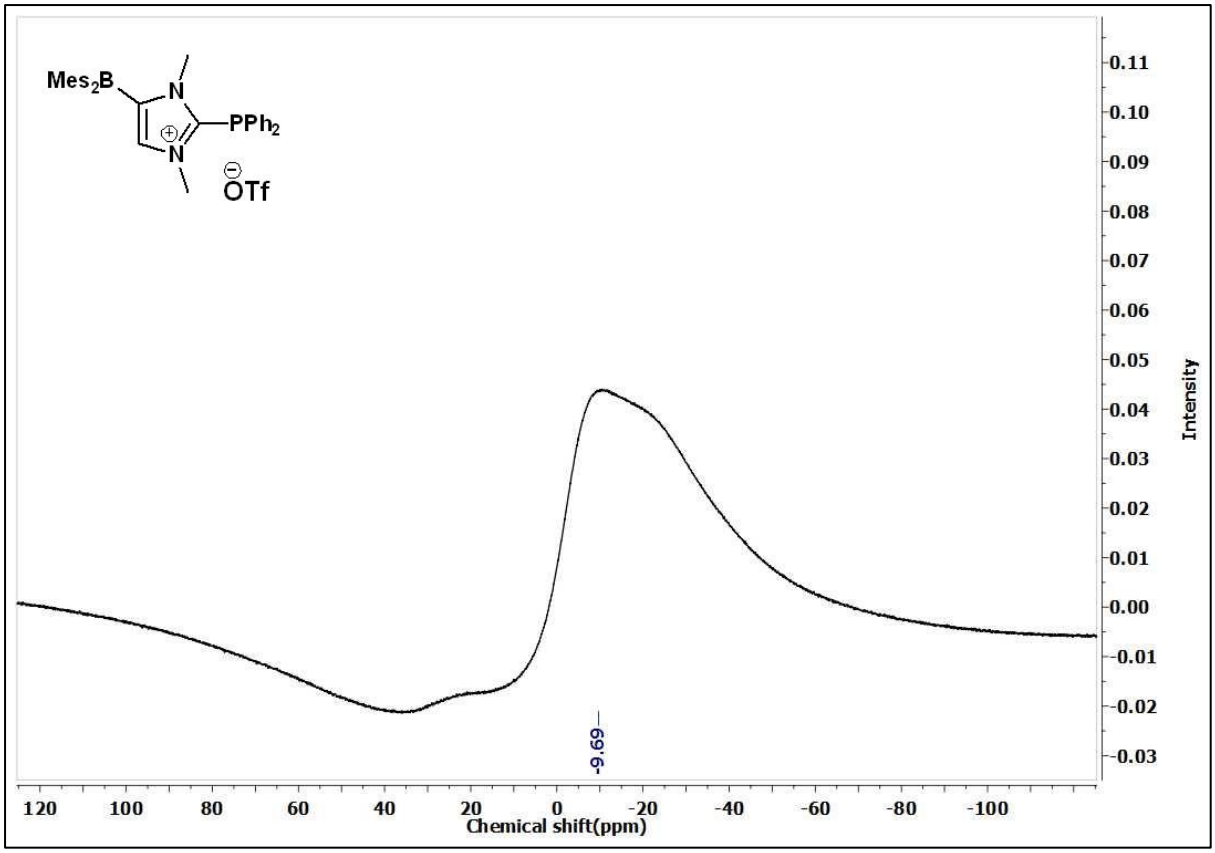


Figure S35: ^{11}B NMR of **11**($CDCl_3$)

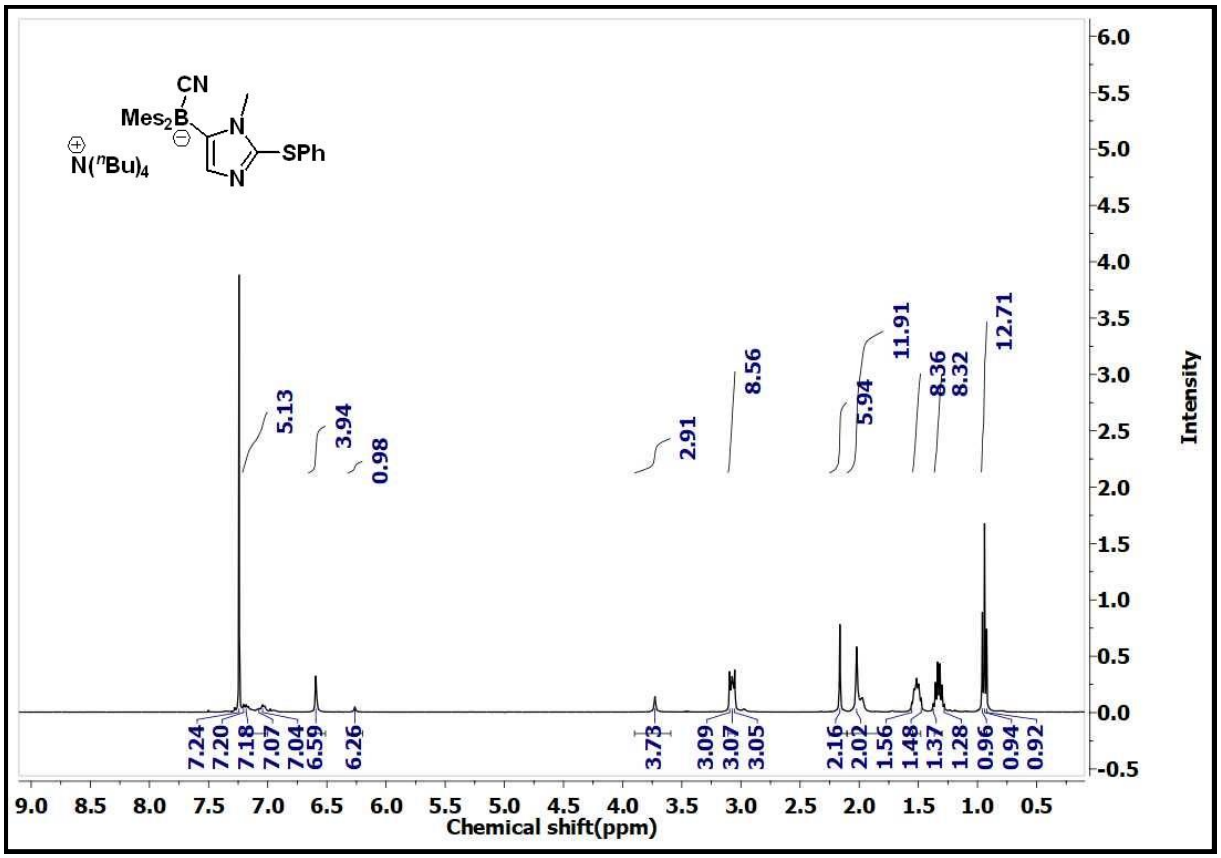


Figure S36: ^{1}H NMR of **7**-[CN] ($CDCl_3$)

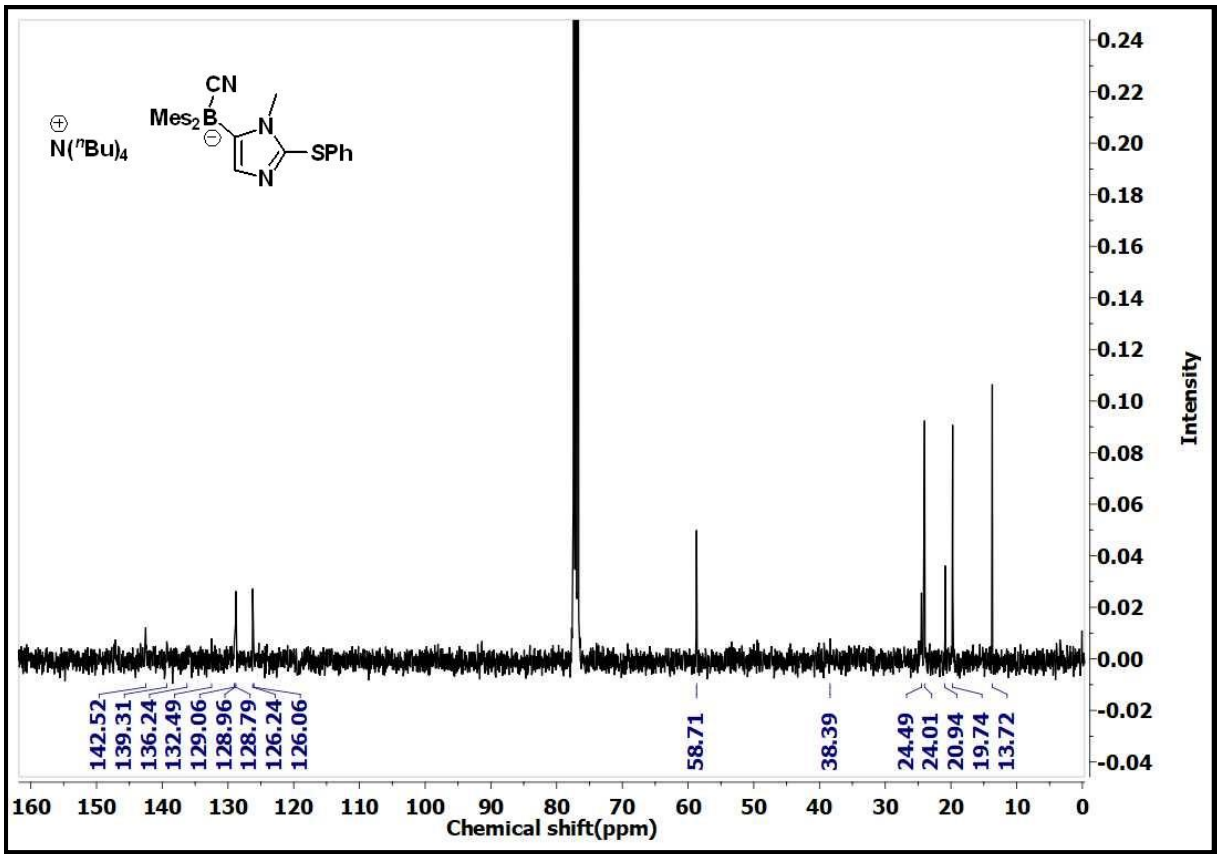


Figure S37: ^{13}C NMR of **7**-[CN] ($CDCl_3$)

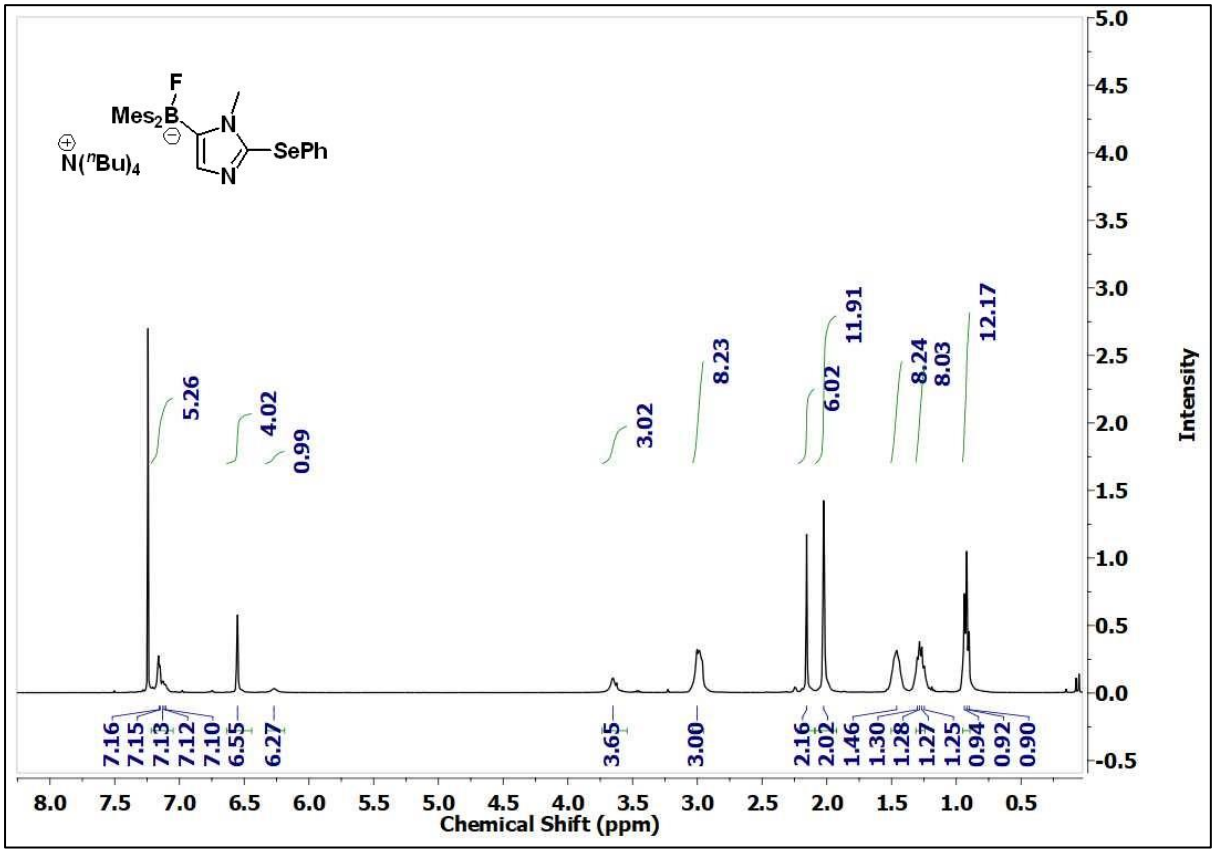


Figure S38: ^{1}H NMR of **8**-[F] ($CDCl_3$)

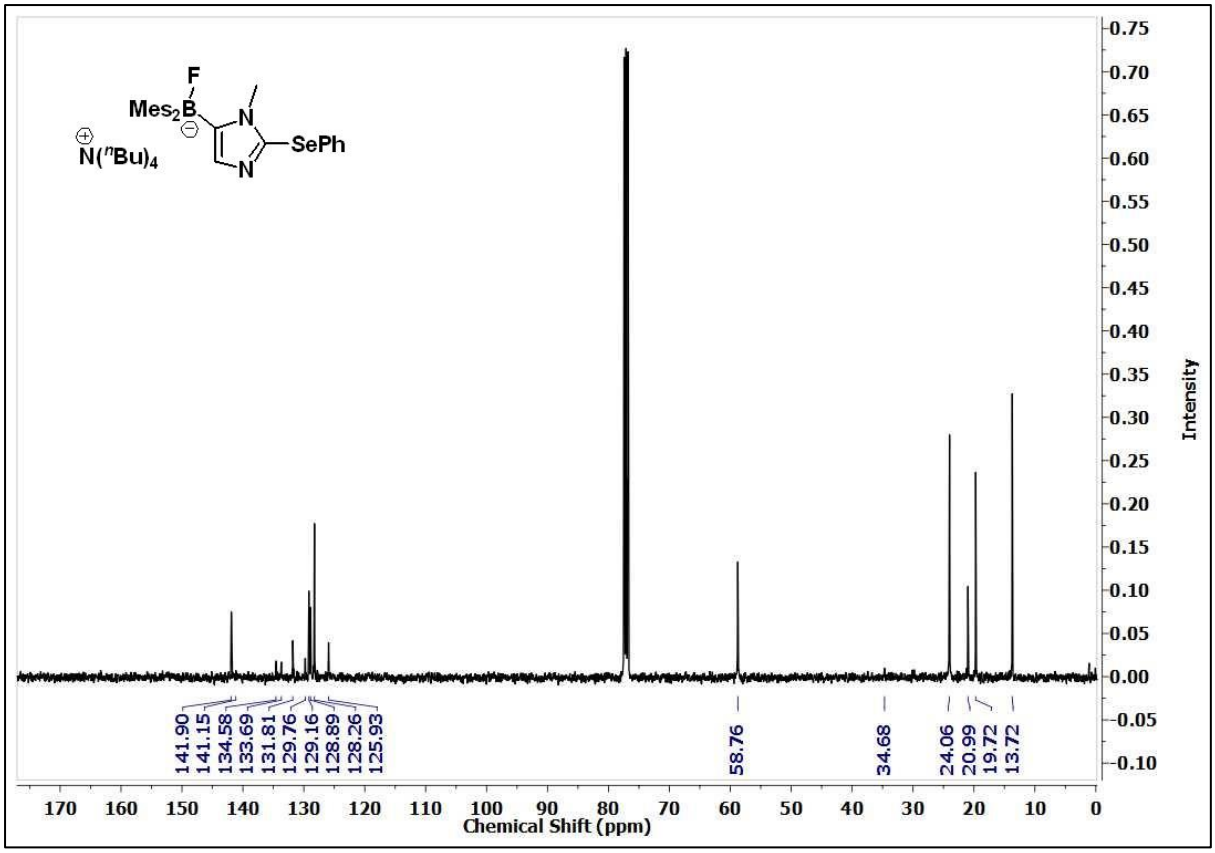


Figure S39: ^{13}C NMR of **8**-[F] ($CDCl_3$)

