FLP Reduction and Hydroborations of Phenanthrene *o*-Iminoquinones and α-Diimines

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Supporting Information

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Characterization

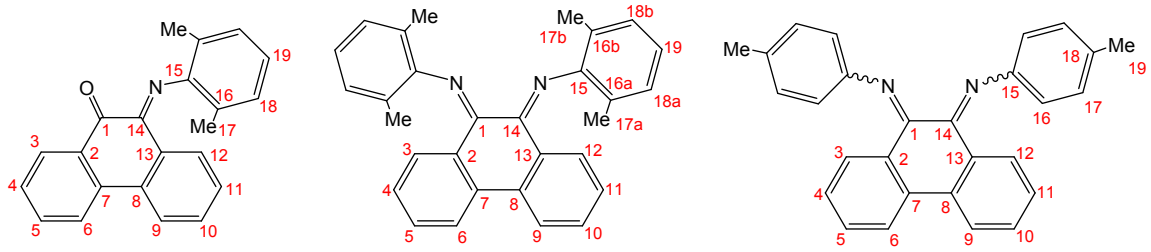


Figure S1. Numbering used for phenanthrene-based *o*-iminoquinone and α-diimine ligands.

N-(2,6-dimethylphenyl)-phenanthren-*o*-iminoquinone-derived products

Compound 2 : $C_{14}H_8O(NC_6H_3Me_2)B(C_6F_5)_3$

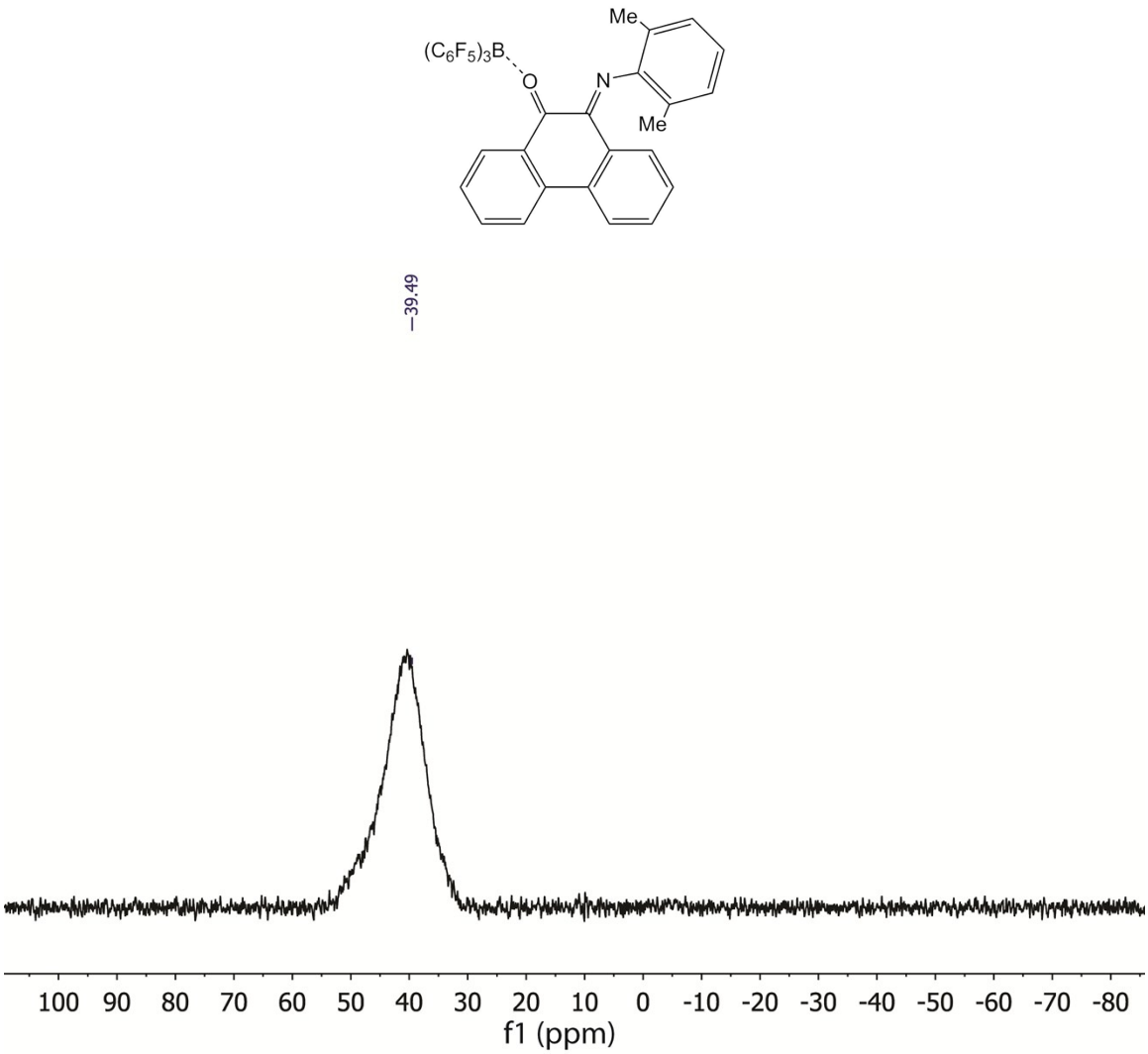


Figure S2. ^{11}B NMR spectrum of crude compound **2** in toluene-d8 at 298 K.

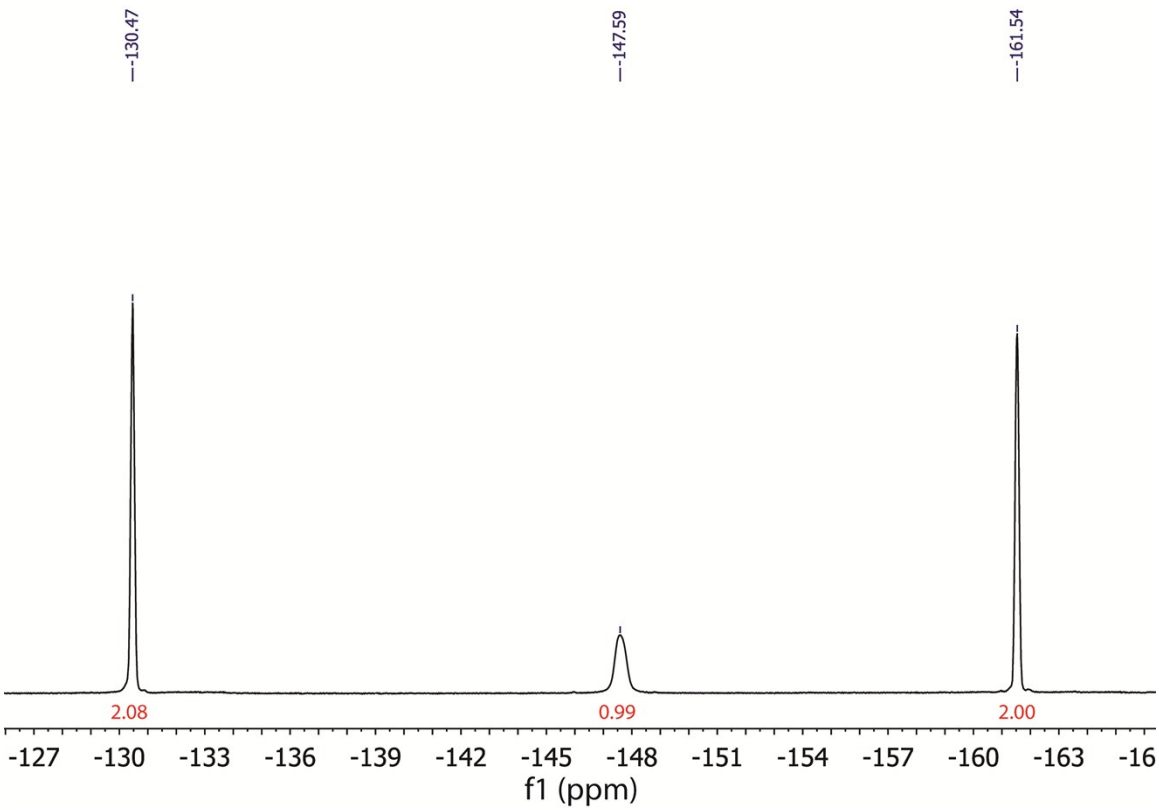
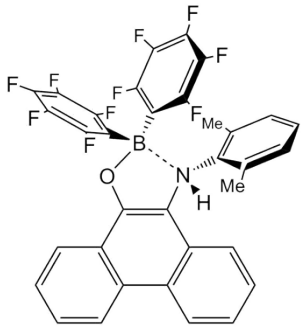


Figure S3. ^{19}F NMR spectrum of crude compound **2** in toluene-d8 at 298 K.

Compound 3 : $C_{14}H_8O(NHC_6H_3Me_2)B(C_6F_5)_2$

Over the course of ~ 1 h in solution a significant amount of compound **5** is produced and hence publication quality ^1H and $^{13}C\{^1H\}$ NMR data could not be obtained.



NMR data in toluene-d8 : ^{11}B NMR (128 MHz, 298 K): δ 10.4 (br s); ^{19}F NMR (377 MHz, 298 K): δ -131.4 (br s, 2F, *o*-C_6F_5), -136.8 (br s, 2F, *o*-C_6F_5), -154.7 (br s, 2F, *p*-C_6F_5), -161.6 (br s, 2F, *m*-C_6F_5), -163.4 (br s, 2F, *m*-C_6F_5).

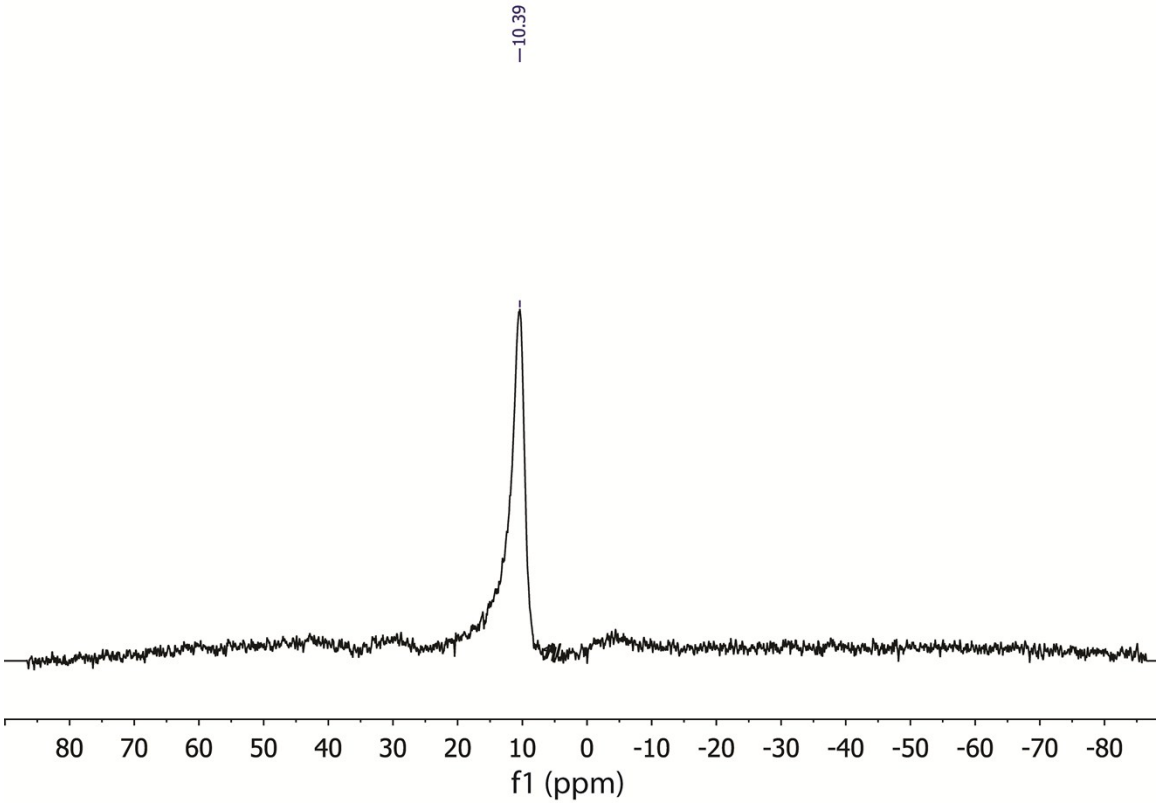


Figure S4. ^{11}B NMR spectrum of compound **3** (from method 2 preparation) in toluene-d8 at 298 K.

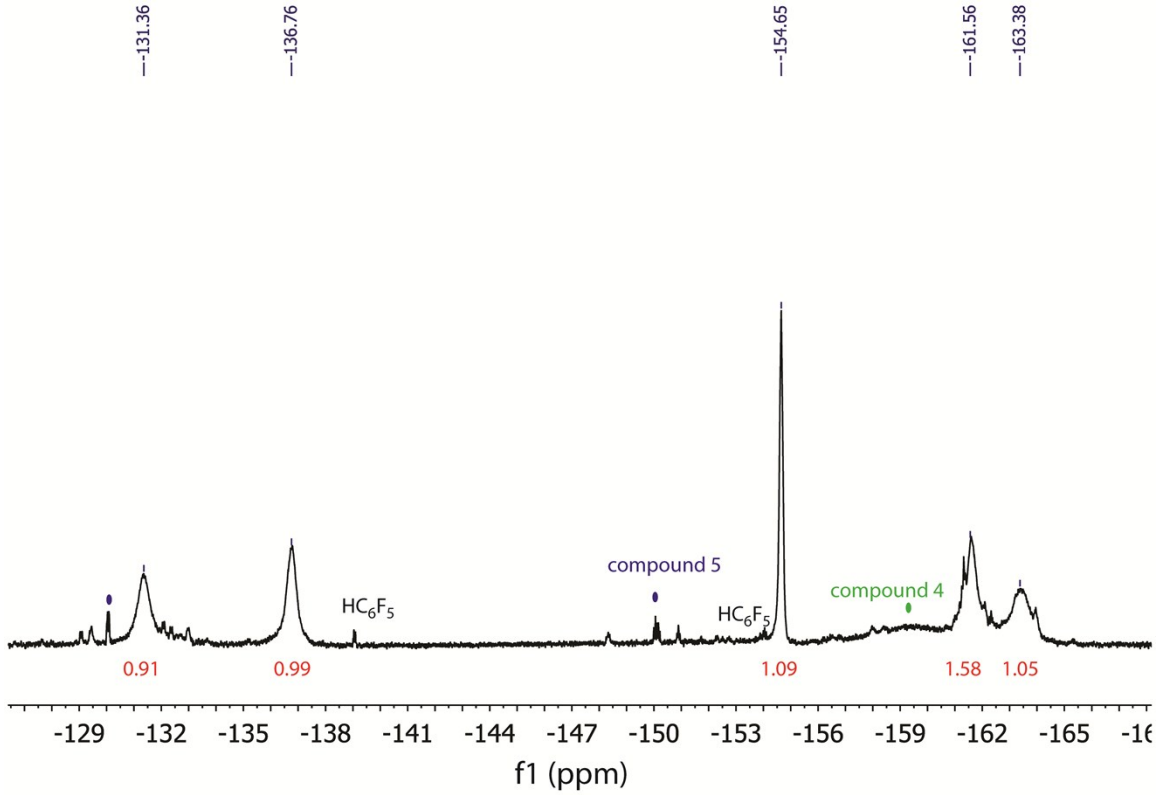


Figure S5. ^{19}F NMR spectrum of compound **3** (from method 2 preparation) in toluene-d8 at 298 K.

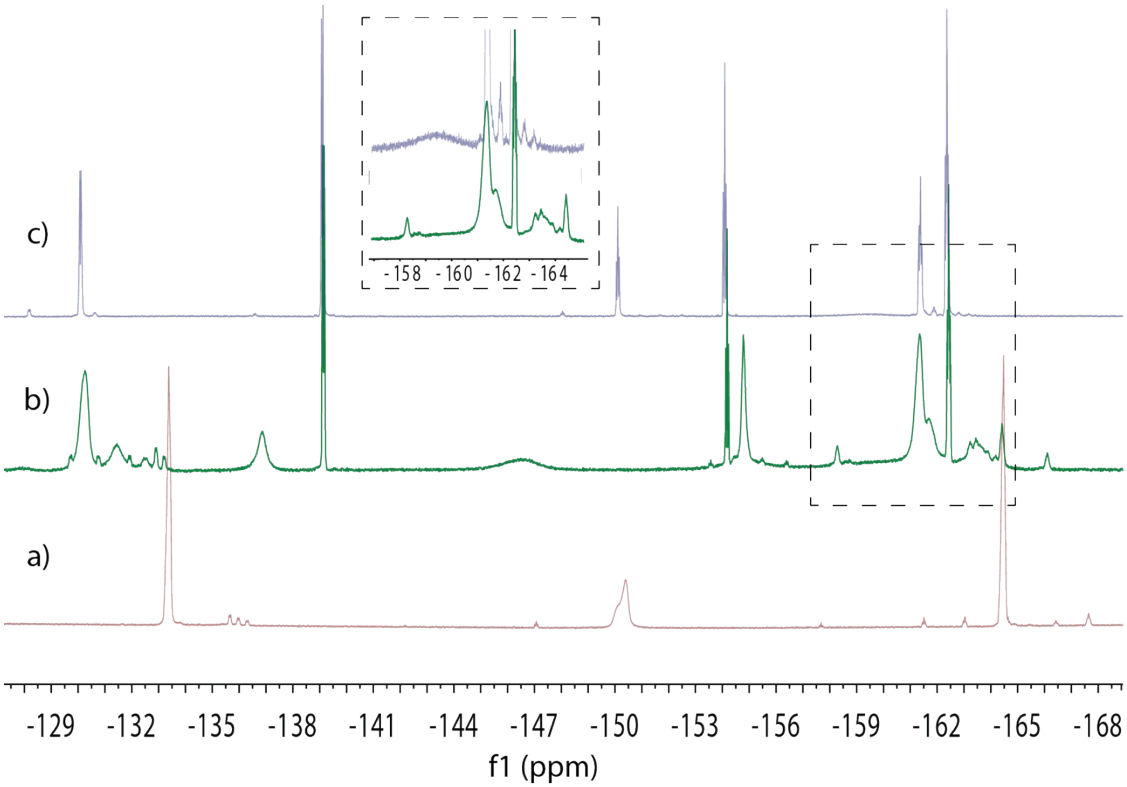
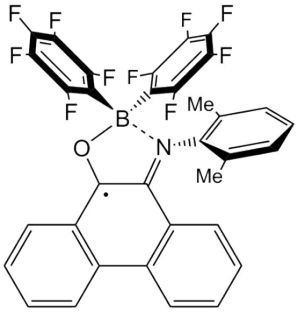


Figure S6. ^{19}F NMR spectra collected at 298K of: a) solution of compound **1**and $B(C_6F_5)_3$; b) solution of compound 1 and $B(C_6F_5)_3$ under 4 atm H_2 heated for **1** h at 100 ºC; and, c) solution of compound **1** and $B(C_6F_5)_3$ under 4 atm H_2 heated for 3 h at 100 ºC (solvent: toluene-d8).

Compound 4 : $[C_{14}H_8O(NC_6H_3Me_2)B(C_6F_5)_2]^{\bullet}$



NMR data in toluene-d8: ^1H NMR (400 MHz, 298 K): NMR silent; ^{19}F NMR (377 MHz, 298 K): δ -159.9 (br s, C_6F_5); ^{11}B NMR (128 MHz, 298 K): NMR silent; $^{13}C\{^1H\}$ NMR (101 MHz, 298 K): NMR silent.

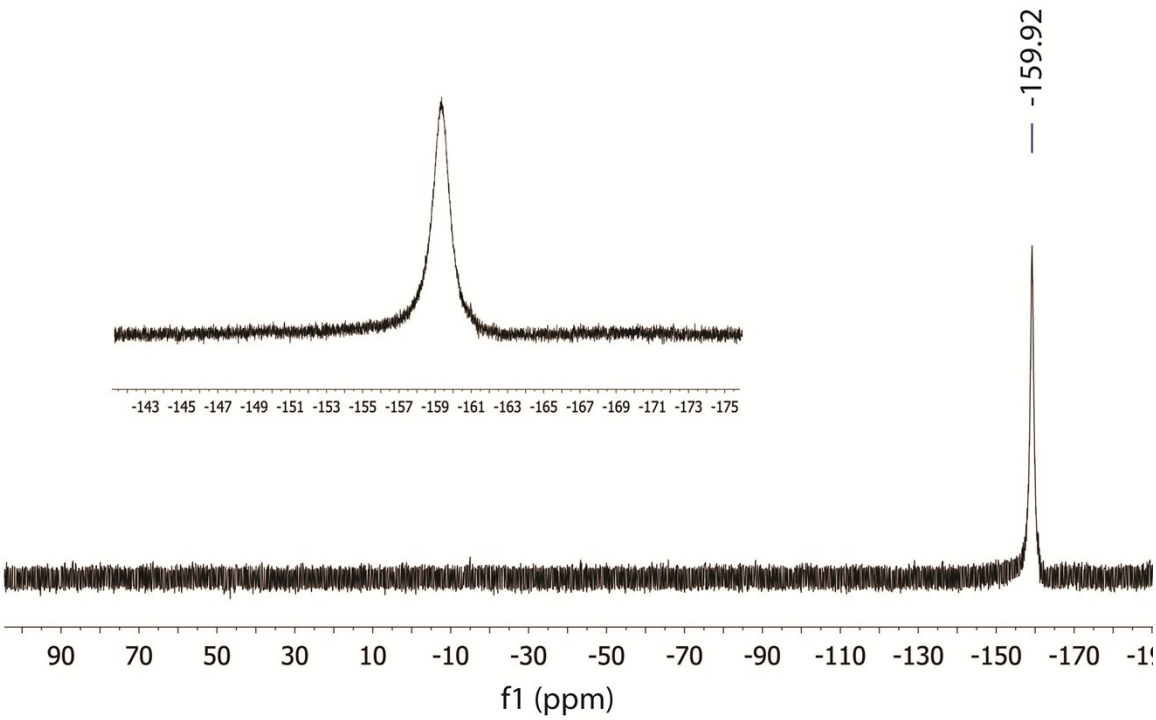
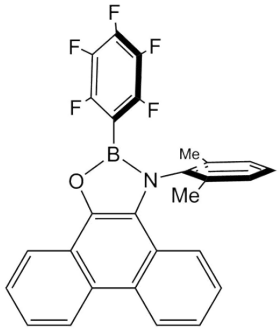


Figure S7. ^{19}F NMR spectrum of **4** in toluene-d8 at 298 K.

Compound 5 : $C_{14}H_8O(NC_6H_3Me_2)BC_6F_5$



NMR data in toluene-d8 : ^{11}B NMR (128 MHz, 298 K): δ 28.6 (br s); ^{19}F NMR (377 MHz, 298 K): δ -130.1 (m, 2F, *o*-C_6F_5), -150.1 (t, $^3J_{FF}$ = 20.6 Hz, 1F, *p*-C_6F_5), -161.3 − -161.5 (m, 2F, *m*-C_6F_5).

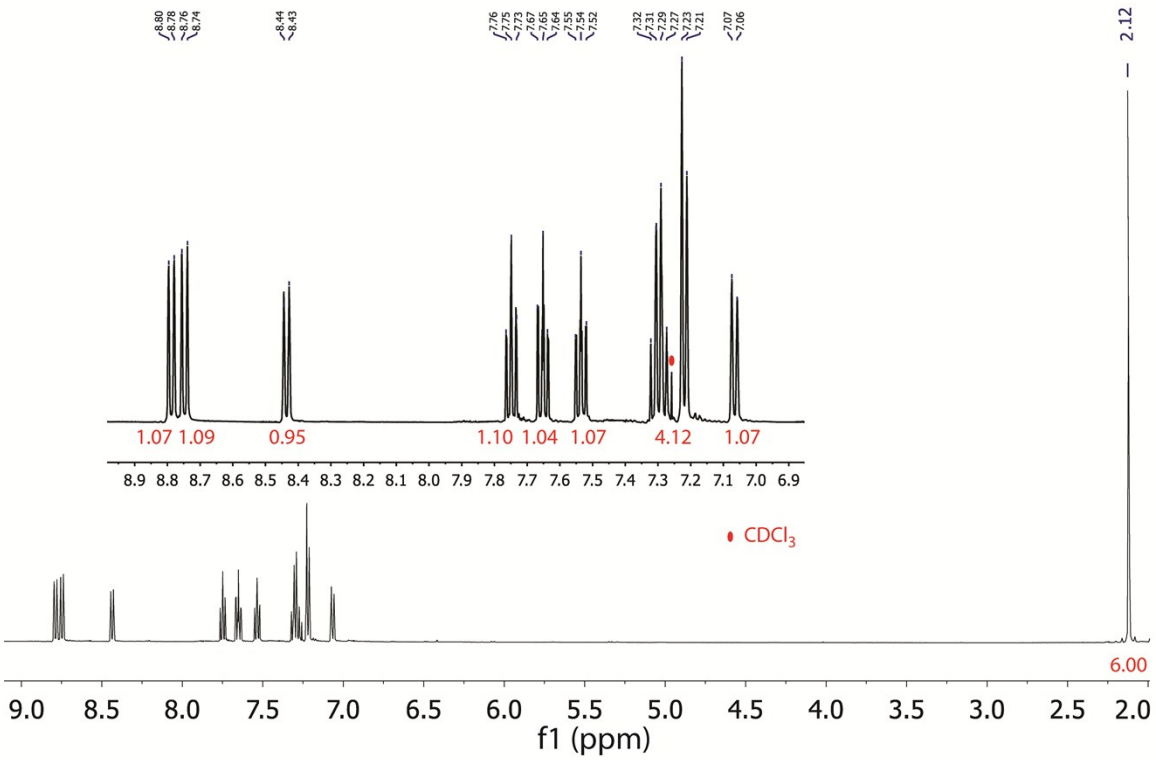


Figure S8. ^{1}H NMR spectrum of **5** in $CDCl_3$ at 298 K.

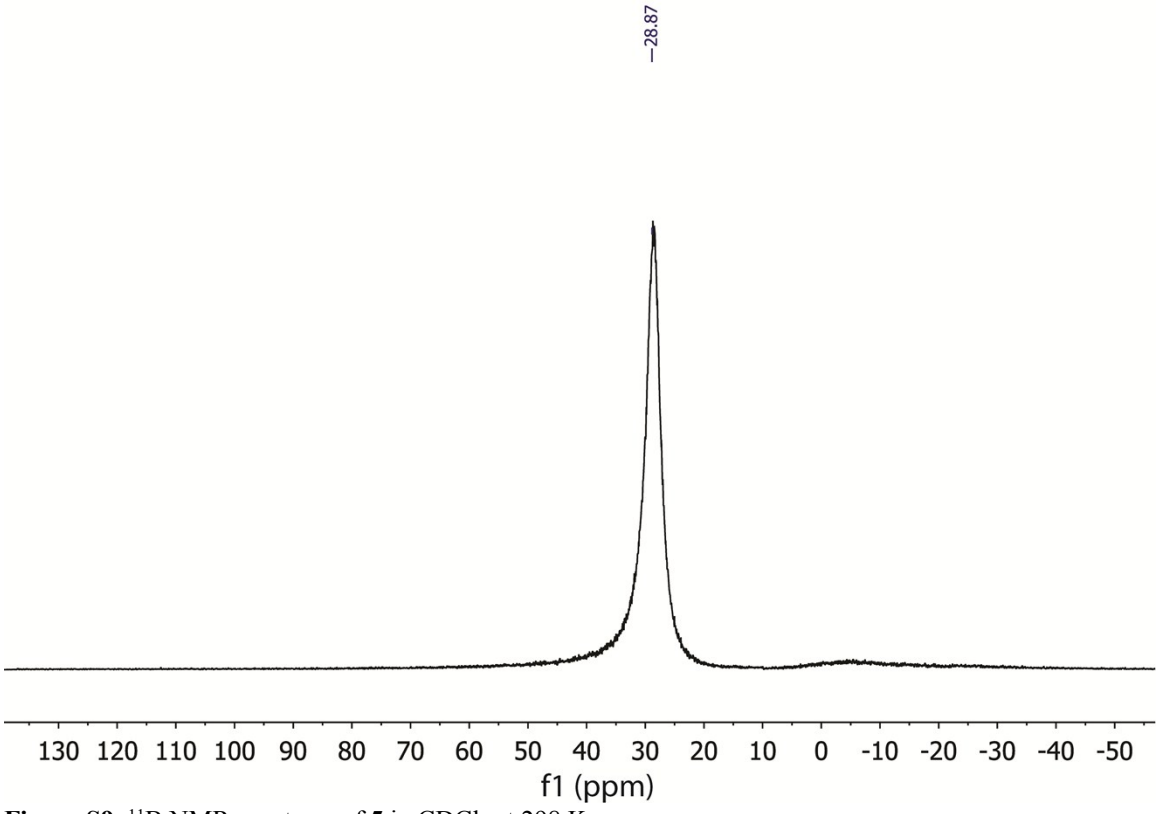


Figure S9. ^{11}B NMR spectrum of **5** in $CDCl_3$ at 298 K.

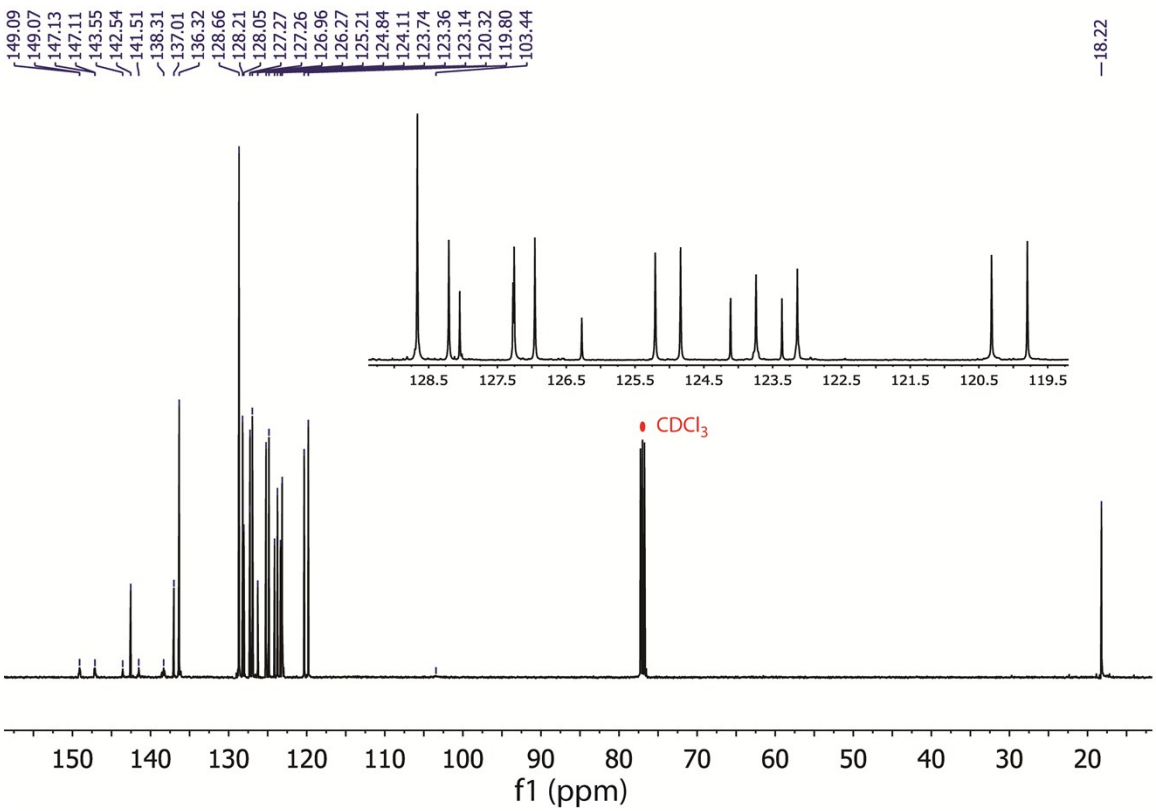


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in $CDCl_3$ at 298 K.

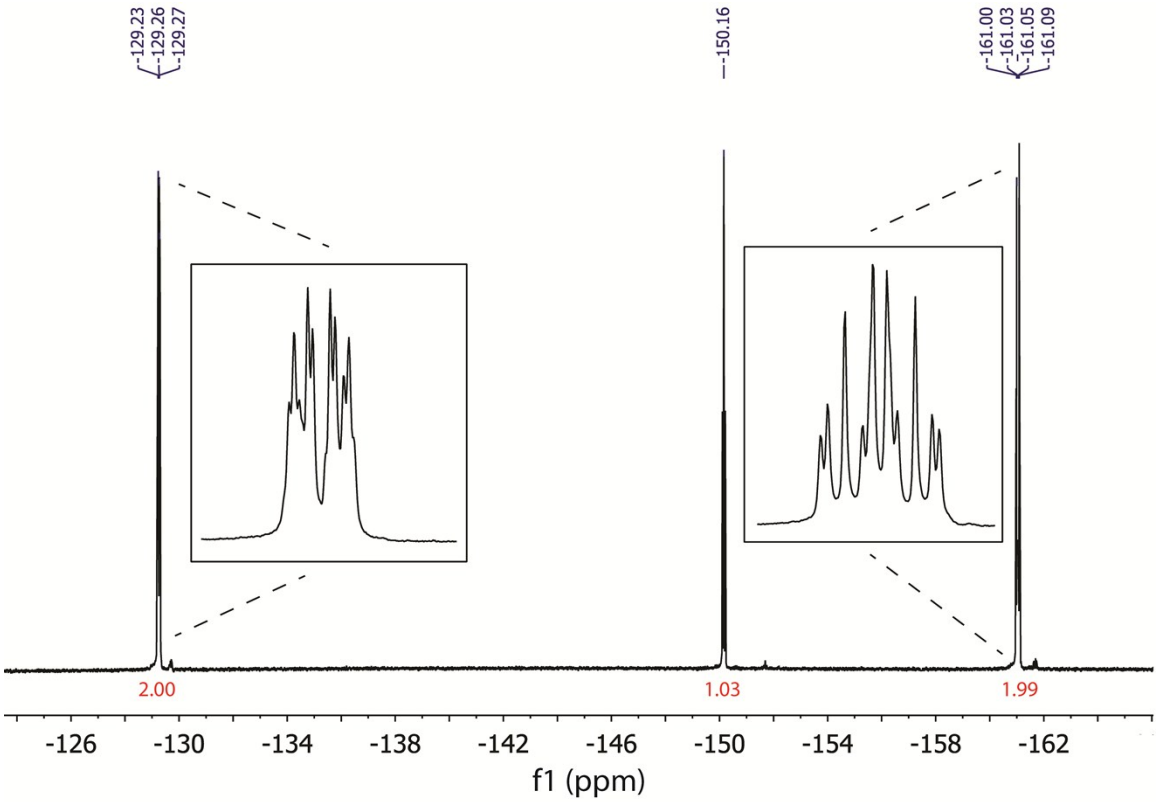
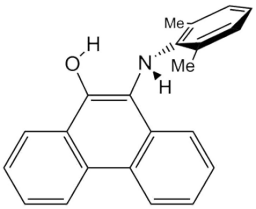


Figure S11. ^{19}F NMR spectrum of **5** in $CDCl_3$ at 298 K.

Compound 6 - $C_{14}H_8OH(NHC_6H_3Me_2)$



NMR data in toluene-d8 : ^{1}H NMR (400 MHz, 298 K): 8.58 (d, $^3J_{H\text{-}H}$ = 7.5 Hz, 1H, H_3), 8.45-8.38 (m, 2H, H_6 & H_9), 7.53-7.40 (m, 3H, H_4 & H_5 & H_{12}), 7.26-7.13 (m, 2H, H_{10} & H_{11}), 6.81 (d, $^3J_{H\text{-}H}$ = 7.4 Hz, 2H, H_{18}), 6.74 (t, $^3J_{H\text{-}H}$ = 7.3 Hz, 1H, H_{19}), 1.82 (s, 3H, H_{17}).

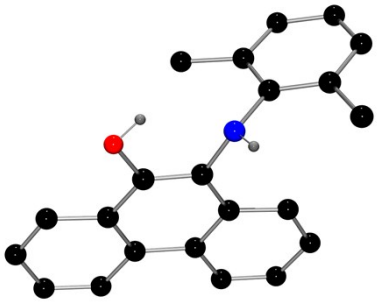


Figure S12. POV-ray depiction of compound **6**. Most H atoms have been omitted for clarity. Atom colour scheme: H: grey, C: black, N: blue, O: red.

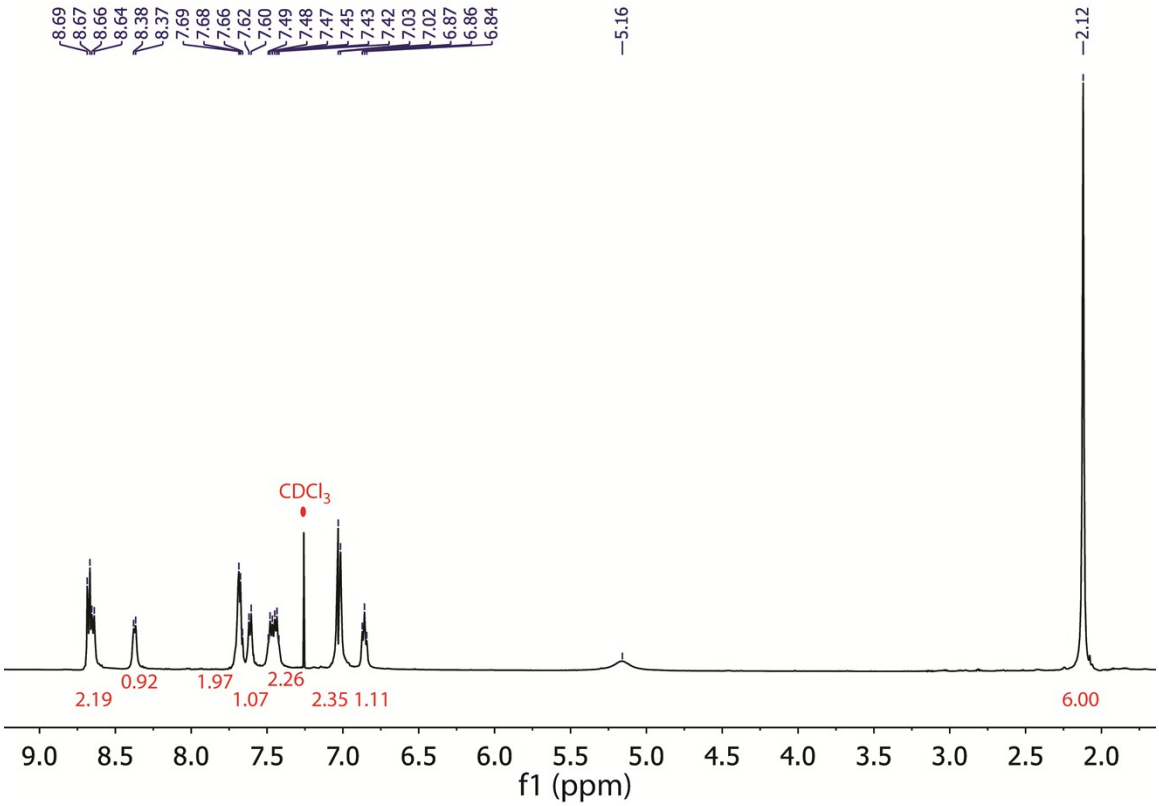


Figure S13. ^{1}H NMR spectrum of **6** in $CDCl_3$ at 298 K.

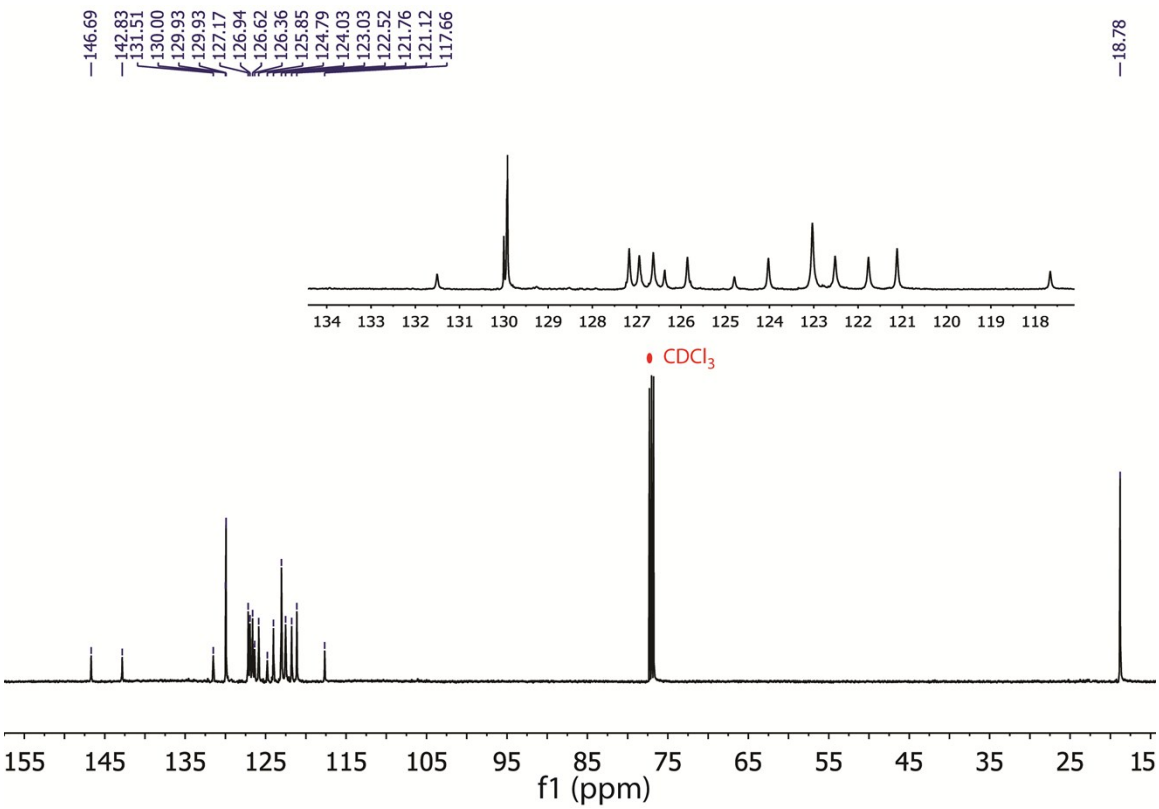


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$ at 298 K.

