Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Structure and electronics in dimeric boron π expanded azine and salphen complexes

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Supporting Information

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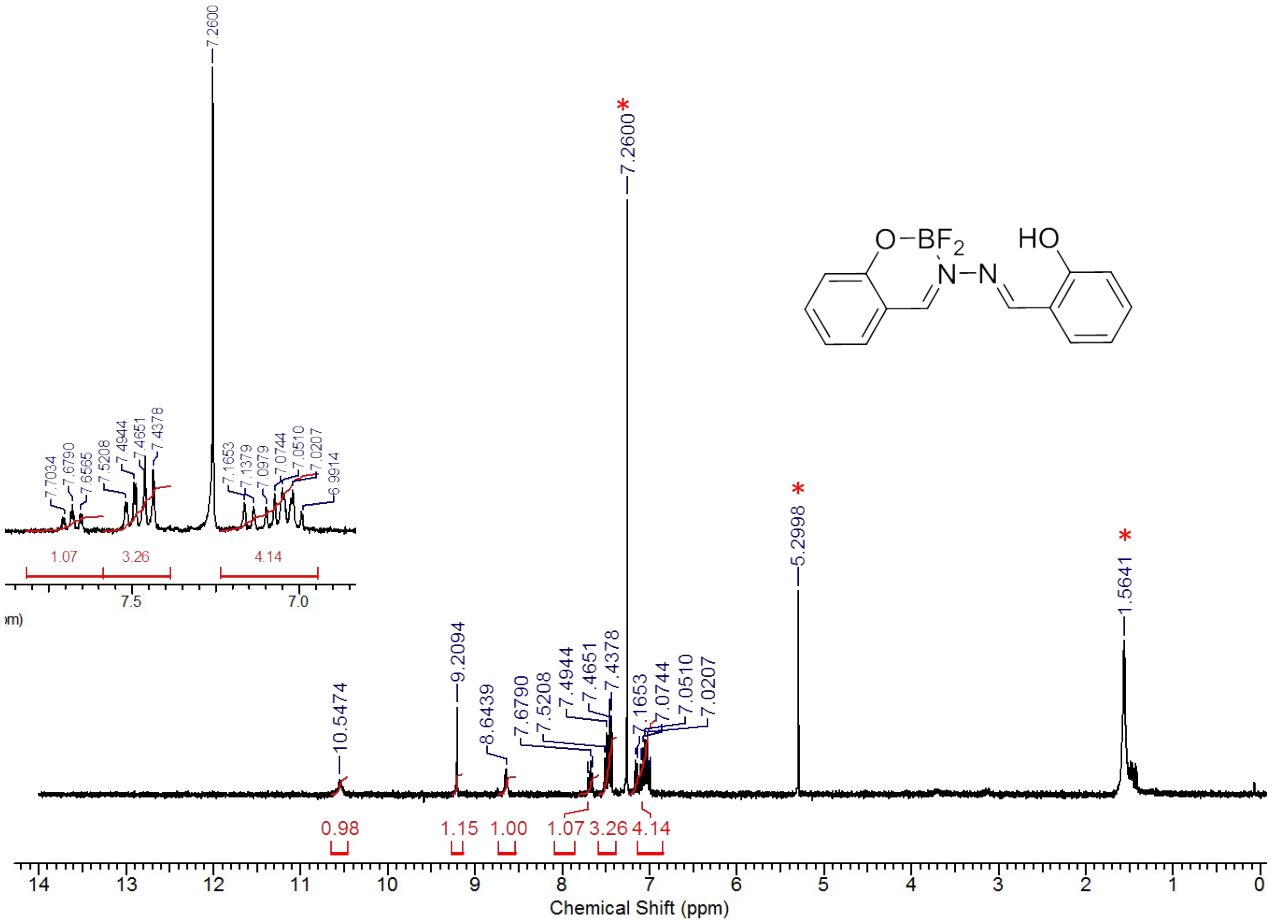


Figure S1: ^{1}H NMR of **1** in $CDCl_3$. * Represents $CDCl_3$, chloroform, and H_2O.

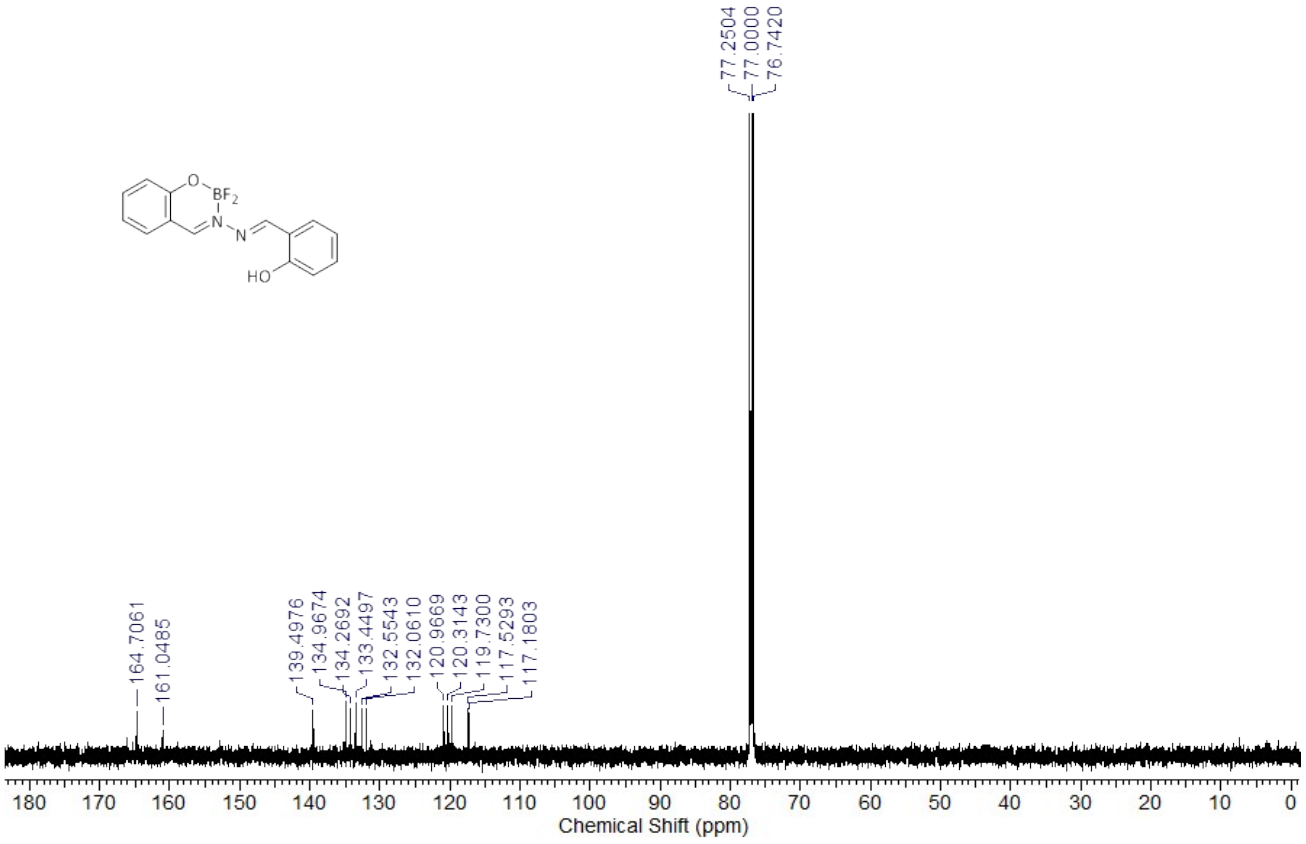


Figure S2: ^{13}C of **1** in $CDCl_3$.

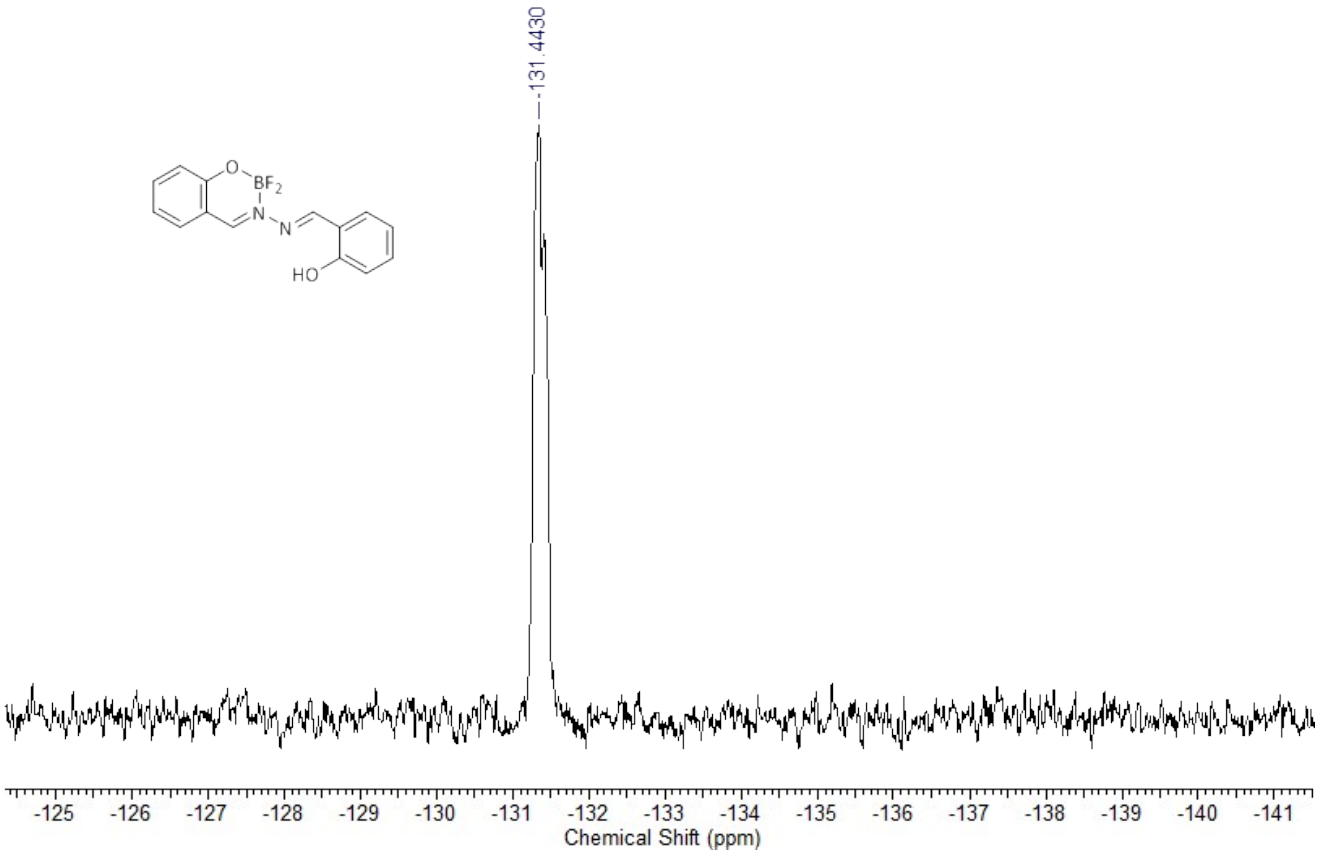


Figure S3: ^{19}F NMR of **1** in $CDCl_3$.

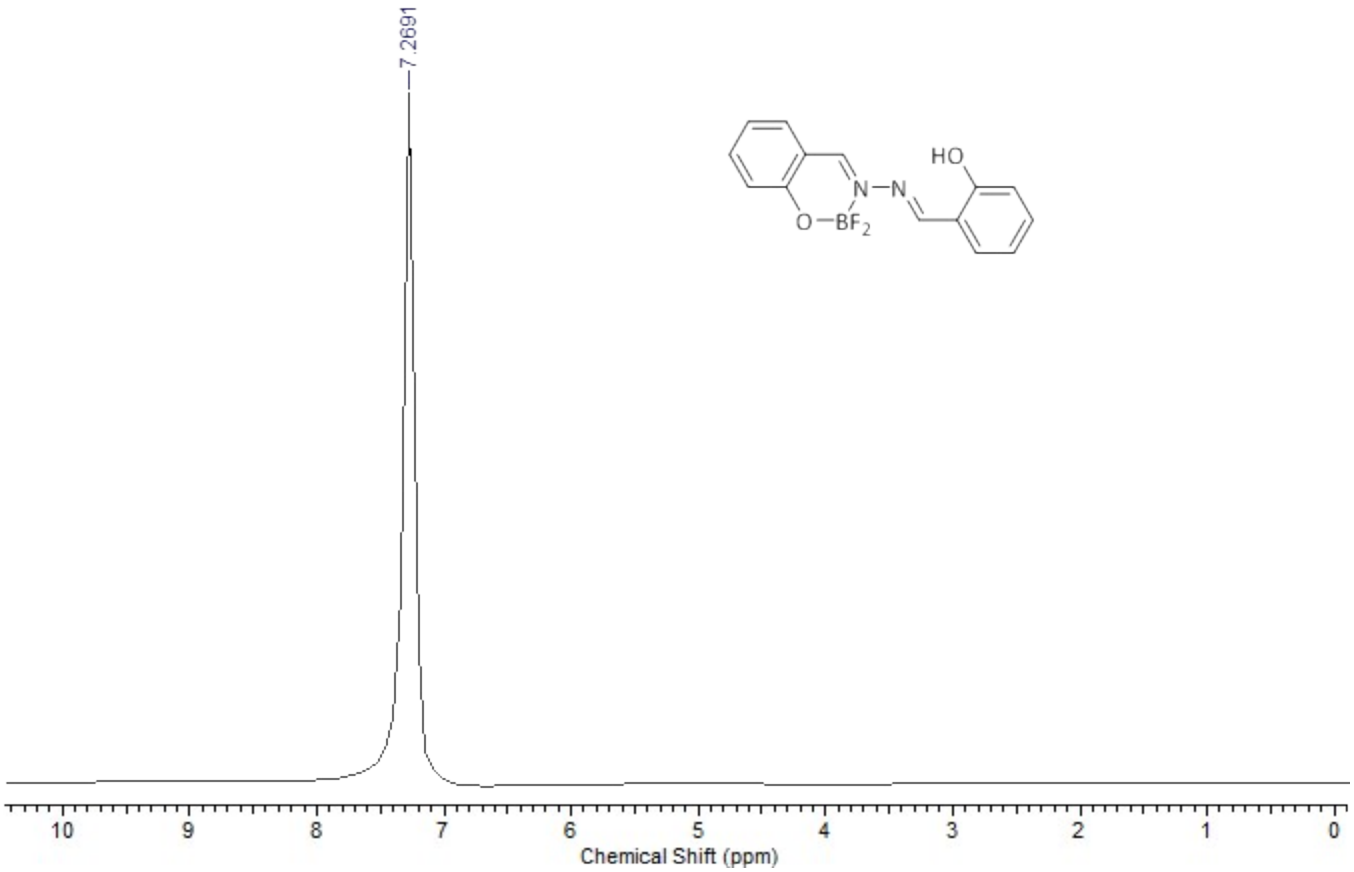


Figure S4: ^{11}B NMR of **1** in DMSO-d_6.

