Electronic Supplementary Material (ESI) for Dalton Transactions.

Triarylborane-A_2H_2 and Triarylborane-Zn-A_2H_2 Porphyrin Conjugates: Synthesis, Structure and Intriguing Optical Properties

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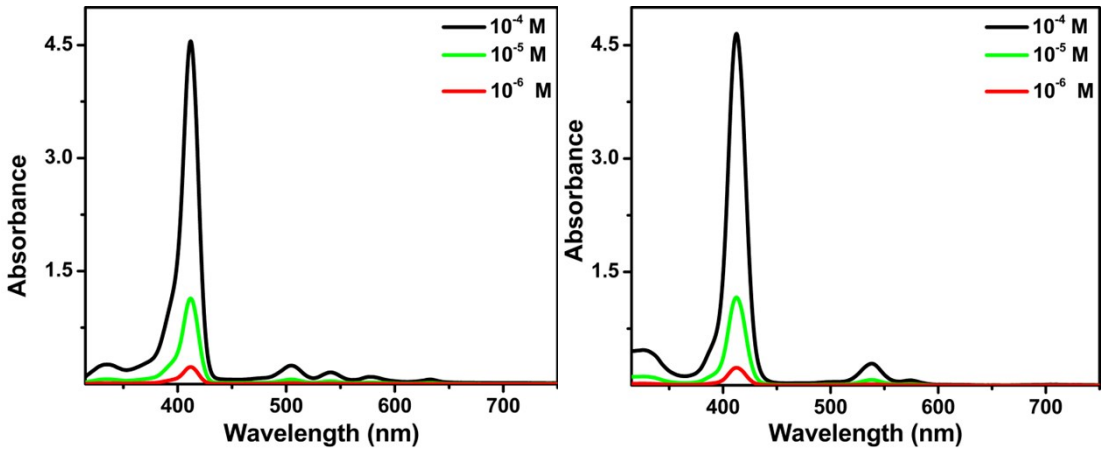


Figure S1: UV-Visible spectra of **1** (left) and **2** (right) in THF at various concentrations (10^{-4}-10^{-6} M).

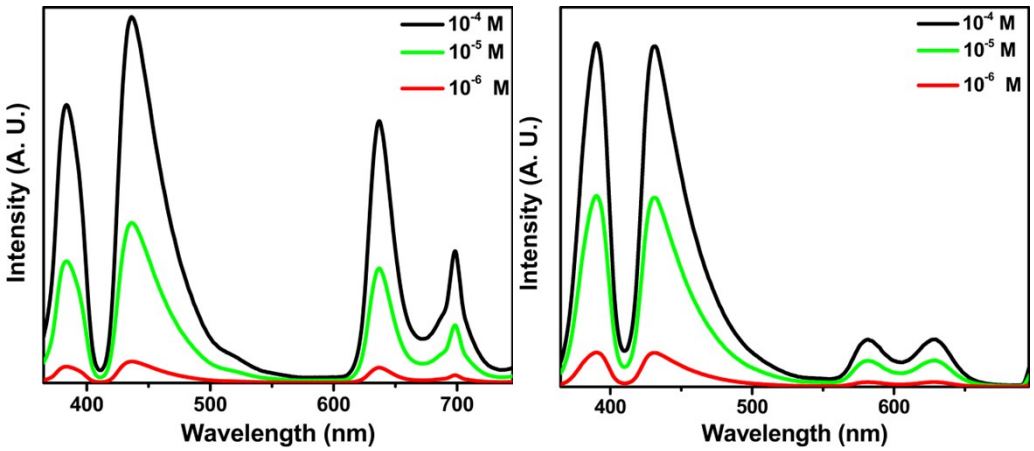


Figure S2: Fluorescence spectra of **1** (left) and **2** (right) in THF at various concentrations (10^{-4}-10^{-6} M) (λ_{ex} at 350 nm).

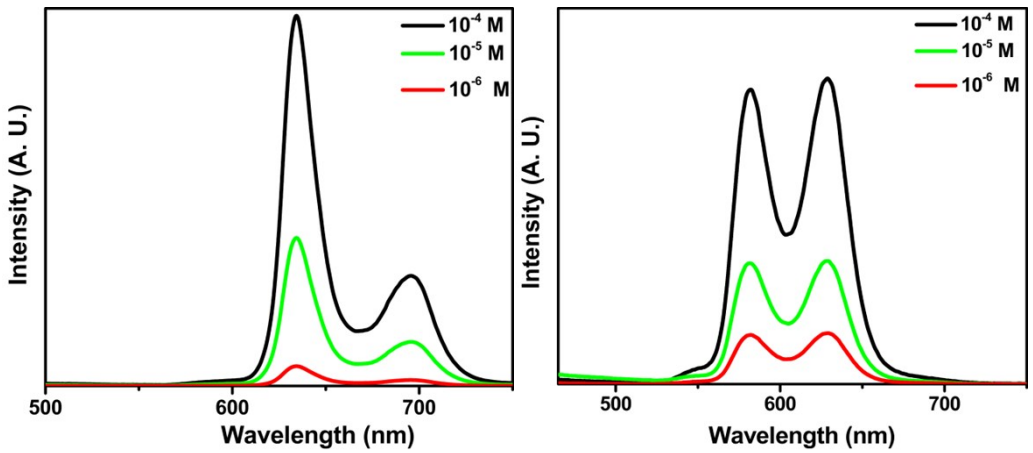


Figure S3: Fluorescence spectra of **1** (left) and **2** (right) in THF at various concentrations (10^{-4}-10^{-6} M) (λ_{ex} at 350 nm).

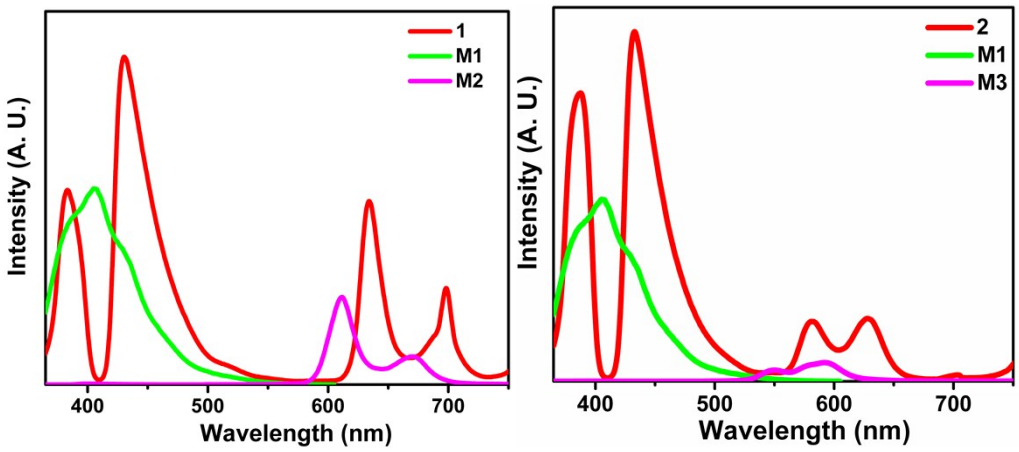


Figure S4: Comparison of emission spectra of **1** (left) and **2** (right) (10 μM THF solution, λ_{ex} = 350 nm) compared to the model building units (i.e. **M1**, **M2** and **M3**).