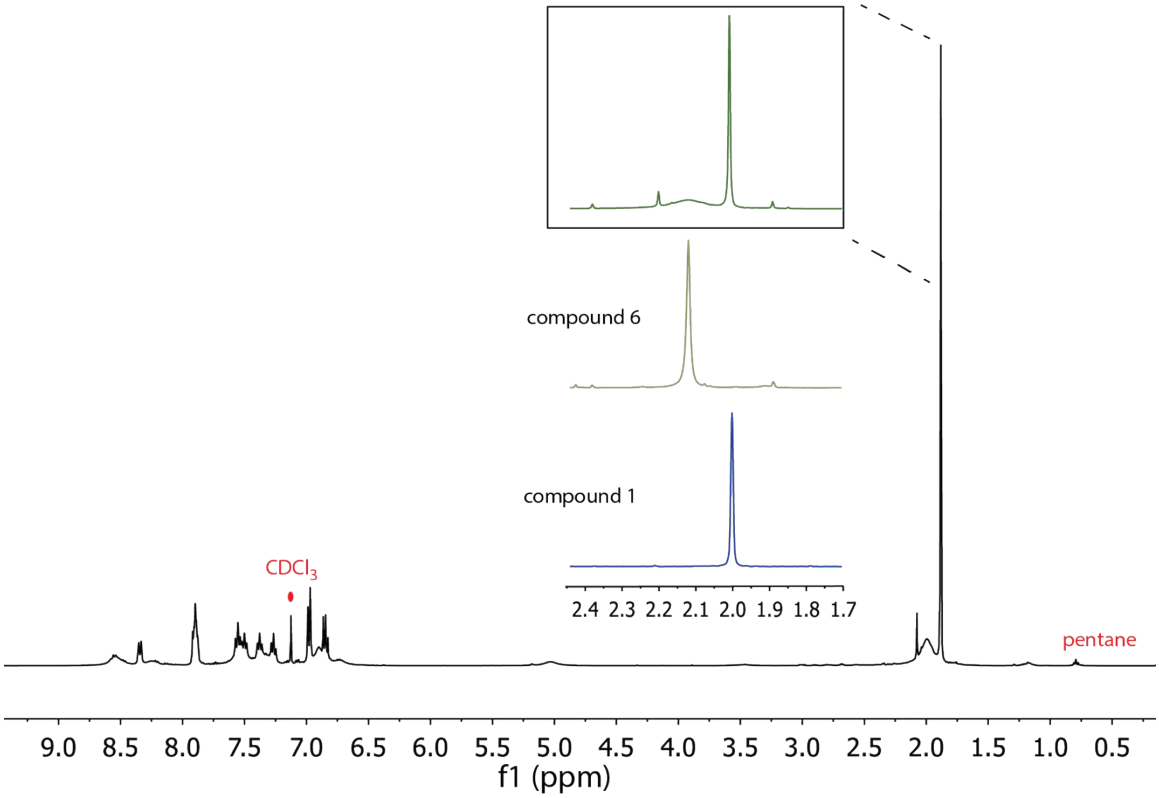


Figure S15. ^{1}H NMR spectrum of equilibrium between compounds **1** and **6** in $CDCl_3$ at 298 K (dark green coloured solution).

***N*,*N*'-(2,6-dimethylphenyl)-phenanthrene-9,10-diimine-derived products**

Compound 8 : $C_{14}H_8(NC_6H_3Me_2)(N(C_6H_3Me_2)B(C_6F_5)_3)$

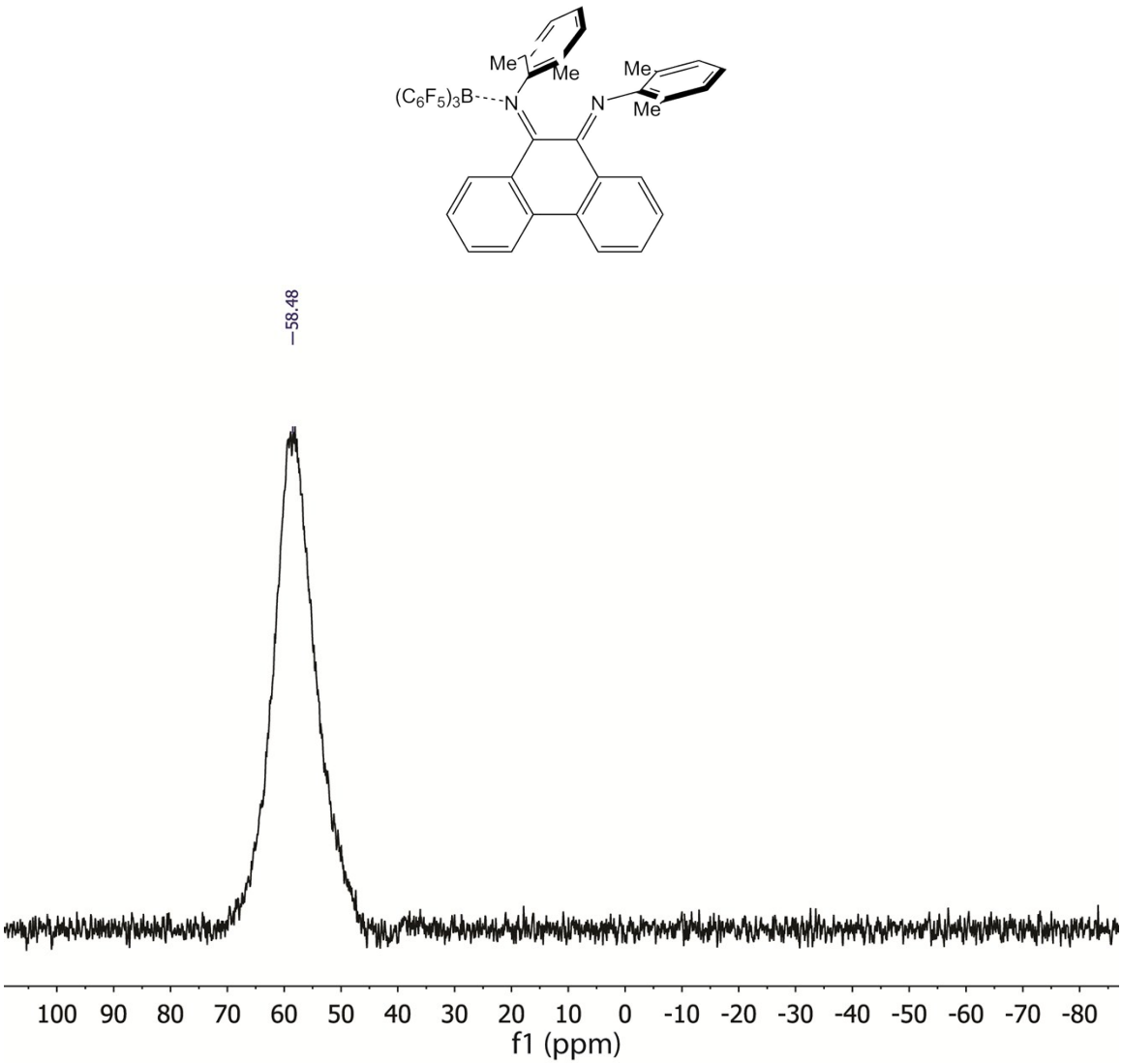


Figure S16. ^{11}B NMR spectrum of compound **8** in toluene-d8 at 298 K.

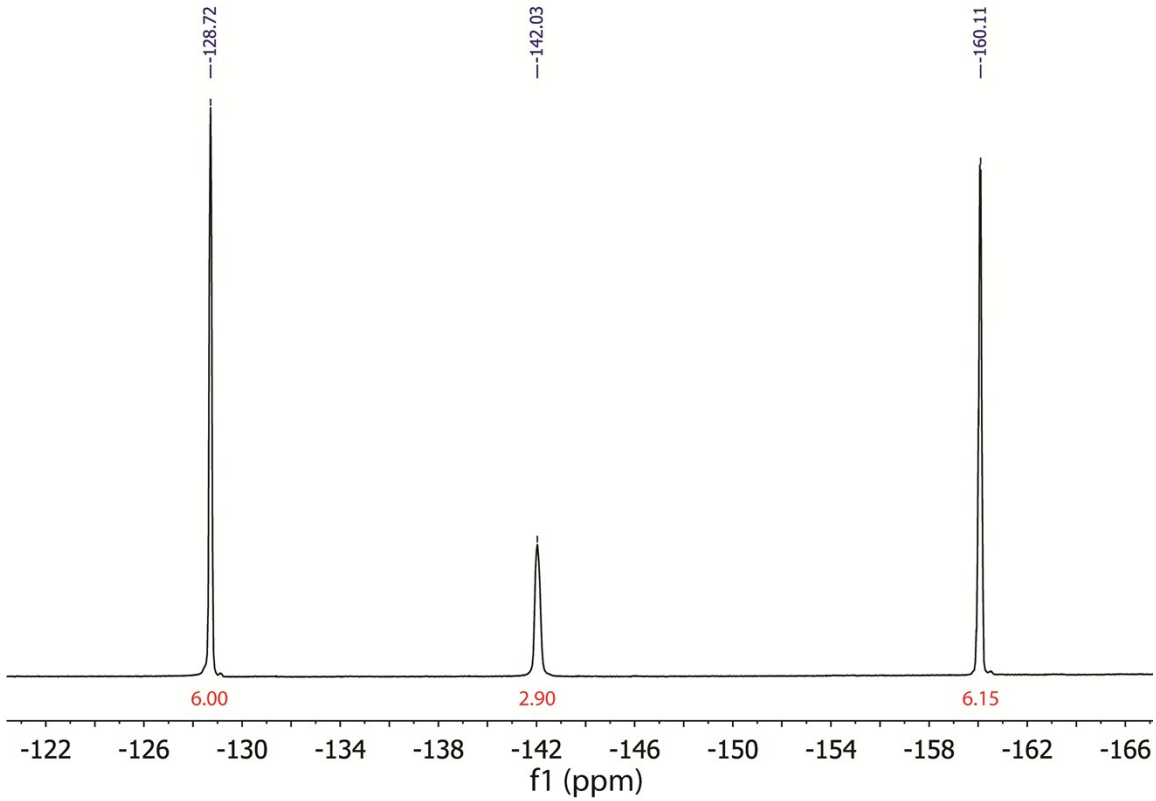
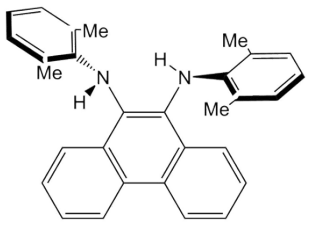


Figure S17. ^{19}F NMR spectrum of compound **8** in toluene-d8 at 298 K.

Compound 9 : $C_{14}H_8(NHC_6H_3Me_2)_2$



NMR data in toluene-d8 : ^1H NMR (400 MHz, 298 K): 8.48 (d, $^3J_{H-H}$ = 8.2 Hz, 2H, H_3/H_{12}), 7.92 (d, 2H, $^3J_{H-H}$ = 8.2 Hz, H_6/H_9), 7.34 (dd, $^3J_{H-H}$ = 8.3 Hz, $^3J_{H-H}$ = 6.9 Hz, 2H, H_4/H_{11}), 7.27 (dd, $^3J_{H-H}$ = 8.1 Hz, $^3J_{H-H}$ = 6.9 Hz, 2H, H_5/H_{10}), 6.86-6.76 (m, 6H, H_{18} & H_{19}), 5.10 (s, N-H), 1.78 (s, 12H, H_{17}).

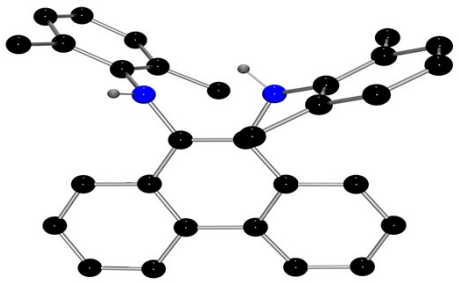


Figure S18. POV-ray depiction of compound **9**. Most H atoms have been omitted for clarity. Atom colour scheme: H: grey, C:black, N: blue.

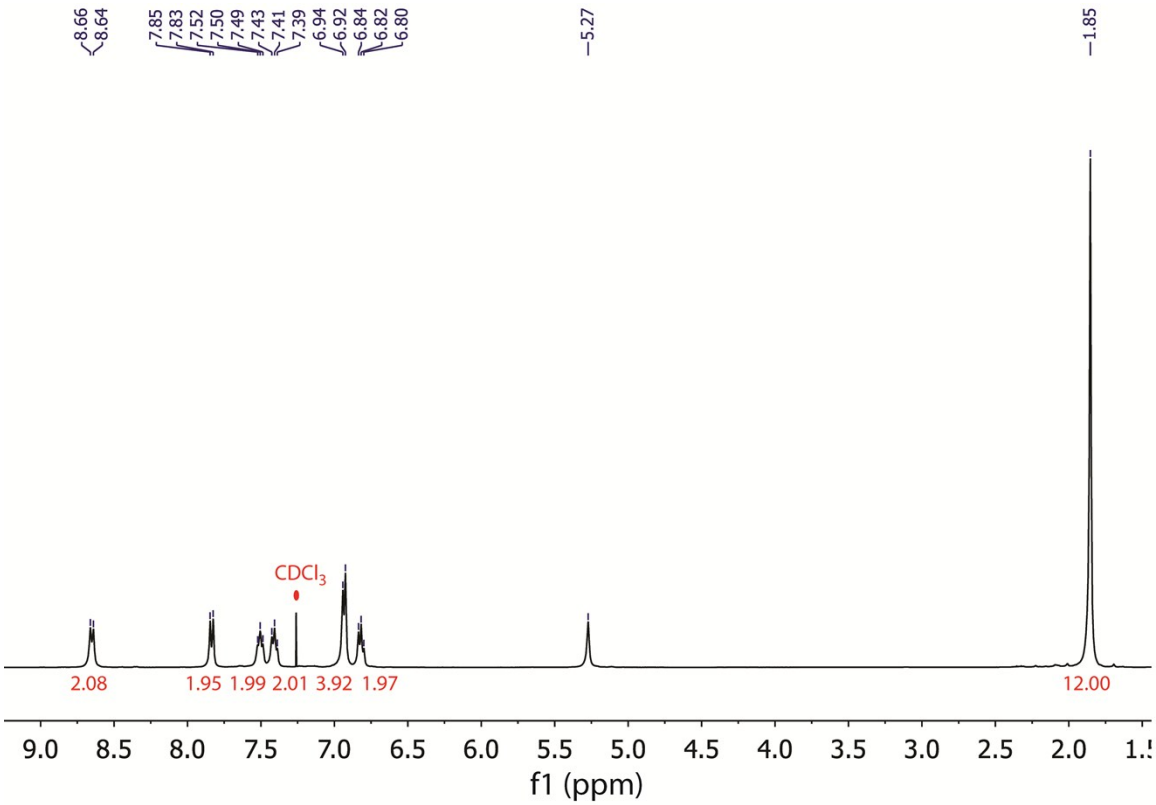


Figure S19. ^{1}H NMR of compound **9** in $CDCl_3$ at 298 K.

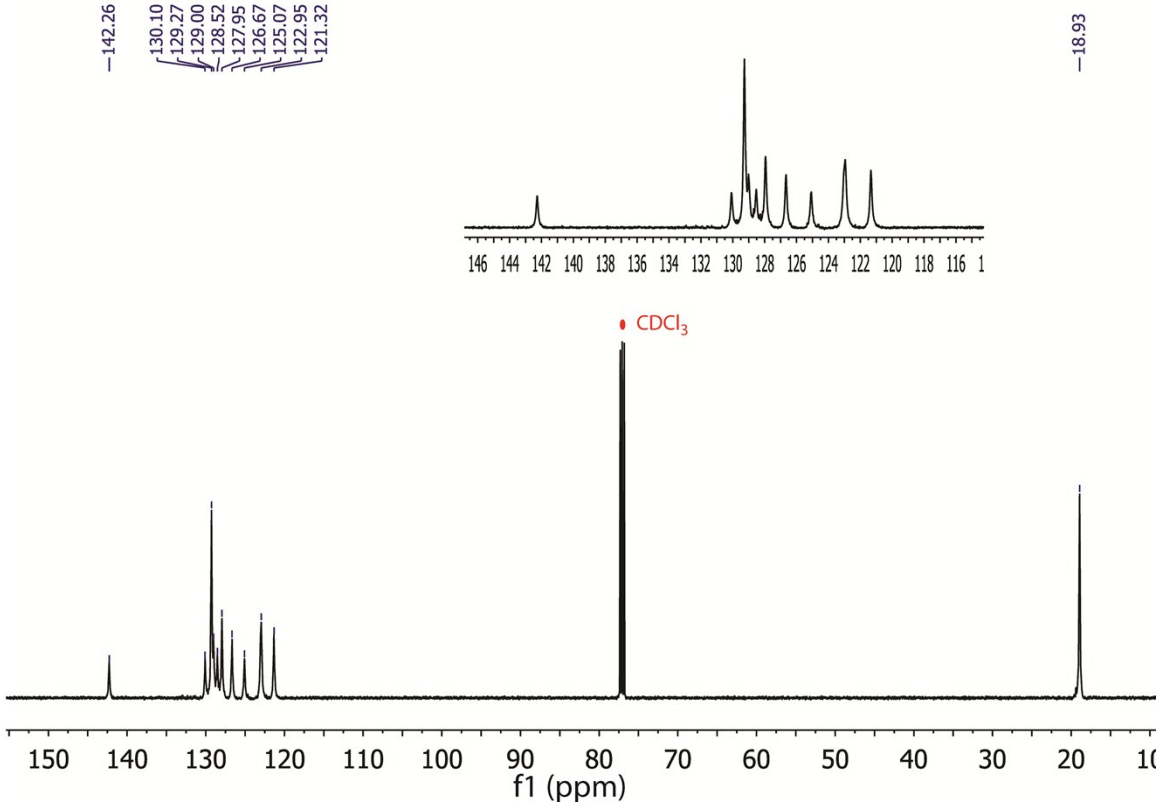


Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of **9** in $CDCl_3$ at 298 K.

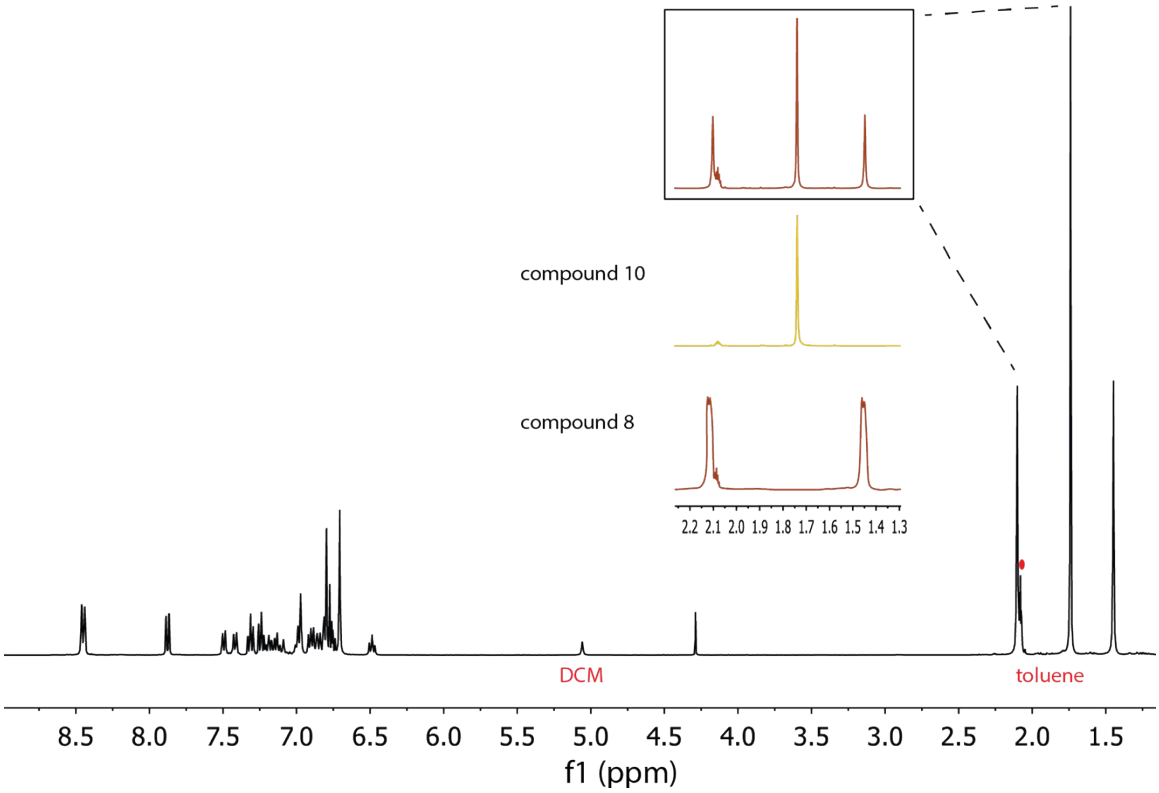
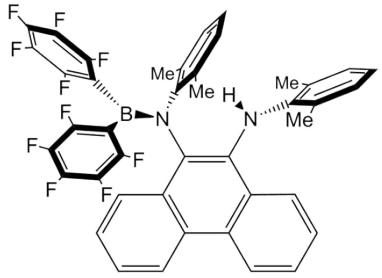


Figure S21. ^{1}H NMR spectrum of non-equilibrium between compounds **7** and **9** in toluene-d8 at 298 K (orange coloured solution).

Compound 10 : $C_{14}H_8(NHC_6H_3Me_2)(N(C_6H_3Me_2)B(C_6F_5)_2)$

Crude material from larger scale syntheses may alternatively be purified by sublimation under reduced pressure with heating (~155 °C).



NMR data in toluene-d8 : ^{11}B NMR (128 MHz, 298 K): δ 39.0 (br s); ^{19}F NMR (377 MHz, 298 K): δ -128.9 (dm, $^{3}J_{FF}$ = 24 Hz, 1F, *o*-C_6F_5(a/b)), -132.0 (dm, $^{3}J_{FF}$ = 24Hz, 1F, *o*-C_6F_5(c/d)), -132.6 (dm, $^{3}J_{FF}$ = 24 Hz, 1F, *o*-C_6F_5(b/a)), -134.1 (dm, $^{3}J_{FF}$ = 24Hz, 1F, *o*-C_6F_5(d/c)), -150.3 (t, $^{3}J_{FF}$ = 21 Hz, 1F, *p*-C_6F_5(a)), -150.7 (t, $^{3}J_{FF}$ = 20 Hz, 1F, *p*-C_6F_5(c)), -161.2 − -162.4 (m, 4F, *m*-C_6F_5(a,b,c,d)).

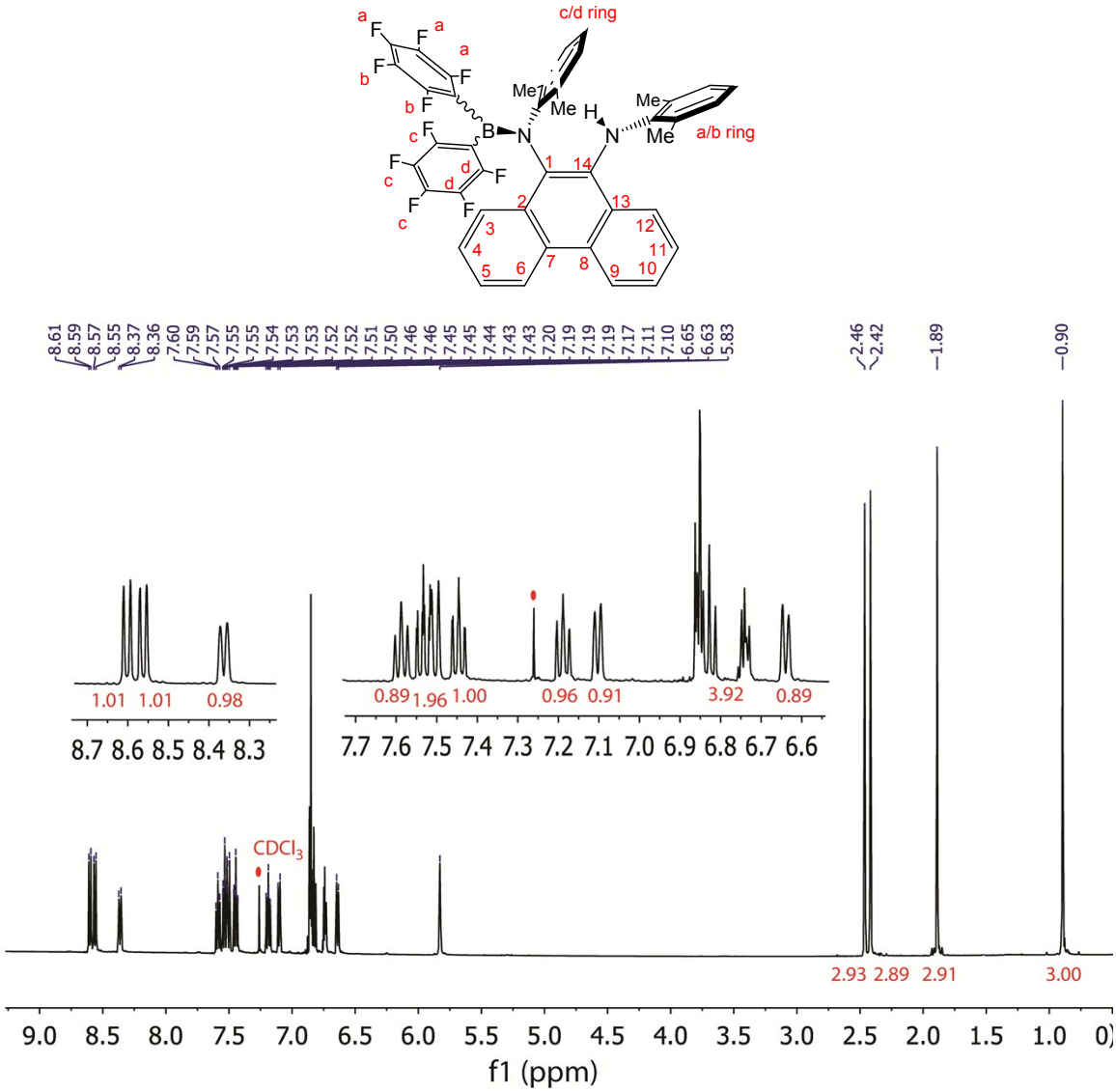


Figure S22. ^{1}H NMR spectrum of compound **10** in $CDCl_3$ at 298 K.

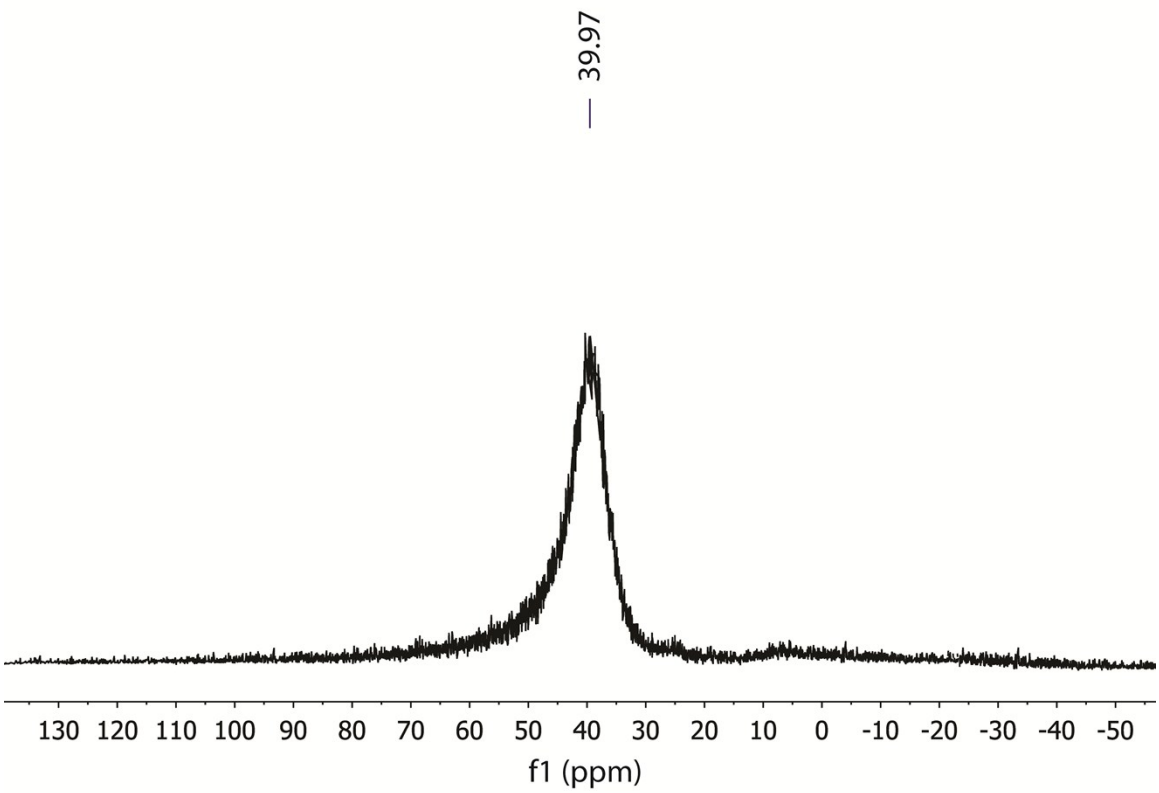


Figure S23. ^{11}B NMR spectrum of compound **10** in $CDCl_3$ at 298 K.

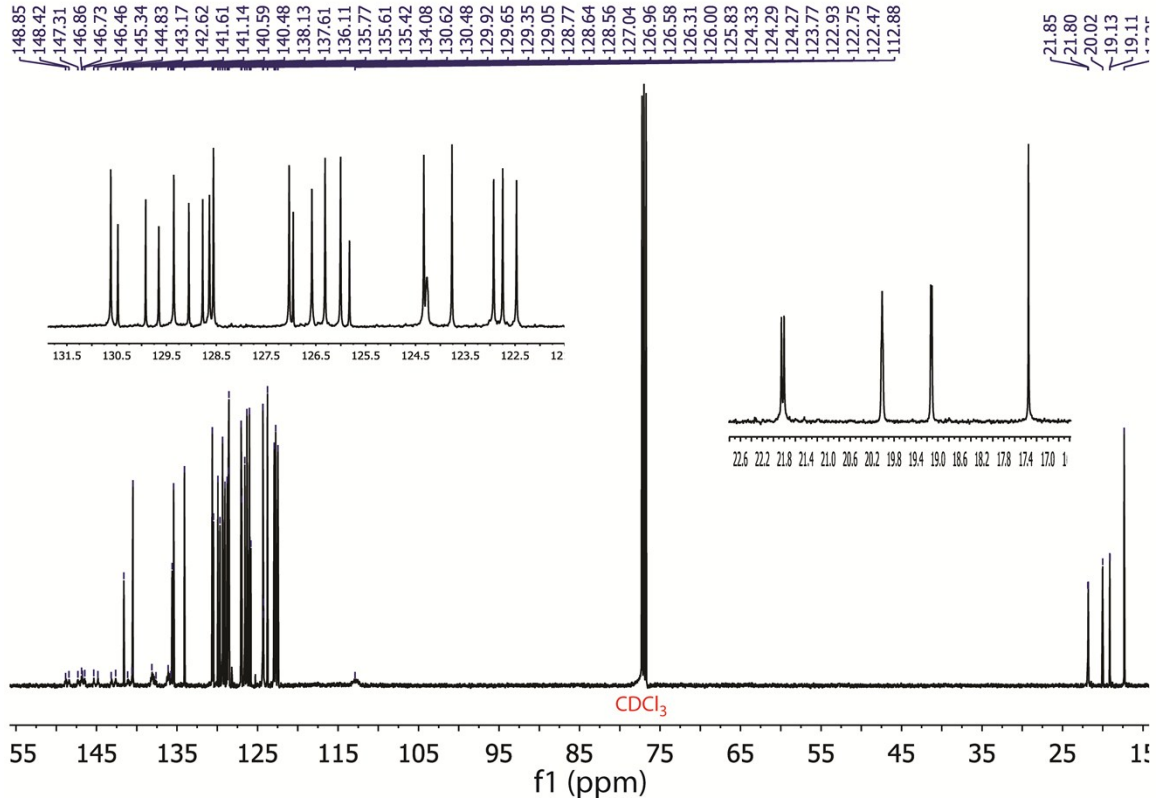


Figure S24. $^{13}C\{^1H\}$ NMR spectrum of compound **10** in $CDCl_3$ at 298 K.

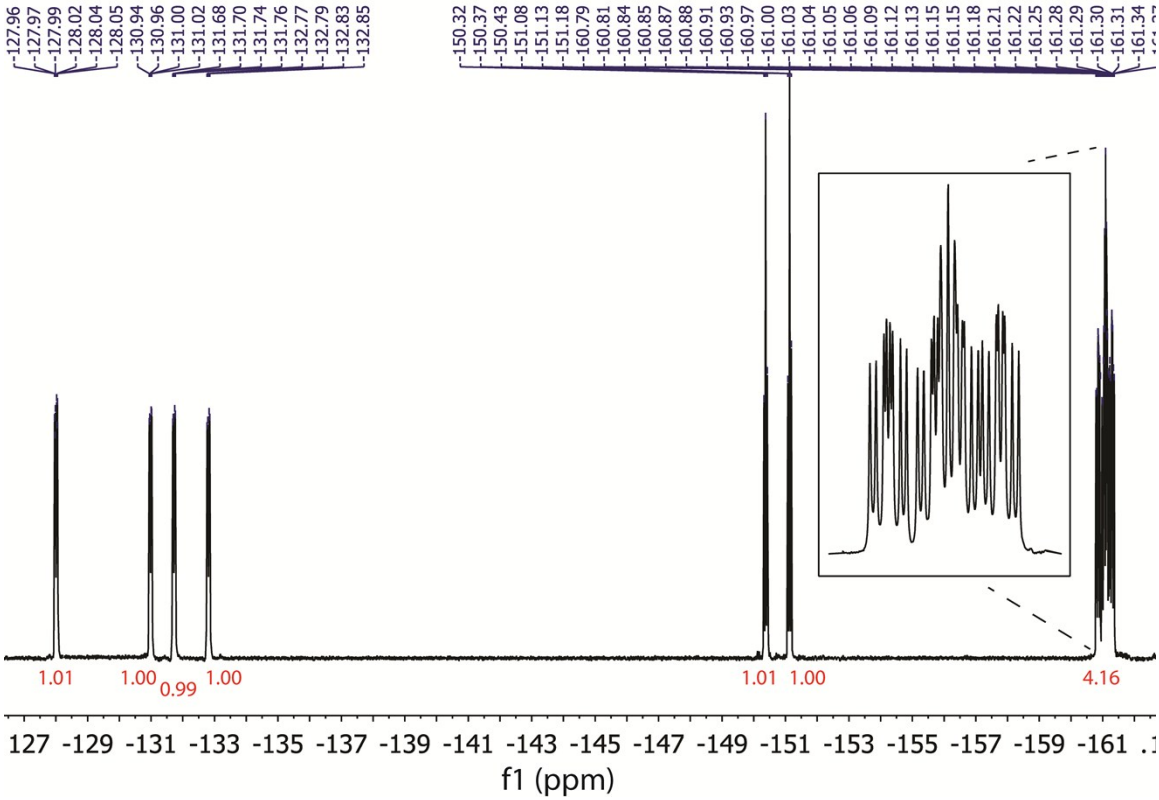
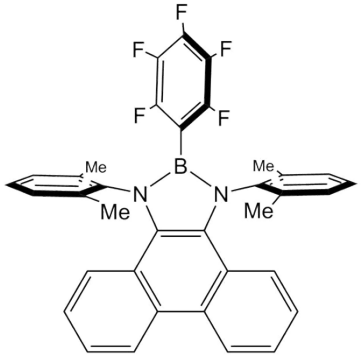


Figure S25. ^{19}F NMR spectrum of compound **10** in $CDCl_3$ at 298 K.

Compound 12 : $C_{14}H_8(NC_6H_3Me_2)_2BC_6F_5$

An adduct between the two substrates and the product of 1,2-hydroboration (compound **11**, $C_{14}H_8(NHC_6H_3Me_2)(NC_6H_3Me_2)BH(C_6F_5)$) were observed by multinuclear NMR spectroscopy (see below) prior to heating and appeared orange in solution.



NMR data in toluene-d8 : ^{11}B NMR (128 MHz, 298 K): δ 25.8 (br s); ^{19}F NMR (377 MHz, 298 K): δ -128.3 (dd, $^3J_{FF}$ = 23 Hz, $^4J_{FF}$ = 9 Hz, 2F, *o*-C_6F_5), -152.4 (t, $^3J_{FF}$ = 20 Hz, 1F, *p*-C_6F_5), -162.1 (td, $^3J_{FF}$ = 23 Hz, $^4J_{FF}$ = 9 Hz, 2F, *m*-C_6F_5).

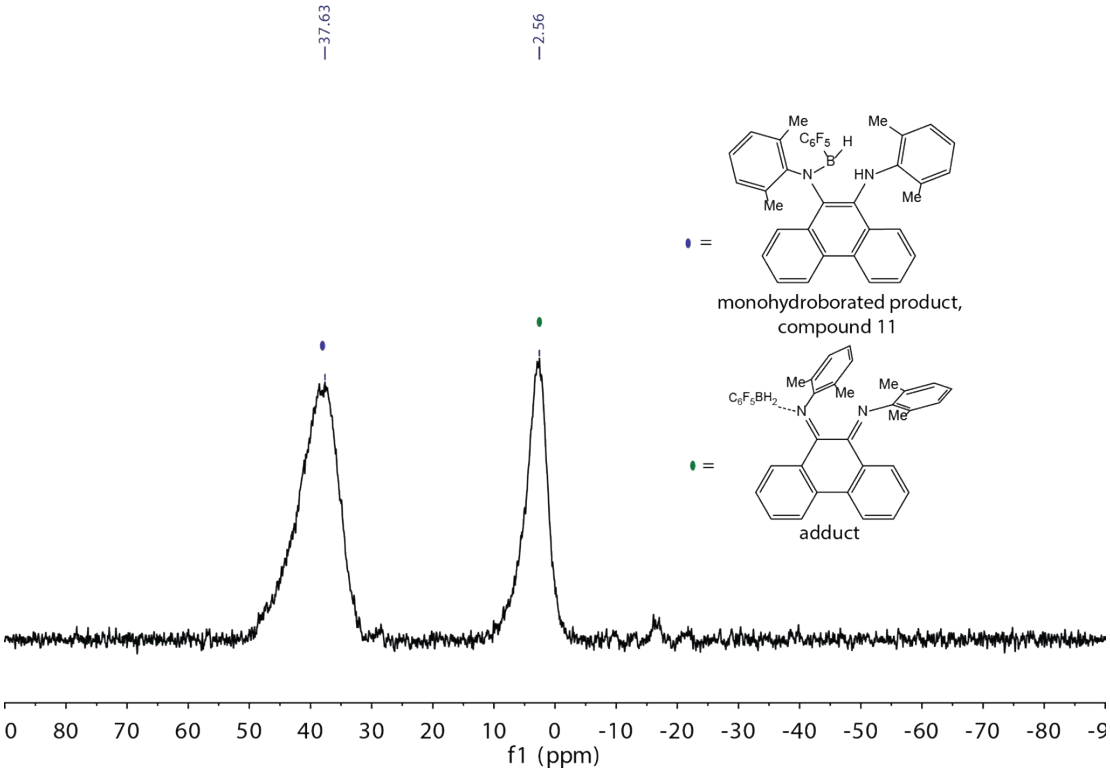


Figure S26. ^{11}B NMR spectrum of compound 7-$H_2B(C_6F_5)$ adduct (green) and the product of 1,2-hydroboration compound **11** (purple) in $CDCl_3$ at 298 K.

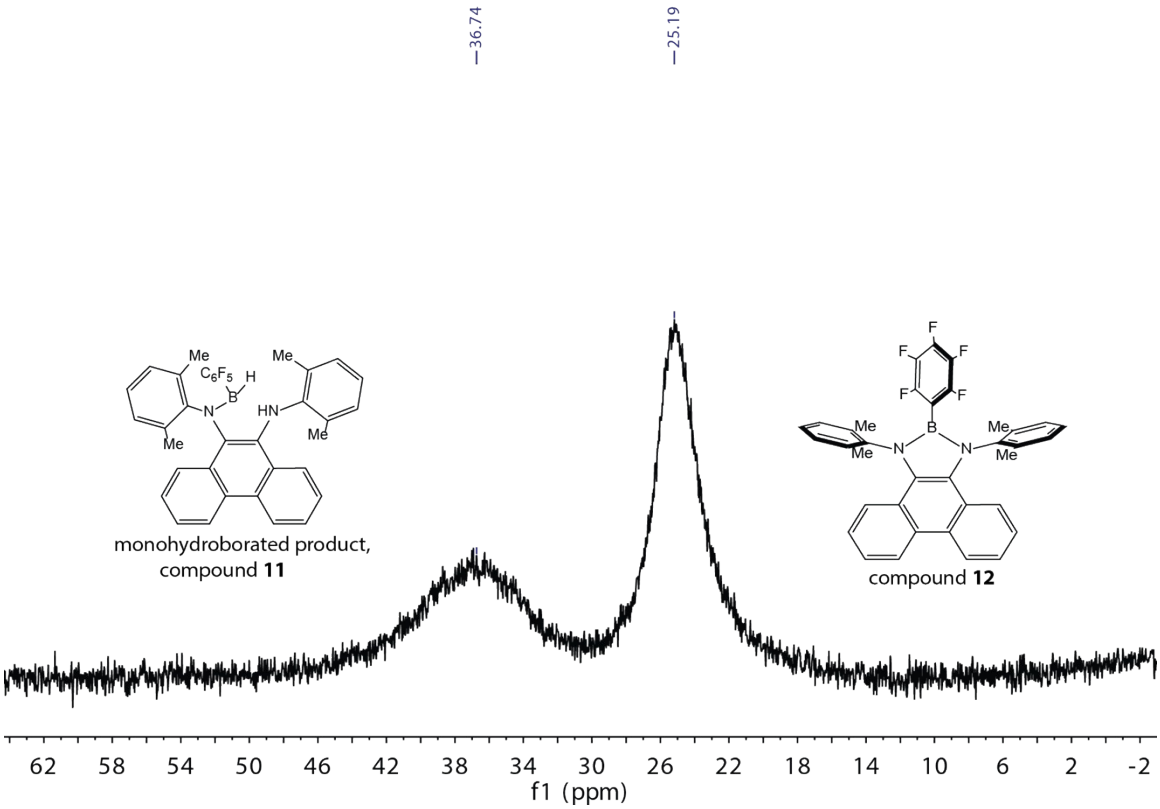


Figure S27.[11]B NMR spectrum of reaction mixture containing compound **11** and compound **12** in toluene at 298 K.