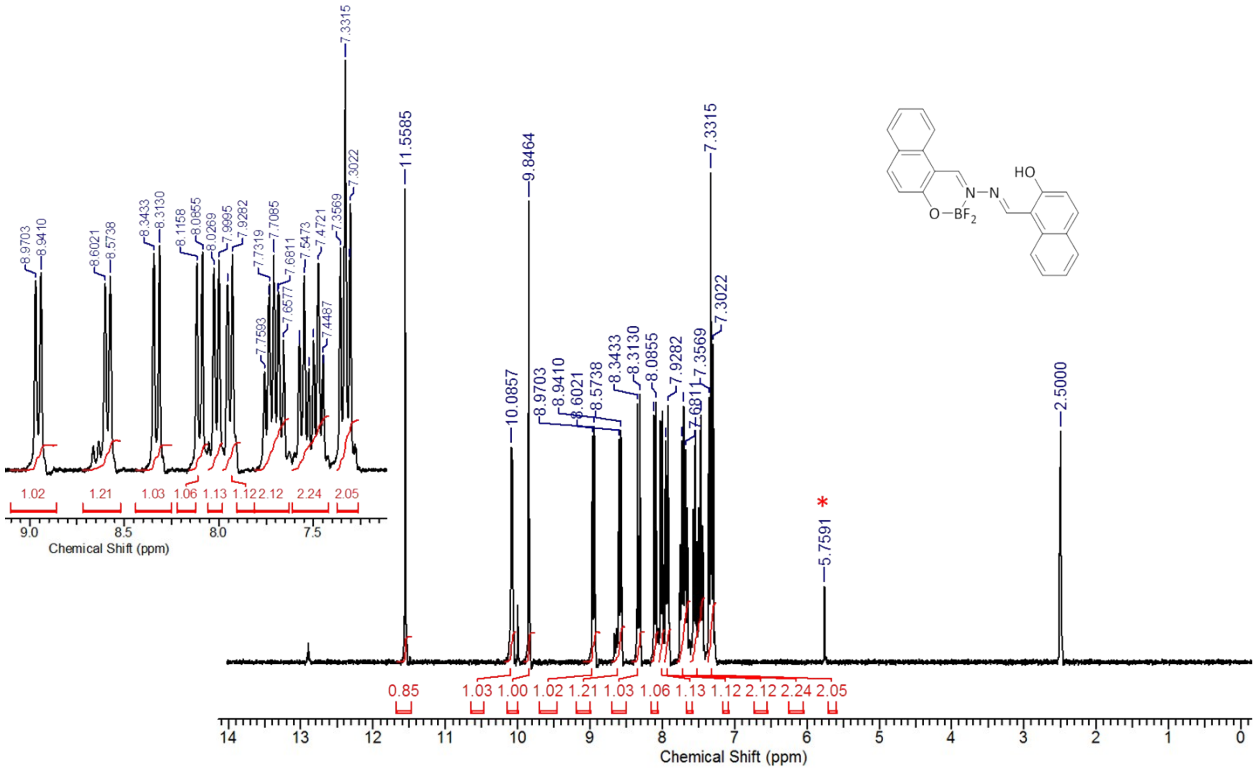


Figure S5: ^{1}H NMR of **2** in DMSO-d_6.

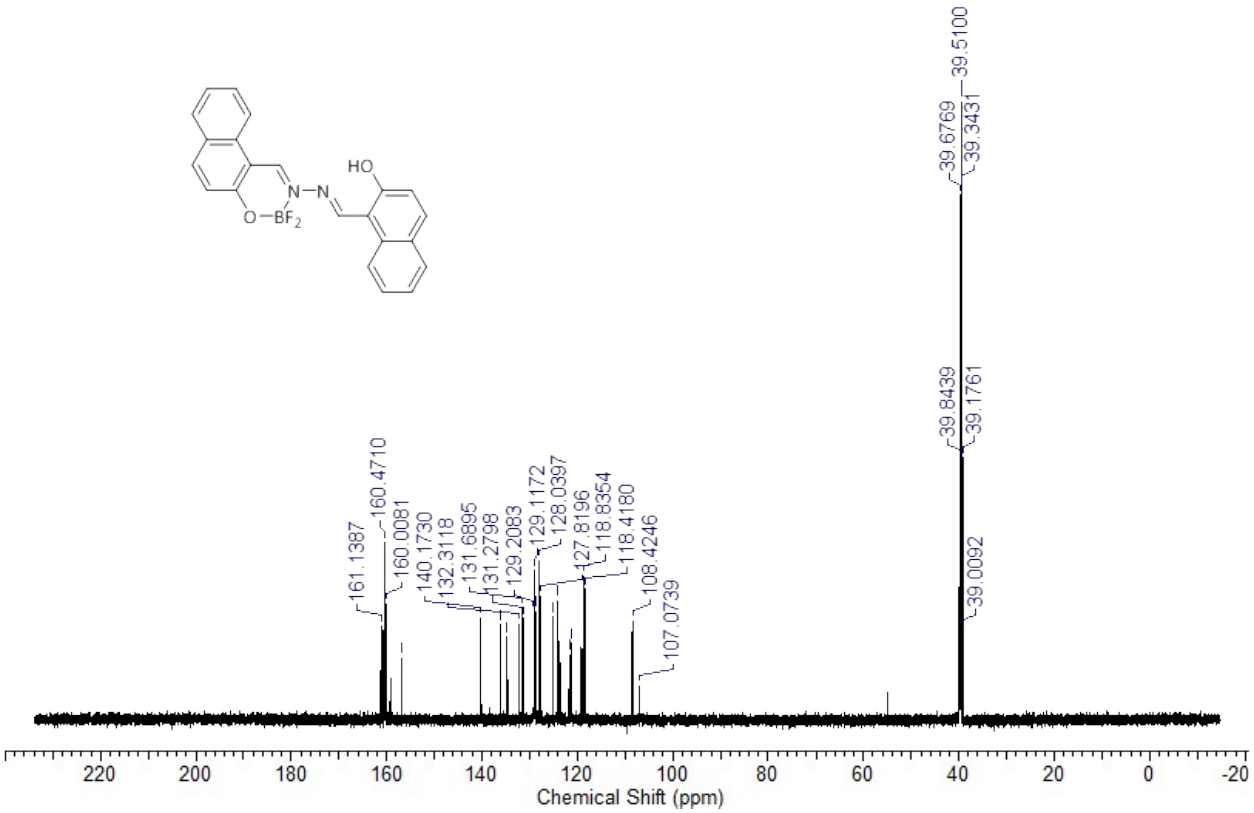


Figure S6: ^{13}C NMR of **2** in DMSO-d_6.

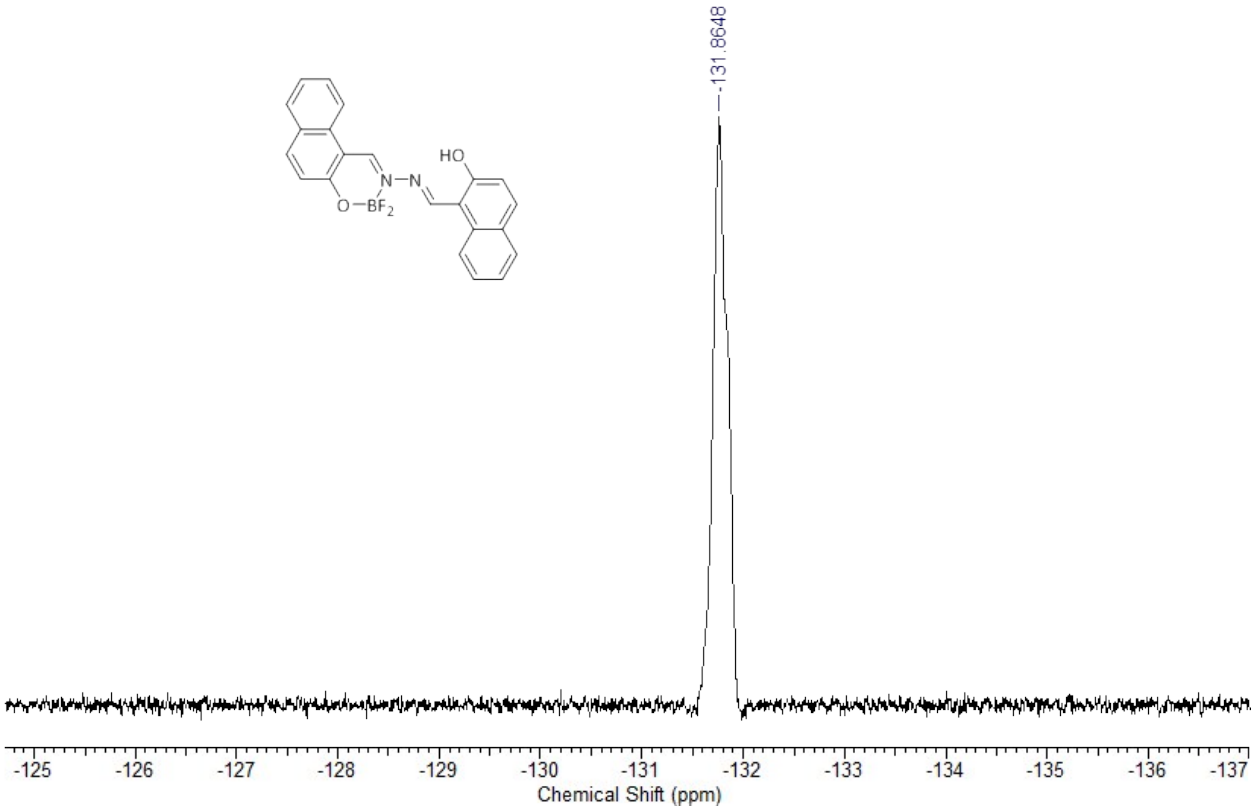


Figure S7: ^{19}F NMR of **2** in DMSO-d_6.

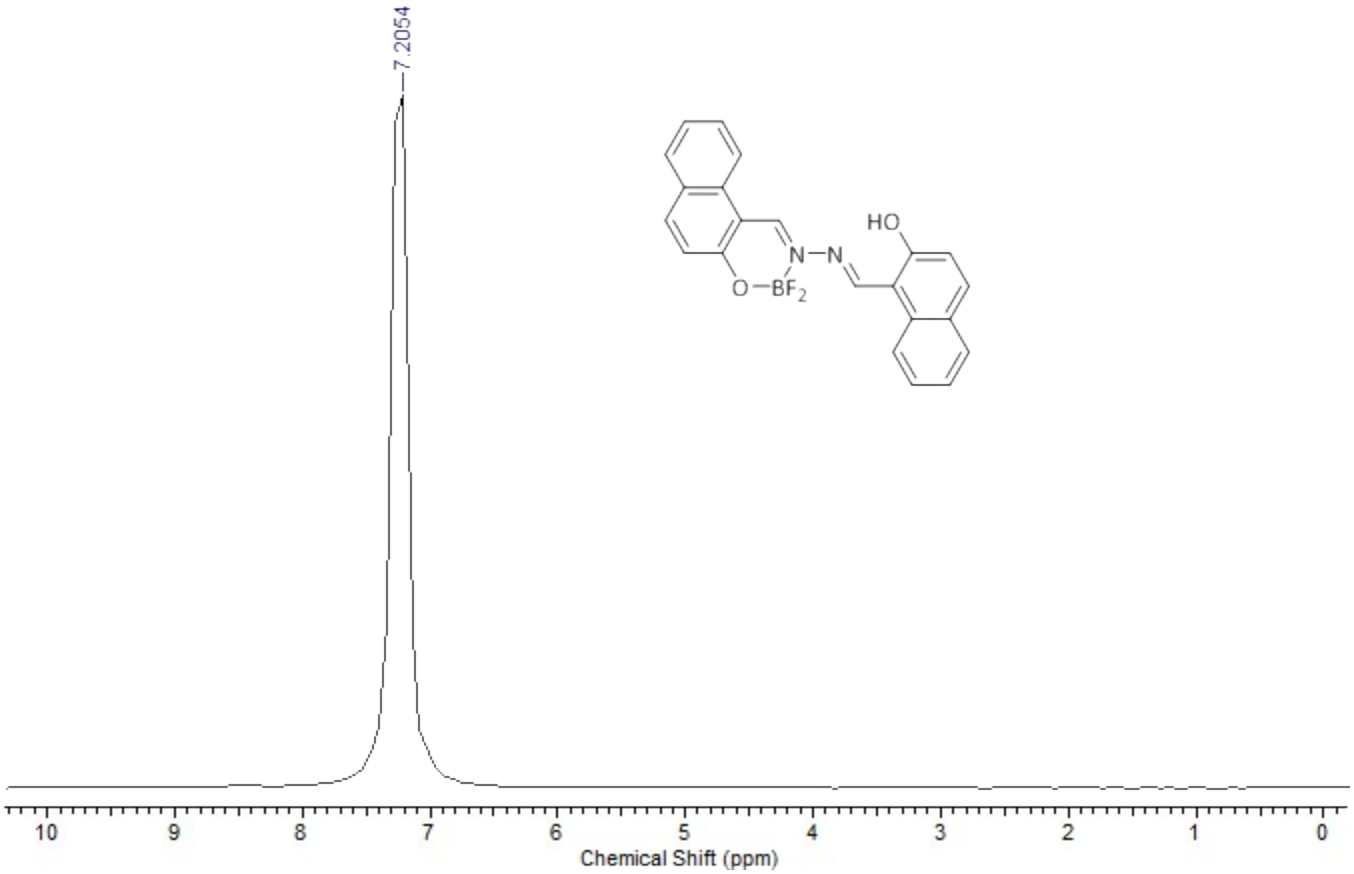


Figure S8: ^{11}B NMR of **2** in DMSO-d_6.

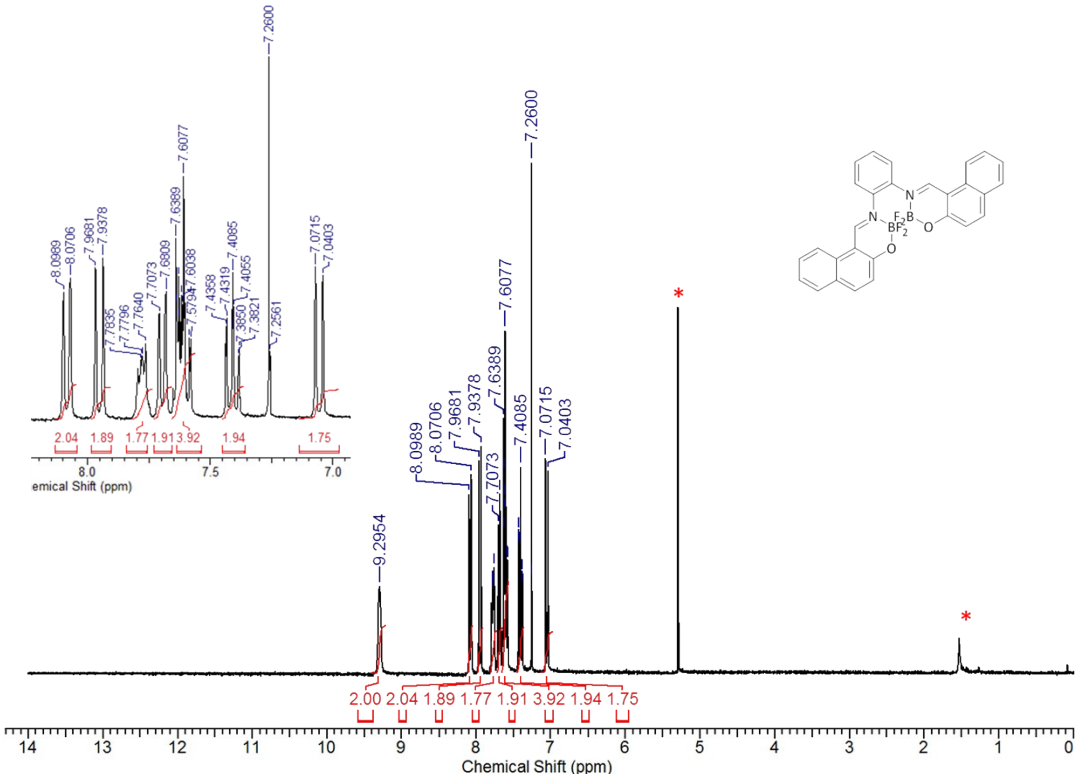


Figure S9: ^{1}H NMR of **3** in $CDCl_3$. * Represents H_2O and dichloromethane.