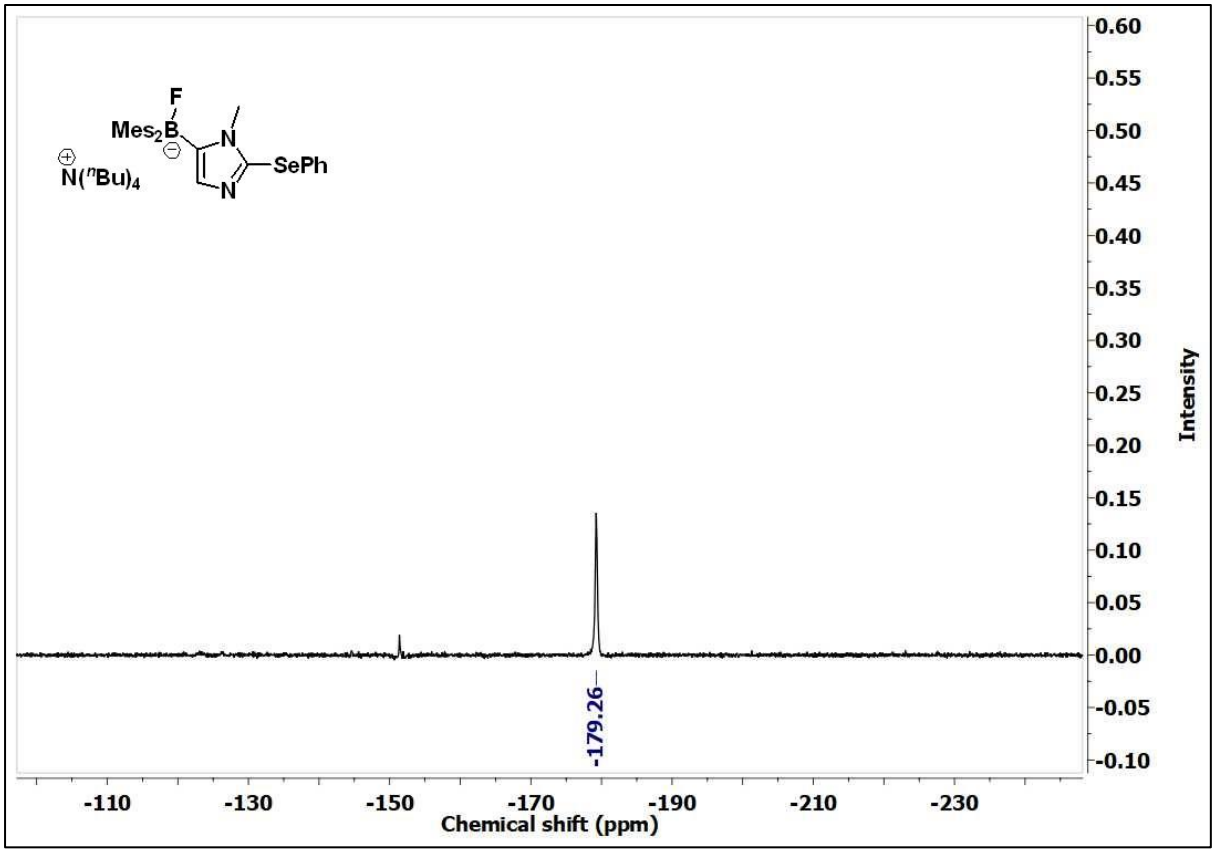


Figure S40: ^{19}F NMR of **8**-[F] ($CDCl_3$)

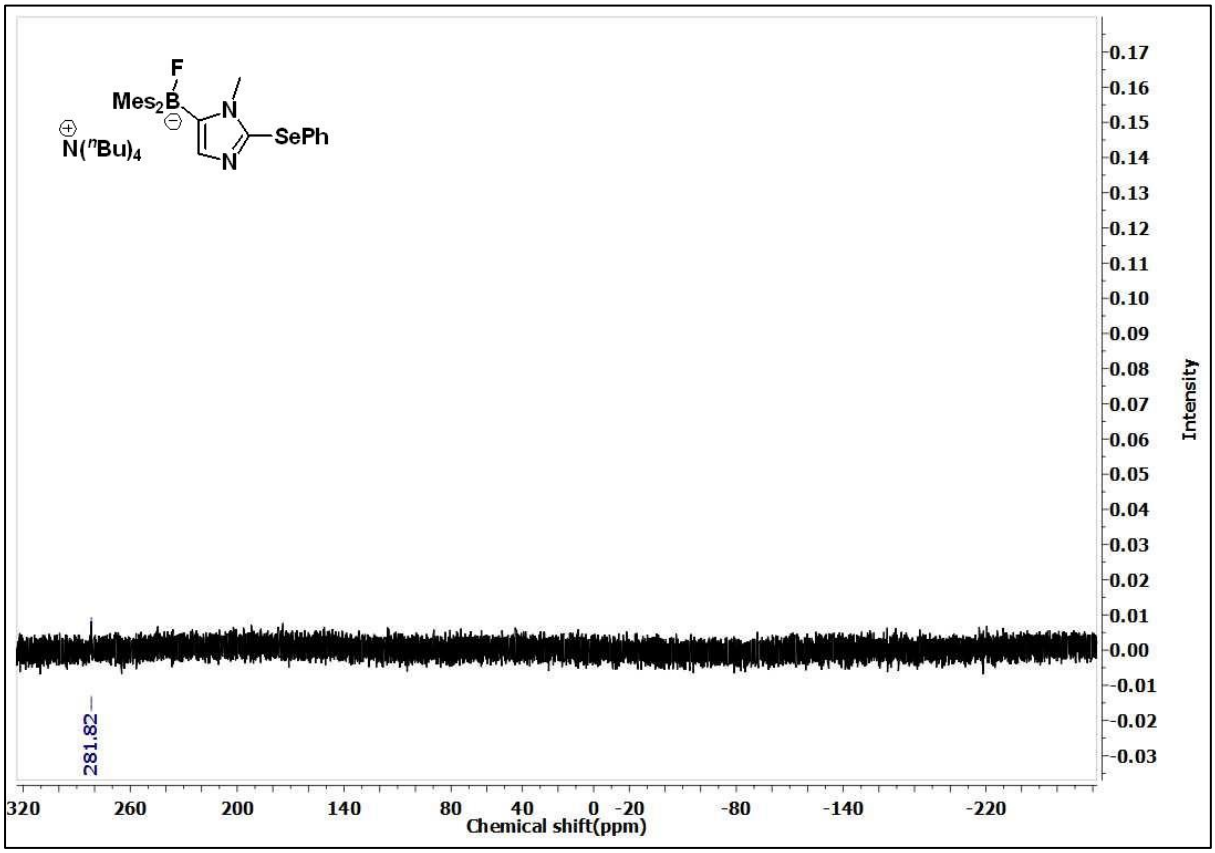


Figure S41: ^{77}Se NMR of **8**-[F] ($CDCl_3$)

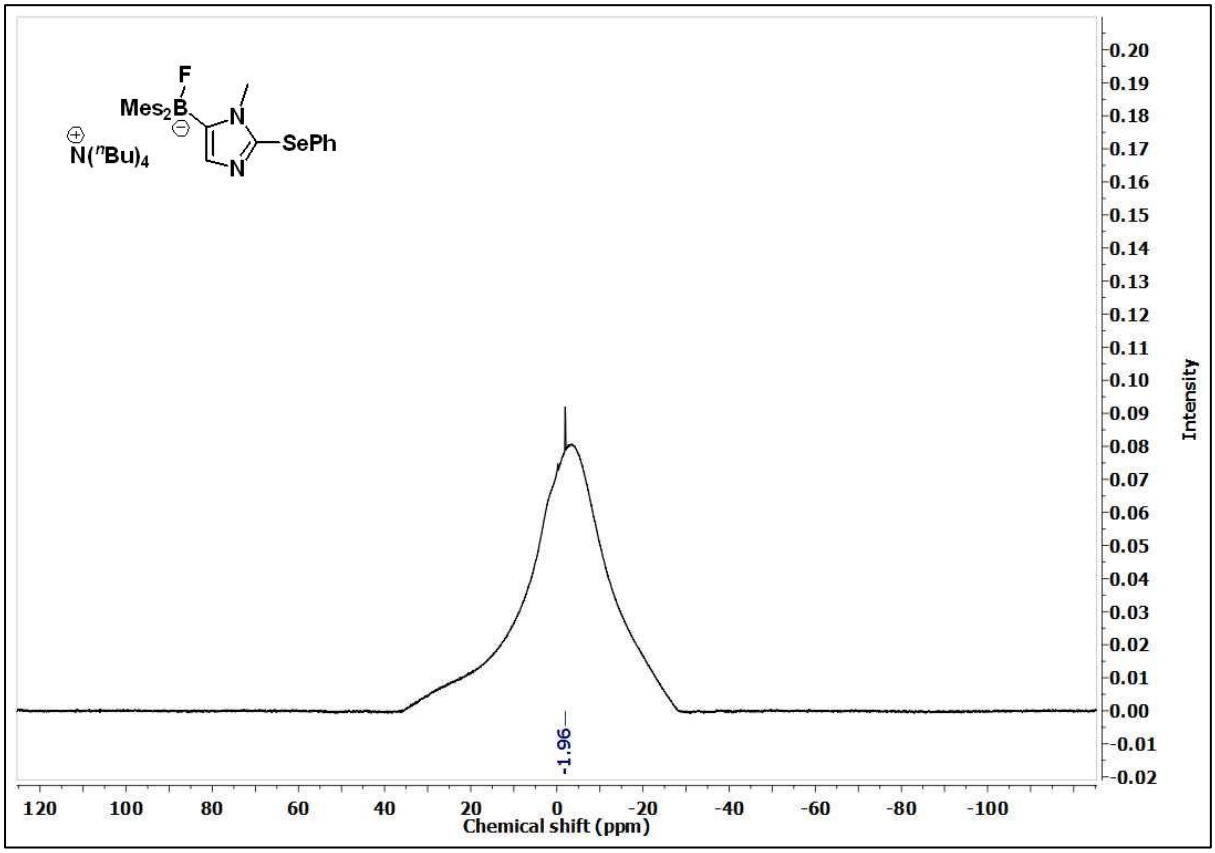


Figure S42: ^{11}B NMR of **8**-[F] ($CDCl_3$).

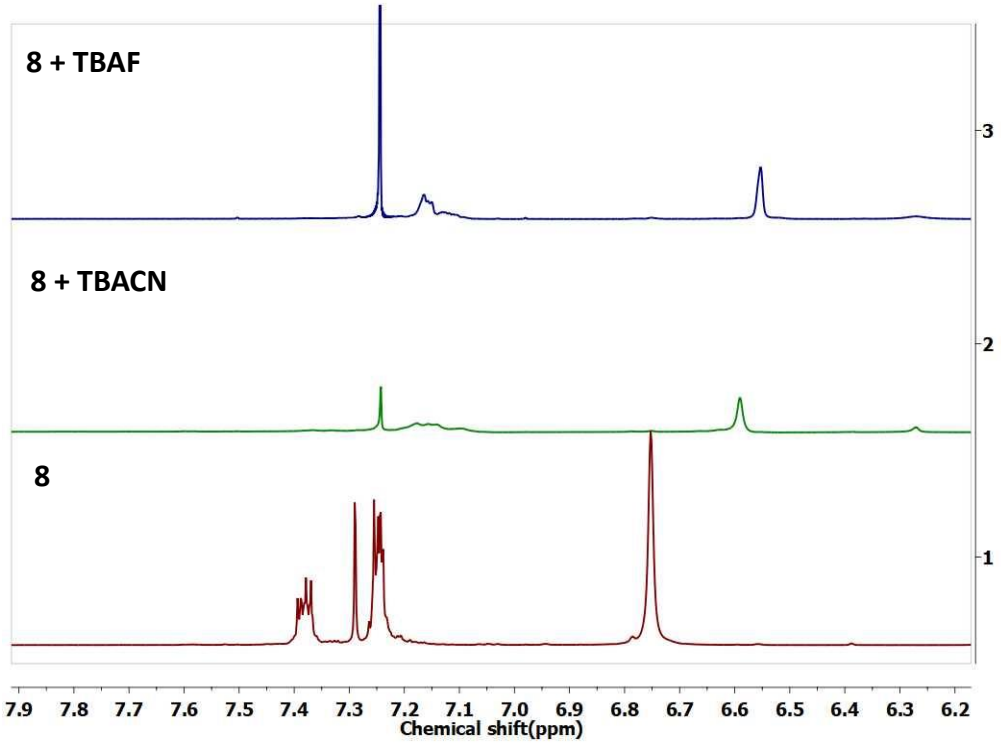


Figure S43: Partial ^{1}H-NMR spectra of (**8**) in the aromatic region upon addition of TBAF and TBACN (1.0 equiv.) in $CDCl_3$ at 400 MHz.

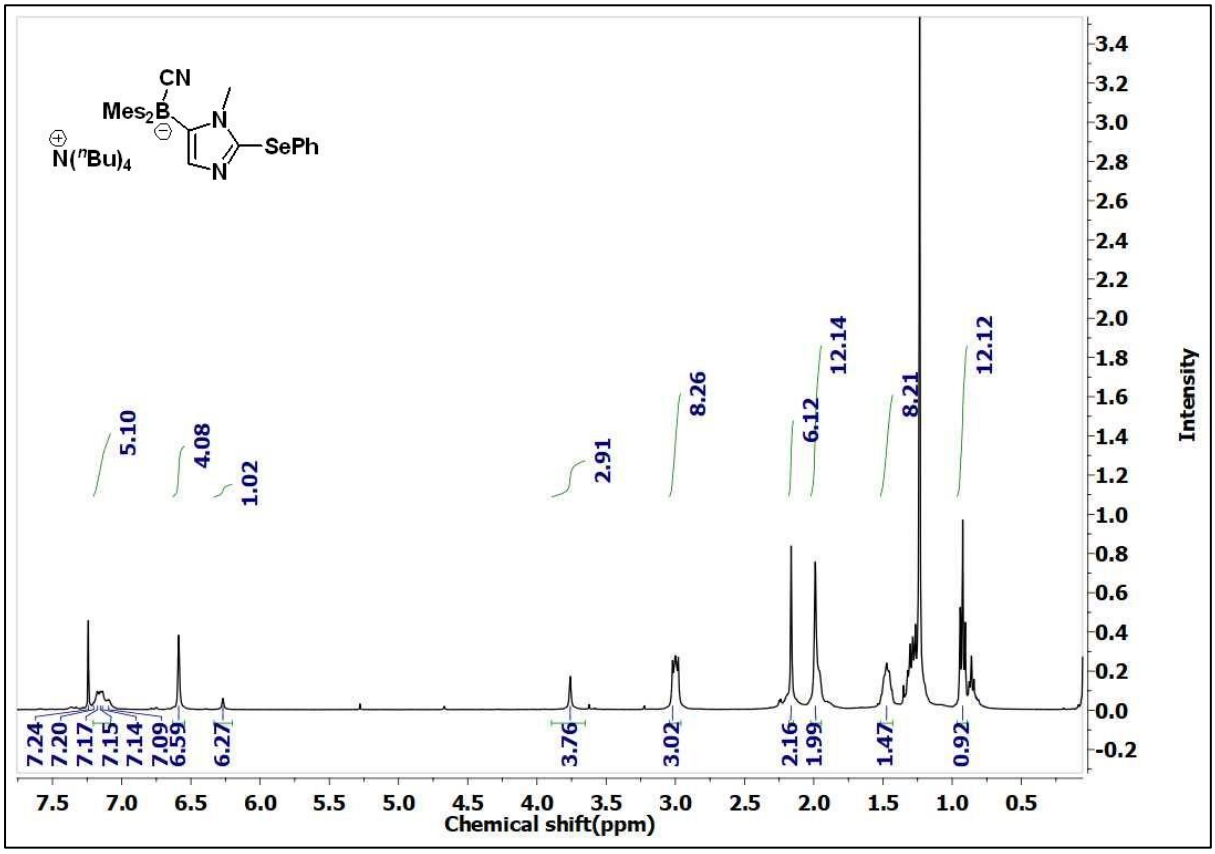


Figure S44: ^{1}H NMR of **8**-[CN] ($CDCl_3$)

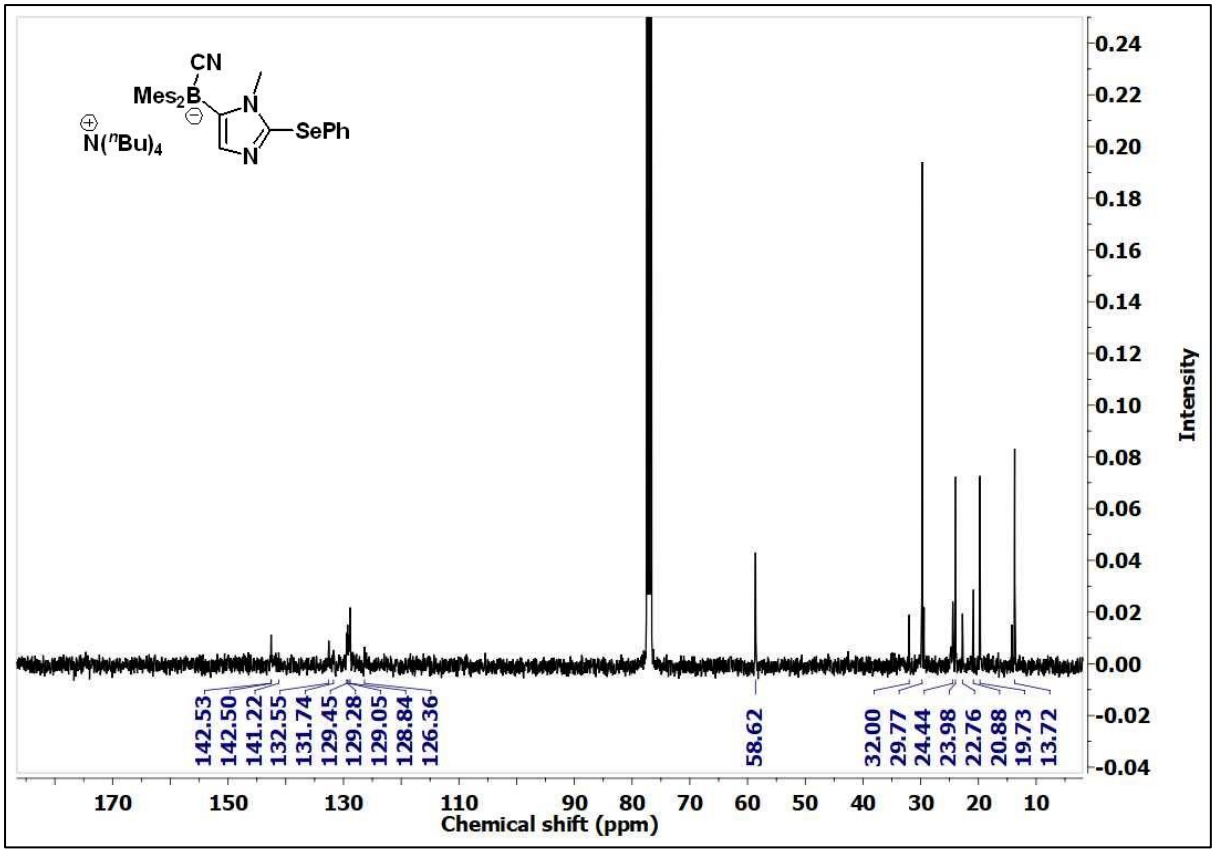


Figure S45: ^{13}C NMR of **8**-[CN] ($CDCl_3$)