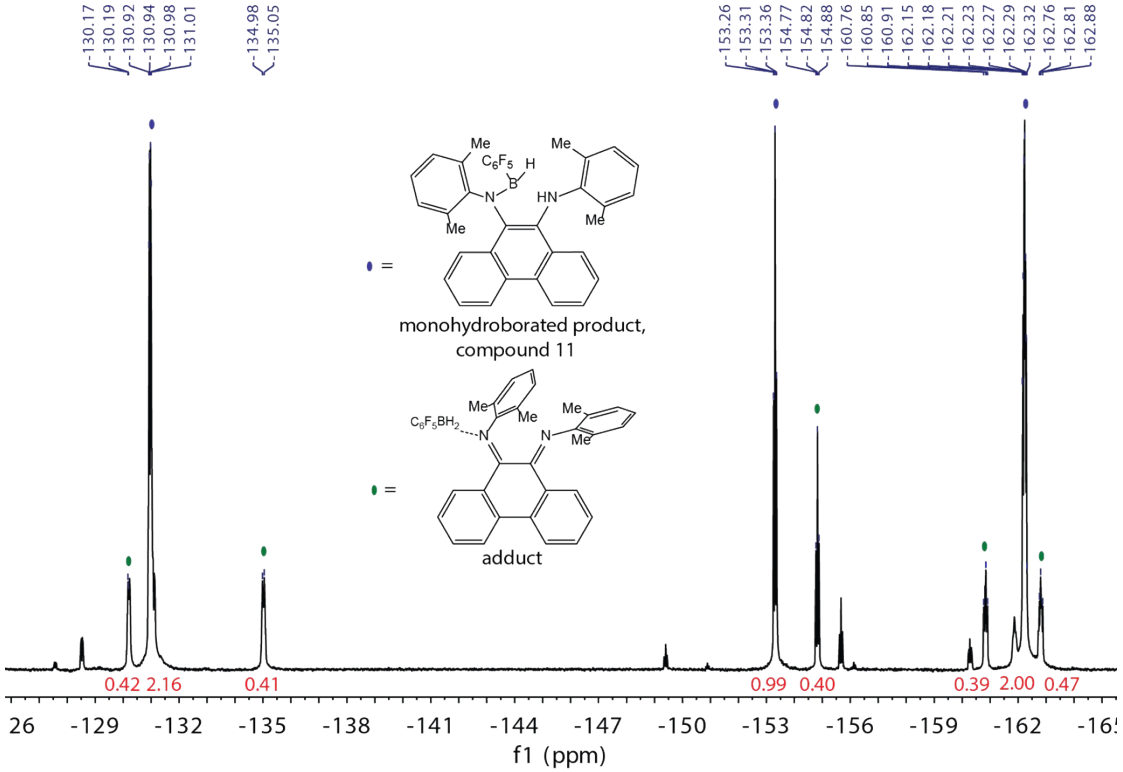


Figure S28. [19]F NMR spectrum of reaction mixture containing compound 7-$H_2B(C_6F_5)$ adduct (green dot) and the product of 1,2-hydroboration compound **11** (purple dot) in $CDCl_3$ at 298 K.

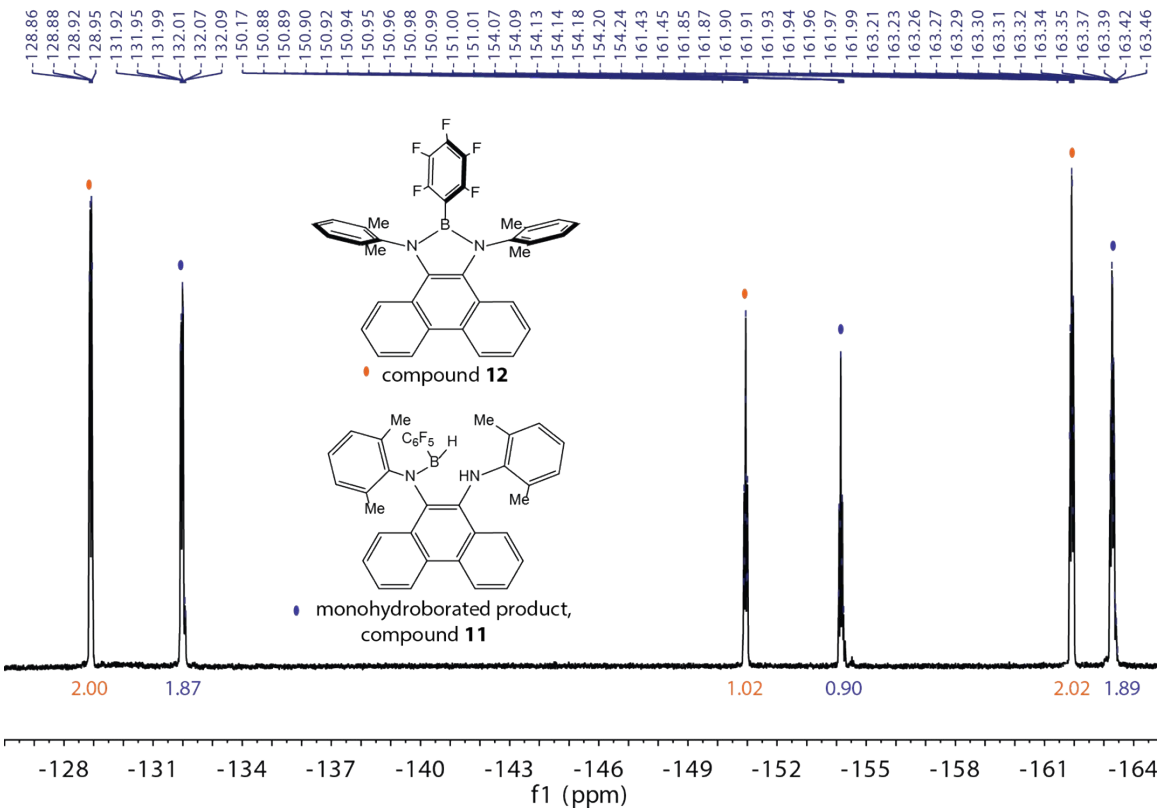


Figure S29. ^{19}F NMR spectrum of reaction mixture containing compound **11** (purple dot) and compound **12** (orange dot) in toluene at 298 K.

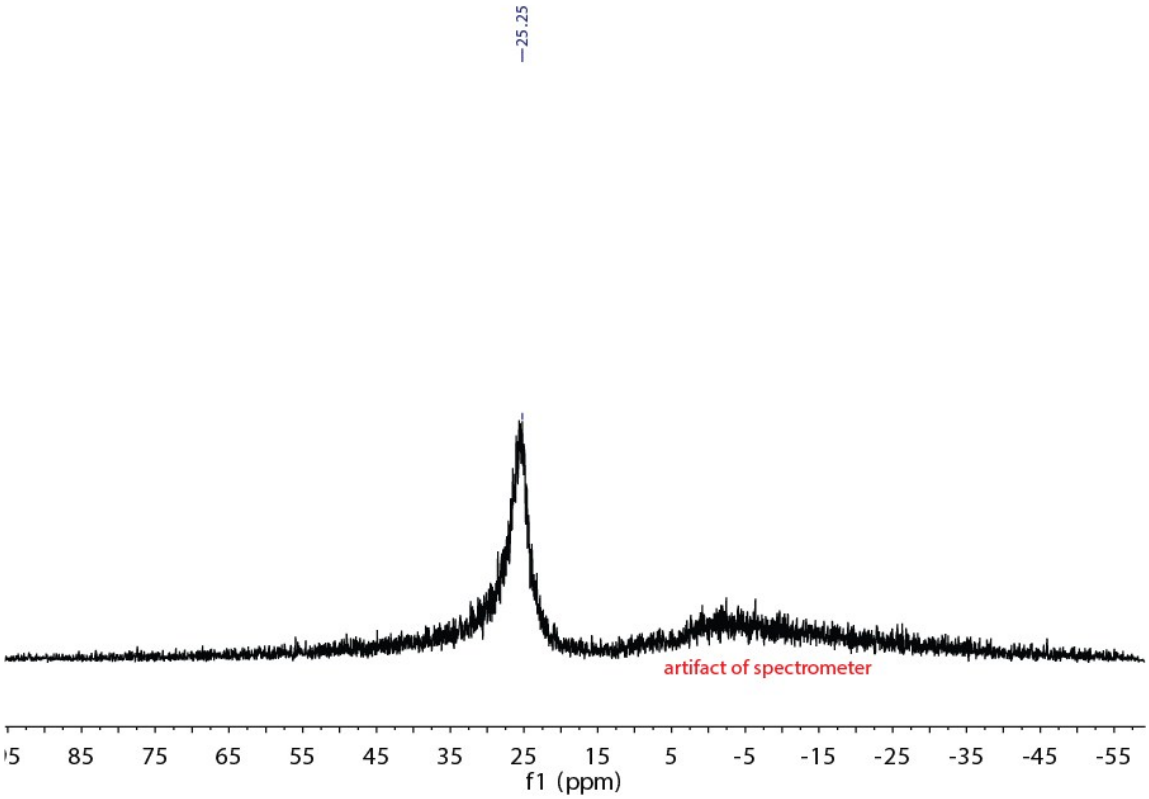


Figure S30. ^{11}B NMR spectrum of compound **12** in $CDCl_3$ at 298 K.

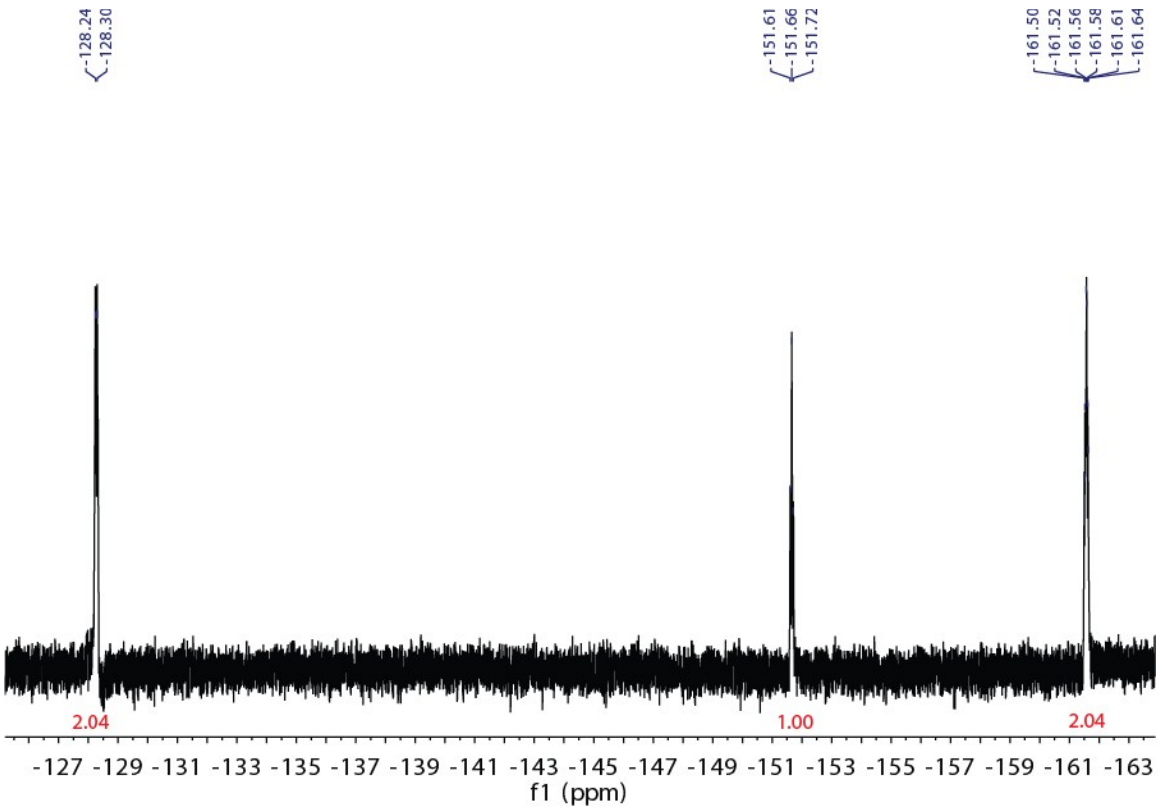
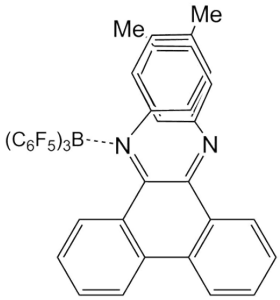


Figure S31. ^{19}F NMR spectrum of compound **12** in CDCl3 at 298 K.

N,*N*'-(*p*-tolyl)-phenanthrene-9,10-diimine-derived products

Compound 14 : $C_{14}H_8(NC_6H_4Me)(NC_6H_4Me(B(C_6F_5)_3))$



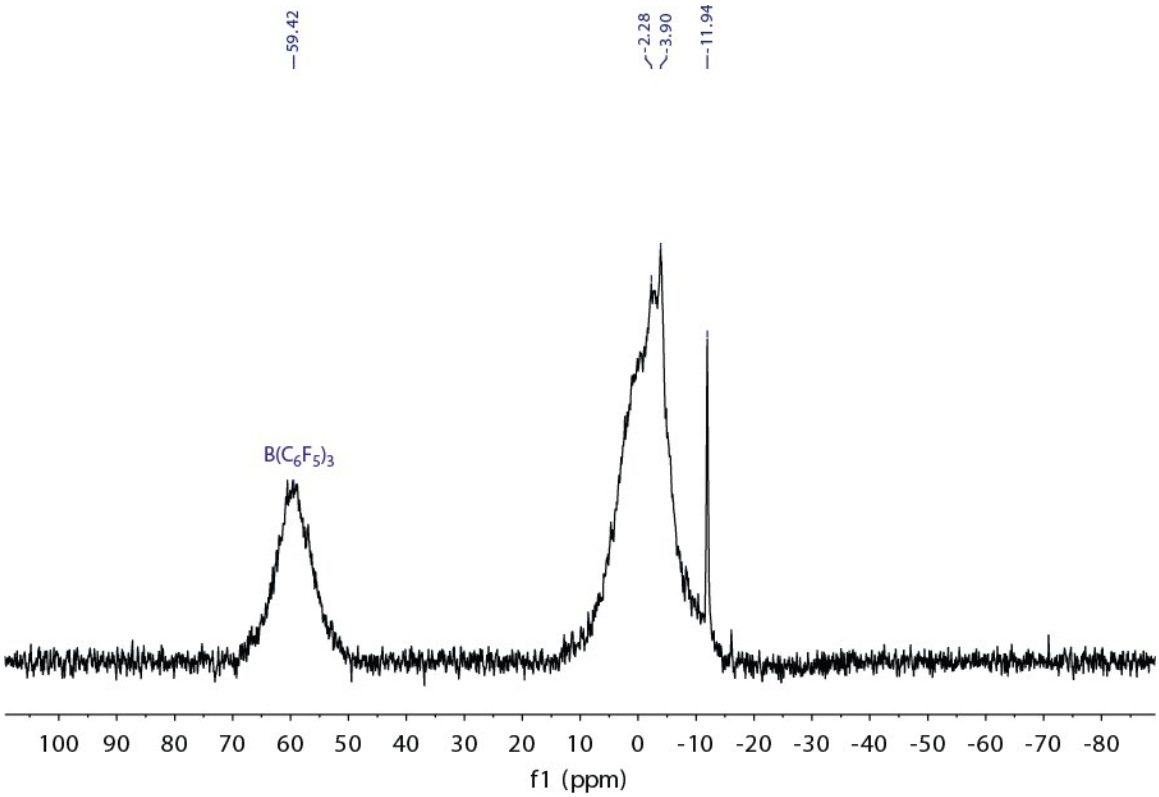


Figure S32. ^{11}B NMR spectrum of crude equimolar mixture of compound **13** and $B(C_6F_5)_3$ in toluene-d8 at 298 K.

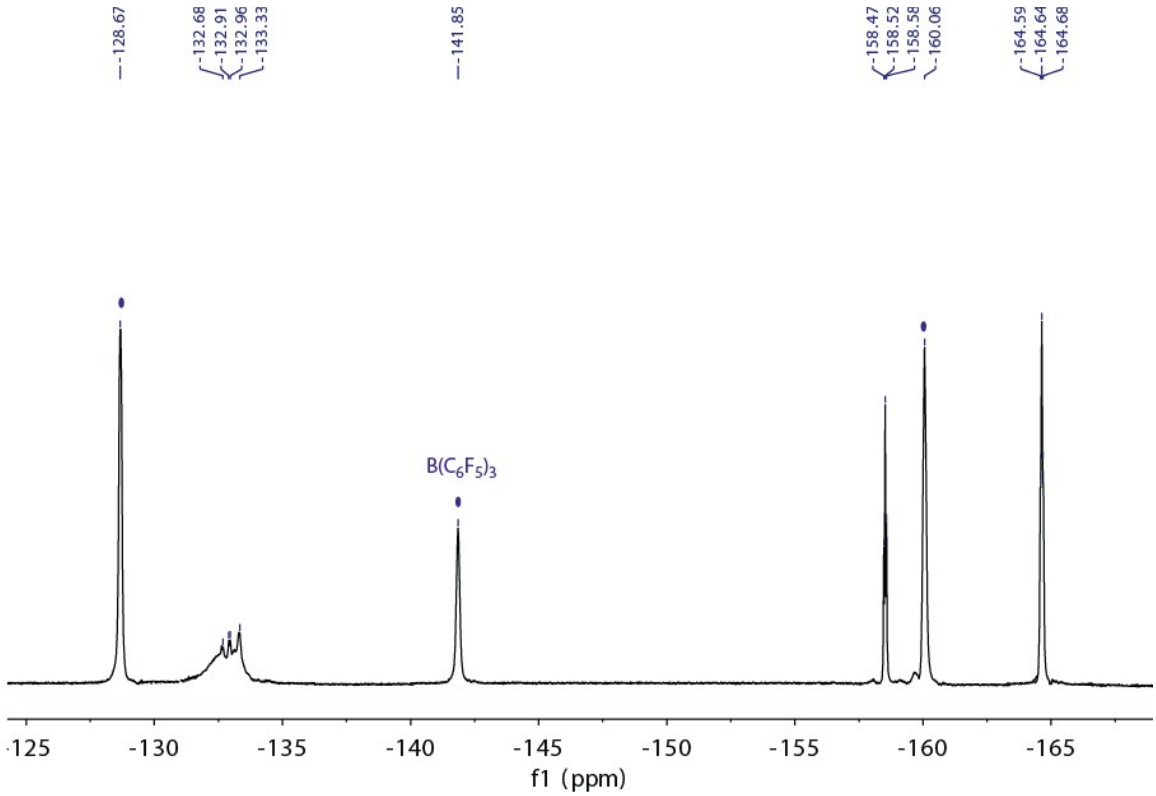
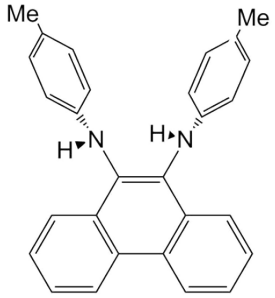


Figure S33. ^{19}F NMR spectrum of crude equimolar mixture of compound **13** and $B(C_6F_5)_3$ in toluene-d8 at 298 K.

Compound 15 : $C_{14}H_8(NHC_6H_4Me)_2$

NMR samples prepared in a variety of solvents (*e.g.* d3-acetonitrile, $CDCl_3$, toluene-d8), using either a 3 mm NMR tube sealed with Teflon tape and Parafilm or a J-young NMR tube, become readily oxidized to the α-diimine **13** in overnight NMR studies. Similarly, solid samples submitted for elemental analysis that were handled in an inert atmosphere glove bag and exposed to the nitrogen atmosphere for > 5 minutes turned orange in colour (compound **13**, according to DART-MS analysis).



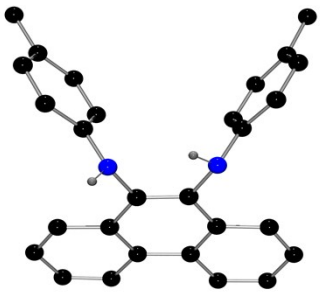


Figure S34. POV-ray depiction of compound **15**. A second molecule in the asymmetric unit, related by global pseudo-symmetry to the one shown, and most H atoms have been omitted for clarity. Atom colour scheme: H: grey, C: black, N: blue.

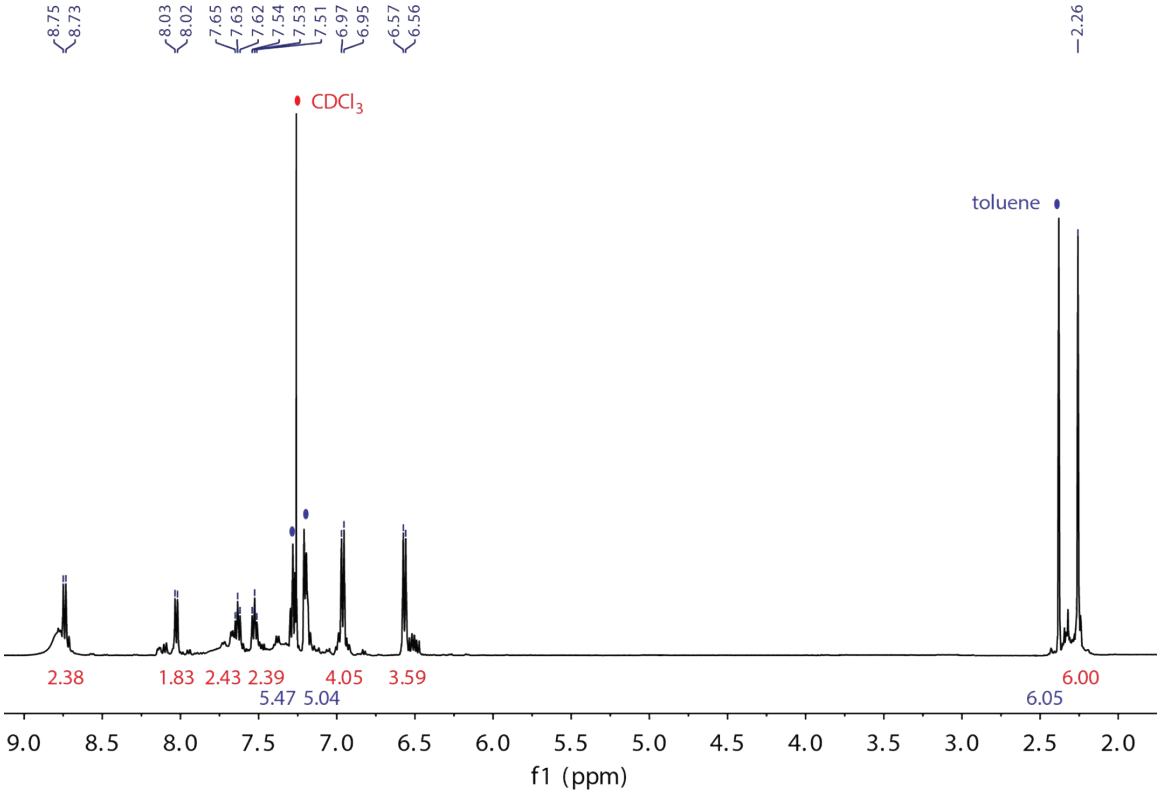


Figure S35. ^{1}H NMR spectrum of compound **15** in CDCl3 at 298 K (note: broadening is due to the formation of the semidiimine radical **S** *via* oxidation of **15** to **13** by trace oxygen).

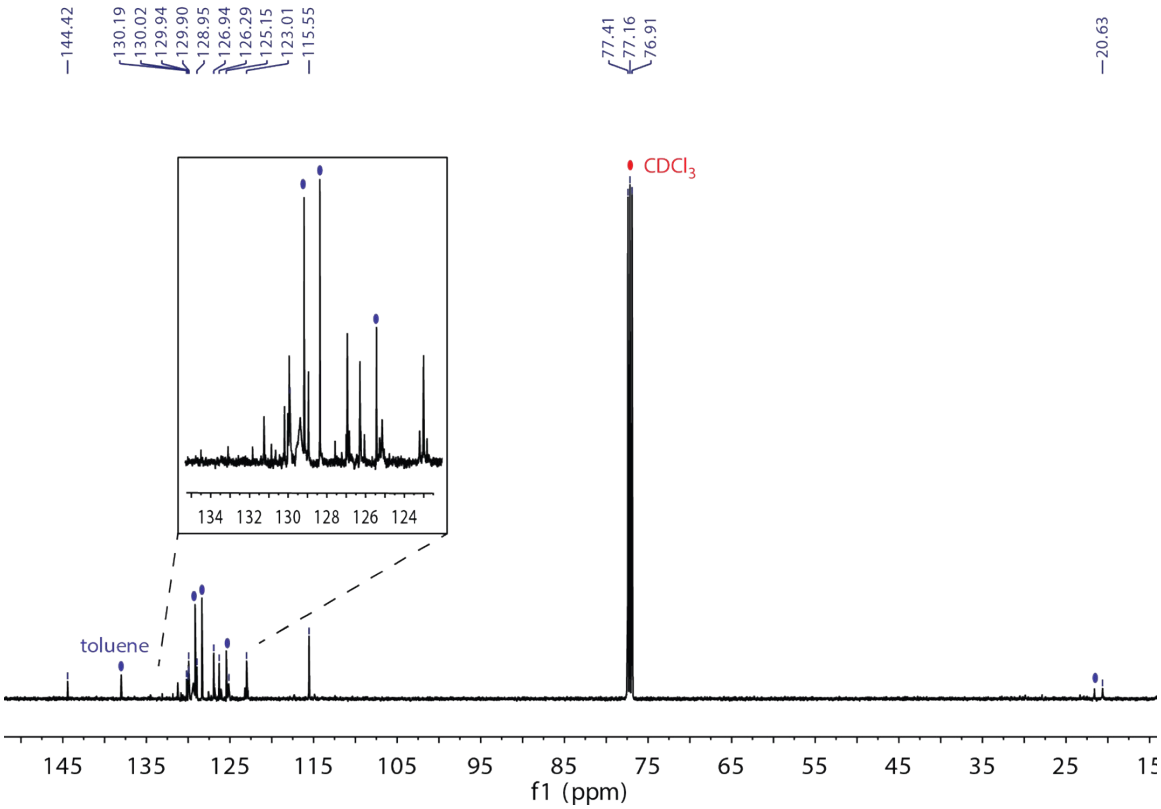


Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum of compound **15** in CDCl3 at 298 K (note: broadening is due to the formation of the semidiimine radical **S** *via* oxidation of **15** to **13** by trace oxygen).

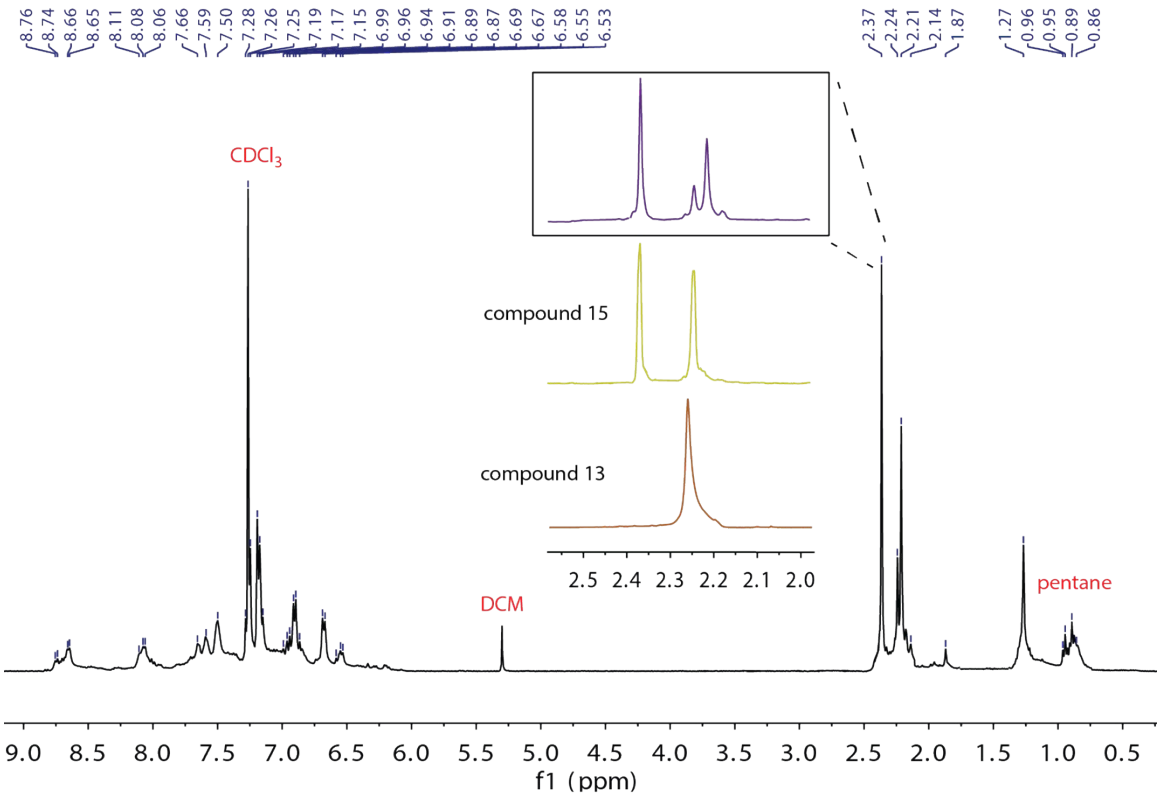
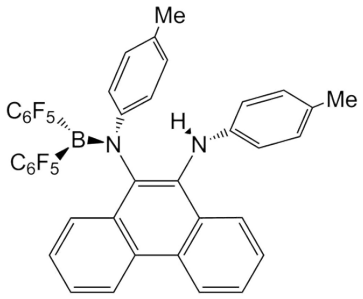


Figure S37. ^{1}H NMR spectrum of equilibrium between compounds **13** and **15** in $CDCl_3$ at 298 K (dark purple coloured solution solution).

Compound 16 : $C_{14}H_8(NHC_6H_4Me)(NC_6H_4Me(B(C_6F_5)_2)$

Compounds **16** and **17** could not be separated by column chromatography, fractional crystallisation, or sublimation (see Figure S38b & Figure S39b). The proposed connectivity of **16** is:



NMR data (partial) in toluene-d8: ^{11}B NMR (128 MHz, 298 K): δ 37.6 (br s); ^{19}F NMR (377 MHz, 298 K): δ -130.2 (dt, $^{3}J_{FF}$ = 23.9 Hz, $^{4}J_{FF}$ = 11.8 Hz, 1F, *o*-C_6F_5), -131.9 (d, $^{3}J_{FF}$ = 22.2 Hz, 1F, *o*-C_6F_5), -133.3 (dt, $^{3}J_{FF}$ = 23.0 Hz, $^{4}J_{FF}$ = 10.4 Hz, 1F, *o*-C_6F_5), -133.9 (d, $^{3}J_{FF}$ = 23.5 Hz, 1F, *o*-C_6F_5), -150.0 (m, 1F, *p*-C_6F_5), -151.7 (m, 1F, *p*-C_6F_5), -159.6 (td, $^{3}J_{FF}$ = 22.5 Hz, $^{4}J_{FF}$ = 9.2 Hz, 1F, *m*-C_6F_5), -160.9 (m, 1F, *m*-C_6F_5), -161.5 (td, $^{3}J_{FF}$ = 22.4 Hz, $^{4}J_{FF}$ = 9.8 Hz, 1F, *m*-C_6F_5), -162.1 (td, $^{3}J_{FF}$ = 23.0 Hz, $^{4}J_{FF}$ = 9.7 Hz, 1F, *m*-C_6F_5).

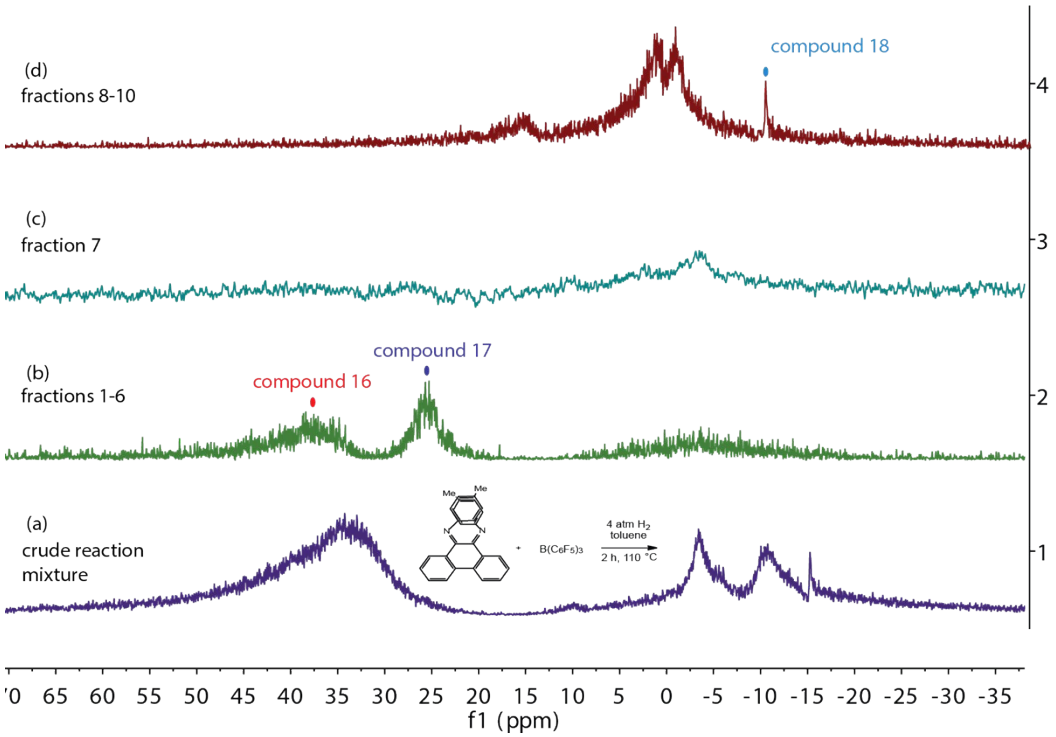


Figure S38. ^{11}B NMR spectra in CDCl3 at 298 K of (a) crude FLP hydrogenation of compound **13** and $B(C_6F_5)_3$ (4 atm H_2) following heating at 110 °C for 2 h in toluene, (b) fractions 1-6, (c) fraction 7, and fractions 8-10 from flash column chromatography (silica gel, 95:5 pentane/CH_2Cl_2 eluent).

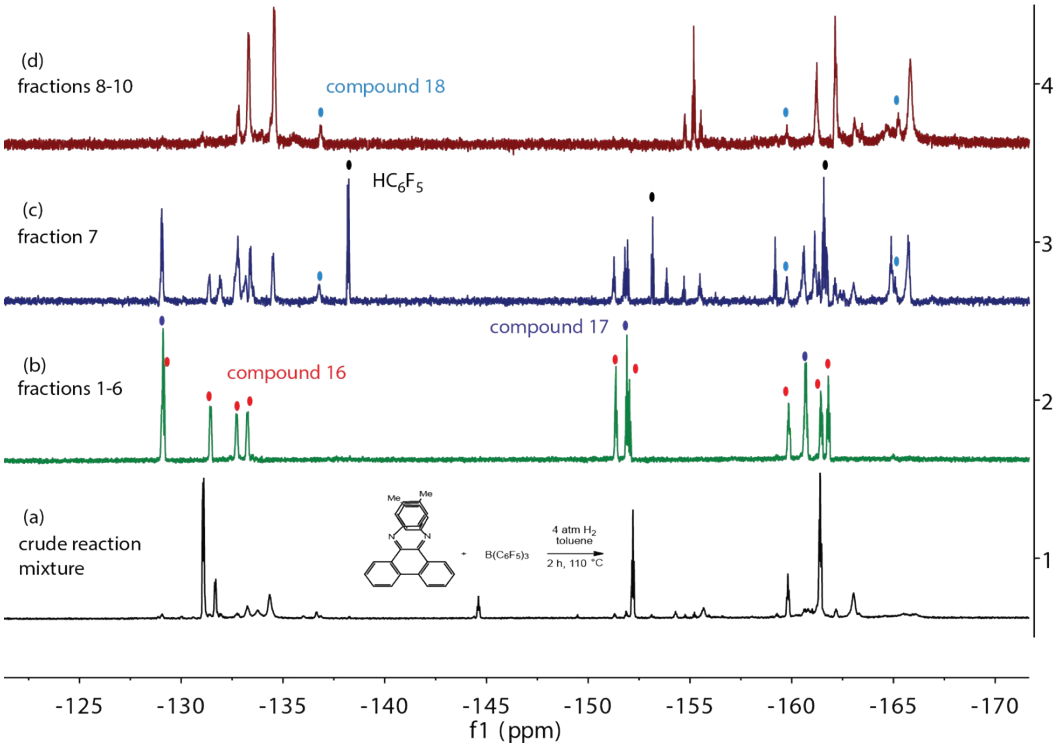
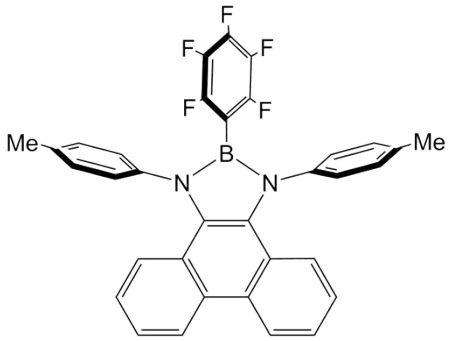


Figure S39. ^{19}F NMR spectra in $CDCl_3$ at 298 K of (a) crude FLP hydrogenation of compound **13** and $B(C_6F_5)_3$ (4 atm H_2) following heating at 110 °C for 2 h in toluene, (b) fractions 1-6, (c) fraction 7, and fractions 8-10 from flash column chromatography (silica gel, 95:5 pentane/CH_2Cl_2 eluent).

Compound 17 : $C_{14}H_8(NC_6H_4Me)_2B(C_6F_5)$

Reactions in toluene heated to 110 ºC resulted in compound **17** as well as its precursor, the product of monohydroboration. Prolonged heating (>10 h) was required at 110 ºC to effect conversion to compound **17**, hence bromobenzene was used instead.



NMR data in toluene-d8 : ^{11}B NMR (128 MHz, 298 K): δ 26.0 (br s); ^{19}F NMR (377 MHz, 298 K): δ -129.4 (dd, , $^3J_{FF}$ = 24.6 Hz, $^4J_{FF}$ = 9.7 Hz, 2F, *o*-C_6F_5), -151.7 (t, $^3J_{FF}$ = 20.5 Hz, 1F, *p*-C_6F_5), -162.1 (ddd, , $^3J_{FF}$ = 24.3 & 19.7 Hz, $^4J_{FF}$ = 9.5 Hz, 2F, *m*-C_6F_5).

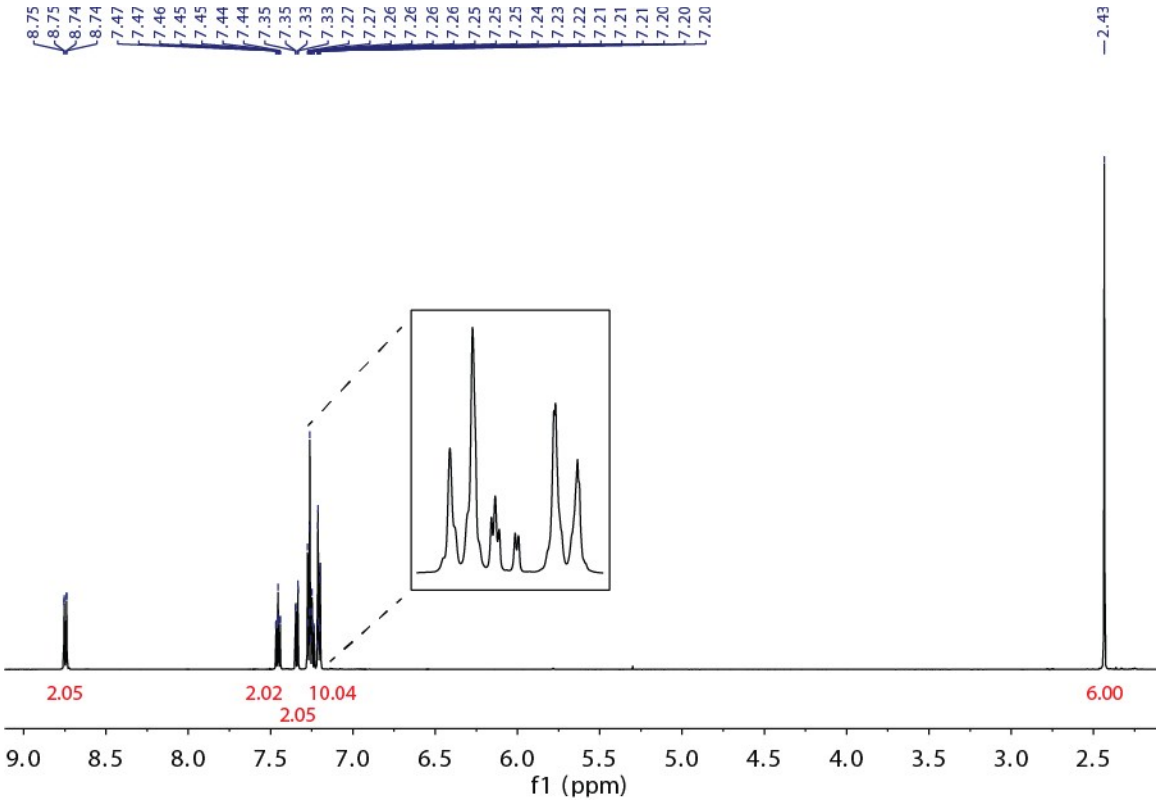


Figure S40. ^{1}H NMR spectrum of compound **17** in $CDCl_3$ at 298 K.

