

Supporting Information

2-Hydroxyphenyl Benzimidazoles and their Boron Complexes: Synthesis, Structure, Aggregation-Induced Emission and Picric acid Sensing

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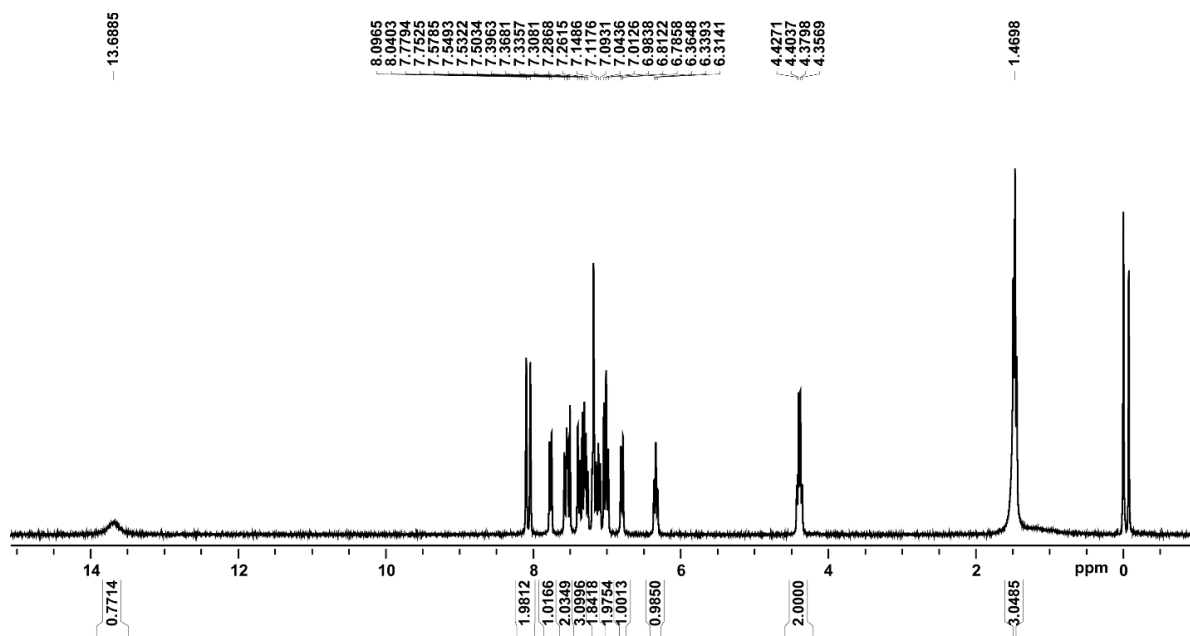