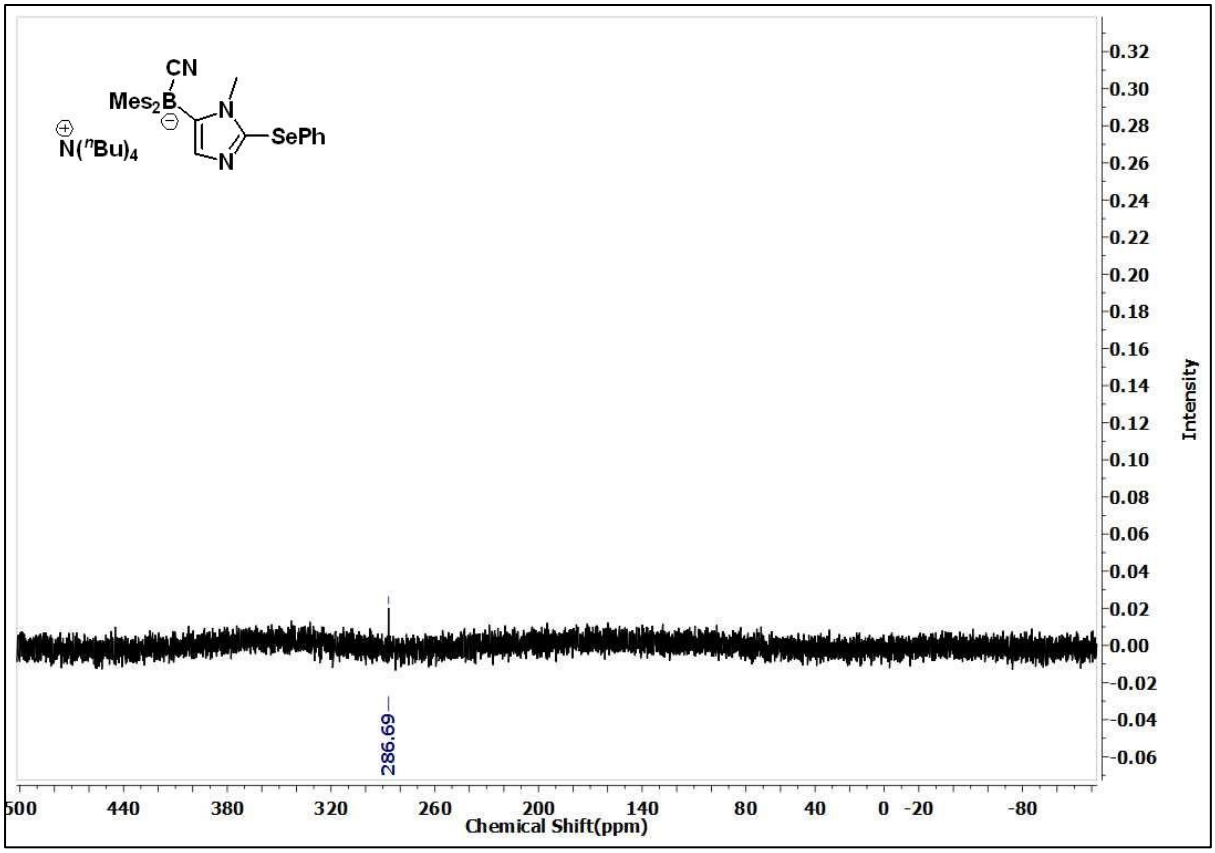


Figure S46: ^{77}Se NMR of **8**-[CN] ($CDCl_3$)

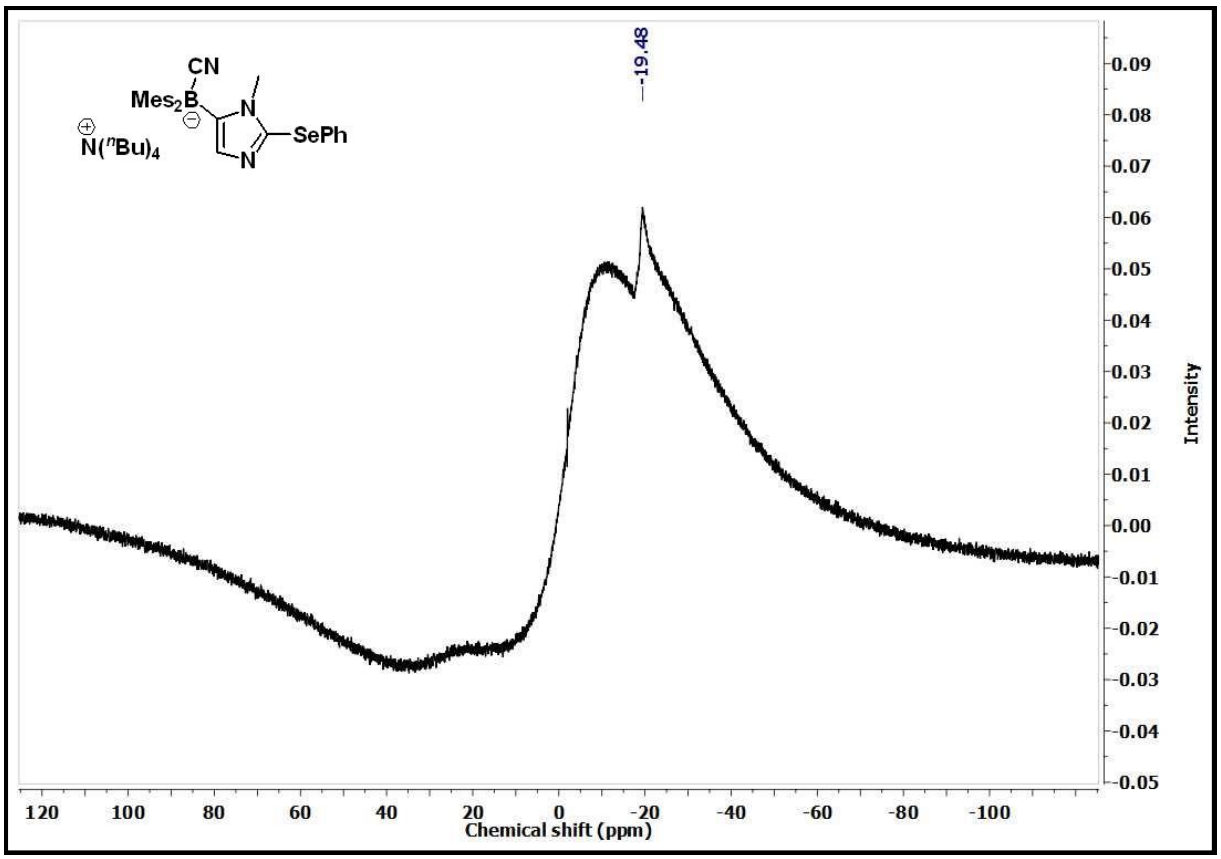


Figure S47: ^{11}B NMR of **8**-[CN] ($CDCl_3$)

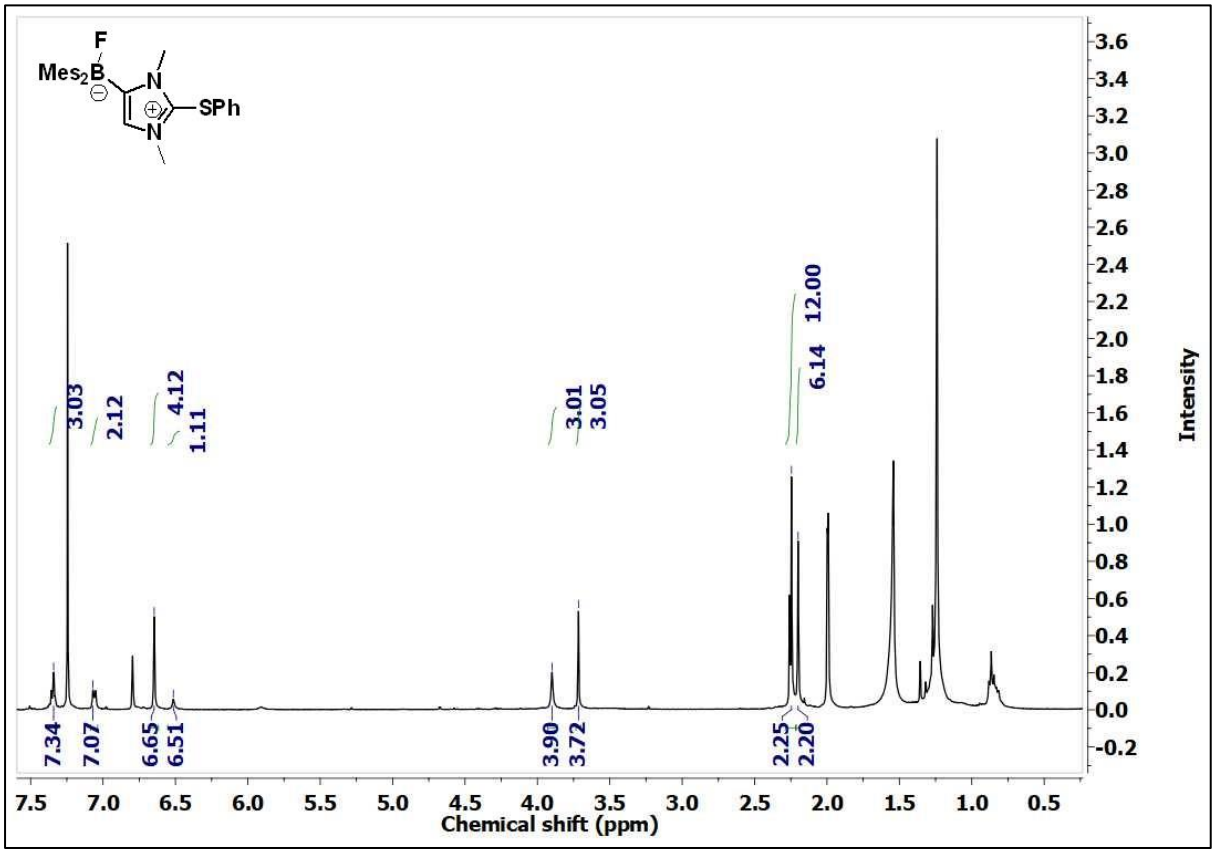


Figure S48: ^{1}H NMR of **9**-[F] ($CDCl_3$)

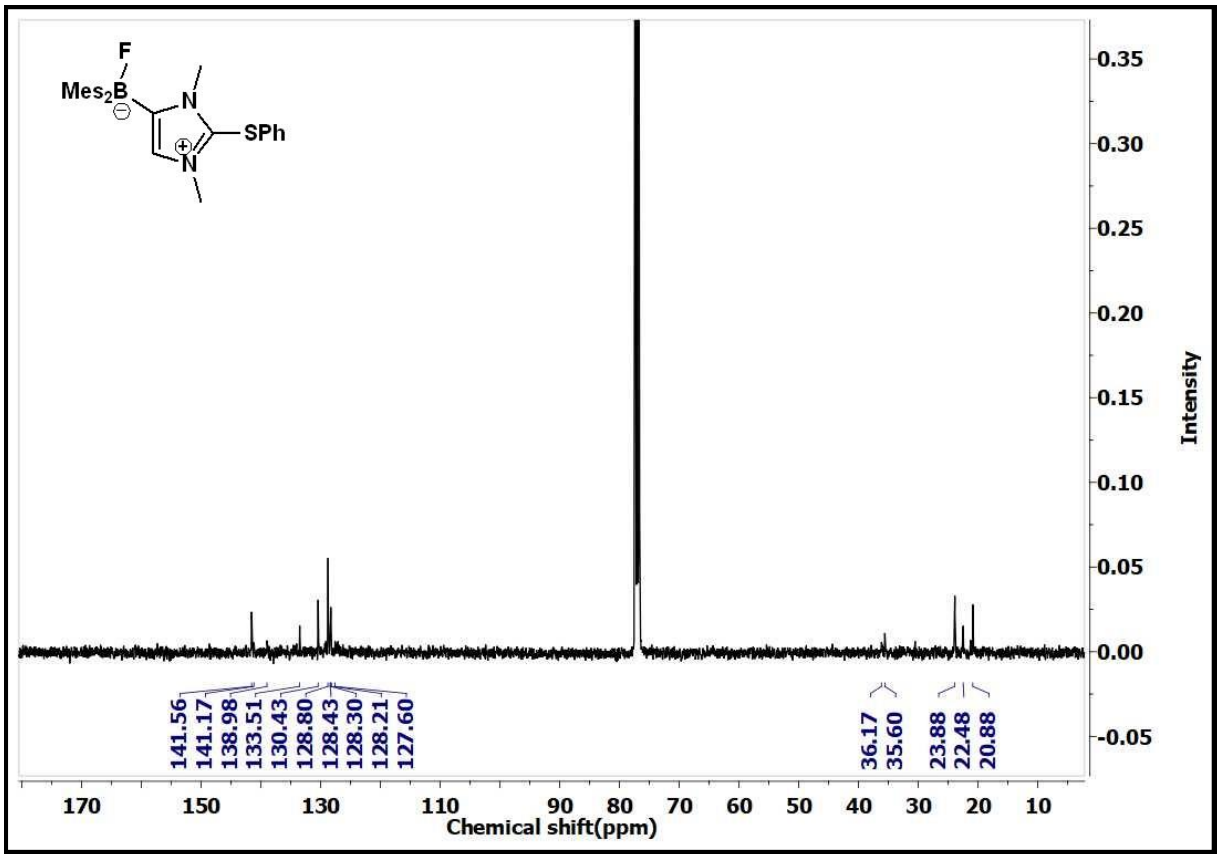


Figure S49: ^{13}C NMR of **9**-[F] ($CDCl_3$)

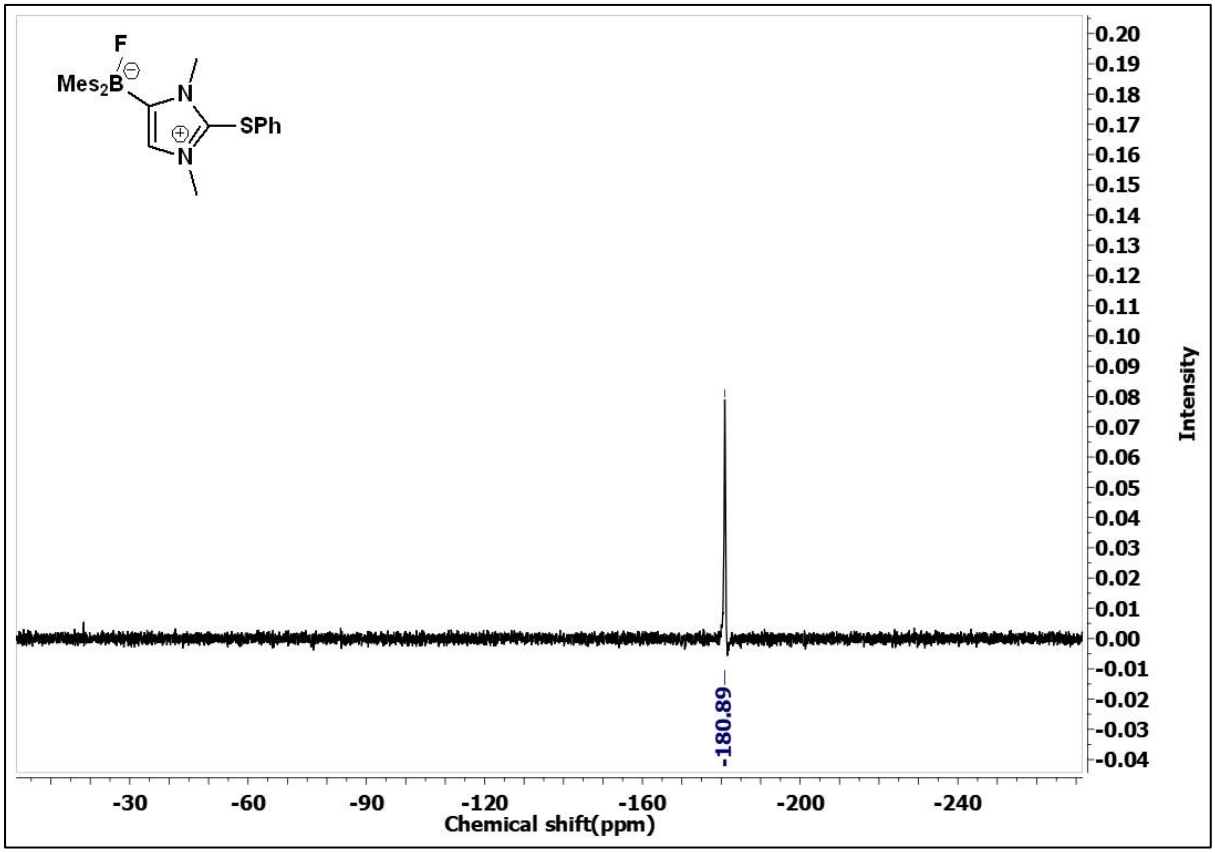


Figure S50: ^{19}F NMR of **9**-[F] ($CDCl_3$)