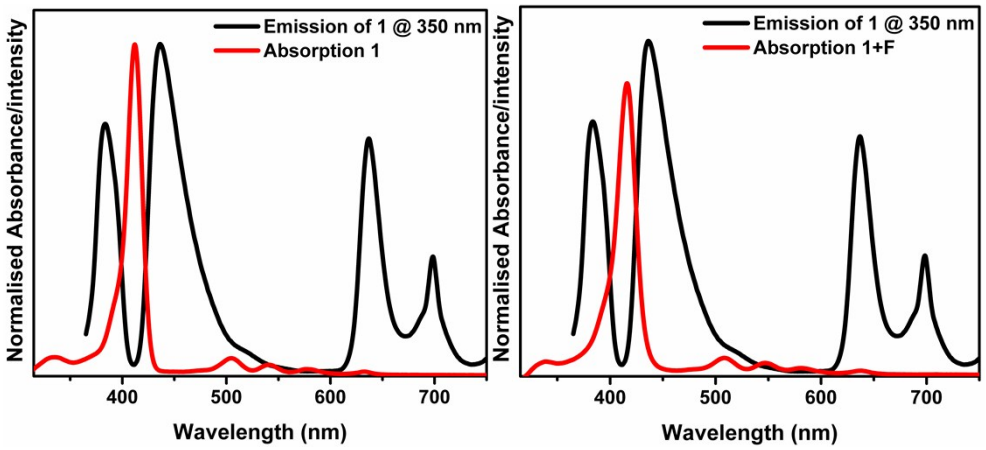


Figure S5: Comparison of UV-Vis absorption spectra and fluorescence emission spectra of **1** in the presence (left) and absence of fluoride ions (**1**+**2F**$^{2-}$) (right). (10 μM THF solution, λ_{ex} = 350 nm)

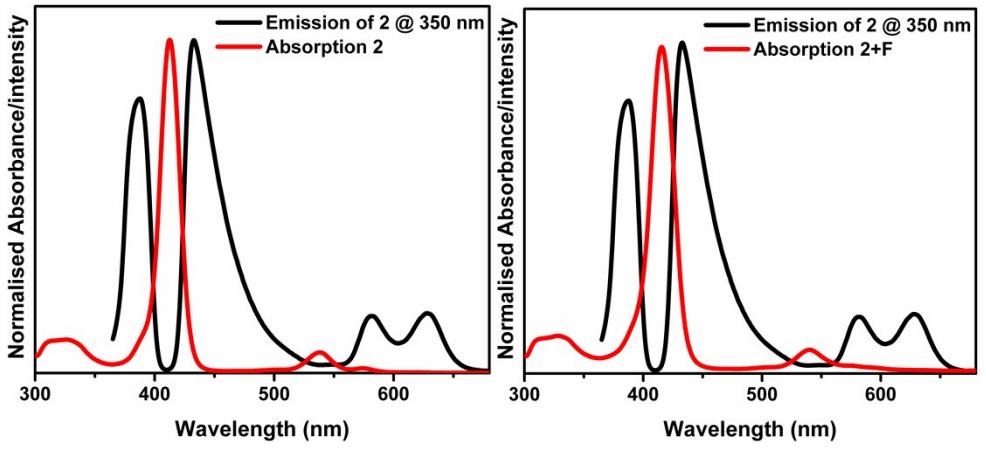


Figure S6: Comparison of UV-Vis absorption spectra and fluorescence emission spectra of **2** in the presence (left) and absence of fluoride ions (**2**+**2F**$^{2-}$) (right). (10 μM THF solution, λ_{ex} = 350 nm)

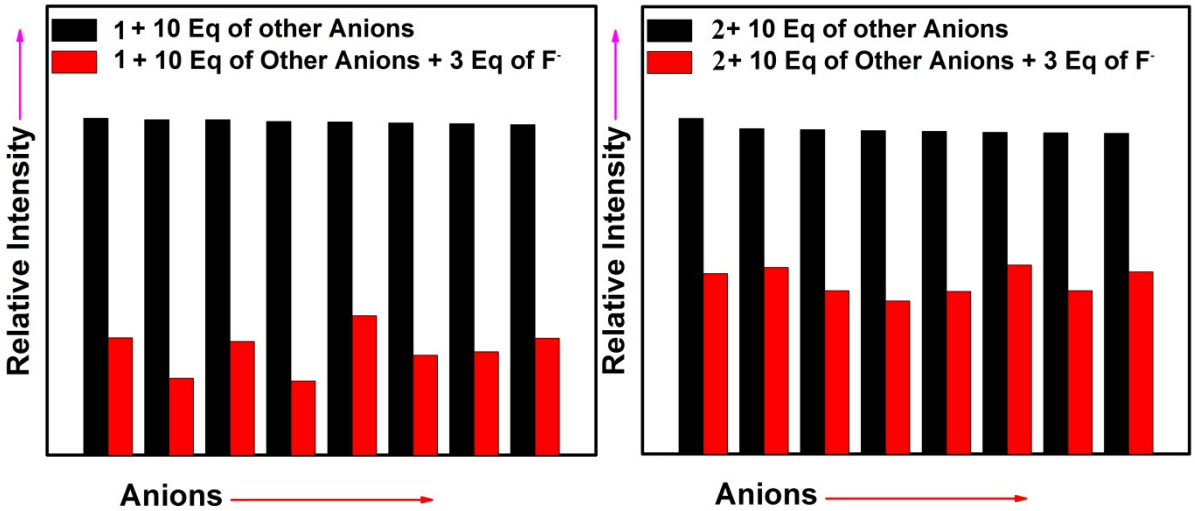


Figure S7:Competitive binding affinity of compound **1** (left) and **2** (right) (10 μM in THF) towards F^- ions in the presence of 50.0 equiv of different anions (Cl^-, Br^-, I^-, ClO_4^-, NO_3^-, CH_3COO^- and CN^- (left to right) (λ_{ex} at 350 nm).

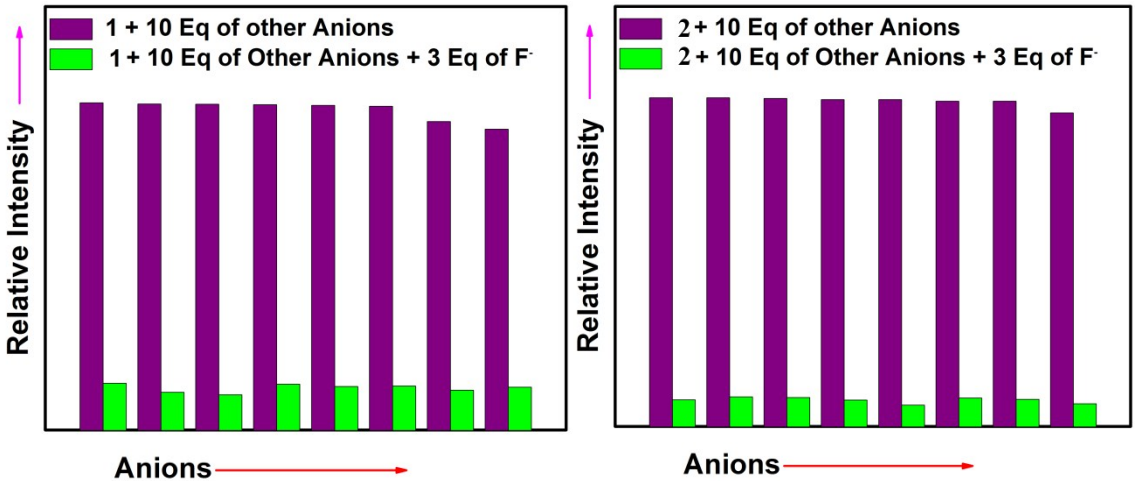


Figure S8:Competitive binding affinity of compound **1** (left) and **2** (right) (10 μM in THF) towards F^- ions in the presence of 50.0 equiv of different anions (Cl^-, Br^-, I^-, ClO_4^-, NO_3^-, CH_3COO^- and CN^- (left to right) (λ_{ex} at 415 nm).

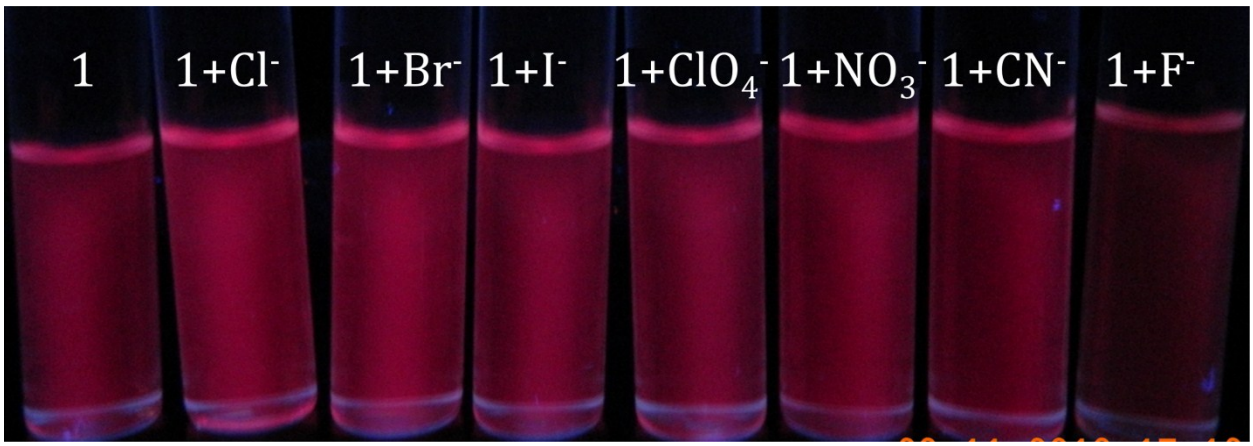


Figure S9: Photograph of **1** with different anions under UV light (260-320 nm). Concentration: 10μM in THF.