Fig. S1a. ¹H NMR spectrum of L1 in CDCl₃

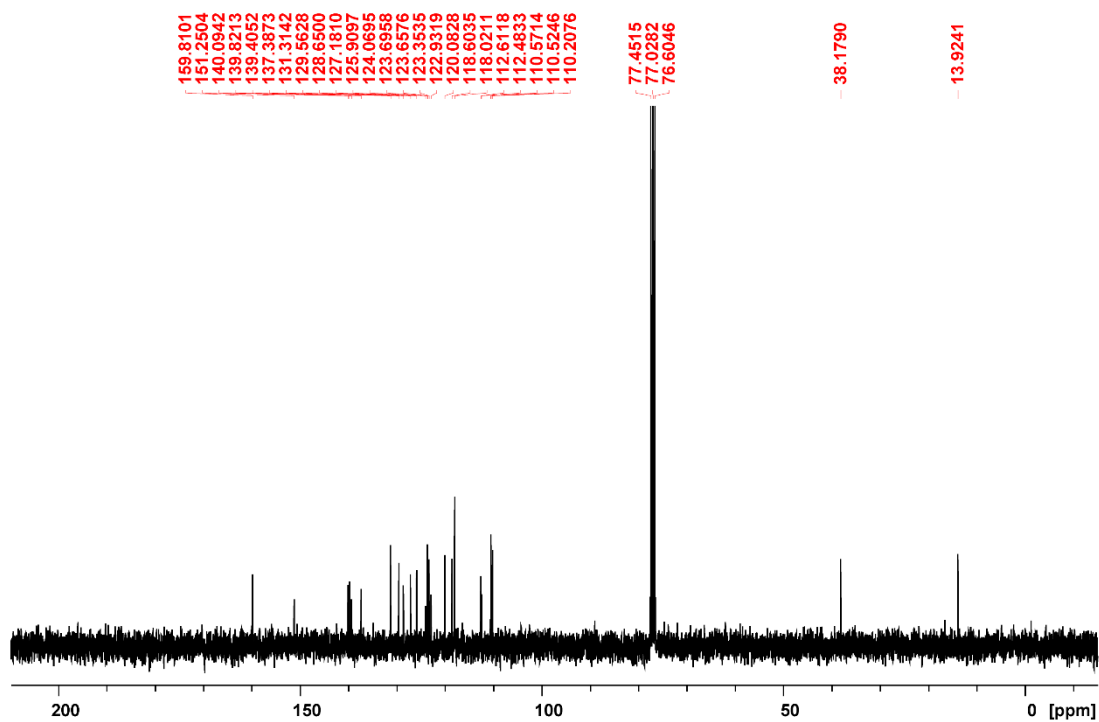


Fig. S1b. ^{13}C NMR spectrum of L1 in CDCl_3

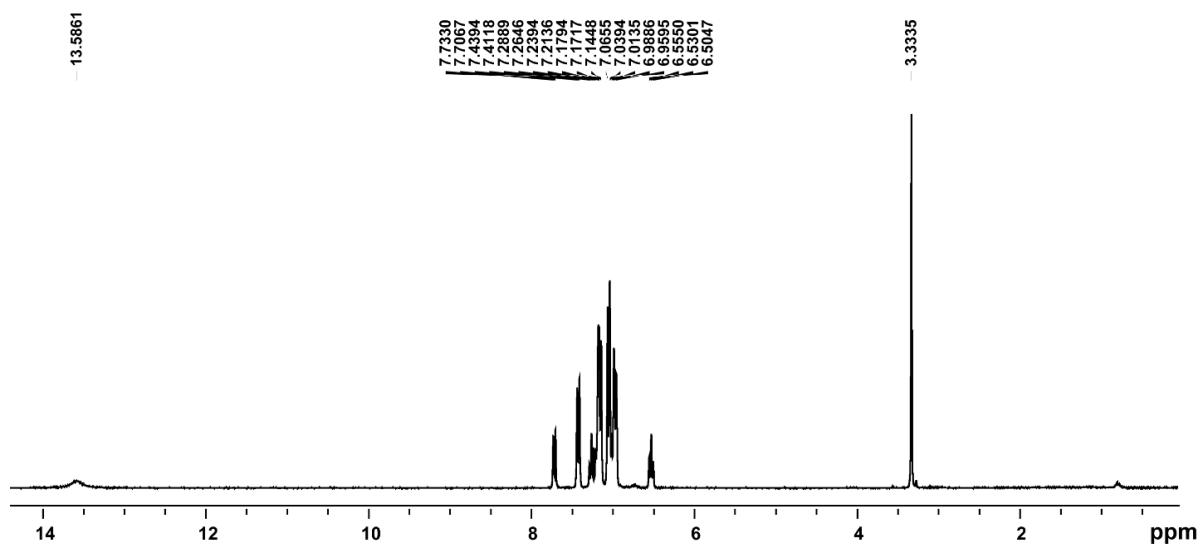


Fig. S2a. ^1H NMR spectrum of L2 in CDCl_3

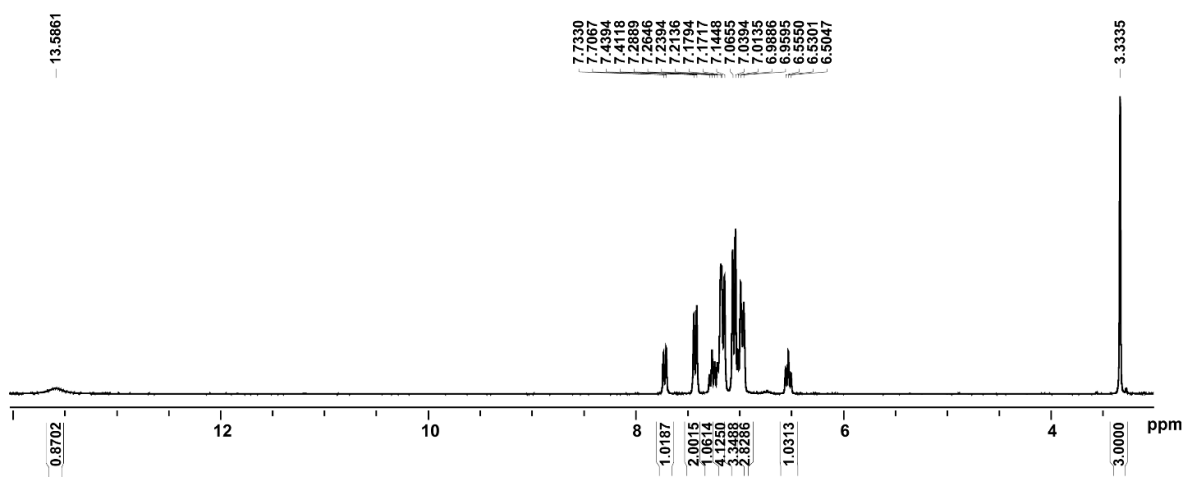


Fig. S2b. Partial ^1H NMR spectrum of **L2** in CDCl_3

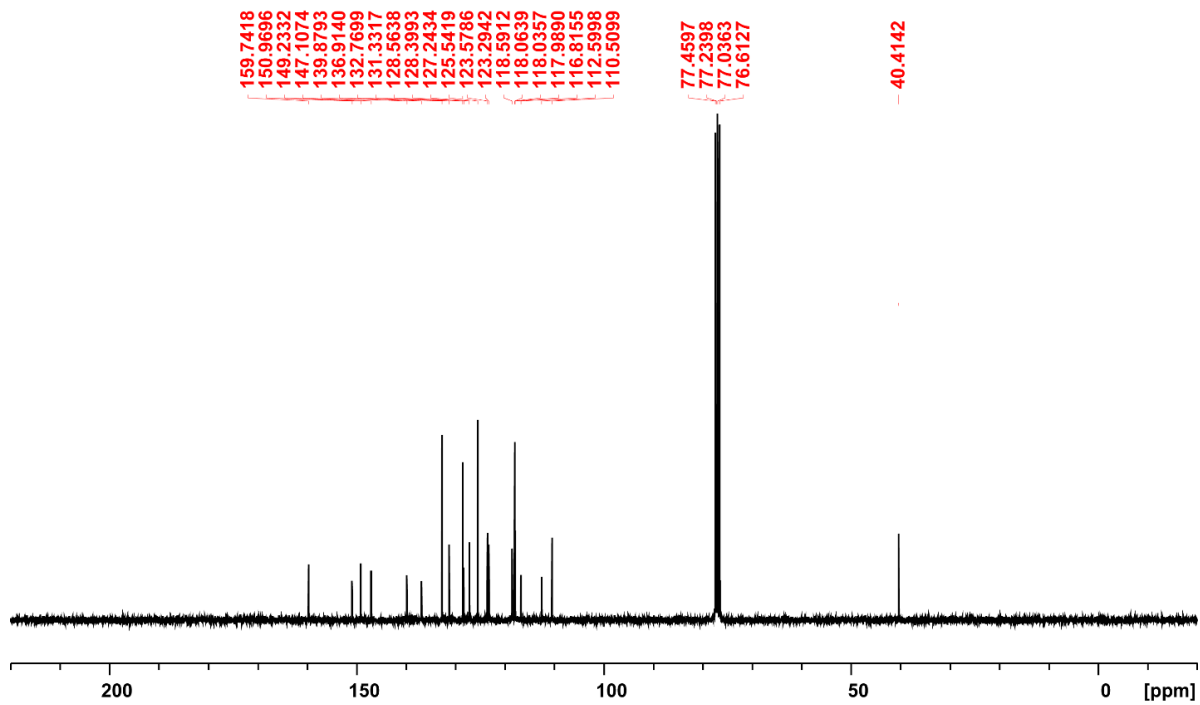


Fig. S2c. ^{13}C NMR spectrum of **L2** in CDCl_3

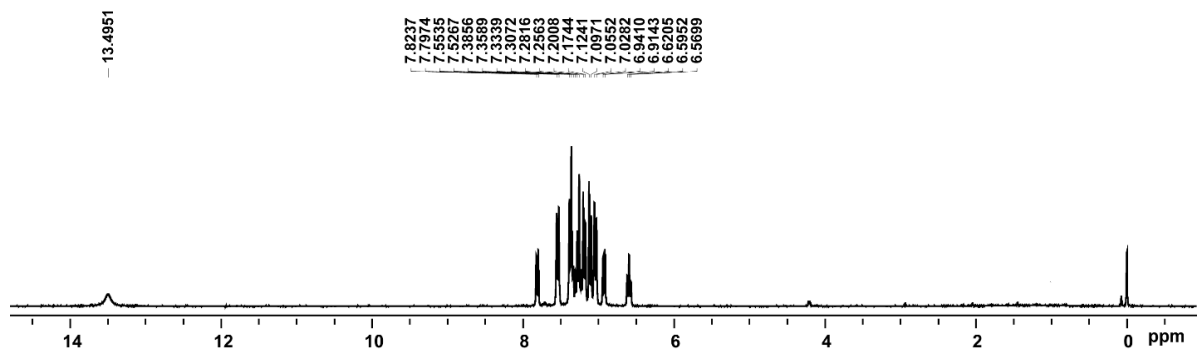


Fig. S3a. ^1H NMR spectrum of **L3** in CDCl_3

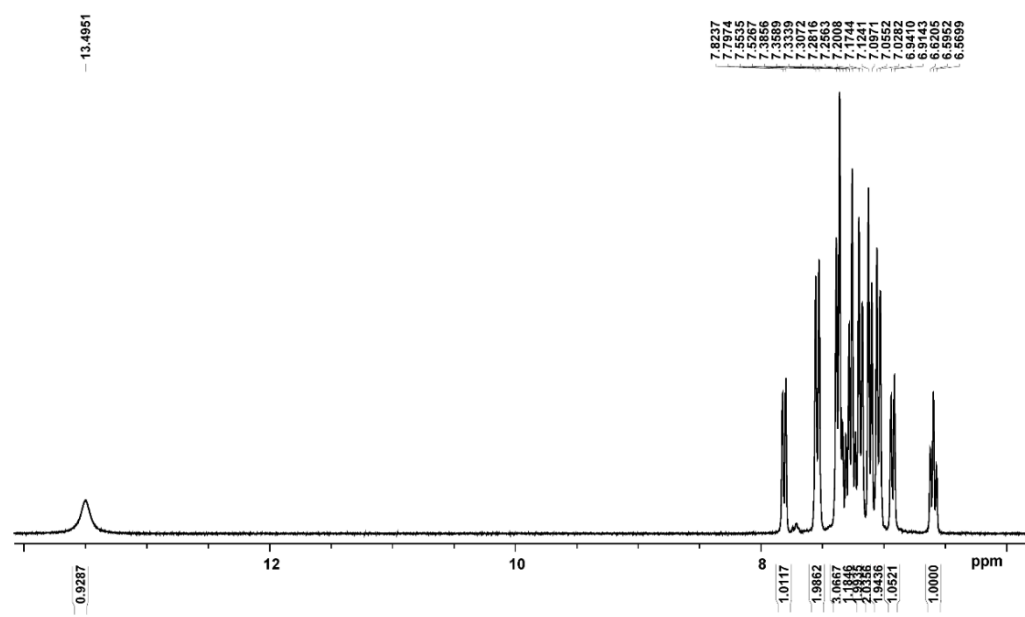


Fig. S3b. Partial ^1H NMR spectrum of **L3** in CDCl_3

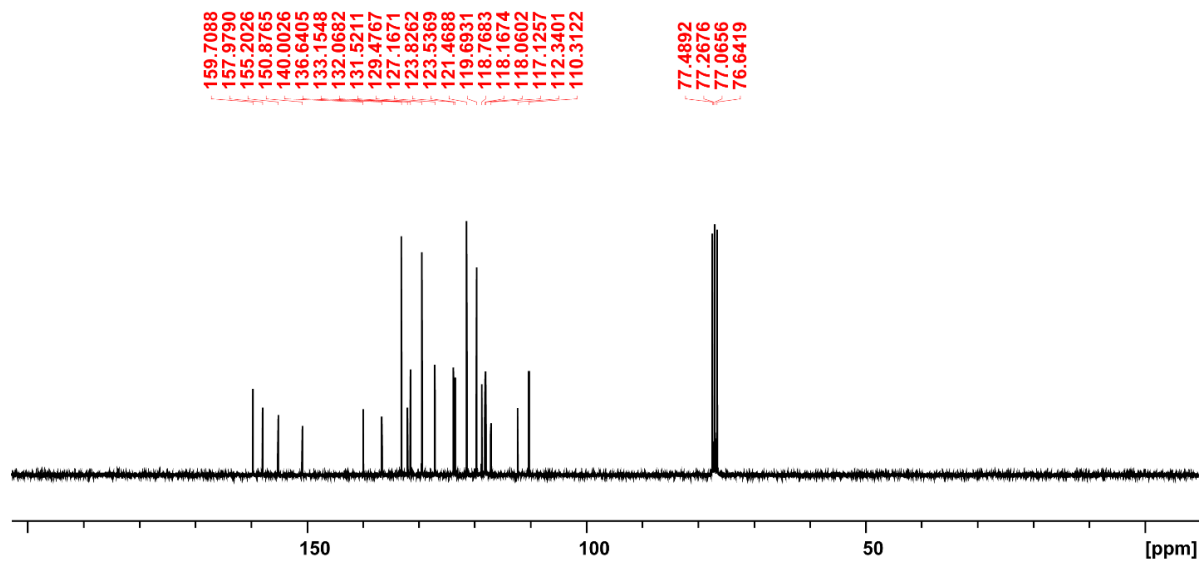


Fig. S3c. ^{13}C NMR spectrum of **L3** in CDCl_3

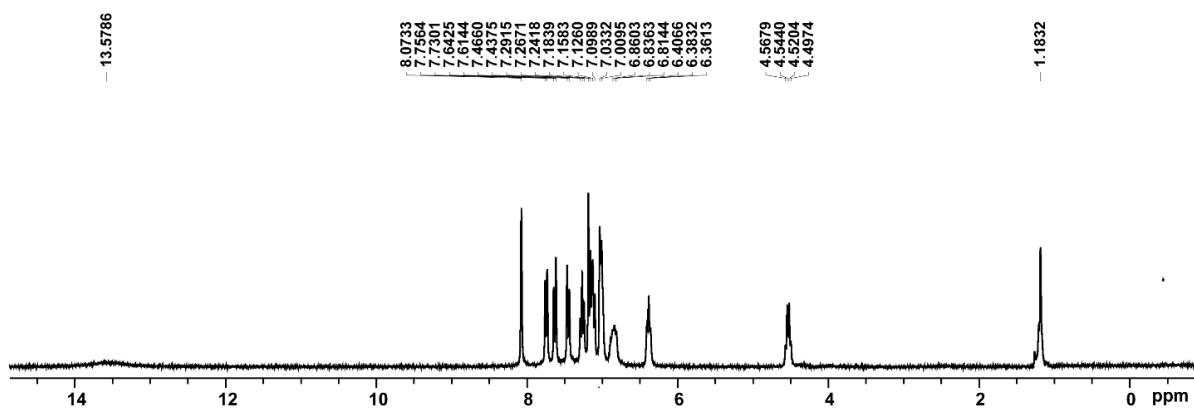


Fig. S4a. ^1H NMR spectrum of **L4** in CDCl_3

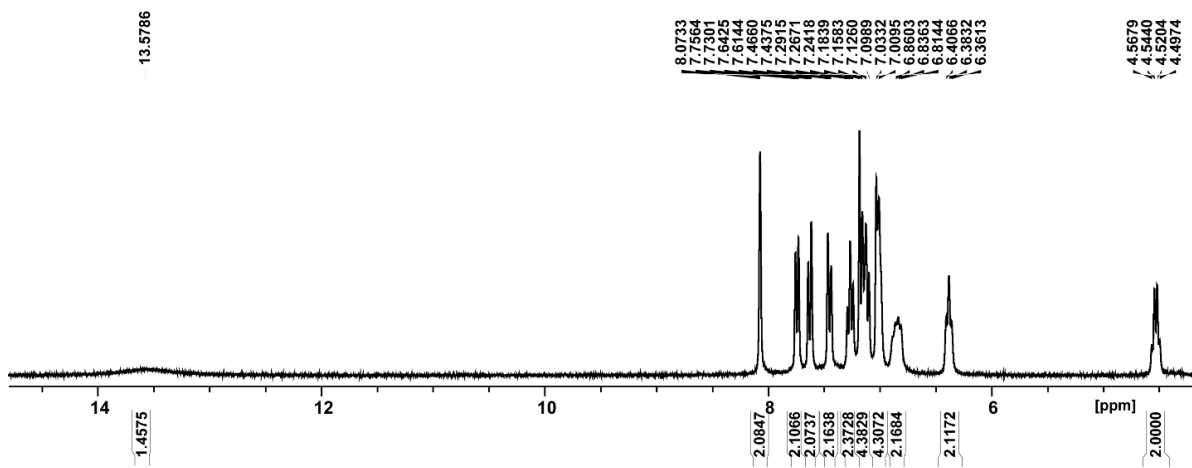


Fig. S4b. Partial ^1H NMR spectrum of **L4** in CDCl_3

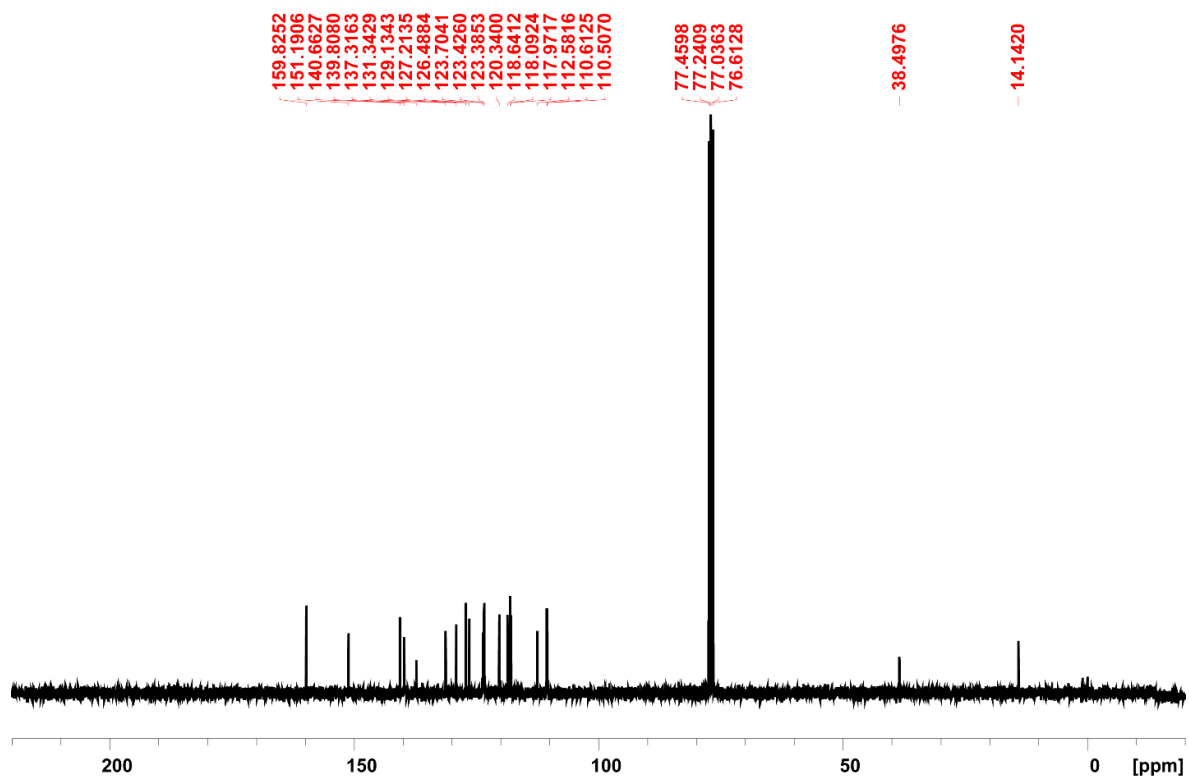


Fig. S4c. ^{13}C NMR spectrum of **L4** in CDCl_3

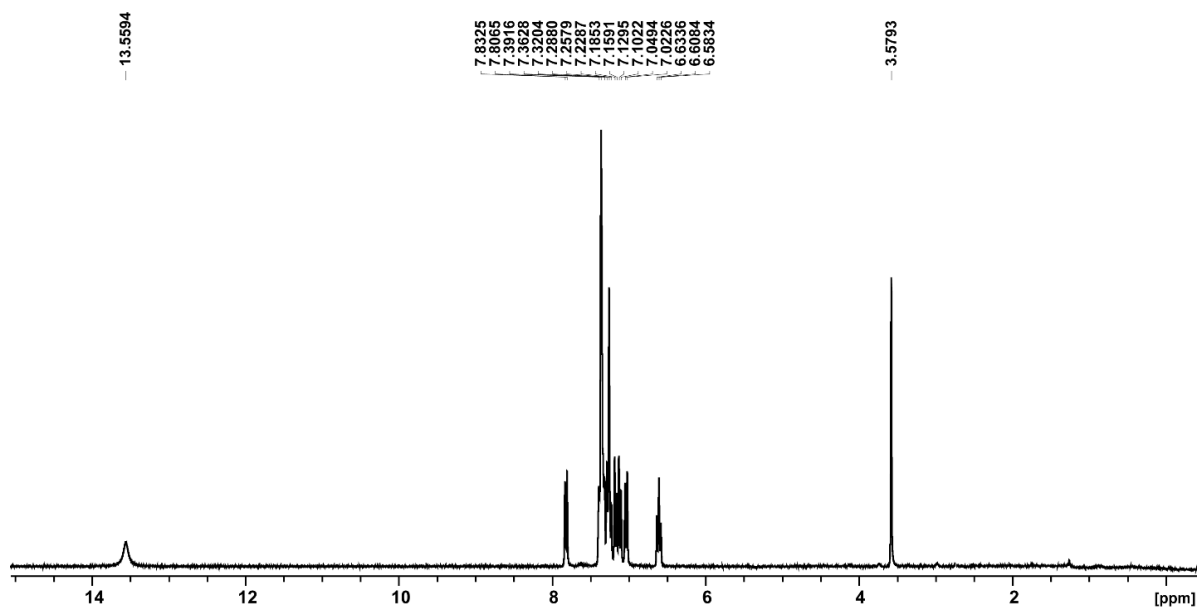


Fig. S5a. ^1H NMR spectrum of L5 in CDCl_3

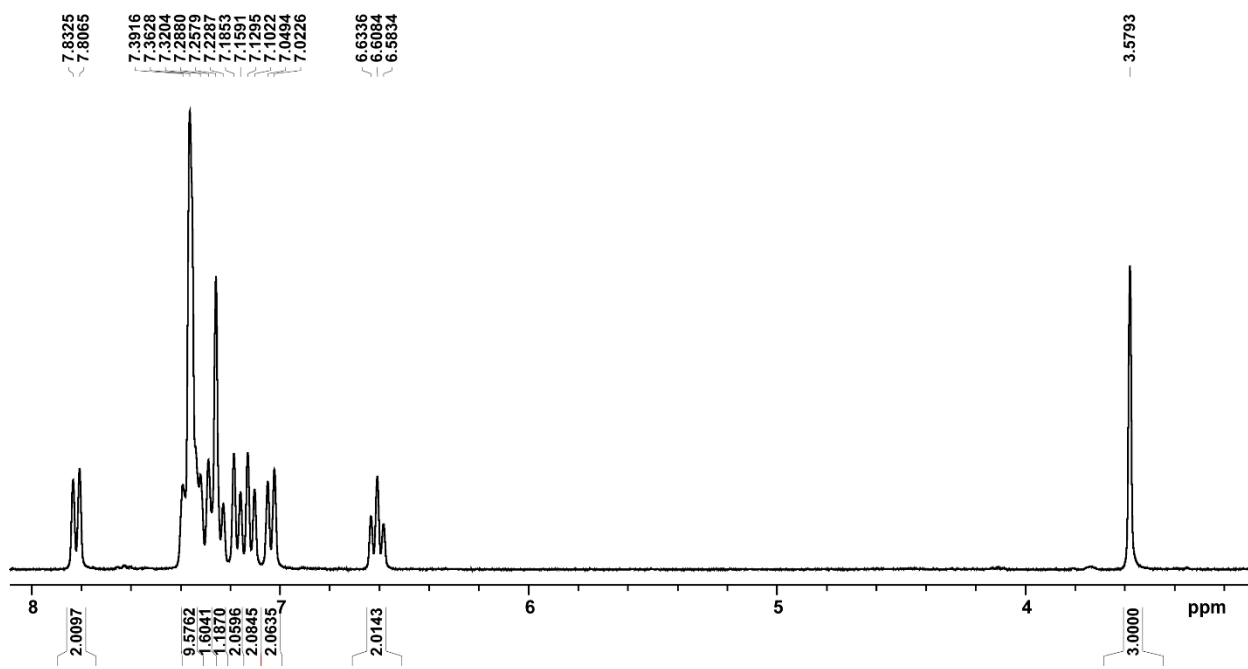


Fig. S5b. Partial ^1H NMR spectrum of L5 in CDCl_3

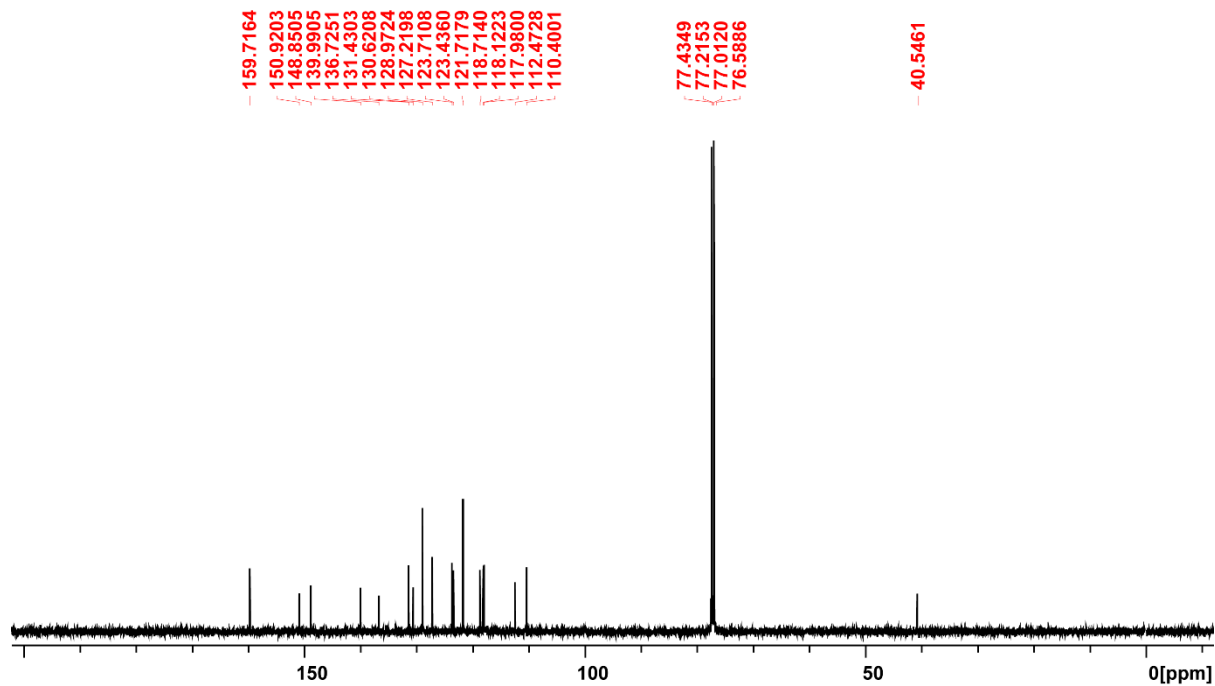


Fig. S5c. ^{13}C NMR spectrum of L5 in CDCl_3

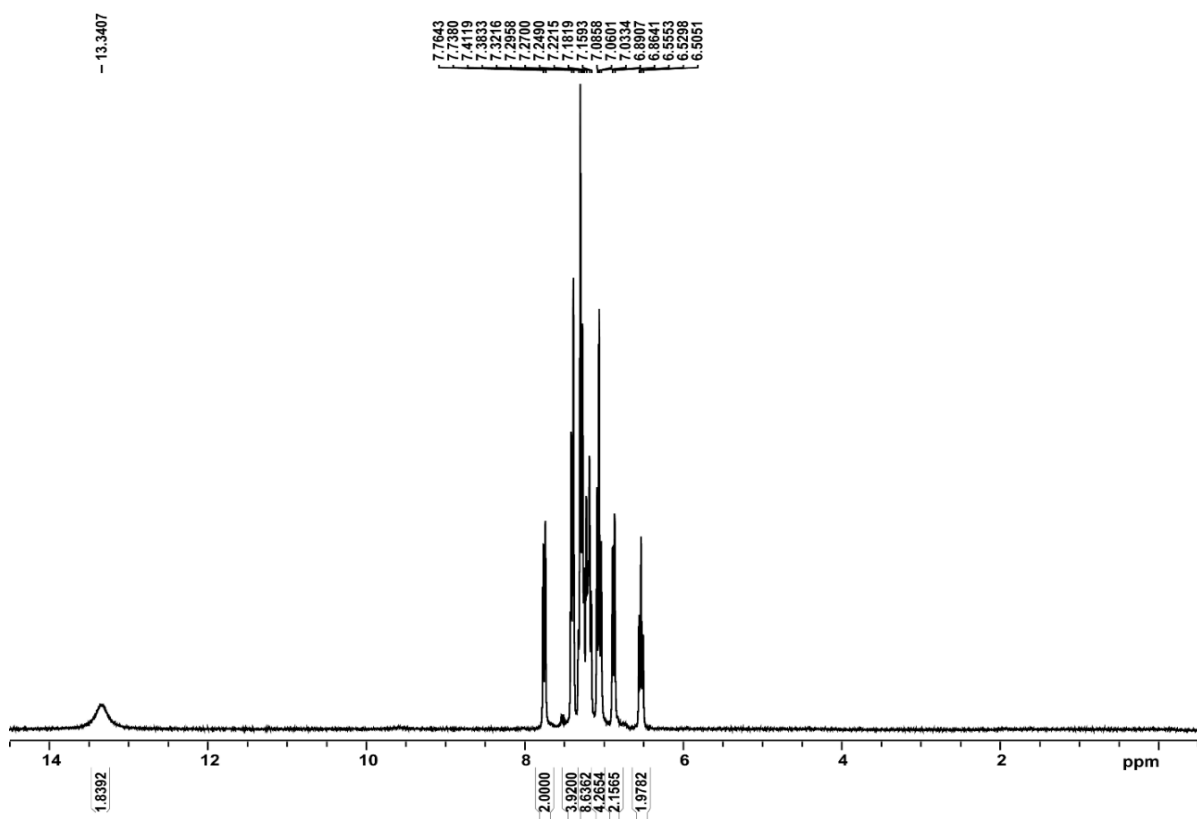


Fig. S6a. ^1H NMR spectrum of L6 in CDCl_3

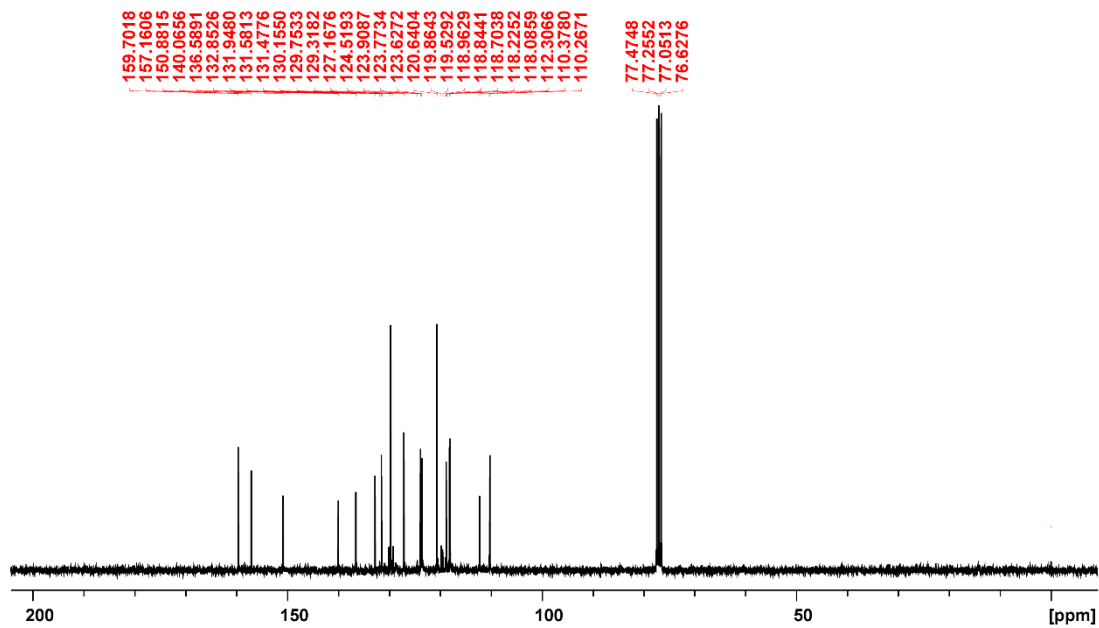


Fig. S6b. ¹³C NMR spectrum of L6 in CDCl₃

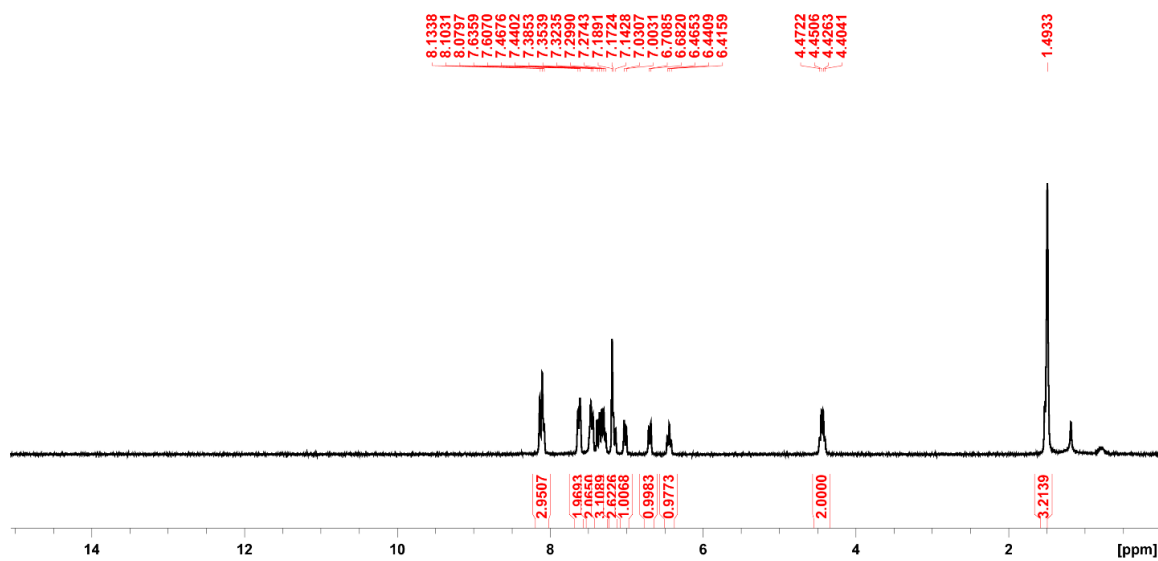


Fig. S7a. ¹H NMR spectrum of 1 in CDCl₃