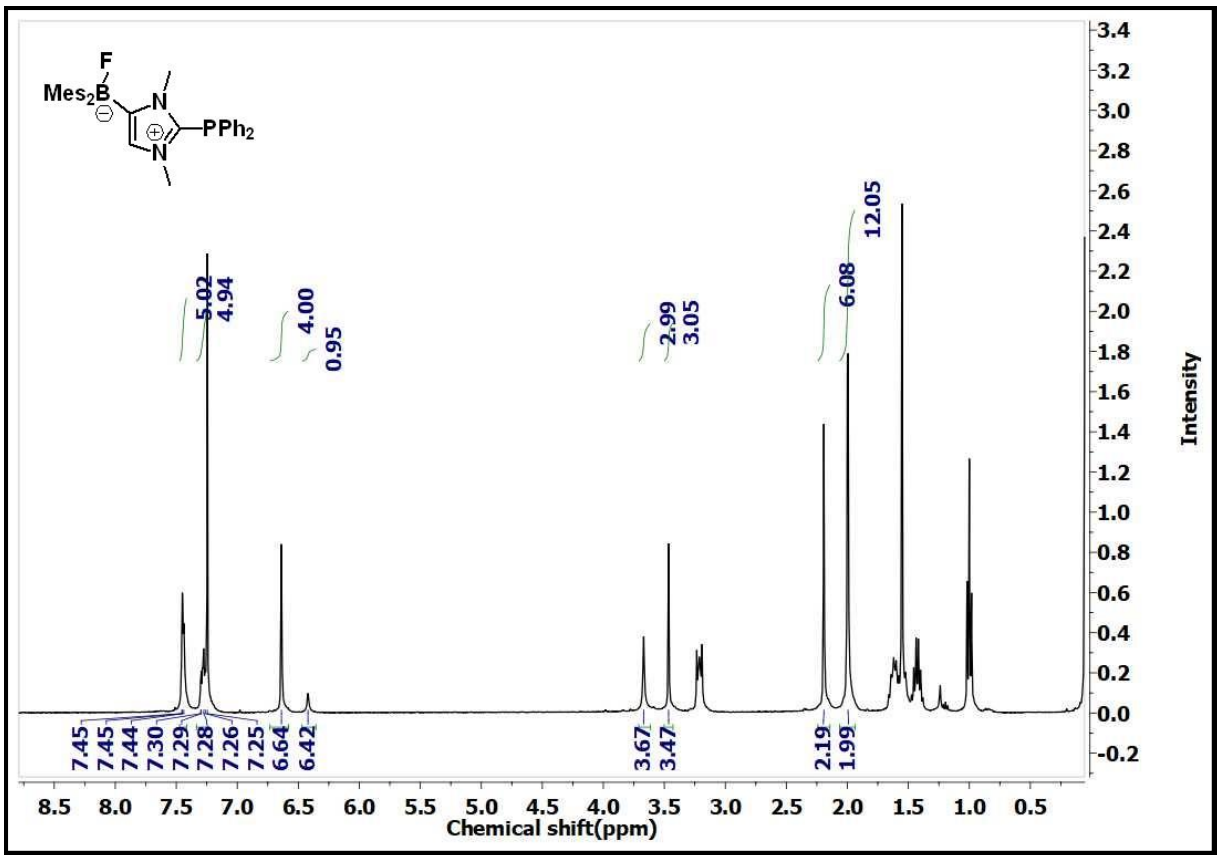


Figure S51: ^{1}H NMR of **11-**[F] ($CDCl_3$)

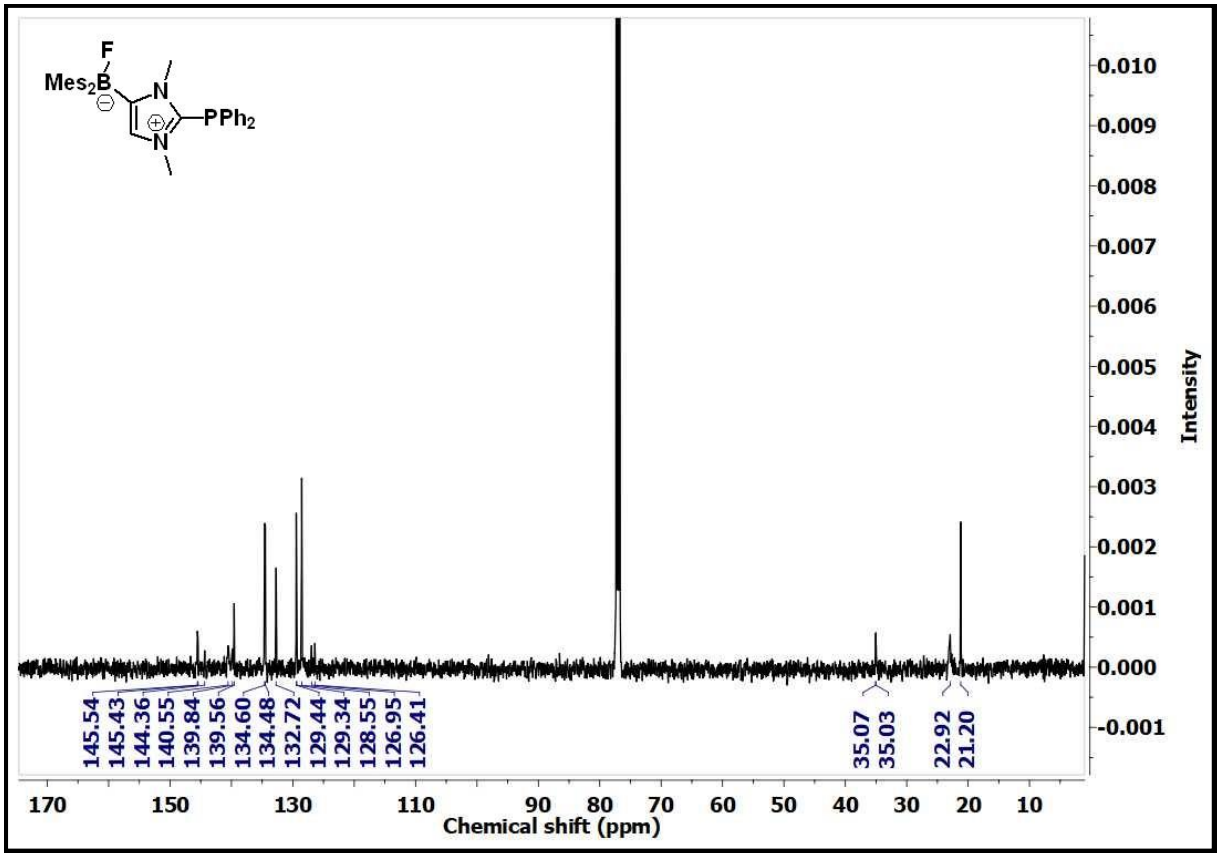


Figure S52: ^{13}C NMR of **11-**[F] ($CDCl_3$)

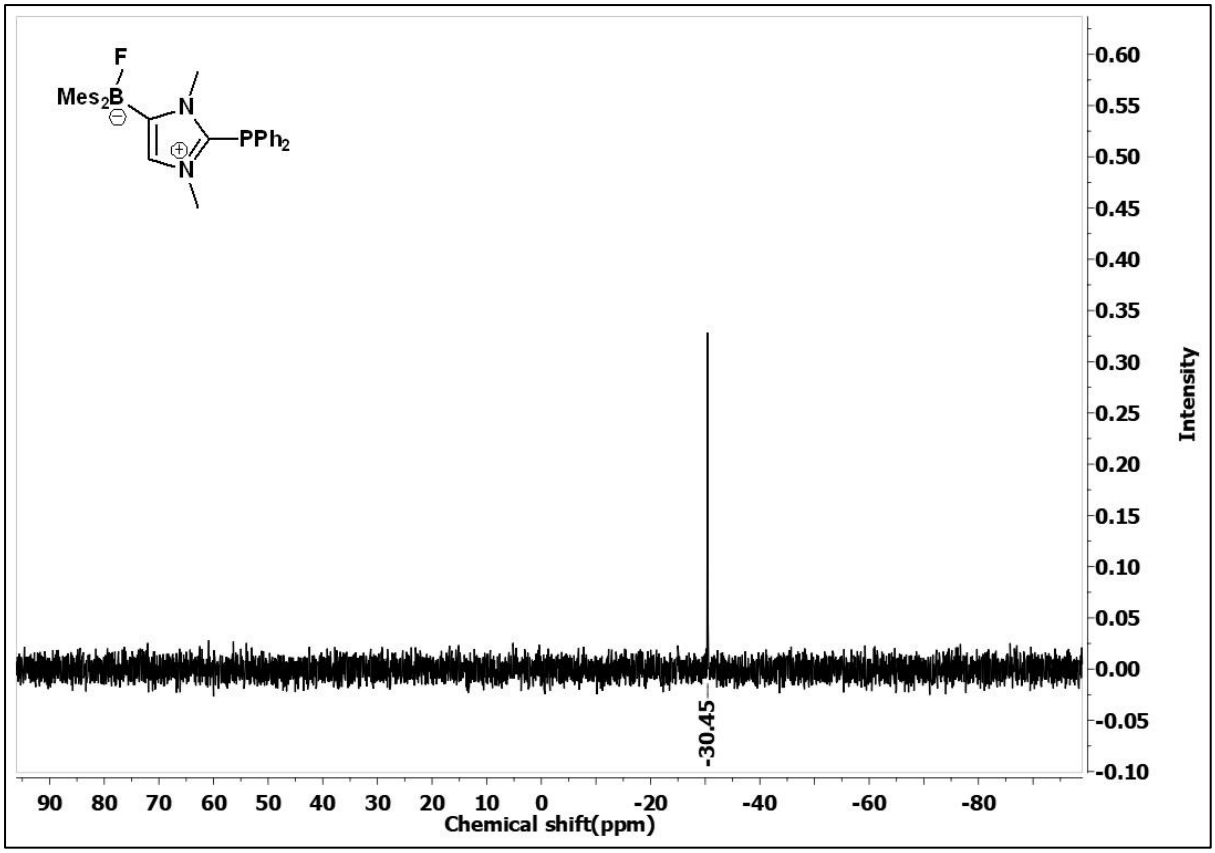


Figure S53: ^{31}P NMR of **11-**[F] ($CDCl_3$)

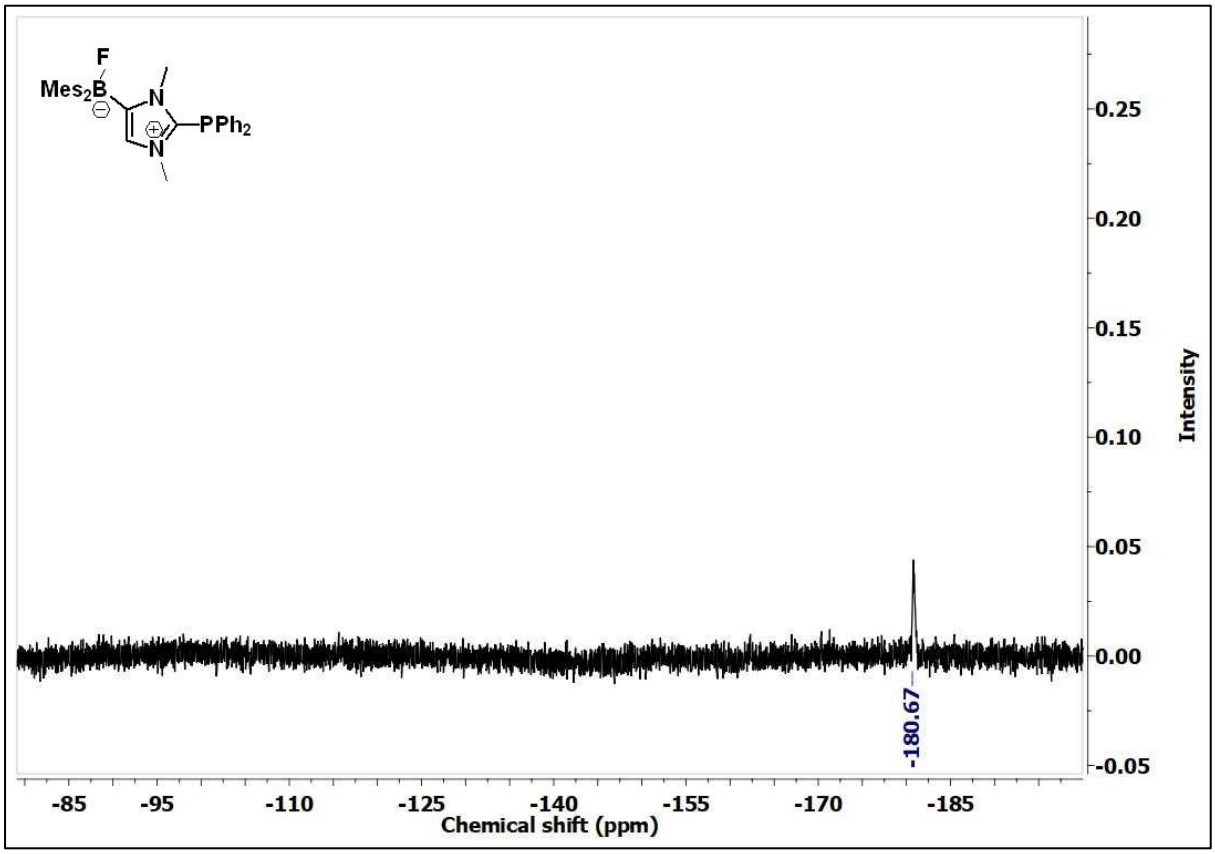


Figure S54: ^{19}F NMR of **11-**[F] ($CDCl_3$)

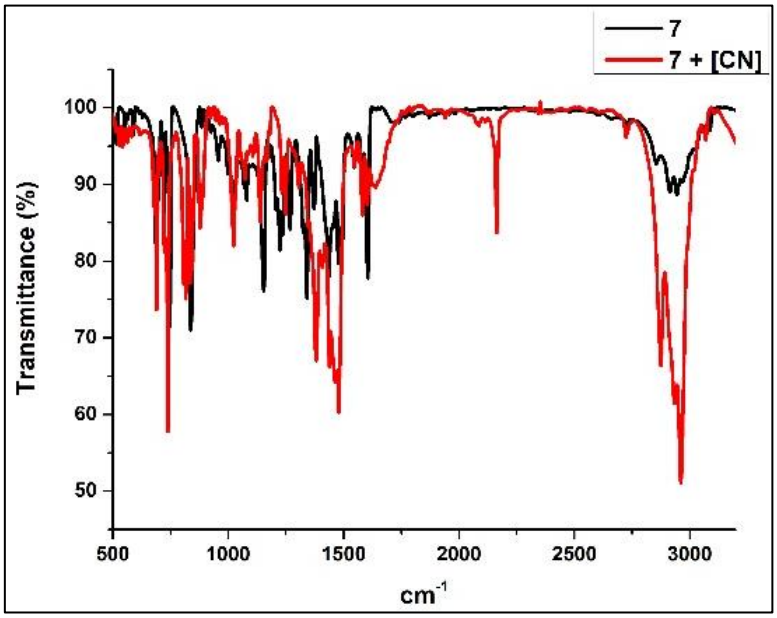


Figure S55: IR spectra of **7** and **7-**[CN]

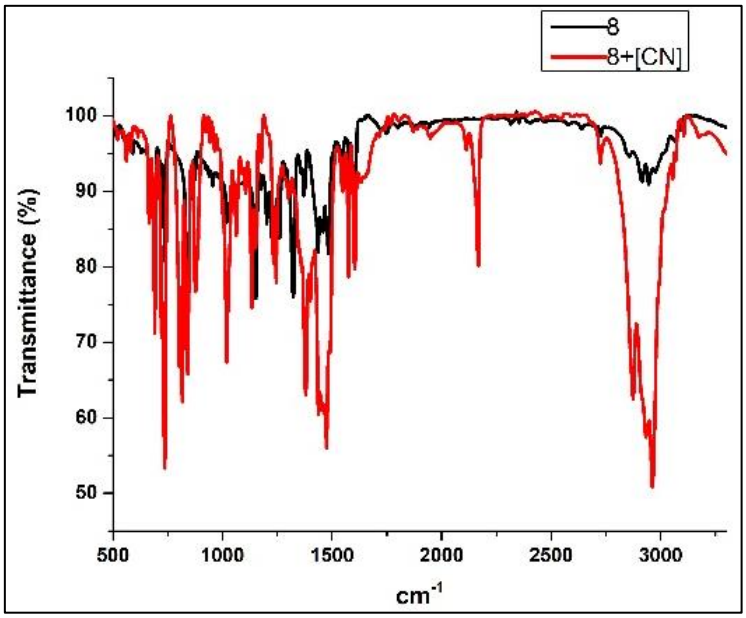


Figure S56: IR spectra of **8** and **8-**[CN]

Selectivity of 7-11 with various anions

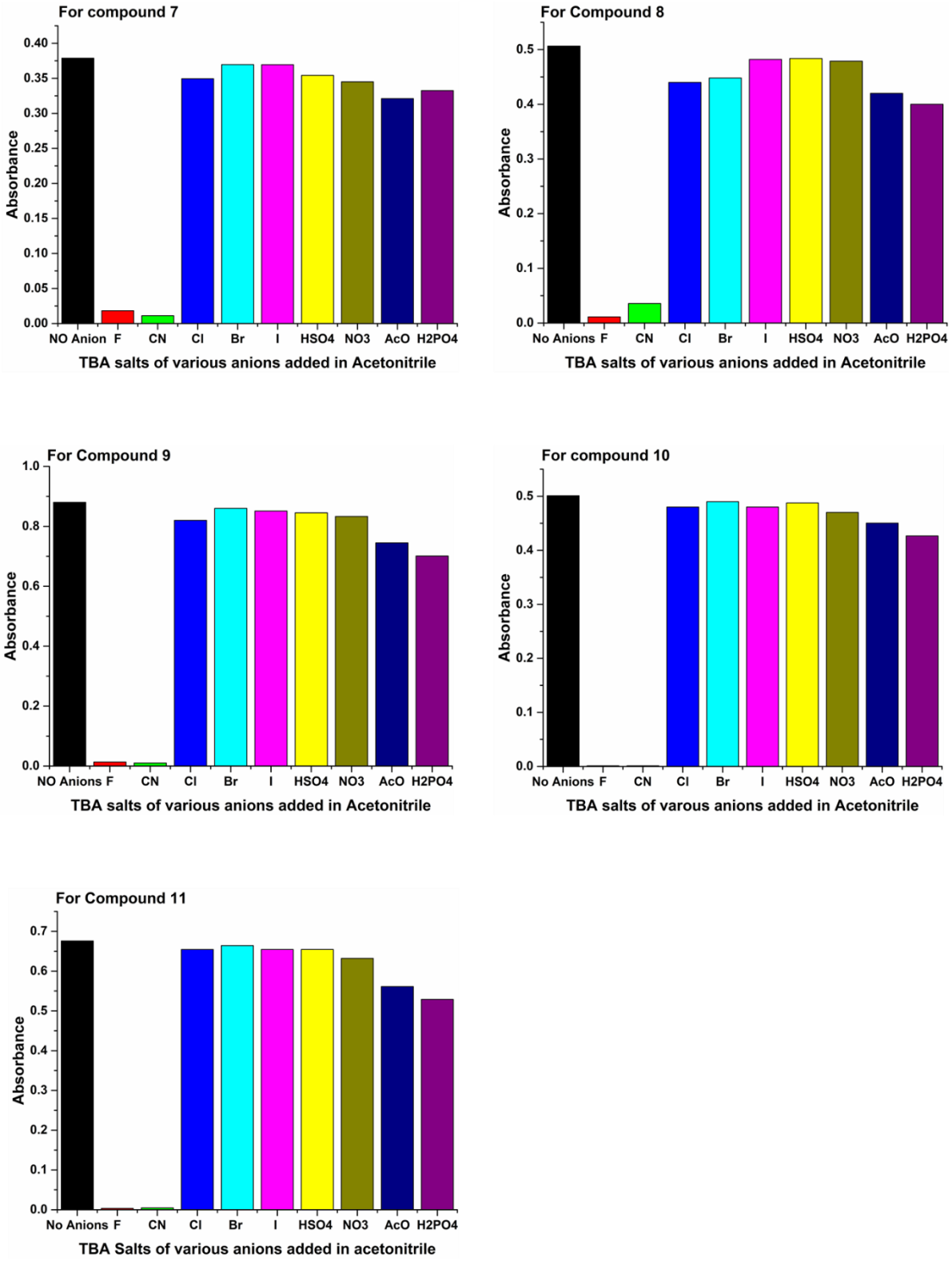


Figure S57: UV- vis titration of compounds **7**-**11** with TBAX (X= F, Cl, Br, I, CN, HSO_4, NO_3, OAc, H_2PO_4) in acetonitrile.