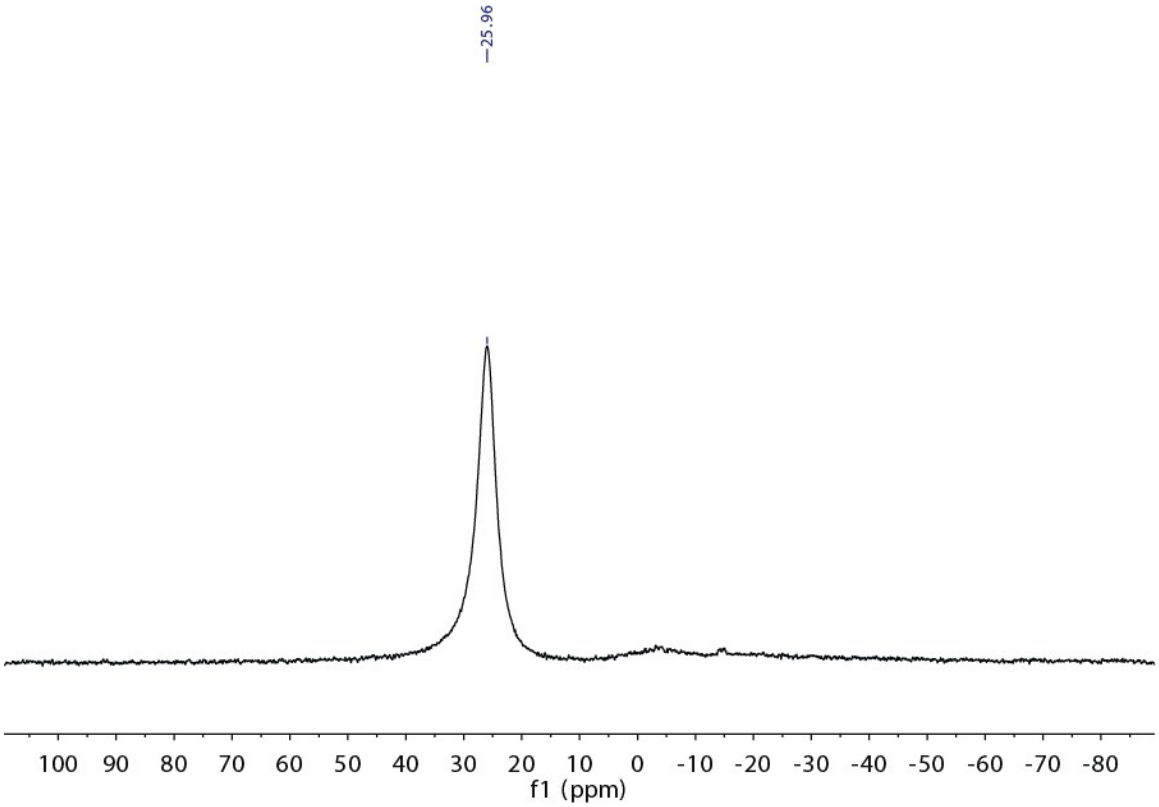


Figure S41. ^{11}B NMR spectrum of compound **17** in $CDCl_3$ at 298 K.

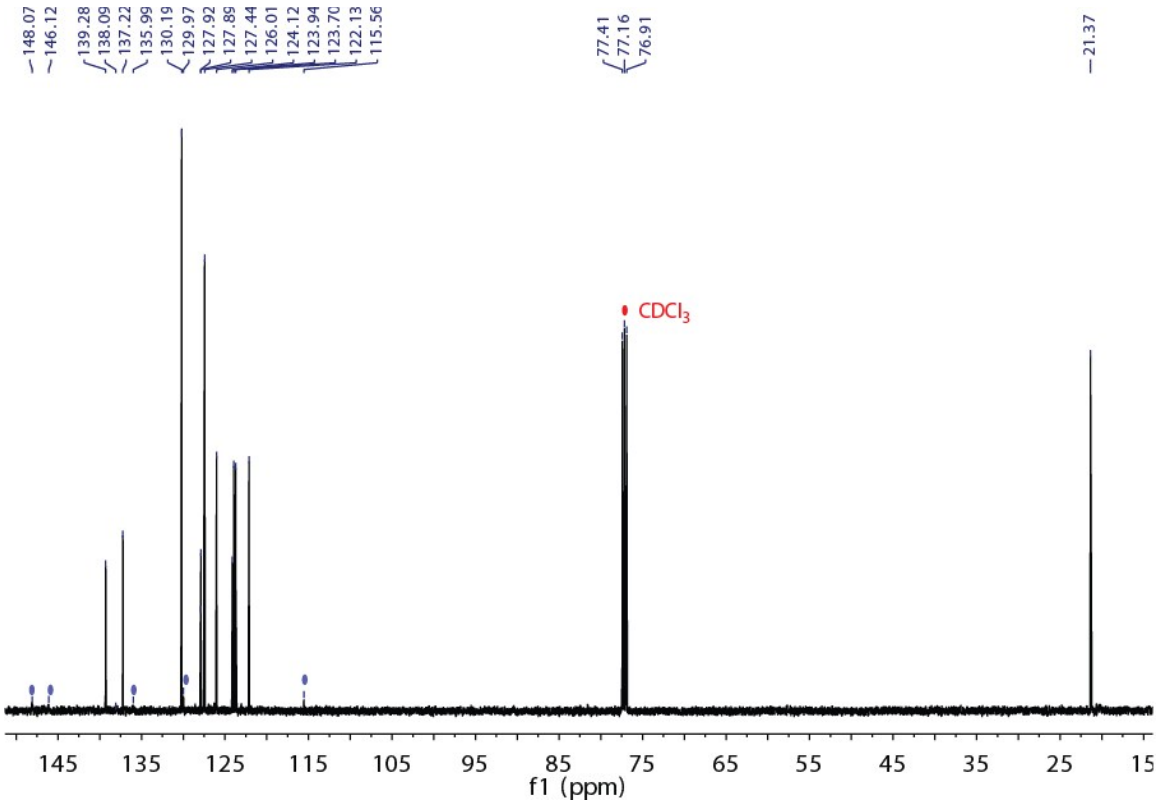


Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of compound **17** in $CDCl_3$ at 298 K (purple markers = partially resolved set of C_6F_5 resonances).

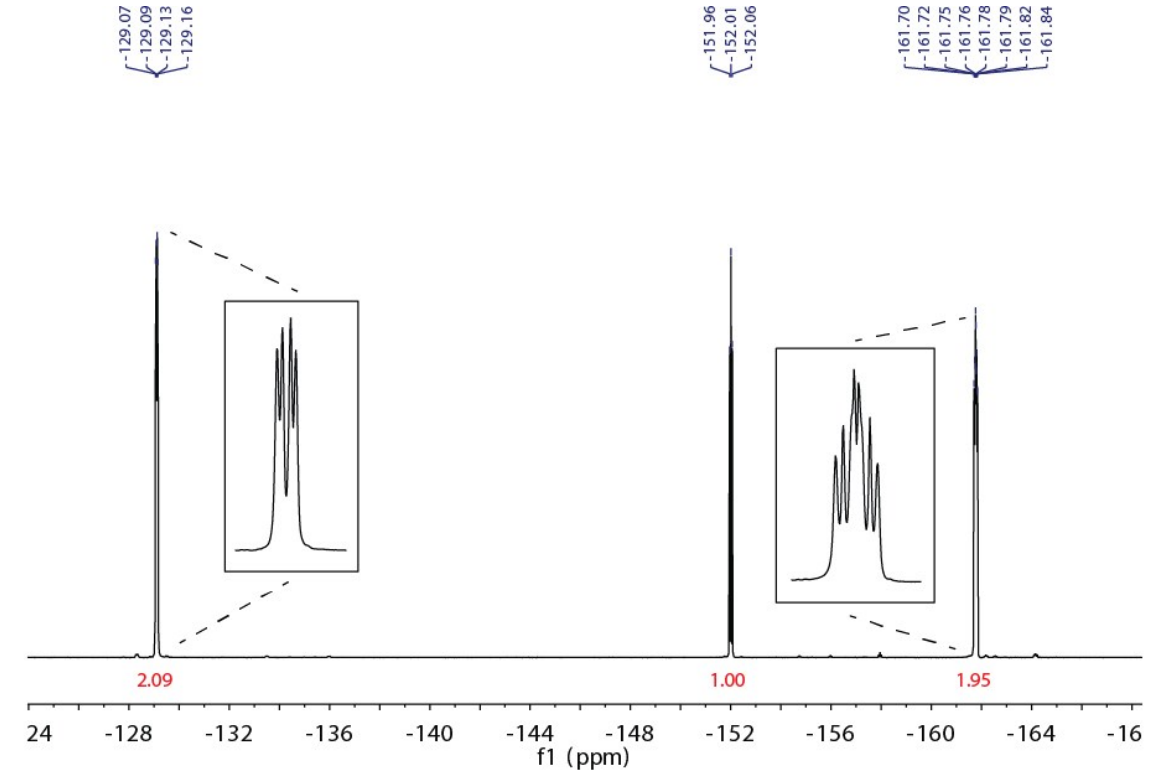
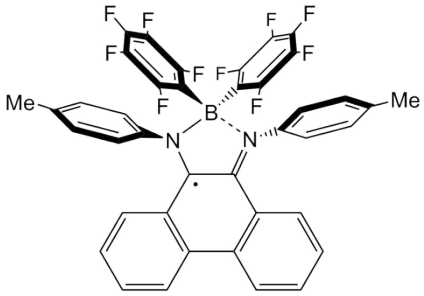


Figure S43. ^{19}F NMR spectrum of compound **17** in $CDCl_3$ at 298 K.

Compound 18 : $[C_{14}H_8(NC_6H_4Me)_2B(C_6F_5)_2]^{\bullet}$



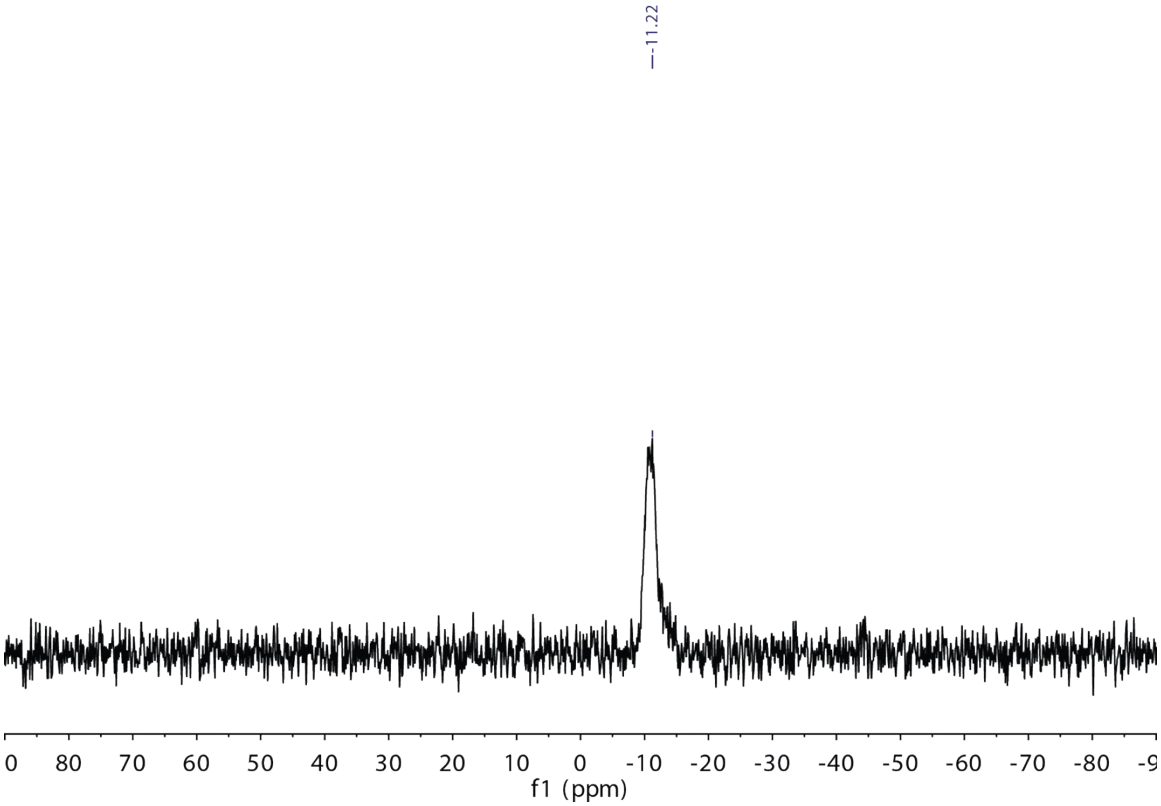


Figure S44. ^{11}B NMR spectrum of compound **18** in $CDCl_3$ at 298 K.

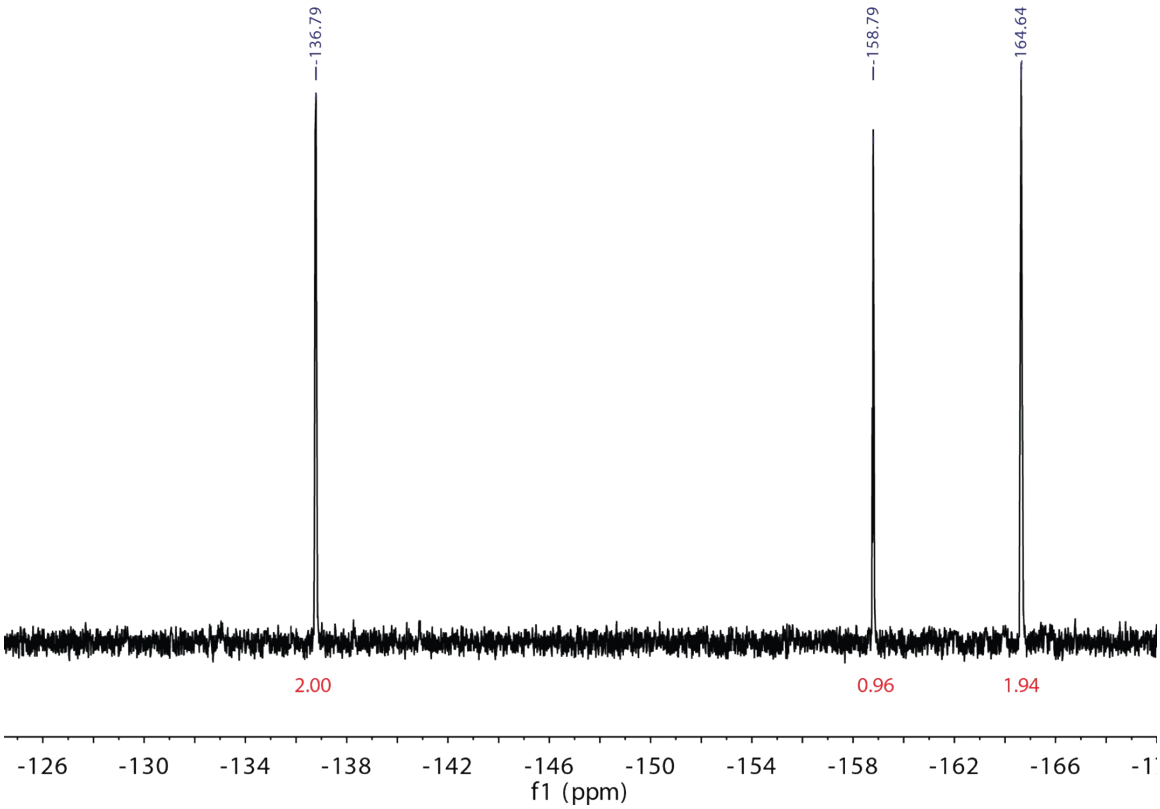
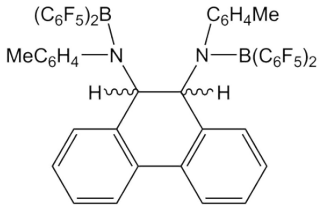


Figure S45. ^{19}F NMR spectrum of compound **18** in $CDCl_3$ at 298 K.

Compounds 19 : $C_{14}H_{10}(N(C_6H_3Me_2)B(C_6F_5)_2)_2$
The proposed connectivity of **19** is:



NMR data in toluene-d8 : ^{11}B NMR (128 MHz, 298 K): δ 38.5 (br s); ^{19}F NMR (377 MHz, 298 K): δ -128.0 (br s, 1F, *o*-C_6F_5), -130.5 (br s, 1F, *o*-C_6F_5), -131.3 (br s, 1F, *o*-C_6F_5), -132.4 (br s, 1F, *o*-C_6F_5), -153.6 (td, $^3J_{FF}$ = 20.2 Hz, $^4J_{FF}$ = 6.7 Hz, 2F, *p*-C_6F_5), -161.1 (br s, 2F, *m*-C_6F_5), -162.2 (td, $^3J_{FF}$ = 22.4 & 21.6 Hz, $^4J_{FF}$ = 9.8 Hz, 2F, *m*-C_6F_5).

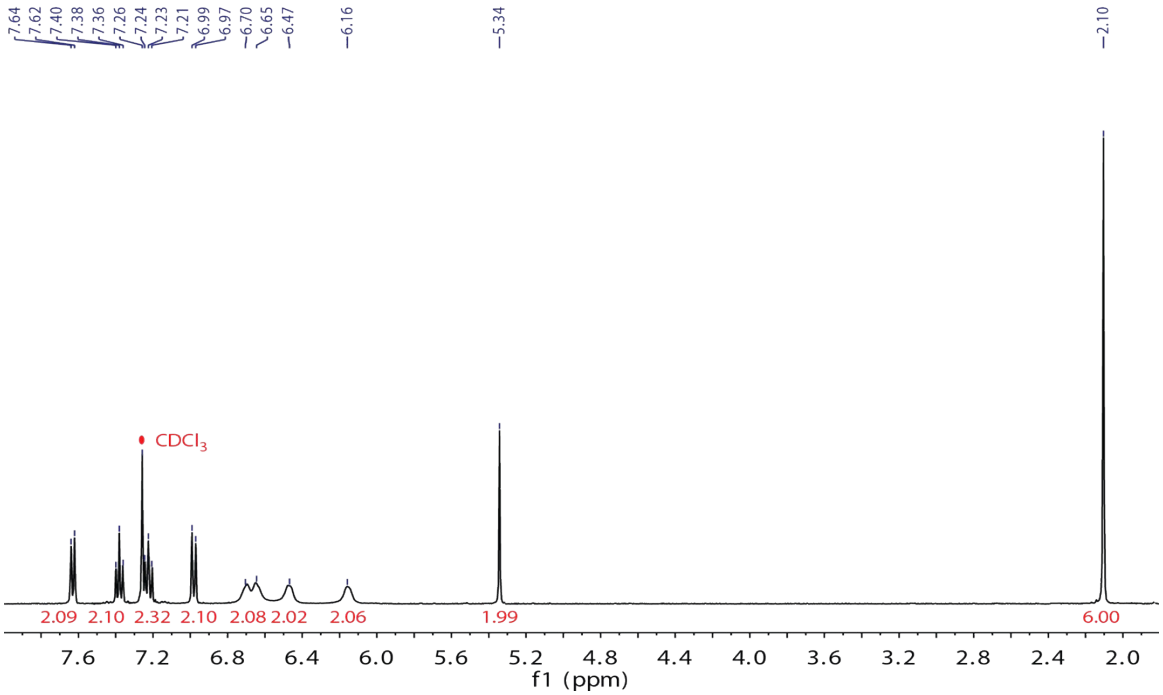


Figure S46. ^{1}H NMR spectrum of compound **19** in $CDCl_3$ at 298 K.

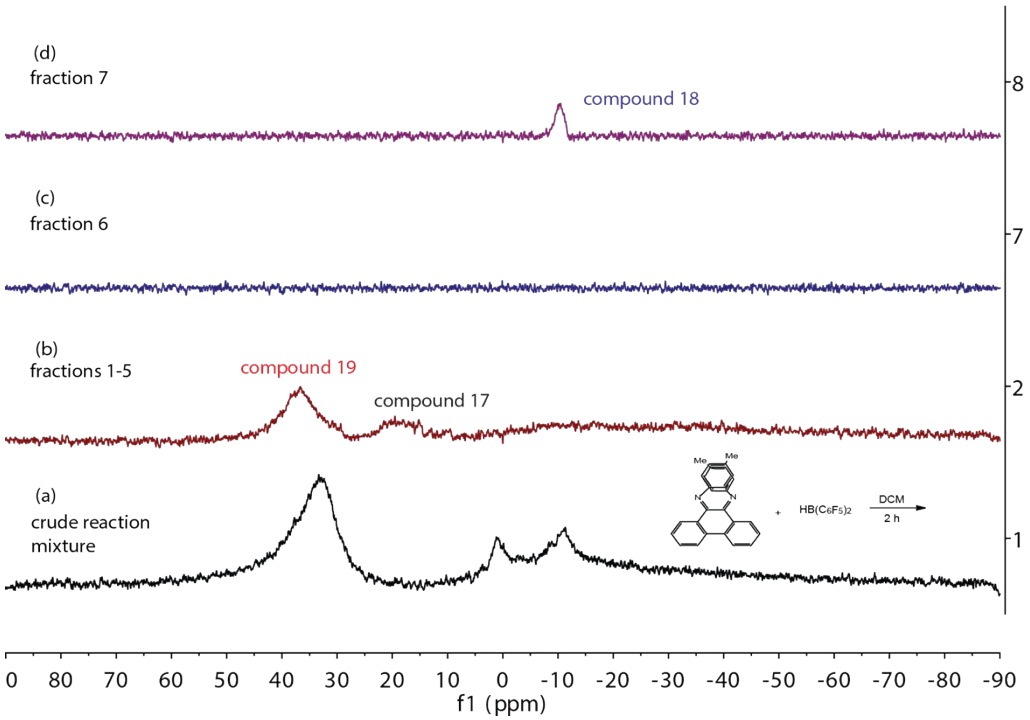


Figure S47. ^{11}B NMR spectra in $CDCl_3$ at 298 K of (a) crude reaction of compound **13** and $HB(C_6F_5)_2$ stirred for 2 h in CH_2Cl_2 (b) fractions 1-5, (c) fraction 6, and fraction 7 from flash column chromatography (silica gel, 95:5 pentane/CH_2Cl_2 eluent).

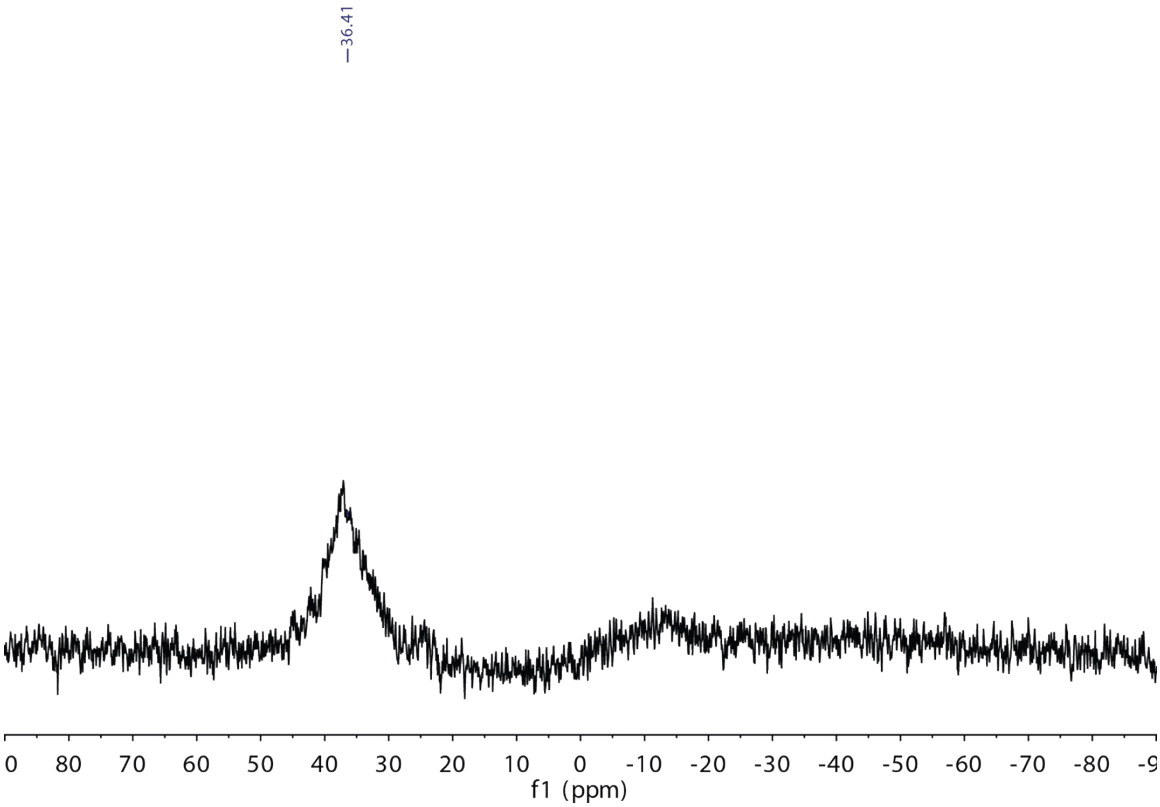


Figure S48. ^{11}B NMR spectrum of compound **19** in $CDCl_3$ at 298 K.

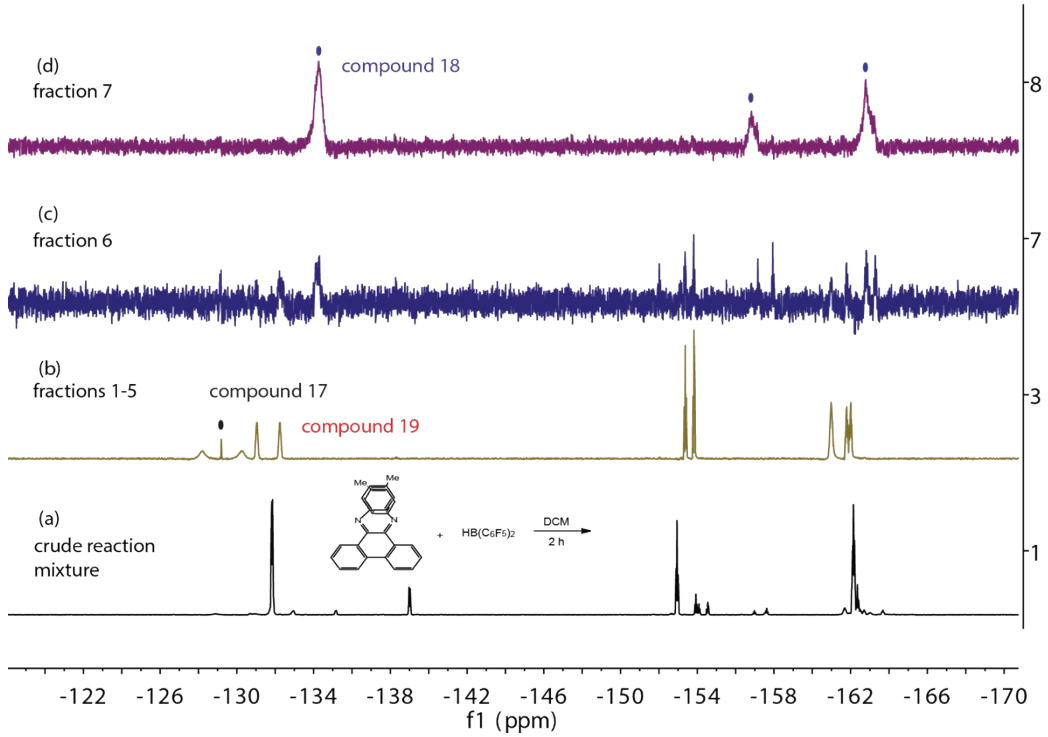


Figure S49. ^{19}F NMR spectra in $CDCl_3$ at 298 K of (a) crude reaction of compound **13** and $HB(C_6F_5)_2$ for 2 h in CH_2Cl_2 (b) fractions 1-5, (c) fraction 6, and fraction 7 from flash column chromatography (silica gel, 95:5 pentane/CH_2Cl_2 eluent).

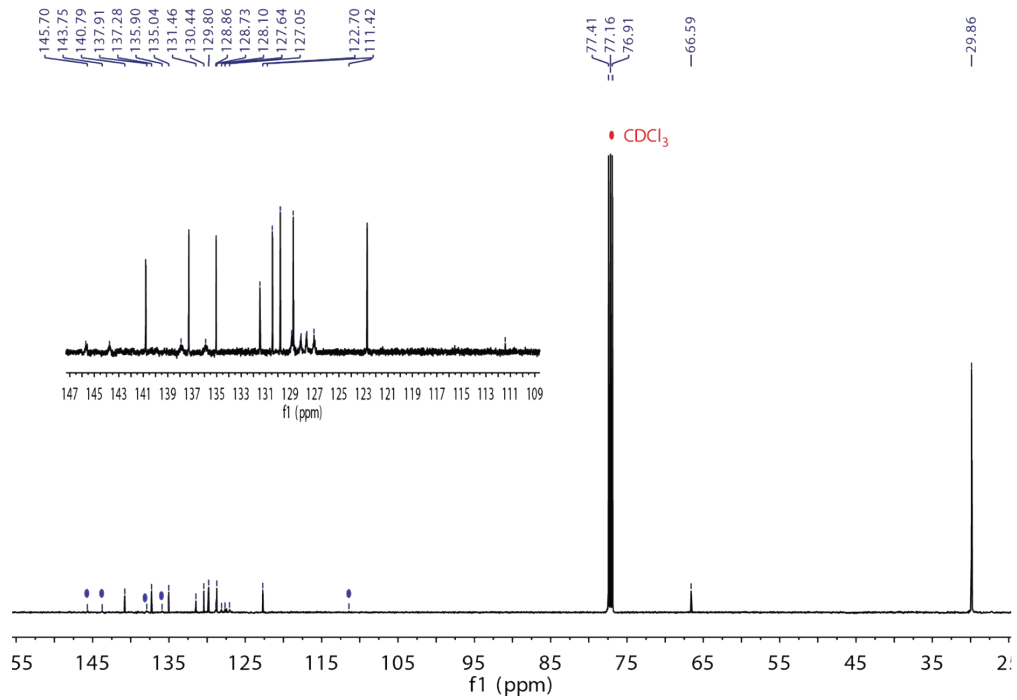


Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum of compound **19** in $CDCl_3$ at 298 K (purple markers = partially resolved set of C_6F_5 resonances).

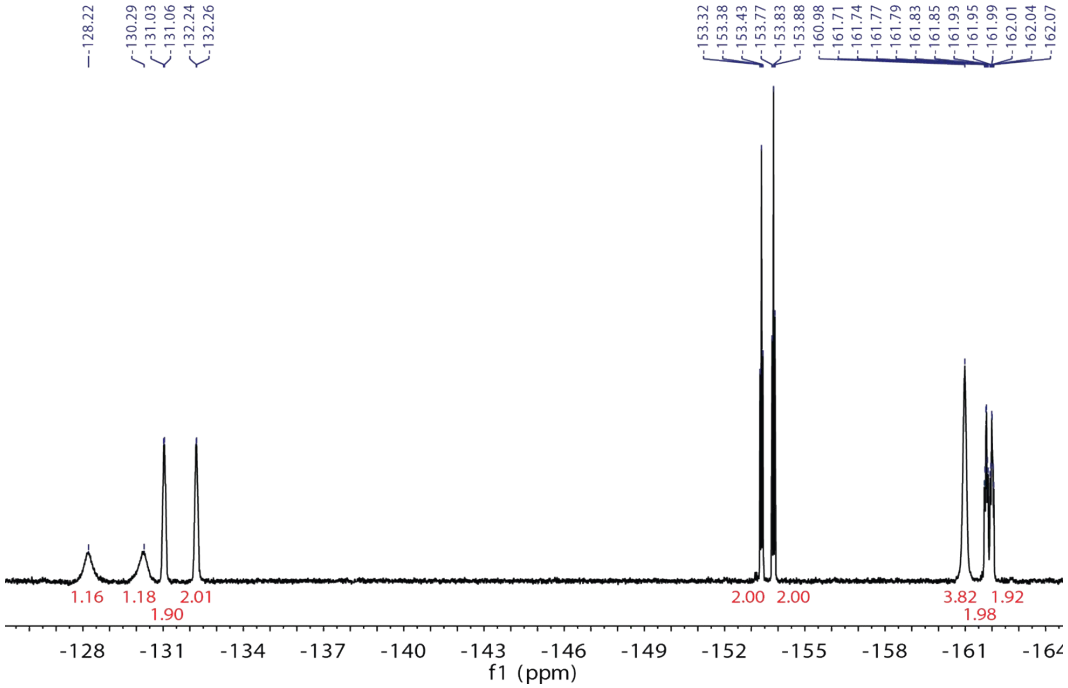


Figure S51. ^{19}F NMR spectrum of compound **19** in $CDCl_3$ at 298 K.

Single-Crystal X-Ray Crystallography

Crystallographic data (CCDC 1535312-1535321) can be obtained free of charge from the Cambridge

Crystallography Data Center at www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal and refinement data

	3	**4**	**5**	**6**	**9**
CCDC #	1535312	1535314	1535313	1535316	1535315
empirical formula	$C_{34}H_{18}BF_{10}NO$	$C_{34}H_{17}BF_{10}NO$	$C_{28}H_{17}BF_5NO$	$C_{22}H_{19}NO$	$C_{30}H_{28}N_2$
formula weight	657.30	656.29	489.23	313.38	416.54
crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic
space group	P21/c	C2/c	P21/n	P21/n	P-1
a (Å)	9.7684(15)	17.968(3)	12.5655(18)	7.9350(9)	8.4010(6)
b (Å)	14.767(3)	22.919(4)	10.2491(16)	9.8367(11)	9.7328(6)
c (Å)	19.986(4)	16.083(3)	17.699(3)	20.542(2)	14.7598(10)
α (°)	90	90	90	90	71.445(2)
β (°)	103.712(6)	122.027(7)	99.760(5)	97.585(5)	79.849(3)
γ (°)	90	90	90	90	86.645(3)
V (Å^3)	2800.8(9)	5615.2(18)	2246.4(6)	1589.3(3)	1126.19(13)
Z	4	8	4	4	2
D_{calc} (g·cm^{-3})	1.559	1.553	1.447	1.310	1.228
μ (mm^{-1})	0.139	0.139	0.116	0.080	0.071
reflections measured	21191	22087	19715	13959	15427
unique reflections, R_{int}	4943, 0.1245	4951, 0.0532	5166, 0.0716	3617, 0.0449	5177, 0.0221
No. of parameters	429	426	327	225	301
R_1, wR_2	0.0542, 0.1546	0.0421, 0.1465	0.500, 0.1493	0.0470, 0.1307	0.0411, 0.1282
GOF on F^2	1.003	1.052	0.994	1.020	1.065

* abbreviated name for 1,1-bis(perfluorophenyl)-3-phenyl-1,3-dihydro-[1,3,2]oxazaborolo[3,4-*a*]pyridine

Table S1. Crystal and refinement data (cont'd)

	10	**12·1/2CH_2Cl_2**	**15**	**17**	**18**
CCDC #	1535316	1535320	1535319	1535321	1535318
empirical	$C_{49}H_{35}BF_{10}N_2$	$C_{73}H_{54}B_2Cl_2F_{10}N_4$	$C_{28}H_{24}N_2$	$C_{34}H_{22}BF_5N_2$	$C_{40}H_{22}BF_{10}N_2$

formula					
formula weight	852.60	1269.72	388.49	564.34	731.40
crystal system	monoclinic	monoclinic	monoclinic	orthorombic	orthorombic
space group	C2/c	P21/n	P21/n	Pbcn	Pbcn
a (Å)	50.971(13)	13.950(3)	20.763(4)	10.3922(19)	9.508(4)
b (Å)	17.609(4)	15.254(5)	5.6764(9)	19.522(3)	21.381(8)
c (Å)	18.424(5)	14.255(3)	35.740(6)	39.998(6)	15.841(6)
α (°)	90	90	90	90	90
β (°)	104.812(15)	91.584(16)	99.442(11)	90	90
γ (°)	90	90	90	90	90
V (Å^3)	15987(7)	3032.2(13)	4155.2(13)	8115(2)	3220(2)
Z	16	2	8	12	4
D_{calc} (g·cm^{-3})	1.417	1.391	1.242	1.386	1.509
μ (mm^{-1})	0.115	0.187	0.072	0.105	0.129
reflections measured	63167	46574	33306	72097	14156
unique reflections, R_{int}	15404, 0.1080	5491, 0.1672	8109, 0.1756	9400, 0.0944	1507, 0.2099
No. of parameters	1173	428	561	573	241
R_1, wR_2	0.0570, 0.1891	0.0595, 0.1402	0.0834, 0.2149	0.0544, 0.1306	0.0578, 0.1971
GOF on F^2	0.967	1.015	1.000	1.014	1.056

EPR Spectroscopy

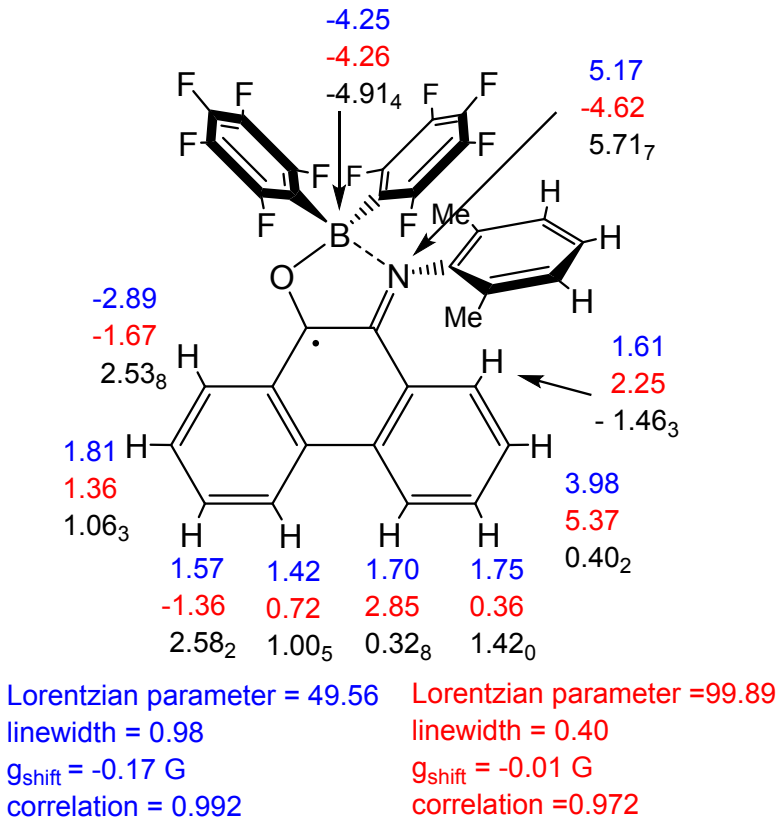


Figure S52. Hyperfine coupling constants (G) for EPR simulations of **4**. DFT-computed values, black; WINSIM optimized values for broad spectrum starting from DFT-computed initial values, blue; WINSIM optimized values for fine spectrum starting form DFT-computed initial values, red.

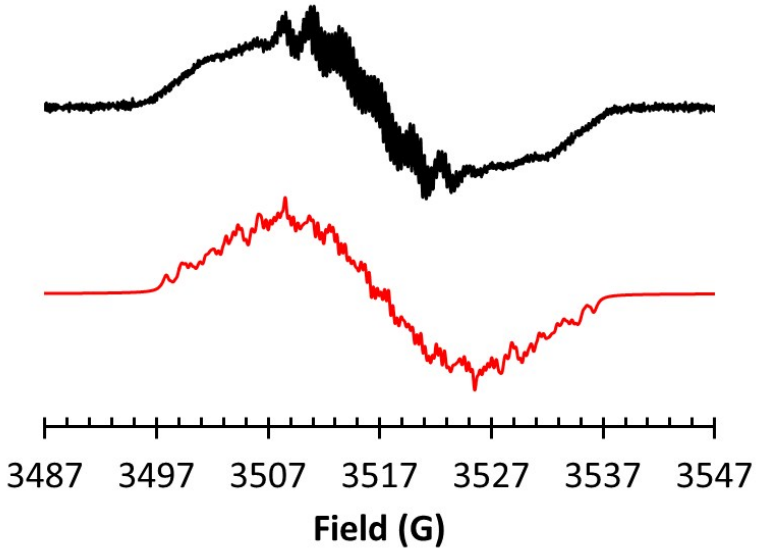


Figure S53. Experimental X-band EPR spectrum of **4** in toluene at 298 K (black: mod. amp. = 0.025 G) and simulated EPR spectrum (red line: g = 2.0038).

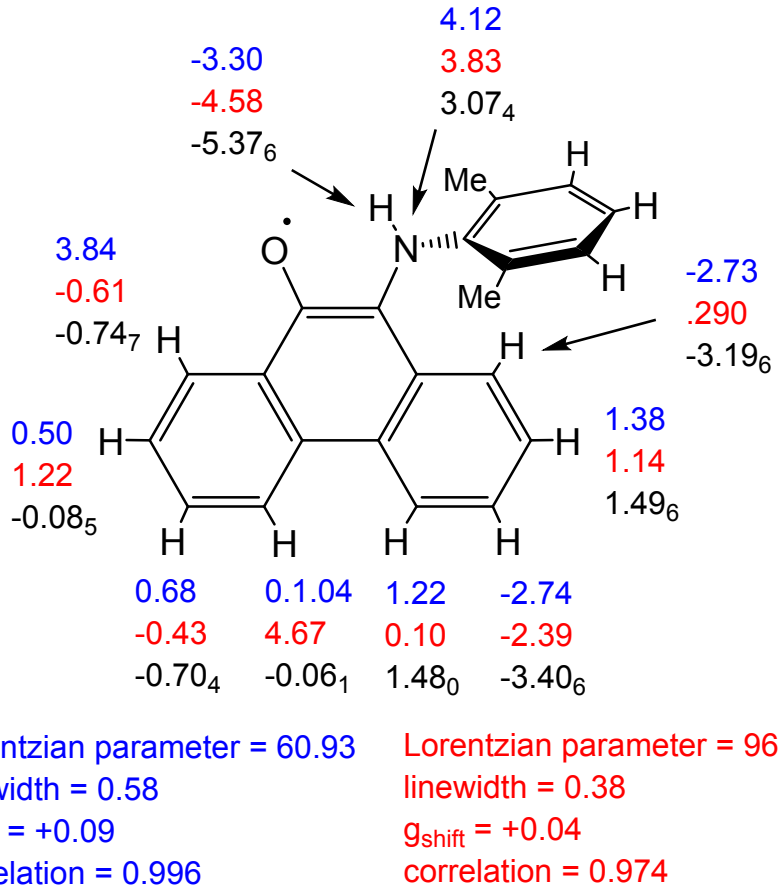


Figure S54. Hyperfine coupling constants (G) for EPR simulations of semiiminoquinone radical. DFT-computed values, black; WINSIM optimized values for broad spectrum starting from DFT-computed initial values, blue; WINSIM optimized values for fine spectrum starting from DFT-computed initial values, red.