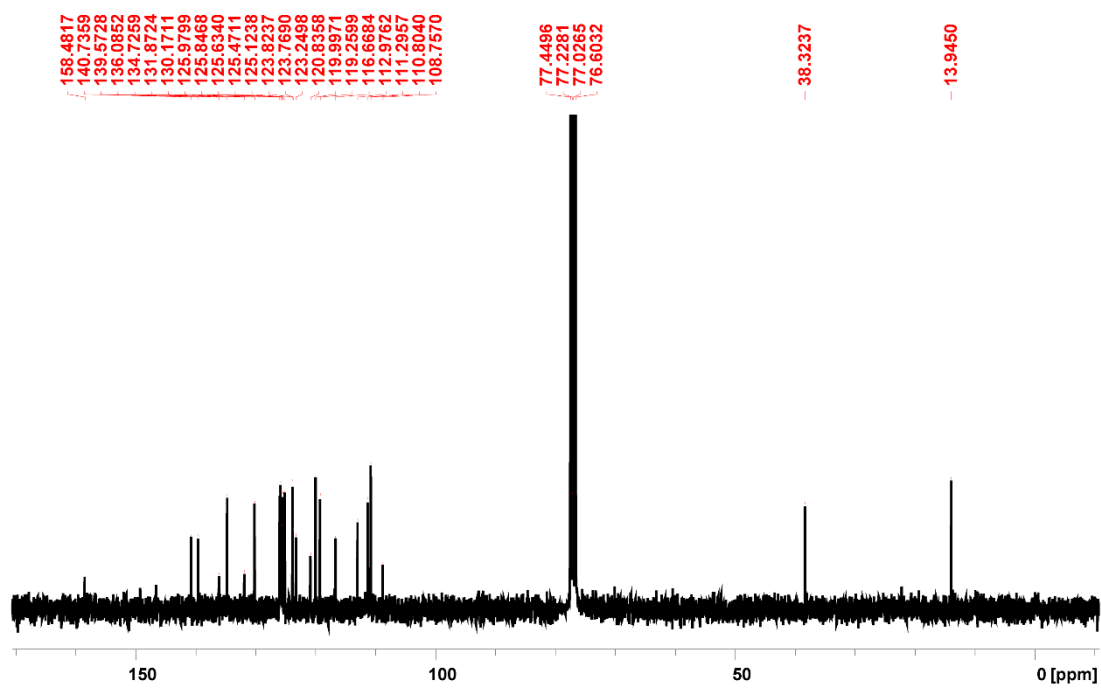


Fig. S7b. ^{13}C NMR spectrum of **1** in CDCl_3

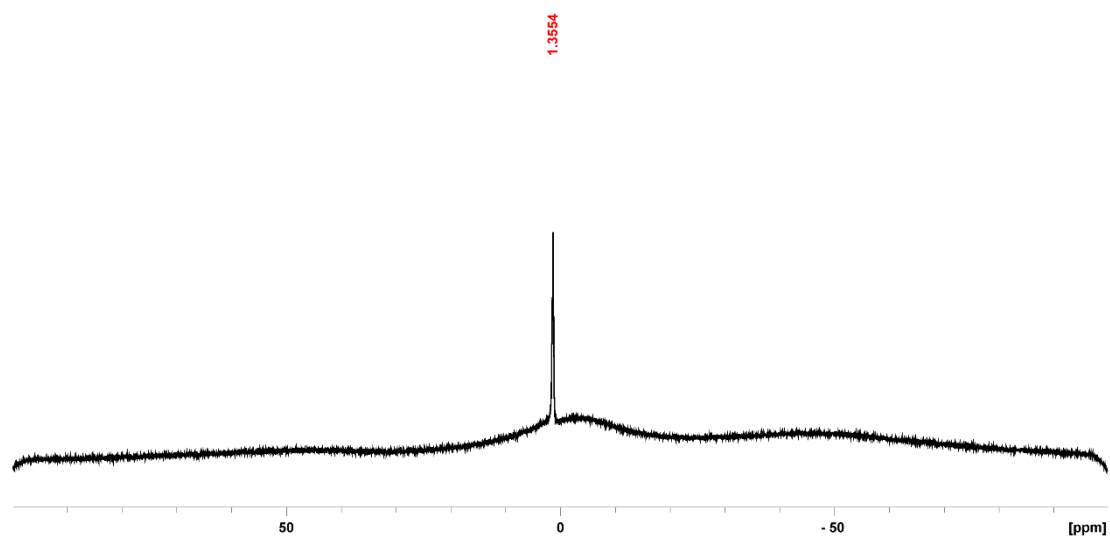


Fig. S8. ^{11}B NMR spectrum of **1** in CDCl_3

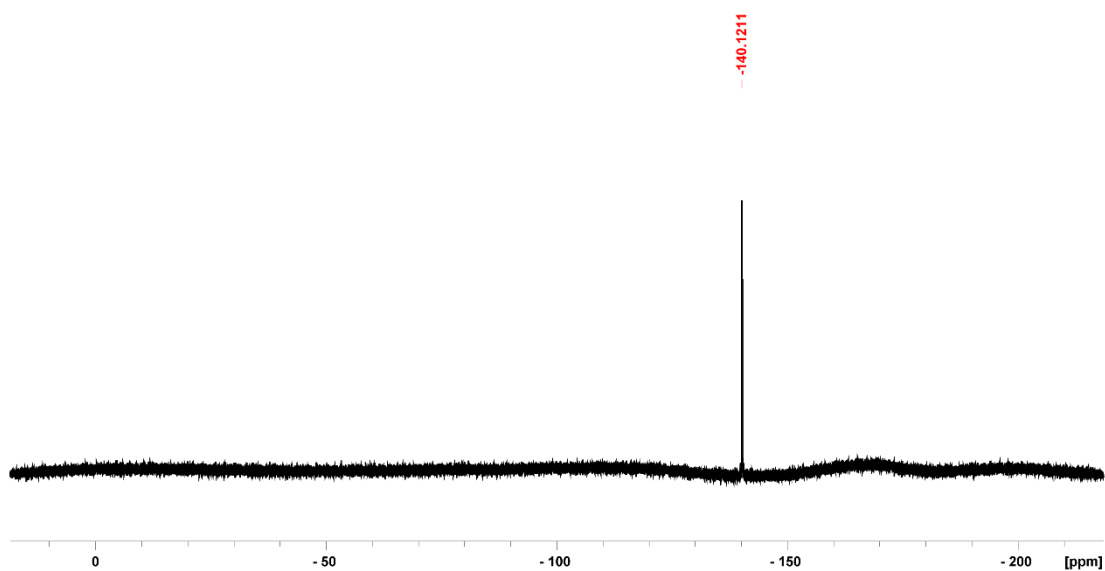


Fig. S9. ^{19}F NMR spectrum of **1** in CDCl_3

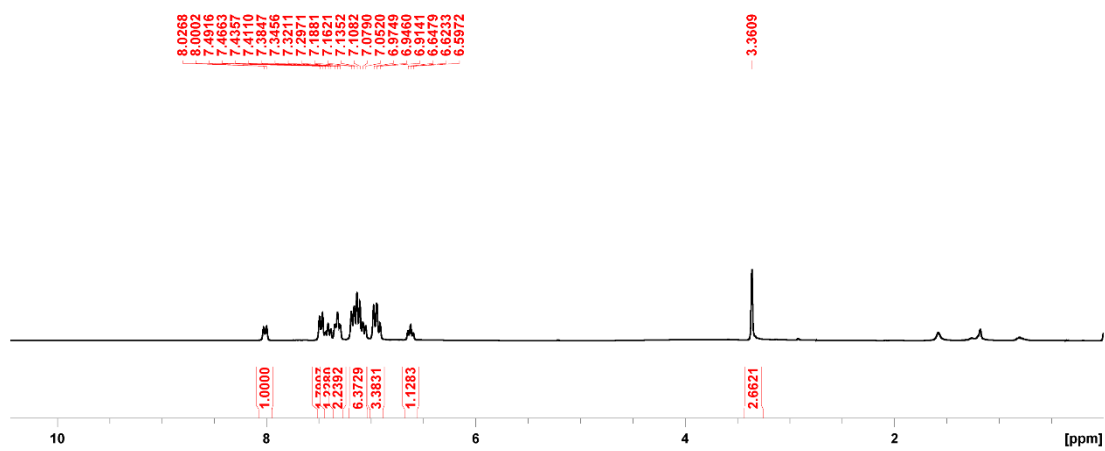


Fig. S10a. ^1H NMR spectrum of **2** in CDCl_3

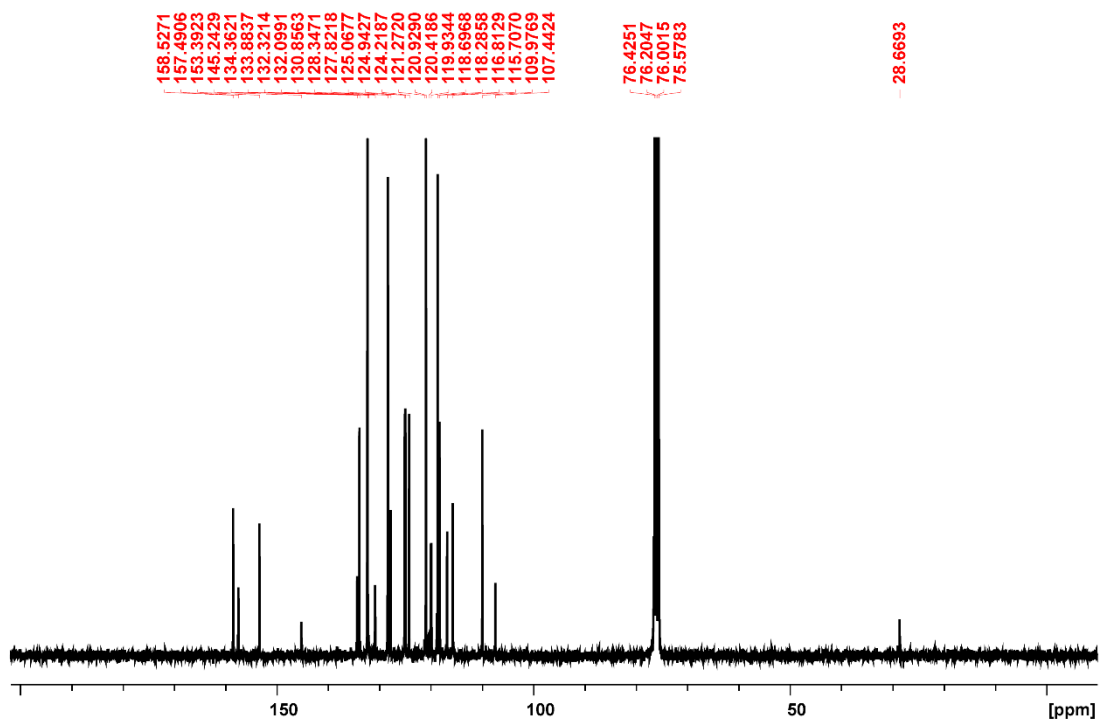


Fig. S10b. ^{13}C NMR spectrum of **2** in CDCl_3

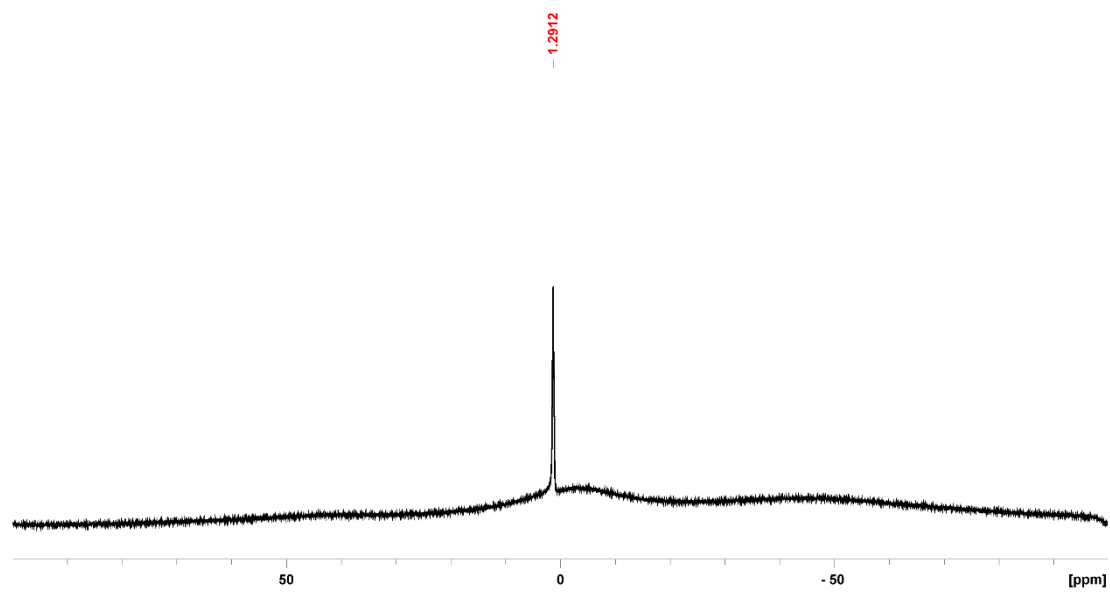


Fig. S11. ^{11}B NMR spectrum of **2** in CDCl_3

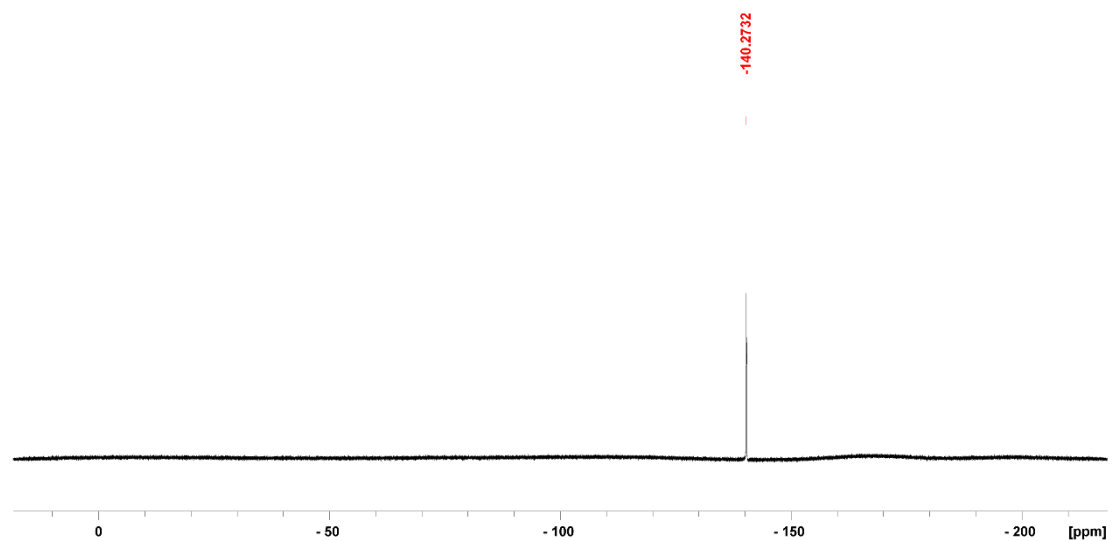


Fig. S12. ^{19}F NMR spectrum of **2** in CDCl_3

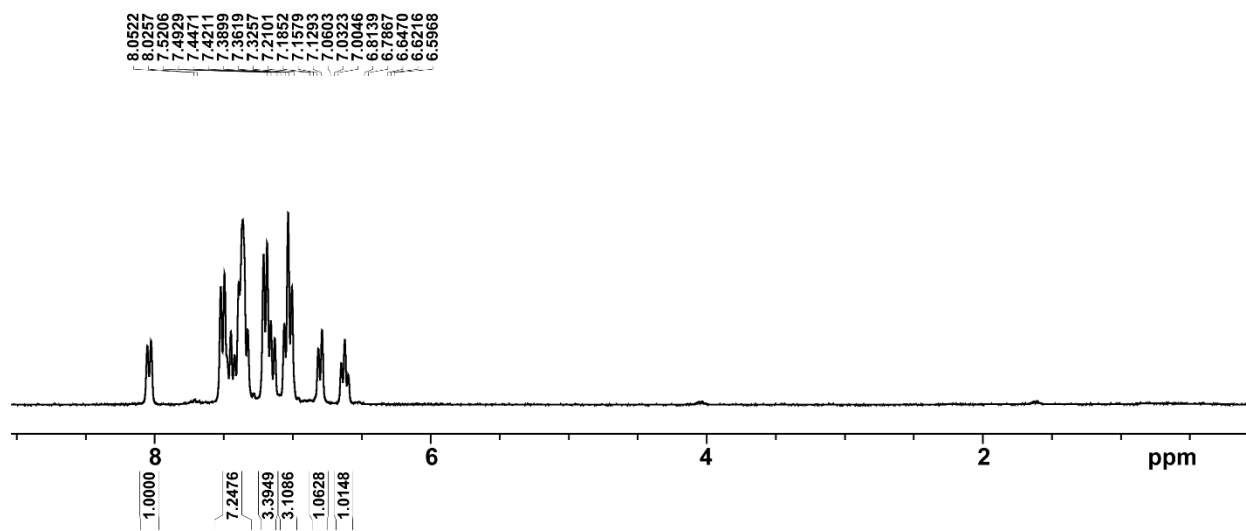


Fig. S13a. ^1H NMR spectrum of **3** in CDCl_3

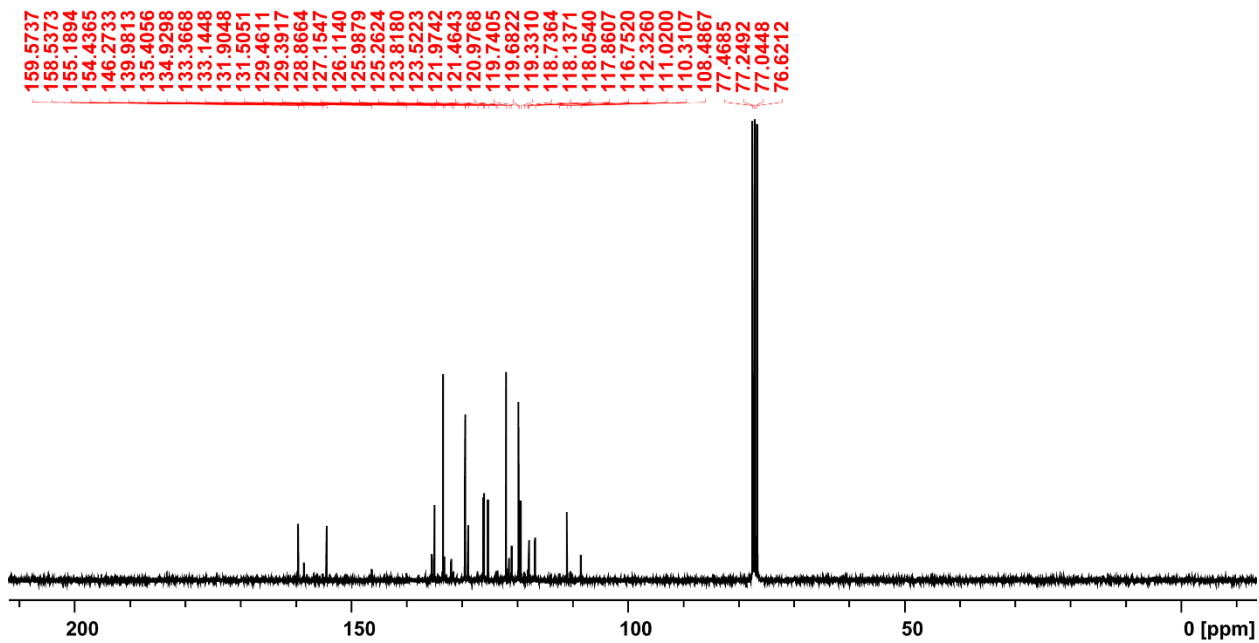


Fig. S13b. ^{13}C NMR spectrum of **3** in CDCl_3

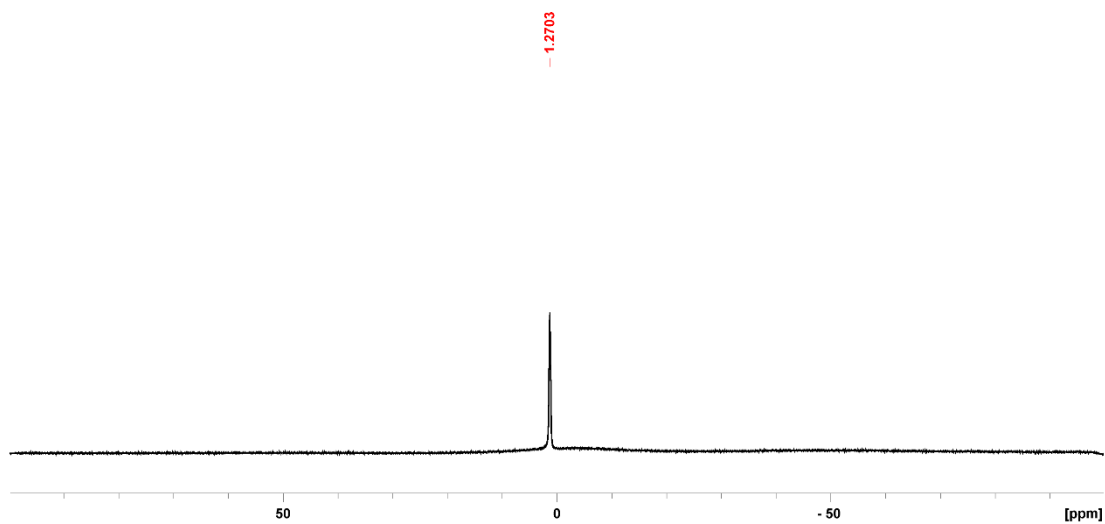


Fig. S14. ^{11}B NMR spectrum of **3** in CDCl_3

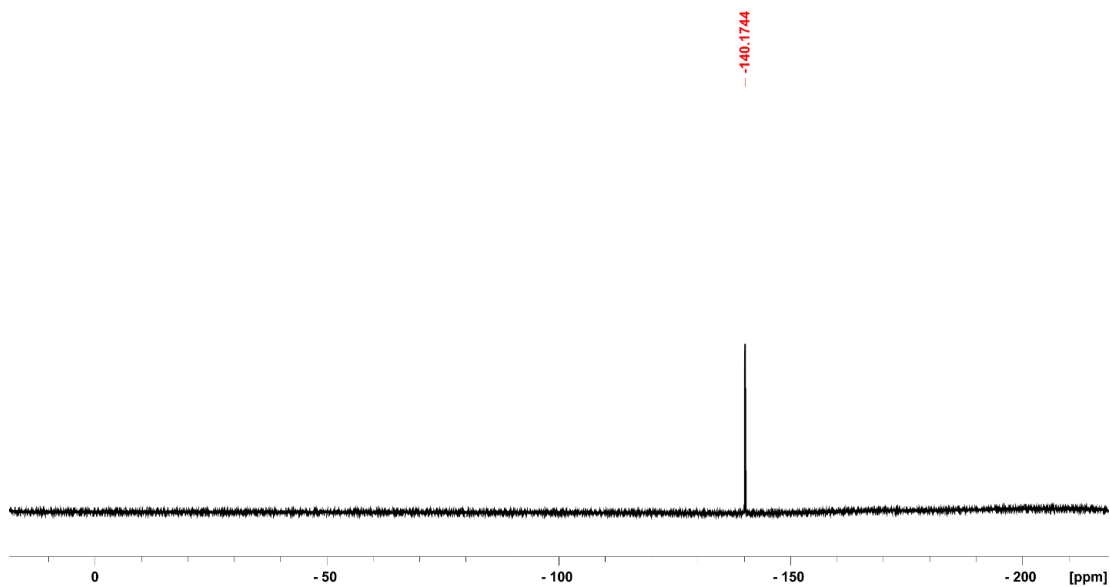


Fig. S15. ^{19}F NMR spectrum of **3** in CDCl_3

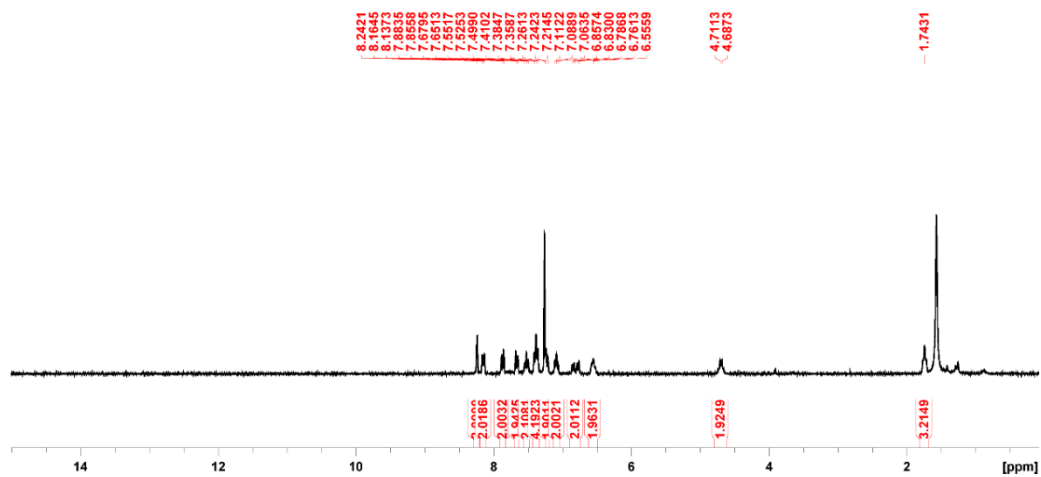


Fig. S16a. ^1H NMR spectrum of **4** in CDCl_3

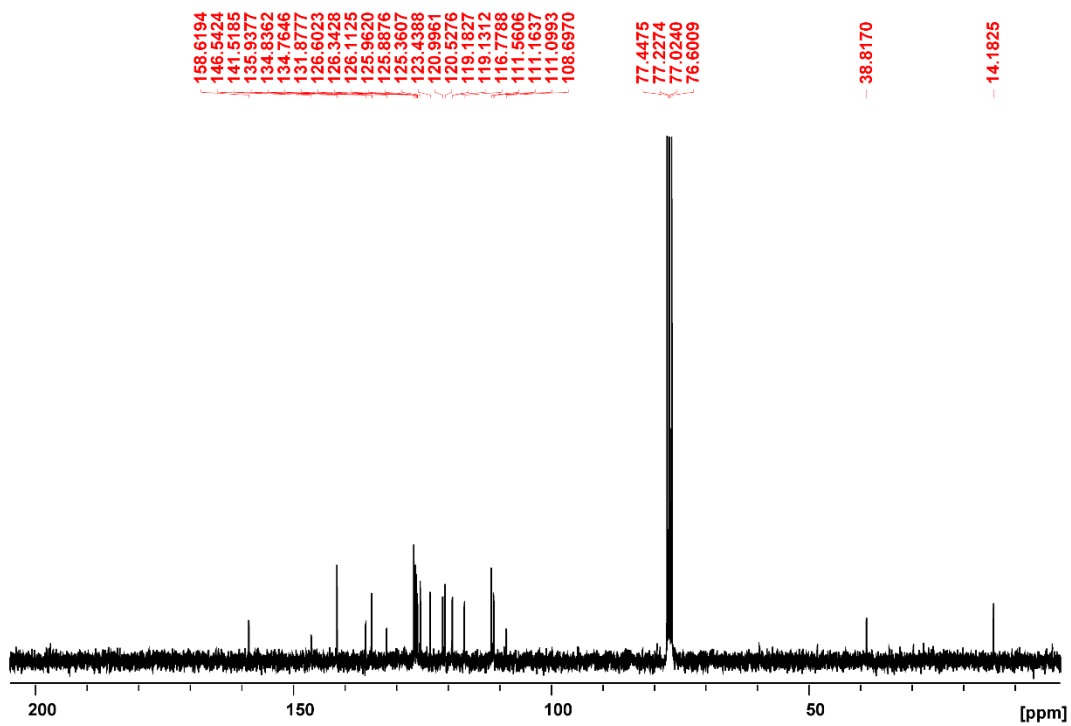


Fig. S16b. ^{13}C NMR spectrum of **4** in CDCl_3

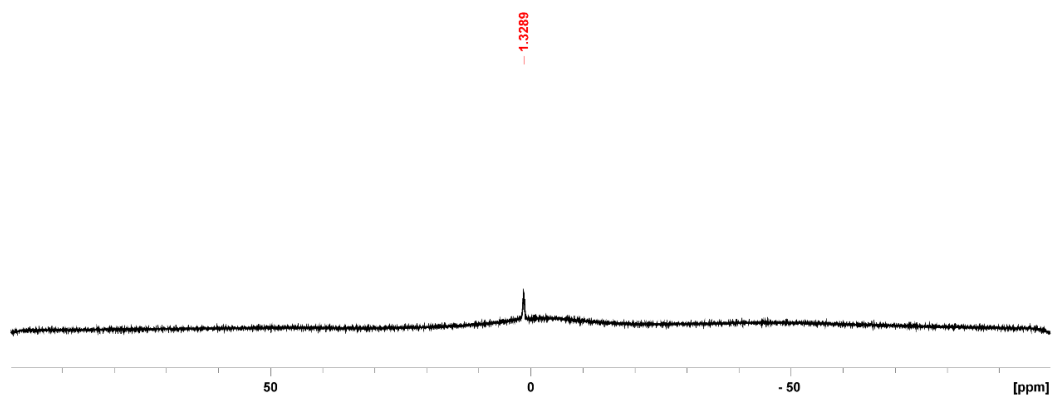


Fig. S17. ^{11}B NMR spectrum of **4** in CDCl_3

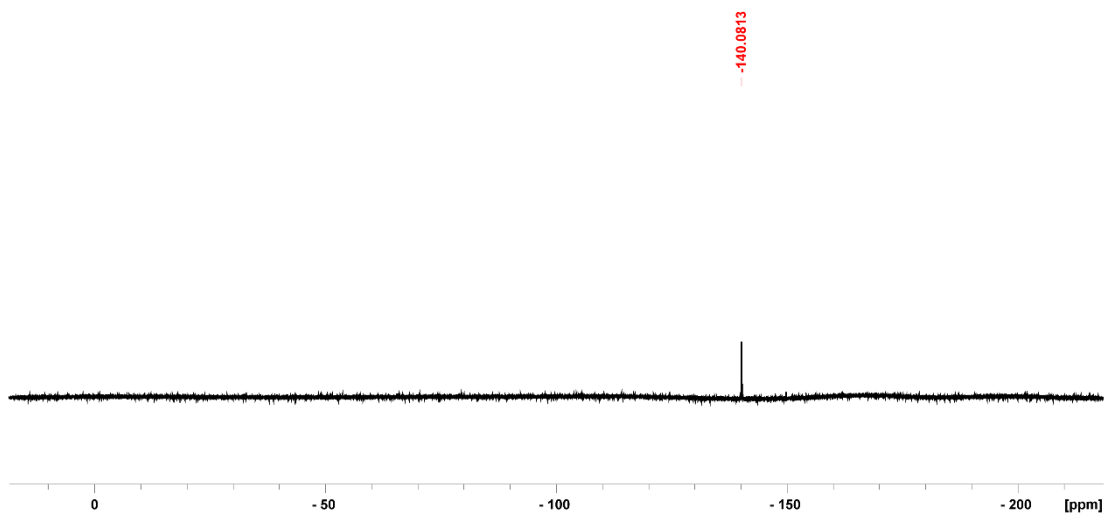


Fig. S18. ^{19}F NMR spectrum of **4** in CDCl_3

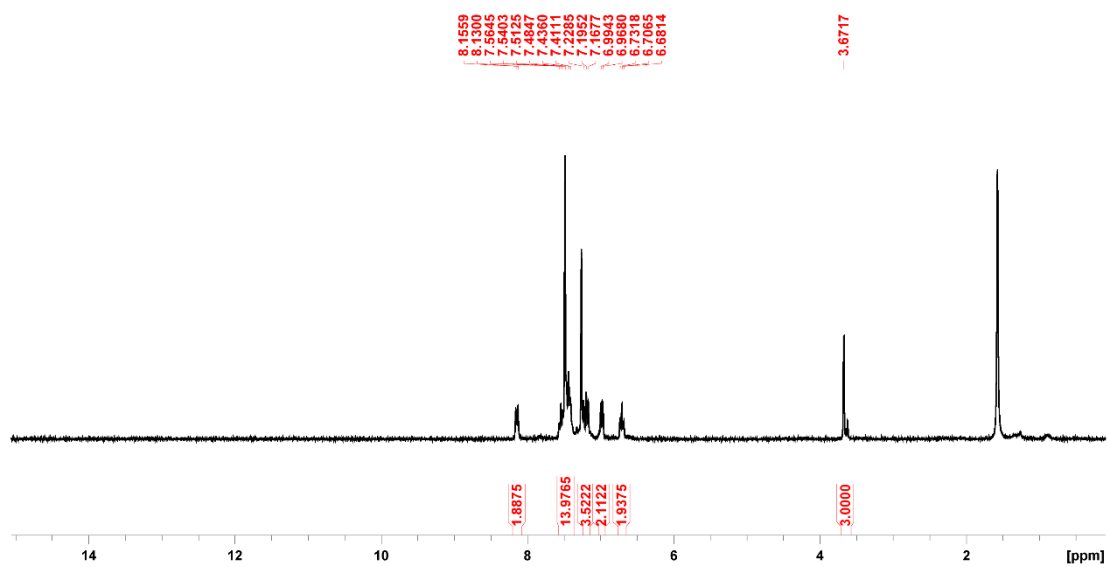


Fig. S19a. ^1H NMR spectrum of **5** in CDCl_3

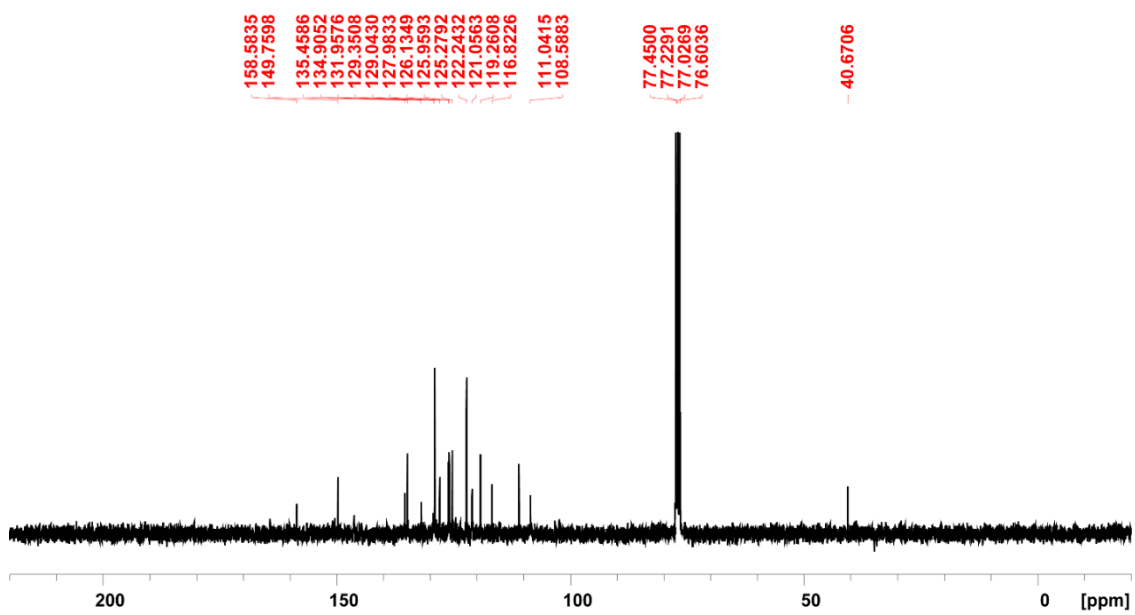