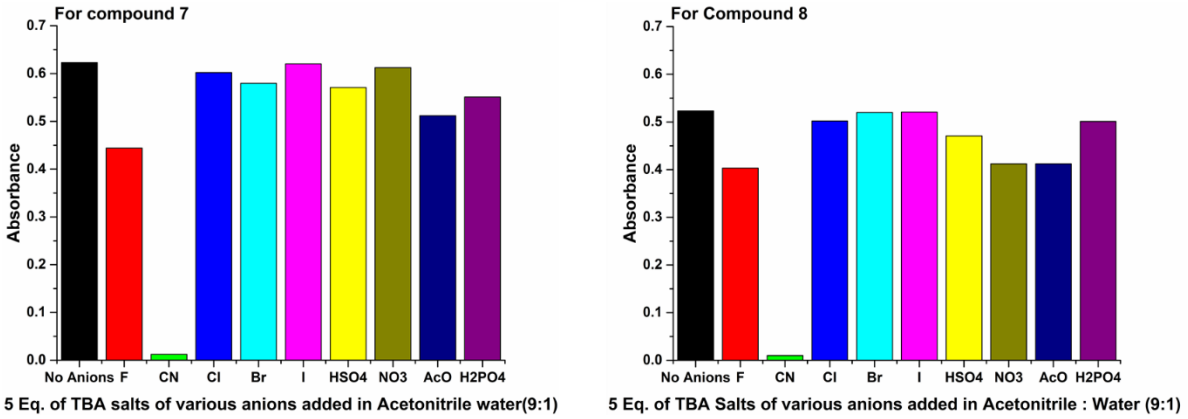


Figure S58: UV- vis titration of compounds **7** and **8** with TBAX (X= F, Cl, Br, I, CN, HSO_4, NO_3, OAc, H_2PO_4) in acetonitrile:water (9:1).

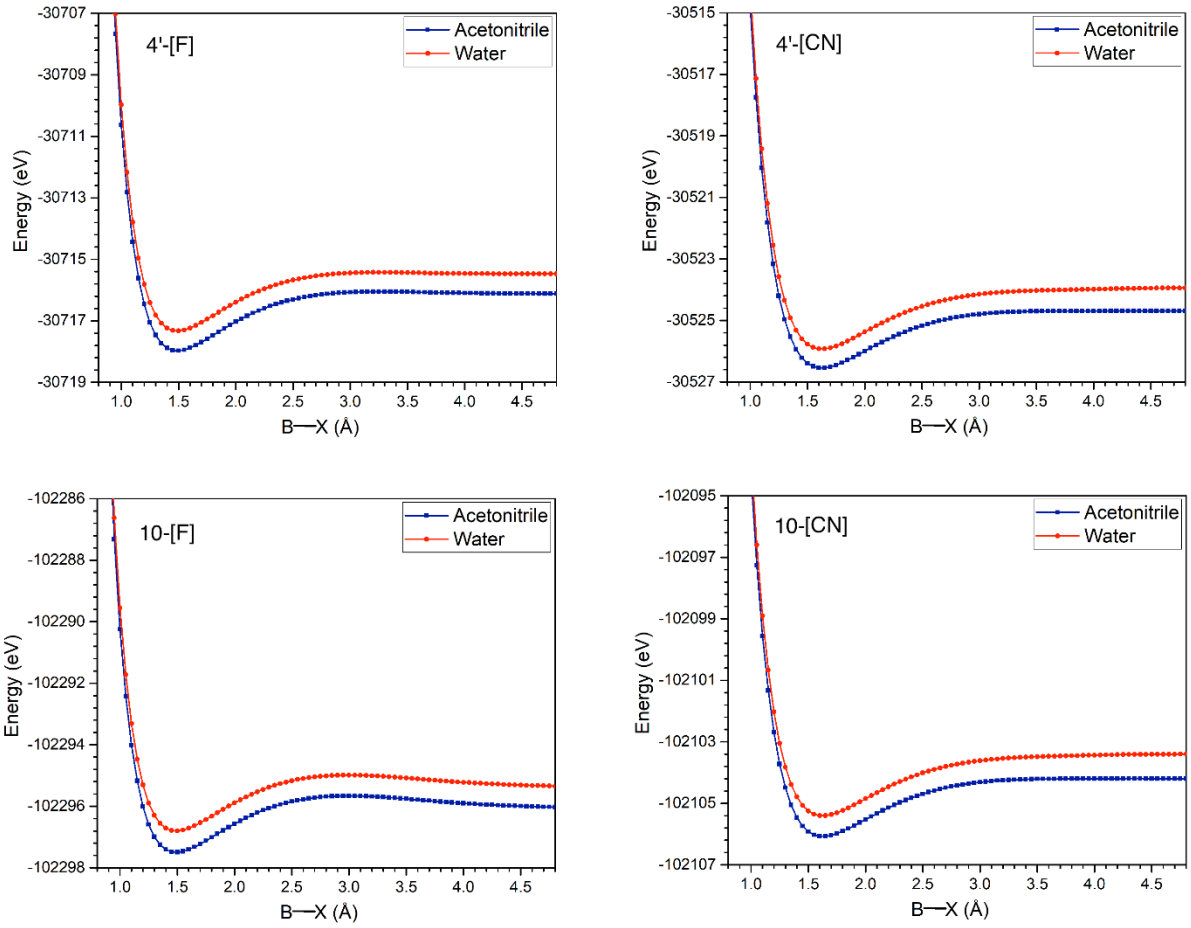


Figure S59. Calculated binding energy curves of B–X (where X is F^-/CN^- anion) in acetonitrile (blue) and water (red) solvent reaction fields for the **4'**-[F]**, 4'**-[CN]**, 10**-[F]**, and 10**-[CN]. The estimated binding energies for B–X in acetonitrile are: **4'**-[F]=1.93 eV, **4'**-[CN]=1.85 eV, **10**-[F]=1.84 eV, **10**-[CN]=1.87 eV. Similar the estimated binding energies for B–X in water are: **4'**-[F]=1.90 eV, **4'**-[CN]=1.98 eV, **10**-[F]=1.82 eV, **10**-[CN]=2.00 eV.

Table S7: Calculated binding energy values of B–X (where X is F^-/CN^- anion) in acetonitrile and water solvent reaction fields for the **1′-**[F]**, 1′-**[CN]**, 7-**[F]**, 7-**[CN]**, 8-**[F]**, 8-**[CN]**, 4′-**[F]**, 4′-**[CN]**, 10-**[F]**, and 10-**[CN] scaffolds.

Compound	**Fluoride binding energy (eV)**		**Cyanide binding energy (eV)**	
	Acetonitrile	Water	Acetonitrile	Water
1′	1.689	1.677	1.646	1.774
7	1.747	1.733	1.699	1.828
8	1.735	1.721	1.671	1.803
4′	1.925	1.904	1.854	1.980
10	1.837	1.816	1.871	2.002

Table S8: Calculated Mulliken charge densities collected for selective atoms of various boron imidazole/imidazolium scaffolds.

Compound / Atoms	Mulliken atomic charge (e)							
	N1	C2	N2	C4	C5	B	F	CN
1′	0.179	0.204	-0.318	-1.310	0.270	0.276	-	-
1′-[F]	0.168	0.150	-0.334	-0.894	-0.586	1.005	-0.514	-
1′-[CN]	0.319	0.176	-0.296	-1.018	-0.798	0.920	-	-0.236
7	0.302	-0.617	-0.106	-1.166	0.241	0.381	-	-
7-[F]	0.343	-0.816	-0.098	-0.830	-0.234	1.142	-0.490	-
7-[CN]	0.547	-0.619	-0.091	-0.954	-0.604	1.026	-	-0.274
8	0.338	-0.471	-0.112	-1.021	0.168	0.326	-	-
8-[F]	0.394	-0.523	-0.125	-0.765	-0.542	1.055	-0.502	-
8-[CN]	0.577	-0.436	-0.104	-0.876	-0.830	0.956	-	-0.309

Note: In case of cyanide charges are reported on carbon atom.

Table S9. Cartesian Coordinates of the optimized imidazole and imidazolium complexes studied at B3LYP/6-31+g(d) level of theory. All the calculations were carried-out in MeCN solvent using SMD solvation model. Molecular formula, total electronic energy (HF), and the number of imaginary frequencies (NImag) are listed as well. Within the harmonic approximation, all the geometries optimized were verified as minima on their potential energy surfaces.

1' [BC22N2H27]
HF = -989.0615658 Ha
NImag= 0

1	-1.875848000	2.492345000	1.221938000
7	-0.581106000	4.123511000	0.735223000
7	0.964637000	2.896554000	-0.306974000
6	-0.858790000	-1.559366000	2.194303000
1	0.025415000	-2.067110000	1.793022000
1	-1.339214000	-2.239673000	2.906116000
1	-0.501575000	-0.689855000	2.758463000
6	2.152418000	2.627505000	-1.115197000
1	2.879925000	2.037949000	-0.554191000
1	2.602042000	3.584213000	-1.390150000
1	1.873934000	2.088933000	-2.024340000
6	-0.958243000	2.810163000	0.742761000
6	4.942997000	-2.809907000	-0.215730000
1	5.594844000	-2.473974000	-1.034084000
1	4.720888000	-3.868837000	-0.398495000
1	5.514861000	-2.736744000	0.715905000
6	-3.734903000	-0.525486000	-0.838990000
1	-4.467203000	-0.282339000	-1.608549000
6	3.679242000	-1.984444000	-0.152158000
6	-2.471834000	0.080387000	-0.893825000
6	3.460057000	-1.062820000	0.876043000
1	4.209452000	-0.954798000	1.659107000
6	-0.022425000	1.991009000	0.109962000
6	0.575763000	4.133079000	0.074167000
1	1.156448000	5.013913000	-0.168160000
6	1.506404000	-1.355406000	-1.095796000
6	-1.481660000	-0.234479000	0.079141000
6	1.292310000	-0.405959000	-0.056575000
6	2.304493000	-0.267421000	0.932307000
6	2.686852000	-2.108776000	-1.132968000
1	2.832093000	-2.818223000	-1.946781000
6	0.497089000	-1.574377000	-2.205521000
1	-0.437671000	-2.002442000	-1.825867000
1	0.896445000	-2.262920000	-2.958245000

1	0.237899000	-0.639607000	-2.715702000
6	-3.112748000	-1.727762000	1.134058000
1	-3.358510000	-2.422915000	1.935628000
6	2.194513000	0.712693000	2.085946000
1	2.898609000	0.446554000	2.882250000
1	1.191951000	0.742720000	2.522600000
1	2.436369000	1.735872000	1.769919000
6	-4.082750000	-1.429324000	0.171048000
6	-5.449650000	-2.072220000	0.204150000
1	-6.245710000	-1.327630000	0.078286000
1	-5.620586000	-2.598360000	1.149702000
1	-5.563607000	-2.802953000	-0.608590000
6	-1.828251000	-1.163738000	1.098029000
5	-0.044144000	0.446989000	0.022839000
6	-2.225513000	1.050254000	-2.036902000
1	-2.832622000	0.775155000	-2.907487000
1	-1.180224000	1.078769000	-2.355262000
1	-2.504644000	2.074925000	-1.758487000

7 [BC28N2H31S]

HF = -1618.3094336 Ha

NImag= 0

7	-1.164388000	-0.978304000	-0.647670000
7	-1.114889000	-2.934708000	0.439858000
6	0.113095000	-1.078797000	-0.086017000
6	2.723302000	-0.630614000	0.150490000
6	3.529832000	-0.255031000	1.263761000
6	0.983832000	1.520997000	-0.152686000
6	0.067263000	2.158754000	0.726852000
6	1.649408000	2.329810000	-1.118333000
6	4.804790000	-0.808532000	1.429807000
1	5.395489000	-0.517670000	2.297851000
6	5.345734000	-1.719257000	0.511209000
6	0.092958000	-2.316669000	0.555771000
1	0.899450000	-2.766049000	1.121365000
6	4.558605000	-2.074982000	-0.586328000
1	4.958886000	-2.771289000	-1.322426000
6	3.263502000	-1.563573000	-0.773333000
6	-4.441535000	-1.013782000	1.281146000
1	-3.688431000	-1.503357000	1.892674000
6	-0.152141000	3.542291000	0.636371000
1	-0.845203000	4.010254000	1.334400000
6	-1.852573000	-2.106330000	-0.305024000
6	-5.327960000	-0.102230000	1.861298000
1	-5.249723000	0.116610000	2.923525000

6	-4.532188000	-1.291402000	-0.090222000
6	-1.656909000	0.085187000	-1.521571000
1	-0.815091000	0.532839000	-2.048423000
1	-2.347119000	-0.344441000	-2.250362000
1	-2.176443000	0.855073000	-0.944523000
6	1.379478000	3.701862000	-1.196104000
1	1.885433000	4.294690000	-1.957260000
6	0.485973000	4.334862000	-0.321944000
6	-6.319980000	0.512043000	1.087216000
1	-7.012555000	1.213590000	1.545256000
6	-0.702735000	1.407308000	1.796972000
1	-1.025525000	2.093919000	2.588211000
1	-1.608554000	0.941625000	1.386389000
1	-0.115459000	0.611614000	2.264306000
6	-5.519075000	-0.675175000	-0.871048000
1	-5.584898000	-0.884830000	-1.935653000
6	6.730226000	-2.290565000	0.709553000
1	6.789044000	-2.876307000	1.636704000
1	7.013859000	-2.946181000	-0.120906000
6	2.511684000	-2.041011000	-2.003925000
1	1.773368000	-1.319787000	-2.362940000
1	3.211418000	-2.239323000	-2.824614000
1	1.976214000	-2.978699000	-1.803569000
6	3.042167000	0.721572000	2.315760000
1	2.078483000	0.418544000	2.740931000
1	3.760937000	0.790319000	3.139669000
1	2.909880000	1.729352000	1.905124000
6	2.643038000	1.752428000	-2.107531000
1	2.237103000	0.889666000	-2.647149000
1	2.926423000	2.505803000	-2.850679000
1	3.560332000	1.416785000	-1.609735000
6	-6.416700000	0.218803000	-0.276341000
1	-7.182175000	0.693120000	-0.885758000
6	0.240937000	5.823190000	-0.404131000
1	1.109893000	6.388262000	-0.039239000
1	0.063284000	6.142644000	-1.438597000
1	-0.624467000	6.119145000	0.198981000
5	1.262749000	-0.036220000	-0.050791000
16	-3.473745000	-2.524718000	-0.880092000
1	7.483088000	-1.495191000	0.786552000

7-[F] [BC28N2H31SF-1]
HF = -1718.3227186 Ha

NImag= 0

16	3.777909000	-2.134319000	0.883998000
7	1.312152000	-0.842041000	0.856741000
7	1.542632000	-2.449164000	-0.677000000
6	-3.184267000	-0.573295000	-1.269728000
6	-2.566880000	-0.897557000	-0.026091000
6	-3.099651000	-2.035454000	0.653086000
1	-3.723113000	0.804395000	1.460108000
6	-4.298334000	-1.289694000	-1.743122000
6	0.084027000	-0.912136000	0.210169000
6	0.275594000	-1.921890000	-0.725768000
1	-0.448505000	-2.296609000	-1.438347000
6	2.152249000	-1.777360000	0.294750000
6	-2.686841000	0.535729000	-2.182061000
1	-1.600026000	0.522126000	-2.297522000
6	-2.508267000	-2.605497000	1.933959000
1	-1.415796000	-2.649426000	1.902409000
6	4.854583000	-0.984415000	0.001508000
1	0.494130000	0.771231000	-1.784800000
6	4.483348000	-0.334281000	-1.182078000
1	3.494248000	-0.484402000	-1.604082000
6	5.394098000	0.511426000	-1.824309000
1	5.095977000	1.015742000	-2.740538000
5	-1.263656000	-0.064542000	0.608542000
6	1.661469000	0.053247000	1.957429000
6	-4.217323000	-2.726436000	0.150650000
1	-4.737701000	-1.003141000	-2.698834000
6	-4.853075000	-2.360667000	-1.038174000
1	-3.127038000	0.427382000	-3.180708000
1	-2.956662000	1.531518000	-1.812257000
1	-2.884060000	-3.622878000	2.097957000
1	-2.774094000	-2.009573000	2.814722000
6	6.139952000	-0.791998000	0.531716000
6	6.678050000	0.702720000	-1.303287000
6	-1.261166000	1.581732000	0.334858000
9	-1.322094000	-0.155785000	2.100272000
1	0.997499000	0.915421000	1.936245000
1	2.693484000	0.392026000	1.846955000
1	1.553451000	-0.456110000	2.920942000
1	-4.592386000	-3.587524000	0.704192000
6	-6.078731000	-3.089356000	-1.540549000
6	7.047137000	0.044450000	-0.124724000
1	6.433004000	-1.288698000	1.453893000
1	7.382774000	1.358130000	-1.808485000