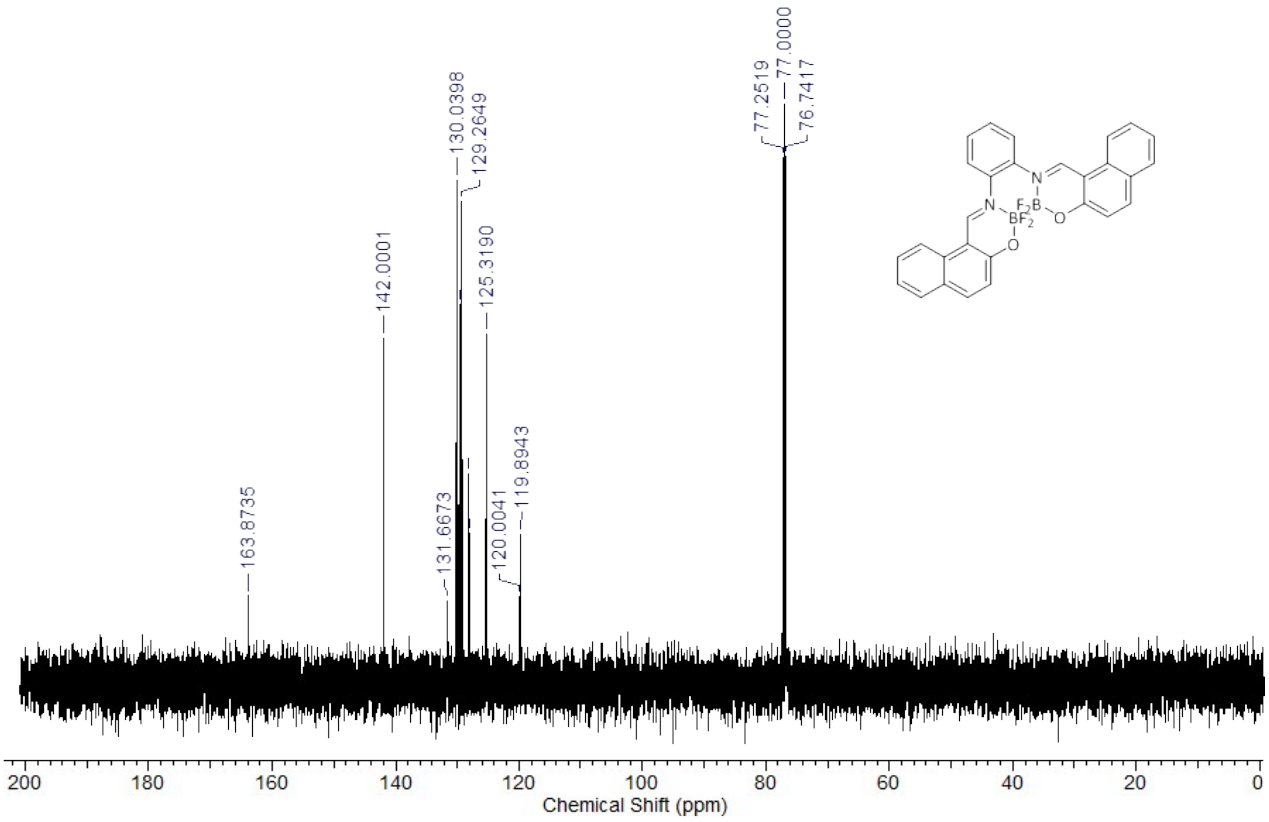


Figure S10: ^{13}C of **3** in $CDCl_3$.

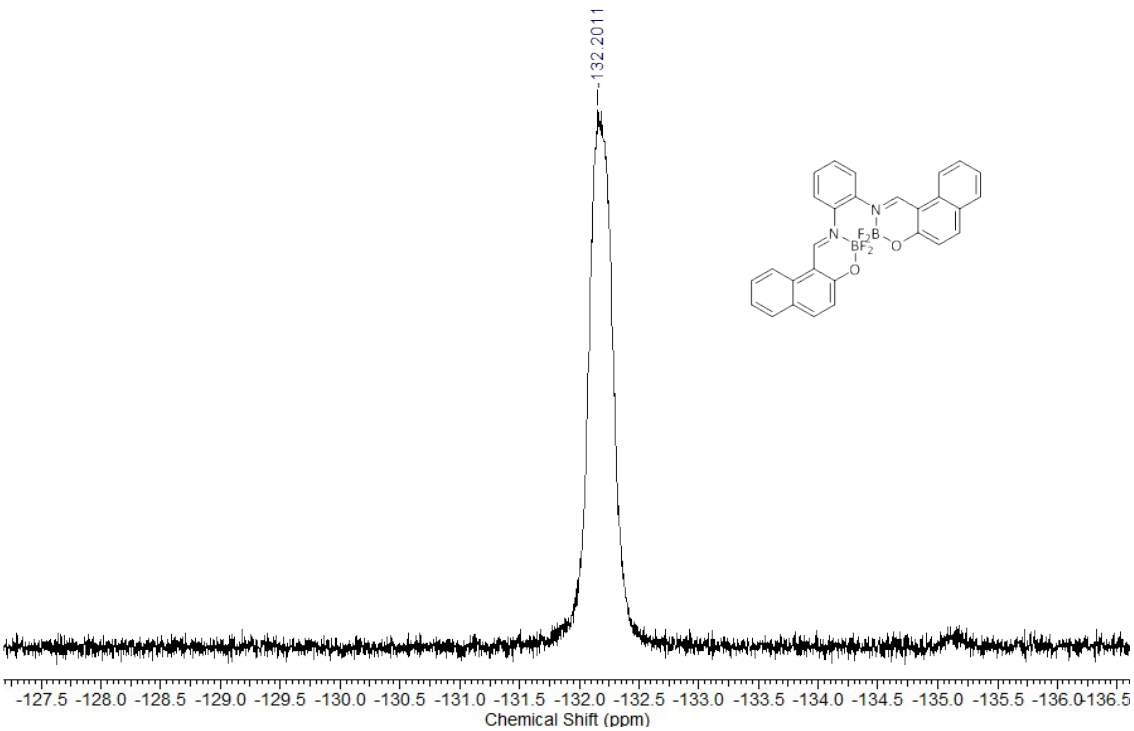


Figure S11: ^{19}F of **14** in $CDCl_3$.

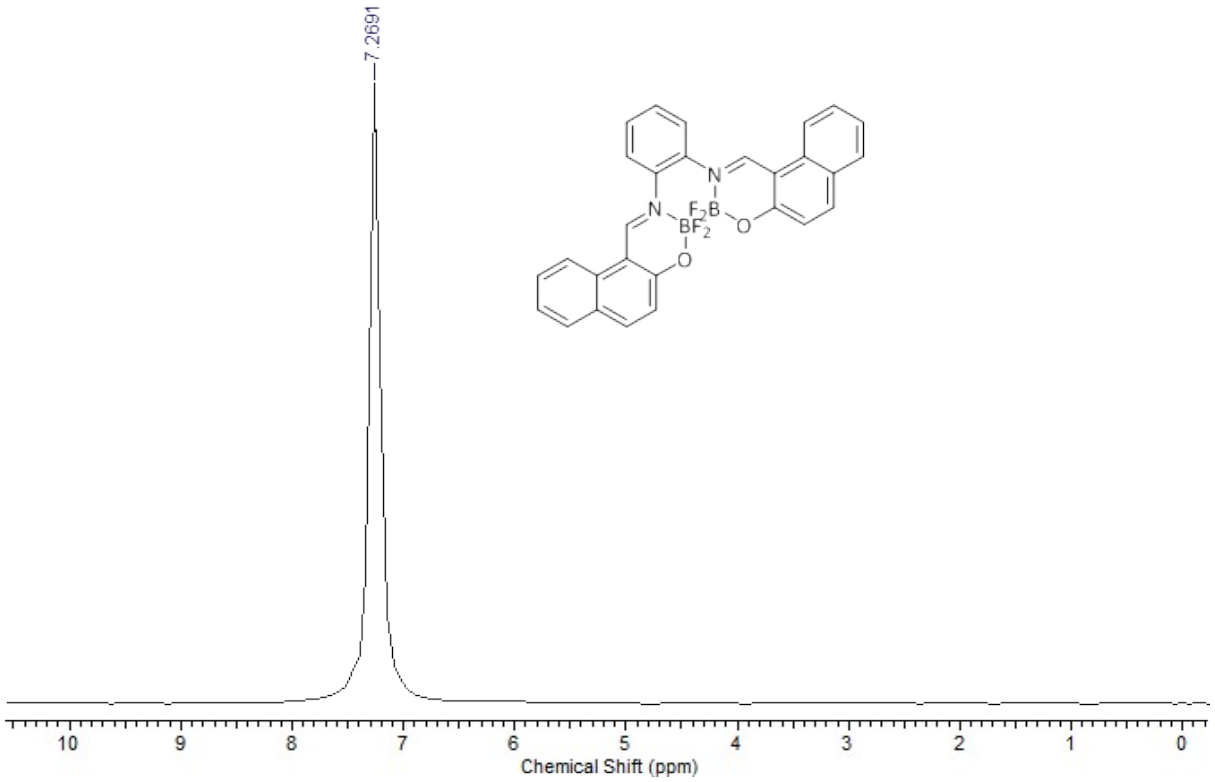


Figure S12: ^{11}B of **3** in $CDCl_3$.

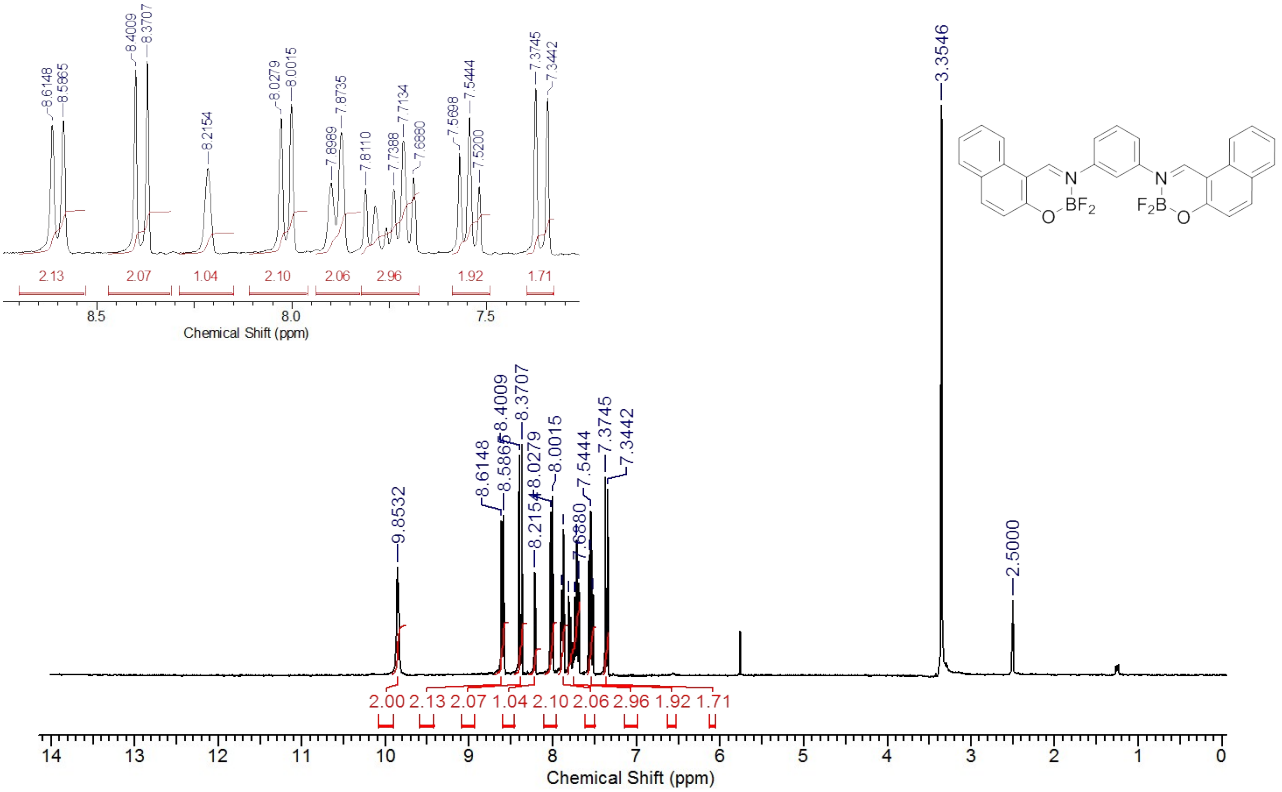


Figure S13: ^{1}H NMR of **4** in DMSO-d_6.

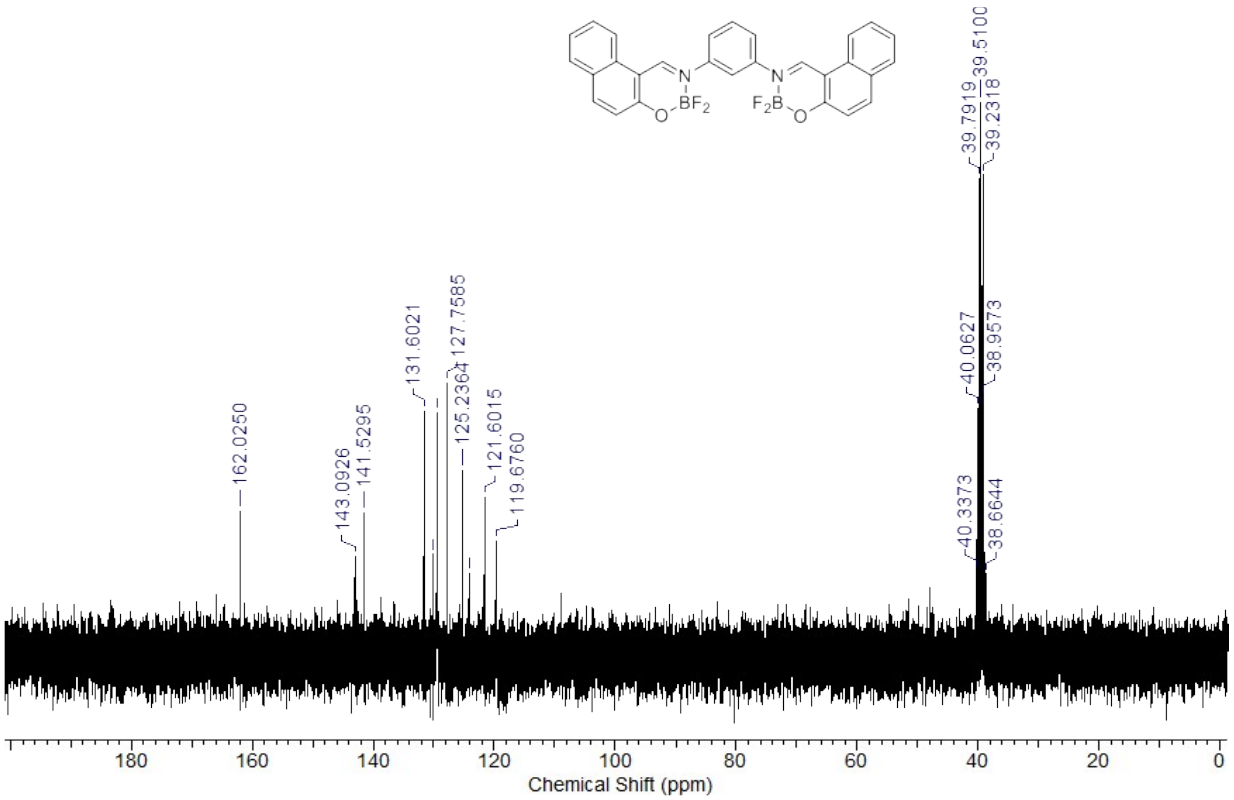


Figure S14: ^{13}C NMR of **4** in DMSO-d_6.

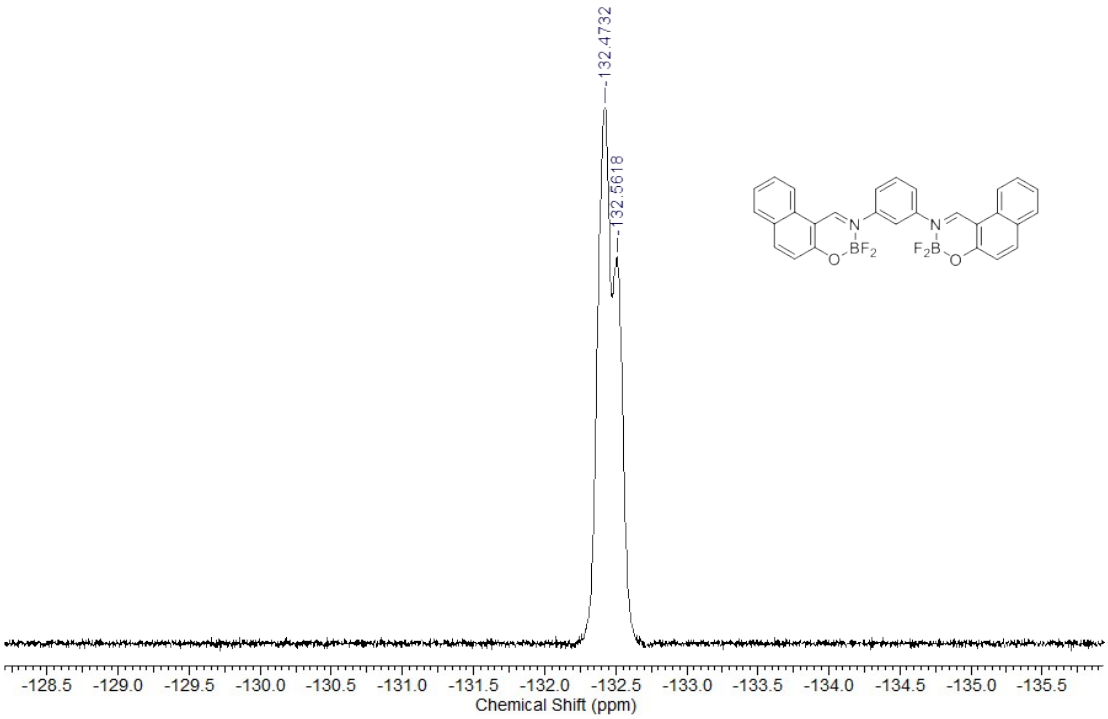


Figure S15: ^{19}F of **4** in DMSO-d_6.