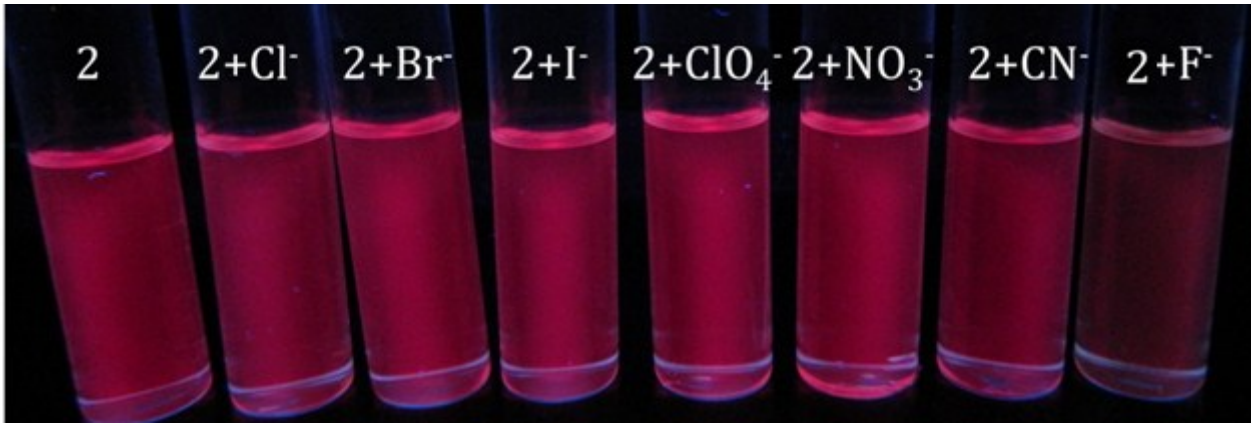


Figure S10: Photograph of **2** with different anions under UV light (260-320 nm). Concentration: 10μM in THF.

Details about the association constant[1]

A THF solution of **1** or **2** (3 mL, 1×10^{-5} M) was placed in the cell and was titrated with incremental amounts of a solution of $^{n}Bu_4NF$ in THF (1×10^{-3} M). The changes associated with a band at 335 nm was monitored.

Sensor + $2F^-$ ⟷ $[F]^2$• Sensor; here sensor is **1** and **2**

$I = K_s[\text{Sensor}] + K_p[F^2\bullet\ \text{Sensor}]$

$I_0 = K_s[\text{Sensor}]_0$

$[\text{Sensor}]_0 = [\text{Sensor}] + [F^2\bullet\ \text{Sensor}]$

$K = [F^2\bullet\ \text{Sensor}]/\ [\text{Sensor}][F]^2$

$I/I_0 = (1 + (K_p/K_s)K[F]^2)/(1 + K[F]^2)\ (1 - I/I_0)/[F]^2 = K(I/I_0) - K(K_p/K_s)$

$K_1 = 2.0\times10^5$ and $K_2 = 2.0\times10^{11}$ for **1** and $K_1 = 2.4\times10^5$ and $K_2 = 5.3\times10^{11}$ for **2**

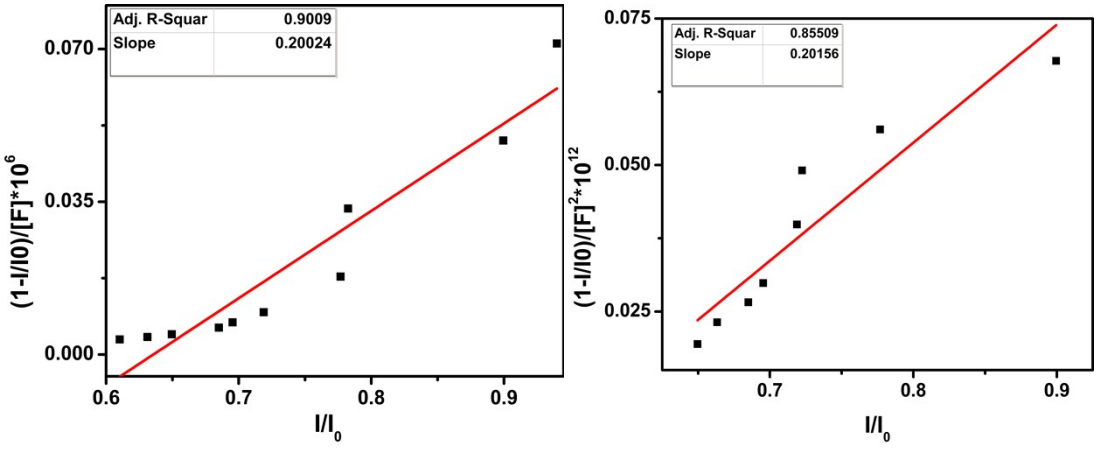


Figure S11: The plot between $(1 - I/I_0)/[F^-]$ and I/I_0 of absorption titration data of **1** with fluoride ions for K_1 (left) K_2 (right).

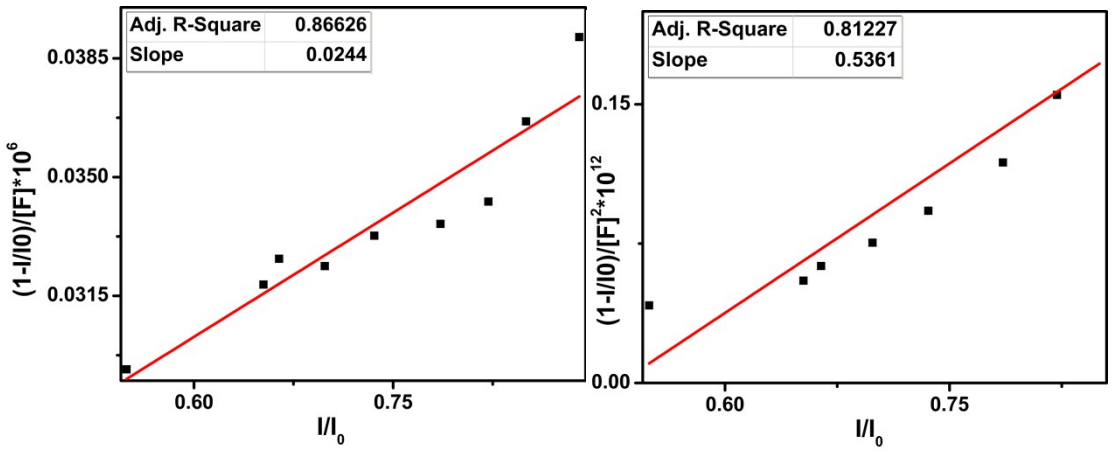


Figure S12: The plot between the $(1 - I/I_0)/[F^-]$ and I/I_0 of absorption titration data of **2** with fluoride ions for K_1 (left) K_2 (right).

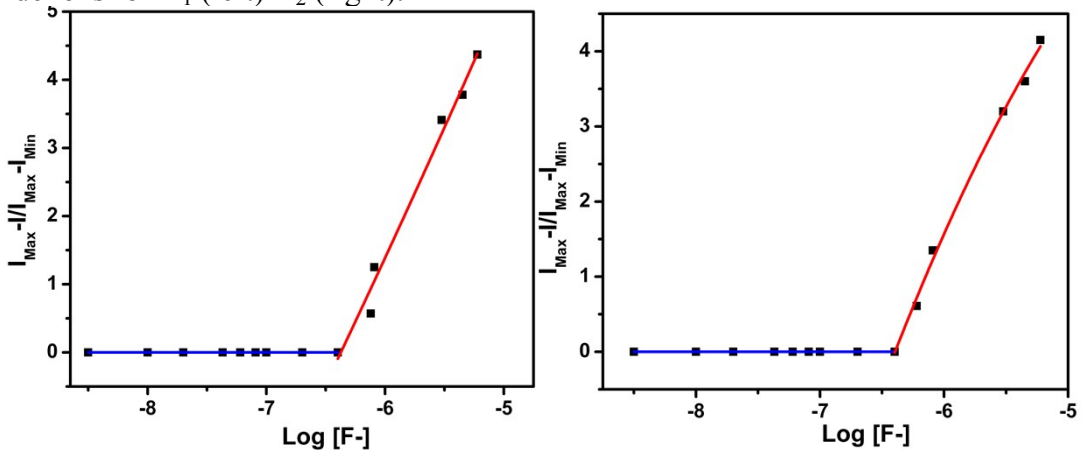


Figure S13: $(I_{max}-I)/(I_{max}-I_{min})$ vs $\log[F^-]$ plots for PL data obtained for acetonitrile solutions of **1** (left) and **2** (right). For **1** and **2**, the lowest detection limit ($[F^-]$) found to be 1.2 and 0.5 ppm respectively.