Fig. S19b. ^{13}C NMR spectrum of **5** in CDCl_3

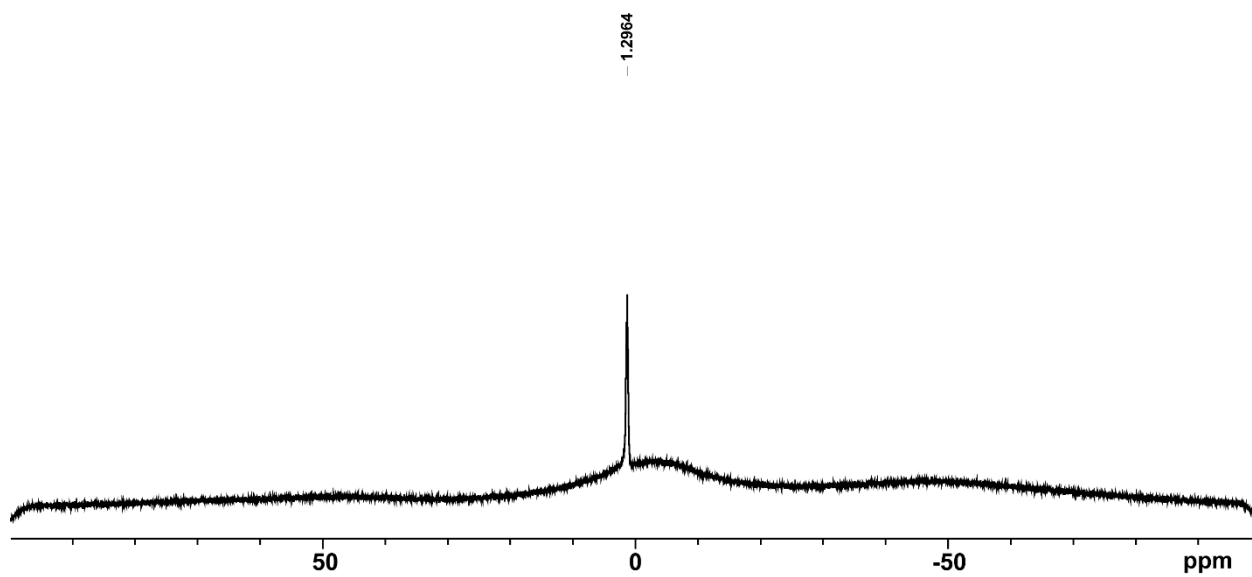


Fig. S20. ^{11}B NMR spectrum of **5** in CDCl_3

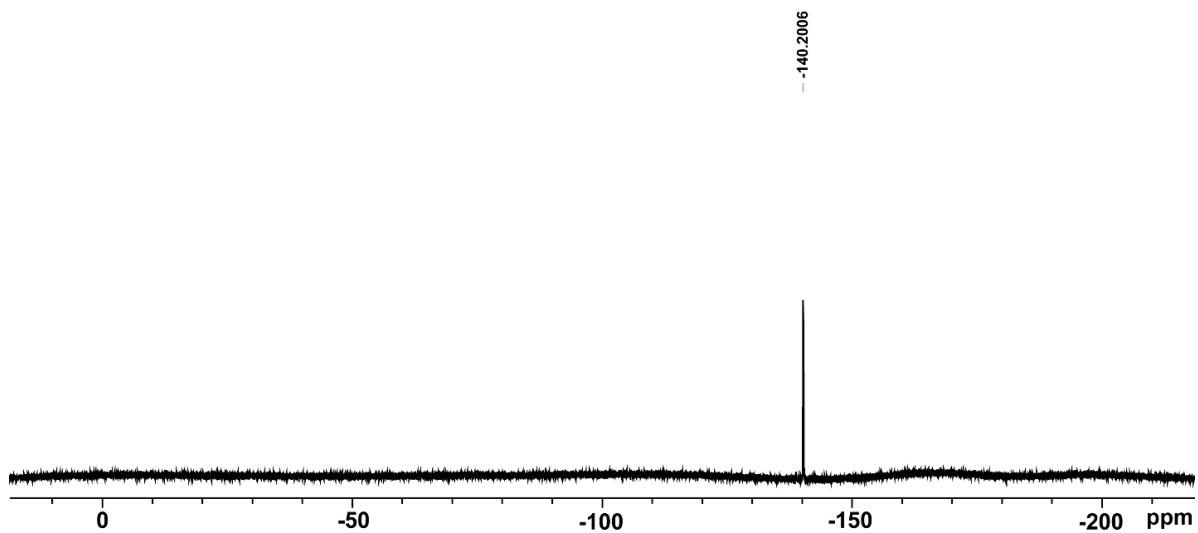


Fig. S21. ^{19}F NMR spectrum of **5** in CDCl_3

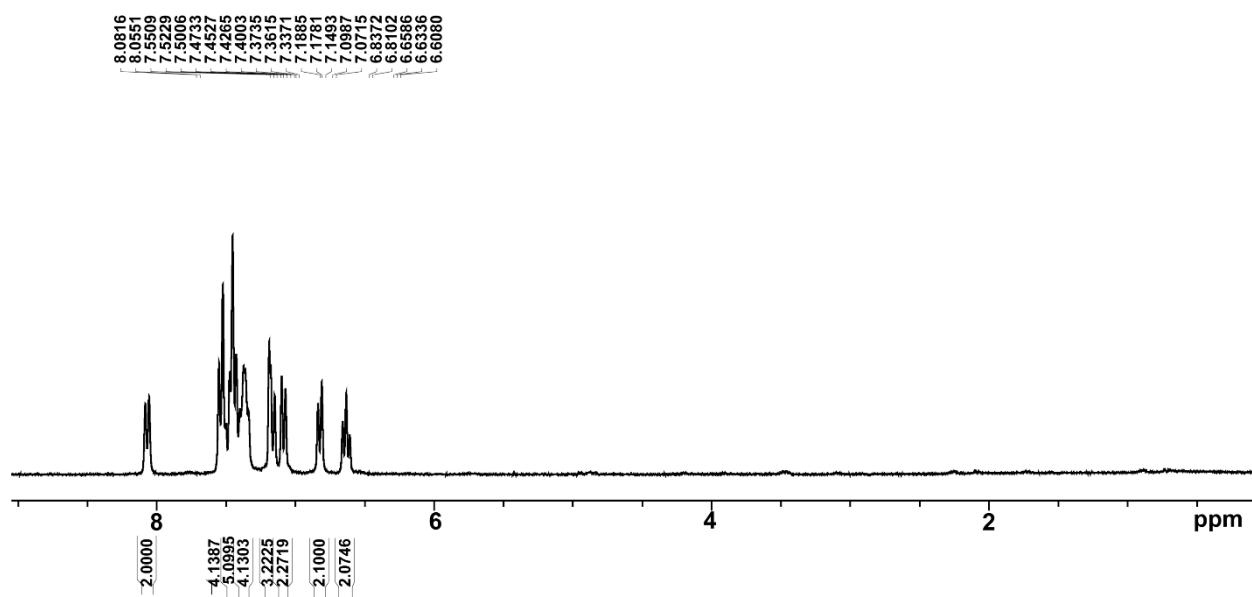


Fig. S22a. ^1H NMR spectrum of **6** in CDCl_3

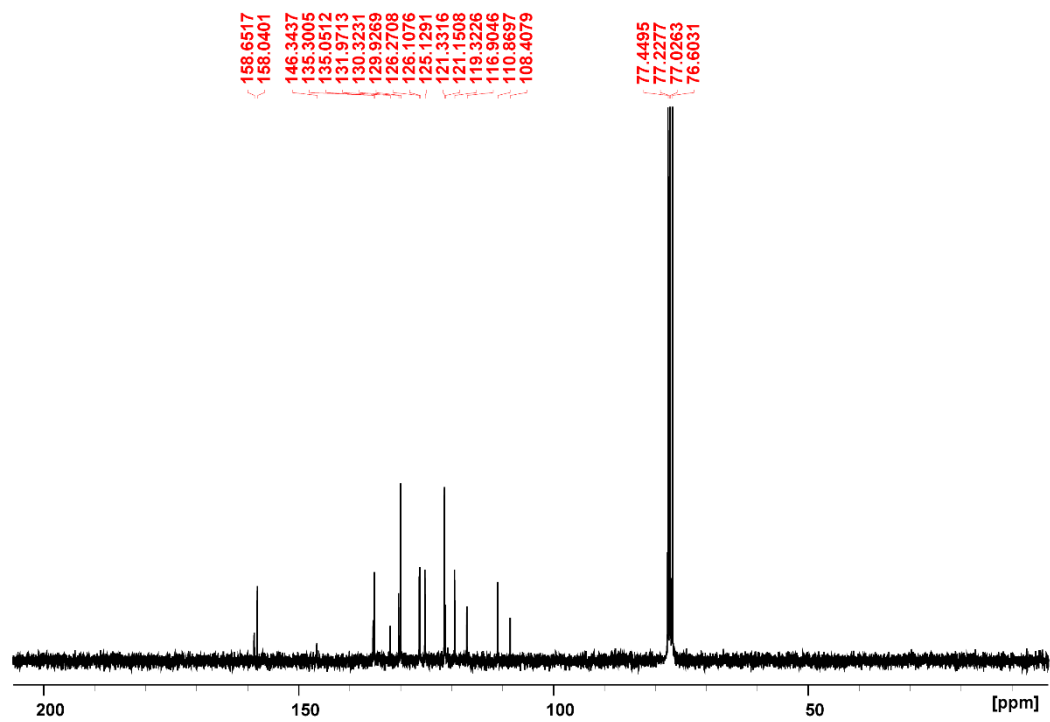


Fig. S22b. ^{13}C NMR spectrum of **6** in CDCl_3

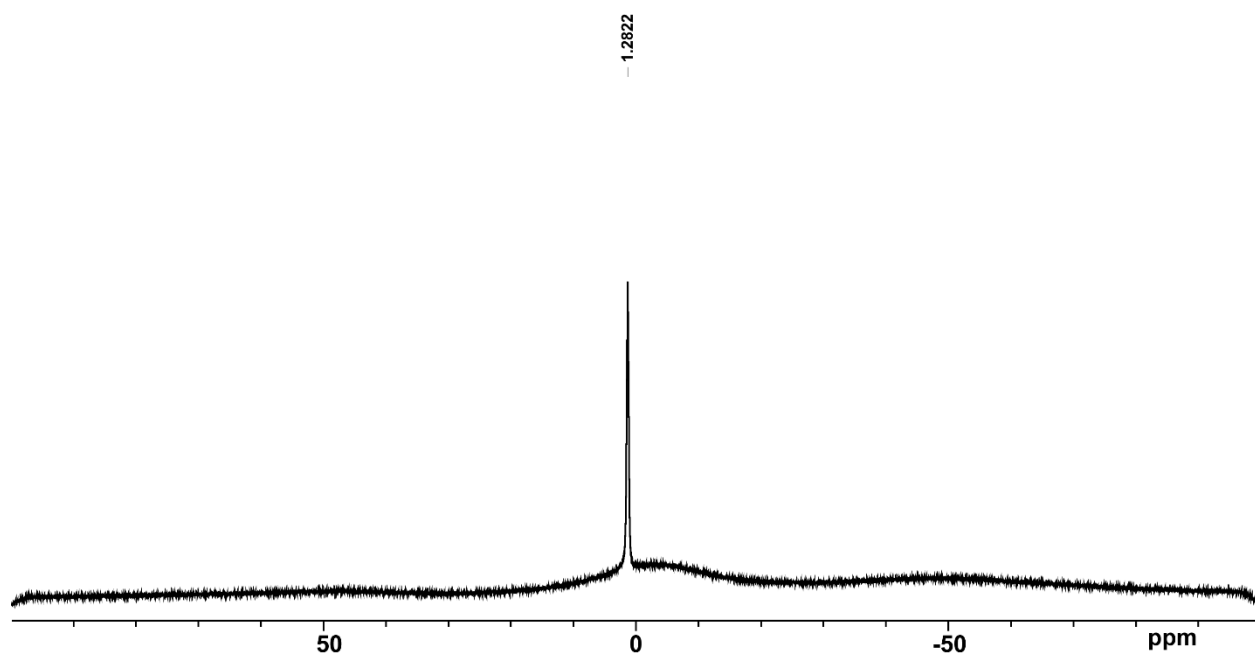


Fig. S23. ^{11}B NMR spectrum of **6** in CDCl_3

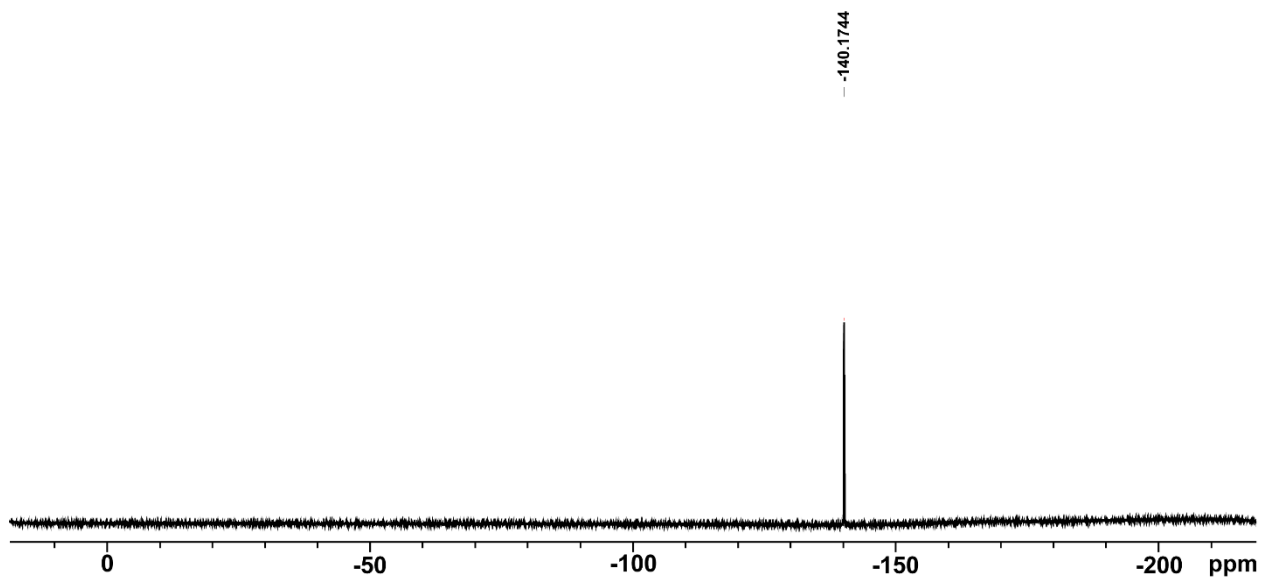


Fig. S24. ^{19}F NMR spectrum of **6** in CDCl_3

Table S1. Intermolecular hydrogen bonds for **L1-L6** [\AA and $^\circ$].

Compounds	D-H...A	$d(\text{D-H})$	$d(\text{H...A})$	$d(\text{D...A})$	$\angle\text{D-H...A}$
L1	O3-H3...N1	0.82	1.89	2.6150	147
L3	O1-H1...N1	0.82	1.91	2.6232	144
L4	O1-H1...N1	0.82	1.90	2.6294	148
L4	O2-H2...N4	0.82	1.86	2.5886	148
L6	O1-H1...N1	0.82	1.83	2.5608	148
L6	O3-H3...N3	0.82	1.81	2.5466	149

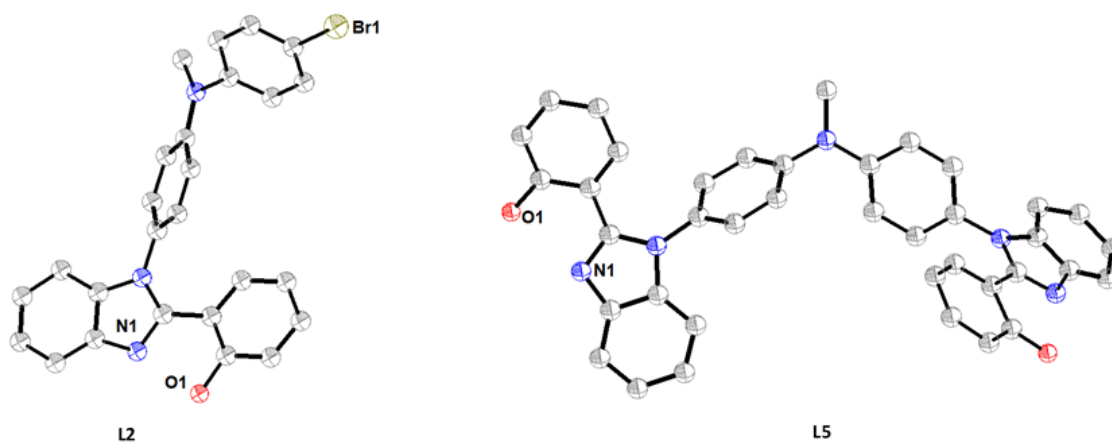


Fig.S25. ORTEP representation of the crystal structure of **L2** and **L5** with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. Color code: carbon (gray), oxygen (red), nitrogen (blue), and bromide (dark yellow).

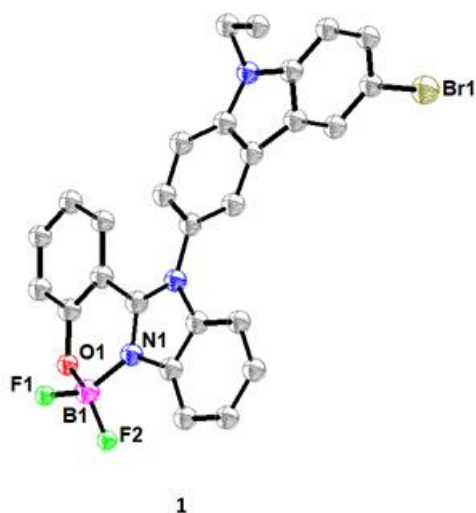


Fig. S26. ORTEP representation of the crystal structure of **1** with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. Color code: carbon (gray), oxygen (red), nitrogen (blue), bromide (dark yellow), boron (pink), and fluoride (bright green).