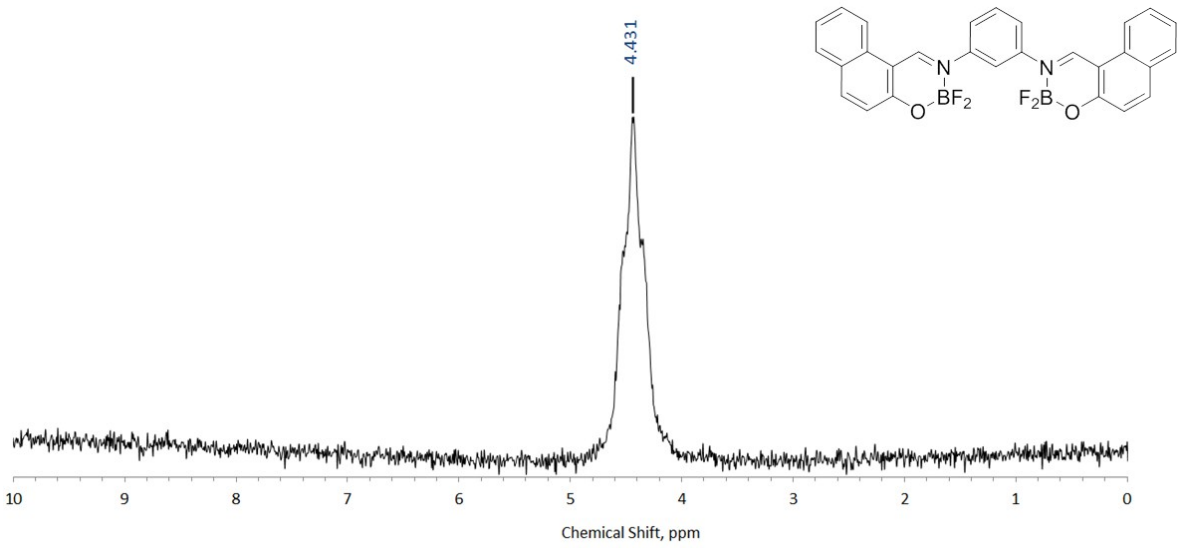


Figure S16: ^{11}B of **4** in DMSO-d_6.

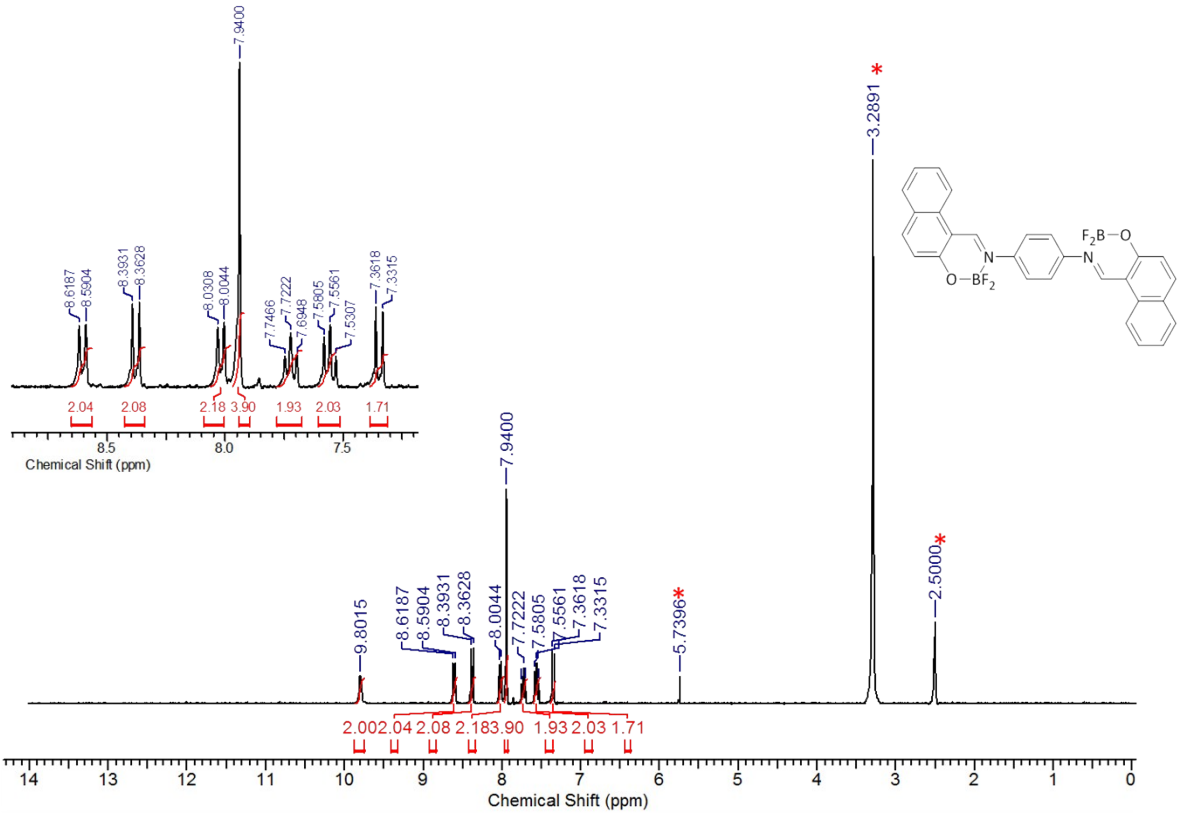


Figure S17: ^{1}H NMR of 5 in DMSO-d_6. * Represents DMSO, H_2O, and dichloromethane.

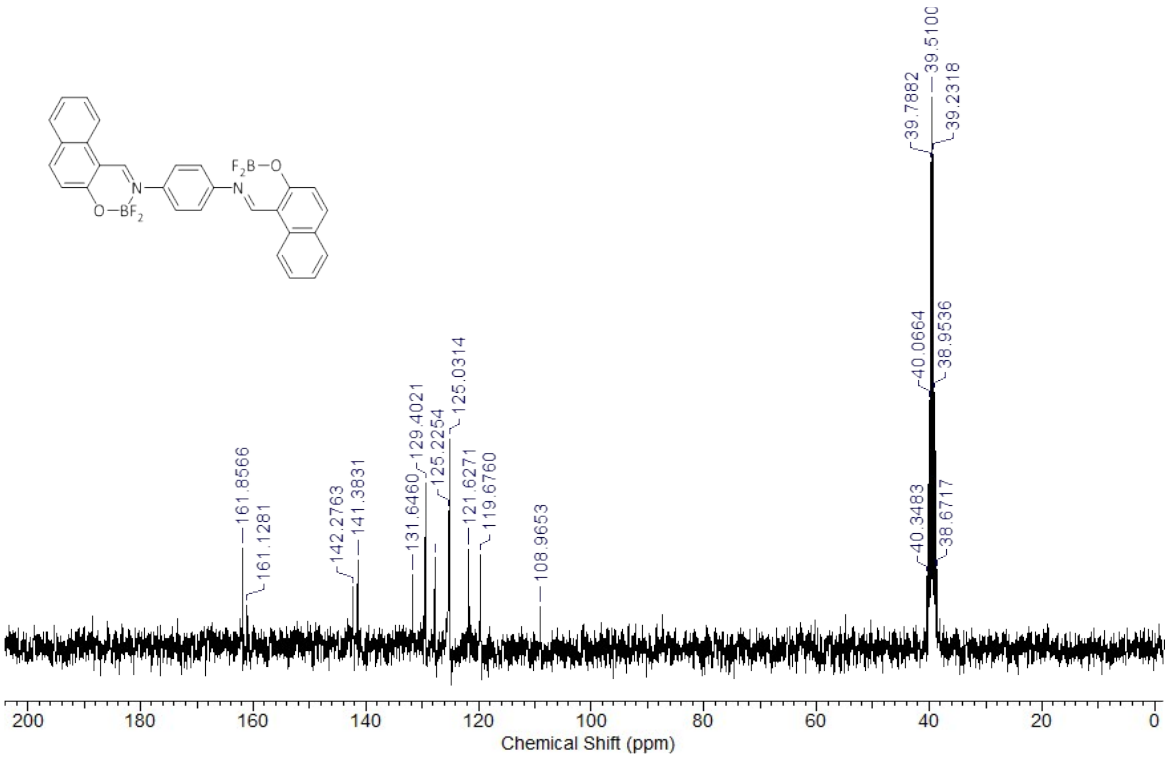


Figure S18: ^{13}C NMR of 5 in DMSO-d_6.

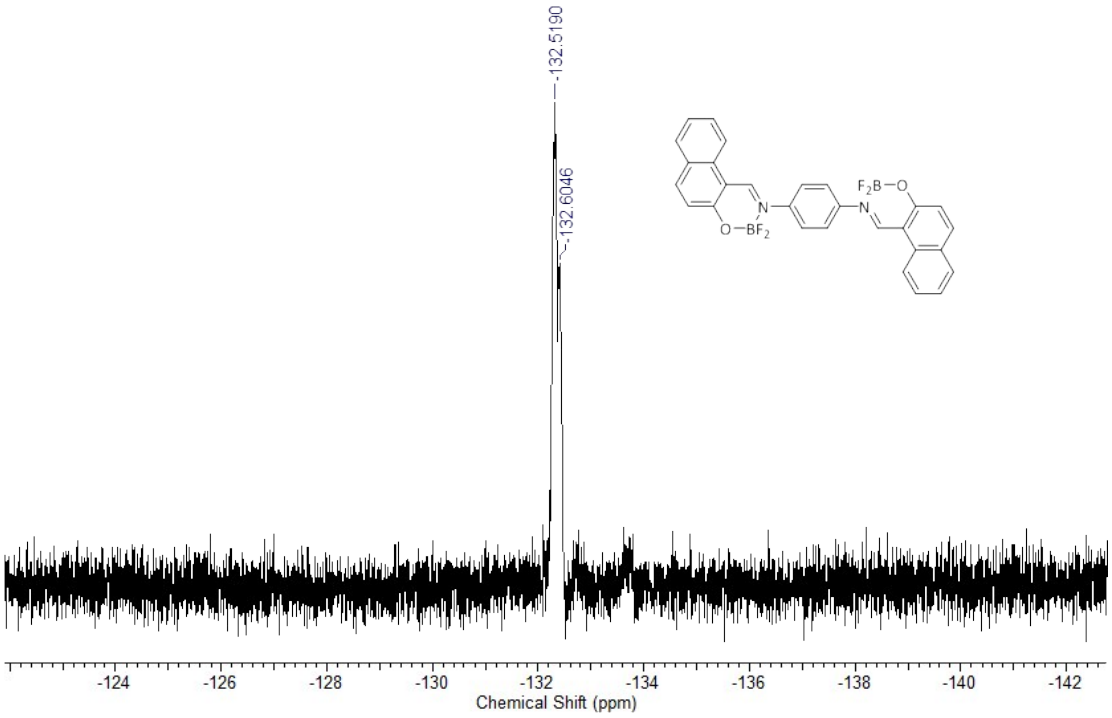


Figure S19: ^{19}F NMR of **5** in DMSO-d_6.

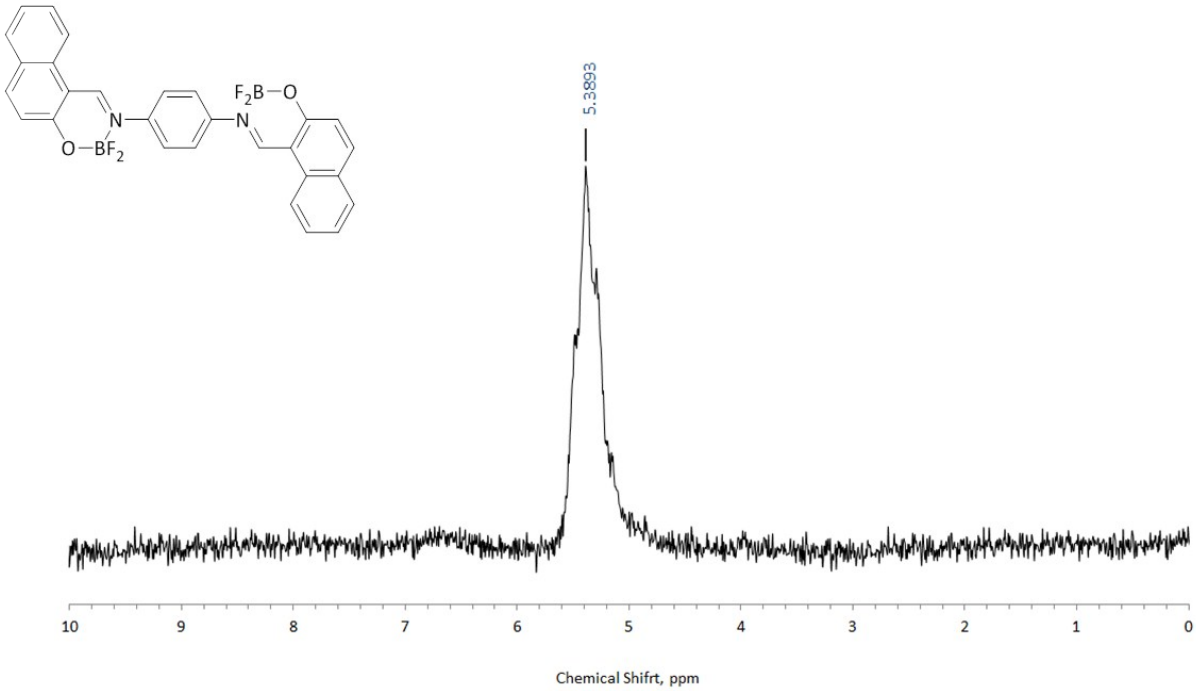
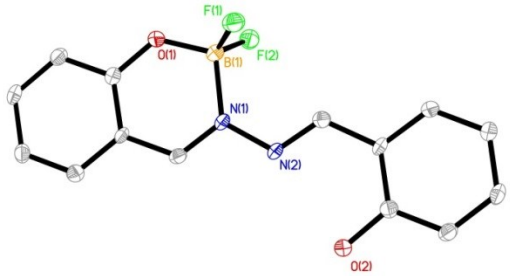


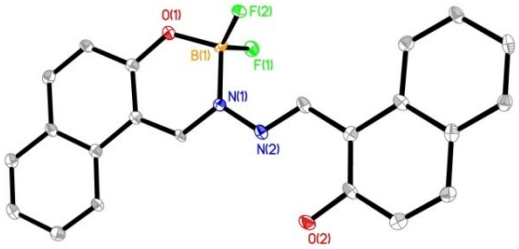
Figure S20: ^{11}B NMR of **5** in DMSO-d_6.

Table S1: Crystal data and refinement parameters for **1**.



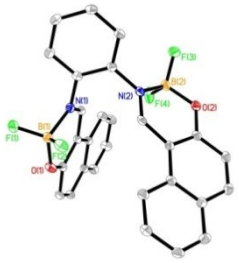
Compound	1	
Empirical formula	**C14 H11 B F2 N2 O2**	
Formula weight	**288.06**	
Temperature	**100(2) K**	
Wavelength	**1.54718 Å**	
Crystal system	**Monoclinic**	
Space group	**P 21/c**	
Unit cell dimensions	a = 6.2396(2) Å	**α=90°**
	b = 15.0244(5) Å	**β= 106.777(2) °**
	c = 13.6239(4) Å	**γ = 90°**
Volume	**1222.83(7) Å^3**	
Z	**4**	
Density (calculated)	**1.565 Mg/m^3**	
Absorption coefficient	**1.066 mm^{-1}**	
F(000)	**592**	
Crystal size	**0.143 x 0.105 x 0.083 mm^3**	
Theta range for data collection	**4.49 to 65.77°**	
Index ranges	**--7<=h<=6, -17<=k<=15, -15<=l<=16**	
Reflections collected	**7595**	
Independent reflections	**2021 [R(int) = 0.0278]**	
Completeness to theta	**95.1 %**	
Absorption correction	**SADABS**	
Max. and min. transmission	**0.7527 and 0.6968**	
Refinement method	**Full-matrix least-squares on F^2**	
Data / restraints / parameters	**2021 / 0 / 190**	
Goodness-of-fit on F2	**1.081**	
Final R indices [I>2sigma(I)]	**R1 = 0.0425, wR2 = 0.1365**	
R indices (all data)	**R1 = 0.0453, wR2 = 0.1391**	
Largest diff. peak and hole	**0.271 and -0.270 e.Å^{-3}**	

Table S2: Crystal data and refinement parameters for **2**.