Table S1: Time resolved fluorescence measurements of **1** and **2**

Compounds	10 μM (THF) τ_f/ns (λ_{em}/nm)
1	6.80 (385) 7.01 (430) 8.72 (630) 7.67 (700)
2	6.83 (385) 6.41 (435) 8.01 (580) 8.23 (630)

All given data are for single exponential fitting of "Time-Resolved Fluorescence" decay profiles. Incorporation of more than one exponential function was not required in any case. (λ_{ex} = 342 nm nano-LED) [$y = A\times\exp(-t/\tau_f) + y_0$] where y is the fluorescence intensity at any given time t. $y_0 = 0$; and A = Pre-exponential constant. τ_f indicates the average fluorescence lifetime of the observed events.]

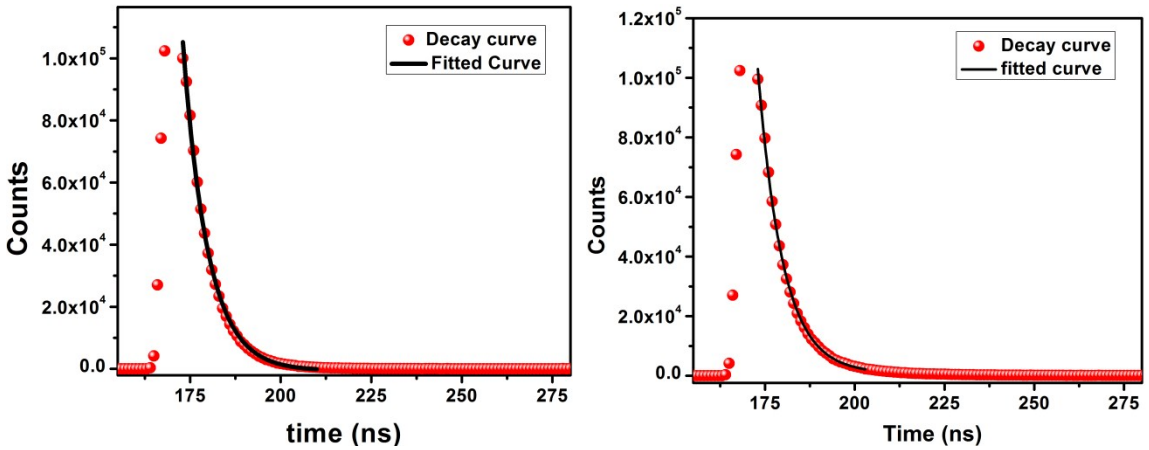


Figure S14: Time resolved fluorescence decay profile of **1** (λ_{ex} = 340 nm, λ_{em} = 385 nm (left) and 430 nm (right) in 10 µM THF.

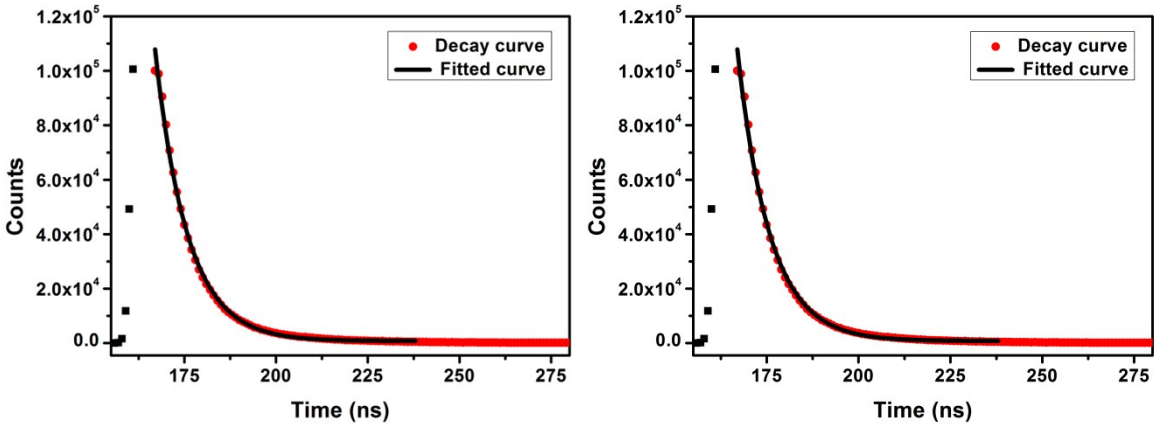


Figure S15: Time resolved fluorescence decay profile of **1** (λ_{ex} = 340 nm, λ_{em} = 630 nm (left) and 700 nm (right)) in 10 µM THF.

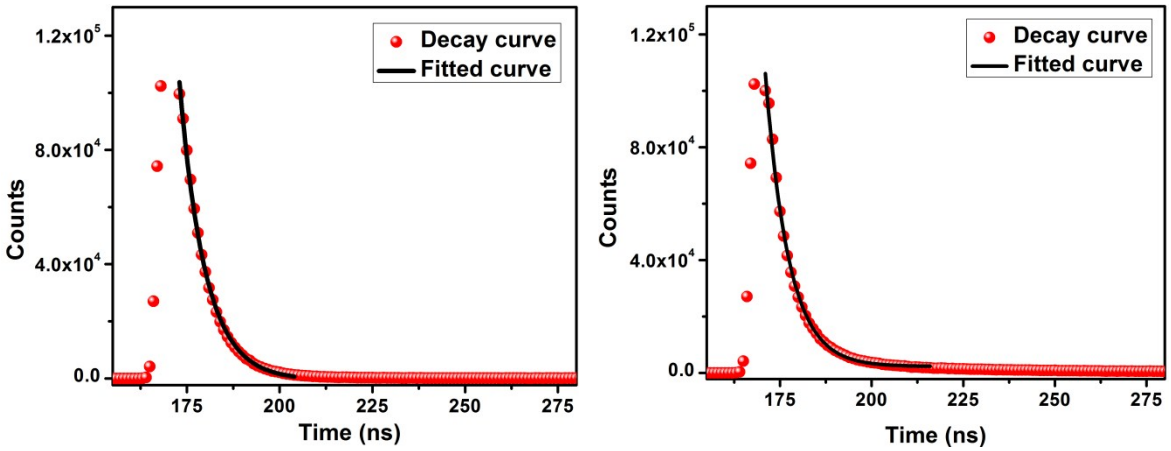


Figure S16: Time resolved fluorescence decay profile of **2** (λ_{ex} = 340 nm, λ_{em} = 385 nm (left) and 435 nm (right)) in 10 µM THF.

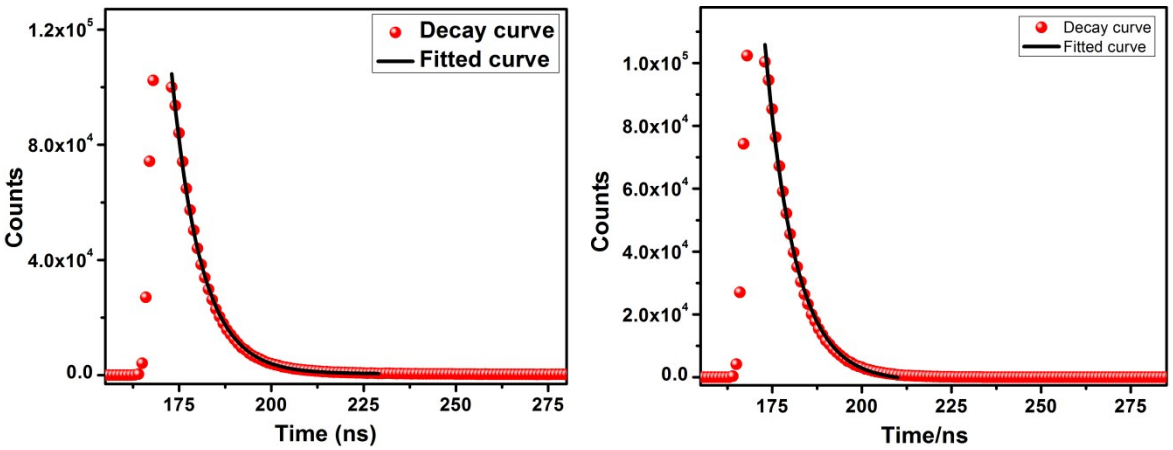


Figure S17: Time resolved fluorescence decay profile of **2** (λ_{ex} = 340 nm, λ_{em} = 580 nm (left) and 630 nm (right)) in 10 µM THF.