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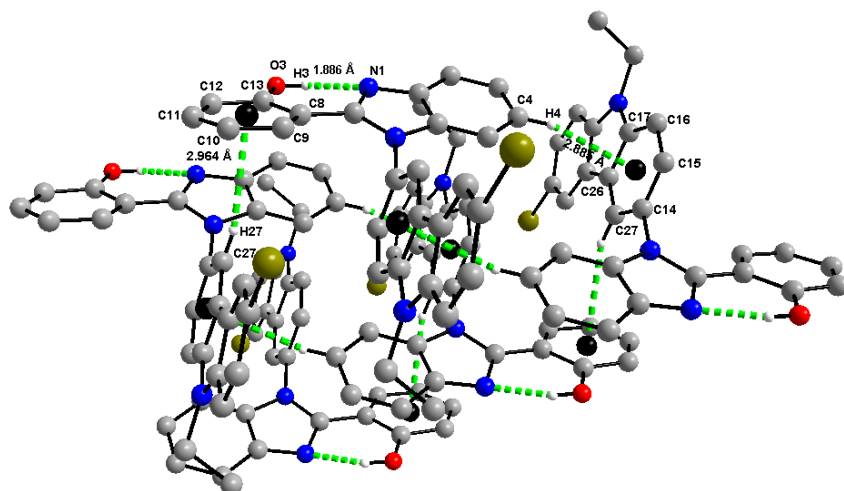


Fig.S27. Hydrogen-bonding and C-H... π (green line) interactions for **L1**. Atom color code: carbon (gray), hydrogen (white), nitrogen (blue), oxygen (red), bromide (dark yellow). Hydrogen atoms are omitted for clarity.

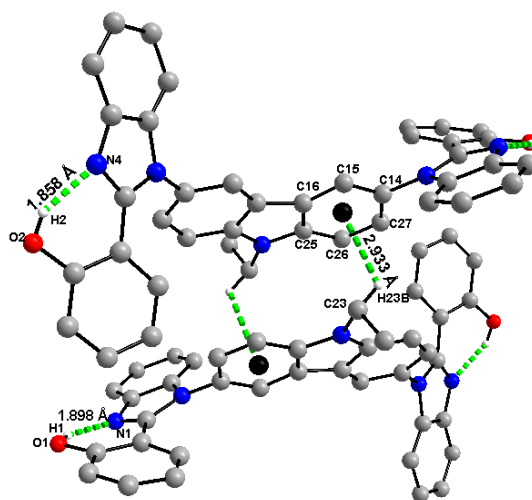


Fig.S28. Hydrogen-bonding and C-H... π (green line) interactions for **L4**. Atom color code: carbon (gray), hydrogen (white), nitrogen (blue), oxygen (red). Hydrogen atoms are omitted for clarity.

Electronic Supporting information

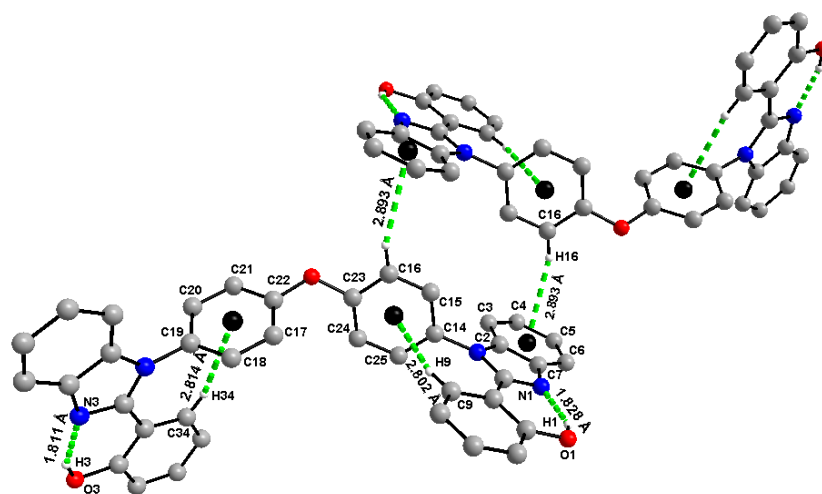


Fig.S29. Hydrogen-bonding and C-H $\cdots\pi$ (green line) interaction for **L6**. Atom color code: carbon (gray), hydrogen (white), nitrogen (blue), oxygen (red). Hydrogen atoms are omitted for clarity

Table S2. Intermolecular hydrogen bonds for **1**, **3**, **4** and **6** [\AA and $^\circ$].

Compounds	D-H \cdots A	$d(\text{D-H})$	$d(\text{H}\cdots\text{A})$	$d(\text{D}\cdots\text{A})$	$\angle\text{D-H}\cdots\text{A}$
3	C18-H18 \cdots Br	0.95	2.79	3.7269	169
	C19-H19 \cdots O1	0.95	2.57	3.4456	154
	C22-H22 \cdots F1	0.95	2.49	3.3777	156
4	C15-H15 \cdots O1	0.93	2.60	3.3681	141
	C24-H24C \cdots F1	0.96	2.44	3.3918	173
	C32-H32 \cdots F1	0.93	2.50	3.2934	143
6	C19-H19 \cdots F2	0.93	2.50	3.3346	149

Electronic Supporting information

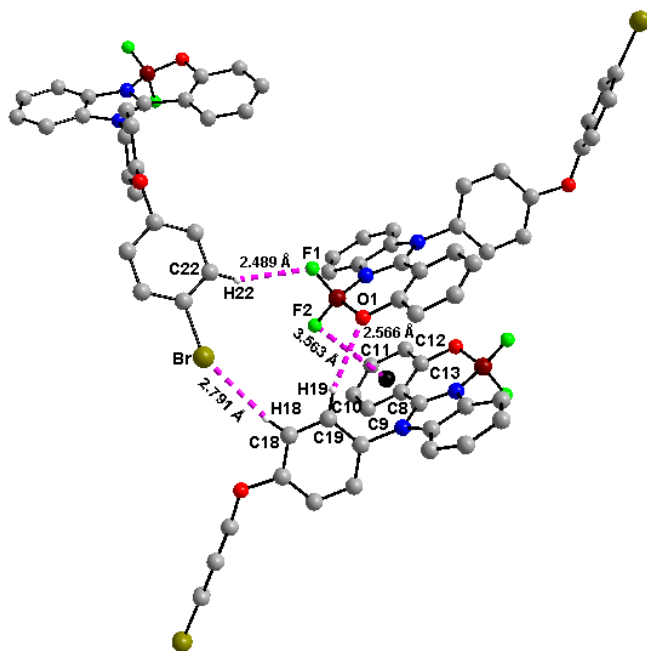


Fig.S30. Hydrogen-bonding and C-H... π (pink line) interactions for **3**. Atom color code: carbon (gray), hydrogen (white), boron (dark red), nitrogen (blue), oxygen (red), fluoride (bright green), bromide (dark yellow). Hydrogen atoms are omitted for clarity.

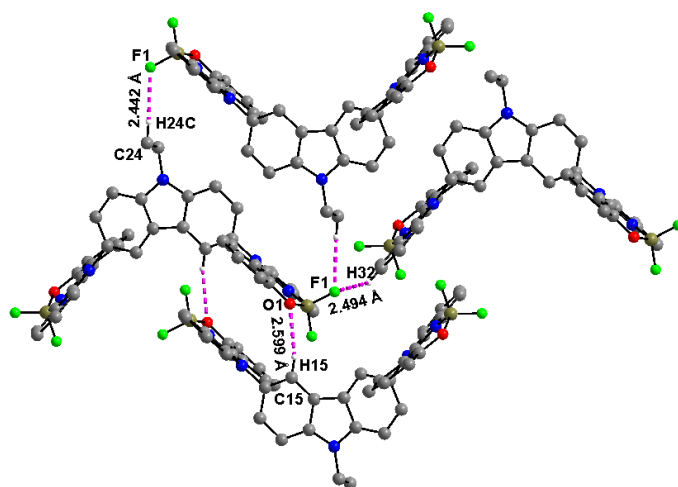


Fig.S31. Hydrogen-bonding (pink line) interactions for **4**. Atom color code: carbon (gray), hydrogen (white), boron (dark red), nitrogen (blue), oxygen (red), fluoride (bright green). Hydrogen atoms are omitted for clarity.

Electronic Supporting information

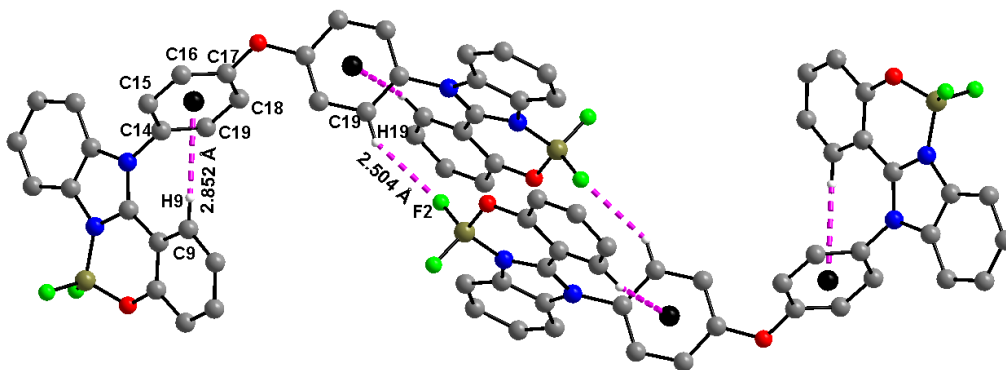


Fig.S32. Hydrogen-bonding and C-H... π (pink line) interactions for **6**. Atom color code: carbon (gray), hydrogen (white), boron (dark red), nitrogen (blue), oxygen (red), fluoride (bright green). Hydrogen atoms are omitted for clarity.

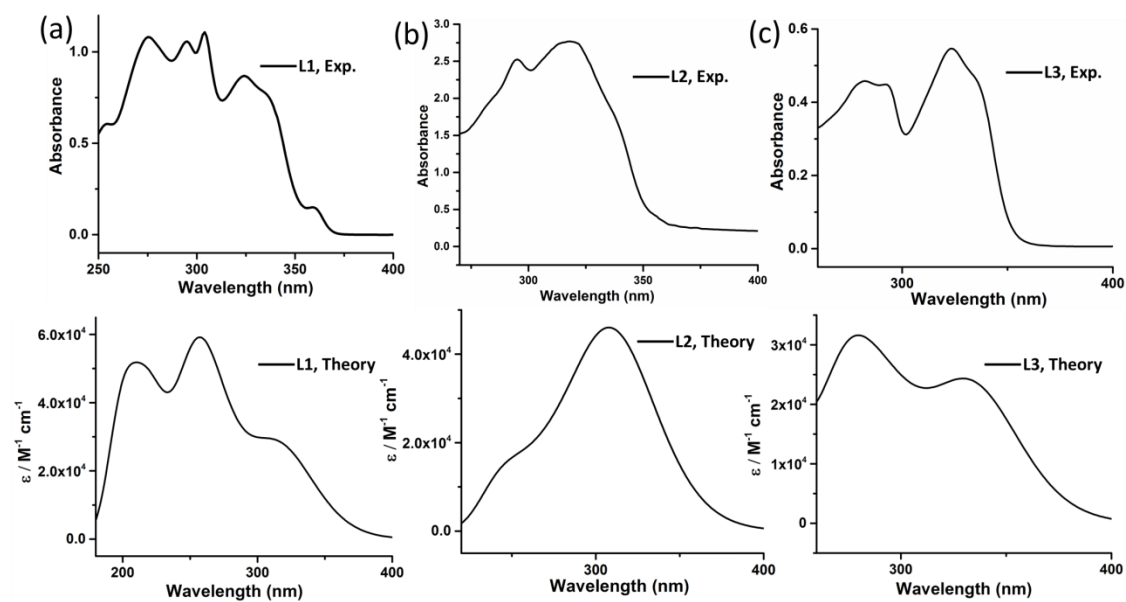


Fig. S33. Experimental and theoretical UV-Vis spectra for ligands, **L1** (a), **L2** (b) and **L3** (c).

Electronic Supporting information

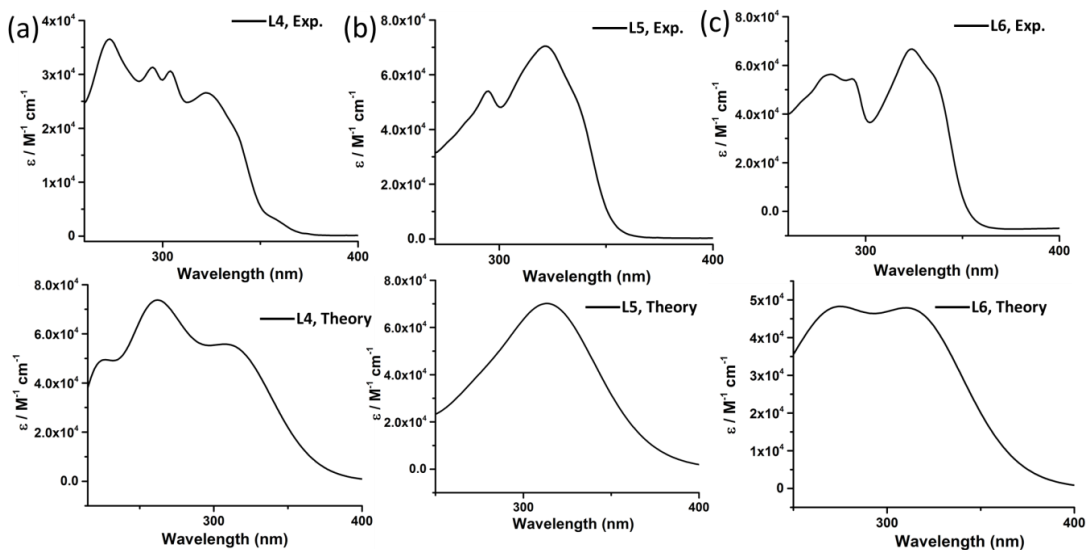


Fig. S34. Experimental and theoretical UV-Vis spectra for ligands, L4 (a), L5 (b) and L6 (c).

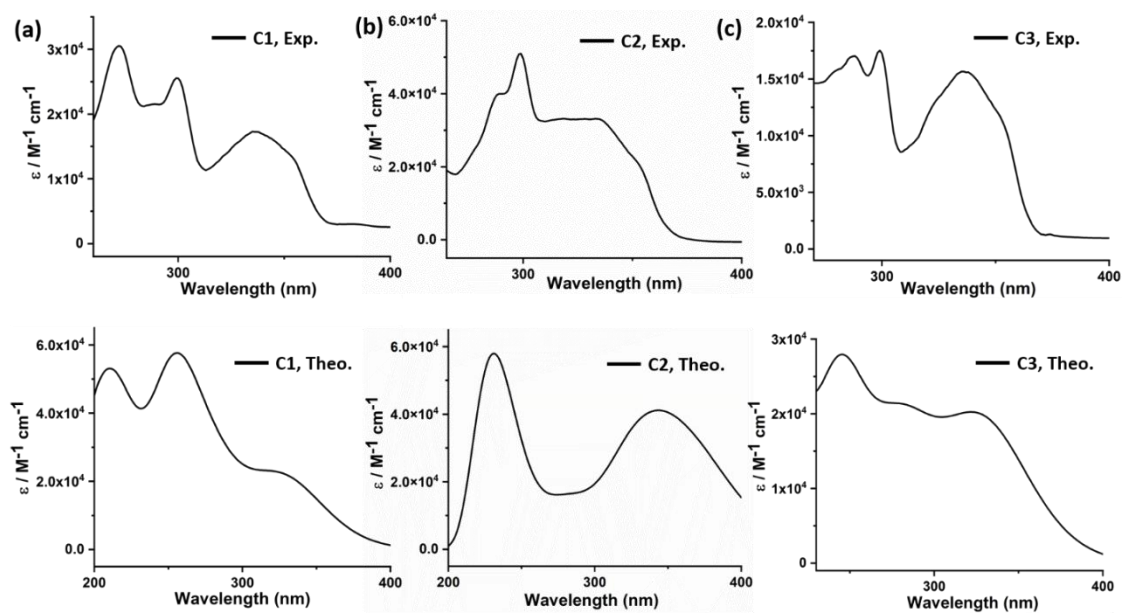


Fig. S35. Experimental and theoretical UV-Vis spectra for complexes, 1 (a), 2 (b) and 3 (c)

Electronic Supporting information

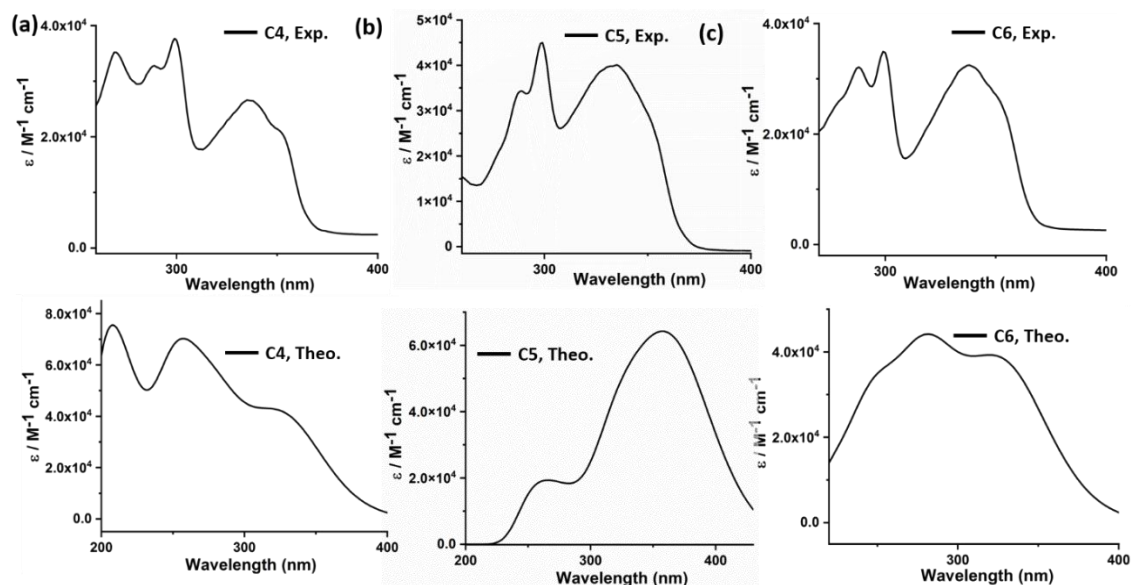


Fig. S36. Experimental and theoretical UV-Vis spectra for complexes, **4** (a), **5** (b) and **6** (c).

Table S3: Summary of photophysical data of ligands and boron complexes in CHCl₃ and THF

Compound	Solvent	λ_{abs} (nm)	ϵ (mol ⁻¹ L cm ⁻¹)	λ_{ems}^a (nm)	Stokes shift (cm ⁻¹)
L1	CHCl ₃	328	17000	484	9826
	THF	325	29800	495	10567
L2	CHCl ₃	318	29000	486	10870
	THF	325	26800	495	10567
L3	CHCl ₃	326	14800	488	10183
	THF	320	17800	500	11250
L4	CHCl ₃	322	31000	485	9962
	THF	325	41200	465	9263
L5	CHCl ₃	333	46000	467	8616
	THF	320	44100	469	9928
L6	CHCl ₃	324	32500	474	9767
	THF	325	35000	490	10361
1	CHCl ₃	340	18800	424	5826
	THF	339	22900	454	7472
2	CHCl ₃	334	19900	474	8843
	THF	335	15500	505	10048
3	CHCl ₃	339	13300	387	3658
	THF	337	18000	388	3900
4	CHCl ₃	340	29900	387	3571
	THF	336	27100	390	4120
5	CHCl ₃	335	36500	449	7579
	THF	333	41700	485	9411
6	CHCl ₃	340	27800	389	3704
	THF	339	45000	390	3857

^a Excited at λ_{max} , Concentration = 1×10^{-5} M

Electronic Supporting information

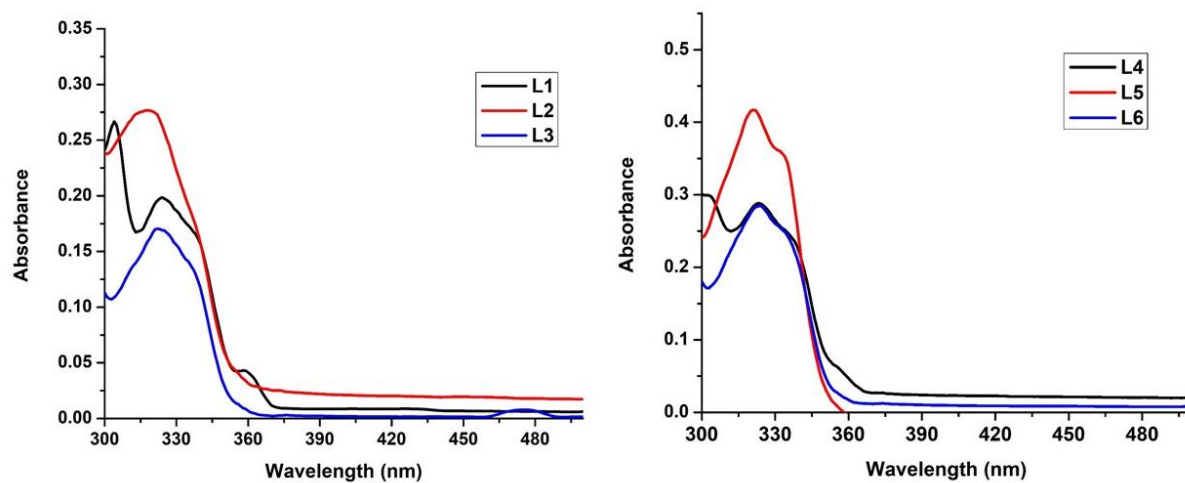


Fig. S37. Absorbance spectra of compounds L1-L3 (left) and L4-L6 (right) in DCM at 1×10^{-5} M concentration

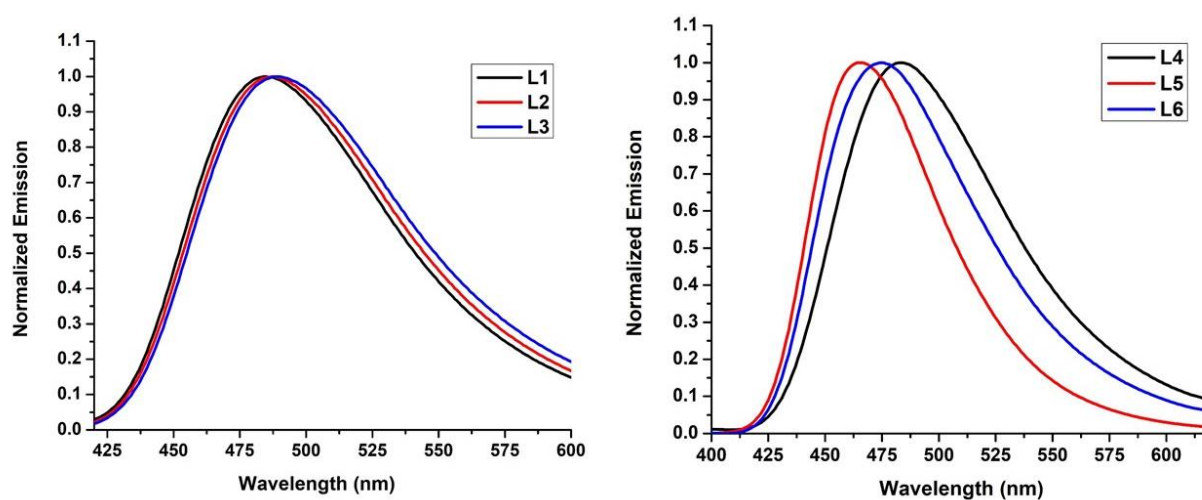


Fig. S38. Normalized emission spectra of compounds L1-L3 (left) and L4-L6 (right) in DCM at 1×10^{-5} M concentration