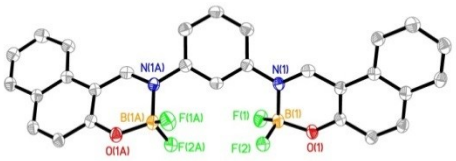
Compound	**2**	
Empirical formula	C22 H15 B F2 N2 O2	
Formula weight	388.17	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.1614(12) Å	α=94.706(7)°
	b = 9.4911(14) Å	β= 101.989(5)°
	c = 11.3018(18) Å	γ = 92.791(7)°
Volume	851.5(2) $Å^3$	
Z	2	
Density (calculated)	1.514 Mg/m^3	
Absorption coefficient	0.112 mm^{-1}	
F(000)	400	
Crystal size	0.49x 0.45 x 0.37 mm^3	
Theta range for data collection	1.85 to 25.15°	
Index ranges	-9<=h<=9, -11<=k<=11, -13<=l<=13	
Reflections collected	8627	
Independent reflections	2951 [R(int) = 0.0453]	
Completeness to theta	96.7 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9596 and 0.9471	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2951/ 0 / 263	
Goodness-of-fit on F2	1.128	
Final R indices [I>2sigma(I)]	R1 = 0.1410, wR2 = 0.4363	
R indices (all data)	R1 = 0.1486, wR2 = 0.4405	
Largest diff. peak and hole	0.843 and -0.767 $e.Å^{-3}$	

Table S3: Crystal data and refinement parameters for **3**.



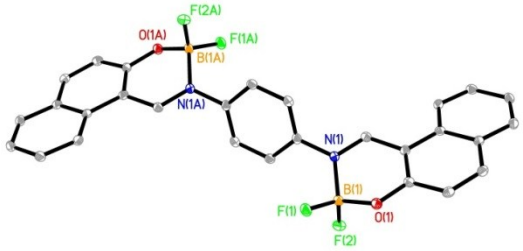
Compound	3	
Empirical formula	C29 H20 B2 Cl2 F4 N2 O2	
Formula weight	596.99	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.2748(14) Å	α= 110.390(3)°
	b = 14.4752(18) Å	β=90.141(3)°
	c = 17.300(2) Å	γ = 100.184(3)°
Volume	2598.6(6) $Å^3$	
Z	4	
Density (calculated)	1.526 Mg/m^3	
Absorption coefficient	0.312 mm^{-1}	
F(000)	1216	
Crystal size	0.31x 0.30 x 0.16 mm^3	
Theta range for data collection	1.26 to 25.21°	
Index ranges	-13<=h<=13, -17<=k<=17, -20<=l<=20	
Reflections collected	31100	
Independent reflections	9279 [R(int) = 0.0288]	
Completeness to theta	99.0 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9527 and 0.9090	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9279 / 0 / 739	
Goodness-of-fit on F2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0513, wR2 = 0.1447	
R indices (all data)	R1 = 0.0654, wR2 = 0.1577	
Largest diff. peak and hole	0.474 and -0.385 $e.Å^{-3}$	

Table S4: Crystal data and refinement parameters for **4**.



Compound	4
Empirical formula	C28 H18 B2 F4 N2 O2
Formula weight	512.06
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	Pcbn
Unit cell dimensions	a = 10.5218(9) Å α= 90°
	b = 12.6033(10) Å β=90°
	c = 16.7317(15) Å γ = 90°
Volume	2218.8(3) $Å^3$
Z	4
Density (calculated)	1.533Mg/m^3
Absorption coefficient	1.002 mm^{-1}
F(000)	1048
Crystal size	0.163x 0.117 x 0.073 mm^3
Theta range for data collection	5.29 to 65.67°
Index ranges	-12<=h<=10, -14<=k<=13, -12<=l<=19
Reflections collected	12464
Independent reflections	1857 [R(int) = 0.0361]
Completeness to theta	96.6 %
Absorption correction	SADABS
Max. and min. transmission	0.7527 and 0.6571
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1857 / 0 / 173
Goodness-of-fit on F2	1.067
Final R indices [I>2sigma(I)]	R1 = 0.0827, wR2 = 0.2133
R indices (all data)	R1 = 0.857, wR2 = 0.2147
Largest diff. peak and hole	0.407 and -0.294 $e.Å^{-3}$

Table S5: Crystal data and refinement parameters for **5**.



Compound	**5**	
Empirical formula	C16 H15 B F2 N O2 S	
Formula weight	334.16	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 9.6836(7) Å	α= 90°
	b = 5.6340(4) Å	β= 96.073(2)°
	c = 27.2833(19) Å	γ = 90°
Volume	1480.15(18) $Å^3$	
Z	4	
Density (calculated)	1.500Mg/m^3	
Absorption coefficient	0.249 mm^{-1}	
F(000)	692	
Crystal size	0.187x 0.138 x 0.101 mm^3	
Theta range for data collection	1.501 to 25.224°	
Index ranges	-11<=h<=11, -6<=k<=6, -32<=l<=32	
Reflections collected	17125	
Independent reflections	2661 [R(int) = 0.0516]	
Completeness to theta	99.2 %	
Absorption correction	SADABS	
Max. and min. transmission	0.7527 and 0.6571	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2661 / 0 / 210	
Goodness-of-fit on F2	0.996	
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.1235	
R indices (all data)	R1 = 0.0451, wR2 = 0.1295	
Largest diff. peak and hole	0.427 and -0.321 e.$Å^{-3}$	

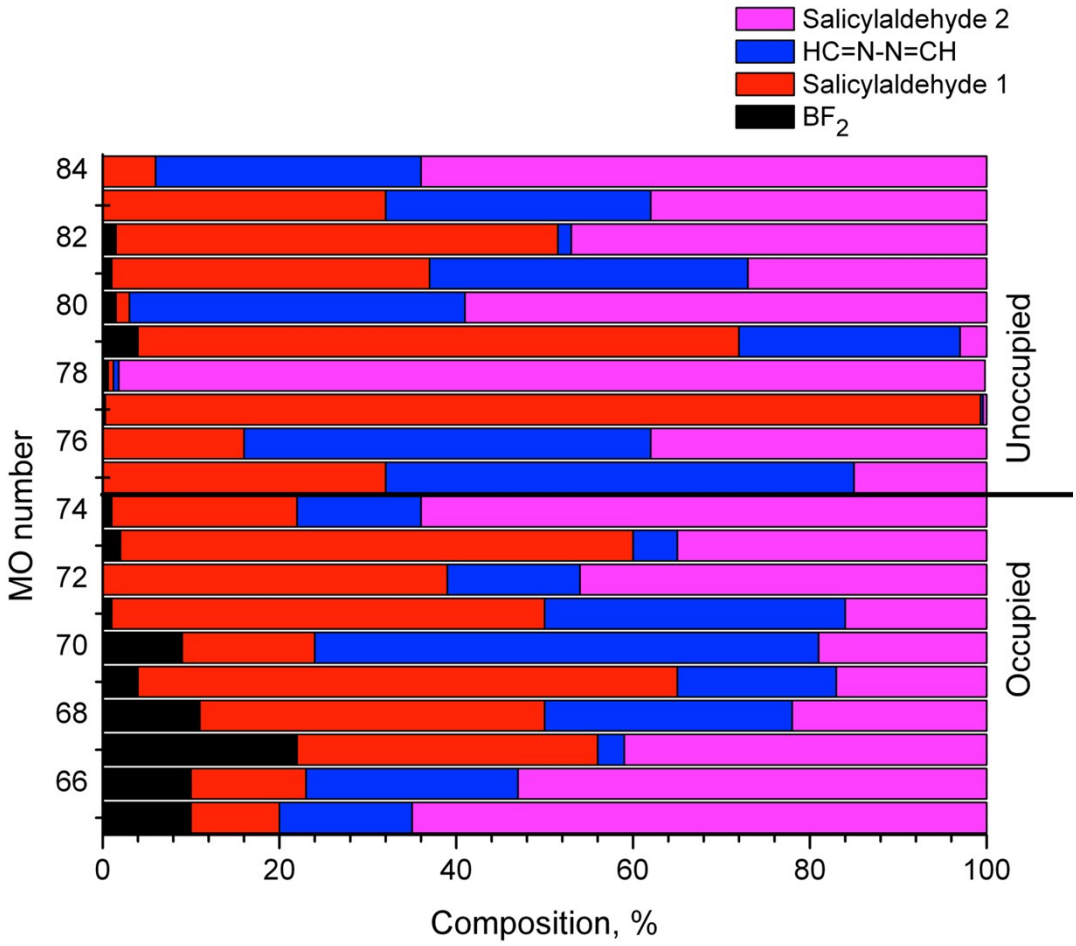


Figure S21: PCM-DFT calculated (TPSSh functional/6-311G(d) basis set) MO compositions of compound **1.**

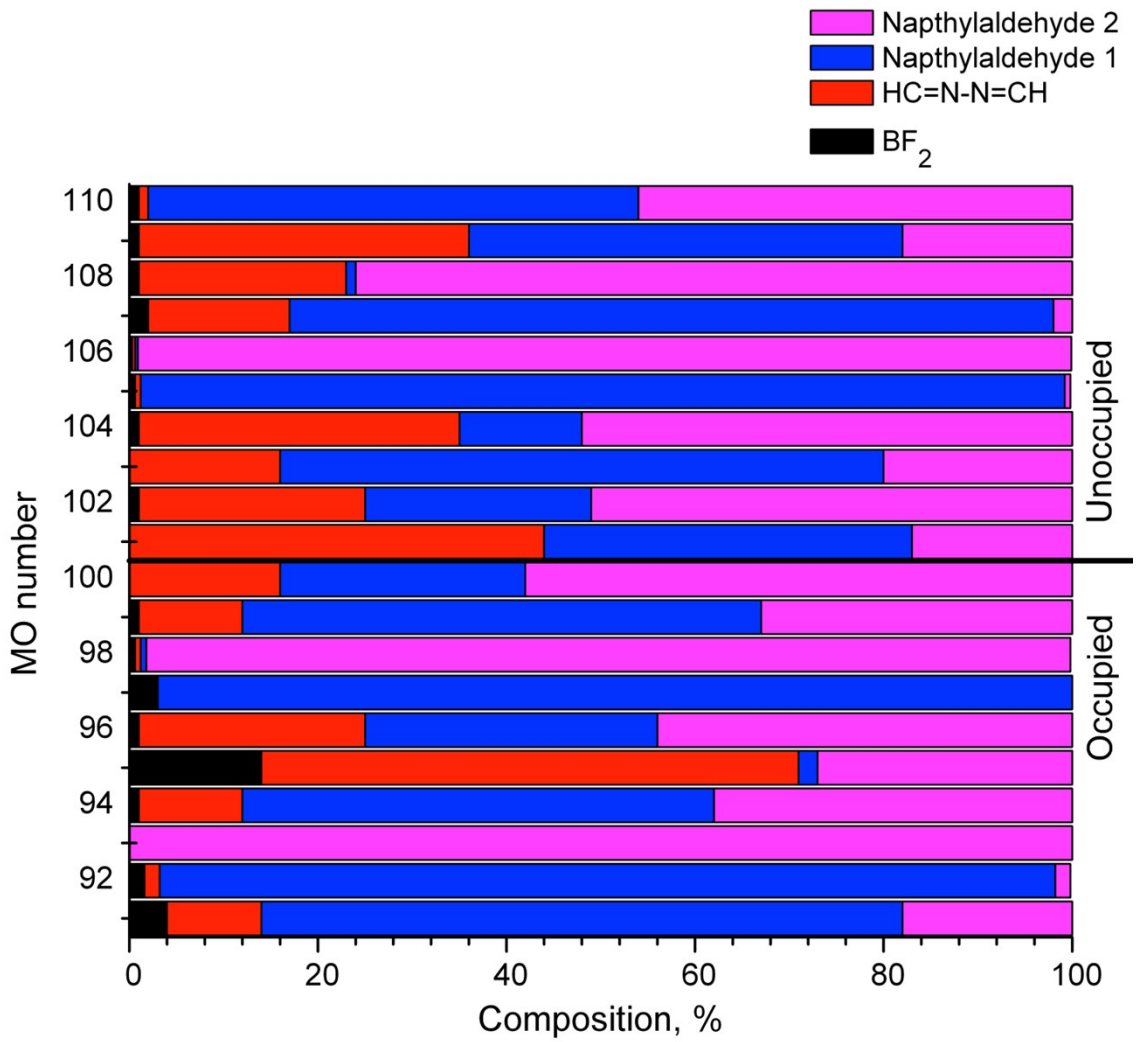


Figure S22: PCM-DFT calculated (TPSSh functional/6-311G(d) basis set) MO compositions of compound **2.**

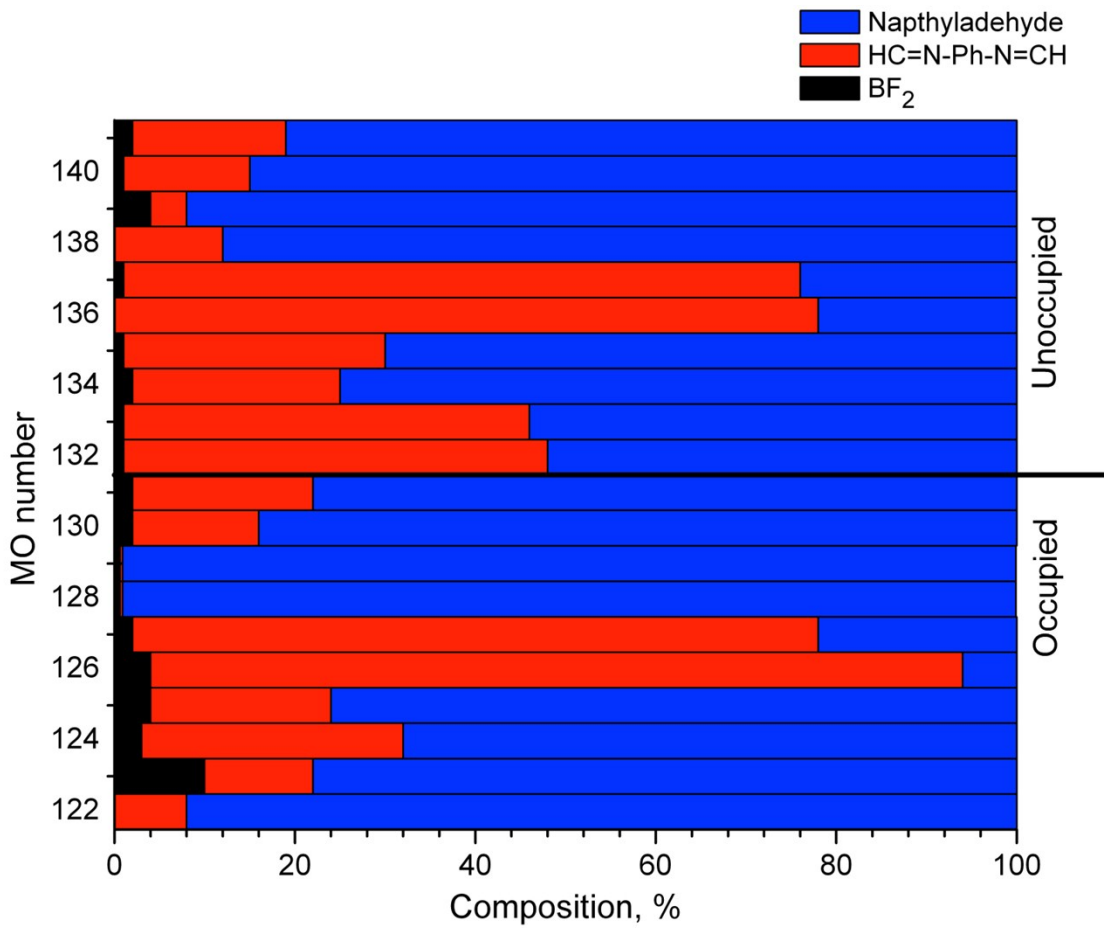


Figure S23: PCM-DFT calculated (TPSSh functional/6-311G(d) basis set) MO compositions of compound **3.**