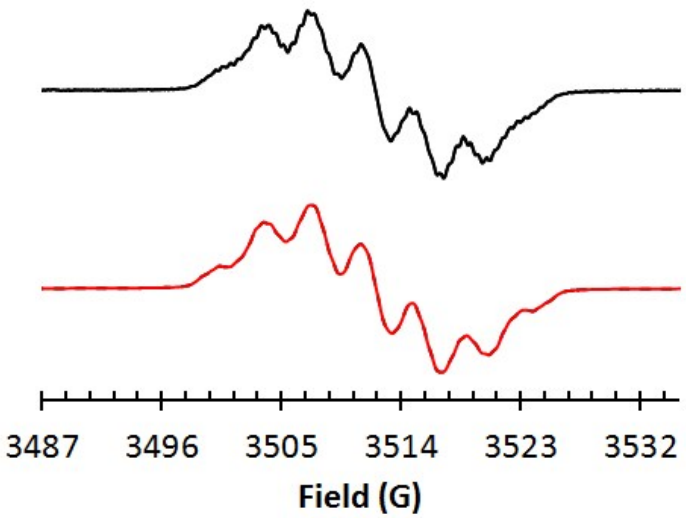


Figure S55. Experimental X-band EPR spectrum of solution containing equimolar mixture of **1** and **6** in toluene at 298 K (black: mod. amp = 1 G) and simulated EPR spectrum (red line: g = 2.0026).

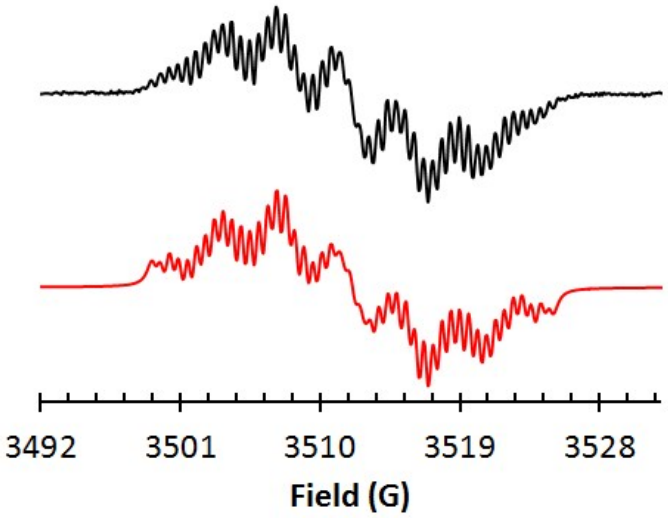


Figure S56. Experimental X-band EPR spectrum of solution containing equimolar mixture of **1** and **6** in toluene at 298 K (black: mod. amp = 0.25 G) and simulated EPR spectrum (red line: g = 2.0026).

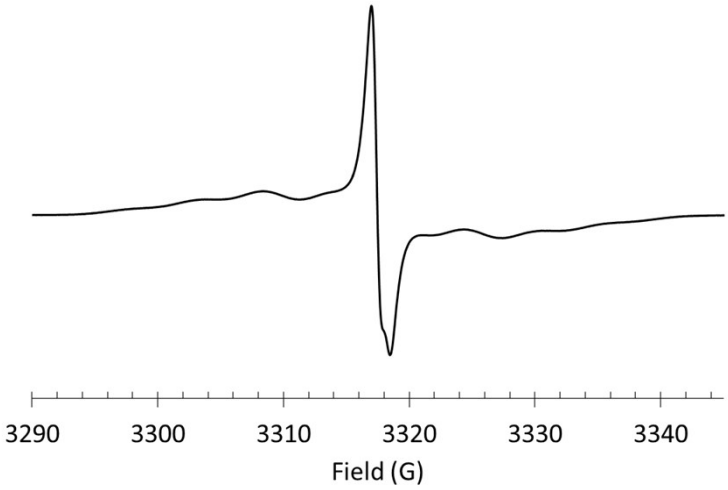


Figure S57. Experimental X-band EPR spectrum of reaction mixture containing $HB(C_6F_5)_2$ and compound **13** in toluene at 298 K (mod. amp. = 0.25 G, g = 2.0044).

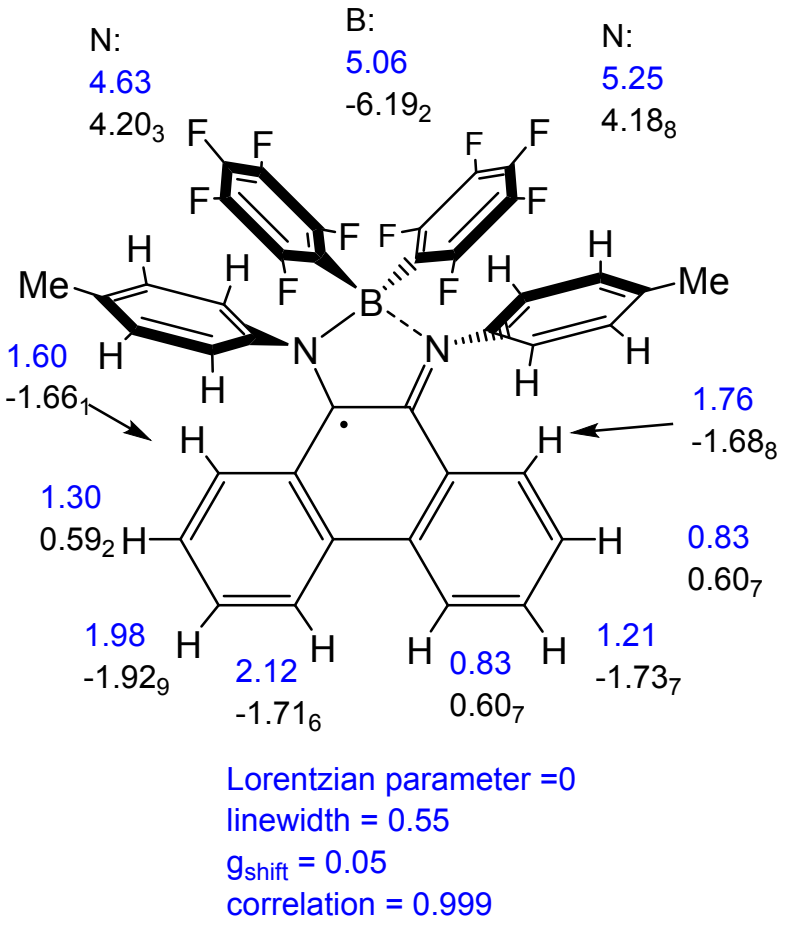


Figure S58. Hyperfine coupling constants (G) for EPR simulations of compound **18**. DFT-computed values, black; WINSIM optimized values for broad spectrum starting from DFT-computed initial values, blue.

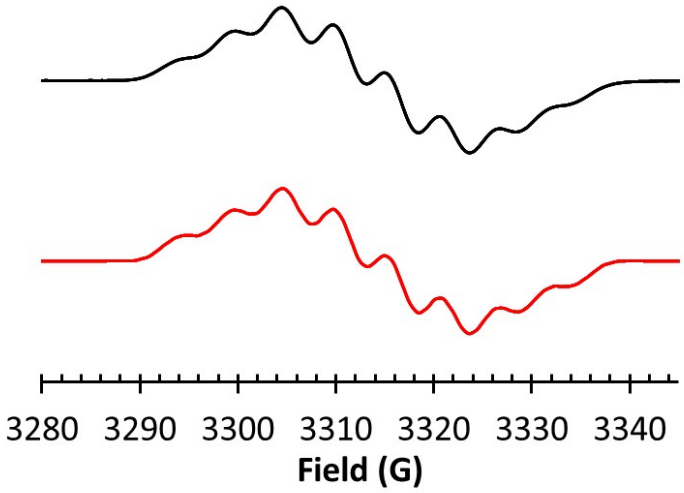


Figure S59. Experimental X-band EPR spectrum of **18** in toluene at 298 K (black: mod. amp. = 1 G) and simulated EPR spectrum (red line: g = 2.0044).

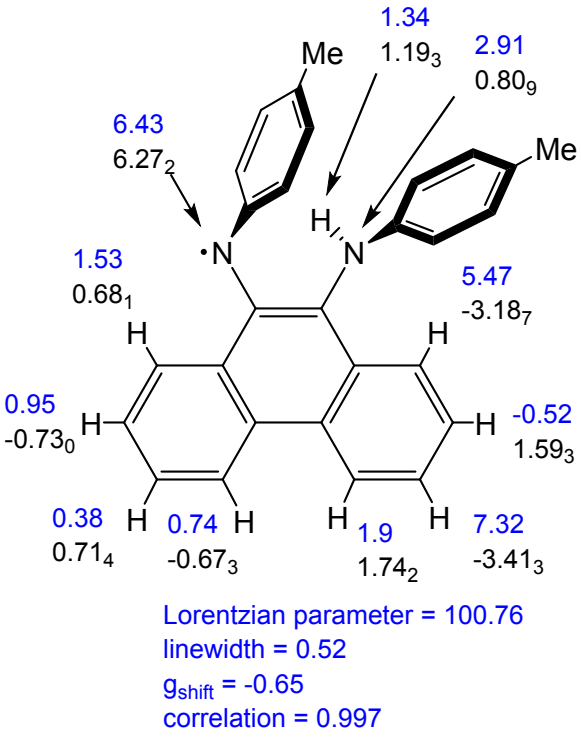


Figure S60. Hyperfine coupling constants (G) for EPR simulations of semidiimine **S**. DFT-computed values, black; WINSIM optimized values for broad spectrum starting from DFT-computed initial values, blue.

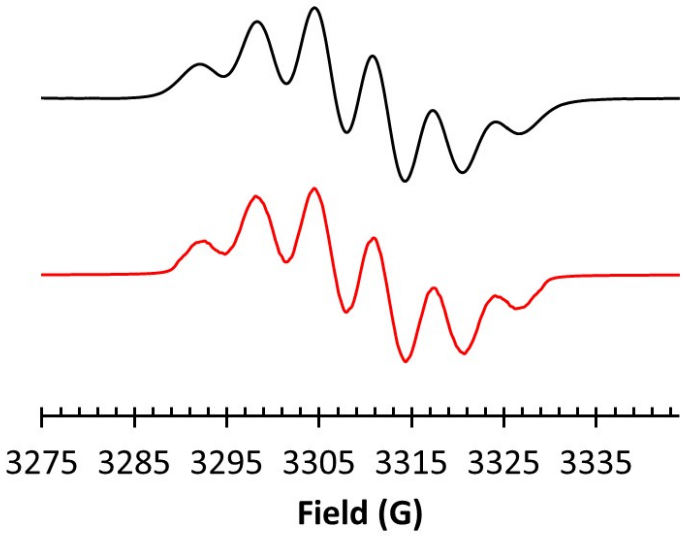


Figure S61. Experimental X-band EPR spectrum of solution containing equimolar mixture of **13** and **15** in toluene at 298 K (black: mod. amp = 1 G) and simulated EPR spectrum (red line: g = 2.0044).

Cyclic Voltammetry

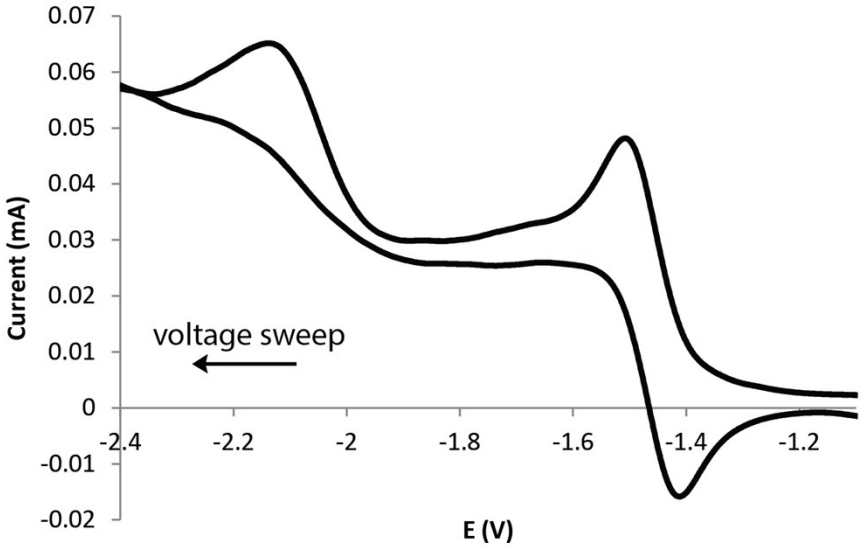


Figure S62. Cyclic voltammogram of compound **1** ($E_{1/2}$ (reversible) = -1.46 V, E_{pc} (irreversible) = -2.14 V) in DCM; x-axis referenced with respect to Fc/Fc^+ couple.

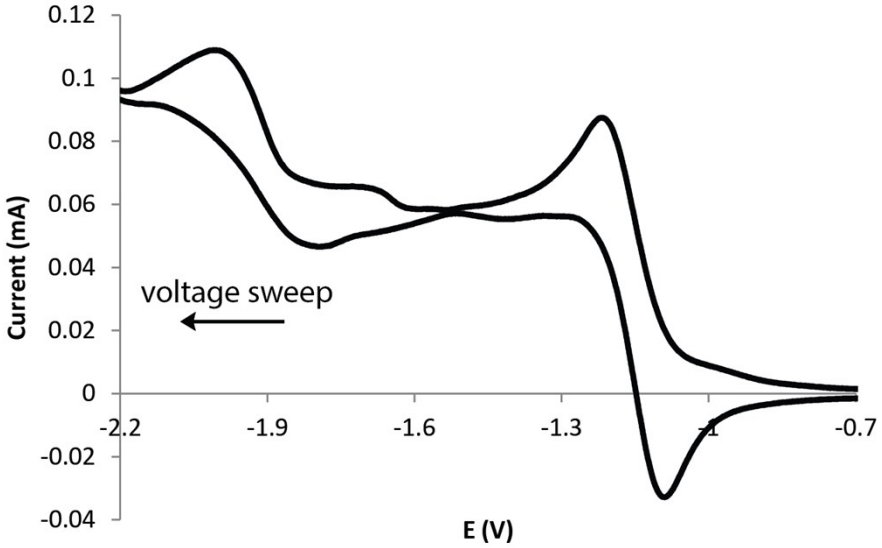


Figure S63. Cyclic voltammogram of 9,10-phenanthrenequinone ($E_{1/2}$ (reversible) = -1.15 V, $E_{1/2}$ (reversible) = -1.90 V) in DCM; x-axis referenced with respect to Fc/Fc^+ couple.

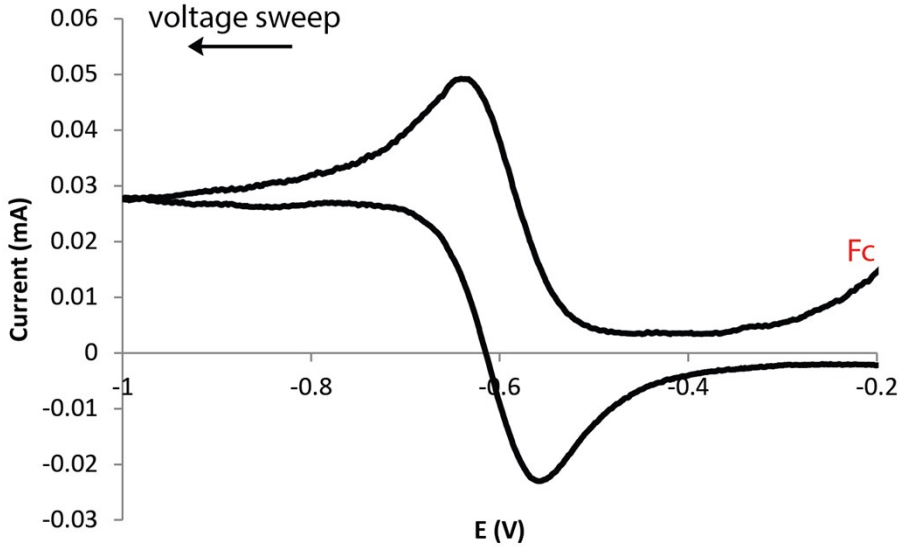


Figure S64. Cyclic voltammogram of compound **4** ($E_{1/2}$ (reversible) = -0.60 V) in DCM; x-axis referenced with respect to Fc/Fc^+ couple.

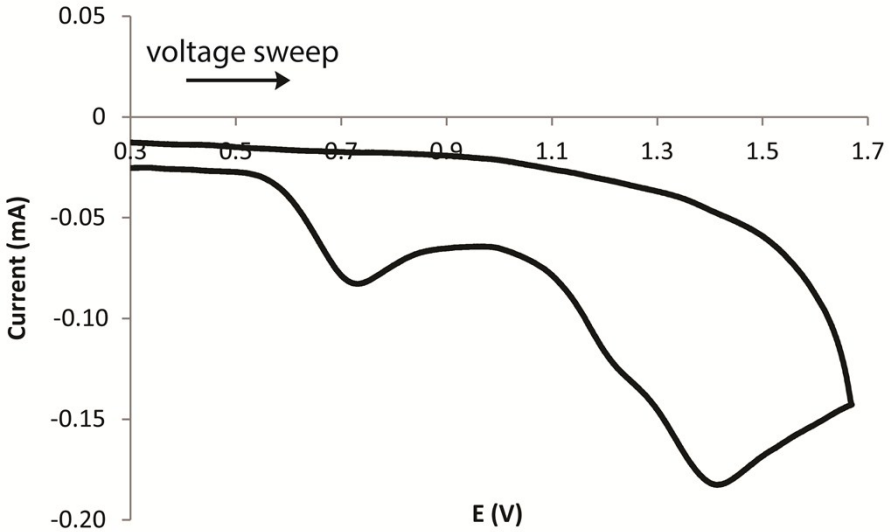


Figure S65. Cyclic voltammogram of compound **5** (E_{pa} (irreversible) = 0.73 V, E_{pa} (irreversible) = 1.41 V) in DCM; x-axis referenced with respect to Fc/Fc^+ couple.

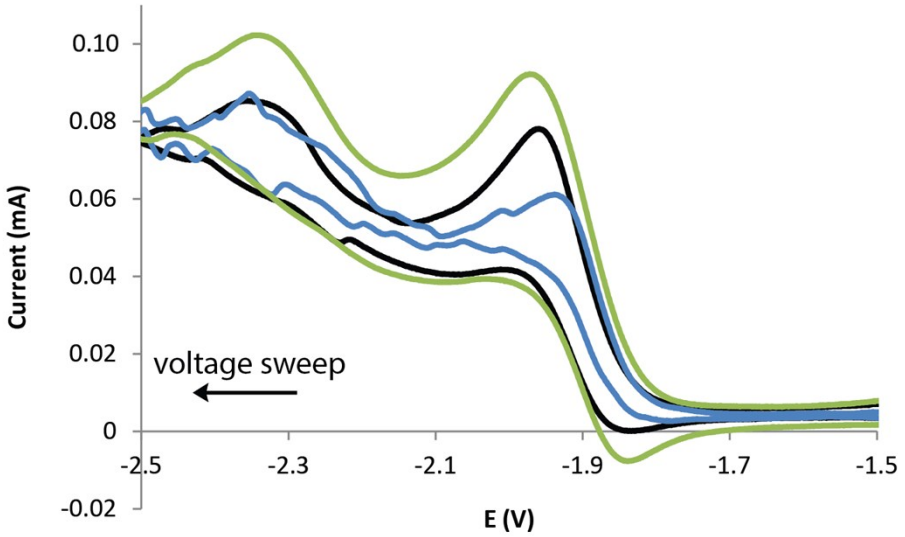


Figure S66. Cyclic voltammogram of compound **7** ($E_{1/2}$ (pseudo-reversible) = -1.90 V, E_{pc} (irreversible) = -2.29 V; 100 mV/s) in DCM; x-axis referenced with respect to Fc/Fc^+ couple. Green: 200 mV/s; black: 100 mV/s; blue: 50 mV/s.

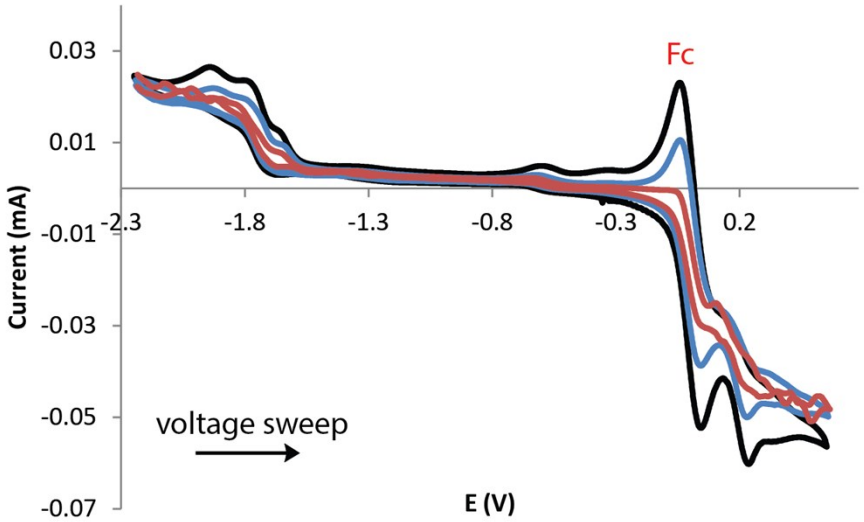


Figure S67. Cyclic voltammogram of compound **13** (E_{pa} (irreversible) = 0.24 V, $E_{1/2}$ (pseudo-reversible) ≈ -1.80 V; 100 mV/s) in DCM; x-axis referenced with respect to Fc/Fc^+ couple. Black: 100 mV/s, blue: 50 mV/s; red: 20 mV/s.

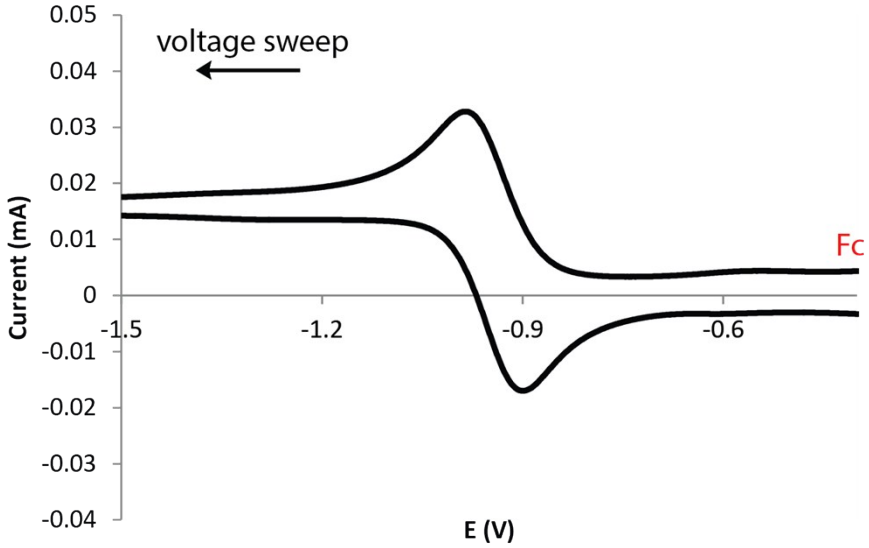


Figure S68. Cyclic voltammogram of compound **18** ($E_{1/2}$ (reversible) = -0.94 V) in DCM; x-axis referenced with respect to Fc/Fc^{+} couple.

UV-Visible Spectroscopy

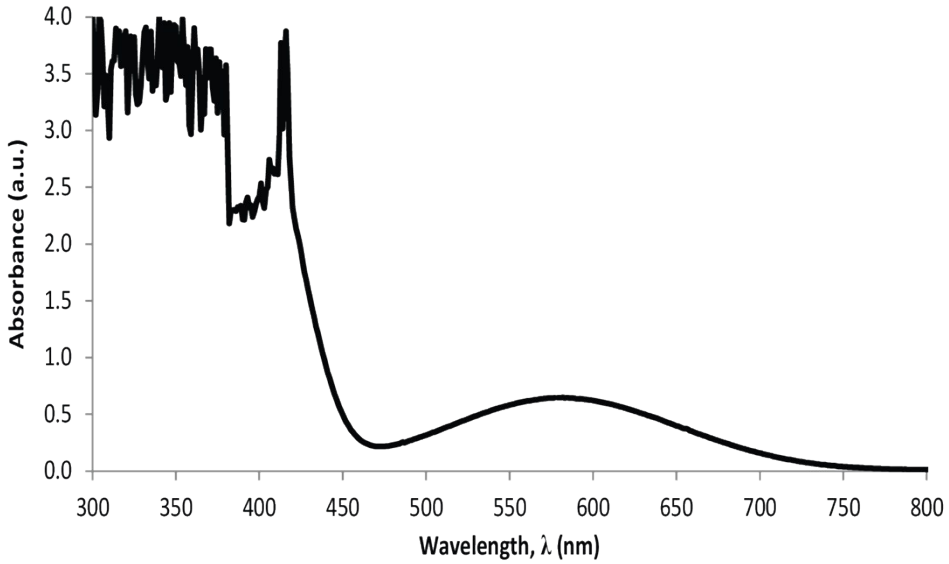


Figure S69. UV-Vis absorption spectrum of compound **1** in dry dichloromethane (1 x 10^{-3} M; λ^{1}_{max} = 416 nm and λ^{2} = 582 nm).

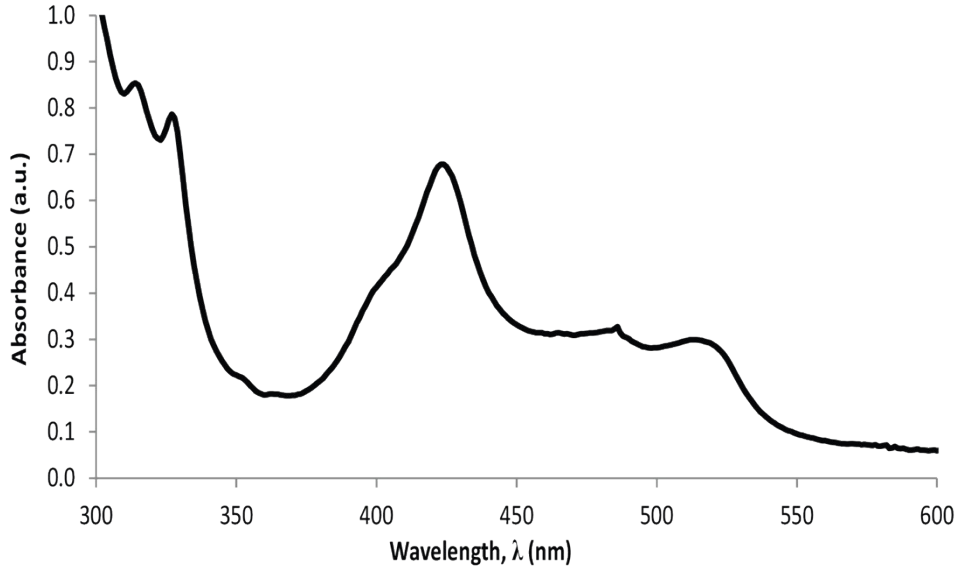


Figure S70. UV-Vis absorption spectrum of compound **4** in dry dichloromethane (6 x 10^{-5} M).

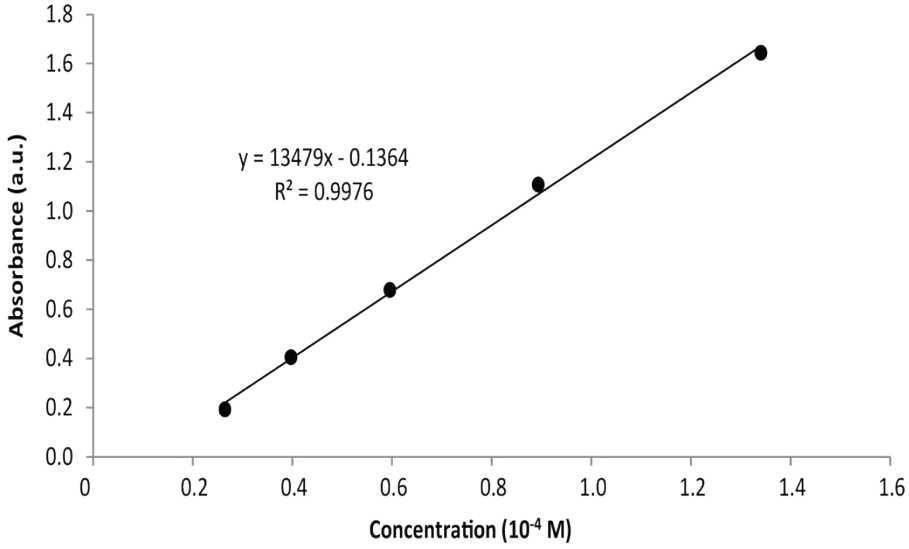


Figure S71. Beer-Lambert plot for compound **4** in dry dichloromethane (λ_{max} = 423 nm, ε = 1.3 x 10^3 $L \cdot cm^{-1} \cdot mol^{-1}$).

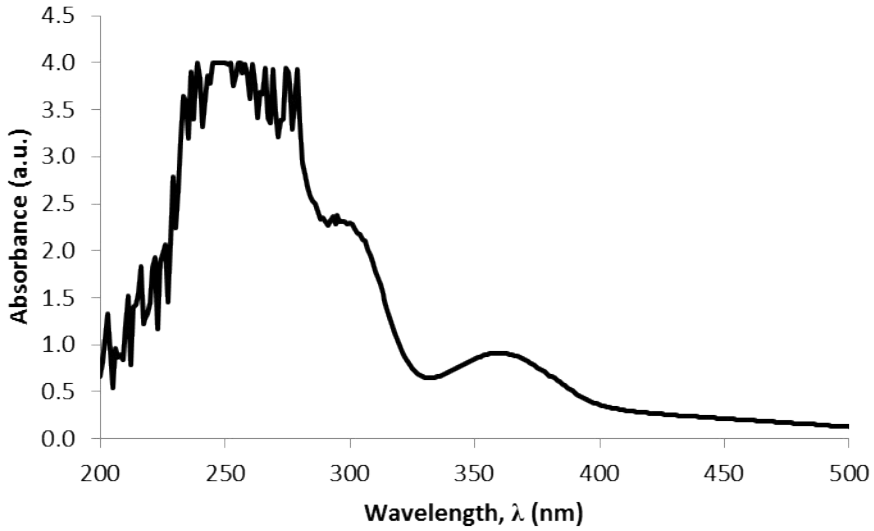


Figure S72. UV-Vis absorption spectrum of compound **7** in dry dichloromethane (4 x 10^{-4} M; λ^1_{max} = 299 nm, λ^2_{max} = 360 nm).

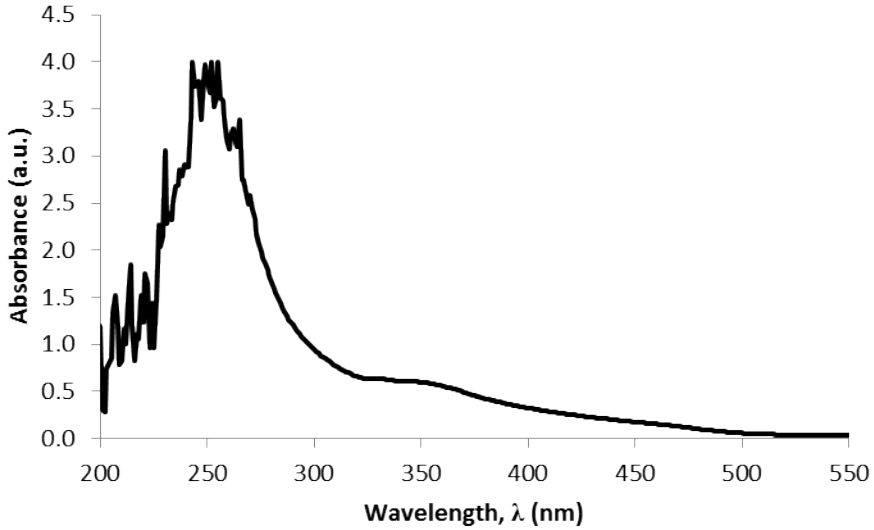


Figure S73. UV-Vis absorption spectrum of compound **13** in dry dichloromethane (1 x 10^{-4} M; λ_{max} = 344 nm).

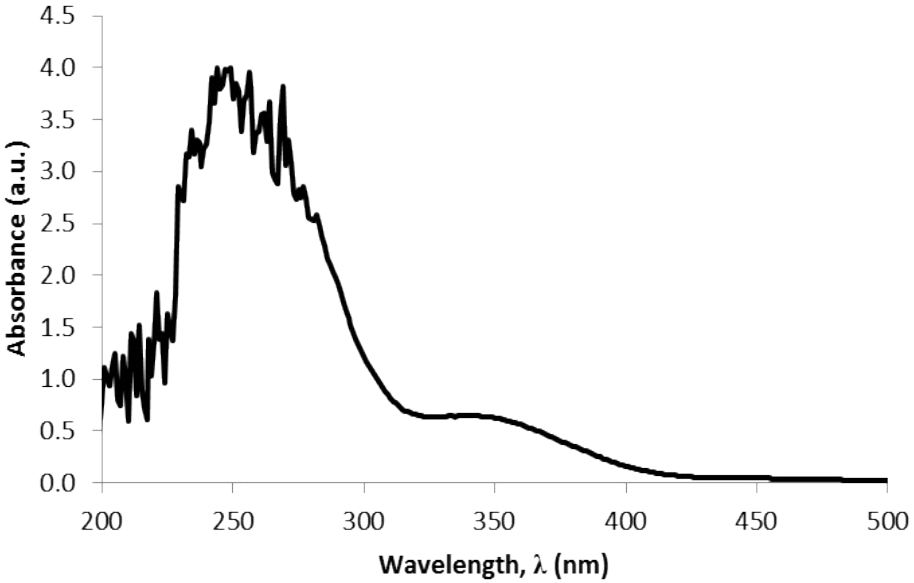


Figure S74. UV-Vis absorption spectrum of compound **15** in dry dichloromethane (9 x 10^{-4} M; λ_{max} = 348 nm).

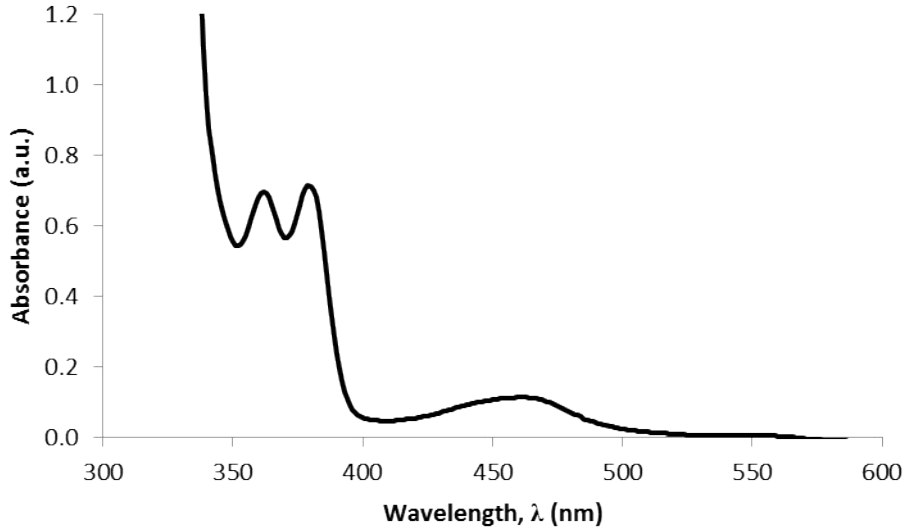


Figure S75.UV-Vis absorption spectrum of compound **17** in dry dichloromethane (3 x 10^{-4} M; λ^1_{max} = 379 nm, λ^2 = 362 nm and λ^3 = 460 nm).

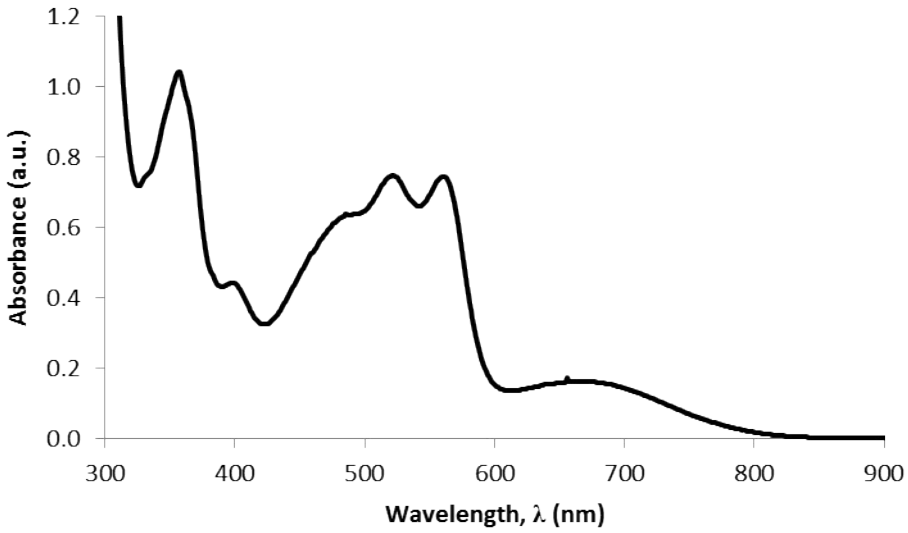


Figure S76. UV-Vis absorption spectrum of compound **18** in dry dichloromethane (2 x 10^{-4} M; λ^1_{max} = 358 nm, λ^2 = 562 nm, λ^3 = 523 nm), and λ^4 = 666 nm).

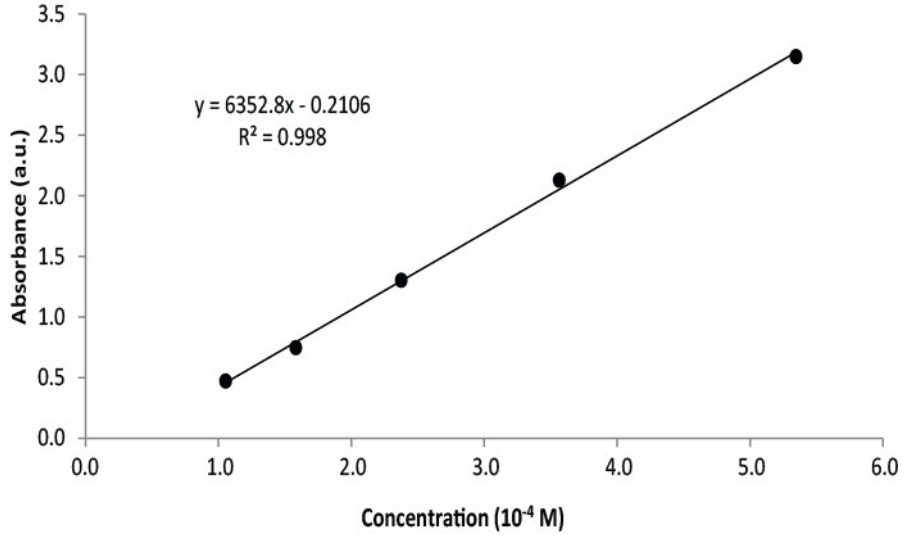


Figure S77. Beer-Lambert plot for compound **18** in dry dichloromethane (λ_{max} = 523 nm, ε = 6.4 x 10^3 $L \cdot cm^{-1} \cdot mol^{-1}$).

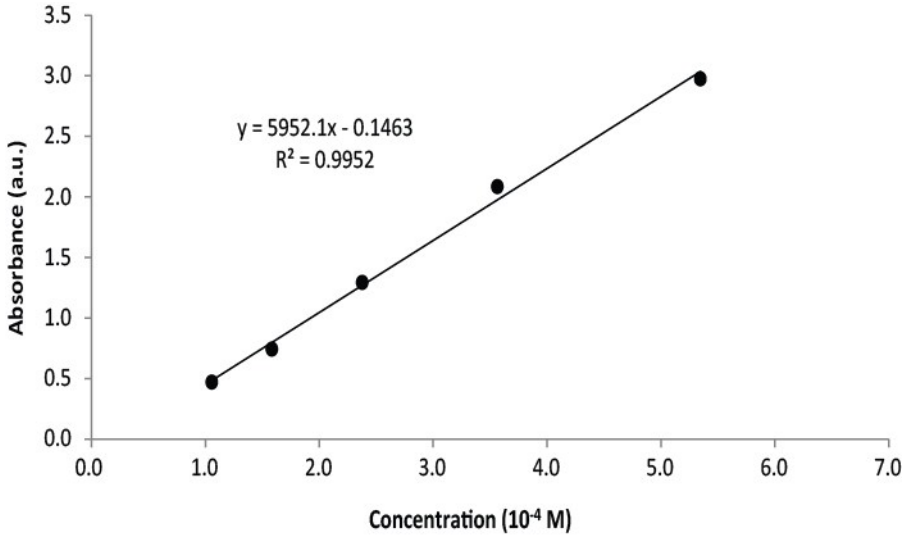


Figure S78. Beer-Lambert plot for compound **18** in dry dichloromethane (λ_{max} = 562 nm, ε = 5.9 x 10^3 $L \cdot cm^{-1} \cdot mol^{-1}$).

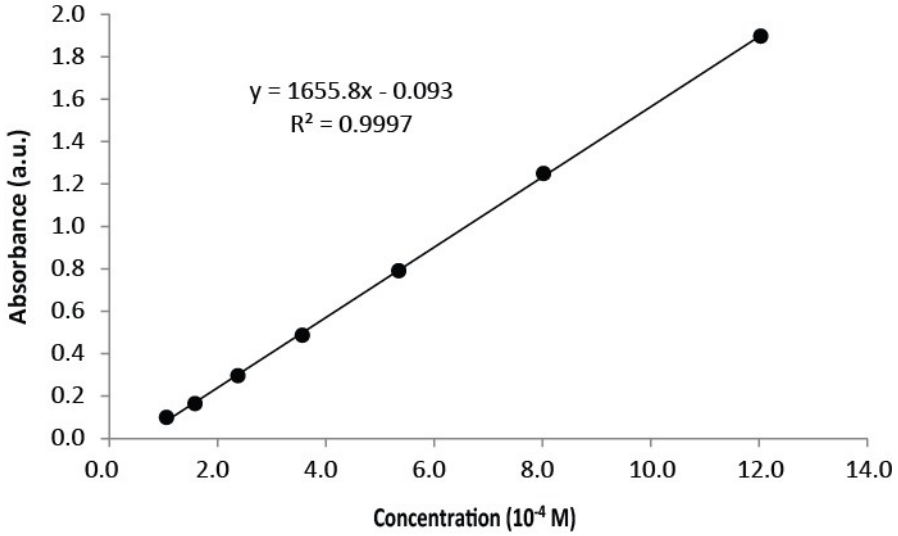


Figure S79. Beer-Lambert plot for compound **18** in dry dichloromethane (λ = 666 nm, ε = 1.7 x 10^3 $L \cdot cm^{-1} \cdot mol^{-1}$).