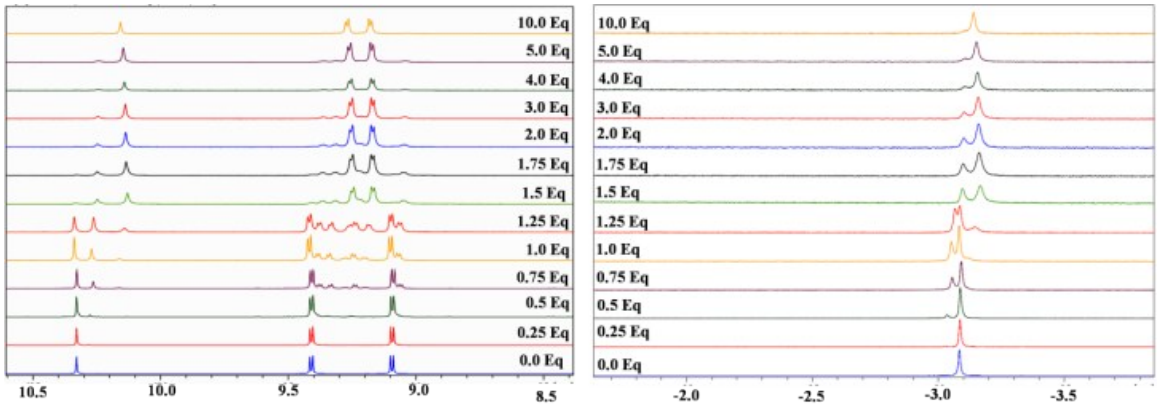


Figure S18: The fluoride binding event of **1** was monitored by ^{1}H NMR. The changes associated with resonance of *meso*, β-protons (left) and N-H proton (right).

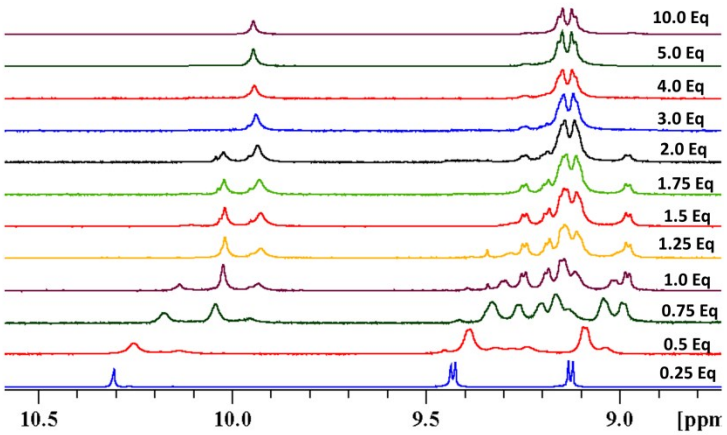


Figure S19: The fluoride binding event of **2** was monitored by ^{1}H NMR. The changes associated with resonance of *meso* and β-protons.

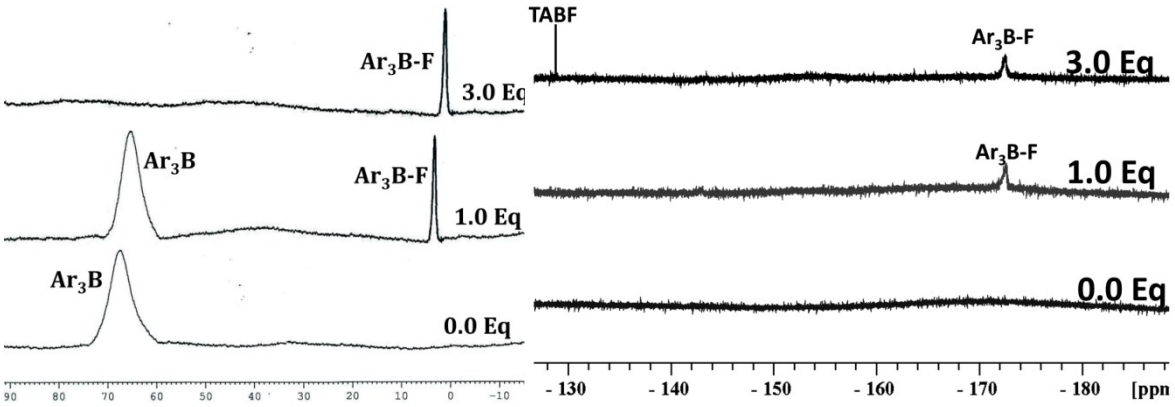


Figure S20: ^{11}B NMR (left) and ^{19}F NMR (right) titration of **2** in presence of increasing amount of fluoride ion.

Table S2: ^{1}H, ^{11}B and ^{19}F NMR data of **1**, **2**, **1**+**2F**$^{2-}$ and **2**+**2F**$^{2-}$

Compound	Meso-Proton (ppm)	β-proton (ppm)	^{11}B NMR (ppm)	^{19}F NMR (ppm)
1	10.33	9.42, 9.09	67	--------
2	9.94	9.14, 8.96	63	---------
1+**2F**$^{2-}$	10.15	9.31, 9. 23	5	-174
2+**2F**$^{2-}$	9.9	9.12, 9.16	4	-172

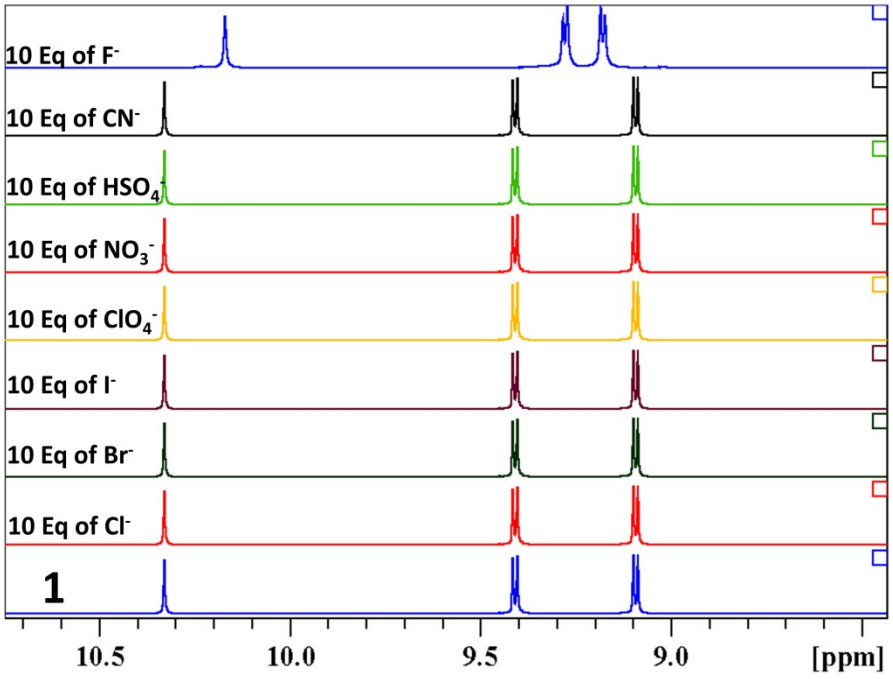


Figure S21: ^{1}H NMR titration of **1** in the presence of different anions ($CDCl_3$). there is no change in chemical shifts of **1** in the presence of other anions, whereas upon addition of fluoride change in chemical shifts of **1**. This results showed that compound **1** selective receptor for fluoride ions.