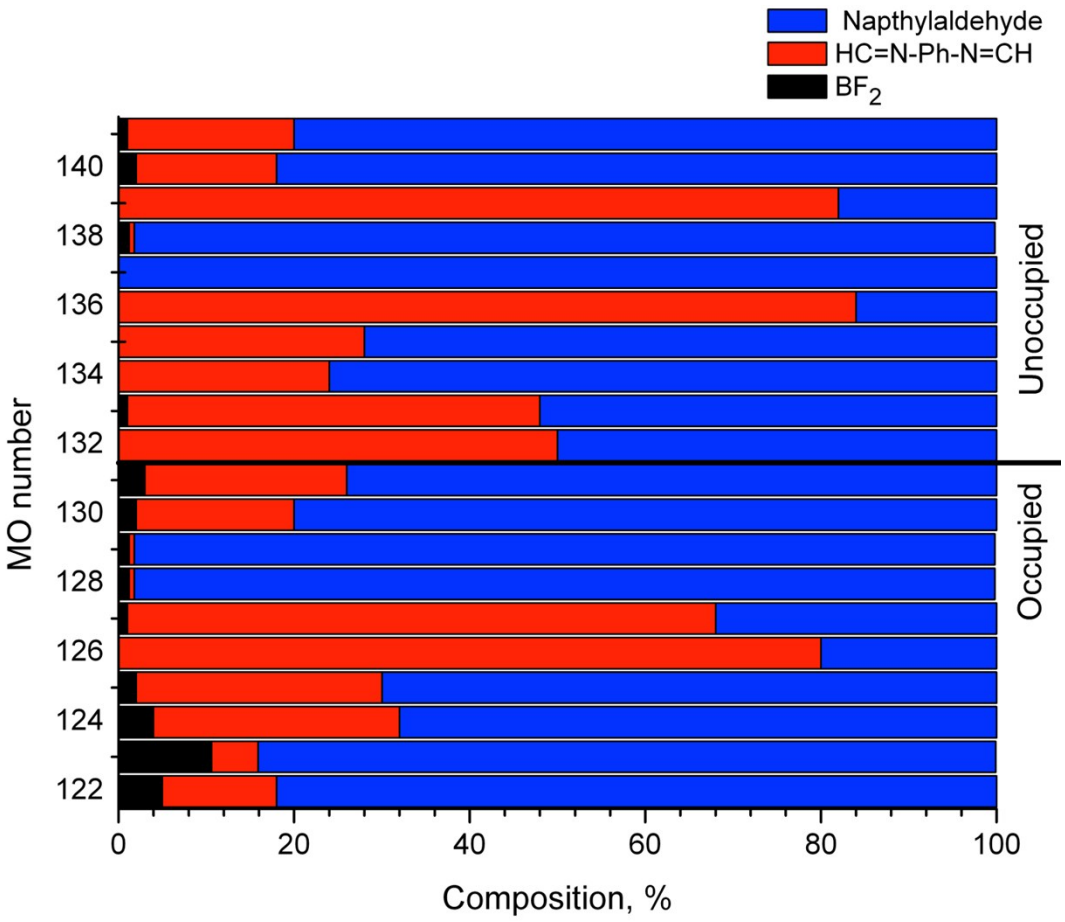


Figure S24: PCM-DFT calculated (TPSSh functional/6-311G(d) basis set) MO compositions of compound **4.**

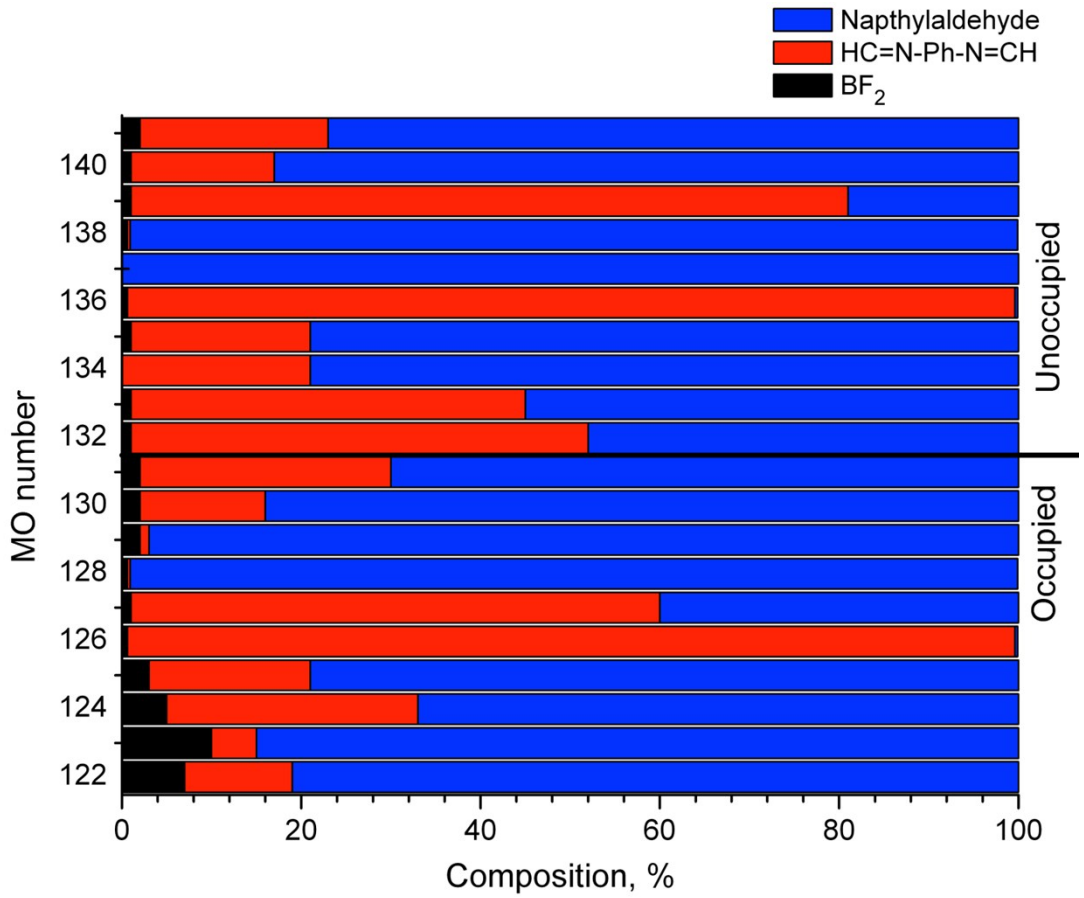


Figure S25: PCM-DFT calculated (TPSSh functional/6-311G(d) basis set) MO compositions of compound **5.**