6	-2.270724000	2.365091000	0.972865000
6	-0.316825000	2.307267000	-0.449429000
1	-6.138212000	-4.104070000	-1.129511000
1	-6.082949000	-3.163744000	-2.635424000
1	-7.001721000	-2.566225000	-1.251012000
1	8.040642000	0.186455000	0.294008000
6	-3.368544000	1.765680000	1.838141000
6	-2.311093000	3.763485000	0.834254000
6	0.814211000	1.656230000	-1.229168000
6	-0.384644000	3.708296000	-0.560238000
1	-4.225431000	2.448492000	1.891494000
1	-3.023396000	1.593985000	2.865461000
1	-3.109082000	4.316935000	1.329974000
6	-1.368980000	4.466076000	0.079080000
1	1.235154000	2.368924000	-1.948385000
1	1.634338000	1.338844000	-0.575294000
1	0.354555000	4.220582000	-1.176481000
6	-1.402673000	5.973662000	-0.030357000
1	-1.069855000	6.313555000	-1.019144000
1	-2.412298000	6.365108000	0.143431000
1	-0.740051000	6.443531000	0.711412000

7-[CN] [BC29N3H31S-1]

HF = -1711.2892865 Ha

NImag= 0

16	3.829104000	-2.084028000	0.897042000
7	1.353414000	-0.810389000	0.884181000
7	1.561289000	-2.468130000	-0.598762000
6	-3.100111000	-0.568908000	-1.348104000
6	-2.524167000	-0.928840000	-0.092967000
6	-3.053278000	-2.108339000	0.514946000
1	-3.760552000	0.753708000	1.277503000
6	-4.190006000	-1.281594000	-1.880037000
6	0.112367000	-0.908712000	0.261309000
6	0.291776000	-1.949452000	-0.642324000
1	-0.443700000	-2.351237000	-1.326918000
6	2.186219000	-1.760676000	0.335831000
6	-2.580438000	0.557692000	-2.225254000
1	-1.489585000	0.564473000	-2.286650000
6	-2.480478000	-2.741050000	1.772802000
1	-1.389345000	-2.682815000	1.812726000
6	4.870846000	-0.956083000	-0.054189000
1	0.621566000	0.734488000	-1.663795000

6	4.486279000	-0.405703000	-1.283411000
1	3.506603000	-0.621241000	-1.699277000
6	5.372158000	0.423973000	-1.979059000
1	5.063884000	0.850825000	-2.930558000
5	-1.261204000	-0.070085000	0.599058000
6	1.737844000	0.127641000	1.937081000
6	-4.144680000	-2.793314000	-0.047855000
1	-4.598318000	-0.967984000	-2.840678000
6	-4.754721000	-2.383839000	-1.234983000
1	-2.968581000	0.444423000	-3.244514000
1	-2.888192000	1.546051000	-1.866293000
1	-2.757362000	-3.801113000	1.813858000
1	-2.862524000	-2.271403000	2.687071000
6	6.144033000	-0.681420000	0.468198000
6	6.644473000	0.696814000	-1.465755000
6	-1.274262000	1.583795000	0.296711000
7	-1.357617000	-0.049270000	3.391230000
6	-1.359642000	-0.100578000	2.223886000
1	1.079433000	0.994043000	1.904637000
1	2.765189000	0.460249000	1.777756000
1	1.662587000	-0.342393000	2.922653000
1	-4.515803000	-3.686155000	0.455352000
6	-5.956165000	-3.105921000	-1.800351000
6	7.027153000	0.137262000	-0.241720000
1	6.445660000	-1.099692000	1.425914000
1	7.329857000	1.339055000	-2.012773000
6	-2.351453000	2.368596000	0.811108000
6	-0.274161000	2.301245000	-0.425607000
1	-5.945552000	-4.170340000	-1.536748000
1	-5.996033000	-3.024401000	-2.893172000
1	-6.894115000	-2.685371000	-1.409735000
1	8.011556000	0.344249000	0.171170000
6	-3.542850000	1.785965000	1.556446000
6	-2.387071000	3.763635000	0.645300000
6	0.900224000	1.650880000	-1.138499000
6	-0.342116000	3.699718000	-0.563173000
1	-4.440134000	2.383694000	1.354365000
1	-3.385306000	1.801765000	2.642965000
1	-3.236761000	4.315665000	1.047920000
6	-1.380138000	4.462292000	-0.022844000
1	1.318340000	2.345137000	-1.876655000
1	1.713035000	1.390853000	-0.451812000
1	0.440233000	4.205486000	-1.128874000
6	-1.410640000	5.967826000	-0.154217000

1	-0.878450000	6.303011000	-1.052388000
1	-2.438830000	6.345828000	-0.204697000
1	-0.930020000	6.453121000	0.707537000

8 [BC28N2H31Se]
HF = -3619.5413041 Ha
NImag= 0

7	0.965981000	-0.790358000	-0.487424000
6	-1.357006000	1.576426000	-0.173624000
6	-0.514272000	2.318556000	0.699552000
6	-1.073334000	4.412110000	-0.448328000
6	-0.401584000	3.710191000	0.557120000
1	0.233637000	4.258676000	1.251279000
6	5.197956000	0.098280000	-0.767730000
1	5.203790000	-0.094981000	-1.836829000
6	-2.050717000	2.290993000	-1.191617000
6	-1.886152000	3.676315000	-1.319942000
1	-2.412173000	4.196367000	-2.119705000
6	1.399347000	0.258920000	-1.407000000
1	1.799453000	1.117604000	-0.860919000
1	0.549980000	0.578368000	-2.010614000
1	2.173528000	-0.143765000	-2.062598000
6	0.276084000	1.671883000	1.821907000
1	0.640542000	2.433396000	2.520184000
1	1.153311000	1.133814000	1.442833000
6	5.941993000	1.161221000	-0.242288000
1	6.529431000	1.786772000	-0.910091000
5	-1.531859000	0.009843000	0.001187000
6	-0.944609000	5.911228000	-0.582968000
1	-1.862893000	6.418295000	-0.255425000
1	-0.770887000	6.205977000	-1.625343000
1	-0.118407000	6.297048000	0.024353000
6	-0.316249000	-0.949681000	0.053343000
6	1.716402000	-1.851164000	-0.080382000
6	4.441049000	-0.706579000	0.090135000
6	-2.959513000	1.596878000	-2.187387000
1	-0.318171000	0.951895000	2.393419000
6	5.923337000	1.422750000	1.131277000
6	-2.955666000	-0.672516000	0.186504000
6	-0.228793000	-2.151958000	0.753462000
7	1.020590000	-2.691902000	0.689557000
34	3.498497000	-2.236110000	-0.648083000
6	4.428614000	-0.458137000	1.467630000

1	-3.277430000	2.294925000	-2.969568000
1	-3.862921000	1.203922000	-1.706769000
1	-2.464126000	0.751834000	-2.678397000
1	6.499147000	2.251059000	1.536336000
6	5.163764000	0.612656000	1.984085000
6	-3.394259000	-1.689994000	-0.702642000
6	-3.832981000	-0.288745000	1.241250000
1	-1.016045000	-2.627925000	1.324644000
1	3.854015000	-1.095988000	2.133412000
1	5.149784000	0.806744000	3.053897000
6	-4.662827000	-2.270786000	-0.540434000
6	-2.557397000	-2.188061000	-1.868880000
6	-3.456279000	0.777750000	2.250712000
6	-5.076884000	-0.914611000	1.387991000
6	-5.518126000	-1.908010000	0.502973000
1	-4.986580000	-3.030563000	-1.250792000
1	-1.905586000	-1.417055000	-2.288221000
1	-3.206483000	-2.550956000	-2.674634000
1	-1.913675000	-3.025616000	-1.570064000
1	-4.220291000	0.855470000	3.031978000
1	-3.357049000	1.764078000	1.783172000
1	-2.501642000	0.557261000	2.742239000
1	-5.723093000	-0.614245000	2.212168000
6	-6.867750000	-2.563044000	0.681742000
1	-7.105148000	-3.223527000	-0.159390000
1	-7.667495000	-1.815916000	0.764950000
1	-6.897004000	-3.165852000	1.599703000

8-[F] [BC28N2H31SeF-1]

HF = -3719.553704 Ha

NImag= 0

9	-1.496374000	-0.157789000	-2.068080000
6	-2.827111000	-0.858266000	0.028864000
6	-3.400702000	-1.961847000	-0.674367000
6	-3.419527000	-0.552005000	1.288288000
6	-0.171780000	-0.866194000	-0.106997000
6	-0.606398000	2.372773000	0.443536000
1	-0.768758000	-2.255667000	1.513766000
6	-1.525004000	1.617639000	-0.339570000
6	-2.529076000	2.376488000	-1.021921000
6	-2.839758000	-2.518955000	-1.974776000
1	-3.066003000	-1.878733000	-2.834928000
1	-3.273450000	-3.506557000	-2.174241000

1	-1.751648000	-2.628597000	-1.944351000
1	0.759403000	0.909601000	-1.868342000
1	-1.788341000	0.481568000	2.305437000
6	-3.591095000	1.743872000	-1.907828000
1	-3.203755000	1.530547000	-2.912002000
1	-4.444092000	2.423651000	-2.024256000
1	-3.962664000	0.798176000	-1.506797000
5	-1.503742000	-0.036693000	-0.577915000
6	-4.532694000	-2.632061000	-0.176369000
6	-4.548147000	-1.248022000	1.757690000
6	-2.877339000	0.517728000	2.221084000
6	-0.014577000	-1.871565000	0.838024000
7	1.090591000	-0.776536000	-0.686943000
6	-0.691315000	3.777699000	0.516617000
6	0.526353000	1.764127000	1.255400000
6	-2.588535000	3.774963000	-0.917721000
1	-4.939494000	-3.466888000	-0.747651000
6	-5.142698000	-2.282199000	1.030846000
1	-4.965472000	-0.976085000	2.727328000
1	-3.292235000	0.386360000	3.227807000
1	-3.140136000	1.529307000	1.890546000
7	1.267328000	-2.372927000	0.862116000
6	1.485449000	0.103538000	-1.783311000
6	1.912187000	-1.689876000	-0.075751000
6	-1.670550000	4.507283000	-0.157470000
1	0.032581000	4.313262000	1.130947000
1	0.845033000	2.462050000	2.039026000
1	0.253073000	0.823329000	1.736185000
1	1.407915000	1.561193000	0.634766000
1	-3.379503000	4.307462000	-1.447047000
6	-6.382914000	-2.990008000	1.527796000
1	2.472625000	0.526592000	-1.586832000
1	1.517237000	-0.449834000	-2.727978000
34	3.703748000	-2.059850000	-0.617542000
6	-1.746569000	6.014875000	-0.068937000
1	-7.297345000	-2.482965000	1.187293000
1	-6.430420000	-4.022137000	1.160174000
1	-6.418754000	-3.016513000	2.623580000
6	4.648047000	-0.554395000	0.175005000
1	-2.721263000	6.348726000	0.311724000
1	-1.613665000	6.483275000	-1.053763000
1	-0.972945000	6.414385000	0.596821000
6	4.533727000	-0.265502000	1.539820000
6	5.495426000	0.207699000	-0.637095000

1	3.885057000	-0.865418000	2.172250000
6	5.255821000	0.798923000	2.086731000
6	6.227647000	1.263183000	-0.080668000
1	5.578179000	-0.011838000	-1.698213000
1	5.160472000	1.024204000	3.146546000
6	6.107140000	1.563547000	1.279805000
1	6.883717000	1.854439000	-0.715089000
1	6.671819000	2.387164000	1.709464000

8-[CN] [BC29N3H31Se-1]

HF = -3712.5206118 Ha

NImag= 1 [methyl rotation of mesityl with -12.8 cm^{-1}]

34	3.767022000	-1.942830000	0.721364000
7	1.126041000	-0.720521000	0.754217000
7	1.324705000	-2.390518000	-0.712725000
6	-2.782004000	-0.902940000	-0.126650000
6	-3.372946000	-0.513033000	-1.367500000
6	-3.308341000	-2.092300000	0.461053000
6	-4.473113000	-1.207157000	-1.899562000
6	-0.137203000	-0.861959000	0.181353000
6	1.960563000	-1.649992000	0.185420000
6	0.035882000	-1.910925000	-0.712343000
1	-0.712437000	-2.344287000	-1.362756000
6	-2.858333000	0.628812000	-2.227921000
1	-1.767861000	0.642339000	-2.290180000
1	-3.981386000	0.708461000	1.365925000
6	-2.723674000	-2.756811000	1.697103000
1	-1.631850000	-2.705358000	1.725232000
6	4.664792000	-0.523277000	-0.260448000
1	0.328835000	0.794423000	-1.636800000
6	4.482921000	-0.370115000	-1.639830000
1	3.806233000	-1.028051000	-2.177805000
5	-1.513757000	-0.054790000	0.567196000
6	5.172915000	0.635706000	-2.322872000
1	5.024415000	0.756086000	-3.393399000
6	1.525426000	0.227554000	1.791324000
6	-4.413768000	-2.757861000	-0.100843000
1	-4.892378000	-0.870374000	-2.847711000
6	-5.036581000	-2.320069000	-1.269898000
1	-3.172107000	1.610670000	-1.856536000
1	-3.246417000	0.528457000	-3.248703000
1	-3.092381000	-2.308529000	2.627463000
1	-3.005121000	-3.816348000	1.716025000

6	5.547645000	0.313625000	0.430845000
6	-1.554046000	1.608640000	0.318585000
7	-1.533004000	-0.122683000	3.361200000
6	-1.571572000	-0.136655000	2.193316000
6	6.060737000	1.473925000	-1.637367000
1	0.794177000	1.031933000	1.845137000
1	2.500949000	0.654074000	1.549858000
1	1.584723000	-0.269066000	2.765169000
1	-4.784887000	-3.657809000	0.389208000
6	-6.246888000	-3.022826000	-1.840527000
6	6.248422000	1.308294000	-0.261645000
1	5.683219000	0.199074000	1.502980000
6	-0.581153000	2.361786000	-0.406347000
6	-2.621407000	2.363509000	0.891832000
1	6.600962000	2.250820000	-2.172522000
1	-7.167207000	-2.452745000	-1.648629000
1	-6.168626000	-3.144405000	-2.928345000
1	-6.379108000	-4.016218000	-1.396193000
1	6.933121000	1.957557000	0.278976000
6	-0.660700000	3.763226000	-0.484643000
6	0.578878000	1.751998000	-1.177514000
6	-2.670035000	3.764551000	0.783881000
6	-3.787617000	1.744337000	1.647338000
6	-1.686552000	4.496463000	0.117640000
1	0.101940000	4.295821000	-1.052995000
1	0.894133000	2.434486000	-1.975669000
1	1.456054000	1.585857000	-0.541385000
1	-3.510426000	4.294047000	1.233447000
1	-4.703446000	2.318464000	1.459479000
1	-3.618132000	1.760024000	2.732212000
6	-1.727128000	6.006163000	0.046589000
1	-1.048306000	6.459136000	0.783149000
1	-2.733378000	6.389315000	0.252248000
1	-1.418161000	6.372351000	-0.940293000

4' [BC23N2H30+1]
HF = -1028.8321512 Ha
NImag= 0

7	-1.173176000	3.708185000	-0.372163000
7	0.493806000	2.729196000	0.630283000
6	-0.068558000	3.906666000	0.360408000
6	-1.304811000	-0.751281000	-0.030240000
6	-1.481953000	-1.695989000	-1.082879000

6	-2.655355000	-2.455248000	-1.152722000
1	-2.779474000	-3.156813000	-1.976839000
6	-0.281944000	1.702542000	0.066663000
6	1.457246000	-0.413641000	0.038683000
6	-1.328089000	2.354762000	-0.549628000
1	-2.160231000	1.955688000	-1.111246000
6	-2.333470000	-0.635912000	0.942620000
6	-2.059411000	4.754533000	-0.890573000
1	-3.081472000	4.551336000	-0.564287000
1	-2.010420000	4.761696000	-1.981834000
1	-1.729691000	5.716637000	-0.498021000
6	-3.481001000	-1.439233000	0.853629000
1	-4.244885000	-1.350651000	1.625027000
6	2.410454000	0.028463000	-0.920637000
6	-3.670503000	-2.347132000	-0.191464000
6	1.861471000	-1.410636000	0.972131000
6	3.168386000	-1.913204000	0.940783000
1	3.460656000	-2.662846000	1.674873000
6	4.105143000	-1.490272000	-0.010698000
6	2.091382000	1.080144000	-1.966881000
1	1.109187000	0.935972000	-2.428341000
1	2.840259000	1.061959000	-2.766295000
1	2.102517000	2.091390000	-1.539406000
6	1.693393000	2.583441000	1.462946000
1	2.534440000	2.251030000	0.852817000
1	1.498164000	1.857920000	2.253774000
1	1.920236000	3.554189000	1.905903000
6	3.698299000	-0.525937000	-0.938808000
1	4.403000000	-0.192296000	-1.699042000
6	-0.439474000	-1.908201000	-2.162843000
1	-0.102356000	-0.965392000	-2.606322000
1	-0.844204000	-2.530091000	-2.968592000
1	0.449837000	-2.415159000	-1.769491000
6	-2.243862000	0.308328000	2.129017000
1	-1.214215000	0.509832000	2.437677000
1	-2.770978000	-0.115333000	2.991790000
1	-2.713308000	1.276023000	1.907994000
6	-4.919951000	-3.189834000	-0.288106000
1	-5.471307000	-2.975899000	-1.213404000
1	-5.592851000	-3.004646000	0.555990000
1	-4.678072000	-4.260643000	-0.301461000
6	0.925571000	-1.953181000	2.034832000
1	0.419481000	-1.155970000	2.590297000
1	1.479454000	-2.562251000	2.757342000