Electronic Supporting information

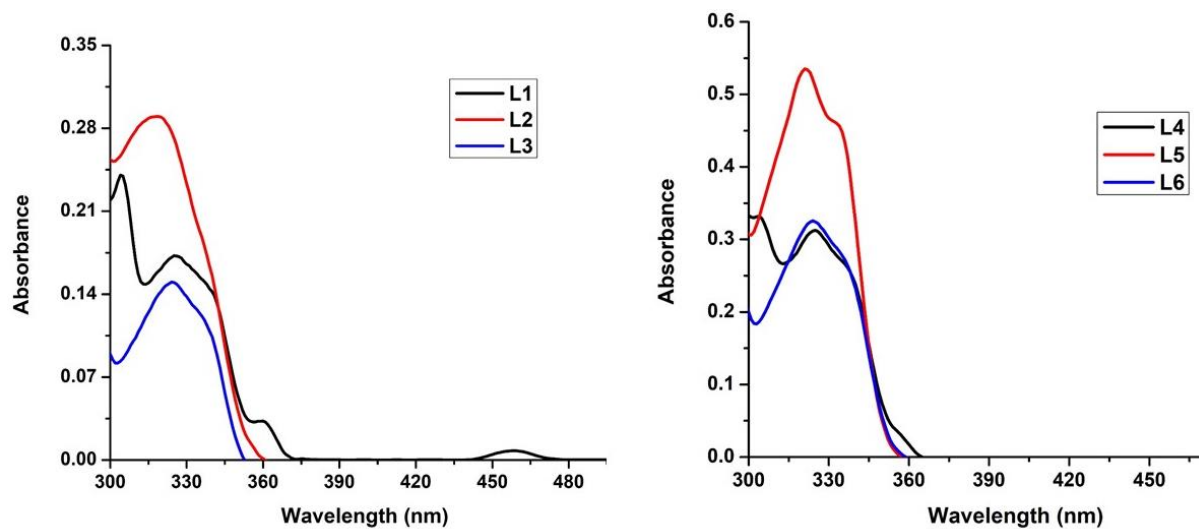


Fig S39: Absorbance spectra of compounds L1-L3 (left) and L4-L6 (right) in CHCl_3 at 1×10^{-5} M concentration

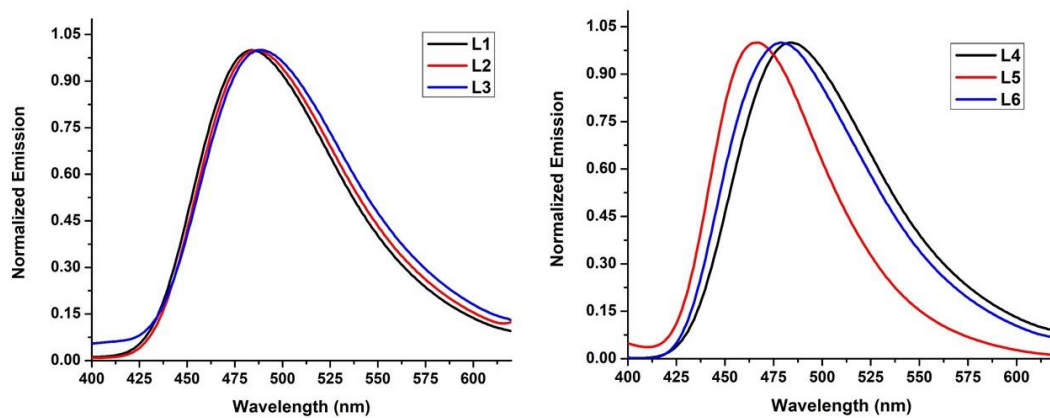


Fig. S40. Normalized emission spectra of compounds L1-L3 (left) and L4-L6 (right) in CHCl_3 at 1×10^{-5} M concentration

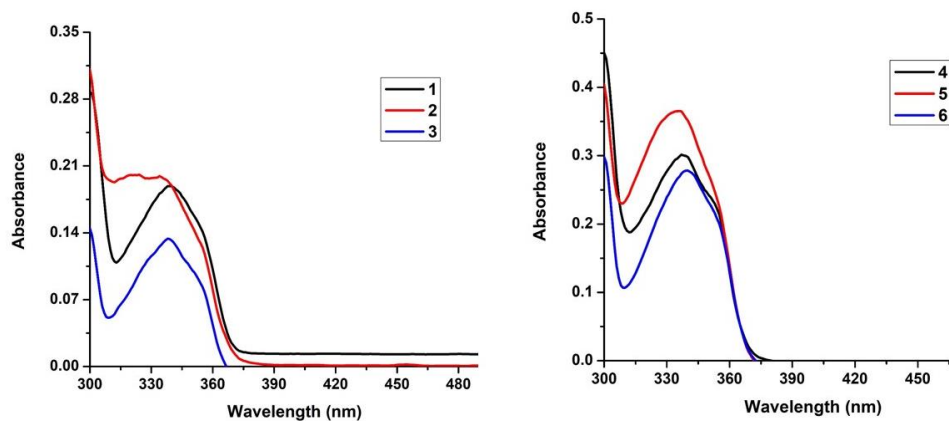


Fig. S41: Absorbance spectra of compounds 1-3 (left) and 4-6 (right) in CHCl_3 at 1×10^{-5} M concentration

Electronic Supporting information

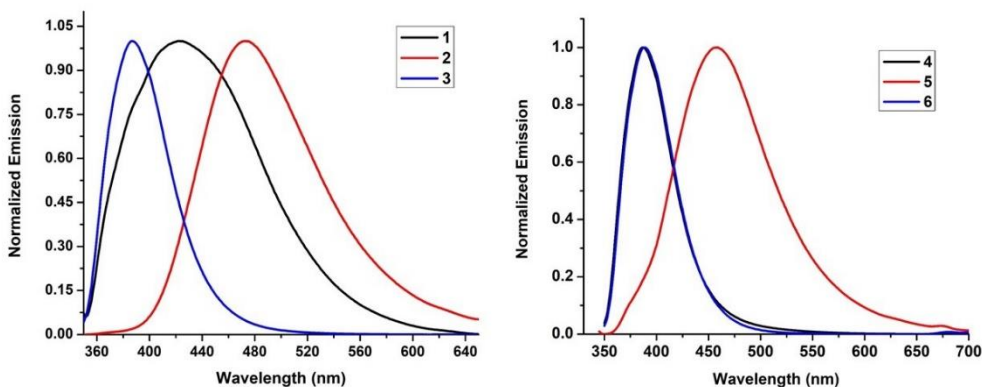


Fig. S42. Normalized emission spectra of compounds 1-3 (left) and 4-6 (right) in CHCl_3 at 1×10^{-5} M concentration

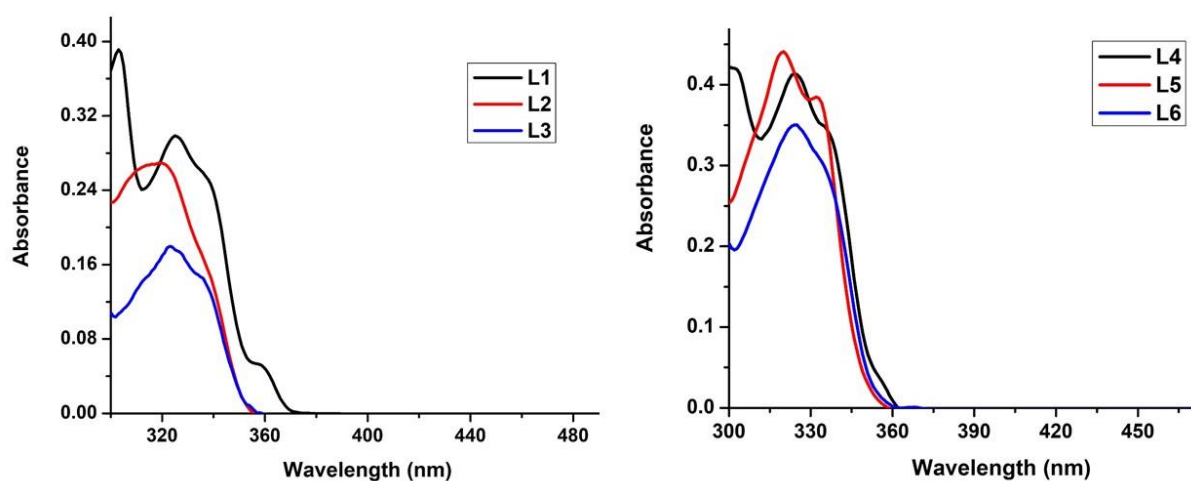


Fig S43: Absorbance spectra of compounds L1-L3 (left) and L4-L6 (right) in THF at 1×10^{-5} M concentration

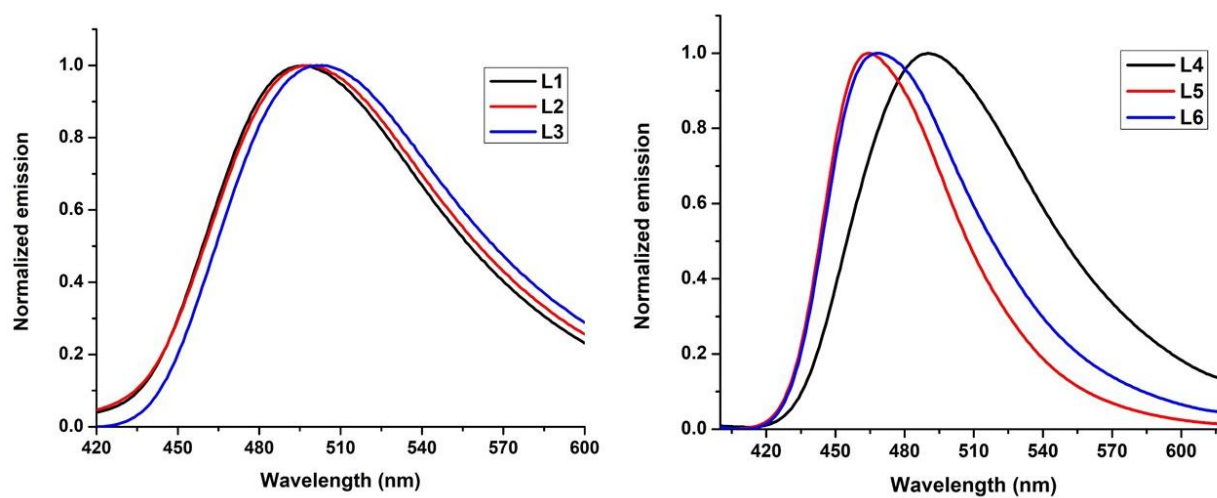


Fig. S44. Normalized Emission spectra of compounds L1-L3 (left) and L4-L6 (right) in THF at 1×10^{-5} M concentration

Electronic Supporting information

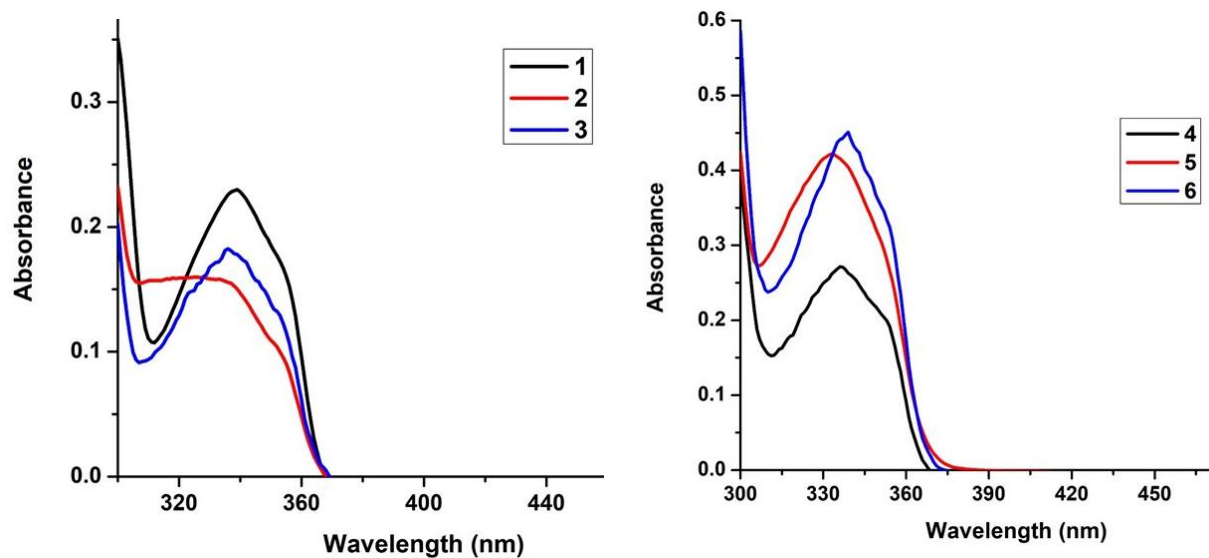


Fig S45: Absorbance spectra of compounds 1-3 (left) and 4-6 (right) in THF at 1×10^{-5} M concentration

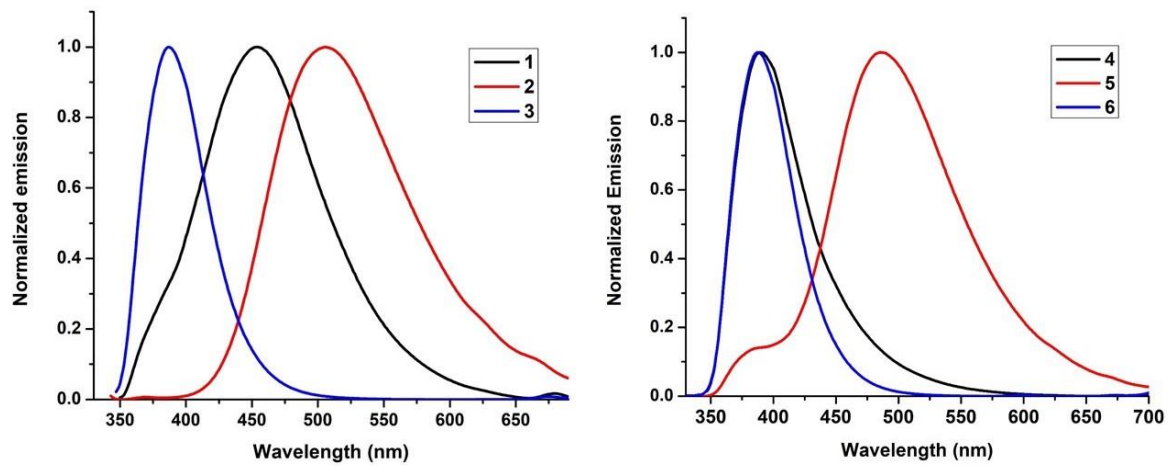


Fig. S46. Normalized Emission spectra of compounds 1-3 (left) and 4-6 (right) in THF at 1×10^{-5} M concentration

Electronic Supporting information

Table S4. Calculated excitation energy (E), oscillator strength (f), and wavelength for absorption in dichloromethane solution for L1-L6 and complexes 1, 3, 4 and 6.

Compound	States	Main Orbital transition (CIC) ^a	Oscillator strength(f)	Excitation energy (E, eV)	Wavelength λ (nm)
Ligand 1 60 root	S0 \rightarrow S2	H \rightarrow L ^b (0.50)	0.4624	3.8854	319.1
	S0 \rightarrow S5	H-2 \rightarrow L (0.37)	0.1077	4.3379	285.82
	S0 \rightarrow S7	H-3 \rightarrow L (0.64)	0.2281	4.5025	275.37
	S0 \rightarrow S11	H \rightarrow L+2 (0.62)	0.1325	4.7544	260.78
Ligand 2 20 root	S0 \rightarrow S2	H-1 \rightarrow L (0.70)	0.5185	3.8974	318.12
	S0 \rightarrow S4	H \rightarrow L+2 (0.67)	0.3634	4.1253	300.55
	S0 \rightarrow S5	H-3 \rightarrow L (0.52)	0.1746	4.4759	277
Ligand 3 40 root	S0 \rightarrow S1	H \rightarrow L (0.69)	0.5388	3.8888	318.82
	S0 \rightarrow S4	H-2 \rightarrow L (0.58)	0.1965	4.4889	276.2
	S0 \rightarrow S9	H \rightarrow L+2 (0.68)	0.4818	4.9267	251.66
Ligand 4 60 root	S0 \rightarrow S2	H-1 \rightarrow L	0.6240	3.8696	320.40
	S0 \rightarrow S10	H-3 \rightarrow L	0.1599	4.3324	286.18
	S0 \rightarrow S12	H-3 \rightarrow L+2	0.1723	4.4483	278.72
Ligand 5 60 root	S0 \rightarrow S3	H-2 \rightarrow L	0.4981	3.8891	318.8
Ligand 6 60 root	S0 \rightarrow S2	H-1 \rightarrow L+1	0.5393	3.8887	318.83
	S0 \rightarrow S11	H-4 \rightarrow L	0.6176	4.4915	276.04
Complex 1 60 root	S0 \rightarrow S2	H-1 \rightarrow L	0.4425	3.7602	329.73
	S0 \rightarrow S7	H-3 \rightarrow L	0.3045	4.3688	283.79
	S0 \rightarrow S8	H-4 \rightarrow L	0.1224	4.5046	275.24
Complex 2 60 roots	S0 \rightarrow S2	H-1 \rightarrow L	0.4468	3.7672	329.11
	S0 \rightarrow S5	H-2 \rightarrow L	0.3518	4.3707	283.67
Complex 3 60 root	S0 \rightarrow S1	H \rightarrow L	0.4464	3.7560	330.1
	S0 \rightarrow S3	H-2 \rightarrow L	0.3611	4.3673	283.89
	S0 \rightarrow S9	H-1 \rightarrow L+2	0.4571	5.0313	246.43
Complex 4 60 root	S0 \rightarrow S2	H-1 \rightarrow L+1	0.4415	3.7552	330.17
	S0 \rightarrow S13	H-3 \rightarrow L+2	0.3643	4.3801	283.06
	S0 \rightarrow S15	H-6 \rightarrow L	0.1415	4.4933	275.93
Complex 5 60 root	S0 \rightarrow S3	H-2 \rightarrow L	0.4823	3.7493	330.68
	S0 \rightarrow S10	H-3 \rightarrow L+1	0.4289	4.3686	283.81
Complex 6 60 root	S0 \rightarrow S2	H \rightarrow L+1	0.4830	3.7555	330.14
	S0 \rightarrow S7	H-4 \rightarrow L	0.6628	4.3740	283.25
	S0 \rightarrow S20	H-2 \rightarrow L+3	0.5626	4.9480	250.58

^aCi expansion coefficients for the main orbital transitions.

^bH denotes HOMO and L denotes LUMO

Electronic Supporting information

Table S5. HOMO-LUMO energies for **L1-L6** obtained from DFT calculation along with respective quantum yields obtained experimentally

Ligands	E _{HOMO} [eV]	E _{LUMO} [eV]	H-L ^o gap [eV] from theory	Quantum yield ^b
Ligand 1	-5.45	-1.43	4.02	31.59%
Ligand 2	-5.43	-1.08	4.35	38.21%
Ligand 3	-5.56	-1.21	4.35	40.53%
Ligand 4	-5.53	-1.62	3.91	14.53%
Ligand 5	-5.52	-1.34	4.18	17.73%
Ligand 6	-5.63	-1.32	4.31	35.01%

^aH denotes HOMO and L denotes LUMO, ^bAbsolute Quantum Yield (Using Integrating Sphere)

Table S6. HOMO-LUMO energies for complexes **1- 6** obtained from DFT calculation along with respective quantum yields obtained experimentally

Complexes	E _{HOMO} [eV]	E _{LUMO} [eV]	H-L ^o gap [eV] from theory	Quantum yield ^b
Complex 1	-5.78	-1.65	4.13	3.79%
Complex 2	-5.77	-1.56	4.21	2.44%
Complex 3	-5.88	-1.69	4.19	6.56%
Complex 4	-5.94	-2.04	3.9	1.62%
Complex 5	-5.93	-1.87	4.06	6.08%
Complex 6	-6.04	-1.86	4.18	14.98%

^aH denotes HOMO and L denotes LUMO, ^bAbsolute Quantum Yield (Using Integrating Sphere)

Electronic Supporting information

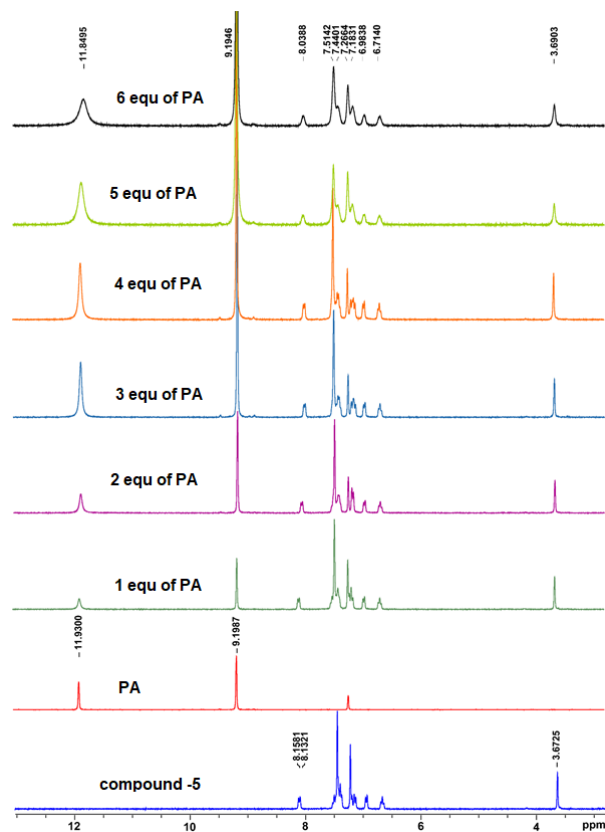


Fig. S47. Partial ^1H NMR spectra of compound **5** and PA with different mol ratio in CDCl_3 .

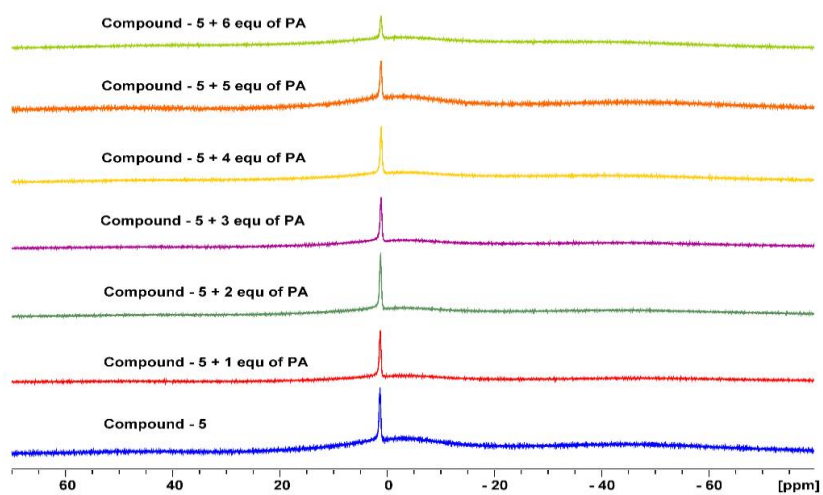


Fig. S48. ^{11}B NMR spectra of compound **5** and PA with different mol ratio in CDCl_3 .