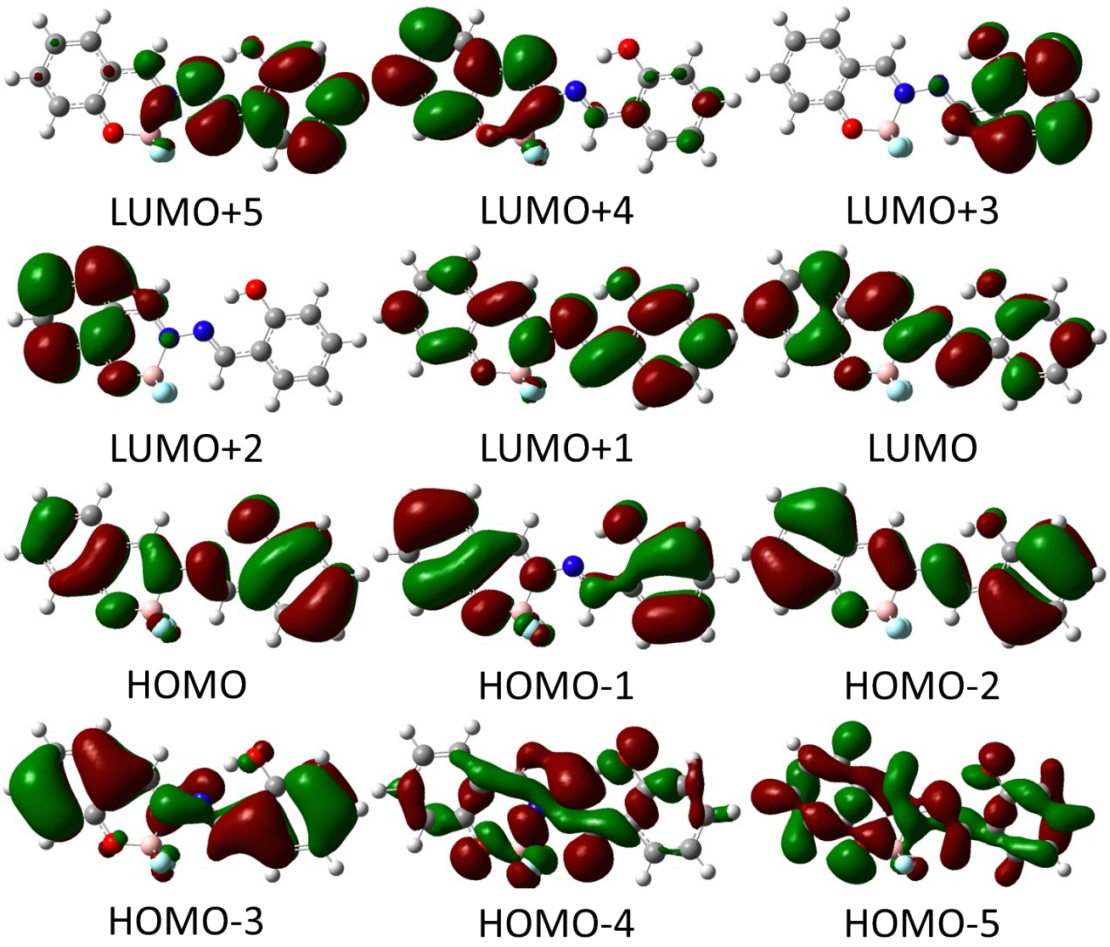


Figure S26: DFT predicted frontier orbital structures for **1.**

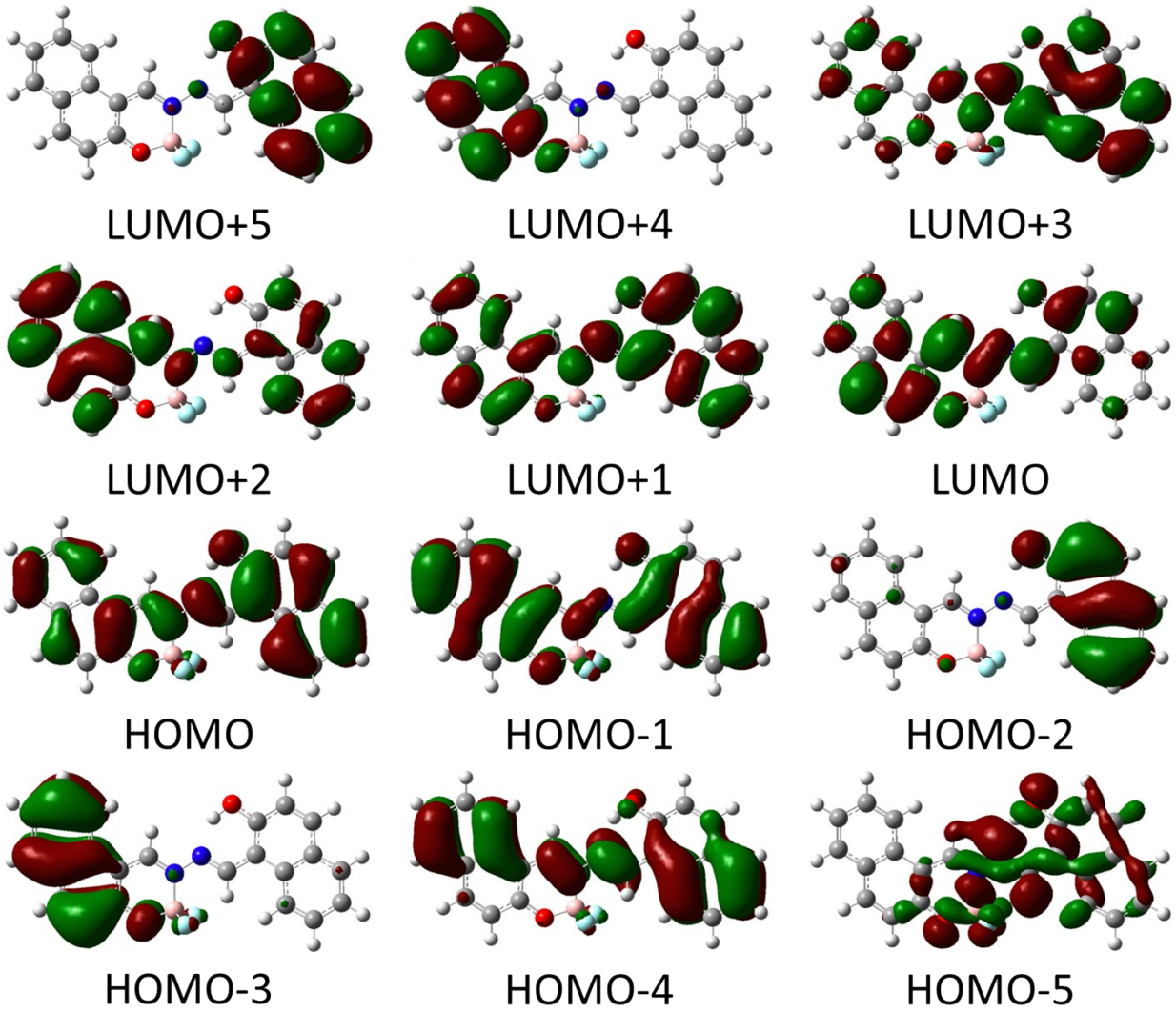


Figure S27: DFT predicted frontier orbital structures for **2.**

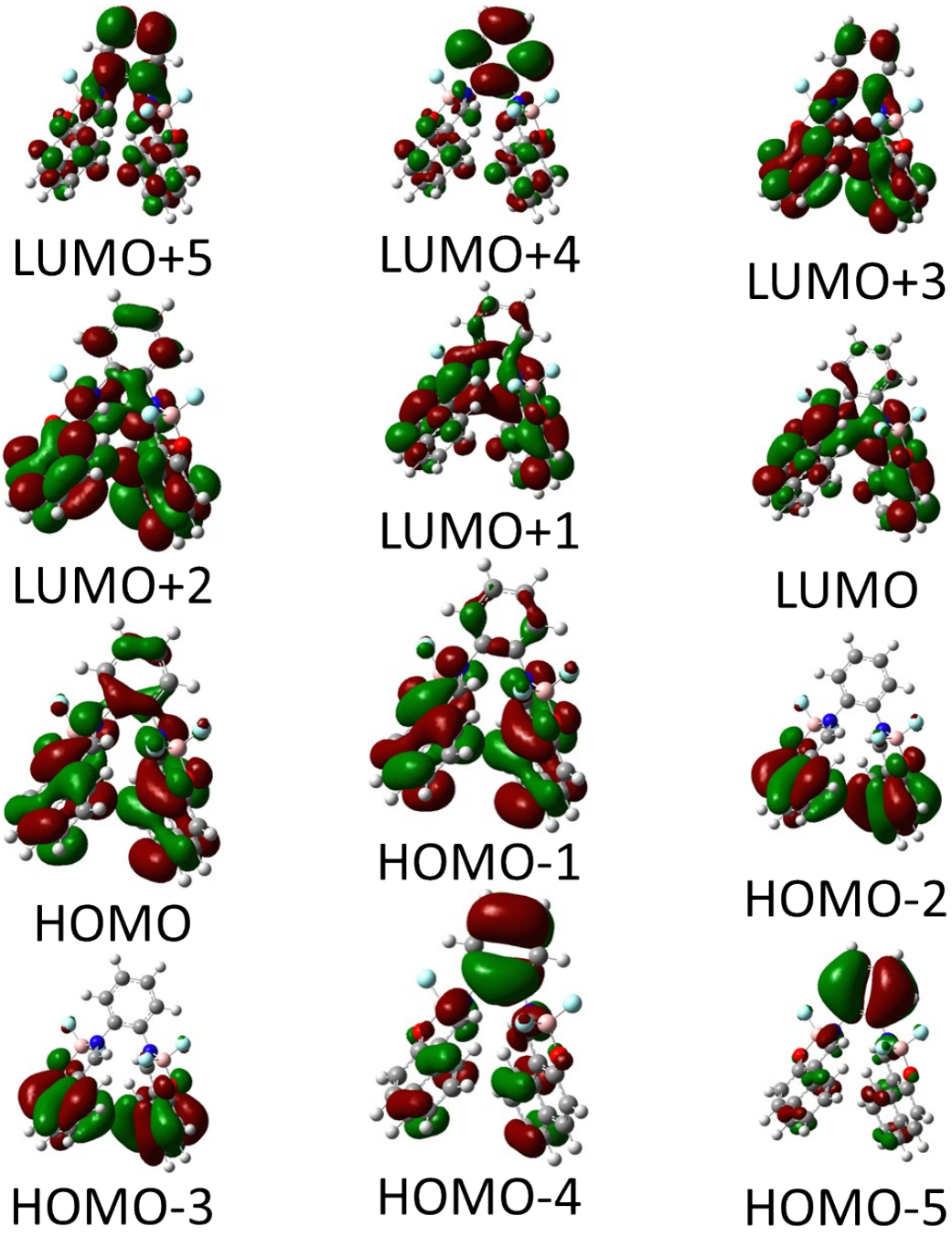


Figure S28: DFT predicted frontier orbital structures for **3.**

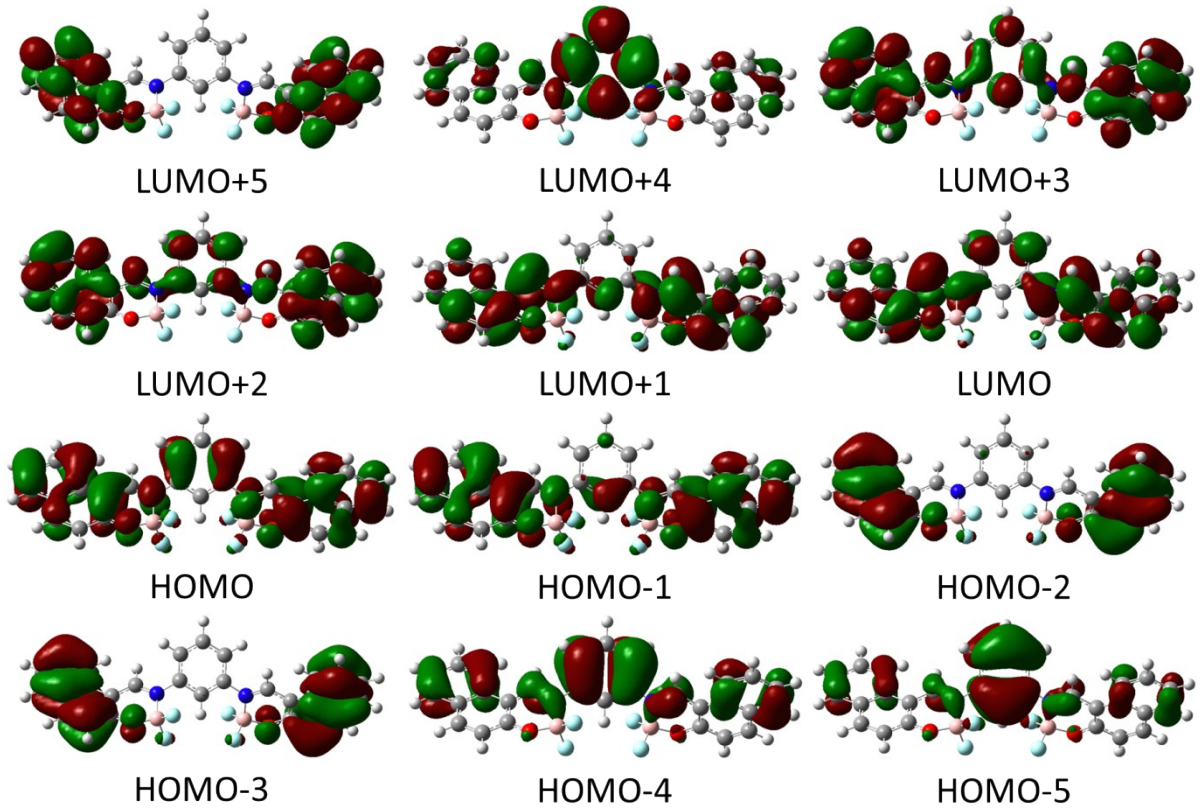


Figure S29: DFT predicted frontier orbital structures for **4.**

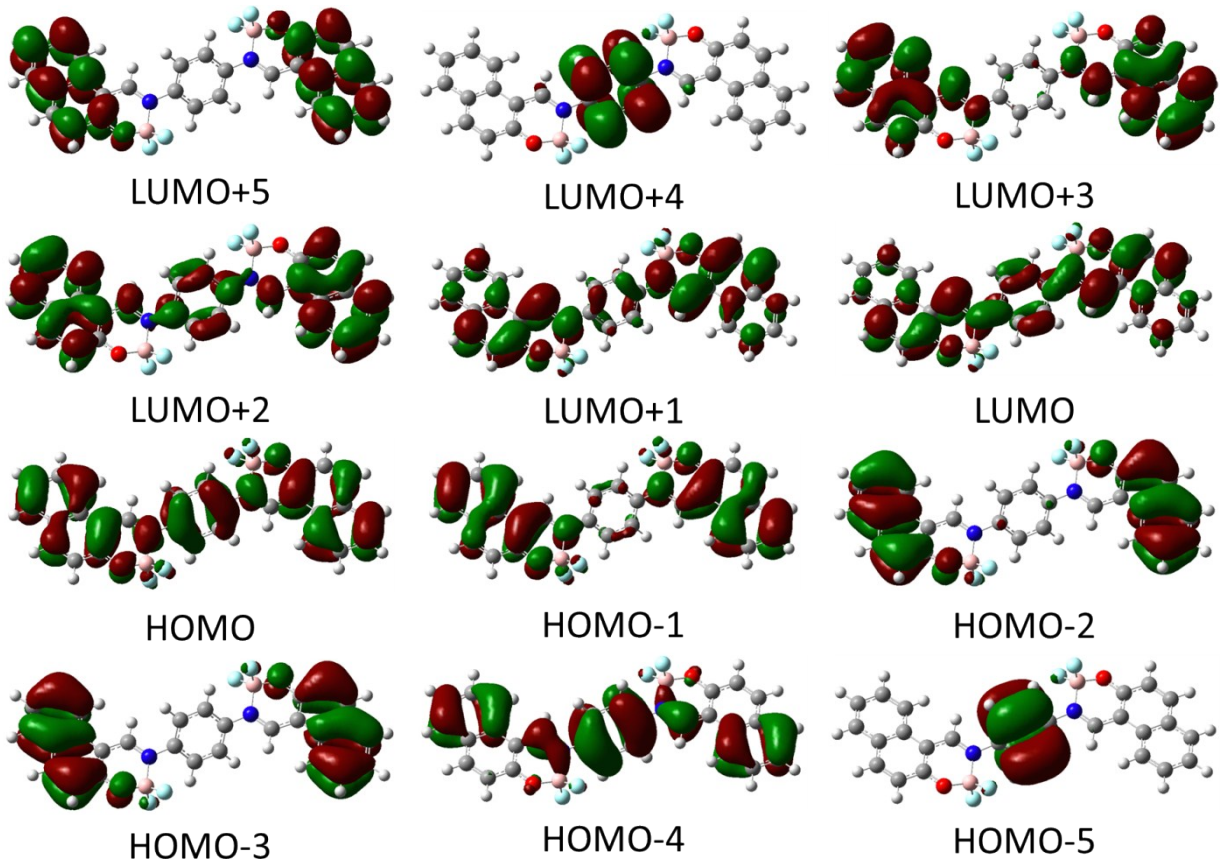


Figure S30: DFT predicted frontier orbital structures for **5.**

PCM-DFT optimized coordinates

Compound 1

F	-0.61230500	-2.13361900	-1.08434600
F	-0.51611700	-2.04655100	1.20868800
O	-2.52310500	-1.52192700	0.12601900
O	2.68940300	2.23419600	0.17566200
H	1.76247600	1.89366700	0.14682300
N	-0.57774100	0.04846500	-0.01330200
N	0.75463700	0.43454800	-0.00030900
C	-3.33832000	-0.47569000	0.04463800
C	-4.72563700	-0.67849400	0.06790000
H	-5.10493500	-1.69089300	0.14524700
C	-5.58036200	0.41197000	-0.00824100
H	-6.65213600	0.24287800	0.00917000
C	-5.08931900	1.72804600	-0.10693100
H	-5.77765200	2.56311700	-0.16421600
C	-3.72541100	1.94138400	-0.12758900
H	-3.32057300	2.94589000	-0.20026800
C	-2.83290600	0.84673300	-0.05392800
C	-1.42861300	1.04483500	-0.06103000
H	-1.00986700	2.04556000	-0.10621900
C	1.66044200	-0.49313800	-0.08396200
H	1.39893600	-1.54304300	-0.18557100
C	3.06291900	-0.15349300	-0.05462600
C	3.52759200	1.18496300	0.07230200
C	4.90401600	1.43981600	0.09297900
H	5.23728700	2.46711300	0.19068700

C	5.81061400	0.39274400	-0.00999600
H	6.87385800	0.60954900	0.00797100
C	5.37089600	-0.93378200	-0.13573100
H	6.08654700	-1.74410300	-0.21472800
C	4.01146000	-1.19459300	-0.15683600
H	3.65145000	-2.21472100	-0.25260800
B	-1.06449500	-1.48010600	0.06255000

Compound 2

F	-0.11222900	-2.19244100	1.35252100
F	-0.07694700	-2.38900600	-0.93375300
C	1.69865500	0.42338200	-0.01390500
H	1.58190200	1.49840600	-0.08146300
O	1.94466200	-2.32488400	0.24393500
C	3.03722500	-1.58294900	0.13951700
O	-1.81422700	2.77511600	0.35778500
H	-1.04157700	2.15421900	0.29342300
C	-6.77536200	-1.25012200	-0.35428200
H	-7.74124900	-1.73462800	-0.44981200
C	4.28604100	-2.24845800	0.18568800
H	4.29225800	-3.32639000	0.29666700
C	-1.72155900	-0.08111300	-0.02445200
H	-1.76792600	-1.15569900	-0.15544300
C	-5.35473900	2.15855800	0.17187000
H	-6.27724300	2.72848100	0.22772500
C	-4.35157200	-1.41153800	-0.31440300

H	-3.47308400	-2.04156700	-0.38675400
C	2.97591500	-0.18048700	-0.00024300
C	-2.94335000	2.06289000	0.22427400
C	-6.69024800	0.11067100	-0.15598900
H	-7.58920000	0.71682700	-0.09284500
C	4.22920100	1.99757700	-0.24811400
H	3.30947900	2.56951700	-0.29369600
C	-4.15104700	2.79779100	0.29451200
H	-4.08615000	3.86912400	0.44749300
N	0.57543200	-0.26158500	0.05740900
C	-4.22572100	-0.01383400	-0.10682600
C	5.43090000	2.67613000	-0.33799900
H	5.42449400	3.75547500	-0.44898400
C	-2.95258800	0.66452100	0.02990000
C	5.44529600	-1.52510000	0.09172200
H	6.40130400	-2.03855100	0.12780500
C	-5.59084300	-2.01034200	-0.43399700
H	-5.64870600	-3.08247500	-0.59220900
C	6.65778200	1.98583600	-0.28873300
H	7.59198800	2.53210200	-0.36125200
C	4.19791000	0.59143400	-0.10187500
C	5.44366800	-0.10578800	-0.05351100
C	-5.43299000	0.75143000	-0.03015200
C	6.65907400	0.61382300	-0.14870500
H	7.59437300	0.06367300	-0.10940500
B	0.56249000	-1.84493100	0.18470500
N	-0.56884600	0.51893400	0.07498700

Compound 3

B	-1.26810200	1.15143300	2.42087800
B	-1.25777900	-1.15987200	-2.42172600
C	0.78221500	2.35907100	1.71731200
C	1.96513800	3.01532700	2.14029200
H	2.16661300	3.07767400	3.20317400
C	2.81147600	3.55523000	1.20998100
H	3.71326300	4.06316700	1.53869400
C	2.55630400	3.46933000	-0.19167700
C	3.46020300	4.02644400	-1.12723500
H	4.34807500	4.53083200	-0.75786000
C	3.22162800	3.92795800	-2.48205300
H	3.91732600	4.35625800	-3.19558700
C	2.07005000	3.25589000	-2.93500600
H	1.88594400	3.16235500	-4.00032200
C	1.16857700	2.70370600	-2.04245000
H	0.30930100	2.17353300	-2.43561100
C	1.37855200	2.80392000	-0.64805500
C	0.47115800	2.25931700	0.34328500
C	-0.75675100	1.65440500	-0.00832900
H	-1.05454400	1.58190300	-1.04844100
C	-2.81585900	0.54706500	0.42924300
C	-4.03295400	1.08039600	0.86141400
H	-4.02027200	1.93526300	1.52409800
C	-5.23542600	0.52801300	0.43032000
H	-6.17219000	0.95751600	0.76766200
C	-5.23098700	-0.56560100	-0.43467100
H	-6.16424800	-1.00197100	-0.77289900
C	-4.02406900	-1.10913200	-0.86460700
H	-4.00447500	-1.96390200	-1.52724900

C	-2.81133600	-0.56683800	-0.43131300
C	-0.74474100	-1.65972900	0.00783700
H	-1.04414800	-1.58986400	1.04765700
C	0.48787600	-2.25552600	-0.34283000
C	1.39764100	-2.79506000	0.64910300
C	1.18416400	-2.69964000	2.04329900
H	0.31996900	-2.17718300	2.43595300
C	2.08821100	-3.24668800	2.93640200
H	1.90126700	-3.15700100	4.00155400
C	3.24591900	-3.90869300	2.48425000
H	3.94354400	-4.33312700	3.19821100
C	3.48788100	-4.00232700	1.12969200
H	4.38035300	-4.49899000	0.76093800
C	2.58145100	-3.45025600	0.19359500
C	2.83993100	-3.53119600	-1.20774700
H	3.74632500	-4.03129000	-1.53580900
C	1.99104300	-2.99618200	-2.13855800
H	2.19498300	-3.05479000	-3.20118300
C	0.80212300	-2.35026300	-1.71647800
F	-1.13861300	-0.18881600	2.82917900
F	-2.28724800	1.77311900	3.13549300
F	-1.14190100	0.18126200	-2.83109800
F	-2.27016300	-1.79270700	-3.13627400
N	-1.59404400	1.15718300	0.88051600
N	-1.58461000	-1.16786800	-0.88158400
O	-0.00783200	1.86620300	2.65519100
O	0.01004900	-1.86155000	-2.65482400

Compound 4

B	-2.33613700	-1.12701300	1.41743000
C	-4.79550000	-1.00438700	1.28498700
C	-6.03019900	-1.54637700	1.72047800
H	-6.01850400	-2.27590600	2.52172000
C	-7.19582500	-1.14755300	1.12339300
H	-8.13911600	-1.57099700	1.45496800
C	-7.21794200	-0.19231700	0.06300800
C	-8.43888300	0.18969500	-0.54246200
H	-9.36121800	-0.25615400	-0.18275200
C	-8.45917200	1.10894100	-1.57070600
H	-9.39753600	1.39786200	-2.03153700
C	-7.24861000	1.66748800	-2.02457500
H	-7.25843000	2.38460200	-2.83883900
C	-6.04149200	1.30998100	-1.45127100
H	-5.13256200	1.75238900	-1.84298700
C	-5.98964500	0.37907000	-0.38876900
C	-4.76130900	-0.03396200	0.25943700
C	-3.51361400	0.56602100	-0.02908500
H	-3.46048900	1.40995100	-0.70821000
C	-1.17690300	0.89402900	0.24935900
C	-1.17985100	2.29297600	0.26726800
H	-2.08616800	2.83601800	0.51094100
C	0.00000800	2.98285700	-0.00002700
H	0.00001200	4.06685200	-0.00004000
C	-0.00000200	0.18646100	0.00000900
H	-0.00000600	-0.89507100	0.00002300
F	-1.50629200	-0.89658100	2.50663900
F	-1.87014700	-2.20415400	0.65218100