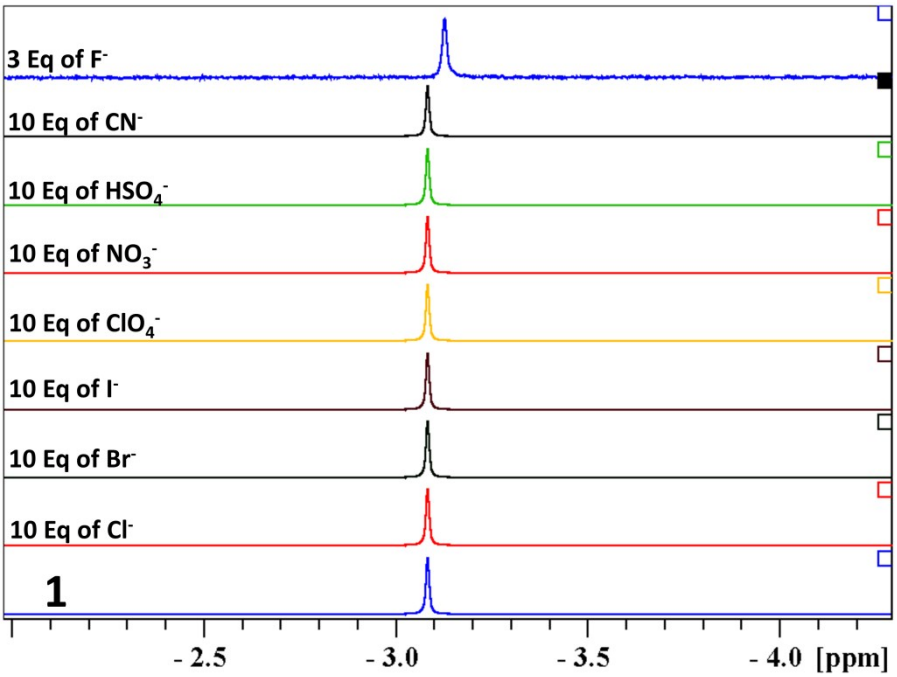


Figure S22: ^{1}H NMR titration of **1** in presence of different anions ($CDCl_3$), there is no change in N-H chemical shifts of **1** in the presence of various other anions, whereas upon addition of fluoride change in chemical shifts of **1**. This results showed that compound **1** selective receptor for fluoride ions.

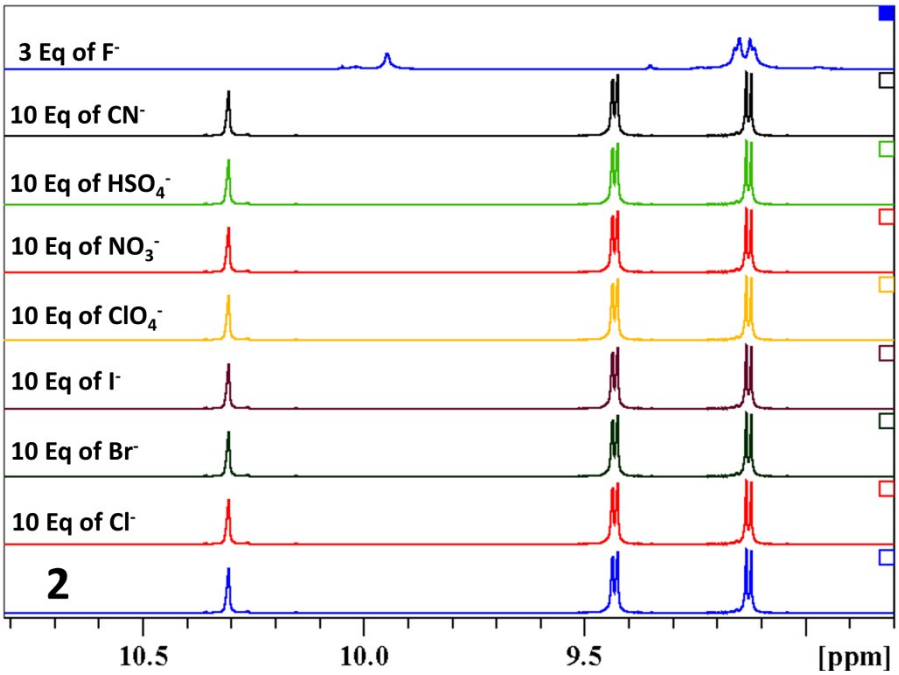


Figure S23: ^{1}H NMR titration of **2** in presence of different anions ($CDCl_3$), there is no change in chemical shifts of **2** in the presence of various other anions, whereas upon addition of fluoride change in chemical shifts of **2**. This results showed that compound **2** selective receptor for fluoride ions.

Table S3: Crystallographic refinement data Table

Compounds	**2**
empirical formula	C68 H62 B2 N4 Zn
Fw	1022.23
T (K)	100 (2) K
crystal system	Triclinic
space group	p -1
a/Å	8.2118(10)
b/Å	14.8870(17)
c/Å	15.0508(18)
α/deg	68.791(6)
β/deg	84.145(7)
γ/deg	75.664(6)
V/Å^3	1661.7(3)
Z	2
ρ_{calcd} (g cm^{-3})	1.021
μ(Mo Kα) (mm^{-1})	0.408
λ/Å	0.71073
F (000)	538.0
collected reflns	26492
unique reflns	5779
GOF *(F^2)*	*1.232*
R_1[I>2σ(I)][a]	0.0636
wR_2[I>2σ(I)][b]	0.1963

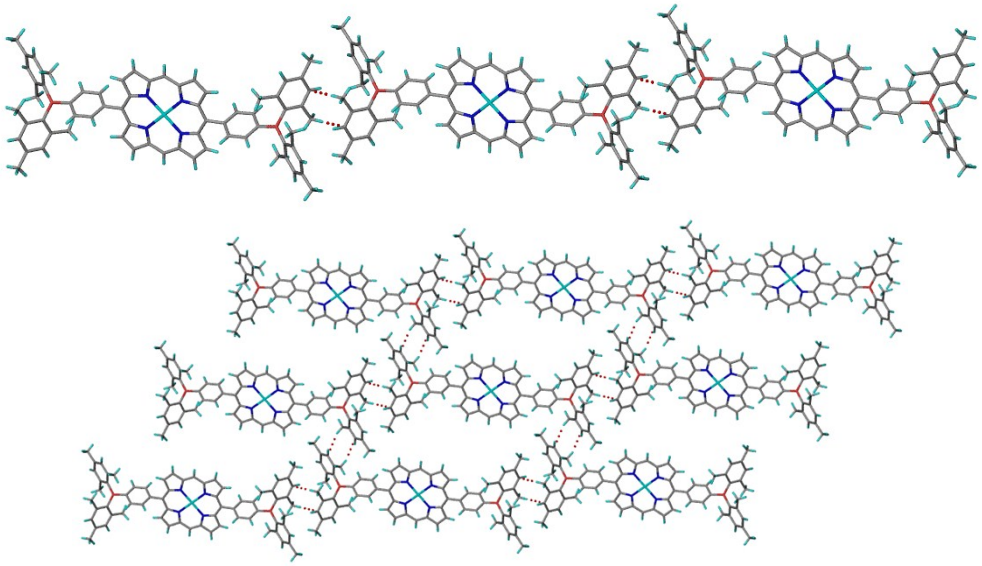


Figure S24: Supramolecular hydrophobic interactions in compound **2** (top). Two tapes of porphyrins are moving in same direction and forms hydrophobic cavity, which contains long alkyl chain and was squeezed by platon commend.

Table S4: Selected bond lengths and bond angles

C5-C11	1.502(5)	C6-C5-C11	118.1(3)
C14-B1	1.573(6)	C4-C5-C11	117.0(3)
C11-C5	1.502(5)	C6-C5-C4	124.9(3)
C5-C6	1.391(7)	C9-C10-C1	126.2(4)
C5-C4	1.403(5)	C1-C10-C9	126.2(4)
C14-B1	1.573(6)	C11-C5-C6	118.1(3)
C9-C10	1.392(7)	C4-C5-C6	124.9(3)
C1-C10	1.386(5)	C11-C5-C4	117.0(3)
C1-C10	1.386(5)	C14-B1-C23	120.4(3)
C10-C9	1.392(7)	C23-B1-C17	122.5(3)
C4-C5	1.403(5)	C17-B1-C14	117.0(3)
C5-C6	1.391(7)		
C23-B1	1.574(5)		
C17-B1	1.573(7)		