Electronic Supporting information

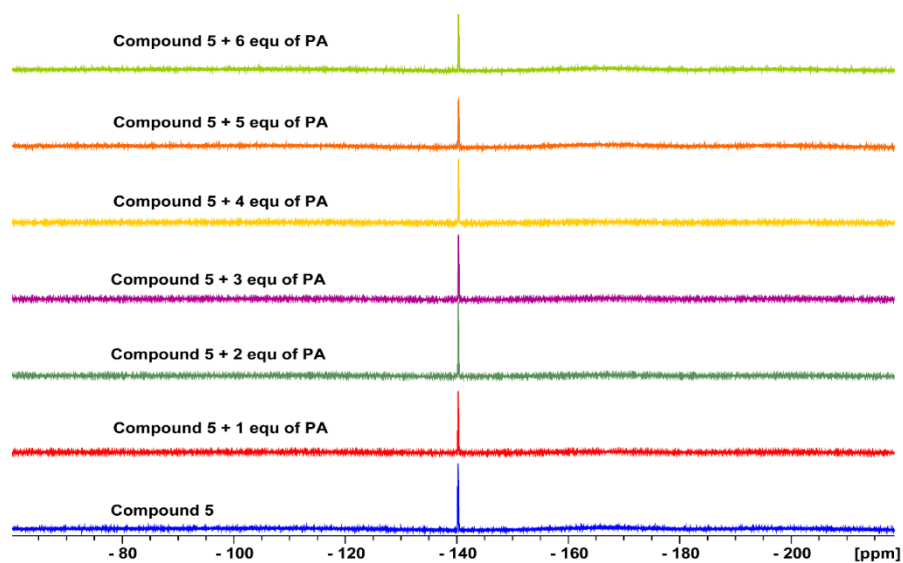
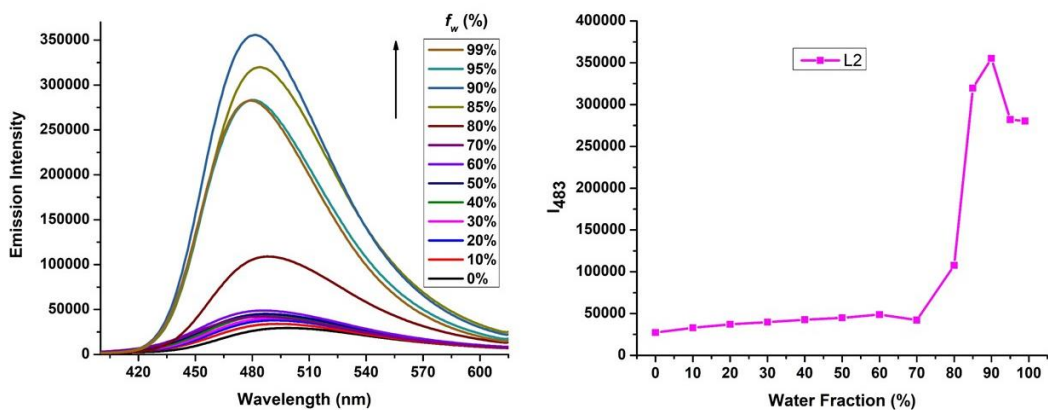
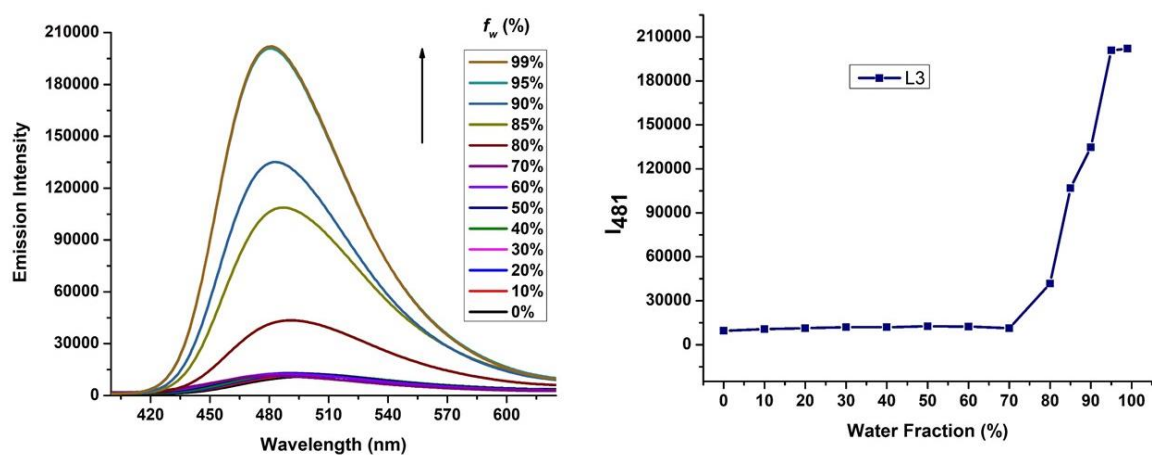


Fig. S49. ^{19}F NMR spectra of compound **5** and PA with different mol ratio in CDCl_3 .

(a)

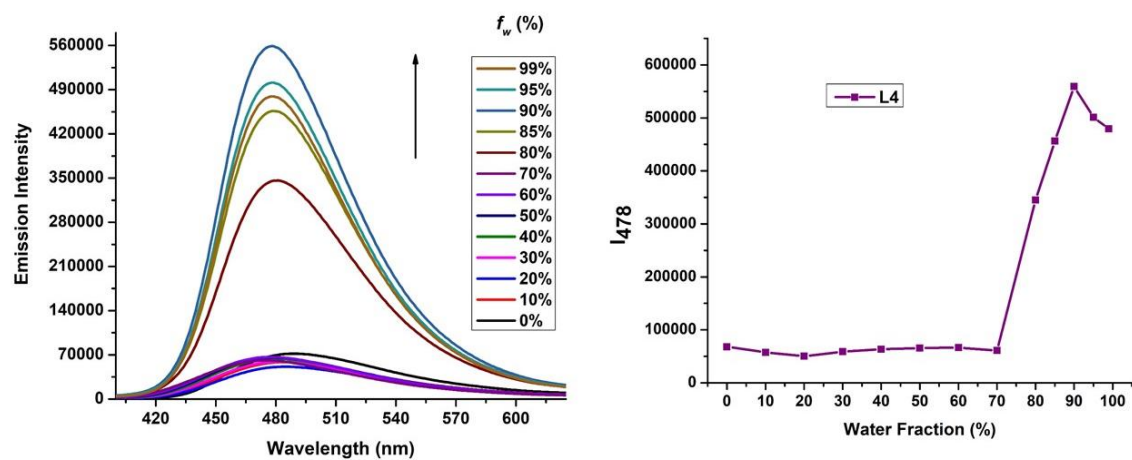


(b)



Electronic Supporting information

(c)



(d)

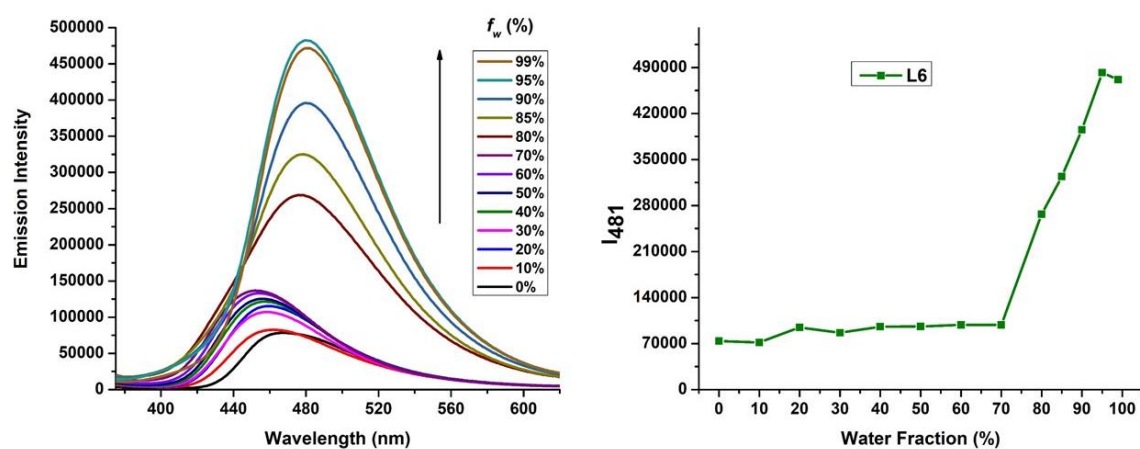


Fig S50: Emission spectrum (Left) of L2-L4 and L6 in THF/water mixtures with different fractions of water (f_w) (concentration = 10 μ M). (Right) Relative intensity vs water fraction (vol %) in THF/Water mixtures; [L2-L4 and L6] = 10 μ M

Electronic Supporting information

Table S7. Optimized geometries for **L1-L6** and complexes **1- 6**

Ligand 1	Br	5.57937847	1.60067816	-2.11044309
	N	-2.42229737	0.66366511	0.32655376
	O	-6.08105412	-0.65792798	-1.36297278
	H	-5.77467705	0.20898800	-0.97200993
	N	2.36710028	-1.85257152	1.67980775
	N	-4.51646980	1.11484579	-0.34789559
	C	1.15914426	-0.30651419	0.49873957
	C	-0.01041378	0.34991367	0.10472488
	H	0.00661215	1.13539997	-0.64400235
	C	2.54965593	-0.18446090	0.11960286
	C	-1.21950988	-0.02717364	0.68611801
	C	-3.53837603	0.21549651	-0.37920231
	C	1.09422276	-1.34225328	1.47100736
	C	3.26130111	-1.15099346	0.87819695
	C	-4.05849614	2.18901837	0.38579709
	C	-2.74306463	1.92922077	0.82108445
	C	-3.69182181	-1.05697852	-1.08697385
	C	3.23366572	0.64188874	-0.77872012
	H	2.71284697	1.38584286	-1.37083567
	C	5.31502750	-0.46594283	-0.14196360
	H	6.38868178	-0.55071187	-0.26237662
	C	-1.27032332	-1.03927933	1.66379385
	H	-2.22878726	-1.29439209	2.10278012
	C	4.60856447	0.48549678	-0.89367848
	C	4.64657758	-1.29444740	0.75480262
	H	5.20047761	-2.02367964	1.33636797
	C	-0.12024622	-1.71131436	2.06076574
	H	-0.17548369	-2.49000461	2.81378605

Electronic Supporting information

	C	-4.99754174	-1.42929375	-1.53164065
	C	2.72250886	-2.88412090	2.64488179
	H	3.56719614	-3.44675548	2.23533272
	H	1.88603599	-3.58713362	2.70523231
	C	-2.61953146	-1.92644291	-1.37470397
	H	-1.61527236	-1.64424778	-1.08908678
	C	-4.68664689	3.39433943	0.72186883
	H	-5.69797694	3.59948507	0.38676177
	C	-2.02143620	2.83393490	1.60014091
	H	-1.01247800	2.61849117	1.93489531
	C	-5.18078421	-2.66138485	-2.18118076
	H	-6.18777149	-2.91723784	-2.49311912
	C	-3.97197837	4.30467226	1.49358222
	H	-4.43203868	5.24856714	1.76963180
	C	-2.81490071	-3.13179104	-2.03382963
	H	-1.96754008	-3.77600085	-2.24464129
	C	-2.66055408	4.02803284	1.92731647
	H	-2.13475147	4.76182382	2.53054759
	C	-4.10659900	-3.50273660	-2.42707431
	H	-4.27103048	-4.44683816	-2.93882602
	C	3.06411440	-2.33073061	4.03170314
	H	2.21468285	-1.78844023	4.45667448
	H	3.91362178	-1.64381125	3.98040052
	H	3.32415805	-3.14816640	4.71156162
Ligand 2	Br	7.22137695	0.45377337	-1.44501203
	N	2.25021654	-0.81922826	1.90820119
	N	-3.00955124	-0.65455319	-0.16095981
	N	-5.09689144	-0.04510437	-0.72158096
	C	0.95280042	-0.73892745	1.39595659

Electronic Supporting information

C	0.70569526	-0.91725611	0.01601587
H	1.53359926	-1.10079694	-0.65824650
C	3.38733464	-0.52540067	1.10077046
O	-6.02427435	2.32439911	-0.37928171
H	-5.99894777	1.34632409	-0.58665839
C	-3.90404076	0.40009831	-0.33855084
C	-3.70679370	-1.82557592	-0.46093773
C	-0.58657811	-0.87310597	-0.48867429
H	-0.75844747	-1.00799864	-1.55192906
C	-0.15706573	-0.53695962	2.24293786
H	-0.01824462	-0.39536037	3.30716501
C	-1.67687611	-0.66032964	0.36260772
C	3.44890416	0.64075320	0.32330218
H	2.60715503	1.32527122	0.31731850
C	-3.32139097	-3.16626974	-0.44530562
H	-2.31620665	-3.46578739	-0.16886316
C	4.48762846	-1.39410845	1.10443647
H	4.44344602	-2.30956748	1.68625568
C	5.66491839	0.05597893	-0.41079192
C	4.57834163	0.92873740	-0.43957795
H	4.62044574	1.83183029	-1.03771482
C	-5.01075944	-1.41847497	-0.80864377
C	2.44597646	-0.85831708	3.35475743
H	2.18628459	0.09542633	3.83765195
H	3.49499158	-1.06439803	3.56468918
H	1.84051727	-1.65126143	3.80494549
C	5.62975308	-1.10362645	0.36059469
H	6.47681112	-1.77992661	0.36798481
C	-1.45139069	-0.51057304	1.73078481

Electronic Supporting information

	H	-2.29359641	-0.35449013	2.39717190
	C	-4.29134918	-4.10089730	-0.80156949
	H	-4.03443077	-5.15581996	-0.80466068
	C	-3.64751516	1.82970334	-0.15103641
	C	-5.97425064	-2.36984693	-1.16504083
	H	-6.97867399	-2.06106480	-1.43522448
	C	-5.59691763	-3.70873510	-1.15721631
	H	-6.32178410	-4.46984334	-1.42948290
	C	-2.36074146	2.37844384	0.02749893
	H	-1.49791976	1.72698715	0.00520485
	C	-4.76227757	2.72386552	-0.16937289
	C	-4.55058622	4.09689715	0.04056606
	H	-5.42148198	4.74362292	0.03182854
	C	-3.27297341	4.59891395	0.23372584
	H	-3.13292927	5.66530537	0.38692973
	C	-2.16772127	3.73942773	0.21732222
	H	-1.16375098	4.12999808	0.34833164
Ligand 3	Br	7.43254	-0.30752	-1.07341
	O	2.27048	0.71864	1.93654
	O	-5.97554	-2.2844	-0.26152
	H	-5.95901	-1.30247	-0.44368
	N	-5.05095	0.09552	-0.5924
	N	-2.93966	0.67239	-0.0905
	C	5.79062	0.01419	-0.15041
	C	-4.96133	1.47158	-0.61988
	C	-3.847	-0.37062	-0.27918
	C	-3.58673	-1.80695	-0.16912
	C	3.40573	0.48237	1.18155

Electronic Supporting information

C	-3.64254	1.8595	-0.30804
C	1.01898	0.67315	1.36557
C	-0.03962	0.37464	2.22979
H	0.17798	0.15567	3.2693
C	-1.34477	0.37445	1.75072
H	-2.1727	0.14852	2.41421
C	-4.70489	-2.69608	-0.14936
C	4.72967	-0.87676	-0.30784
H	4.84	-1.74839	-0.94259
C	-1.59625	0.6488	0.40202
C	0.77401	0.97356	0.02187
H	1.59409	1.21902	-0.6427
C	5.67242	1.13353	0.67115
H	6.50624	1.81618	0.78674
C	-3.25198	3.1972	-0.24453
H	-2.23615	3.48337	0.00589
C	4.47061	1.36936	1.33742
H	4.35018	2.23215	1.98347
C	-0.53608	0.95493	-0.45484
H	-0.74001	1.17782	-1.49709
C	3.53177	-0.6454	0.36617
H	2.70365	-1.33813	0.26308
C	-4.48713	-4.0766	-0.00615
H	-5.35981	-4.72041	0.01903
C	-5.93472	2.44031	-0.89219
H	-6.95044	2.14618	-1.13482
C	-2.29353	-2.36549	-0.10377
H	-1.43054	-1.71628	-0.1646
C	-4.23228	4.14922	-0.5169

Electronic Supporting information

	H	-3.9717	5.20253	-0.48027
	C	-2.09514	-3.7332	0.01892
	H	-1.08694	-4.13201	0.063
	C	-5.55237	3.77663	-0.83746
	H	-6.28474	4.55095	-1.04419
	C	-3.20192	-4.58899	0.07989
	H	-3.05753	-5.6608	0.18218
Ligand 4	N	0.00462	-0.65192	3.26688
	O	-7.62078	-0.58594	-1.6267
	H	-7.16303	0.29071	-1.76802
	N	3.94652	-0.72999	-0.67765
	N	-3.92876	1.03194	-0.31038
	N	5.81645	-0.39646	-1.87589
	N	-5.79184	1.22416	-1.54958
	O	7.65371	1.26708	-1.17942
	H	7.19301	0.53385	-1.67743
	C	0.71191	-0.35669	1.10845
	C	1.10347	-0.73262	2.42203
	C	-1.09705	-0.25312	2.52186
	C	-1.64224	0.36448	0.22598
	H	-1.37087	0.51852	-0.81348
	C	2.97216	-0.70109	0.37176
	C	-0.70015	-0.05029	1.1722
	C	3.34479	-1.09351	1.67196
	H	4.37394	-1.38228	1.85578
	C	1.65873	-0.33877	0.07977
	H	1.39229	-0.04361	-0.93005
	C	2.42091	-1.10649	2.71018
	H	2.72351	-1.40921	3.70673

Electronic Supporting information

C	-3.99795	2.36096	-0.73369
C	4.01198	-1.75829	-1.62033
C	-2.95813	0.56942	0.63597
C	-5.04625	0.38537	-0.83832
C	-2.41888	-0.04459	2.93128
H	-2.72993	-0.20114	3.95844
C	-5.17252	2.45585	-1.50734
C	-0.00961	-1.01151	4.67939
H	-0.74288	-0.37098	5.17878
H	0.96551	-0.74737	5.09979
C	-3.33813	0.37823	1.97844
H	-4.37045	0.55594	2.25967
C	5.07042	0.07085	-0.88068
C	-3.16648	3.45652	-0.50017
H	-2.26948	3.37245	0.10382
C	-5.4176	-1.02178	-0.67884
C	5.4471	1.27824	-0.14337
C	5.19102	-1.5274	-2.3577
C	4.57762	1.96599	0.72817
H	3.56215	1.61471	0.85201
C	-6.72838	-1.42385	-1.08043
C	6.76188	1.80351	-0.33452
C	3.17389	-2.84465	-1.87231
H	2.27335	-3.01596	-1.2925
C	-7.12544	-2.75985	-0.90389
H	-8.13223	-3.02653	-1.20718
C	-4.54662	-2.00827	-0.17218
H	-3.53384	-1.73696	0.09353
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Electronic Supporting information

	H	6.4603	-2.21972	-3.96599
	C	-5.53876	3.67738	-2.08523
	H	-6.44042	3.75419	-2.68374
	C	-4.9483	-3.32794	-0.02189
	H	-4.25207	-4.06431	0.36612
	C	-3.54507	4.66521	-1.08077
	H	-2.92555	5.54337	-0.92671
	C	-6.25032	-3.6988	-0.37987
	H	-6.57652	-4.72817	-0.26082
	C	4.98424	3.09765	1.42053
	H	4.28913	3.60695	2.08002
	C	4.72174	-3.47776	-3.65618
	H	4.97695	-4.16791	-4.45446
	C	-4.71193	4.77355	-1.8625
	H	-4.96892	5.73416	-2.29825
	C	6.28986	3.57636	1.25571
	H	6.61991	4.45825	1.79749
	C	7.16377	2.93909	0.3884
	H	8.17341	3.30216	0.22855
	C	3.55041	-3.69989	-2.90586
	H	2.92568	-4.55701	-3.13774
	C	-0.32394	-2.48951	4.92902
	H	-1.30801	-2.75326	4.53133
	H	-0.32059	-2.69982	6.00305
	H	0.41936	-3.13408	4.45131
Ligand 5	N	4.62328	0.75292	-0.46144
	N	-7.04878	0.80822	-0.01839
	N	6.75474	1.45262	-0.57661
	N	0.03862	-2.53822	-0.03043

Electronic Supporting information

O	8.74928	-0.07266	0.02999
H	8.24696	0.71071	-0.32981
O	-7.03236	3.08255	1.18297
H	-7.35075	2.32273	0.61722
C	3.47197	-0.0861	-0.33851
C	1.17524	-1.69162	-0.14541
N	-5.24049	-0.51485	-0.17223
C	1.27501	-0.49708	0.58559
H	0.46285	-0.2005	1.24028
C	5.95087	0.50467	-0.11007
C	2.41031	0.30298	0.48345
H	2.48951	1.21831	1.06103
C	4.61898	1.94422	-1.19222
C	-1.56556	-0.82609	-0.71987
H	-0.77973	-0.29572	-1.24436
C	-1.26234	-2.02101	-0.02939
C	6.46362	-0.62029	0.67321
C	5.96462	2.36049	-1.25121
C	3.37944	-1.26917	-1.07738
H	4.1959	-1.5571	-1.73104
C	-6.19413	-1.02845	-1.05289
C	5.64654	-1.46883	1.44794
H	4.5832	-1.2765	1.5043
C	-2.86099	-0.33262	-0.75761
H	-3.07792	0.58234	-1.29925
C	-5.21172	1.48126	1.43589
C	-3.89909	-1.00976	-0.10668
C	2.24081	-2.06262	-0.98125
H	2.16452	-2.96801	-1.57469

Electronic Supporting information

C	-5.81549	0.60256	0.43226
C	-5.2979	3.59002	2.67508
H	-5.82035	4.51985	2.87305
C	7.87235	-0.85402	0.67658
C	6.30935	3.53624	-1.92841
H	7.34341	3.86132	-1.9737
C	3.58871	2.65893	-1.80347
H	2.55797	2.32406	-1.76038
C	-5.87273	2.71029	1.74255
C	-2.32067	-2.70431	0.60195
H	-2.1376	-3.62446	1.14218
C	-7.31665	-0.18341	-0.93861
C	7.55197	-2.78273	2.11528
H	7.97432	-3.61928	2.66472
C	6.17417	-2.53579	2.16103
H	5.52023	-3.16738	2.75343
C	3.948	3.82613	-2.47432
H	3.17704	4.41471	-2.96196
C	5.28697	4.2591	-2.53417
H	5.52282	5.17569	-3.06596
C	8.38814	-1.95134	1.3859
H	9.46093	-2.1087	1.35404
C	-4.02586	1.17353	2.1342
H	-3.53255	0.22841	1.95187
C	-3.6205	-2.20269	0.55885
H	-4.42256	-2.73409	1.06129
C	-6.16466	-2.11841	-1.92306
H	-5.2909	-2.75553	-2.00757
C	0.25731	-3.90585	0.43439

Electronic Supporting information

	H	1.28457	-4.19703	0.21936
	H	-0.41459	-4.59858	-0.08135
	H	0.0994	-4.00737	1.51815
	C	-8.46284	-0.42725	-1.70485
	H	-9.32991	0.21919	-1.61855
	C	-8.44416	-1.5157	-2.57082
	H	-9.31822	-1.73068	-3.17793
	C	-4.11811	3.26513	3.32648
	H	-3.69678	3.9572	4.05016
	C	-7.31217	-2.3472	-2.6795
	H	-7.33345	-3.18563	-3.36899
	C	-3.48127	2.04543	3.06626
	H	-2.57045	1.77632	3.59134
Ligand 6	O	-0.04021	0.72531	-2.65522
	N	4.90972	-0.39942	-0.31291
	O	7.60924	1.90156	2.00892
	H	7.67715	1.01464	1.55628
	N	6.89973	-0.21058	0.71051
	N	-5.14355	0.25058	-0.4232
	N	-6.88134	-0.24333	0.91092
	O	-6.70849	-1.92981	2.85633
	H	-7.08075	-1.21361	2.26933
	C	-1.26248	0.56629	-2.03695
	C	1.13944	0.44125	-1.99918
	C	5.70585	-1.4483	-0.78006
	C	3.62702	-0.09595	-0.86824
	C	6.94605	-1.30723	-0.12504
	C	5.68836	0.32084	0.59432
	C	-2.32023	0.15169	-2.84931