Computational Details

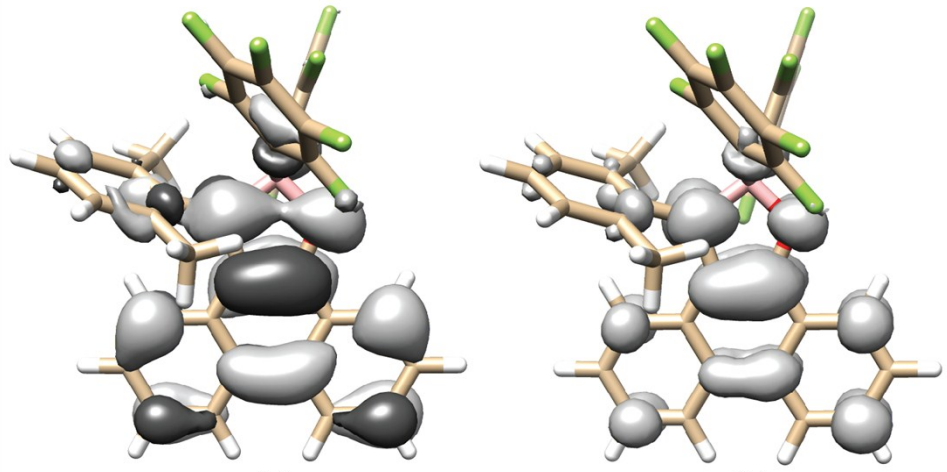


Figure S80. Calculated SOMO (a) and spin density (b) at a contour surface value of 0.03 a.u. (computational level: PW6B95/def2-TZVP //TPSS-D3/def2-TZVP) for compound **4**.

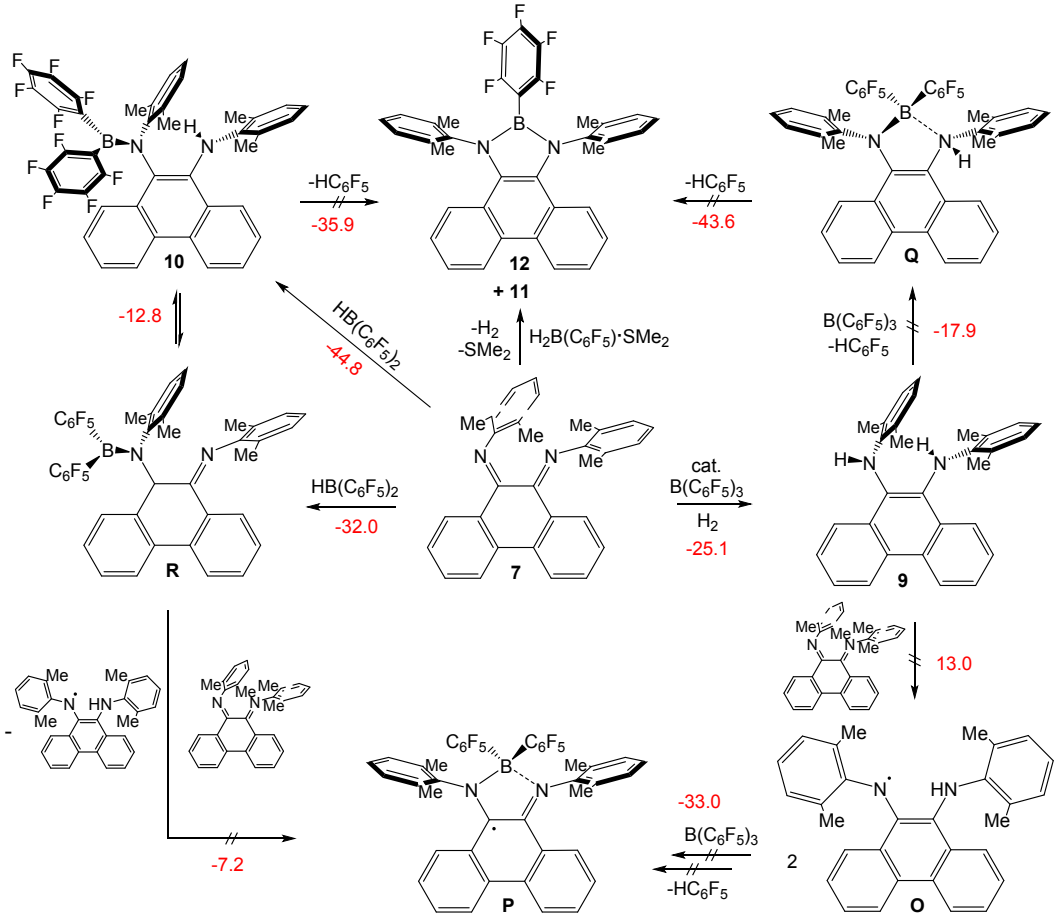


Figure S81. Proposed reaction pathways involving compound **7** and its derivatives with DFT-computed Gibbs energies of reaction (red, kcal·mol^{-1}, computational level: PW6B95/def2-TZVP (COSMO-RS, toluene)//PBEh-3c).

Computed Hyperfine Coupling Constants

Table S2. Cartesian coordinates (PBEh-3c), and the computed hyperfine coupling constants (PBE0/def2-QZVP) for compound **4**.

Element	Atom #	Cartesian coordinates (Å)			HFC (MHz)
f	1	-2.6250102	-5.2397023	3.2974070	-0.3128
f	2	-3.1685018	4.6798476	2.8537603	-0.0583
f	3	-3.0153034	1.7335394	-0.7414927	-1.2777
f	4	-0.8419418	0.6643998	3.3013505	3.9621
o	5	-1.7212585	-0.5373838	-0.7722780	-15.8366
f	6	-3.3282251	-0.6713906	2.8112309	1.2783
f	7	-0.7726080	-5.1871876	1.3135580	1.5908
f	8	-0.1854934	-2.9018706	0.0936272	5.1388
f	9	-3.8479839	4.0067284	0.3200899	0.6823
f	10	-1.6457503	2.9915397	4.3348442	1.8132
f	11	-3.8902252	-2.9547025	4.0125431	2.0467
n	12	0.2906751	-0.0802852	0.3581249	16.0103
c	13	-2.3231651	-4.0970189	2.6993685	-0.3117
c	14	-2.9597085	-2.9284903	3.0658818	2.2660
c	15	-2.6297642	-1.7397300	2.4331017	-0.8393
c	16	-1.6568027	-1.6505846	1.4490978	33.2036
b	17	-1.2733965	-0.2915139	0.6333792	-13.7596
c	18	0.5153684	-0.2579157	-0.9477308	-9.4377
c	19	1.7341793	-0.2395207	-1.7154183	-7.5037
c	20	1.6292528	-0.3886634	-3.1213982	1.0439
c	21	2.8116471	-0.3832968	-3.8693929	-3.7655
c	22	4.0470750	-0.2509960	-3.2753510	4.4881
c	23	-2.7540650	3.5314517	2.3379716	-0.1601
c	24	-3.0999157	3.1842227	1.0477294	1.6167
c	25	-2.6560804	1.9827603	0.5181495	-1.4080
c	26	-1.8711511	1.0925465	1.2331396	27.8664
c	27	-1.5587118	1.4812056	2.5267056	-0.9127
c	28	-1.9745857	2.6709192	3.0893512	1.6603
c	29	-0.7156995	-0.5091979	-1.5848535	12.0559
c	30	1.1957966	0.6078641	1.2149342	-9.8601
c	31	1.8202122	-0.0691556	2.2674670	11.5588
c	32	2.6724906	0.6476359	3.0978665	-0.6025
c	33	2.8981495	1.9978906	2.8996332	0.9111
c	34	2.2836094	2.6470711	1.8455721	1.7070
c	35	1.4316927	1.9692576	0.9798483	16.2260
c	36	0.8534980	2.7102314	-0.1902434	-1.1059
c	37	1.6231246	-1.5346336	2.5069417	-0.4281
c	38	3.0028179	-0.1271274	-1.1254490	4.3125
c	39	4.1442445	-0.1310357	-1.8927687	-4.2857
c	40	0.3298125	-0.5692473	-3.7689379	7.7071
c	41	0.1814794	-0.6685932	-5.1563926	-8.3788
c	42	-1.0574163	-0.8503909	-5.7350056	9.1421
c	43	-2.2065296	-0.9404338	-4.9486504	-8.5074
c	44	-2.1000499	-0.8421395	-3.5828627	8.9698
c	45	-0.8424265	-0.6565938	-2.9893558	-16.5922
c	46	-1.3775865	-4.0665114	1.6911169	0.8562
c	47	-1.0828894	-2.8612542	1.0846760	-1.4254
h	48	2.3801393	-1.9123960	3.1923576	0.4849

h	49	0.6511793	-1.7369552	2.9564094	1.9101
h	50	1.6923735	-2.1144720	1.5884924	0.1750
h	51	0.8417085	3.7811320	0.0070724	-0.1902
h	52	1.4556345	2.5549581	-1.0883085	0.4463
h	53	-0.1649850	2.4155160	-0.4294550	1.1512
h	54	3.1634437	0.1334274	3.9144038	1.3614
h	55	3.5568633	2.5419506	3.5632488	-0.8085
h	56	2.4653991	3.7019896	1.6826593	2.3097
h	57	3.0983432	-0.0430771	-0.0542987	-4.0972
h	58	5.1113182	-0.0459353	-1.4165621	1.1268
h	59	4.9389957	-0.2535485	-3.8871275	-3.9763
h	60	2.7746708	-0.4978054	-4.9424473	0.9201
h	61	1.0394227	-0.5981684	-5.8083076	2.8165
h	62	-1.1346788	-0.9202711	-6.8117016	-7.2302
h	63	-3.1736759	-1.0803266	-5.4114349	2.9775
h	64	-2.9790316	-0.8985623	-2.9558867	-7.1078

Table S3. Cartesian coordinates (PBEh-3c), and the computed hyperfine coupling constants (PBE0/def2-QZVP) for semiiminoquinone **E**.

Element	Atom #	Cartesian coordinates (Å)			HFC(MHz)
C	1	0.326805	-0.150352	5.302920	1.6153
C	2	-0.585192	-1.190860	5.140988	-1.4518
H	3	-1.033277	-1.663237	6.004831	-0.2387
C	4	-0.916923	-1.606606	3.871618	1.2730
H	5	-1.630594	-2.404654	3.720690	-2.0916
C	6	-0.343878	-0.998475	2.751412	-4.1990
C	7	0.589071	0.038143	2.901238	-2.5301
C	8	0.901499	0.449975	4.203678	-1.2171
C	9	1.217050	0.626773	1.719704	11.9416
C	10	-0.773465	-1.438096	1.424256	-14.4767
C	11	-0.228199	-0.741831	0.276311	18.4973
C	12	0.827668	0.214380	0.419075	-21.0092
C	13	2.240190	1.571441	1.835722	-11.7032
C	14	1.524689	0.730541	-0.692431	11.7062
C	15	2.531919	1.653362	-0.540847	-11.2197
C	16	2.884810	2.090840	0.732957	12.2747
O	17	-1.603182	-2.337423	1.261737	-14.7967
N	18	-0.771515	-1.140430	-0.896272	8.6077
H	19	-1.379764	-1.943540	-0.769966	-15.0546
C	20	-0.880935	-0.445515	-2.119471	-6.2455
C	21	-1.441441	0.836029	-2.167519	12.7125
C	22	-0.450980	-1.101959	-3.277909	8.8167
C	23	-0.564582	-0.443445	-4.495215	-1.5515
C	24	-1.086814	0.837656	-4.559959	1.7619
C	25	-1.522405	1.464619	-3.405462	0.0749
C	26	-1.957557	1.525073	-0.939873	-1.3627
C	27	0.134467	-2.480531	-3.196314	-0.0400
H	28	2.559982	1.903408	2.812559	4.1465
H	29	3.673290	2.819612	0.863608	-9.5379
H	30	3.050670	2.029033	-1.412452	4.1891
H	31	1.284171	0.393699	-1.688912	-8.9496

H	32	-0.230963	-0.938045	-5.398993	1.0139
H	33	-1.163885	1.344068	-5.512958	-1.4353
H	34	-1.949671	2.458112	-3.462199	2.0143
H	35	-1.150127	1.959109	-0.347307	0.6384
H	36	-2.631974	2.335174	-1.213470	0.1839
H	37	-2.505456	0.843732	-0.289029	3.1071
H	38	0.525856	-2.795214	-4.162342	1.2757
H	39	0.947231	-2.529924	-2.470596	0.4304
H	40	-0.607046	-3.222164	-2.891807	3.6566
H	41	0.588764	0.192262	6.295278	-1.9716
H	42	1.601690	1.255263	4.372724	-0.1728

Table S4. Cartesian coordinates (PBEh-3c) and the computed hyperfine coupling constants (PBE0/def2-QZVP) for compound **18**.

Element	Atom #	Cartesian coordinates (Å)			HFC(MHz)
N	1	0.823015	-0.12135	-0.83697	11.7686
F	2	-1.0356	-2.56141	0.692494	-3.749
F	3	-2.05693	-4.71942	-0.45807	1.2837
F	4	-2.95878	-4.61872	-3.01467	-0.3404
F	5	-2.82595	-2.2898	-4.39543	3.0002
F	6	-1.84225	-0.10375	-3.2498	4.5784
C	7	0.635878	-0.10383	1.416177	-1.2785
C	8	1.11028	-0.33602	2.754151	-9.9605
C	9	0.238277	-0.50378	3.843597	5.2287
H	10	-0.82779	-0.41949	3.706075	-4.7271
C	11	0.718291	-0.80317	5.095943	-5.4941
H	12	0.028151	-0.93502	5.917929	1.7005
C	13	2.088103	-0.95138	5.294626	5.9065
C	14	2.954329	-0.81315	4.233699	-5.3738
H	15	4.006526	-0.97435	4.414997	1.7327
C	16	2.500163	-0.50551	2.945514	3.7287
C	17	3.424052	-0.38943	1.820609	3.5999
C	18	4.810449	-0.38005	2.015564	-5.288
H	19	5.219441	-0.45803	3.011944	1.6919
C	20	5.6902	-0.2432	0.96576	5.817
H	21	6.75517	-0.23688	1.155109	-4.805
C	22	5.204963	-0.08986	-0.32988	-5.4037
H	23	5.887184	0.045701	-1.15787	1.6578
H	24	3.495527	0.053538	-1.56427	-4.6518
C	25	2.937536	-0.25987	0.499628	-9.8024
C	26	1.512506	-0.20106	0.307185	-1.6634
C	27	1.277706	-0.57769	-2.0914	-9.1489
C	28	1.224748	0.247865	-3.20347	10.1162

C	29	1.622468	-0.23433	-4.44192	-1.4382
H	30	1.577804	0.424256	-5.30046	1.2182
C	31	2.072879	-1.53837	-4.60125	2.2139
C	32	2.111843	-2.35853	-3.47368	-1.3426
H	33	2.447514	-3.38422	-3.569	2.2084
C	34	1.715022	-1.89254	-2.23568	9.6085
C	35	-1.6478	0.676434	1.775115	-8.8719
C	36	-1.44853	1.903922	2.396823	9.6939
C	37	-2.48183	2.503752	3.095188	-1.4133
H	38	-2.31199	3.463852	3.566832	2.2399
C	39	-3.7356	1.906518	3.183114	2.2622
C	40	-3.91928	0.680313	2.550515	-1.4959
H	41	-4.88596	0.193517	2.598427	1.2168
C	42	-2.89288	0.066164	1.853677	9.8315
C	43	-1.44317	-1.20718	-1.2037	37.7759
C	44	-1.50186	-2.4294	-0.55424	-2.0178
C	45	-2.013	-3.57676	-1.13582	1.6798
C	46	-2.47008	-3.52945	-2.4378	-0.3806
C	47	-2.40502	-2.33914	-3.1368	2.7099
C	48	-1.89716	-1.21418	-2.5139	-0.8849
B	49	-0.69618	0.09041	-0.55696	-17.3403
N	50	-0.61801	0.106689	0.998774	11.7283
C	51	-1.29912	1.544093	-0.97799	35.2297
C	52	-0.51903	2.688938	-0.99293	-1.9001
C	53	-2.66019	1.757085	-1.13458	-0.7891
C	54	-1.03409	3.958758	-1.18715	1.54
C	55	-3.21762	3.008414	-1.32219	2.5537
C	56	-2.39554	4.118092	-1.35424	-0.3712
F	57	-3.51278	0.73307	-1.08152	4.1454
F	58	-4.52979	3.155185	-1.46449	2.7918
F	59	0.800539	2.613306	-0.78749	-3.4103
F	60	-0.23702	5.022303	-1.19983	1.1568
F	61	-2.91013	5.326692	-1.53325	-0.3427
C	62	3.849544	-0.09464	-0.55698	5.143
H	63	-3.05831	-0.89084	1.379888	-1.892
H	64	-0.48429	2.391503	2.325296	-2.2087
H	65	2.474879	-1.19304	6.2754	-4.866
C	66	-4.86365	2.561902	3.923666	-0.87
H	67	-5.24555	1.919145	4.718158	2.2324
H	68	-5.69869	2.781044	3.256797	2.6986
H	69	-4.55316	3.500519	4.380203	0.0951

H	70	1.737959	-2.54686	-1.37324	-2.0819
H	71	0.886261	1.26926	-3.10557	-1.9666
C	72	2.49145	-2.06412	-5.94236	-0.8511
H	73	2.463031	-1.28728	-6.70498	0.0628
H	74	1.835081	-2.87107	-6.27173	2.3985
H	75	3.505875	-2.46409	-5.91528	2.4627

Table S5. Cartesian coordinates (PBEh-3c) and the computed hyperfine coupling constants (PBE0/def2-QZVP) for semidiimine **S**.

Element	Atom #	Cartesian coordinates (Å)			HFC(MHz)
N	1	0.44858	-1.10202	-0.09993	2.2674
H	2	1.119033	-1.28234	0.630781	3.3404
N	3	2.139443	1.136657	0.622766	17.5636
C	4	1.720923	0.905064	-0.60612	-35.4703
C	5	2.280738	1.780361	-1.64163	8.0751
C	6	3.217921	2.757038	-1.28216	-4.4703
H	7	3.536432	2.808633	-0.25118	1.9081
C	8	3.718733	3.634868	-2.21454	3.3147
H	9	4.44718	4.37904	-1.92123	-2.0467
C	10	3.277793	3.565666	-3.53491	-3.5637
H	11	3.659288	4.256796	-4.27478	1.9995
C	12	2.35586	2.613386	-3.90131	3.9518
H	13	2.038927	2.580316	-4.93349	-1.8858
C	14	1.841112	1.696423	-2.97196	-8.4425
C	15	0.904572	0.650226	-3.35571	14.4468
C	16	0.460031	0.496648	-4.67451	-12.4182
H	17	0.753099	1.208842	-5.43179	4.8781
C	18	-0.33964	-0.55953	-5.05085	12.7199
H	19	-0.66514	-0.64792	-6.07872	-9.5585
C	20	-0.7021	-1.52609	-4.11214	-11.4754
H	21	-1.29617	-2.37986	-4.40871	4.4612
C	22	-0.29605	-1.3949	-2.80781	12.0415
H	23	-0.56752	-2.15767	-2.09371	-8.9248
C	24	0.474785	-0.28995	-2.38992	-22.4806
C	25	0.844632	-0.13684	-1.01378	36.5948
C	26	-0.86499	-1.35788	0.295109	11.5906
C	27	-1.09265	-2.35453	1.240506	1.2709
C	28	-2.37389	-2.61792	1.691747	-2.1891
H	29	-2.5175	-3.39297	2.435162	0.902
C	30	-3.47388	-1.91697	1.20998	2.7606
C	31	-3.23353	-0.9264	0.262473	-2.2085

H	32	-4.06375	-0.34982	-0.12887	1.1795
C	33	-1.95711	-0.63868	-0.18848	1.3829
C	34	1.498864	0.75352	1.780745	-21.7271
C	35	2.248899	0.197312	2.820589	20.4509
C	36	1.63877	-0.17177	4.00866	-3.9755
H	37	2.238646	-0.62646	4.788239	2.9784
C	38	0.28164	0.040931	4.225566	6.1791
C	39	-0.44939	0.648298	3.205706	-4.2292
H	40	-1.50753	0.836893	3.344025	4.2069
C	41	0.136798	0.998065	2.006779	17.5033
H	42	-0.45534	1.472837	1.234813	-5.0697
C	43	-0.38426	-0.36339	5.507354	-2.3703
H	44	-1.16396	-1.10655	5.330346	7.8927
H	45	-0.85777	0.487622	5.999467	6.1065
H	46	0.326826	-0.79431	6.211201	0.2341
H	47	3.310106	0.041015	2.67575	-4.9539
H	48	-0.25688	-2.91635	1.640324	-1.6153
H	49	-1.81454	0.155335	-0.90935	-2.1295
C	50	-4.86694	-2.21331	1.683599	-0.98
H	51	-5.48268	-2.62774	0.883264	3.1171
H	52	-5.36981	-1.31427	2.043029	2.3488
H	53	-4.86663	-2.93534	2.49958	0.0937

Cartesian Coordinates (Å)

H_2

H	0.0000000	0.0000000	-0.3712431
H	0.0000000	0.0000000	0.3712431

$B(C_6F_5)_3$

C	3.6763842	1.8318463	1.4207575
C	1.6081168	1.9818818	0.2455755
F	1.9913154	-1.3271259	1.5753920
F	4.2660690	-0.1936608	2.4455204
F	4.7956314	2.3863327	1.8468907
F	3.0506713	3.8387668	0.3814725
B	-0.0097117	-0.0049448	0.0044319
F	0.7728590	2.7123195	-0.4858657
F	-1.9840905	0.1163575	-2.0695759
F	2.0331608	-1.0106914	-1.7465915
C	0.0250716	-1.4388969	-0.5994175

C	-0.9738398	-2.3679489	-0.3344643
C	-0.9485814	-3.6501205	-0.8464074
C	0.0988180	-4.0242410	-1.6714939
C	1.1084380	-3.1250091	-1.9710082
C	1.0606921	-1.8573339	-1.4262942
F	-1.9805539	-2.0429857	0.4690852
F	-1.9056995	-4.5194317	-0.5600913
F	0.1349518	-5.2432693	-2.1750938
F	2.1006209	-3.4881302	-2.7693948
C	-1.3529606	0.7768532	0.0946602
C	-1.6944831	1.5130589	1.2214062
C	-2.8812535	2.2125130	1.3169203
C	-3.7570683	2.2002916	0.2443874
C	-3.4495646	1.4859220	-0.9014381
C	2.7786306	2.5762457	0.6743176
C	-2.2640507	0.7803337	-0.9530329
F	-0.8795962	1.5265476	2.2709716
F	-3.1889425	2.8904410	2.4121199
F	-4.8902207	2.8731465	0.3144256
F	-4.2876956	1.4887413	-1.9267759
C	1.3050371	0.6542369	0.5164986
C	2.2357763	-0.0595420	1.2594879
C	3.4060683	0.5074959	1.7226243

$HB(C_6F_5)_2$

C	-1.5160981	-1.1329254	2.0392686
C	-0.5794719	-0.8647506	1.0456837
C	0.7590717	-0.9392765	1.4188260
C	1.1547149	-1.2518738	2.7035935
C	0.1874107	-1.4889391	3.6668021
C	-1.1564252	-1.4255959	3.3404784
B	-1.0450218	-0.5806871	-0.4072150
C	-0.3061175	0.3613576	-1.3936086
C	0.3852587	1.5011252	-0.9915076
C	0.9746673	2.3670057	-1.8904325
C	0.8883799	2.0922941	-3.2455978
C	0.2122995	0.9694397	-3.6915367
C	-0.3828910	0.1350596	-2.7653433
F	0.4603818	1.8117248	0.2964487
F	1.6139895	3.4517356	-1.4785329
F	1.4522296	2.9076225	-4.1160796
F	0.1410898	0.7144071	-4.9894792
F	-1.0234879	-0.9327744	-3.2200518
F	1.7098777	-0.7442647	0.5135746
F	2.4375076	-1.3292209	3.0253477

F	0.5494937	-1.7785316	4.9021142
F	-2.0728285	-1.6473689	4.2708957
F	-2.8098507	-1.0791566	1.7535997
H	-2.0341798	-1.1164065	-0.7872478

HC_6F_5

C	1.1889035	0.0000000	0.7118744
C	1.2019607	0.0000000	-0.6716160
C	-0.0000000	0.0000000	-1.3582605
C	-1.2019607	0.0000000	-0.6716160
C	-1.1889035	0.0000000	0.7118744
F	2.3443398	0.0000000	1.3650606
F	2.3456533	0.0000000	-1.3409899
F	-0.0000000	0.0000000	-2.6811070
F	-2.3456533	0.0000000	-1.3409899
F	-2.3443398	0.0000000	1.3650606
C	0.0000000	0.0000000	1.4133529
H	0.0000000	0.0000000	2.4943936

Compound 1

O	1.7861306	-0.6119948	-2.7413863
C	1.6581462	-0.5295153	-1.5481450
C	0.3154034	-0.2679586	-0.9092318
C	0.0969754	-0.8642089	0.4222584
C	1.2121533	-1.1090453	1.2408110
C	2.5708589	-0.7948489	0.7607444
C	2.7960957	-0.5813725	-0.6052342
C	1.0022408	-1.6857122	2.4923449
C	-0.2688965	-2.0147552	2.9263038
C	-1.3633758	-1.7881794	2.1058604
C	-1.1777956	-1.2178366	0.8604025
C	4.0836608	-0.3832639	-1.0937559
C	5.1609031	-0.3546887	-0.2293428
C	4.9454544	-0.5293850	1.1312555
C	3.6695428	-0.7510681	1.6183517
N	-0.4567182	0.4689523	-1.5888750
C	-1.6939926	0.9513356	-1.1650196
C	-2.8207292	0.5319997	-1.8851202
C	-4.0632682	1.0316434	-1.5221198
C	-4.1885694	1.9523907	-0.4941158
C	-3.0579091	2.3875458	0.1758613
C	-1.7950601	1.8992998	-0.1386206
C	-2.6656230	-0.4569017	-3.0007165
C	-0.5844915	2.3977774	0.5943573

H	-3.5927348	-0.5631148	-3.5622853
H	-1.8764608	-0.1527410	-3.6894062
H	-2.3895445	-1.4476814	-2.6322653
H	-0.8134833	3.3181120	1.1302098
H	-0.2257387	1.6760279	1.3311291
H	0.2439494	2.6085099	-0.0828279
H	-4.9419539	0.7011206	-2.0626440
H	-5.1616390	2.3438599	-0.2292961
H	-3.1512819	3.1259259	0.9631605
H	-2.0341520	-1.0587715	0.2215024
H	-2.3579661	-2.0622867	2.4297912
H	-0.4018081	-2.4660436	3.9004984
H	1.8417365	-1.9119151	3.1347043
H	3.5378547	-0.8767133	2.6840442
H	5.7786524	-0.4923719	1.8205255
H	6.1600187	-0.1862678	-0.6073738
H	4.2234154	-0.2358586	-2.1563343

Compound 2

O	1.7861306	-0.6119948	-2.7413863
C	1.6581462	-0.5295153	-1.5481450
C	0.3154034	-0.2679586	-0.9092318
C	0.0969754	-0.8642089	0.4222584
C	1.2121533	-1.1090453	1.2408110
C	2.5708589	-0.7948489	0.7607444
C	2.7960957	-0.5813725	-0.6052342
C	1.0022408	-1.6857122	2.4923449
C	-0.2688965	-2.0147552	2.9263038
C	-1.3633758	-1.7881794	2.1058604
C	-1.1777956	-1.2178366	0.8604025
C	4.0836608	-0.3832639	-1.0937559
C	5.1609031	-0.3546887	-0.2293428
C	4.9454544	-0.5293850	1.1312555
C	3.6695428	-0.7510681	1.6183517
N	-0.4567182	0.4689523	-1.5888750
C	-1.6939926	0.9513356	-1.1650196
C	-2.8207292	0.5319997	-1.8851202
C	-4.0632682	1.0316434	-1.5221198
C	-4.1885694	1.9523907	-0.4941158
C	-3.0579091	2.3875458	0.1758613
C	-1.7950601	1.8992998	-0.1386206
C	-2.6656230	-0.4569017	-3.0007165
C	-0.5844915	2.3977774	0.5943573
H	-3.5927348	-0.5631148	-3.5622853
H	-1.8764608	-0.1527410	-3.6894062

H	-2.3895445	-1.4476814	-2.6322653
H	-0.8134833	3.3181120	1.1302098
H	-0.2257387	1.6760279	1.3311291
H	0.2439494	2.6085099	-0.0828279
H	-4.9419539	0.7011206	-2.0626440
H	-5.1616390	2.3438599	-0.2292961
H	-3.1512819	3.1259259	0.9631605
H	-2.0341520	-1.0587715	0.2215024
H	-2.3579661	-2.0622867	2.4297912
H	-0.4018081	-2.4660436	3.9004984
H	1.8417365	-1.9119151	3.1347043
H	3.5378547	-0.8767133	2.6840442
H	5.7786524	-0.4923719	1.8205255
H	6.1600187	-0.1862678	-0.6073738
H	4.2234154	-0.2358586	-2.1563343

TS A‡

C	2.4223979	2.5736384	-2.3057163
C	2.1726376	1.2234655	-2.1066386
C	3.2798050	0.4543611	-1.7802235
C	4.5470609	0.9793005	-1.6105574
C	4.7458683	2.3327461	-1.8030534
C	3.6785232	3.1346155	-2.1603179
B	0.7273944	0.5483948	-2.3298456
C	-0.5629310	1.4589191	-2.0708386
C	-0.6016201	2.3225757	-0.9855527
C	-1.6680655	3.1485341	-0.7039683
C	-2.7797370	3.1074573	-1.5229857
C	-2.7949038	2.2582654	-2.6110430
C	-1.6976766	1.4543613	-2.8683024
F	0.4271167	2.3519986	-0.1346788
F	-1.6461719	3.9583620	0.3476375
F	-3.8292614	3.8675867	-1.2563575
F	-3.8698062	2.2057200	-3.3888611
F	-1.7905219	0.6495844	-3.9244603
F	3.1429492	-0.8613794	-1.6066119
F	5.5671108	0.1987607	-1.2706965
F	5.9522326	2.8573304	-1.6515746
F	3.8680327	4.4325796	-2.3613148
F	1.4425557	3.3969029	-2.6687935
C	0.7173022	-0.4441236	-3.5949778
C	0.4431664	-1.8006544	-3.6011804
C	0.4861399	-2.5672674	-4.7538454
C	0.8102967	-1.9730805	-5.9572267
C	1.0868080	-0.6183940	-5.9974199

C	1.0348758	0.1097115	-4.8257772
F	0.1086529	-2.4338076	-2.4772496
F	0.2141911	-3.8658832	-4.7106416
F	0.8494784	-2.6946195	-7.0672902
F	1.3886571	-0.0356690	-7.1507683
F	1.2812417	1.4186101	-4.9029128
O	1.4124801	-2.4046016	0.3020839
C	1.0955898	-1.9172287	1.3544018
C	-0.2829541	-1.3502970	1.5915295
C	-0.8548603	-1.6531498	2.9123586
C	0.0311758	-1.7708662	3.9966067
C	1.4820251	-1.6063441	3.7872503
C	2.0099626	-1.7426938	2.4968243
C	-0.4954227	-2.0686444	5.2505601
C	-1.8554045	-2.2536757	5.4280321
C	-2.7202625	-2.1607098	4.3478145
C	-2.2197281	-1.8605635	3.0946252
C	3.3804331	-1.6878774	2.2686758
C	4.2451856	-1.4578337	3.3227287
C	3.7325968	-1.2943393	4.6026034
C	2.3690656	-1.3731391	4.8342270
N	-0.7781427	-0.6407625	0.6586196
C	-1.9907337	0.0651939	0.8097074
C	-3.0313911	-0.2611695	-0.0701338
C	-4.2276476	0.4335167	0.0354701
C	-4.3858186	1.4408252	0.9742520
C	-3.3369757	1.7647740	1.8142834
C	-2.1214394	1.0895525	1.7553512
C	-2.8717658	-1.3694199	-1.0658112
C	-1.0199455	1.4953807	2.6909730
H	-3.7489235	-1.4441282	-1.7061831
H	-2.0063117	-1.2215276	-1.7085181
H	-2.7332862	-2.3378717	-0.5810631
H	-1.0691895	2.5654758	2.8866554
H	-1.1107594	0.9845825	3.6513087
H	-0.0255613	1.2860249	2.3026042
H	-5.0426994	0.1828416	-0.6319086
H	-5.3198649	1.9822794	1.0377665
H	-3.4528486	2.5669236	2.5323586
H	-2.8961755	-1.8002117	2.2543575
H	-3.7804987	-2.3271161	4.4785863
H	-2.2386475	-2.4899377	6.4115679
H	0.1614389	-2.1881599	6.1008375
H	2.0031692	-1.2354124	5.8422433
H	4.4012280	-1.1008228	5.4307941
H	5.3104172	-1.3940077	3.1486345

H	3.7543027	-1.7993547	1.2589756
H	0.8554819	-0.4389103	-1.2983397
H	0.2189065	-0.3554975	-0.7896665

Intermediate B

O	1.1571238	-2.6390535	0.3262429
C	1.0257205	-2.0250203	1.3465689
C	-0.3091433	-1.3985449	1.6888287
C	-0.7637778	-1.5819515	3.0508404
C	0.2337310	-1.6532053	4.0426250
C	1.6578721	-1.5192672	3.6790232
C	2.0557311	-1.7629068	2.3566065
C	-0.1729844	-1.8596354	5.3562004
C	-1.5129220	-2.0074546	5.6732429
C	-2.4857826	-1.9608196	4.6833169
C	-2.1124215	-1.7408891	3.3731354
C	3.3927211	-1.7267567	1.9814628
C	4.3556690	-1.4062665	2.9227982
C	3.9749879	-1.1429415	4.2302428
C	2.6414270	-1.2060069	4.6088182
N	-0.9104758	-0.7693631	0.7435546
C	-2.1165043	-0.0115529	0.8143976
C	-3.0944973	-0.3324761	-0.1337238
C	-4.2737884	0.3954900	-0.1066133
C	-4.4609567	1.4068124	0.8225693
C	-3.4612183	1.7184000	1.7247319
C	-2.2539858	1.0269248	1.7382336
C	-2.8796126	-1.4248209	-1.1377271
C	-1.1809325	1.4635586	2.6904455
H	-3.7603896	-1.5459925	-1.7644252
H	-2.0432795	-1.2093539	-1.8029058
H	-2.6758089	-2.3880289	-0.6668325
H	-1.1993677	2.5475395	2.7857316
H	-1.3369044	1.0436922	3.6857856
H	-0.1769730	1.1965345	2.3686291
H	-5.0481671	0.1721619	-0.8286138
H	-5.3828311	1.9722023	0.8244677
H	-3.5997846	2.5378702	2.4176008
H	-2.8666833	-1.7115858	2.5993972
H	-3.5282637	-2.0998586	4.9322070
H	-1.7991407	-2.1770546	6.7024457
H	0.5614829	-1.9372079	6.1453551
H	2.3797606	-0.9875202	5.6350633
H	4.7223460	-0.8790051	4.9663258
H	5.3948339	-1.3448383	2.6317476

H	3.6661026	-1.9113818	0.9520913
B	0.6055227	0.3990830	-2.2839884
F	1.5255972	3.2808329	-2.4860243
F	-1.7563055	0.7892556	-4.1435801
F	1.3719114	1.5412609	-4.8123991
C	0.7037505	-0.4075277	-3.6874551
C	0.4417013	-1.7591605	-3.8220060
C	0.5796513	-2.4425187	-5.0191512
C	0.9962304	-1.7611974	-6.1452920
C	1.2661285	-0.4075940	-6.0602788
C	1.1165013	0.2317310	-4.8449118
F	0.0180722	-2.4816476	-2.7772363
F	0.3120631	-3.7448701	-5.0951908
F	1.1318343	-2.3987115	-7.3030278
F	1.6574900	0.2578803	-7.1433325
C	-0.6427263	1.4401275	-2.1596430
C	-0.7507677	2.2496471	-1.0398293
C	-1.7925691	3.1227641	-0.8072118
C	-2.8306870	3.1850792	-1.7156369
C	-2.7877176	2.3860926	-2.8393440
C	-1.7056443	1.5421414	-3.0429183
F	0.1860647	2.1739948	-0.0803395
F	-1.8210050	3.8805445	0.2893209
F	-3.8677502	3.9864241	-1.4938484
F	-3.7940518	2.4225418	-3.7095914
C	2.0624786	1.0474098	-1.9387514
C	3.0812571	0.2193958	-1.4955282
C	4.3338077	0.6698992	-1.1225561
C	4.6241540	2.0161314	-1.2216474
C	3.6550222	2.8794985	-1.6947672
C	2.4086595	2.3852005	-2.0442474
F	2.8736058	-1.0994986	-1.3966458
F	5.2557120	-0.1800848	-0.6617435
F	5.8206145	2.4730035	-0.8665423
F	3.9272352	4.1771106	-1.8024099
H	0.4101335	-0.4423000	-1.4085690
H	-0.4288869	-0.7523653	-0.1835681

TS C‡

O	1.0573331	-1.4121671	-0.3708690
C	0.9534885	-1.3713015	0.8811891
C	-0.3653672	-1.2544813	1.4643376
C	-0.5614920	-1.6383755	2.8392051
C	0.5639512	-1.7075866	3.6867423
C	1.9023763	-1.4316247	3.1667176

C	2.0941832	-1.3353049	1.7778895
C	0.3542838	-2.0909012	5.0143153
C	-0.9018183	-2.4157311	5.4806562
C	-2.0007461	-2.3904353	4.6252292
C	-1.8294198	-2.0032499	3.3177896
C	3.3801970	-1.1835435	1.2557332
C	4.4658346	-1.0719695	2.0983769
C	4.2812354	-1.1257073	3.4755988
C	3.0171427	-1.3122423	3.9988012
N	-1.3195965	-0.8159447	0.6637597
C	-2.5597843	-0.2046253	0.9761627
C	-3.6684831	-0.5954676	0.2139728
C	-4.8701335	0.0673754	0.4160297
C	-4.9699630	1.0859154	1.3477767
C	-3.8647035	1.4490604	2.0941435
C	-2.6342589	0.8215520	1.9301078
C	-3.5775147	-1.6915845	-0.8060222
C	-1.4793765	1.2929378	2.7625626
H	-4.5701210	-2.0642979	-1.0518789
H	-3.1332627	-1.3406912	-1.7381037
H	-2.9836645	-2.5378468	-0.4608144
H	-1.6210417	2.3349121	3.0399597
H	-1.3995324	0.7207070	3.6881899
H	-0.5189581	1.2266896	2.2554857
H	-5.7352167	-0.2195674	-0.1676648
H	-5.9095595	1.6030385	1.4868252
H	-3.9442089	2.2555389	2.8115034
H	-2.6829351	-2.0007888	2.6555975
H	-2.9795746	-2.6800764	4.9807860
H	-1.0261756	-2.7149500	6.5127617
H	1.1901360	-2.1680702	5.6938793
H	2.9062255	-1.3519988	5.0731413
H	5.1269227	-1.0254853	4.1422059
H	5.4552877	-0.9342854	1.6842427
H	3.5177952	-1.1409107	0.1868326
B	0.8963665	0.6651235	-2.2413134
F	1.1404578	3.6386868	-2.3650290
F	-1.6358349	0.7178665	-3.8592959
F	2.5015733	0.8421553	-4.7137466
C	0.9176660	-0.3840055	-3.4532910
C	0.1275683	-1.5249786	-3.4634845
C	0.1686940	-2.4837154	-4.4545994
C	1.0340692	-2.3141079	-5.5194752
C	1.8212806	-1.1813590	-5.5771764
C	1.7467751	-0.2452768	-4.5602171
F	-0.7622523	-1.7293511	-2.4828622

F	-0.6133580	-3.5574516	-4.4009500
F	1.0960408	-3.2230203	-6.4818844
F	2.6354324	-0.9961787	-6.6099002
C	-0.4926760	1.3965113	-1.9002353
C	-0.6136458	2.1577588	-0.7416721
C	-1.7401426	2.8782763	-0.4086619
C	-2.8499802	2.8162877	-1.2326582
C	-2.7938207	2.0566975	-2.3825339
C	-1.6263516	1.3786399	-2.7029674
F	0.4138611	2.2111174	0.1134056
F	-1.7781542	3.6257794	0.6903105
F	-3.9497768	3.4858335	-0.9208872
F	-3.8528682	1.9939773	-3.1821334
C	2.2220760	1.5547940	-2.0947136
C	3.4619670	0.9490285	-1.9376526
C	4.6394040	1.6443398	-1.7548005
C	4.6128313	3.0269320	-1.7636545
C	3.4120829	3.6799434	-1.9635625
C	2.2529244	2.9420176	-2.1293232
F	3.5543858	-0.3846387	-1.9690245
F	5.7916956	1.0036058	-1.5790788
F	5.7317205	3.7173245	-1.5941490
F	3.3826240	5.0074906	-2.0019713
H	1.0383179	-0.2196429	-1.1476180
H	-1.0504379	-0.7729752	-0.3163481

Compound 6

O	-0.7028145	-2.7821358	-0.7439294
H	-0.1513480	-2.4751764	-1.4824991
N	0.1860636	-0.4240591	-1.6333789
H	-0.4143951	-0.1697072	-2.4038180
C	2.2913800	-1.0935176	0.3234258
H	1.6702122	-0.6653423	1.1109940
H	3.2543280	-1.3414298	0.7686816
H	1.8280546	-2.0328633	0.0200578
C	0.6585210	1.2908188	-3.8575867
H	1.0276674	1.9873050	-4.6082529
H	-0.2164779	1.7581075	-3.3965620
H	0.3108303	0.4055788	-4.3975378
C	-0.9782584	-1.6912712	-0.0188391
C	-1.7338982	-1.8740540	1.1834900
C	-2.1784756	-3.1521524	1.5625918
H	-1.9545565	-4.0018742	0.9335719
C	-2.8918618	-3.3258963	2.7213491
H	-3.2313022	-4.3122356	3.0076268