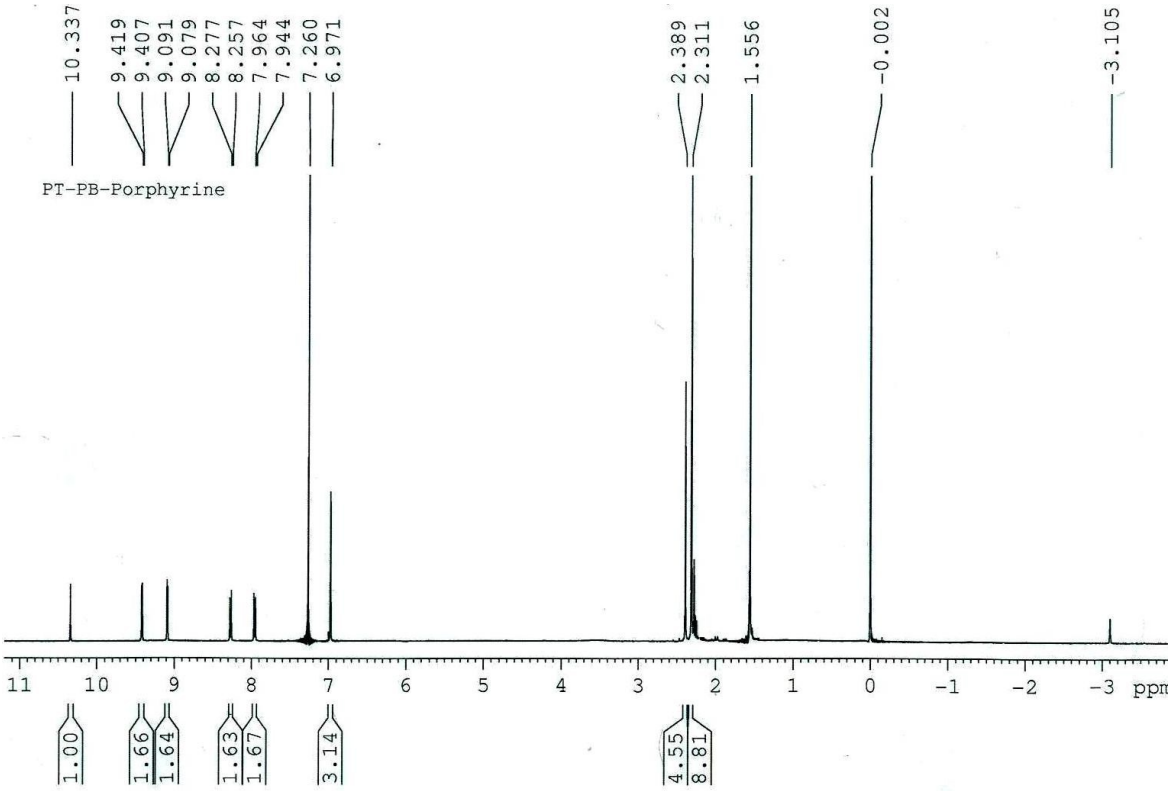


Figure S25: ^{1}H NMR of **1**

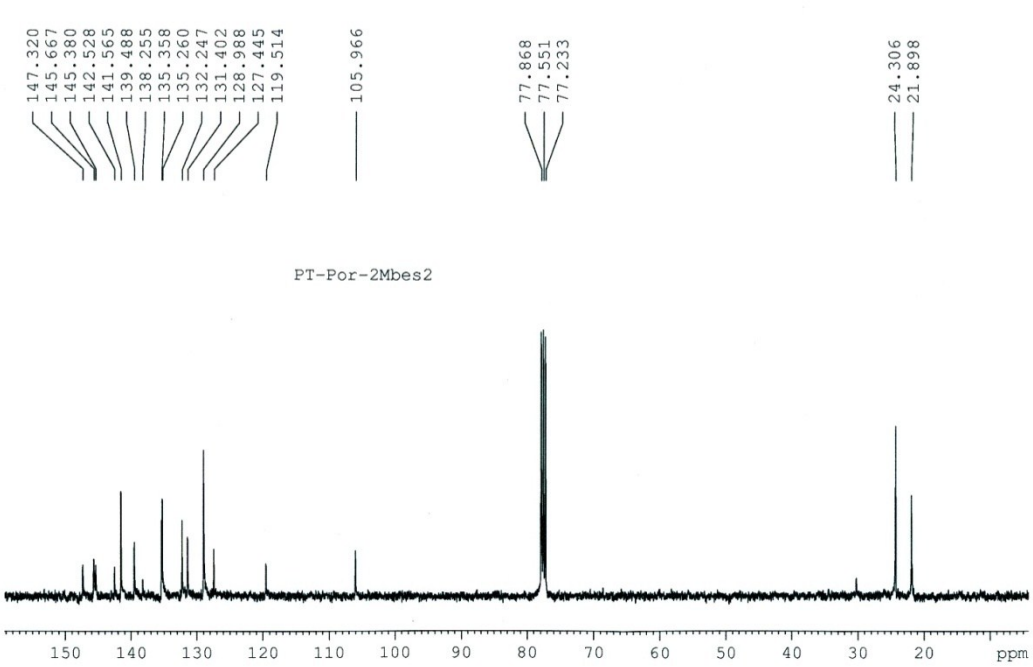


Figure S26: ^{13}C NMR of **1**

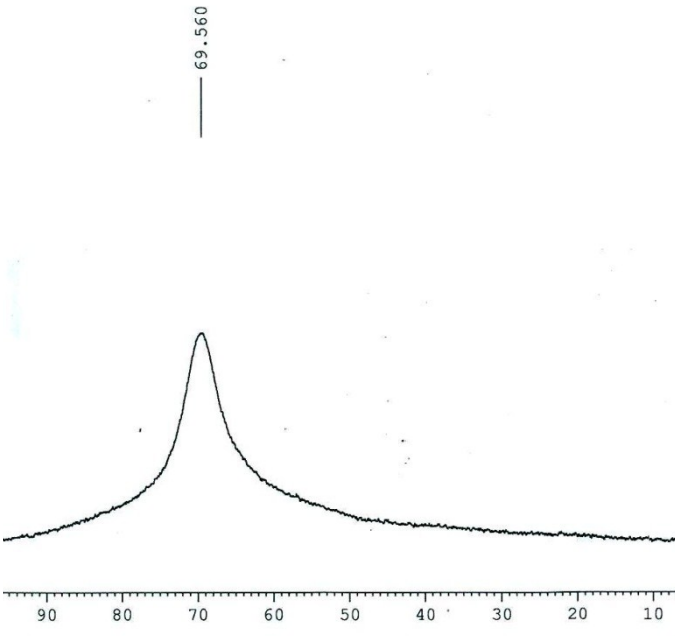


Figure S27: ^{11}B NMR of **1**

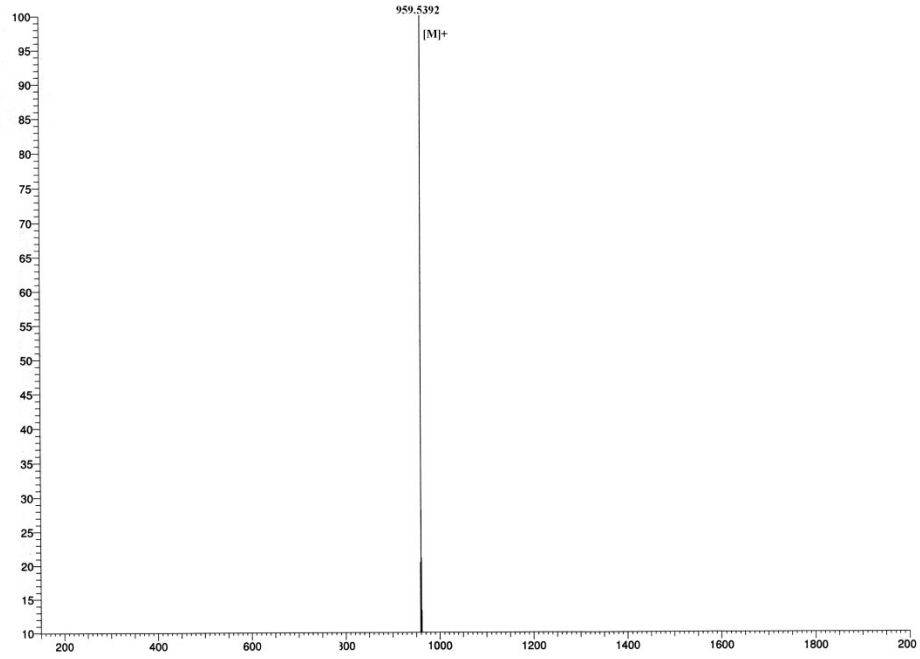


Figure S28: HRMS of **1**