1	0.144560000	-2.587327000	1.598489000
6	5.509504000	-2.045228000	-0.018974000
1	6.118869000	-1.584833000	0.771349000
1	6.009537000	-1.853446000	-0.974667000
1	5.513655000	-3.126905000	0.161907000
5	-0.012855000	0.156662000	0.046180000
1	0.294673000	4.868152000	0.692728000

9 [BC29N2H34S+1]

HF = -1658.0747842 Ha

NImag= 1 [methyl rotation of mesityl with -11.4 cm^{-1}]

7	1.117563000	-0.798096000	-0.709414000
7	1.110326000	-2.726171000	0.323416000
6	-1.069786000	1.657344000	-0.098158000
6	-2.764227000	-0.543358000	0.093496000
6	-5.334850000	-1.753688000	0.403593000
6	-3.244552000	-1.491721000	-0.847400000
6	1.861675000	-1.888146000	-0.432697000
6	-4.853546000	-0.823146000	1.336215000
6	-1.758829000	2.488399000	-1.028170000
6	1.563020000	0.305043000	-1.567752000
1	2.064472000	1.069120000	-0.969912000
1	0.694051000	0.733314000	-2.063712000
1	2.251588000	-0.087674000	-2.316932000
6	-3.605552000	-0.207184000	1.194798000
6	-4.516017000	-2.064540000	-0.684471000
1	-4.872929000	-2.771397000	-1.432438000
6	0.627329000	1.492317000	1.836705000
1	0.033607000	0.705914000	2.312491000
1	0.987792000	2.160456000	2.626559000
1	1.510703000	1.011856000	1.396438000
6	-0.156565000	2.274669000	0.799872000
6	-0.119192000	-2.156809000	0.505334000
1	-0.885589000	-2.655690000	1.079529000
6	-3.187065000	0.793302000	2.254048000
1	-2.197625000	0.568444000	2.667496000
1	-3.901996000	0.794061000	3.084032000
1	-3.144237000	1.812857000	1.852854000
6	1.520220000	-4.039567000	0.836871000
1	2.465780000	-3.946802000	1.372998000
1	1.624627000	-4.746664000	0.010850000
1	0.742098000	-4.383687000	1.518148000
6	-0.143161000	-0.925473000	-0.115007000

6	0.035035000	3.663830000	0.762925000
1	0.722250000	4.118136000	1.475064000
6	-2.457003000	-1.910431000	-2.076706000
1	-3.132788000	-2.056627000	-2.928528000
1	-1.704534000	-1.175927000	-2.376830000
6	-0.624568000	4.480054000	-0.161048000
6	-2.752606000	1.932171000	-2.029030000
1	-3.685238000	1.624667000	-1.541122000
5	-1.329826000	0.103011000	-0.060981000
6	4.534457000	-0.891465000	1.195641000
1	3.923355000	-1.538174000	1.818771000
6	4.487131000	-0.994033000	-0.201067000
6	5.290676000	-0.180701000	-1.008182000
6	6.148906000	0.747049000	-0.407494000
1	6.775699000	1.377828000	-1.032151000
6	6.189433000	0.869677000	0.984301000
1	6.851883000	1.596425000	1.447169000
6	5.379188000	0.053863000	1.782596000
1	5.412148000	0.141668000	2.865530000
6	-6.696410000	-2.384863000	0.572552000
1	-5.472027000	-0.566248000	2.195333000
6	-1.512367000	3.866107000	-1.054547000
1	-1.937807000	-2.865021000	-1.912109000
6	-0.404140000	5.973673000	-0.191138000
1	-2.363876000	1.056913000	-2.560286000
1	-3.006761000	2.691001000	-2.777033000
1	5.248112000	-0.264419000	-2.090444000
1	-6.897693000	-3.116751000	-0.217068000
1	-6.780102000	-2.896303000	1.540400000
1	-7.491341000	-1.627592000	0.542215000
1	-2.032943000	4.478906000	-1.789396000
1	-0.174365000	6.322097000	-1.205953000
1	0.420160000	6.269103000	0.466790000
1	-1.303904000	6.512694000	0.135671000
16	3.480721000	-2.265370000	-1.007751000

9-[F] [BC29N2H34SF]

HF = -1758.099327 Ha

NImag= 1 [methyl rotation of mesityl with -9.8 cm^{-1}]

16	-3.715349000	-2.047508000	0.893774000
9	1.313009000	0.058497000	2.103165000
7	-1.262607000	-0.709601000	0.827783000
7	-1.417680000	-2.341784000	-0.609726000

6	1.321632000	1.705114000	0.251899000
6	2.637035000	-0.797596000	0.075430000
6	4.927554000	-2.357411000	-0.759160000
6	3.095589000	-1.927553000	0.820704000
6	-2.100842000	-1.649864000	0.326355000
6	4.450038000	-1.291212000	-1.524409000
6	2.294625000	2.528541000	0.898035000
6	-1.645466000	0.238946000	1.879073000
1	-2.651063000	0.615235000	1.686867000
1	-0.939677000	1.065415000	1.869269000
1	-1.616720000	-0.254481000	2.854419000
6	3.334535000	-0.525697000	-1.136867000
6	4.216246000	-2.666805000	0.403201000
1	4.533819000	-3.519431000	1.003478000
6	-0.670203000	1.673797000	-1.415949000
1	-0.310144000	0.771743000	-1.918378000
1	-1.063950000	2.346595000	-2.186557000
1	-1.520947000	1.375890000	-0.791716000
6	0.411587000	2.376989000	-0.611670000
6	-0.142608000	-1.831958000	-0.678223000
1	0.578884000	-2.253269000	-1.361472000
6	2.934259000	0.577241000	-2.102486000
1	1.860869000	0.579227000	-2.310537000
1	3.456132000	0.449151000	-3.058170000
1	3.187936000	1.573004000	-1.722191000
6	-1.915507000	-3.476947000	-1.391428000
1	-2.864305000	-3.217774000	-1.864036000
1	-2.047745000	-4.349065000	-0.746601000
1	-1.174249000	-3.699356000	-2.159179000
6	-0.014579000	-0.788386000	0.213068000
6	0.472189000	3.772516000	-0.789552000
1	-0.239812000	4.245050000	-1.465831000
6	2.420979000	-2.434388000	2.086883000
1	2.655854000	-1.812409000	2.958480000
1	1.330642000	-2.453538000	2.000708000
6	1.416811000	4.570547000	-0.141823000
6	3.355061000	1.980695000	1.839930000
1	3.738746000	1.008615000	1.521280000
5	1.327176000	0.083562000	0.615960000
6	-4.643856000	-0.414675000	-1.208829000
1	-3.870248000	-0.852216000	-1.833361000
6	-4.762741000	-0.776844000	0.138963000
6	-5.769118000	-0.223401000	0.939922000

6 -6.664861000 0.696129000 0.31 -7.446479000 1.124123000 1.005480000
6 -6.544806000 1.073968000 -0.957405000
1 -7.236535000 1.795191000 -1.384507000
6 -5.530630000 0.521355000 -1.747801000
1 -5.433406000 0.808320000 -2.791877000
6 6.156088000 -3.138686000 -1.165956000
1 4.954225000 -1.046213000 -2.458915000
6 2.328961000 3.917271000 0.691567000
1 2.759118000 -3.453823000 2.307037000
6 1.446889000 6.071338000 -0.322079000
1 2.962867000 1.848873000 2.856160000
1 4.200948000 2.675829000 1.905000000
1 -5.853348000 -0.499862000 1.987781000
1 6.081396000 -4.191120000 -0.866618000
1 6.314755000 -3.102757000 -2.250227000
1 7.061811000 -2.733489000 -0.692208000
1 3.097586000 4.503638000 1.196163000
1 0.975989000 6.585612000 0.528018000
1 0.908000000 6.376413000 -1.226656000
1 2.474531000 6.448287000 -0.394256000

9-[CN] [BC30N3H34S]
HF = -1751.0643175 Ha
NImag= 0
16 -3.773356000 -2.003350000 0.946384000
6 1.373903000 0.117243000 2.244432000
7 -1.304368000 -0.692257000 0.887412000
7 -1.431207000 -2.398581000 -0.464596000
6 1.309005000 1.697973000 0.226861000
6 2.595212000 -0.820967000 -0.001167000
6 4.849395000 -2.327472000 -1.017267000
6 3.107898000 -1.969203000 0.676777000
6 -2.132929000 -1.657001000 0.416345000
6 4.302837000 -1.256588000 -1.727315000
6 2.358733000 2.526755000 0.728299000
6 -1.719436000 0.306768000 1.878325000
1 -2.738502000 0.630412000 1.665254000
1 -1.053070000 1.163551000 1.813561000
1 -1.670521000 -0.121337000 2.882828000
6 3.201258000 -0.519088000 -1.257393000
6 4.211056000 -2.680411000 0.173061000
1 4.569880000 -3.547308000 0.727639000

6	-0.821303000	1.644778000	-1.273382000
1	-0.513458000	0.702089000	-1.731952000
1	-1.217928000	2.284993000	-2.069516000
1	-1.659907000	1.421588000	-0.603976000
6	0.318111000	2.354805000	-0.560747000
6	-0.154960000	-1.894769000	-0.534986000
1	0.578363000	-2.351984000	-1.180653000
6	2.706648000	0.566246000	-2.198238000
1	1.618614000	0.562849000	-2.298582000
1	3.131370000	0.413737000	-3.197372000
1	2.995907000	1.570431000	-1.869690000
6	-1.909800000	-3.576504000	-1.194412000
1	-2.871809000	-3.359980000	-1.661035000
1	-2.009069000	-4.424906000	-0.512704000
1	-1.174215000	-3.809129000	-1.964512000
6	-0.041816000	-0.805169000	0.301467000
6	0.365668000	3.744922000	-0.770819000
1	-0.408191000	4.204745000	-1.385025000
6	2.509230000	-2.538295000	1.952766000
1	2.872064000	-2.020933000	2.848799000
1	1.417280000	-2.483097000	1.970065000
6	1.373910000	4.553898000	-0.242429000
6	3.538965000	2.004005000	1.532547000
1	3.784150000	0.964276000	1.308755000
5	1.320157000	0.069218000	0.620220000
6	-4.646428000	-0.575333000	-1.316052000
1	-3.920407000	-1.141084000	-1.893000000
6	-4.760051000	-0.762744000	0.067577000
6	-5.708491000	-0.048162000	0.809212000
6	-6.550822000	0.859230000	0.156991000
1	-7.288344000	1.412420000	0.732741000
6	-6.433359000	1.064205000	-1.220610000
1	-7.082721000	1.776468000	-1.722876000
6	-5.477758000	0.349841000	-1.952800000
1	-5.384448000	0.502033000	-3.025093000
6	6.063110000	-3.075277000	-1.518679000
1	4.736822000	-0.988025000	-2.690137000
6	2.374321000	3.910786000	0.488886000
1	2.787859000	-3.593674000	2.053825000
6	1.382326000	6.050669000	-0.451739000
1	3.351173000	2.068058000	2.612331000
1	4.429903000	2.609217000	1.325820000
1	-5.788539000	-0.191520000	1.883387000
1	6.037307000	-4.129742000	-1.218948000

1	6.138538000	-3.031018000	-2.611581000
1	6.990051000	-2.646182000	-1.111850000
1	3.202829000	4.499088000	0.883751000
1	0.907751000	6.572900000	0.391432000
1	0.833234000	6.331776000	-1.358017000
1	2.404464000	6.438920000	-0.536314000
7	1.344131000	0.226129000	3.406659000

10 [BC29N2H34Se+1]
HF = -3659.3109464 Ha
NImag= 0

7	0.921856000	-0.640983000	-0.486820000
7	1.000603000	-2.488393000	0.674265000
6	-1.454850000	1.697536000	-0.084606000
6	-2.994152000	-0.615284000	0.092535000
6	-5.496016000	-1.984981000	0.252876000
6	-3.329515000	-1.636154000	-0.837512000
6	1.720964000	-1.659435000	-0.118690000
6	-5.155851000	-0.986210000	1.175741000
6	-2.164386000	2.443784000	-1.069902000
6	1.315002000	0.430214000	-1.406798000
1	1.716392000	1.279253000	-0.849199000
1	0.439141000	0.741156000	-1.973829000
1	2.073019000	0.045792000	-2.090259000
6	-3.942156000	-0.292488000	1.105086000
6	-4.571381000	-2.283737000	-0.752250000
1	-4.819787000	-3.042975000	-1.492612000
6	0.164249000	1.729227000	1.924274000
1	-0.416152000	0.964021000	2.450062000
1	0.498742000	2.462288000	2.666282000
1	1.062873000	1.239827000	1.528451000
6	-0.629931000	2.412884000	0.827300000
6	-0.269928000	-1.992084000	0.780781000
1	-1.022052000	-2.501789000	1.364358000
6	-3.679259000	0.782457000	2.141560000
1	-2.692833000	0.678194000	2.606266000
1	-4.429350000	0.738256000	2.938851000
1	-3.724127000	1.786094000	1.701533000
6	1.484846000	-3.724562000	1.299567000
1	2.370981000	-3.507017000	1.898501000
1	1.729707000	-4.459988000	0.530502000
1	0.687435000	-4.107394000	1.936765000
6	-0.350090000	-0.810385000	0.077170000

6	-0.546974000	3.811134000	0.752083000
1	0.071676000	4.339772000	1.475573000
6	-2.407858000	-2.053693000	-1.970581000
1	-2.993442000	-2.435932000	-2.814739000
1	-1.789194000	-1.231912000	-2.342911000
6	-1.230635000	4.544770000	-0.222183000
6	-3.065461000	1.781657000	-2.094037000
1	-3.997907000	1.425762000	-1.639519000
5	-1.603161000	0.130566000	0.007509000
6	4.467069000	-0.150572000	1.307759000
1	3.976041000	-0.790781000	2.034587000
6	4.395684000	-0.444703000	-0.057983000
6	5.048756000	0.355306000	-0.999930000
6	5.777487000	1.468447000	-0.566532000
1	6.287242000	2.092666000	-1.296086000
6	5.842440000	1.780632000	0.794918000
1	6.405873000	2.648449000	1.127811000
6	5.185126000	0.971917000	1.729565000
1	5.238621000	1.207027000	2.789627000
6	-6.813065000	-2.717096000	0.354391000
1	-5.859366000	-0.736022000	1.968783000
6	-2.028207000	3.835586000	-1.130044000
1	-1.727247000	-2.857006000	-1.659483000
6	-1.122580000	6.049169000	-0.296336000
1	-2.589426000	0.917934000	-2.569963000
1	-3.333830000	2.492040000	-2.883575000
1	4.987029000	0.119609000	-2.058284000
1	-7.006838000	-3.317482000	-0.541081000
1	-6.821663000	-3.395037000	1.219061000
1	-7.649135000	-2.019171000	0.487051000
1	-2.564339000	4.383121000	-1.904203000
1	-0.769767000	6.374114000	-1.283788000
1	-0.428752000	6.437377000	0.457000000
1	-2.098819000	6.525250000	-0.134076000
34	3.495643000	-2.050080000	-0.677837000

10-[F] [BC29N2H34SeF]

HF = -3759.3341711 Ha

NImag= 1 [methyl rotation of mesityl with -3.3 cm^{-1}]

34	-3.718917000	-1.727531000	0.897487000
9	1.617655000	-0.001418000	2.115177000
7	-1.038753000	-0.566401000	0.834853000
7	-1.275382000	-2.214222000	-0.567818000

6	1.649159000	1.702896000	0.314591000
6	2.857167000	-0.834622000	0.016594000
6	5.068577000	-2.422723000	-0.966326000
6	3.342173000	-1.977190000	0.724719000
6	-1.924460000	-1.458544000	0.337723000
6	4.559826000	-1.345652000	-1.695120000
6	2.677227000	2.463471000	0.954216000
6	-1.383699000	0.413139000	1.869858000
1	-2.245803000	1.001600000	1.549380000
1	-0.527481000	1.062468000	2.027510000
1	-1.625389000	-0.106945000	2.800658000
6	3.481472000	-0.567780000	-1.236274000
6	4.424503000	-2.729492000	0.235413000
1	4.764204000	-3.591683000	0.809553000
6	-0.394783000	1.814442000	-1.290104000
1	-0.116505000	0.874897000	-1.772595000
1	-0.730747000	2.502688000	-2.074476000
1	-1.266953000	1.606735000	-0.658926000
6	0.745024000	2.439917000	-0.501101000
6	0.031644000	-1.785567000	-0.631998000
1	0.732978000	-2.265085000	-1.297430000
6	3.033419000	0.540191000	-2.174359000
1	1.948071000	0.566843000	-2.297531000
1	3.475087000	0.393728000	-3.166859000
1	3.339598000	1.531806000	-1.822968000
6	-1.835598000	-3.339843000	-1.320279000
1	-2.743149000	-3.025863000	-1.838516000
1	-2.068816000	-4.163297000	-0.641292000
1	-1.087978000	-3.660476000	-2.046569000
6	0.212319000	-0.732661000	0.237443000
6	0.863789000	3.836500000	-0.640133000
1	0.153903000	4.360321000	-1.279330000
6	2.733089000	-2.484588000	2.023388000
1	3.009180000	-1.861958000	2.882151000
1	1.640238000	-2.505821000	1.990012000
6	1.864403000	4.572066000	-0.003399000
6	3.737002000	1.841929000	1.850693000
1	4.078455000	0.870569000	1.485714000
5	1.596038000	0.070548000	0.627664000
6	-4.486403000	-0.223444000	-1.488524000
1	-3.904395000	-0.958701000	-2.036488000
6	-4.573737000	-0.287764000	-0.093295000
6	-5.336563000	0.644045000	0.617430000
6	-6.016191000	1.651285000	-0.078092000