Electronic Supporting information

H	-2.12519	-0.07764	-3.89104
C	2.23429	1.25103	-2.31226
H	2.09599	2.08057	-2.99675
C	3.47928	0.97414	-1.75672
H	4.33744	1.59231	-1.99744
C	-3.8221	0.337	-0.96382
C	-5.6617	-0.61539	0.54063
C	2.52957	-0.90664	-0.56459
H	2.6553	-1.74122	0.11732
C	-6.12233	1.21929	-0.65913
C	-7.19911	0.88818	0.18831
C	-5.01263	-1.79649	1.11133
C	5.29422	1.50621	1.35687
C	1.28362	-0.64665	-1.1329
H	0.43457	-1.28084	-0.90493
C	-3.60016	0.03984	-2.31181
H	-4.42826	-0.29113	-2.92979
C	-1.47985	0.88262	-0.69177
H	-0.65911	1.22413	-0.0715
C	5.45953	-2.46471	-1.70318
H	4.50457	-2.55717	-2.20918
C	-2.76215	0.76982	-0.16123
H	-2.94657	1.0182	0.87852
C	7.98383	-2.2118	-0.37928
H	8.93905	-2.10827	0.12454
C	6.31563	2.25279	2.01996
C	3.95935	1.93932	1.49455
H	3.1639	1.36077	1.04413
C	-8.35592	1.67662	0.19788

Electronic Supporting information

	H	-9.18798	1.42409	0.84666
	C	7.74443	-3.23288	-1.29306
	H	8.52963	-3.9503	-1.51071
	C	6.50257	-3.35615	-1.94616
	H	6.3537	-4.1638	-2.65622
	C	-6.14846	2.33054	-1.50188
	H	-5.30952	2.58124	-2.1421
	C	-8.39342	2.78275	-0.6447
	H	-9.27714	3.41315	-0.66003
	C	-5.5865	-2.38354	2.28005
	C	3.63376	3.08125	2.21209
	H	2.59636	3.3859	2.30375
	C	5.97148	3.41767	2.72577
	H	6.77428	3.968	3.20461
	C	4.65082	3.82884	2.81874
	H	4.40721	4.72794	3.37755
	C	-7.30613	3.1057	-1.47991
	H	-7.37027	3.97916	-2.12145
	C	-3.86701	-2.40334	0.55676
	H	-3.44673	-2.0081	-0.35855
	C	-3.27395	-3.51235	1.14289
	H	-2.39707	-3.96152	0.68801
	C	-3.82029	-4.04864	2.31564
	H	-3.35986	-4.91276	2.78606
	C	-4.96156	-3.49314	2.8732
	H	-5.41573	-3.90393	3.76853
Complex 1	Br	5.49605639	2.41902819	-2.00047909
	F	-6.14756201	0.35685118	0.53192041
	F	-5.80951454	1.28527537	-1.54081861

Electronic Supporting information

O	-4.74597001	2.23779347	0.31576811
N	-3.99997031	0.07070701	-0.52508214
N	-2.02873325	-0.85843556	-0.12000474
C	3.44459353	0.81655454	-0.81139542
H	2.77069403	1.38523120	-1.44201940
C	1.65490163	-0.70540616	0.33521777
C	2.97220558	-0.18213943	0.04728757
C	-2.90494989	0.13955900	0.24236198
C	0.37532000	-0.40995860	-0.13914637
H	0.21180172	0.36138040	-0.88469819
N	3.17313633	-1.82532258	1.63243991
C	-0.52711509	-2.13956557	1.32953201
H	-1.39647150	-2.67670255	1.69380327
C	-2.76513954	1.18554934	1.23222285
C	-3.85651300	-0.97805552	-1.41925858
C	-0.70626547	-1.12356960	0.37289824
C	-2.61298482	-1.57909911	-1.16981426
C	-4.25091590	-2.53891095	-3.16601028
H	-4.87470307	-2.93457907	-3.96120751
C	-4.69880152	-1.44583839	-2.43103198
H	-5.64497507	-0.95700665	-2.62542547
C	-3.73535653	2.23236830	1.17609521
C	4.81069948	1.06336623	-0.83670045
C	-2.15774936	-2.67089040	-1.90780681
H	-1.19331728	-3.12591899	-1.71221397
C	-3.60004983	3.32936837	2.04771544
H	-4.33962824	4.11913244	1.97582841
C	-3.00385734	-3.14141789	-2.90957492
H	-2.69115823	-3.99000556	-3.50988709

Electronic Supporting information

	C	1.82877945	-1.72490096	1.31366872
	C	0.74022735	-2.45116023	1.81051114
	H	0.86674428	-3.23807766	2.54597093
	C	-1.63695408	2.33046105	3.05837853
	H	-0.84207977	2.36322226	3.79598178
	C	-2.56988318	3.37613032	2.97173952
	H	-2.49252963	4.22660206	3.64317405
	C	-1.73422310	1.25302687	2.19440053
	H	-1.01404655	0.44907601	2.26629032
	C	3.88033731	-0.90611299	0.86281805
	C	5.71123362	0.34565024	-0.03410825
	H	6.76991393	0.57054888	-0.08887719
	B	-5.26743801	1.01119102	-0.30518256
	C	5.25409509	-0.64959534	0.82464061
	H	5.95736952	-1.20321709	1.43745390
	C	3.76155714	-2.79149854	2.55115885
	H	4.63027926	-2.31865525	3.01949465
	H	3.04010654	-2.97073898	3.35410694
	C	4.16036391	-4.10830039	1.87829748
	H	4.89625103	-3.93672362	1.08769702
	H	3.29094380	-4.59914253	1.43172289
	H	4.59910887	-4.79018093	2.61337017
Complex 2	C	1.59825700	0.84049900	-1.43074000
	C	1.30225200	0.89492000	-0.04869400
	C	-0.00954400	0.85833500	0.40180000
	C	-1.06897400	0.77161800	-0.50761400
	C	-0.79787800	0.74169300	-1.87490500
	C	0.51558400	0.76580600	-2.33408500
	H	2.10801200	0.97776600	0.67036200

Electronic Supporting information

H	-0.21914200	0.90000200	1.46604200
H	0.69161300	0.72073900	-3.40106200
N	2.91309200	0.91259600	-1.88600000
C	4.01301000	0.55488200	-1.05026700
C	4.04846100	-0.67868000	-0.38422900
C	5.09983100	1.42923900	-0.91744200
C	5.14137900	-1.02853200	0.40567700
H	3.21578200	-1.36683400	-0.48671400
C	6.20639000	1.07903500	-0.14572800
H	5.07335000	2.39377500	-1.41496000
C	6.21664900	-0.14780700	0.51466000
H	5.16490900	-1.98327300	0.91845600
H	7.04466700	1.75895700	-0.04652900
Br	7.72292200	-0.62868100	1.58546600
N	-2.42350800	0.76791900	-0.03546700
C	-3.29147600	-0.29211900	0.09396300
C	-3.12710800	1.93596900	0.28629700
C	-4.43437700	1.53694800	0.60533100
N	-4.49183300	0.15811800	0.48021200
C	-2.73579000	3.27399400	0.30940600
C	-5.41275200	2.47023800	0.95720500
C	-3.71051300	4.20146800	0.67038500
C	-5.02470500	3.80588000	0.98763700
H	-3.45108100	5.25499400	0.70334000
H	-5.75348800	4.56367300	1.25721800
H	-1.72489000	3.57370500	0.05698300
H	-6.42237500	2.14838300	1.17883000
C	-3.08255600	-1.70097300	-0.16295200
C	-1.82705300	-2.29849800	-0.40601400

Electronic Supporting information

	C	-4.25893000	-2.50984200	-0.20326600
	C	-1.72776800	-3.64541700	-0.71154100
	H	-0.92819900	-1.69965600	-0.34408700
	C	-4.13467900	-3.87044900	-0.54201200
	C	-2.89132700	-4.42703800	-0.79060400
	H	-0.75433700	-4.09083400	-0.88819000
	H	-5.04335100	-4.46091400	-0.58158000
	H	-2.81796800	-5.48262500	-1.03663900
	H	-1.61774500	0.68244700	-2.58355400
	O	-5.47434300	-2.03184800	0.03321200
	B	-5.70793400	-0.81291200	0.82258100
	C	3.17354500	1.05388500	-3.31631700
	H	2.89717000	0.15159500	-3.88110400
	H	2.62210700	1.90464200	-3.72927900
	H	4.23855900	1.22889300	-3.46460100
	F	-6.86988300	-0.19188200	0.42243800
	F	-5.68070300	-1.07623100	2.17647900
Complex 3	Br	7.97225825	0.35978619	-1.24657311
	O	2.94295403	-0.62251525	1.99369575
	F	-5.66653143	0.82369357	-2.15237091
	O	-5.44944154	1.94030817	-0.08938946
	C	4.05042918	-0.39769805	1.18959987
	F	-6.79906065	0.03963658	-0.31471697
	C	1.67790226	-0.62733895	1.46041902
	C	4.20082128	0.79480289	0.47843583
	H	3.41583224	1.54316336	0.50068900
	N	-2.31964300	-0.76129852	0.12223852

Electronic Supporting information

C	0.63101110	-0.47214053	2.37731670
H	0.86963701	-0.32660102	3.42495128
C	5.36752474	1.01761424	-0.25081162
H	5.49842515	1.93893168	-0.80643095
C	5.05763275	-1.36094489	1.18944513
H	4.91973902	-2.27356354	1.75902823
C	6.37254278	0.05049221	-0.25032300
N	-4.41343209	-0.24926559	-0.39388086
C	6.22947674	-1.13536870	0.46749707
H	7.02093662	-1.87569454	0.46141854
C	-0.68627407	-0.51459465	1.93726378
H	-1.50415333	-0.39749922	2.64033477
C	-2.99588132	-1.97056539	-0.09158447
C	-3.22013290	0.26265574	-0.07006286
C	1.40720860	-0.82804158	0.10250759
H	2.21712766	-0.96137524	-0.60454245
C	-4.24394500	2.46895586	0.07881971
C	-2.56856767	-3.29556426	-0.01709973
H	-1.54574820	-3.54989609	0.23713479
C	-0.96142786	-0.69305951	0.57751027
C	-3.04549456	1.69186371	0.07031577
C	0.08319227	-0.85825840	-0.33340561
H	-0.14134664	-1.00817154	-1.38446495
C	-4.31960611	-1.63179326	-0.41223837

Electronic Supporting information

	C	-3.52457583	-4.27349924	-0.28277930
	H	-3.23705292	-5.31917286	-0.23750503
	C	-5.27858968	-2.61490619	-0.66858024
	H	-6.30074120	-2.33759350	-0.89286481
	C	-4.85476393	-3.93833059	-0.60214234
	H	-5.56757666	-4.73360554	-0.79540617
	C	-1.80226609	2.34097449	0.23112363
	H	-0.88703464	1.76555654	0.18816303
	C	-4.15143750	3.85445305	0.30960064
	H	-5.07569076	4.42123352	0.32825886
	C	-2.91921517	4.46228673	0.48115435
	H	-2.87077517	5.53521106	0.64395904
	C	-1.73504523	3.70947675	0.42956616
	H	-0.77118456	4.19411863	0.54396675
	B	-5.66375801	0.66104937	-0.78301642
Complex 4	F	7.88921801	1.35869645	0.85847134
	F	-6.23249560	2.10453098	2.84071113
	F	6.77561608	2.25920654	2.65393614
	F	-7.71297648	2.36999668	1.10482988
	N	4.11694569	-0.75752604	0.47710227
	N	5.64009410	0.61921820	1.31135153
	O	6.11854913	2.86782942	0.48991991
	O	-7.23305870	0.20761861	1.86532285
	N	-3.80633895	0.56167619	-0.42633554

Electronic Supporting information

N	-0.03189841	-2.96585739	-2.51987934
N	-5.54248053	1.45609326	0.62234142
C	-0.63578825	-1.22426744	-1.16025630
C	0.78320511	-1.45518510	-1.00324250
C	4.83070763	0.40177588	0.26810937
C	1.77681303	-0.85971627	-0.22264384
H	1.55439999	-0.03611068	0.44793066
C	-1.53643146	-0.32236018	-0.58641182
H	-1.21732569	0.40652250	0.15158169
C	5.46467449	-0.39743934	2.23668991
C	-5.15466420	-0.85531856	1.22279998
C	3.08099368	-1.33709186	-0.32910687
C	-1.09626152	-2.17337697	-2.11324009
C	1.11425141	-2.53563472	-1.86702366
C	4.50525056	-1.28075785	1.71809778
C	-4.81127792	0.34361209	0.48984691
C	-2.87269597	-0.37931932	-0.97497096
C	4.77121003	1.34543538	-0.82700432
C	3.40094842	-2.41061767	-1.18085252
H	4.42934711	-2.75254743	-1.22934599
C	2.42410747	-3.01907534	-1.96162023
H	2.68461965	-3.83882706	-2.62195463
C	6.05171970	-0.61523617	3.48564059
H	6.77372041	0.08760641	3.88151454

Electronic Supporting information

C	4.09421889	-2.41769728	2.41247699
H	3.34844599	-3.09266974	2.00780595
C	-6.42660665	-0.84617676	1.87232607
C	-3.92622021	1.88150556	-0.88500436
C	-3.31722592	-1.30755213	-1.93524780
H	-4.36394569	-1.30814558	-2.21946081
C	-2.43791568	-2.21768416	-2.50931176
H	-2.79297955	-2.92908481	-3.24667989
C	-4.34594831	-2.00926432	1.30593949
H	-3.36331351	-2.00927648	0.85284820
C	-5.03058984	2.43302113	-0.21694979
C	5.43405592	2.59260307	-0.61266069
C	4.68841188	-2.63761974	3.65322795
H	4.39949860	-3.51051046	4.23005339
C	4.08520778	1.13024127	-2.04201461
H	3.61104703	0.17594931	-2.22882768
C	5.64879457	-1.75181768	4.17937183
H	6.08015552	-1.95906129	5.15344965
C	-6.86378347	-2.01607655	2.52167515
H	-7.83998087	-1.99171358	2.99313983
C	5.33182179	3.59265579	-1.59825778
H	5.82951765	4.53666228	-1.40601235
C	4.63896066	3.35920426	-2.77396503
H	4.58547071	4.14058328	-3.52671426

Electronic Supporting information

	C	-6.05705191	-3.14043041	2.57191898
	H	-6.40840152	-4.02700384	3.09210958
	C	-4.78582717	-3.13851493	1.97536672
	H	-4.14842375	-4.01416476	2.03847173
	C	4.02158629	2.11989496	-3.00803873
	H	3.49746026	1.93496098	-3.93981033
	C	-0.09221425	-4.01867772	-3.52818578
	H	-1.07299580	-4.49714295	-3.45011524
	H	0.64356405	-4.78148993	-3.25649554
	C	-3.18612376	2.60940593	-1.81569955
	H	-2.33716715	2.17572038	-2.33206409
	B	6.68763978	1.82113077	1.35256488
	C	-3.59489411	3.92089337	-2.04763325
	H	-3.04656096	4.52635798	-2.76236424
	C	-5.44440176	3.74528377	-0.45896544
	H	-6.31131835	4.14861487	0.04875008
	C	-4.70387032	4.47750748	-1.38132196
	H	-4.98985808	5.50188142	-1.59745426
	B	-6.73879958	1.57989988	1.67094545
	C	0.15237145	-3.51255221	-4.95250724
	H	1.14126852	-3.05407458	-5.04178198
	H	-0.59494826	-2.76674566	-5.23772428
	H	0.09496021	-4.34360897	-5.66204728
Complex 5	C	-1.20305000	-0.37450400	-2.22376300

Electronic Supporting information

C	-1.25916800	0.44726000	-1.07578500
C	-2.47090600	0.73578600	-0.46348900
C	-3.66480800	0.22382100	-0.98207900
C	-3.63134700	-0.56455100	-2.13129500
C	-2.41783400	-0.87007200	-2.74106700
H	-0.34770000	0.87065000	-0.67165000
H	-2.49713300	1.36687700	0.41914000
H	-2.42547600	-1.50096800	-3.62045300
N	0.01317800	-0.63484800	-2.86460100
C	1.24910000	-0.61108900	-2.16553100
C	1.38858700	-1.22044000	-0.90747900
C	2.37202100	-0.00137400	-2.74922000
C	2.61355400	-1.20772500	-0.24596500
H	0.53394000	-1.70613700	-0.44977700
C	3.60415000	-0.01296500	-2.10323700
H	2.27536300	0.49136700	-3.71101600
C	3.72289600	-0.60325300	-0.84269200
H	2.71678400	-1.67584100	0.72759400
H	4.46882700	0.45620400	-2.56056300
N	-4.91600500	0.55670400	-0.36660500
C	-5.71871100	-0.22245400	0.43616800
C	-5.59387000	1.75973400	-0.60789800
C	-6.81877800	1.66702200	0.07098300
N	-6.85311000	0.43493700	0.70443500

Electronic Supporting information

C	-5.24686800	2.88295000	-1.35743400
C	-7.75599900	2.70200100	0.02202700
C	-6.17894300	3.91764100	-1.39622300
C	-7.41066100	3.82764100	-0.71900300
H	-5.95122500	4.81272800	-1.96646200
H	-8.10943600	4.65567200	-0.78216800
H	-4.30101700	2.94479000	-1.88379800
H	-8.70551500	2.60576000	0.53308800
C	-5.50931400	-1.56372100	0.93667300
C	-4.28890500	-2.26949400	0.86638900
C	-6.65264400	-2.20297800	1.50599700
C	-4.19759300	-3.57786700	1.30993400
H	-3.40897000	-1.77955200	0.47094800
C	-6.54176500	-3.54254300	1.92432600
C	-5.33587700	-4.21615100	1.82822100
H	-3.25015200	-4.10387600	1.25686300
H	-7.42718800	-4.01215200	2.33825200
H	-5.26974400	-5.24484200	2.17096300
H	-4.55691600	-0.95489800	-2.54176900
O	-7.82909700	-1.60222600	1.63111500
B	-7.96962800	-0.13882100	1.68791500
C	-0.00350800	-1.22436300	-4.20264900
H	-0.35464600	-2.26585100	-4.18965900
H	-0.64933100	-0.64664500	-4.87072000

Electronic Supporting information

H	1.00656400	-1.21990300	-4.60914000
F	-9.19767000	0.24943100	1.20268000
F	-7.71549800	0.34346900	2.95443300
C	5.82388700	-1.77006300	-0.18014900
C	5.68769400	0.39134200	0.41454300
C	7.02581600	-1.37596500	0.42814800
C	5.62953100	-3.06270000	-0.66487000
C	8.09177700	-2.26711200	0.57395800
C	6.69061500	-3.95208000	-0.50892200
H	4.70126600	-3.35933000	-1.14008200
C	7.89895900	-3.56049200	0.09918600
H	9.02007400	-1.94120000	1.02565600
H	6.58357200	-4.97019900	-0.86955700
H	8.70121500	-4.28517700	0.19408500
C	5.30138200	1.76822200	0.62900500
C	3.99384300	2.27424100	0.46520600
C	6.35257100	2.65898900	1.00518800
C	3.72860200	3.62330700	0.62608600
H	3.18356600	1.59845100	0.22441500
C	6.06393500	4.03072200	1.13377200
C	4.77552600	4.50251300	0.94770300
H	2.71680300	3.99582300	0.50596800
H	6.88089900	4.69110500	1.40255300
H	4.57251400	5.56283900	1.06764600

Electronic Supporting information

	N	4.99376100	-0.63907200	-0.18164700
	N	6.89786300	-0.04249300	0.78334400
	O	7.60040900	2.25669500	1.20895800
	B	7.93271500	0.87320000	1.58342000
	F	7.74485700	0.65533800	2.93112000
	F	9.19874900	0.54560900	1.15613600
Complex 6	F	-0.44402900	8.39196800	-2.29553300
	F	1.60921000	8.41976700	-1.26604100
	O	0.00000000	0.00000000	3.20413300
	N	-0.18502200	5.03882600	0.79817500
	N	0.00000000	6.75509600	-0.59160400
	O	1.08876500	6.68747000	-2.77578900
	C	0.44842200	5.52355200	-0.32533200
	C	-0.11358800	3.72879600	1.37487900
	C	0.60102600	3.53104100	2.55935800
	H	1.12696800	4.36363800	3.01462700
	C	1.42004700	4.88963500	-1.18868100
	C	-1.07440400	6.02629900	1.24715700
	C	-0.02800100	1.20306300	2.53222400
	C	0.64787700	2.26538700	3.13762900
	H	1.19905100	2.08540400	4.05379500
	C	-0.80233200	2.66733600	0.78212900
	H	-1.37031600	2.83724600	-0.12639500
	C	-0.95001600	7.10317900	0.35565600

Electronic Supporting information

C	-0.76055000	1.39962200	1.35672800
H	-1.29937800	0.57585700	0.90303700
C	2.09860600	3.68721600	-0.89435700
H	1.95552600	3.21194100	0.06733300
C	-1.96244700	6.05374600	2.32147900
H	-2.05866300	5.21591600	3.00290200
C	1.66235700	5.54016400	-2.43698000
C	-1.71974900	8.25969900	0.50290300
H	-1.62779200	9.07262500	-0.20609600
C	-2.72151900	7.21239200	2.47154000
H	-3.42546700	7.27938900	3.29495700
C	2.96217300	3.11553400	-1.81290900
H	3.48517000	2.19706300	-1.56803900
C	-2.60184100	8.29450100	1.57814000
H	-3.21809600	9.17482300	1.72998200
C	2.52123600	4.92352400	-3.36637900
H	2.67614600	5.42593300	-4.31472200
B	0.58956900	7.64642200	-1.77767300
C	3.15890200	3.73371400	-3.05857400
H	3.82987800	3.28387400	-3.78472600
F	0.44402900	-8.39196800	-2.29553300
F	-1.60921000	-8.41976700	-1.26604100
N	0.18502200	-5.03882600	0.79817500
N	0.00000000	-6.75509600	-0.59160400

Electronic Supporting information

O	-1.08876500	-6.68747000	-2.77578900
C	-0.44842200	-5.52355200	-0.32533200
C	0.11358800	-3.72879600	1.37487900
C	-0.60102600	-3.53104100	2.55935800
H	-1.12696800	-4.36363800	3.01462700
C	-1.42004700	-4.88963500	-1.18868100
C	1.07440400	-6.02629900	1.24715700
C	0.02800100	-1.20306300	2.53222400
C	-0.64787700	-2.26538700	3.13762900
H	-1.19905100	-2.08540400	4.05379500
C	0.80233200	-2.66733600	0.78212900
H	1.37031600	-2.83724600	-0.12639500
C	0.95001600	-7.10317900	0.35565600
C	0.76055000	-1.39962200	1.35672800
H	1.29937800	-0.57585700	0.90303700
C	-2.09860600	-3.68721600	-0.89435700
H	-1.95552600	-3.21194100	0.06733300
C	1.96244700	-6.05374600	2.32147900
H	2.05866300	-5.21591600	3.00290200
C	-1.66235700	-5.54016400	-2.43698000
C	1.71974900	-8.25969900	0.50290300
H	1.62779200	-9.07262500	-0.20609600
C	2.72151900	-7.21239200	2.47154000
H	3.42546700	-7.27938900	3.29495700

Electronic Supporting information

C	-2.96217300	-3.11553400	-1.81290900
H	-3.48517000	-2.19706300	-1.56803900
C	2.60184100	-8.29450100	1.57814000
H	3.21809600	-9.17482300	1.72998200
C	-2.52123600	-4.92352400	-3.36637900
H	-2.67614600	-5.42593300	-4.31472200
B	-0.58956900	-7.64642200	-1.77767300
C	-3.15890200	-3.73371400	-3.05857400
H	-3.82987800	-3.28387400	-3.78472600