C	-3.1775184	-2.2223117	3.5299328
H	-3.7395321	-2.3533812	4.4451804
C	-2.7484340	-0.9685327	3.1701018
H	-2.9876901	-0.1397852	3.8207240
C	-2.0150664	-0.7524759	1.9901781
C	-1.5503213	0.5600058	1.5861108
C	-1.8145292	1.7137763	2.3423399
H	-2.3735208	1.6404924	3.2643889
C	-1.3819691	2.9540263	1.9421173
H	-1.6007978	3.8236937	2.5469503
C	-0.6616320	3.0860640	0.7532898
H	-0.3171390	4.0599131	0.4316344
C	-0.3851673	1.9791266	-0.0094989
H	0.1848686	2.1003724	-0.9192661
C	-0.8161846	0.6988497	0.3847579
C	-0.5311892	-0.4637414	-0.4025747
C	1.4720327	0.1376838	-1.7550406
C	1.7330135	0.9709757	-2.8554746
C	3.0016378	1.5118244	-3.0116086
H	3.1979212	2.1533402	-3.8621413
C	4.0049752	1.2539926	-2.0953295
H	4.9881624	1.6865888	-2.2211224
C	3.7363763	0.4239907	-1.0222760
H	4.5211308	0.2019067	-0.3093455
C	2.4869039	-0.1564903	-0.8334129

TS D‡

C	0.1927465	-2.0143747	2.2553837
C	-0.5637633	-2.0747993	1.0714320
C	-1.9312957	-2.4081944	1.1126597
C	-2.5273699	-2.6715551	2.3362742
C	-1.7901344	-2.6351770	3.5092835
C	-0.4447933	-2.3110291	3.4548428
N	-0.0105624	-1.7807521	-0.1685671
C	1.2421888	-2.1197478	-0.6576246
C	1.9154011	-1.1144497	-1.3811796
C	3.1959564	-1.4484150	-1.9866512
C	3.8037571	-2.6964657	-1.7605372
C	3.1005003	-3.7054146	-0.9891567
C	1.8042666	-3.4206569	-0.4845274
C	3.6416372	-4.9784448	-0.7683273
C	2.9470243	-5.9619033	-0.1035436
C	1.6520049	-5.6997974	0.3465511
C	1.0945199	-4.4611456	0.1566618
C	3.8496026	-0.4795116	-2.7617591

C	5.0874964	-0.7261706	-3.3046400
C	5.7050757	-1.9564496	-3.0740217
C	5.0732042	-2.9170809	-2.3189330
O	1.4681543	0.0654055	-1.4820651
C	-2.7211319	-2.4953830	-0.1591465
C	1.6361356	-1.6095102	2.2703490
O	-1.4063504	0.3449253	-2.0682218
C	-1.8542104	1.4306642	-1.7325011
C	-3.0417727	1.9998005	-2.3620122
C	-3.6617143	3.1383234	-1.8320532
C	-3.0496678	3.8420565	-0.7013374
C	-1.8463832	3.3789645	-0.1091892
C	-1.2366246	2.1585445	-0.5948280
C	-4.8466673	3.5712308	-2.4353138
C	-5.3781040	2.9138327	-3.5266361
C	-4.7434050	1.7935808	-4.0539144
C	-3.5849766	1.3367688	-3.4656784
C	-1.2392090	4.1730267	0.8824660
C	-1.8118951	5.3418907	1.3253225
C	-3.0203167	5.7630547	0.7848460
C	-3.6117993	5.0253633	-0.2186068
N	-0.1372931	1.5972978	-0.1400279
C	0.4672648	1.7689994	1.1292187
C	1.7911663	2.2234735	1.1822724
C	2.4029849	2.2972610	2.4265650
C	1.7249548	1.9314264	3.5775069
C	0.4137954	1.4963158	3.4998645
C	-0.2464083	1.4102297	2.2801556
C	2.5139204	2.6574050	-0.0551005
C	-1.6748852	0.9618342	2.2414781
H	-0.5838742	-1.2515155	-0.8081952
H	0.3707267	0.8631669	-0.7469860
H	-2.3570823	1.8155148	2.2496086
H	-1.9037665	0.3441032	3.1076723
H	-1.9043001	0.3647653	1.3620054
H	3.4567693	3.1386378	0.1989149
H	1.9242694	3.3661073	-0.6389552
H	2.7266543	1.8078795	-0.7052899
H	-3.0822206	0.4594956	-3.8483723
H	-5.1587743	1.2823297	-4.9114959
H	-6.2951075	3.2773768	-3.9707499
H	-5.3762564	4.4342719	-2.0599790
H	-4.5308805	5.3995167	-0.6430692
H	-3.4897005	6.6739984	1.1308838
H	-1.3162228	5.9245048	2.0894106
H	-0.2977663	3.8799591	1.3160500

H	3.4246341	2.6499107	2.4894481
H	2.2207490	1.9866237	4.5377113
H	-0.1125209	1.2020823	4.3991641
H	-3.7194239	-2.8878278	0.0285036
H	-2.8458588	-1.5240039	-0.6465693
H	-2.2344824	-3.1482713	-0.8863949
H	1.9322848	-1.3149194	3.2761724
H	2.2942420	-2.4218585	1.9567038
H	1.8294973	-0.7632463	1.6119033
H	-3.5791314	-2.9295786	2.3659374
H	-2.2605440	-2.8567189	4.4581092
H	0.1324198	-2.2674226	4.3709137
H	0.0868145	-4.2932385	0.5051968
H	1.0804194	-6.4730042	0.8429282
H	3.3966338	-6.9334813	0.0514599
H	4.6309534	-5.2135009	-1.1345321
H	5.5803261	-3.8590769	-2.1656807
H	6.6822061	-2.1612010	-3.4918452
H	5.5797279	0.0264386	-3.9064493
H	3.3555612	0.4669352	-2.9311658

Semiiminoquinone E

O	1.9041552	0.4580150	-2.4047981
C	1.7563702	0.0016216	-1.2674410
C	0.4284912	-0.0982450	-0.6959682
C	0.2080787	-0.7353327	0.5669540
C	1.3251642	-1.1098360	1.3577252
C	2.6848891	-0.9040778	0.8619816
C	2.8866974	-0.4054901	-0.4333201
C	1.0869902	-1.7161502	2.5939853
C	-0.1890064	-1.9736422	3.0488203
C	-1.2833618	-1.6461076	2.2528861
C	-1.0862727	-1.0417367	1.0343407
C	4.1790678	-0.2485636	-0.9414539
C	5.2766770	-0.5702014	-0.1759498
C	5.0901457	-1.0509369	1.1181038
C	3.8189378	-1.2139253	1.6244731
N	-0.5365582	0.4043902	-1.4993159
C	-1.8069087	0.9197502	-1.1645007
C	-2.9116418	0.4285110	-1.8689484
C	-4.1694255	0.9345076	-1.5681970
C	-4.3270426	1.9001480	-0.5881215
C	-3.2205241	2.3857741	0.0868957
C	-1.9410753	1.9181620	-0.1928895
C	-2.7354203	-0.6323684	-2.9144832

C	-0.7576366	2.4906085	0.5281421
H	-3.6992947	-1.0027224	-3.2599390
H	-2.2016740	-0.2569441	-3.7902829
H	-2.1640237	-1.4802538	-2.5352388
H	-1.0146154	3.4467071	0.9820234
H	-0.4114816	1.8329903	1.3278384
H	0.0866476	2.6576549	-0.1406496
H	-5.0335807	0.5592314	-2.1020621
H	-5.3125892	2.2819955	-0.3569384
H	-3.3450721	3.1557853	0.8381992
H	-1.9501872	-0.8162372	0.4285956
H	-2.2882541	-1.8713680	2.5834874
H	-0.3326728	-2.4458438	4.0112841
H	1.9168554	-2.0138251	3.2180256
H	3.7181787	-1.5866249	2.6334983
H	5.9449195	-1.2992571	1.7333343
H	6.2750460	-0.4452328	-0.5731645
H	4.2990300	0.1361083	-1.9448149
H	-0.1680222	0.6529621	-2.4121165

Compound 6

O	1.4480840	-0.1571118	-0.1360317
C	0.9927002	-0.5772346	0.9745304
C	-0.3777308	-0.8872780	1.2274969
C	-0.7645033	-1.5143868	2.4685733
C	0.1699468	-1.6286848	3.5168110
C	1.5324001	-1.1472152	3.3281578
C	1.9398184	-0.6852062	2.0634231
C	-0.2325262	-2.2564062	4.6997203
C	-1.5006274	-2.7739163	4.8473101
C	-2.4057623	-2.7031136	3.7921978
C	-2.0391585	-2.0864937	2.6196659
C	3.2626158	-0.2639745	1.8622524
C	4.1706141	-0.2903794	2.8941878
C	3.7705587	-0.7335392	4.1517938
C	2.4738439	-1.1519730	4.3613346
N	-1.2775129	-0.5999616	0.2713701
C	-2.6083495	-0.1476998	0.3912671
C	-3.5182013	-0.6458620	-0.5522551
C	-4.8106427	-0.1447598	-0.5493879
C	-5.1934246	0.8187158	0.3689140
C	-4.2827793	1.2862695	1.2984458
C	-2.9719423	0.8212822	1.3363408
C	-3.1072170	-1.7054082	-1.5328283
C	-2.0440539	1.3801692	2.3738428

H	-3.9775095	-2.1175850	-2.0396731
H	-2.4478677	-1.3127819	-2.3090109
H	-2.5821440	-2.5307177	-1.0496187
H	-2.3488097	2.3894337	2.6460338
H	-2.0623902	0.7772437	3.2843215
H	-1.0067628	1.4353997	2.0506693
H	-5.5235641	-0.5158126	-1.2743859
H	-6.2022076	1.2084325	0.3574806
H	-4.5848725	2.0455764	2.0086515
H	-2.7482415	-2.0663522	1.8062981
H	-3.3900353	-3.1410038	3.8842738
H	-1.7796794	-3.2558849	5.7743705
H	0.4623869	-2.3679871	5.5187013
H	2.1973518	-1.4806533	5.3522399
H	4.4754109	-0.7483298	4.9721214
H	5.1868708	0.0392412	2.7284603
H	3.5670150	0.0983074	0.8930933
B	1.1743091	0.4875335	-1.5009401
F	1.8695302	3.3272474	-2.3627284
F	-1.4401313	0.8861978	-3.0487863
F	1.0942412	0.9464215	-4.2862427
C	0.8502616	-0.6770720	-2.6063010
C	0.6328208	-2.0225899	-2.3640269
C	0.4500941	-2.9590973	-3.3697070
C	0.4990868	-2.5589497	-4.6881206
C	0.7244195	-1.2258558	-4.9837576
C	0.8932379	-0.3272592	-3.9503656
F	0.5657734	-2.5021221	-1.1136867
F	0.2272021	-4.2346704	-3.0709838
F	0.3262211	-3.4403070	-5.6621846
F	0.7686039	-0.8288964	-6.2491195
C	-0.0069045	1.6055202	-1.2992382
C	0.1201034	2.5339135	-0.2733008
C	-0.8178706	3.5085424	0.0013730
C	-1.9645123	3.5814402	-0.7684538
C	-2.1399789	2.6859527	-1.8016288
C	-1.1678391	1.7293727	-2.0474678
F	1.1995120	2.5045501	0.5133535
F	-0.6439838	4.3594214	1.0071711
F	-2.8874210	4.4949809	-0.5069673
F	-3.2399522	2.7333517	-2.5415721
C	2.6254809	1.1327007	-1.8937165
C	3.7429622	0.3077302	-1.8971114
C	5.0163552	0.7440459	-2.2137173
C	5.2070534	2.0665066	-2.5661271
C	4.1229608	2.9203023	-2.6009189

C	2.8640085	2.4439809	-2.2728652
F	3.6183533	-0.9863307	-1.5880321
F	6.0511633	-0.0897210	-2.1864926
F	6.4186550	2.5078416	-2.8742813
F	4.2954431	4.1900962	-2.9508605
H	-0.9103604	-0.5071372	-0.6633553

TS G‡

O	1.6101630	-0.1316280	-0.0064544
C	1.0002558	-0.5384294	1.0872082
C	-0.3760667	-0.8780771	1.1294639
C	-0.8821308	-1.5051313	2.3532141
C	-0.0999362	-1.5011120	3.5247632
C	1.2512525	-0.9606600	3.4976913
C	1.8112504	-0.5690924	2.2642103
C	-0.6233531	-2.0907126	4.6829678
C	-1.8562649	-2.7001903	4.6883916
C	-2.5942204	-2.7693294	3.5110500
C	-2.1091994	-2.1848109	2.3642995
C	3.1520835	-0.1430717	2.2067220
C	3.9122356	-0.0726530	3.3479346
C	3.3495716	-0.4169432	4.5767397
C	2.0445667	-0.8556482	4.6441883
N	-1.1134766	-0.6099329	0.0562435
C	-2.5000916	-0.4061577	0.0940621
C	-3.3005828	-1.0978924	-0.8299245
C	-4.6611694	-0.8363926	-0.8655219
C	-5.2283116	0.1112163	-0.0298771
C	-4.4282746	0.7914055	0.8682518
C	-3.0629194	0.5446987	0.9648697
C	-2.7198429	-2.1380293	-1.7432081
C	-2.2808285	1.2962659	2.0036992
H	-3.5045546	-2.7806472	-2.1401126
H	-2.2172353	-1.6847769	-2.5986584
H	-1.9962113	-2.7778926	-1.2374455
H	-2.7485239	2.2602397	2.2016364
H	-2.2565116	0.7503113	2.9492565
H	-1.2471197	1.4875693	1.7211014
H	-5.2838402	-1.3816691	-1.5640843
H	-6.2886209	0.3185929	-0.0807792
H	-4.8685010	1.5365505	1.5192965
H	-2.6944641	-2.2720976	1.4633247
H	-3.5434459	-3.2867821	3.4880739
H	-2.2322152	-3.1488248	5.5979801
H	-0.0443711	-2.1005082	5.5946219

H	1.6424275	-1.1150265	5.6124450
H	3.9369597	-0.3449565	5.4821448
H	4.9398868	0.2591337	3.2931965
H	3.5858183	0.1310229	1.2574805
B	1.2116034	0.6629602	-1.1141502
F	1.6947695	3.1618696	-2.6475939
F	-1.7436924	1.5012795	-1.8455952
F	-0.1576776	1.1195636	-3.7703150
C	0.2998127	-0.6546454	-2.2690064
C	0.7433487	-1.9811853	-2.1959975
C	1.0278643	-2.7529691	-3.3029755
C	0.8724498	-2.1975824	-4.5594805
C	0.4376078	-0.8885275	-4.6945449
C	0.1507824	-0.1499391	-3.5666634
F	0.8567598	-2.5767099	-1.0176501
F	1.4301692	-4.0092509	-3.1810360
F	1.1471543	-2.9106422	-5.6327162
F	0.3235623	-0.3608095	-5.9048834
C	0.2814850	1.9151469	-0.6806800
C	0.9073161	2.7963606	0.1936900
C	0.3147543	3.9416868	0.6881655
C	-0.9777251	4.2453991	0.3052664
C	-1.6438773	3.4008620	-0.5596082
C	-1.0129792	2.2631782	-1.0357767
F	2.1685787	2.5632600	0.5676308
F	0.9721664	4.7470042	1.5125376
F	-1.5744712	5.3321961	0.7718047
F	-2.8919672	3.6759334	-0.9150033
C	2.4699154	1.0025543	-2.0577934
C	3.4992017	0.0857799	-2.2485441
C	4.5979838	0.3340126	-3.0494577
C	4.7024913	1.5494687	-3.6996946
C	3.7033350	2.4895003	-3.5458978
C	2.6143930	2.2048582	-2.7393109
F	3.4536783	-1.1116317	-1.6657414
F	5.5482041	-0.5800483	-3.1998514
F	5.7496843	1.8078905	-4.4660348
F	3.7952858	3.6572023	-4.1681864
H	-0.4461553	-0.4719564	-1.2553691

Compound 4

F	-2.6250102	-5.2397023	3.2974070
F	-3.1685018	4.6798476	2.8537603
F	-3.0153034	1.7335394	-0.7414927
F	-0.8419418	0.6643998	3.3013505

O	-1.7212585	-0.5373838	-0.7722780
F	-3.3282251	-0.6713906	2.8112309
F	-0.7726080	-5.1871876	1.3135580
F	-0.1854934	-2.9018706	0.0936272
F	-3.8479839	4.0067284	0.3200899
F	-1.6457503	2.9915397	4.3348442
F	-3.8902252	-2.9547025	4.0125431
N	0.2906751	-0.0802852	0.3581249
C	-2.3231651	-4.0970189	2.6993685
C	-2.9597085	-2.9284903	3.0658818
C	-2.6297642	-1.7397300	2.4331017
C	-1.6568027	-1.6505846	1.4490978
B	-1.2733965	-0.2915139	0.6333792
C	0.5153684	-0.2579157	-0.9477308
C	1.7341793	-0.2395207	-1.7154183
C	1.6292528	-0.3886634	-3.1213982
C	2.8116471	-0.3832968	-3.8693929
C	4.0470750	-0.2509960	-3.2753510
C	-2.7540650	3.5314517	2.3379716
C	-3.0999157	3.1842227	1.0477294
C	-2.6560804	1.9827603	0.5181495
C	-1.8711511	1.0925465	1.2331396
C	-1.5587118	1.4812056	2.5267056
C	-1.9745857	2.6709192	3.0893512
C	-0.7156995	-0.5091979	-1.5848535
C	1.1957966	0.6078641	1.2149342
C	1.8202122	-0.0691556	2.2674670
C	2.6724906	0.6476359	3.0978665
C	2.8981495	1.9978906	2.8996332
C	2.2836094	2.6470711	1.8455721
C	1.4316927	1.9692576	0.9798483
C	0.8534980	2.7102314	-0.1902434
C	1.6231246	-1.5346336	2.5069417
C	3.0028179	-0.1271274	-1.1254490
C	4.1442445	-0.1310357	-1.8927687
C	0.3298125	-0.5692473	-3.7689379
C	0.1814794	-0.6685932	-5.1563926
C	-1.0574163	-0.8503909	-5.7350056
C	-2.2065296	-0.9404338	-4.9486504
C	-2.1000499	-0.8421395	-3.5828627
C	-0.8424265	-0.6565938	-2.9893558
C	-1.3775865	-4.0665114	1.6911169
C	-1.0828894	-2.8612542	1.0846760
H	2.3801393	-1.9123960	3.1923576
H	0.6511793	-1.7369552	2.9564094
H	1.6923735	-2.1144720	1.5884924

H	0.8417085	3.7811320	0.0070724
H	1.4556345	2.5549581	-1.0883085
H	-0.1649850	2.4155160	-0.4294550
H	3.1634437	0.1334274	3.9144038
H	3.5568633	2.5419506	3.5632488
H	2.4653991	3.7019896	1.6826593
H	3.0983432	-0.0430771	-0.0542987
H	5.1113182	-0.0459353	-1.4165621
H	4.9389957	-0.2535485	-3.8871275
H	2.7746708	-0.4978054	-4.9424473
H	1.0394227	-0.5981684	-5.8083076
H	-1.1346788	-0.9202711	-6.8117016
H	-3.1736759	-1.0803266	-5.4114349
H	-2.9790316	-0.8985623	-2.9558867

TS H‡

O	1.4293842	-0.1648446	0.0045664
C	0.9413587	-0.6244605	1.1918781
C	-0.3510709	-1.0019258	1.3628759
C	-0.7582340	-1.6002887	2.6089487
C	0.1407129	-1.6621398	3.6922276
C	1.4959520	-1.1865821	3.5132317
C	1.9095990	-0.7164383	2.2485016
C	-0.3096755	-2.2183624	4.9017180
C	-1.5845018	-2.7093550	5.0341479
C	-2.4613473	-2.6734883	3.9472936
C	-2.0532888	-2.1284663	2.7562582
C	3.2478198	-0.3248463	2.0624343
C	4.1459126	-0.3575429	3.0986177
C	3.7344949	-0.7909763	4.3600203
C	2.4392517	-1.2001037	4.5544601
N	-1.2590321	-0.8749472	0.2976874
C	-2.4792515	-0.1966883	0.3181693
C	-3.4038981	-0.5687976	-0.6816959
C	-4.5906523	0.1323810	-0.8151974
C	-4.9005151	1.1808670	0.0327980
C	-4.0106880	1.5040509	1.0374945
C	-2.7978699	0.8398478	1.2140955
C	-3.1255190	-1.7269165	-1.5992770
C	-1.9577934	1.2814871	2.3850156
H	-3.9667675	-1.8934994	-2.2691652
H	-2.2499383	-1.5685753	-2.2321109
H	-2.9727680	-2.6617345	-1.0513482
H	-2.2383335	2.2927594	2.6771211
H	-2.1235609	0.6432714	3.2546957

H	-0.8881834	1.2895249	2.2019178
H	-5.2811401	-0.1517289	-1.5996403
H	-5.8236320	1.7315165	-0.0830336
H	-4.2525303	2.3109146	1.7189654
H	-2.7437033	-2.1021095	1.9257573
H	-3.4615201	-3.0744662	4.0416385
H	-1.9034573	-3.1331873	5.9767574
H	0.3528535	-2.2794829	5.7528606
H	2.1518401	-1.5388126	5.5389172
H	4.4358763	-0.8125283	5.1829973
H	5.1698966	-0.0506000	2.9346818
H	3.6013548	-0.0011079	1.0942638
B	0.9211694	0.4035377	-1.3256107
F	1.9607796	3.4281644	-1.5479313
F	-1.5181863	0.7741979	-2.9882808
F	1.0511788	1.1032334	-4.0546216
C	0.8199839	-0.6576652	-2.5189619
C	0.7287847	-2.0296483	-2.3693017
C	0.7004388	-2.9043123	-3.4435194
C	0.7907125	-2.4056276	-4.7277058
C	0.9064315	-1.0399969	-4.9244484
C	0.9190819	-0.2047422	-3.8274595
F	0.6579552	-2.5821722	-1.1550077
F	0.5955650	-4.2119729	-3.2462354
F	0.7705172	-3.2254818	-5.7657792
F	1.0056886	-0.5541728	-6.1541223
C	-0.1937884	1.5320613	-1.1752813
C	-0.1351738	2.4675859	-0.1496936
C	-1.0781967	3.4543049	0.0417688
C	-2.1671882	3.5208205	-0.8066538
C	-2.2860374	2.6043127	-1.8299314
C	-1.3122584	1.6351036	-1.9931385
F	0.8865544	2.4406351	0.7140841
F	-0.9647656	4.3190857	1.0434518
F	-3.0949606	4.4454730	-0.6251816
F	-3.3336672	2.6483880	-2.6402193
C	2.6212915	1.1494053	-1.5765360
C	3.6042650	0.2689492	-2.0575221
C	4.6543074	0.6581062	-2.8584093
C	4.7651887	1.9946629	-3.2056733
C	3.8386855	2.9133850	-2.7464101
C	2.8006100	2.4885588	-1.9398127
F	3.5482294	-1.0162212	-1.7346342
F	5.5538990	-0.2124812	-3.2905257
F	5.7622220	2.3920186	-3.9672783
F	3.9608064	4.1887511	-3.0814797

H	-1.2402800	-1.6588710	-0.3323717
H	2.2527211	0.6610071	-0.3311121

Compound 3

F	4.8827761	3.0376772	2.5168083
F	2.7632453	-4.1711324	3.9726807
N	-0.4590077	0.2327085	0.4605596
H	-0.7913167	1.0930235	0.8884992
C	1.0256136	2.8938593	1.2707041
C	1.7419030	1.7106419	1.2299401
C	1.7221429	-0.9870037	1.5314488
C	3.0603285	1.8208317	1.6534751
C	1.5369586	4.0930604	1.7321614
C	2.4551554	-2.0672892	1.0622151
C	2.8463461	4.1430557	2.1665020
C	1.4058355	-1.0293547	2.8790334
C	1.7317549	-2.0786374	3.7149016
F	0.7537693	-0.0000248	3.4297534
B	1.2550674	0.2692681	0.6337192
F	-0.2509591	2.9383153	0.8394480
F	3.8665527	0.7619423	1.6049673
F	0.7857174	5.1867010	1.7541460
F	2.8679401	-2.1271437	-0.2015180
F	3.3589477	5.2790046	2.6126978
F	3.4963385	-4.1586640	1.3683398
F	1.3855869	-2.0661322	4.9963048
O	1.6581892	0.1876837	-0.7670910
C	2.8052632	-3.1396185	1.8659396
C	3.6179089	2.9973060	2.1206631
C	2.4360241	-3.1487221	3.1967512
C	0.6224606	0.3692955	-1.5674842
C	0.7667089	0.4932074	-2.9812459
C	2.0325535	0.4460551	-3.5832244
H	2.9090647	0.3197837	-2.9627804
C	2.1516088	0.5578908	-4.9454046
H	3.1265506	0.5214298	-5.4121524
C	1.0039054	0.7187421	-5.7270950
H	1.0928231	0.8076467	-6.8016945
C	-0.2402698	0.7640639	-5.1456116
H	-1.0998935	0.8868708	-5.7880926
C	-0.4038655	0.6514354	-3.7543134
C	-1.7072093	0.6900749	-3.1113453
C	-2.8947976	0.8622232	-3.8389539
H	-2.8583803	0.9772239	-4.9126523
C	-4.1235101	0.8930837	-3.2246035

H	-5.0187457	1.0284641	-3.8158446
C	-4.2118482	0.7480045	-1.8393639
H	-5.1770044	0.7656385	-1.3511126
C	-3.0722856	0.5802349	-1.0922429
H	-3.1619954	0.4523252	-0.0225939
C	-1.8071135	0.5528572	-1.7034231
C	-0.5957103	0.3914379	-0.9799230
C	-1.1973383	-0.8551330	1.0986978
C	-1.1457162	-2.1617453	0.6071096
C	-1.8067560	-3.1450492	1.3387736
H	-1.7676760	-4.1665068	0.9826903
C	-2.5065318	-2.8514781	2.4927746
H	-3.0014339	-3.6391510	3.0444396
C	-2.5874182	-1.5416110	2.9248242
H	-3.1588102	-1.2980090	3.8111615
C	-1.9456025	-0.5218896	2.2343889
C	-2.1254762	0.8966139	2.7077229
H	-2.7841930	0.9182558	3.5733116
H	-2.5950500	1.5323083	1.9516717
H	-1.1976526	1.3764412	3.0150738
C	-0.4887435	-2.5769100	-0.6784688
H	-1.0881861	-2.2720136	-1.5379191
H	-0.4042982	-3.6620894	-0.7120889
H	0.5097543	-2.1813793	-0.8260559

TS I‡

F	4.1411245	3.2722345	2.8796720
F	3.9665460	-3.8532734	4.2058335
N	-0.3472901	-0.2900292	0.4529730
H	0.0029485	0.6401020	0.9997272
C	0.7868259	2.9030429	0.6264569
C	1.2653810	1.7514689	1.2208837
C	1.9222278	-1.4955116	1.5017504
C	2.4031564	1.9369648	1.9783432
C	1.3645556	4.1530314	0.7595848
C	3.0059755	-2.2815856	1.1196008
C	2.5086542	4.2753391	1.5261060
C	1.5762547	-1.5452829	2.8459305
C	2.2458549	-2.3276916	3.7632978
F	0.5865996	-0.7937374	3.3048947
B	1.1752600	-0.6299890	0.4506279
F	-0.3390493	2.8574389	-0.1173351
F	2.9839568	0.9005667	2.6121942
F	0.8445142	5.2308620	0.1752473
F	3.4102703	-2.3078306	-0.1424954

F	3.0915508	5.4594127	1.6737692
F	4.7191820	-3.8196511	1.6099513
F	1.8850741	-2.3387064	5.0378997
O	1.6335933	-0.4519132	-0.8184893
C	3.6975767	-3.0780114	2.0136304
C	3.0382350	3.1567969	2.1418011
C	3.3137563	-3.0989216	3.3412139
C	0.6181450	0.0366551	-1.5786037
C	0.7994461	0.4211786	-2.9281499
C	2.0519246	0.3525860	-3.5579107
H	2.9103590	0.0006535	-3.0025136
C	2.1802389	0.7372983	-4.8674266
H	3.1434510	0.6891276	-5.3567329
C	1.0597187	1.1976039	-5.5665714
H	1.1592534	1.5052490	-6.5988600
C	-0.1686577	1.2672188	-4.9562234
H	-1.0045310	1.6323107	-5.5343661
C	-0.3443208	0.8800835	-3.6163717
C	-1.6294211	0.9314874	-2.9406021
C	-2.7878028	1.3701047	-3.6032140
H	-2.7332202	1.6809298	-4.6360377
C	-4.0073789	1.4206899	-2.9762785
H	-4.8776275	1.7658755	-3.5176222
C	-4.1204521	1.0229944	-1.6435681
H	-5.0799036	1.0531583	-1.1451701
C	-3.0131907	0.5883004	-0.9605425
H	-3.1274334	0.2674731	0.0624110
C	-1.7536234	0.5390183	-1.5811998
C	-0.5641943	0.0984450	-0.9329317
C	-1.3236153	-1.1188772	1.1333620
C	-1.4902391	-2.4434841	0.7330574
C	-2.4360108	-3.2077973	1.4093255
H	-2.5831968	-4.2399251	1.1180564
C	-3.1871598	-2.6679310	2.4366191
H	-3.9168980	-3.2780861	2.9517342
C	-3.0131297	-1.3433067	2.7989031
H	-3.6113631	-0.9189069	3.5948461
C	-2.0813763	-0.5397990	2.1541567
C	-1.9462460	0.9072295	2.5339671
H	-2.6892008	1.1722798	3.2837027
H	-2.0951581	1.5738316	1.6821461
H	-0.9677316	1.1442598	2.9504448
C	-0.7148507	-3.0501418	-0.3992429
H	-0.8833925	-2.5245684	-1.3398718
H	-1.0141477	-4.0855504	-0.5506910
H	0.3602024	-3.0627942	-0.2150996

Compound 5

F	-5.2872847	-0.3287666	-4.6377550
F	-3.6505237	-2.4803907	-4.5679612
F	-1.7584345	-2.6602129	-2.6581746
F	-3.1956360	1.4225198	-0.8556378
F	-5.0538303	1.6240090	-2.7816253
O	-1.1623914	-1.8041726	0.2319035
N	-0.2499490	0.1884387	-0.3479198
C	0.2497515	3.9176231	-2.1606828
H	0.3674242	4.8825177	-2.6359576
C	0.6134048	2.7655640	-2.8356602
H	1.0220944	2.8321370	-3.8361180
C	0.4685901	1.5162248	-2.2418300
C	-0.0595381	1.4579269	-0.9511118
C	0.5138758	-0.3783661	0.6796057
C	-0.0731778	-1.5636123	1.0013663
C	0.3860180	-2.4284974	2.0206286
C	1.5331391	-2.0156183	2.7350265
C	1.9849698	-2.8600088	3.7642245
H	2.8550937	-2.5933020	4.3466788
C	1.3455313	-4.0385083	4.0617930
H	1.7211712	-4.6636784	4.8607075
C	-4.3655748	-0.4245909	-3.6939053
C	-3.5282184	-1.5262622	-3.6553374
C	-2.5690174	-1.6065303	-2.6631032
C	-2.4106491	-0.6201243	-1.7027014
C	-3.2719581	0.4613384	-1.7695424
C	-4.2421850	0.5764388	-2.7473576
C	-0.2599518	3.8373730	-0.8754247
H	-0.5393638	4.7414360	-0.3490031
C	-0.4244372	2.6089498	-0.2473340
C	-0.9345597	2.5364151	1.1602419
H	-1.6706314	1.7458976	1.2964362
H	-1.3990476	3.4771777	1.4514267
H	-0.1224538	2.3410220	1.8638213
C	0.8885982	0.2731031	-2.9690932
H	0.0310738	-0.3061013	-3.3151306
H	1.4877636	-0.3849481	-2.3397471
H	1.4820568	0.5228714	-3.8472219
C	1.7073855	0.0531822	1.3375871
C	2.1998644	-0.7721020	2.3845492
C	-0.2592509	-3.6373801	2.3282838
H	-1.1329224	-3.9319654	1.7629284
C	0.2157725	-4.4337435	3.3380539

H	-0.2817953	-5.3645923	3.5749820
C	3.3605838	-0.3491867	3.0549065
H	3.7635423	-0.9438396	3.8616350
C	4.0176431	0.8069767	2.7154402
H	4.9081826	1.0985469	3.2558772
C	3.5410792	1.5960725	1.6675310
H	4.0628953	2.5001015	1.3835512
C	2.4074553	1.2234071	0.9907356
H	2.0604603	1.8398908	0.1751578
B	-1.2926387	-0.7306606	-0.6197433

TS J‡

C	-1.0468817	2.5015477	3.0459518
C	-1.3970604	2.2665379	1.7080905
C	-2.6222949	2.7050873	1.1833421
C	-3.5300498	3.3078694	2.0410514
C	-3.2169113	3.5218146	3.3740983
C	-1.9784040	3.1390407	3.8576101
N	-0.5058318	1.6846767	0.8066759
C	-0.0065943	0.5280399	0.9408066
C	1.0981967	0.2235707	-0.0147140
C	2.2178567	-0.5195502	0.5173035
C	2.0430085	-1.2962900	1.6776612
C	0.7064285	-1.4291344	2.2738848
C	-0.3106441	-0.5296528	1.9184321
C	0.4062357	-2.4536242	3.1695930
C	-0.8640123	-2.5865978	3.6989489
C	-1.8679259	-1.7029422	3.3306124
C	-1.5912144	-0.6797821	2.4431365
C	3.4534481	-0.4470249	-0.1307494
C	4.5396575	-1.1231424	0.3831318
C	4.3843214	-1.8732462	1.5427859
C	3.1575427	-1.9596008	2.1800864
O	1.1507231	0.7716144	-1.1592003
B	0.3726170	-0.4323637	-1.8492327
C	-0.9191663	0.1061015	-2.6193883
C	-1.1153064	1.4022039	-3.0693147
C	-2.2665733	1.7903590	-3.7344955
C	-3.2655661	0.8659555	-3.9722540
C	-3.1046657	-0.4403142	-3.5476308
C	-1.9428750	-0.7906500	-2.8863615
F	-0.1970139	2.3410039	-2.8758059
F	-2.4225958	3.0466033	-4.1398443
F	-4.3712700	1.2274456	-4.6085479
F	-4.0595744	-1.3356398	-3.7758749

F	-1.8172820	-2.0612398	-2.5008536
C	-2.9328339	2.5085255	-0.2690170
C	0.2942189	2.1299687	3.6093301
C	1.4499066	-1.2826003	-2.6819035
C	1.9117862	-2.5243149	-2.2752734
C	2.8608298	-3.2393854	-2.9854014
C	3.3701819	-2.7104170	-4.1561034
C	2.9316655	-1.4764796	-4.6024843
C	1.9888610	-0.7896399	-3.8597144
F	1.4627101	-3.0785092	-1.1495181
F	1.6000379	0.3995536	-4.3125600
F	3.4215795	-0.9696957	-5.7278054
F	4.2806224	-3.3813823	-4.8475226
F	3.2895412	-4.4207881	-2.5533990
H	-3.9079031	2.9231024	-0.5195480
H	-2.1848422	3.0009440	-0.8916808
H	-2.9381156	1.4550950	-0.5547125
H	0.5265421	2.7536274	4.4716572
H	0.3246590	1.0920069	3.9460062
H	1.1003272	2.2632411	2.8875987
H	-4.4884873	3.6283493	1.6521451
H	-3.9281594	4.0079275	4.0282574
H	-1.7201890	3.3392134	4.8903240
H	-2.3823505	-0.0065730	2.1461462
H	-2.8686177	-1.8175191	3.7236697
H	-1.0758091	-3.3949110	4.3855941
H	1.1588271	-3.1810395	3.4391211
H	3.0836627	-2.5495833	3.0823777
H	5.2328263	-2.4003503	1.9585583
H	5.5015266	-1.0648234	-0.1063655
H	3.5494610	0.1565043	-1.0225956
H	-0.0227874	-1.1387237	-0.9141163

Intermediate K

C	-0.6656129	-1.4695777	-3.1075649
C	-0.5567648	-0.1069744	-2.8729098
C	-0.9116447	0.6906755	-3.9506487
C	-1.3962006	0.1841045	-5.1468956
C	-1.5239805	-1.1801776	-5.3090821
C	-1.1499310	-2.0204912	-4.2773817
F	-1.9882081	-1.6804246	-6.4448425
F	-1.7276921	0.9983027	-6.1418851
F	-0.7772299	2.0150419	-3.8997734
B	0.1346806	0.4596934	-1.4974342
C	-0.0990201	2.0480219	-1.2253696

C	0.9145044	2.9565848	-0.9643454
C	0.6723390	4.2906301	-0.6725350
C	-0.6252865	4.7590555	-0.6366523
C	-1.6680973	3.8920633	-0.9047690
C	-1.3816368	2.5745167	-1.1979206
F	-0.8707370	6.0307153	-0.3523532
F	1.6797283	5.1210011	-0.4210626
F	2.1942748	2.5898235	-0.9696443
F	-2.4216092	1.7895176	-1.4946859
F	-2.9205319	4.3341200	-0.8860170
F	-1.2518675	-3.3378910	-4.4219668
F	-0.2944551	-2.3457129	-2.1601352
O	1.5137216	0.0169198	-1.4681475
C	1.7587368	-0.9625919	-0.5348582
C	0.5389913	-1.0542601	0.3162642
C	0.5863087	-1.8814221	1.5089375
C	1.8449488	-2.0231851	2.1248818
C	2.9969604	-1.2467616	1.6314885
C	2.9565559	-0.6926087	0.3485696
C	1.9382544	-2.8773646	3.2205860
C	0.8285464	-3.5537140	3.6965919
C	-0.4097118	-3.3962243	3.0897422
C	-0.5290363	-2.5583807	1.9981472
C	4.0211491	0.0527184	-0.1300550
C	5.1353570	0.2635333	0.6667050
C	5.1826200	-0.2684489	1.9462810
C	4.1198281	-1.0140488	2.4243891
N	-0.4030656	-0.3071856	-0.1302669
C	-1.5396058	0.0348247	0.6714577
C	-2.8132239	-0.4404924	0.3501285
C	-3.8762421	-0.0478356	1.1528818
C	-3.6884710	0.8007746	2.2294526
C	-2.4190732	1.2530990	2.5317181
C	-1.3183622	0.8736274	1.7698203
C	-3.0675610	-1.3653870	-0.8010259
C	0.0452715	1.3429849	2.1873358
H	-4.0900311	-1.7373716	-0.7680028
H	-2.9388787	-0.8588697	-1.7563462
H	-2.4063094	-2.2315982	-0.7957850
H	-0.0333243	2.2565295	2.7745309
H	0.5396702	0.6000680	2.8171198
H	0.7103426	1.5550948	1.3538301
H	-4.8694094	-0.4099220	0.9194658
H	-4.5324167	1.1067993	2.8330014
H	-2.2679962	1.9125837	3.3769451
H	-1.4874494	-2.4483085	1.5125111

H	-1.2737539	-3.9308091	3.4586255
H	0.9334318	-4.2164547	4.5452431
H	2.8926652	-3.0357413	3.7026141
H	4.1610441	-1.3921396	3.4370234
H	6.0426459	-0.0933994	2.5783576
H	5.9596689	0.8555264	0.2925477
H	3.9715786	0.4772106	-1.1224351
H	1.9206037	-1.9503877	-1.0043967

TS L‡

C	3.7820265	0.1471381	1.3988386
C	2.4451247	-0.2215320	1.2203358
C	1.5326126	0.7550359	0.7772737
C	1.9792001	2.0510803	0.5016512
C	3.3048019	2.3861660	0.6872163
C	4.2129840	1.4321199	1.1395468
C	0.1378518	0.3798134	0.5784202
C	-0.3291906	-0.6919092	1.3639747
C	0.5640822	-1.8028068	1.6349237
C	1.9519065	-1.5639257	1.5204722
C	2.8179434	-2.6457305	1.7074517
C	2.3426518	-3.9018098	2.0156443
C	0.9749657	-4.1245702	2.1436225
C	0.0957285	-3.0810581	1.9565153
O	-0.8160527	1.3563567	0.5110417
B	-2.0295590	0.9660171	1.2387933
C	-2.3528209	1.8667597	2.5694304
C	-1.5275061	2.8636393	3.0615081
C	-1.7813599	3.5378801	4.2460667
C	-2.9022993	3.2215135	4.9857118
C	-3.7642526	2.2435728	4.5262437
C	-3.4761612	1.6040048	3.3372604
F	-0.4152966	3.2257223	2.4186812
F	-0.9500376	4.4830629	4.6809144
F	-3.1540226	3.8548543	6.1259382
F	-4.8531521	1.9391928	5.2259694
F	-4.3637935	0.6975760	2.9158322
N	-1.5745743	-0.4974251	1.7677275
C	-2.0970765	-1.1843903	2.9008620
C	-3.2198832	-2.0126360	2.7806915
C	-3.7218537	-2.6262557	3.9207106
C	-3.1375928	-2.4266814	5.1590436
C	-2.0235026	-1.6179125	5.2625088
C	-1.4789691	-0.9910982	4.1451389
C	-3.8812897	-2.2758784	1.4629595