1	-6.609484000	2.376794000	0.473022000
6	-5.923267000	1.731606000	-1.471052000
1	-6.446921000	2.518196000	-2.007636000
6	-5.155095000	0.794817000	-2.173332000
1	-5.082584000	0.849614000	-3.256881000
6	6.256904000	-3.219195000	-1.454870000
1	5.007921000	-1.103199000	-2.658726000
6	2.770035000	3.853999000	0.783955000
1	3.084406000	-3.503816000	2.226487000
6	1.966328000	6.073143000	-0.151297000
1	3.360965000	1.682924000	2.868943000
1	4.608240000	2.503947000	1.923092000
1	-5.396058000	0.592224000	1.700904000
1	6.191344000	-4.269543000	-1.146307000
1	6.338084000	-3.188202000	-2.547932000
1	7.197824000	-2.821619000	-1.048645000
1	3.579634000	4.390224000	1.279703000
1	1.616905000	6.589378000	0.754073000
1	1.359624000	6.433880000	-0.989750000
1	3.003067000	6.391517000	-0.319863000

10-[CN] [BC30N3H34Se]

HF = -3752.2995694 Ha

NImag= 0

34	-3.752149000	-1.722516000	0.847752000
6	1.628650000	0.051288000	2.227437000
7	-1.080641000	-0.553820000	0.805113000
7	-1.279366000	-2.210455000	-0.594508000
6	1.656870000	1.704622000	0.265515000
6	2.820362000	-0.866577000	-0.041270000
6	5.007250000	-2.447115000	-1.091658000
6	3.265857000	-2.064203000	0.597402000
6	-1.953377000	-1.451285000	0.291561000
6	4.523321000	-1.324447000	-1.766441000
6	2.741044000	2.463550000	0.803269000
6	-1.450825000	0.429638000	1.828529000
1	-2.422170000	0.861433000	1.586947000
1	-0.703204000	1.218866000	1.843386000
1	-1.497845000	-0.052599000	2.808202000
6	3.455216000	-0.549768000	-1.279501000
6	4.338353000	-2.810852000	0.078415000

1	4.646916000	-3.714433000	0.603898000
6	-0.463371000	1.810246000	-1.250610000
1	-0.204719000	0.864265000	-1.731910000
1	-0.812503000	2.493366000	-2.033337000
1	-1.321891000	1.618908000	-0.597020000
6	0.706064000	2.435708000	-0.506736000
6	0.027311000	-1.780312000	-0.628651000
1	0.743977000	-2.259777000	-1.277160000
6	3.026357000	0.593150000	-2.183978000
1	1.940879000	0.644996000	-2.298719000
1	3.458322000	0.458777000	-3.182637000
1	3.357088000	1.569310000	-1.812945000
6	-1.792464000	-3.318205000	-1.403337000
1	-2.852828000	-3.453242000	-1.196062000
1	-1.246416000	-4.229831000	-1.148112000
1	-1.645920000	-3.085904000	-2.460978000
6	0.187205000	-0.724779000	0.239598000
6	0.823689000	3.828137000	-0.667704000
1	0.079039000	4.346701000	-1.271233000
6	2.626373000	-2.648529000	1.846434000
1	3.006510000	-2.183464000	2.763872000
1	1.538655000	-2.538181000	1.857219000
6	1.865380000	4.568243000	-0.104339000
6	3.886861000	1.855453000	1.597108000
1	4.084638000	0.814288000	1.336375000
5	1.585455000	0.064186000	0.602144000
6	-4.547455000	-0.223030000	-1.531222000
1	-3.984877000	-0.968128000	-2.086066000
6	-4.608773000	-0.278533000	-0.134785000
6	-5.347652000	0.664626000	0.585937000
6	-6.028651000	1.676020000	-0.101584000
1	-6.602744000	2.410975000	0.457030000
6	-5.961872000	1.747598000	-1.496271000
1	-6.487188000	2.537449000	-2.026870000
6	-5.219139000	0.798429000	-2.208738000
1	-5.168090000	0.846421000	-3.293657000
6	6.188227000	-3.235645000	-1.608623000
1	4.981045000	-1.043228000	-2.714415000
6	2.826421000	3.852500000	0.611965000
1	2.850584000	-3.719694000	1.910360000
6	1.948698000	6.068977000	-0.263354000
1	3.691668000	1.888118000	2.676967000
1	4.807850000	2.424457000	1.420856000
1	-5.386858000	0.618755000	1.670450000

1	6.112231000	-4.295836000	-1.339293000
1	6.271915000	-3.164042000	-2.699501000
1	7.131626000	-2.861299000	-1.185937000
1	3.678881000	4.385889000	1.033104000
1	1.477567000	6.585842000	0.585076000
1	1.436191000	6.404756000	-1.172550000
1	2.989592000	6.410834000	-0.310710000
7	1.594619000	0.115768000	3.392948000

1'-[F] [BC22N2H27F-1]

HF = -1089.0723928 Ha

NImag= 0

9	0.026898000	0.723215000	1.951427000
6	3.564654000	-0.831440000	-0.858736000
1	4.317740000	-0.549144000	-1.594439000
6	2.397804000	-0.048542000	-0.751518000
6	1.375832000	-0.373056000	0.187171000
6	-1.442051000	-0.313155000	0.098439000
6	3.788510000	-1.960439000	-0.069236000
6	2.784679000	-2.298089000	0.843066000
1	2.912279000	-3.184984000	1.464801000
6	1.612701000	-1.537032000	0.984208000
6	-2.618434000	-0.126750000	0.889781000
6	2.327849000	1.127421000	-1.713418000
1	3.115391000	1.040393000	-2.471691000
6	1.610719000	3.185010000	1.275523000
1	1.158433000	3.117017000	2.268947000
1	2.330835000	2.371688000	1.162213000
6	-3.805626000	-0.823179000	0.605070000
1	-4.677334000	-0.653108000	1.237587000
6	-2.792915000	-1.848814000	-1.286195000
6	-1.586031000	-1.170519000	-1.029489000
6	0.637420000	-2.041070000	2.036531000
1	-0.405178000	-1.919863000	1.736789000
1	0.812951000	-3.105252000	2.238127000
1	0.757913000	-1.506383000	2.986993000
6	-3.915514000	-1.711866000	-0.468754000
6	-2.694865000	0.836514000	2.065297000
1	-2.235176000	1.802644000	1.836177000
1	-3.742615000	1.015992000	2.334665000
1	-2.185126000	0.449474000	2.954990000
6	-0.482038000	-1.402248000	-2.048060000
1	0.291307000	-2.086473000	-1.679551000

1	5.740784000	-2.573965000	0.652687000
5	-0.024818000	0.493543000	0.471709000
6	5.056839000	-2.776060000	-0.183785000
1	2.474758000	2.088163000	-1.207422000
1	1.369956000	1.193564000	-2.236595000
1	2.135748000	4.139648000	1.185500000
7	0.592212000	3.113687000	0.233580000
1	-2.853976000	-2.496063000	-2.160595000
6	-5.194341000	-2.472843000	-0.737446000
1	0.021154000	-0.475056000	-2.333284000
1	-0.899123000	-1.845322000	-2.960764000
6	-0.142558000	1.994541000	-0.166630000
1	5.597371000	-2.547540000	-1.109459000
1	4.846791000	-3.853063000	-0.170468000
6	0.177102000	4.188256000	-0.494699000
1	-6.077896000	-1.833801000	-0.612676000
1	-5.312625000	-3.319409000	-0.046060000
1	-5.210677000	-2.878367000	-1.756046000
6	-0.984603000	2.510705000	-1.138993000
1	0.602059000	5.174417000	-0.353650000
7	-0.781434000	3.863922000	-1.348829000
1	-1.729980000	1.970801000	-1.710212000

1'-[CN] [BC23N3H27-1]

HF = -1082.0392659 Ha

NImag= 0

6	0.092313000	0.772225000	2.010387000
6	3.565371000	-0.824382000	-0.913813000
1	4.310172000	-0.532378000	-1.654059000
6	2.386472000	-0.063006000	-0.811773000
6	1.371870000	-0.401319000	0.134071000
6	-1.463447000	-0.334881000	0.069079000
6	3.810950000	-1.948298000	-0.121637000
6	2.803567000	-2.314620000	0.772178000
1	2.935911000	-3.208723000	1.382020000
6	1.616226000	-1.575368000	0.910576000
6	-2.671282000	-0.067212000	0.783290000
6	2.285887000	1.080656000	-1.808862000
1	3.018078000	0.938006000	-2.612279000
6	1.658332000	3.270944000	0.973881000
1	1.256878000	3.417750000	1.980728000
1	2.303439000	2.390696000	0.977095000
6	-3.854031000	-0.777543000	0.511201000

1	-4.749370000	-0.540219000	1.085909000
6	-2.773950000	-1.969014000	-1.237530000
6	-1.571484000	-1.280702000	-0.994083000
6	0.634749000	-2.136500000	1.928666000
1	-0.403482000	-1.883223000	1.708573000
1	0.712983000	-3.230208000	1.961294000
1	0.850518000	-1.769582000	2.940757000
6	-3.927988000	-1.757933000	-0.480048000
6	-2.799498000	1.007171000	1.850834000
1	-2.228899000	1.907977000	1.608534000
1	-3.850616000	1.299440000	1.960241000
1	-2.456001000	0.661955000	2.833359000
6	-0.444625000	-1.594429000	-1.964028000
1	0.314266000	-2.253363000	-1.527602000
1	5.856158000	-2.344664000	0.478297000
5	-0.037641000	0.477674000	0.414512000
6	5.102886000	-2.726063000	-0.226196000
1	2.499000000	2.054029000	-1.353195000
1	1.297259000	1.155565000	-2.267478000
1	2.252311000	4.145416000	0.695615000
7	0.583303000	3.107153000	0.000480000
1	-2.808072000	-2.683296000	-2.060090000
6	-5.195830000	-2.542548000	-0.728455000
1	0.071336000	-0.693278000	-2.304001000
1	-0.846588000	-2.100297000	-2.850028000
6	-0.166325000	1.959012000	-0.277711000
1	5.534840000	-2.653401000	-1.231468000
1	4.952713000	-3.787327000	0.005714000
6	0.130100000	4.118931000	-0.792194000
1	-6.086896000	-1.957810000	-0.470422000
1	-5.223174000	-3.458828000	-0.121125000
1	-5.279663000	-2.848589000	-1.778120000
6	-1.055673000	2.398216000	-1.246313000
1	0.562554000	5.111049000	-0.755038000
7	-0.867214000	3.729033000	-1.570085000
1	-1.822018000	1.814584000	-1.740273000
7	0.284918000	1.006717000	3.138943000

4'-[F] [BC23N2H30F]

HF = -1128.8558837 Ha

NImag= 0

6	3.732994000	-0.108868000	-0.982166000
1	4.358727000	0.417953000	-1.702397000

6	2.423967000	0.359192000	-0.754529000
6	1.559674000	-0.293924000	0.169468000
6	-1.213688000	-0.854609000	0.164706000
6	4.255102000	-1.227025000	-0.330280000
6	3.407338000	-1.886941000	0.564637000
1	3.770682000	-2.777947000	1.077568000
6	2.099716000	-1.445773000	0.822237000
6	-2.372655000	-0.986276000	0.990787000
6	2.027872000	1.576020000	-1.576222000
1	2.755745000	1.740200000	-2.379272000
6	1.066867000	3.038585000	1.721795000
1	0.672947000	2.749864000	2.698004000
1	1.915169000	2.401072000	1.471525000
6	-3.414327000	-1.865215000	0.646839000
1	-4.278619000	-1.935587000	1.307420000
6	-2.287443000	-2.473219000	-1.358167000
6	-1.224264000	-1.605670000	-1.045684000
6	1.317429000	-2.275792000	1.828028000
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4'-[CN] [BC24N3H30]

HF = -1121.8211859 Ha

NImag= 0

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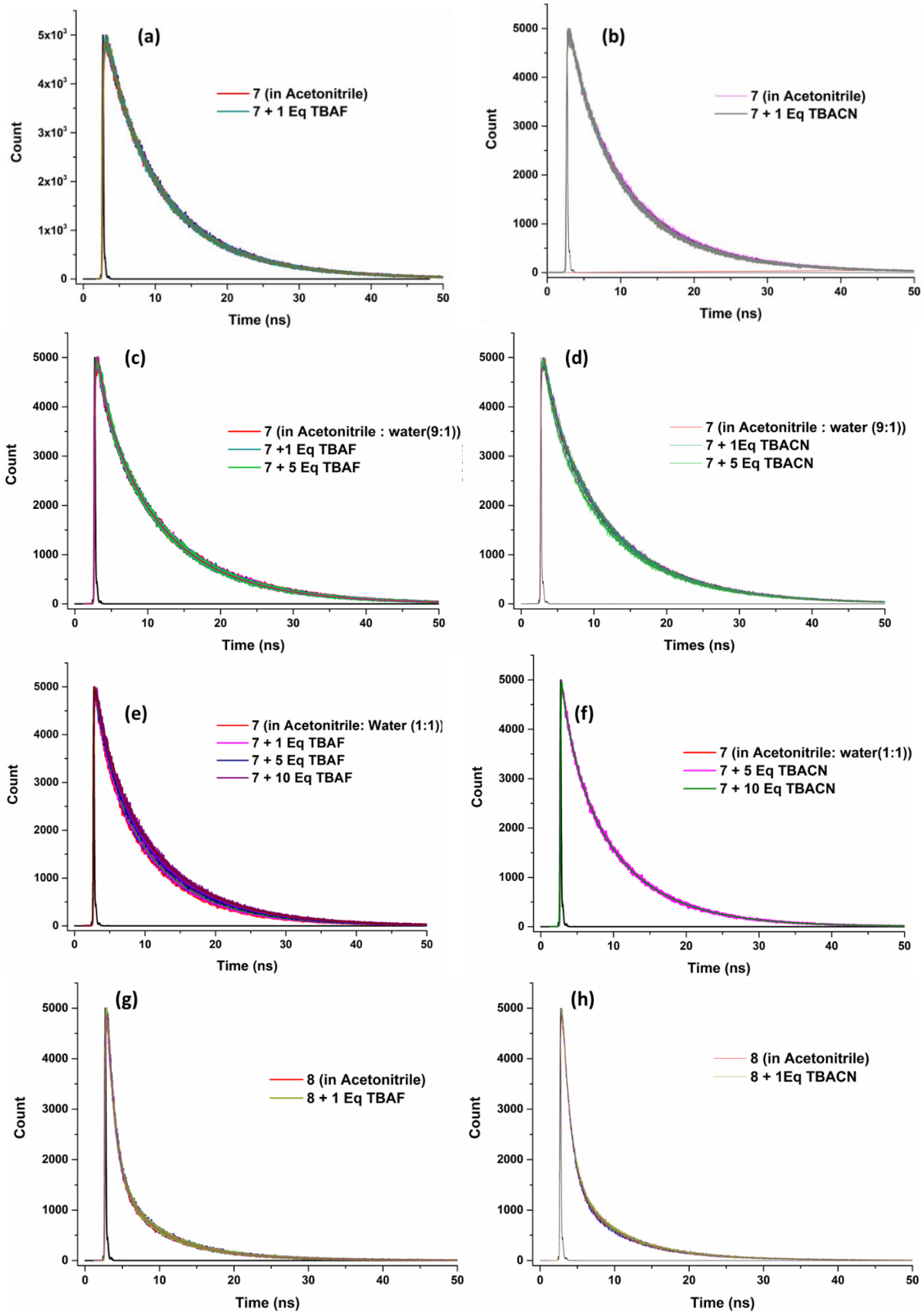

Figure S60: Lifetime change spectra of the compounds **7(a-f)** and **8(g-h)** upon complexation with TBAF and TBACN

Table S10: Average lifetime of **7** and **8** with TBAF and TBACN

Compound	Solvent	Avg. lifetime (τ_{av}) (only compound) (ns)	Avg. lifetime τ_{av} (in presence of anions) (ns)
7	acetonitrile	9.21	9.12 (1 eq. fluoride)
7	acetonitrile	9.14	9.01 (1 eq. cyanide
7	acetonitrile:water(9:1)	9.16	9.19 (5 eq. fluoride)
7	acetonitrile:water(9:1)	9.30	9.16 (5 eq. cyanide)
7	acetonitrile: water(1:1)	7.66	8.10 (10 eq. fluoride)
7	acetonitrile: water(1:1)	7.64	7.90 (10 eq. cyanide
8	acetonitrile	5.73	5.71 (1 eq. fluoride)
8	acetonitrile	5.78	5.80 (1 eq. cyanide)

Image showing competitive binding of anions

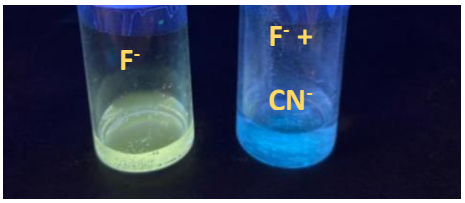

Figure S61: Images taken under UV light (365 nm) upon addition of solution of **7** in acetonitrile:water (9:1) to (a) aq. TBAF solution (25 μM; left) and (b) first aq. TBAF solution (25 μM) and then aq. TBACN solution (25 μM; right).

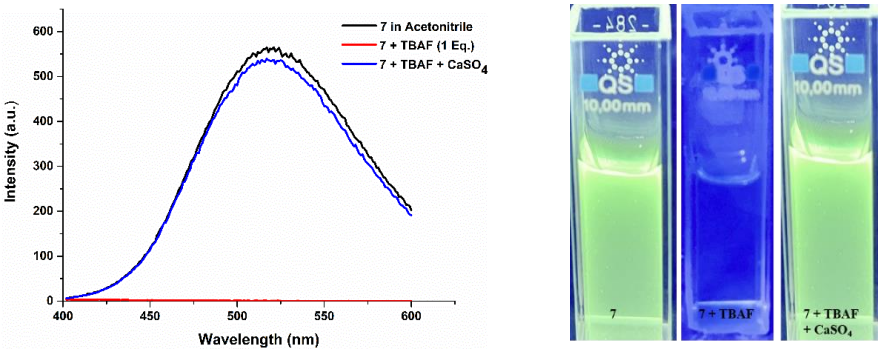

Figure S62: Experiments studies on reversibility of compound **7**.