N	-2.37973300	0.16273000	0.50585200
O	-3.69633200	-1.40870900	1.90059700
B	2.33612800	-1.12706500	-1.41737800
C	4.79549100	-1.00443200	-1.28495800
C	6.03018800	-1.54643100	-1.72044600
H	6.01848700	-2.27598300	-2.52166700
C	7.19581800	-1.14758700	-1.12338400
H	8.13910800	-1.57103800	-1.45495600
C	7.21794300	-0.19231800	-0.06302800
C	8.43889000	0.18971400	0.54241900
H	9.36122200	-0.25614400	0.18271400
C	8.45918600	1.10899100	1.57063500
H	9.39755400	1.39792800	2.03144800
C	7.24862700	1.66754900	2.02449900
H	7.25845400	2.38468800	2.83874100
C	6.04150400	1.31002200	1.45121800
H	5.13257800	1.75244000	1.84292900
C	5.98964900	0.37907800	0.38874400
C	4.76130800	-0.03397800	-0.25943700
C	3.51361400	0.56601000	0.02908100
H	3.46049400	1.40996300	0.70817800
C	1.17690400	0.89401500	-0.24936000
C	1.17986200	2.29296100	-0.26730400
H	2.08618300	2.83599000	-0.51099000
F	1.50627300	-0.89666500	-2.50658700
F	1.87014700	-2.20418700	-0.65209700
N	2.37973000	0.16270300	-0.50583600
O	3.69631900	-1.40877300	-1.90054800

Compound 5

B	2.31959700	-2.37074800	1.96840400
C	0.49997200	-2.76447000	4.18782600
C	1.60519200	-3.61640000	3.96860800
C	1.92053200	-4.63973400	4.89606900
H	2.76392200	-5.28597500	4.68298900
C	1.16929200	-4.78238400	6.03138300
H	1.41923600	-5.56170100	6.74497500
C	0.06232300	-3.92951000	6.32102800
C	-0.68428200	-4.09398100	7.51194500
H	-0.39892900	-4.88299600	8.20109500
C	-1.75268400	-3.26872400	7.79436600
H	-2.32153300	-3.39859000	8.70867000
C	-2.09867700	-2.24860900	6.88701700
H	-2.93387000	-1.59207600	7.10804600
C	-1.38364200	-2.06442900	5.71704300
H	-1.67377700	-1.25618400	5.05525000
C	-0.28989700	-2.90024800	5.39544500
C	0.15794600	-1.86086200	3.15486500
H	-0.76204600	-1.28972900	3.21548500
C	0.44054600	-0.83295800	1.02887900
C	-0.89991600	-0.86035300	0.62724800
H	-1.59309100	-1.56089000	1.07969600
C	1.34238700	0.02558200	0.39136100
H	2.37320300	0.06654400	0.71905300
F	2.51284700	-2.81827200	0.66850900
F	3.30448500	-1.44207000	2.33063100
N	0.90360600	-1.67606500	2.08420800

O	2.35475700	-3.52143000	2.88180600
B	-2.31959700	2.37074800	-1.96840400
C	-0.49997200	2.76447000	-4.18782600
C	-1.60519200	3.61640000	-3.96860800
C	-1.92053200	4.63973400	-4.89606900
H	-2.76392200	5.28597500	-4.68298900
C	-1.16929200	4.78238400	-6.03138300
H	-1.41923600	5.56170100	-6.74497500
C	-0.06232300	3.92951000	-6.32102800
C	0.68428200	4.09398100	-7.51194500
H	0.39892900	4.88299600	-8.20109500
C	1.75268400	3.26872400	-7.79436600
H	2.32153300	3.39859000	-8.70867000
C	2.09867700	2.24860900	-6.88701700
H	2.93387000	1.59207600	-7.10804600
C	1.38364200	2.06442900	-5.71704300
H	1.67377700	1.25618400	-5.05525000
C	0.28989700	2.90024800	-5.39544500
C	-0.15794600	1.86086200	-3.15486500
H	0.76204600	1.28972900	-3.21548500
C	-0.44054600	0.83295800	-1.02887900
C	0.89991600	0.86035300	-0.62724800
H	1.59309100	1.56089000	-1.07969600
C	-1.34238700	-0.02558200	-0.39136100
H	-2.37320300	-0.06654400	-0.71905300
F	-2.51284700	2.81827200	-0.66850900
F	-3.30448500	1.44207000	-2.33063100
N	-0.90360600	1.67606500	-2.08420800
O	-2.35475700	3.52143000	-2.88180600

PCM-TDDFT expansion coefficients

Compound 1

Excited State 1: Singlet-A 2.8435 eV 436.03 nm f=0.0182 <S**2>=0.000

73 -> 75 0.10520

74 -> 75 0.69179

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1024.95228129

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1415 eV 394.67 nm f=0.1076 <S**2>=0.000

73 -> 75 0.69142

74 -> 75 -0.10120

Excited State 3: Singlet-A 3.5588 eV 348.39 nm f=0.6281 <S**2>=0.000

72 -> 75 0.69143

Excited State 4: Singlet-A 4.0915 eV 303.03 nm f=0.0700 <S**2>=0.000

70 -> 75 -0.26514

71 -> 75 -0.39886

74 -> 76 0.50884

Excited State 5: Singlet-A 4.1664 eV 297.58 nm f=0.0178 <S**2>=0.000

70 -> 75 0.61149

74 -> 76 0.33904

Excited State 6: Singlet-A 4.3922 eV 282.28 nm f=0.0629 <S**2>=0.000

70 -> 75 -0.10262

71 -> 75 0.19931

73 -> 76 0.63804

74 -> 76 0.11161

Excited State 7: Singlet-A 4.5090 eV 274.97 nm f=0.0370 <S**2>=0.000

70 -> 75 -0.19415

71 -> 75 0.46582

72 -> 76 0.33801

73 -> 76 -0.25088

74 -> 76 0.23985

Excited State 8: Singlet-A 5.0241 eV 246.78 nm f=0.0256 <S**2>=0.000

71 -> 75 -0.18888

72 -> 76 0.47210

74 -> 76 -0.17774

74 -> 77 -0.37652

74 -> 78 0.21330

Compound 2

Excited State 1: Singlet-A 2.7600 eV 449.21 nm f=0.7237 <S**2>=0.000

99 ->101 0.10201

100 ->101 0.69304

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1332.33834210

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0113 eV 411.73 nm f=0.1021 <S**2>=0.000

99 ->101 0.66967

100 ->102 -0.19286

Excited State 3: Singlet-A 3.1667 eV 391.53 nm f=0.0222 <S**2>=0.000

98 ->101 0.69619

Excited State 4: Singlet-A 3.3097 eV 374.61 nm f=0.0786 <S**2>=0.000

97 ->101 0.69330

Excited State 5: Singlet-A 3.5713 eV 347.17 nm f=0.0220 <S**2>=0.000

94 ->101 -0.11012

99 ->101 0.18347

100 ->102 0.65976

Excited State 6: Singlet-A 3.9658 eV 312.63 nm f=0.2502 <S**2>=0.000

96 ->101 0.10684

99 ->102 0.61891

100 ->103 0.30166

Excited State 7: Singlet-A 4.0166 eV 308.68 nm f=0.0793 <S**2>=0.000

95 ->101 0.25773

96 ->101 0.59057

99 ->102 -0.19562

100 ->103 0.19147

Excited State 8: Singlet-A 4.1001 eV 302.39 nm f=0.0385 <S**2>=0.000

95 ->101 -0.42752

98 ->102 -0.24623

99 ->102 -0.16858

100 ->103 0.42980

100 ->106 0.14086

Excited State 9: Singlet-A 4.1240 eV 300.64 nm f=0.082 <S**2>=0.000

95 ->101 0.49311

96 ->101 -0.32410

98 ->102 -0.23508

100 ->103 0.25336

100 ->106 0.10546

Excited State 10: Singlet-A 4.1798 eV 296.63 nm f=0.0070 <S**2>=0.000

96 ->101 -0.13369

97 ->102 -0.11063

98 ->102 0.52808

99 ->102 -0.12179

100 ->103 0.30438

100 ->104 -0.13291

100 ->106 -0.20246

Excited State 11: Singlet-A 4.3010 eV 288.27 nm f=0.0028 <S**2>=0.000

97 ->102 0.61809

100 ->103 0.12718

100 ->105 -0.26872

Excited State 12: Singlet-A 4.4538 eV 278.38 nm f=0.0124 <S**2>=0.000

94 ->101 -0.13828

96 ->102 0.11710

98 ->102 0.10900

100 ->104 0.65198

Excited State 13: Singlet-A 4.5687 eV 271.38 nm f=0.0442 <S**2>=0.000

97 ->102 0.25758

97 ->103 -0.21445

99 ->103 -0.28875

100 ->105 0.52717

Excited State 14: Singlet-A 4.6836 eV 264.72 nm f=0.0223 <S**2>=0.000

97 ->105 -0.10215

98 ->103 0.16077

99 ->103 0.51696

99 ->105 0.14071

100 ->105 0.28071

100 ->106 0.23203

Excited State 15: Singlet-A 4.7710 eV 259.87 nm f=0.0434 <S**2>=0.000

94 ->101 0.22792

98 ->102 0.15522

98 ->103 0.36170

98 ->104 0.11648

99 ->103 -0.21774

99 ->104 0.12973

100 ->106 0.39893

Compound 3

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8387 eV 436.77 nm f=0.0104 <S**2>=0.000

130 ->133 -0.41738

131 ->132 0.56993

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1787.66073268

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.8486 eV 435.24 nm f=0.0010 <S**2>=0.000

130 ->132 -0.49031

131 ->133 0.50890

Excited State 3: Singlet-A 3.0613 eV 405.00 nm f=0.1597 <S**2>=0.000

130 ->132 0.50175

131 ->133 0.48258

Excited State 4: Singlet-A 3.1874 eV 388.98 nm f=0.3218 <S**2>=0.000

130 ->133 0.56271

131 ->132 0.40853

Excited State 5: Singlet-A 3.3712 eV 367.77 nm f=0.0038 <S**2>=0.000

128 ->133 0.29784

129 ->132 0.63923

Excited State 6: Singlet-A 3.3733 eV 367.54 nm f=0.0107 <S**2>=0.000

128 ->132 0.62392

129 ->133 0.32890

Excited State 7: Singlet-A 3.4657 eV 357.74 nm f=0.0496 <S**2>=0.000

128 ->133 0.63229

129 ->132 -0.28446

Excited State 8: Singlet-A 3.4755 eV 356.74 nm f=0.2952 <S**2>=0.000

128 ->132 -0.31113

129 ->133 0.61398

Excited State 9: Singlet-A 3.8290 eV 323.80 nm f=0.0300 <S**2>=0.000

126 ->133 0.17978

127 ->132 0.68029

Excited State 10: Singlet-A 3.8558 eV 321.55 nm f=0.0092 <S**2>=0.000

126 ->132 0.66193

127 ->133 -0.24058

Excited State 11: Singlet-A 3.8882 eV 318.88 nm f=0.0175 <S**2>=0.000

126 ->132 0.24225

127 ->133 0.66029

Excited State 12: Singlet-A 3.9390 eV 314.76 nm f=0.0754 <S**2>=0.000

126 ->133 0.67826

127 ->132 -0.17427

Excited State 13: Singlet-A 4.3645 eV 284.08 nm f=0.0042 <S**2>=0.000

130 ->135 -0.23763

131 ->134 0.65551

Excited State 14: Singlet-A 4.3873 eV 282.60 nm f=0.0054 <S**2>=0.000

130 ->134 -0.32201

131 ->135 0.62387

Excited State 15: Singlet-A 4.4459 eV 278.87 nm f=0.0356 <S**2>=0.000

128 ->134 -0.11452

128 ->138 0.10193

129 ->135 0.10941

129 ->139 0.10028

130 ->134 0.59074

131 ->135 0.27841

131 ->139 -0.11078

Compound 4

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8881 eV 429.29 nm f=0.0057 <S**2>=0.000

130 ->132 0.54399

131 ->133 -0.44962

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1787.66363555

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.9016 eV 427.30 nm f=0.0086 <S**2>=0.000

130 ->133 -0.38200

131 ->132 0.59407

Excited State 3: Singlet-A 3.0186 eV 410.74 nm f=0.8165 <S**2>=0.000

130 ->132 0.44464

131 ->133 0.53907

Excited State 4: Singlet-A 3.1536 eV 393.15 nm f=0.0482 <S**2>=0.000

130 ->133 0.58760

131 ->132 0.37415

Excited State 5: Singlet-A 3.4171 eV 362.83 nm f=0.0987 <S**2>=0.000

128 ->132 0.69484

Excited State 6: Singlet-A 3.4173 eV 362.81 nm f=0.0114 <S**2>=0.000

129 ->132 0.69715

Excited State 7: Singlet-A 3.4892 eV 355.34 nm f=0.2756 <S**2>=0.000

129 ->133 0.69544

Excited State 8: Singlet-A 3.4959 eV 354.66 nm f=0.0125 <S**2>=0.000

128 ->133 0.69687

Excited State 9: Singlet-A 3.8584 eV 321.34 nm f=0.0110 <S**2>=0.000

126 ->132 0.60810

127 ->133 0.34893

Excited State 10: Singlet-A 3.9008 eV 317.85 nm f=0.0259 <S**2>=0.000

127 ->132 0.69473

Excited State 11: Singlet-A 3.9147 eV 316.72 nm f=0.1036 <S**2>=0.000

126 ->132 -0.34238

127 ->133 0.60604

Excited State 12: Singlet-A 3.9813 eV 311.41 nm f=0.0010 <S**2>=0.000

126 ->133 0.69699

Excited State 13: Singlet-A 4.3870 eV 282.62 nm f=0.0002 <S**2>=0.000

131 ->134 0.66849

Excited State 14: Singlet-A 4.3935 eV 282.20 nm f=0.1431 <S**2>=0.000

128 ->134 -0.10214

130 ->134 -0.17921

131 ->135 0.63920

Excited State 15: Singlet-A 4.4056 eV 281.43 nm f=0.0307 <S**2>=0.000

130 ->134 0.65049

131 ->135 0.22724

Compound 5

Excitation energies and oscillator strengths:

Excited State 1: Singlet-AU 2.6752 eV 463.46 nm f=0.0194 <S**2>=0.000

131 ->132 0.58911

131 ->133 0.38941

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1787.67194076

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-AG 2.8892 eV 429.13 nm f=0.8194 <S**2>=0.000

131 ->132 0.70434

Excited State 3: Singlet-AG 3.1582 eV 392.58 nm f=0.0000 <S**2>=0.000

130 ->132 -0.38162

131 ->133 0.58262

Excited State 4: Singlet-AU 3.2554 eV 380.85 nm f=0.0509 <S**2>=0.000

129 ->132 0.43429

130 ->133 0.55031

Excited State 5: Singlet-AG 3.3018 eV 375.51 nm f=0.0000 <S**2>=0.000

128 ->132 0.69941

Excited State 6: Singlet-AU 3.3089 eV 374.70 nm f=0.0564 <S**2>=0.000

129 ->132 0.54921

130 ->133 -0.42949

Excited State 7: Singlet-AG 3.6313 eV 341.43 nm f=0.0000 <S**2>=0.000

129 ->133 0.69621

Excited State 8: Singlet-AU 3.6413 eV 340.49 nm f=0.0933 <S**2>=0.000

128 ->133 0.69535

Excited State 9: Singlet-AU 3.6872 eV 336.25 nm f=0.2824 <S**2>=0.000

127 ->132 0.69469

Excited State 10: Singlet-AU 3.9035 eV 317.63 nm f=0.0105 <S**2>=0.000

126 ->132 0.69128

131 ->136 -0.12446

Excited State 11: Singlet-AG 3.9909 eV 310.67 nm f=0.0000 <S**2>=0.000

127 ->133 0.69616

Excited State 12: Singlet-AG 4.2097 eV 294.52 nm f=0.0000 <S**2>=0.000

126 ->133 0.70480

Excited State 13: Singlet-AU 4.2545 eV 291.42 nm f=0.1115 <S**2>=0.000

131 ->134 0.68309

Excited State 14: Singlet-AG 4.3860 eV 282.68 nm f=0.0000 <S**2>=0.000

125 ->132 0.17486

131 ->135 0.66163

Excited State 15: Singlet-AG 4.4846 eV 276.47 nm f=0.0000 <S**2>=0.000

128 ->134 0.11490

130 ->134 0.64946

131 ->137 0.15314

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(S1) Gaussian 09, Revision B.0.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.