C	-0.2311433	-0.1768811	4.3351868
C	-3.2600122	0.9583647	0.1488474
C	-3.2780720	0.0333801	-0.8806632
C	-4.2147738	0.0121375	-1.8935512
C	-5.1937063	0.9853157	-1.9210795
C	-5.2036231	1.9565565	-0.9404327
C	-4.2441182	1.9306578	0.0596958
F	-2.3286062	-0.9084158	-0.9492842
F	-4.3012905	2.9359176	0.9362952
F	-6.1262170	2.9150199	-0.9730194
F	-6.1032156	0.9970472	-2.8889425
F	-4.1678337	-0.9153532	-2.8489469
O	-1.3179417	1.3401996	-2.4623567
C	-0.1542962	1.4422887	-2.7231669
C	0.7532937	0.2429003	-2.8660589
C	1.4961524	0.2271270	-4.1267995
C	1.9277782	1.4713427	-4.6216002
C	1.6231824	2.7081881	-3.8747567
C	0.5567814	2.7072309	-2.9676840
C	2.3153681	3.8986929	-4.0670556
C	1.9465663	5.0457676	-3.3804930
C	0.8719744	5.0339480	-2.5018847
C	0.1666730	3.8599465	-2.3005445
C	1.7529892	-0.9479944	-4.8257525
C	2.4506315	-0.9042412	-6.0185865
C	2.8975595	0.3148195	-6.5070837
C	2.6351665	1.4879336	-5.8186654
N	0.8363091	-0.5881798	-1.9022906
C	1.7479380	-1.6824026	-1.8623185
C	3.1297301	-1.4611280	-1.8787406
C	3.9561565	-2.5741182	-1.7640522
C	3.4376121	-3.8504461	-1.6504093
C	2.0669615	-4.0390720	-1.6353798
C	1.1971417	-2.9617199	-1.7294314
C	3.7564918	-0.1069402	-2.0188551
C	-0.2846765	-3.1817836	-1.7058947
H	-4.5994351	-3.0895294	1.5550579
H	-4.4248031	-1.4018026	1.1064365
H	-3.1652404	-2.5527873	0.6914232
H	-0.2271670	0.2841607	5.3225070
H	0.6568321	-0.8098647	4.2710801
H	-0.1077563	0.6210868	3.6085566
H	-4.5905866	-3.2667381	3.8323461
H	-3.5497028	-2.9024193	6.0391767
H	-1.5588970	-1.4616171	6.2283905
H	-0.9661585	-3.2601415	2.0435767

H	0.6000666	-5.1109312	2.3804000
H	3.0392161	-4.7193910	2.1470810
H	3.8831679	-2.5100017	1.5857565
H	4.4949803	-0.5722896	1.7788123
H	5.2488960	1.6975914	1.3022243
H	3.6321405	3.3998352	0.4965056
H	1.2674850	2.7983736	0.1818927
H	0.3524162	-0.2566579	-0.7741266
H	-0.5122768	-4.2416012	-1.8048861
H	-0.7163662	-2.8455197	-0.7641178
H	-0.8045496	-2.6533347	-2.5044189
H	4.7191498	-0.0863404	-1.5127125
H	3.9358913	0.1365214	-3.0679885
H	3.1595407	0.6948746	-1.5867587
H	1.6578274	-5.0366305	-1.5404707
H	4.1025060	-4.6996967	-1.5654529
H	5.0290838	-2.4267138	-1.7677632
H	1.3965773	-1.8951576	-4.4458819
H	2.6394697	-1.8163674	-6.5671074
H	3.4420652	0.3559467	-7.4408574
H	2.9659069	2.4274197	-6.2397042
H	3.1589330	3.9407984	-4.7427071
H	2.5062048	5.9587063	-3.5341586
H	0.5923810	5.9326023	-1.9696108
H	-0.6623627	3.8156241	-1.6056656

Compound 7

N	-0.8151366	0.0882590	0.6021542
N	1.8169516	1.3660638	0.7197976
C	-0.8992381	-2.0281798	2.4361751
H	-0.5512942	-1.1442983	2.9717139
H	-0.0426541	-2.3922569	1.8641060
H	-1.1518888	-2.7928474	3.1692622
C	-3.0031072	0.8074829	-1.1603810
H	-2.4317126	0.5546740	-2.0560310
H	-2.5350712	1.6870599	-0.7171701
H	-4.0018848	1.0944695	-1.4868256
C	3.1015591	-1.1862437	0.8510555
H	2.3730665	-1.5552825	0.1245411
H	3.7138819	-2.0360123	1.1499813
H	3.7444248	-0.4803997	0.3230790
C	0.4165423	2.5529607	2.8610193
H	0.0704688	2.9411235	3.8180231
H	-0.4556922	2.4112510	2.2195108
H	1.0420509	3.3157358	2.3934944

C	1.1025557	1.1175846	-0.2916787
C	1.8451077	3.1711552	-1.4745799
H	2.1515718	3.5631611	-0.5142646
C	1.9822459	3.9230303	-2.6259526
H	2.3991285	4.9198639	-2.5770225
C	1.5664663	3.3965295	-3.8419721
H	1.6529479	3.9841821	-4.7462014
C	1.0366171	2.1204348	-3.9043926
H	0.7130876	1.7370076	-4.8624498
C	0.9004797	1.3431320	-2.7548806
C	0.4074236	-0.0451199	-2.7995196
C	0.3902323	-0.7810552	-3.9825116
H	0.7561744	-0.3419625	-4.9004316
C	-0.0587815	-2.0896142	-4.0030219
H	-0.0562454	-2.6413728	-4.9336490
C	-0.4914599	-2.6971841	-2.8338219
H	-0.8286000	-3.7245582	-2.8422746
C	-0.4816974	-1.9845197	-1.6484796
H	-0.8082764	-2.4647343	-0.7372489
C	-0.0421462	-0.6638764	-1.6222601
C	-0.0048417	0.1170199	-0.3695539
C	-1.9869955	-0.6756044	0.6230759
C	-2.0717221	-1.7142657	1.5586759
C	-3.2478429	-2.4478517	1.6269564
H	-3.3180168	-3.2630970	2.3369351
C	-4.3275271	-2.1448454	0.8127889
H	-5.2419568	-2.7184611	0.8848567
C	-4.2365296	-1.0902632	-0.0788035
H	-5.0858722	-0.8380514	-0.7022033
C	-3.0723393	-0.3390922	-0.1949834
C	1.7680060	0.6625463	1.9269437
C	2.4451338	-0.5549812	2.0438797
C	2.5039396	-1.1599146	3.2945927
H	3.0313856	-2.1007493	3.3976432
C	1.9061389	-0.5808855	4.4002946
H	1.9651198	-1.0631259	5.3669202
C	1.2352889	0.6246803	4.2608967
H	0.7607691	1.0811983	5.1213826
C	1.1572719	1.2639794	3.0319312
C	1.2924928	1.8961212	-1.5291213

Compound 9

N	-0.0413192	-1.2009413	0.2457357
H	0.6972404	-1.2831216	0.9242825
N	1.9902895	0.6602317	0.5930728

C	0.0377684	-3.9092164	0.9125115
H	0.7723316	-3.5934117	1.6588445
H	0.5065744	-3.7928686	-0.0659515
H	-0.1428898	-4.9702643	1.0773984
C	-2.4869877	0.4471654	0.4798011
H	-2.4030325	0.6810662	-0.5827961
H	-1.6793354	0.9607036	0.9995340
H	-3.4256688	0.8726007	0.8324062
C	2.8444327	-1.0146088	2.7389088
H	2.9736540	-1.5865433	3.6560956
H	3.8322222	-0.6321129	2.4666722
H	2.5581008	-1.7254101	1.9578122
C	0.2202493	2.9508234	0.9858959
H	-0.3445256	3.7847228	1.4011500
H	-0.3680521	2.5323727	0.1686555
H	1.1270831	3.3572509	0.5370842
C	1.2560179	0.5955452	-0.6135840
C	1.6417410	1.4753408	-1.6782538
C	2.7050705	2.3833248	-1.5085101
H	3.2379321	2.3946711	-0.5681892
C	3.0584760	3.2580663	-2.5043957
H	3.8774612	3.9485349	-2.3513216
C	2.3554041	3.2600161	-3.7120657
H	2.6274892	3.9481240	-4.5010910
C	1.3150778	2.3829892	-3.8956856
H	0.7913985	2.4049620	-4.8404897
C	0.9322055	1.4723319	-2.8959415
C	-0.1358896	0.5136428	-3.0780558
C	-0.8500610	0.4270688	-4.2864743
H	-0.6555061	1.1351650	-5.0784667
C	-1.7869989	-0.5502067	-4.5057109
H	-2.3171017	-0.5889281	-5.4480470
C	-2.0286965	-1.5077274	-3.5198100
H	-2.7328463	-2.3096069	-3.6963577
C	-1.3673682	-1.4354453	-2.3201010
H	-1.5670345	-2.1971192	-1.5838377
C	-0.4432706	-0.4067423	-2.0496079
C	0.2378675	-0.3157784	-0.7747533
C	-1.2618406	-1.7671006	0.6584194
C	-1.2381980	-3.1256253	1.0079211
C	-2.4116970	-3.7362379	1.4281152
H	-2.3954276	-4.7854704	1.6964755
C	-3.5982337	-3.0255778	1.4858036
H	-4.5114529	-3.5126819	1.8006774
C	-3.6048070	-1.6832856	1.1508450
H	-4.5267189	-1.1187289	1.2188557

C	-2.4458796	-1.0245396	0.7534928
C	1.4433514	0.8979597	1.8563075
C	1.8365168	0.0840132	2.9325965
C	1.2896541	0.3076635	4.1889436
H	1.5927794	-0.3244115	5.0148511
C	0.3565592	1.3081767	4.3925800
H	-0.0759047	1.4633188	5.3715977
C	0.0004271	2.1228329	3.3319241
H	-0.7006602	2.9330526	3.4927207
C	0.5447989	1.9569124	2.0636299
H	2.8872304	0.2030626	0.5778799

Intermediate Q

N	0.1087786	-0.8108054	-0.9993822
F	-2.8515764	-1.5008172	-0.7990065
F	-4.9904121	-2.1922790	-2.2521579
F	-5.2255181	-1.3326759	-4.8076506
F	-3.3025984	0.2268780	-5.9003994
F	-1.1442111	0.9011621	-4.4548408
C	0.7007660	-1.7529390	-3.7435821
H	1.0831588	-0.7905613	-3.4143212
H	-0.0695898	-1.5726306	-4.4924940
H	1.5218599	-2.2531668	-4.2594380
C	-0.4586971	-2.7913767	1.1347360
H	-1.1317456	-1.9574722	1.3146969
H	0.5089702	-2.5323791	1.5628177
H	-0.8437925	-3.6386663	1.6996606
C	-3.2659021	1.6932652	1.6780393
H	-3.5091376	0.9467322	0.9187108
H	-2.6832533	2.4749551	1.1914498
H	-4.2086661	2.1334671	1.9982246
C	0.7866798	-0.6285096	3.7618348
H	1.5756183	0.0923818	3.9822726
H	1.0372331	-1.0926815	2.8136413
H	0.8364601	-1.4068885	4.5231307
C	0.5795720	0.4864136	0.9893773
C	1.4946463	1.3870066	1.6538331
C	1.0117630	2.4951527	2.3735545
H	-0.0494907	2.6871543	2.4241020
C	1.8751235	3.3629927	2.9934533
H	1.4866217	4.2163966	3.5324772
C	3.2527811	3.1492517	2.9112387
H	3.9385093	3.8298530	3.3979446
C	3.7407400	2.0950937	2.1796694
H	4.8114257	1.9849015	2.0864779

C	2.8810404	1.1972158	1.5243241
C	3.3688405	0.1245060	0.6882597
C	4.7293950	-0.2170998	0.6470751
H	5.4242177	0.2682118	1.3177434
C	5.2101730	-1.1663453	-0.2191487
H	6.2625834	-1.4153400	-0.2255912
C	4.3256367	-1.8005851	-1.0906162
H	4.6869955	-2.5439824	-1.7887604
C	2.9870046	-1.4985852	-1.0603967
H	2.3373969	-2.0322811	-1.7310454
C	2.4611713	-0.5543963	-0.1579319
C	1.0463672	-0.3072125	-0.0345118
C	-0.0039563	-2.2112123	-1.3071844
C	0.2002644	-2.6340823	-2.6317015
C	0.0019061	-3.9751135	-2.9475556
H	0.1541773	-4.2963883	-3.9708816
C	-0.3605943	-4.8941128	-1.9854752
H	-0.5138421	-5.9322709	-2.2479553
C	-0.5005534	-4.4760590	-0.6749421
H	-0.7608939	-5.1939708	0.0924937
C	-0.3228753	-3.1470789	-0.3121045
C	-1.2498673	0.5523871	2.6831747
C	-2.5309751	1.1114411	2.8464968
C	-3.1149755	1.1361905	4.1027658
H	-4.1031909	1.5647406	4.2144381
C	-2.4455831	0.6391536	5.2069305
H	-2.9011893	0.6713415	6.1874468
C	-1.1905840	0.0928169	5.0370279
H	-0.6655408	-0.3114817	5.8942025
C	-0.5705709	0.0181718	3.7898967
C	-1.8897035	-0.3269542	-2.5961940
C	-2.9099065	-1.1017694	-2.0694307
C	-4.0331894	-1.4516449	-2.7934213
C	-4.1594267	-1.0051981	-4.0967836
C	-3.1758412	-0.2069012	-4.6536982
C	-2.0717624	0.1269846	-3.8930044
B	-0.6408737	0.1243761	-1.7461244
N	-0.7528340	0.5525725	1.3533691
C	-0.3237226	1.6682456	-1.6992475
C	0.9435517	2.2014813	-1.8875146
C	-1.3431287	2.5848156	-1.4951072
C	1.2019479	3.5565861	-1.8127023
C	-1.1248084	3.9459820	-1.4023121
C	0.1602739	4.4310090	-1.5579602
F	-2.5999682	2.1570422	-1.3658411
F	-2.1284681	4.7827233	-1.1704524

F	1.9610675	1.4023705	-2.1860546
F	2.4271358	4.0274212	-1.9949285
F	0.3912781	5.7308997	-1.4795856
H	-1.3897155	0.1221706	0.7024497

Compound 12

B	-0.8975082	-0.0478538	-0.4817170
N	0.2684163	-0.8041102	-0.7732933
N	-0.5645797	0.7940209	0.6122001
F	-3.3614509	-0.9596370	0.6874337
F	-5.7259353	-1.0769058	-0.5751870
F	-5.9039668	-0.3522970	-3.1769336
F	-3.7094262	0.5235963	-4.4980319
F	-1.3573302	0.6945368	-3.2187210
C	1.8051285	0.1300312	-3.0169745
H	2.7499411	0.0790563	-2.4717710
H	1.2093656	0.9110132	-2.5482969
H	2.0310056	0.4464277	-4.0342872
C	-0.8714685	-3.4258366	-0.6318672
H	-1.8545296	-2.9705871	-0.5077574
H	-0.3031162	-3.2138060	0.2739082
H	-1.0220411	-4.5030593	-0.6858887
C	-1.3169136	3.3099080	-0.5261233
H	-1.7011919	2.7660490	-1.3893787
H	-0.2311946	3.2110577	-0.5425744
H	-1.5578663	4.3612990	-0.6762699
C	-1.4907474	-0.1190016	3.1763085
H	-0.5222205	0.0407188	3.6553840
H	-1.3595571	-0.9226757	2.4541019
H	-2.1811368	-0.4675666	3.9432024
C	0.7663227	0.5551700	0.9517920
C	1.5859663	1.2135725	1.9218794
C	1.1566933	2.3203262	2.6812714
H	0.1626479	2.7174346	2.5516022
C	1.9889371	2.9293576	3.5855601
H	1.6328722	3.7793024	4.1523016
C	3.2900967	2.4580552	3.7632480
H	3.9527513	2.9344432	4.4732471
C	3.7334050	1.3925110	3.0213852
H	4.7517411	1.0648294	3.1684818
C	2.9123117	0.7409699	2.0841550
C	3.3986261	-0.3762360	1.2949326
C	4.6855889	-0.9084787	1.4880485
H	5.3381684	-0.4868263	2.2381428
C	5.1526375	-1.9712529	0.7569107

H	6.1484693	-2.3536450	0.9362308
C	4.3324197	-2.5605310	-0.2057444
H	4.6833180	-3.4088208	-0.7781208
C	3.0701177	-2.0703810	-0.4240307
H	2.4521992	-2.5570401	-1.1613737
C	2.5767075	-0.9693259	0.3042623
C	1.2620639	-0.4326625	0.1311848
C	0.4144106	-1.6589515	-1.8958251
C	1.1156689	-1.2010767	-3.0150560
C	1.2067233	-2.0410530	-4.1185279
H	1.7438400	-1.7033944	-4.9961041
C	0.6207206	-3.2956414	-4.1096319
H	0.6994701	-3.9354712	-4.9786023
C	-0.0582075	-3.7347278	-2.9862079
H	-0.5027720	-4.7220636	-2.9756888
C	-0.1702304	-2.9264312	-1.8600961
C	-1.4924230	1.5989200	1.3216189
C	-1.9019368	2.8108210	0.7618417
C	-2.8457794	3.5668797	1.4482981
H	-3.1731406	4.5112074	1.0314233
C	-3.3600541	3.1314301	2.6573849
H	-4.0940490	3.7303382	3.1802486
C	-2.9294307	1.9334620	3.2021077
H	-3.3283315	1.5990081	4.1516582
C	-1.9900501	1.1464228	2.5468902
C	-2.2766331	-0.1283576	-1.2215424
C	-3.4242785	-0.5668290	-0.5824887
C	-4.6489755	-0.6460058	-1.2187668
C	-4.7407228	-0.2795088	-2.5495045
C	-3.6173996	0.1631390	-3.2247769
C	-2.4121564	0.2327336	-2.5514849

Semidiimine O

N	-0.4367945	-0.5497690	0.5690703
H	0.0126949	-0.3621373	1.4533211
N	1.6200451	1.5066843	0.6878675
C	-0.6902944	-2.8137724	2.1877247
H	-0.2877362	-2.1486510	2.9567751
H	0.1264376	-3.0169538	1.4923755
H	-0.9534022	-3.7492986	2.6788933
C	-2.7294908	0.7658431	-0.7545415
H	-2.3978207	0.5822877	-1.7780957
H	-2.0309656	1.4767253	-0.3124135
H	-3.7015186	1.2542935	-0.8113919
C	3.2160948	-0.8478475	1.1136525

H	2.6081856	-1.3603198	0.3648238
H	3.9075717	-1.5811940	1.5267736
H	3.7999238	-0.0947408	0.5831717
C	-0.0029197	2.7012257	2.6406407
H	-0.4525519	3.1161916	3.5416030
H	-0.8128040	2.4624186	1.9472295
H	0.5952099	3.4794483	2.1643705
C	1.0957282	1.0513910	-0.4100959
C	1.4013330	1.8031022	-1.6380751
C	2.1052605	3.0079844	-1.5374699
H	2.4418128	3.3259167	-0.5612282
C	2.3527573	3.7791792	-2.6502070
H	2.8909779	4.7126973	-2.5529870
C	1.8982587	3.3571816	-3.8972925
H	2.0743125	3.9626647	-4.7765145
C	1.2207172	2.1646029	-4.0122181
H	0.8722639	1.8639523	-4.9900324
C	0.9683900	1.3573473	-2.8946240
C	0.3095961	0.0621739	-3.0065464
C	0.0639911	-0.5375872	-4.2448734
H	0.3528859	-0.0328782	-5.1554925
C	-0.5168069	-1.7840803	-4.3452335
H	-0.6912431	-2.2207656	-5.3193533
C	-0.8475061	-2.4861919	-3.1884687
H	-1.2710858	-3.4792733	-3.2533624
C	-0.6193060	-1.9215116	-1.9561902
H	-0.8555934	-2.4964636	-1.0737100
C	-0.0598250	-0.6343430	-1.8334835
C	0.1791342	-0.0507960	-0.5414273
C	-1.7315946	-1.0912740	0.6746866
C	-1.8799288	-2.2218340	1.4911894
C	-3.1416920	-2.7796177	1.6366299
H	-3.2637319	-3.6558204	2.2612341
C	-4.2358237	-2.2367814	0.9832403
H	-5.2139930	-2.6852181	1.0947166
C	-4.0752991	-1.1062491	0.2025076
H	-4.9365646	-0.6642566	-0.2834655
C	-2.8330911	-0.4998257	0.0438705
C	1.5885194	0.8993570	1.9317438
C	2.3820777	-0.2310967	2.1972416
C	2.3852026	-0.7519658	3.4858365
H	2.9995710	-1.6189280	3.6980050
C	1.6226501	-0.1863856	4.4949590
H	1.6368654	-0.6091165	5.4906078
C	0.8526103	0.9336896	4.2223468
H	0.2582178	1.3842250	5.0081122

C	0.8300868	1.4963614	2.9535732

Diazaborocyclic Radical P

N	0.3981468	-0.5736278	-0.9093536
F	-2.7961068	-1.1022829	1.3898475
F	-4.7295226	-2.7519390	0.7649680
F	-5.2768140	-3.3372128	-1.8305337
F	-3.8061073	-2.1694691	-3.7938799
F	-1.8912444	-0.4677896	-3.1971103
C	1.2276644	-0.0762798	-3.6846921
H	1.9511713	0.3883120	-3.0164505
H	0.3931907	0.6129295	-3.8045353
H	1.7031046	-0.1776405	-4.6591344
C	-0.0527304	-3.2399076	0.0654302
H	-0.7961907	-2.5972195	0.5284643
H	0.8757125	-3.1210641	0.6285632
H	-0.3830992	-4.2683210	0.2024881
C	-2.0588683	3.3069110	0.9033639
H	-2.8250196	3.0980634	0.1593183
H	-1.1006557	3.3758100	0.3951270
H	-2.2819900	4.2906618	1.3150837
C	-0.4243556	-0.9672540	3.2182085
H	0.5576015	-0.7534203	3.6455684
H	-0.2604383	-1.4614213	2.2654960
H	-0.9107484	-1.6874300	3.8751285
C	0.8239452	0.5360592	1.0110288
C	1.6891639	1.0972240	2.0139300
C	1.3161017	2.1929590	2.8114373
H	0.3571956	2.6653796	2.6751861
C	2.1656025	2.6996237	3.7647049
H	1.8572759	3.5466514	4.3621090
C	3.4210781	2.1266773	3.9472124
H	4.0960807	2.5158114	4.6975277
C	3.8197591	1.0820116	3.1450754
H	4.8194755	0.6969071	3.2777698
C	2.9814417	0.5493590	2.1576864
C	3.4467650	-0.4905445	1.2460028
C	4.6914395	-1.1038170	1.4288453
H	5.2832187	-0.8780458	2.3031604
C	5.2003812	-2.0044875	0.5212009
H	6.1653496	-2.4601201	0.6979815
C	4.4748585	-2.3095880	-0.6249952
H	4.8734440	-2.9922383	-1.3627603
H	2.6975444	-2.0114203	-1.7142611
C	2.6753475	-0.8607372	0.1175818

C	1.3377693	-0.3292349	0.0081582
C	0.4439270	-1.6480471	-1.8467348
C	0.7804675	-1.4163555	-3.1842467
C	0.7510200	-2.4903921	-4.0673304
H	1.0041570	-2.3202802	-5.1062694
C	0.4111446	-3.7613098	-3.6425005
H	0.3839272	-4.5813133	-4.3476277
C	0.1305663	-3.9826143	-2.3066898
H	-0.1042557	-4.9818711	-1.9623495
C	0.1536332	-2.9398318	-1.3882705
C	-1.2940234	1.1130875	1.9835070
C	-2.0599405	2.2851473	2.0000600
C	-2.8207328	2.5735776	3.1306314
H	-3.4131544	3.4801786	3.1386720
C	-2.8131332	1.7504627	4.2370500
H	-3.4098280	1.9938533	5.1059224
C	-2.0208289	0.6180995	4.2254859
H	-1.9986515	-0.0309517	5.0921947
C	-1.2556046	0.2797132	3.1186943
C	-2.2046493	-0.6872376	-0.8630199
C	-2.9975289	-1.3056191	0.0887516
C	-4.0238641	-2.1887133	-0.2104652
C	-4.3023386	-2.4928884	-1.5248098
C	-3.5489167	-1.9005681	-2.5193856
C	-2.5406444	-1.0243741	-2.1723796
B	-0.9062083	0.2832329	-0.6095354
N	-0.4976639	0.7415565	0.8561994
C	-0.9547593	1.6446951	-1.5558176
C	0.1760538	2.4140736	-1.7984345
C	-2.1146074	2.1563753	-2.1229135
C	0.1874719	3.5547592	-2.5811182
C	-2.1531000	3.2953838	-2.9079514
C	-0.9896657	3.9981591	-3.1487253
F	-3.3029512	1.5956853	-1.8839423
F	-3.3018474	3.7301187	-3.4128784
F	1.3544713	2.0889271	-1.2563007
F	1.3164432	4.2248557	-2.7850963
F	-1.0053348	5.0899876	-3.8985195
C	3.2350123	-1.7484006	-0.8198038

Compound 10

B	2.0819787	0.4839627	0.3308835
N	-1.2180476	-1.3292138	0.2604491
H	-0.3703428	-1.5280641	0.7596819
N	0.6921042	0.6734849	0.3451949

F	1.5172656	-2.1724364	-0.7275584
F	2.7511857	-3.2856362	-2.8236591
F	4.7271469	-1.9471594	-4.1003597
F	5.4600630	0.5201255	-3.2603947
F	4.2142799	1.6447890	-1.1626033
F	4.0063627	-1.1606321	1.6341083
F	5.6374942	-0.3985691	3.6247397
F	5.5067747	2.1305177	4.5826574
F	3.7594021	3.8992243	3.5159616
F	2.1528474	3.1510045	1.5118111
C	-1.0671889	-3.9941911	1.1129215
H	-0.2261236	-3.6450972	1.7180232
H	-0.7382897	-3.9726732	0.0725314
H	-1.2393828	-5.0334450	1.3877682
C	-3.6550764	0.3219242	0.5389229
H	-3.7471937	0.4067185	-0.5456459
H	-2.7870042	0.9025427	0.8451512
H	-4.5329025	0.7957481	0.9763123
C	0.8307090	-0.9968194	2.8144975
H	0.1594688	-1.7670119	3.1999839
H	1.6517047	-0.9109373	3.5274760
H	1.2640523	-1.3734275	1.8918085
C	-0.9352989	3.1589915	0.3456706
H	-1.4523280	4.0728168	0.6342242
H	-1.5256622	2.6871740	-0.4403757
H	0.0114996	3.4534053	-0.0991425
C	-0.0880114	0.4518158	-0.8392832
C	0.1776757	1.2474910	-2.0095430
C	1.1638881	2.2535289	-2.0241138
H	1.7265545	2.4759905	-1.1306614
C	1.4078656	3.0125818	-3.1388038
H	2.1736447	3.7761589	-3.1092411
C	0.6637498	2.8020261	-4.3008785
H	0.8540946	3.3897948	-5.1885274
C	-0.3197585	1.8467448	-4.3053825
H	-0.8858756	1.7055935	-5.2142468
C	-0.5950143	1.0560763	-3.1751956
C	-1.6240871	0.0403181	-3.1864487
C	-2.4137429	-0.2036498	-4.3247660
H	-2.3093496	0.4195620	-5.2004670
C	-3.3216519	-1.2301944	-4.3669211
H	-3.9137677	-1.3905723	-5.2579949
C	-3.4577287	-2.0790271	-3.2674396
H	-4.1412612	-2.9164585	-3.3040315
C	-2.7182520	-1.8531884	-2.1350439
H	-2.8360529	-2.5320697	-1.3058159

C	-1.8208897	-0.7708320	-2.0492208
C	-1.0560700	-0.5220291	-0.8470475
C	-2.3775977	-1.8535403	0.8476664
C	-2.3096194	-3.1759883	1.3162289
C	-3.4204372	-3.7297039	1.9372258
H	-3.3686352	-4.7491403	2.2997123
C	-4.5930707	-3.0067610	2.0717421
H	-5.4576104	-3.4510041	2.5464442
C	-4.6485105	-1.7091060	1.5954032
H	-5.5608555	-1.1362770	1.7080522
C	-3.5516179	-1.1021856	0.9934540
C	-0.0011558	1.0885419	1.5362678
C	0.0887390	0.3062887	2.6961330
C	-0.5702106	0.7276419	3.8484633
H	-0.5018187	0.1158083	4.7398603
C	-1.3108467	1.8886260	3.8685340
H	-1.8171082	2.2013028	4.7718279
C	-1.4033261	2.6463521	2.7155023
H	-1.9836549	3.5602680	2.7202643
C	-0.7633644	2.2704642	1.5417243
C	2.7933660	-0.2047496	-0.8985371
C	2.4613441	-1.4684661	-1.3530994
C	3.0947811	-2.0690070	-2.4237668
C	4.1093474	-1.3886152	-3.0726169
C	4.4845881	-0.1291826	-2.6399920
C	3.8311128	0.4312955	-1.5596320
C	2.9950059	0.9565800	1.5254735
C	3.9273851	0.0932532	2.0794843
C	4.7730053	0.4638017	3.1072577
C	4.7061037	1.7556201	3.5988394
C	3.8060938	2.6560833	3.0578398
C	2.9731100	2.2450219	2.0342777

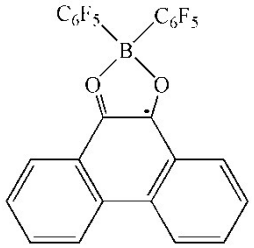
Intermediate R

C	3.3114169	-1.6819566	2.3199814
C	2.0986832	-2.1108138	1.8041774
C	1.5683753	-3.2521092	2.3865108
C	2.1630538	-3.9027664	3.4511183
C	3.3591483	-3.4218426	3.9513446
C	3.9426078	-2.3070819	3.3793578
B	1.4324080	-1.4251202	0.5344694
C	1.2512783	-2.3904766	-0.7040762
C	0.0571869	-3.0265306	-0.9850969
C	-0.0656243	-3.9360573	-2.0189502
C	1.0370336	-4.2221284	-2.8028497

C	2.2541627	-3.6192142	-2.5365309
C	2.3407110	-2.7312847	-1.4832183
F	-1.0205961	-2.7653805	-0.2510369
F	-1.2280534	-4.5252230	-2.2749088
F	0.9288949	-5.0768050	-3.8104950
F	3.3109914	-3.8982691	-3.2884852
F	3.5208560	-2.1721100	-1.2147765
F	0.4251032	-3.7586363	1.9266200
F	1.6031964	-4.9773743	3.9910652
F	3.9485192	-4.0331806	4.9659390
F	5.1027515	-1.8577448	3.8388551
F	3.9390753	-0.6484174	1.7684252
N	1.0778188	-0.0749266	0.5563226
C	1.0848119	0.6287724	1.8106684
C	0.1142830	0.3103356	2.7689367
C	0.1548068	0.9527205	4.0016410
C	1.1122184	1.9087161	4.2785923
C	2.0399098	2.2418064	3.3093675
C	2.0439415	1.6187399	2.0666898
C	-0.9799758	-0.6873168	2.5258548
C	3.0755850	2.0643658	1.0695276
C	0.6937711	0.7864248	-0.5850735
C	1.0668109	0.2524049	-1.9434117
C	0.1040988	-0.3395738	-2.7698636
C	-1.2693875	-0.5247538	-2.2713670
C	-1.7034154	0.2086056	-1.1582322
C	-0.7652271	1.1867914	-0.5781662
C	0.4923438	-0.7709040	-4.0373164
C	1.8010572	-0.6418519	-4.4693491
C	2.7484685	-0.0536997	-3.6462628
C	2.3705062	0.4015636	-2.3950901
C	-2.9856955	0.0242832	-0.6528442
C	-3.8460308	-0.8842471	-1.2415439
C	-3.4289082	-1.6039799	-2.3513660
C	-2.1552816	-1.4247088	-2.8595051
N	-1.0268861	2.3512387	-0.1559541
C	-2.2895825	2.9504278	-0.2203501
C	-2.9073927	3.2962958	0.9885353
C	-4.1314495	3.9486457	0.9494626
C	-4.7224297	4.2843033	-0.2577276
C	-4.0763712	3.9754591	-1.4415856
C	-2.8568258	3.3074283	-1.4512683
C	-2.2594043	2.9388804	2.2907735
C	-2.1782952	3.0110542	-2.7564949
H	-1.1987156	3.1916278	2.2964049
H	-2.3189361	1.8670568	2.4903782

H	-2.7407192	3.4519538	3.1225482
H	-2.3558123	1.9850184	-3.0846903
H	-1.0983151	3.1494636	-2.7011662
H	-2.5538402	3.6687888	-3.5395492
H	-1.8538674	-0.4366831	3.1271818
H	-0.6885149	-1.6965958	2.8135155
H	-1.2985324	-0.7298541	1.4878740
H	3.9973412	2.3452916	1.5776459
H	2.7316938	2.9466027	0.5242404
H	3.3296119	1.2988031	0.3425911
H	3.1041928	0.8753516	-1.7559605
H	3.7710722	0.0590340	-3.9792859
H	2.0773292	-0.9905033	-5.4553758
H	-0.2354381	-1.2040342	-4.7097736
H	-1.8496715	-2.0147044	-3.7127582
H	-4.0938523	-2.3186683	-2.8173565
H	-4.8374387	-1.0310103	-0.8355185
H	-3.3116184	0.5880472	0.2105690
H	-4.6207787	4.2057695	1.8812592
H	-5.6718230	4.8026608	-0.2748541
H	-4.5227875	4.2600843	-2.3869031
H	-0.5896589	0.7030234	4.7476532
H	1.1309188	2.3997887	5.2424589
H	2.7876030	2.9971589	3.5178105
H	1.2315046	1.7237508	-0.4499782

phenanthrene dioxoborocyclic radical[1]



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C	-1.4780035	-0.0914556	-4.4617990
C	-2.8552309	-0.1886117	-4.4385280
C	-3.5481111	-0.2511774	-3.2304119
C	-2.8484712	-0.2159353	-2.0475781
C	-1.4512224	-0.1182595	-2.0649709
C	-0.7315057	-0.0531033	-3.2816221
C	-0.7006125	-0.0657872	-0.8617030
C	0.7315057	0.0531033	-3.2816221
C	1.4512224	0.1182595	-2.0649709
C	0.7006125	0.0657872	-0.8617030

C	2.8484712	0.2159353	-2.0475781
C	1.4780035	0.0914556	-4.4617990
C	2.8552309	0.1886117	-4.4385280
C	3.5481111	0.2511774	-3.2304119
O	-1.1644441	-0.1196699	0.3386810
O	1.1644441	0.1196699	0.3386810
H	-0.9878682	-0.0416224	-5.4230205
H	-3.3998310	-0.2135530	-5.3727386
H	-4.6267357	-0.3235158	-3.2239390
H	-3.3649098	-0.2566204	-1.0981891
H	3.3649098	0.2566204	-1.0981891
H	0.9878682	0.0416224	-5.4230205
H	3.3998310	0.2135530	-5.3727386
H	4.6267357	0.3235158	-3.2239390
C	0.0638001	-1.3536111	2.1816181
C	-0.0638001	1.3536111	2.1816181
C	0.9203161	1.5694692	3.1324946
C	0.9590720	2.6897125	3.9404943
C	-0.0204308	3.6548535	3.7944824
C	-1.0131884	3.4858869	2.8489943
C	-1.0199150	2.3471812	2.0610005
F	1.8865326	0.6642092	3.2906181
F	1.9188811	2.8511748	4.8430094
F	-0.0032800	4.7399261	4.5541589
F	-1.9492897	4.4162633	2.7017427
F	-2.0001409	2.2507349	1.1638781
C	1.0199150	-2.3471812	2.0610005
C	1.0131884	-3.4858869	2.8489943
C	0.0204308	-3.6548535	3.7944824
C	-0.9590720	-2.6897125	3.9404943
C	-0.9203161	-1.5694692	3.1324946
F	2.0001409	-2.2507349	1.1638781
F	1.9492897	-4.4162633	2.7017427
F	0.0032800	-4.7399261	4.5541589
F	-1.9188811	-2.8511748	4.8430094
F	-1.8865326	-0.6642092	3.2906181

Compound 18

N	0.8230152	-0.1213461	-0.8369679
F	-1.0356019	-2.5614143	0.6924943
F	-2.0569338	-4.7194212	-0.4580689
F	-2.9587794	-4.6187208	-3.0146658
F	-2.8259494	-2.2897986	-4.3954287
F	-1.8422547	-0.1037513	-3.2498012
C	0.6358780	-0.1038253	1.4161771
C	1.1102798	-0.3360193	2.7541505

C	0.2382774	-0.5037825	3.8435965
H	-0.8277853	-0.4194865	3.7060746
C	0.7182907	-0.8031681	5.0959432
H	0.0281514	-0.9350220	5.9179287
C	2.0881029	-0.9513846	5.2946258
C	2.9543286	-0.8131502	4.2336994
H	4.0065262	-0.9743473	4.4149974
C	2.5001626	-0.5055097	2.9455135
C	3.4240520	-0.3894307	1.8206086
C	4.8104489	-0.3800506	2.0155635
H	5.2194412	-0.4580296	3.0119439
C	5.6902003	-0.2431979	0.9657599
H	6.7551703	-0.2368783	1.1551089
C	5.2049628	-0.0898580	-0.3298760
H	5.8871837	0.0457006	-1.1578742
H	3.4955273	0.0535376	-1.5642717
C	2.9375363	-0.2598729	0.4996284
C	1.5125057	-0.2010604	0.3071848
C	1.2777057	-0.5776889	-2.0913953
C	1.2247479	0.2478654	-3.2034715
C	1.6224682	-0.2343309	-4.4419178
H	1.5778041	0.4242555	-5.3004627
C	2.0728788	-1.5383677	-4.6012534
C	2.1118425	-2.3585256	-3.4736829
H	2.4475141	-3.3842188	-3.5690029
C	1.7150219	-1.8925399	-2.2356812
C	-1.6477981	0.6764336	1.7751148
C	-1.4485295	1.9039216	2.3968228
C	-2.4818252	2.5037520	3.0951875
H	-2.3119881	3.4638524	3.5668324
C	-3.7355972	1.9065180	3.1831142
C	-3.9192834	0.6803125	2.5505145
H	-4.8859614	0.1935171	2.5984266
C	-2.8928820	0.0661639	1.8536773
C	-1.4431723	-1.2071753	-1.2037030
C	-1.5018591	-2.4294036	-0.5542405
C	-2.0130024	-3.5767567	-1.1358239
C	-2.4700847	-3.5294456	-2.4378001
C	-2.4050247	-2.3391380	-3.1368026
C	-1.8971554	-1.2141833	-2.5138974
B	-0.6961838	0.0904104	-0.5569580
N	-0.6180134	0.1066894	0.9987741
C	-1.2991242	1.5440930	-0.9779891
C	-0.5190337	2.6889380	-0.9929343
C	-2.6601898	1.7570853	-1.1345837
C	-1.0340910	3.9587578	-1.1871490

C	-3.2176213	3.0084136	-1.3221884
C	-2.3955395	4.1180922	-1.3542401
F	-3.5127827	0.7330699	-1.0815195
F	-4.5297902	3.1551853	-1.4644898
F	0.8005388	2.6133063	-0.7874914
F	-0.2370219	5.0223026	-1.1998347
F	-2.9101342	5.3266918	-1.5332549
C	3.8495444	-0.0946373	-0.5569764
H	-3.0583092	-0.8908427	1.3798875
H	-0.4842913	2.3915030	2.3252960
H	2.4748786	-1.1930422	6.2754002
C	-4.8636489	2.5619021	3.9236660
H	-5.2455479	1.9191446	4.7181581
H	-5.6986904	2.7810436	3.2567972
H	-4.5531616	3.5005190	4.3802029
H	1.7379587	-2.5468583	-1.3732434
H	0.8862606	1.2692596	-3.1055749
C	2.4914498	-2.0641219	-5.9423566
H	2.4630312	-1.2872776	-6.7049815
H	1.8350813	-2.8710719	-6.2717338
H	3.5058750	-2.4640850	-5.9152820

Semidiimine S

N	0.8230152	-0.1213461	-0.8369679
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F	-2.0569338	-4.7194212	-0.4580689
F	-2.9587794	-4.6187208	-3.0146658
F	-2.8259494	-2.2897986	-4.3954287
F	-1.8422547	-0.1037513	-3.2498012
C	0.635878	-0.1038253	1.4161771
C	1.1102798	-0.3360193	2.7541505
C	0.2382774	-0.5037825	3.8435965
H	-0.8277853	-0.4194865	3.7060746
C	0.7182907	-0.8031681	5.0959432
H	0.0281514	-0.935022	5.9179287
C	2.0881029	-0.9513846	5.2946258
C	2.9543286	-0.8131502	4.2336994
H	4.0065262	-0.9743473	4.4149974
C	2.5001626	-0.5055097	2.9455135
C	3.424052	-0.3894307	1.8206086
C	4.8104489	-0.3800506	2.0155635
H	5.2194412	-0.4580296	3.0119439
C	5.6902003	-0.2431979	0.9657599
H	6.7551703	-0.2368783	1.1551089
C	5.2049628	-0.089858	-0.329876
H	5.8871837	0.0457006	-1.1578742

H	3.4955273	0.0535376	-1.5642717
C	2.9375363	-0.2598729	0.4996284
C	1.5125057	-0.2010604	0.3071848
C	1.2777057	-0.5776889	-2.0913953
C	1.2247479	0.2478654	-3.2034715
C	1.6224682	-0.2343309	-4.4419178
H	1.5778041	0.4242555	-5.3004627
C	2.0728788	-1.5383677	-4.6012534
C	2.1118425	-2.3585256	-3.4736829
H	2.4475141	-3.3842188	-3.5690029
C	1.7150219	-1.8925399	-2.2356812
C	-1.6477981	0.6764336	1.7751148
C	-1.4485295	1.9039216	2.3968228
C	-2.4818252	2.503752	3.0951875
H	-2.3119881	3.4638524	3.5668324
C	-3.7355972	1.906518	3.1831142
C	-3.9192834	0.6803125	2.5505145
H	-4.8859614	0.1935171	2.5984266
C	-2.892882	0.0661639	1.8536773
C	-1.4431723	-1.2071753	-1.203703
C	-1.5018591	-2.4294036	-0.5542405
C	-2.0130024	-3.5767567	-1.1358239
C	-2.4700847	-3.5294456	-2.4378001
C	-2.4050247	-2.339138	-3.1368026
C	-1.8971554	-1.2141833	-2.5138974
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C	-0.5190337	2.688938	-0.9929343
C	-2.6601898	1.7570853	-1.1345837
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C	-3.2176213	3.0084136	-1.3221884
C	-2.3955395	4.1180922	-1.3542401
F	-3.5127827	0.7330699	-1.0815195
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F	0.8005388	2.6133063	-0.7874914
F	-0.2370219	5.0223026	-1.1998347
F	-2.9101342	5.3266918	-1.5332549
C	3.8495444	-0.0946373	-0.5569764
H	-3.0583092	-0.8908427	1.3798875
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H	2.4748786	-1.1930422	6.2754002
C	-4.8636489	2.5619021	3.923666
H	-5.2455479	1.9191446	4.7181581
H	-5.6986904	2.7810436	3.2567972
H	-4.5531616	3.500519	4.3802029

H	1.7379587	-2.5468583	-1.3732434
H	0.8862606	1.2692596	-3.1055749
C	2.4914498	-2.0641219	-5.9423566
H	2.4630312	-1.2872776	-6.7049815
H	1.8350813	-2.8710719	-6.2717338
H	3.505875	-2.464085	-5.915282

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