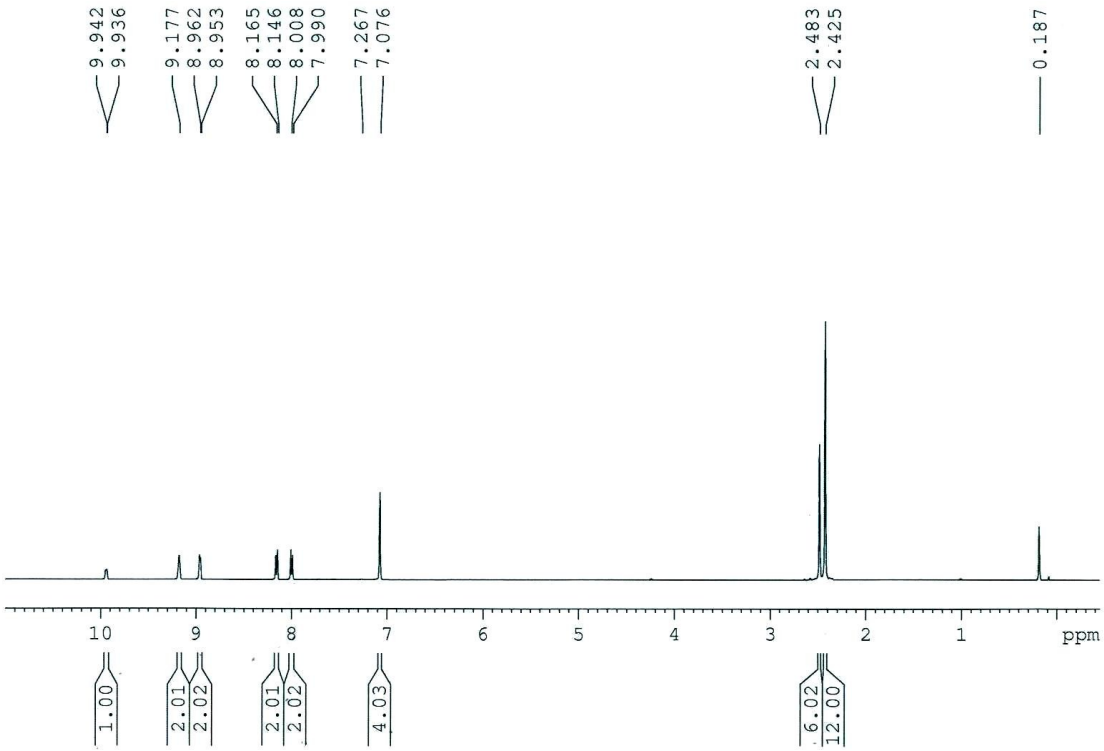


Figure S29: ^{1}H NMR of **2**

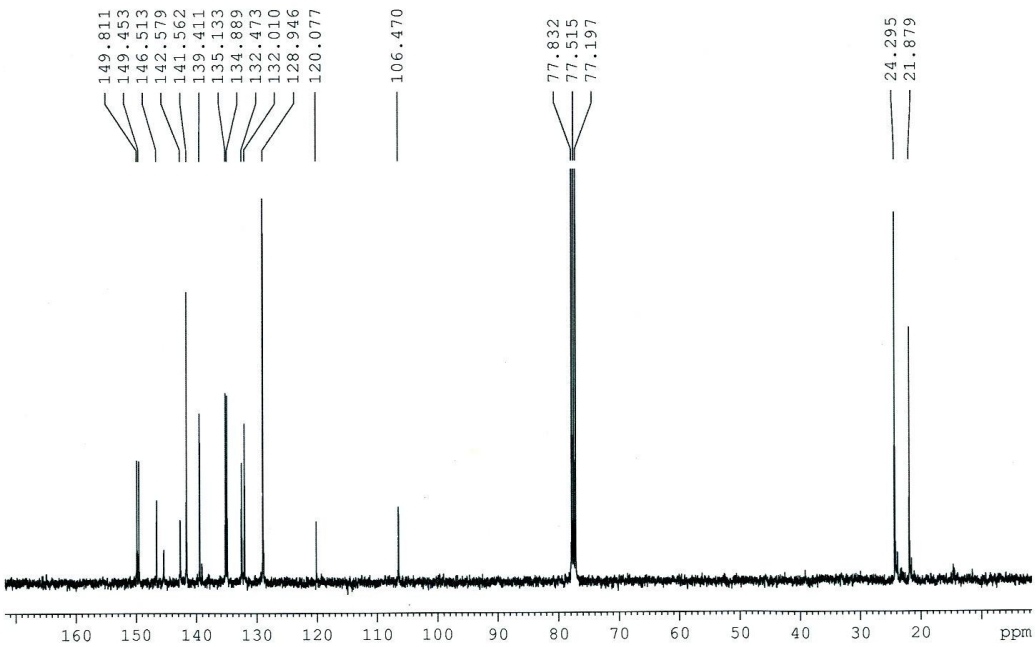


Figure S30: ^{13}C NMR of **2**

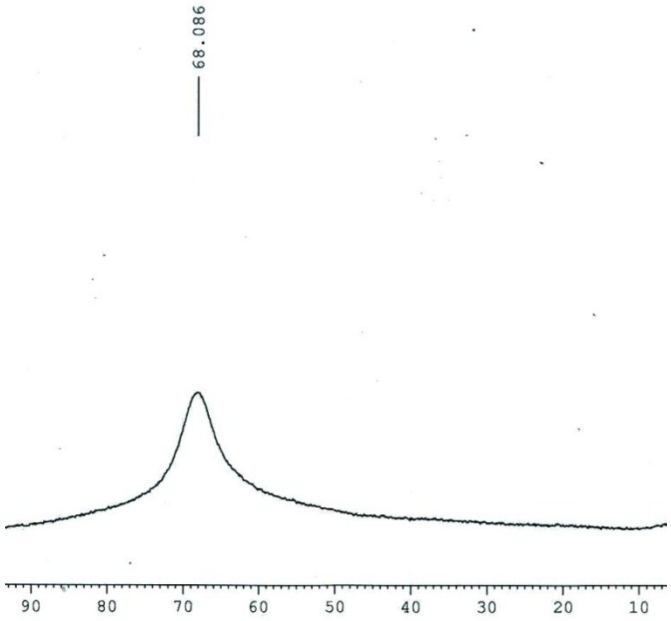


Figure S31: ^{11}B NMR of **2**

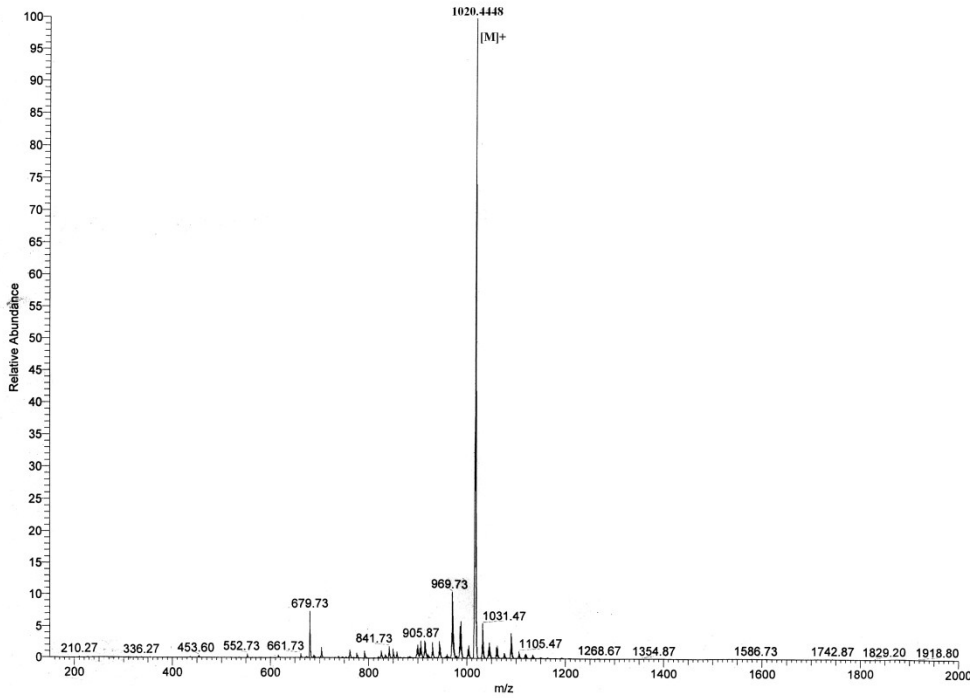


Figure S32: HRMS of **2**

DFT-computational data[2]

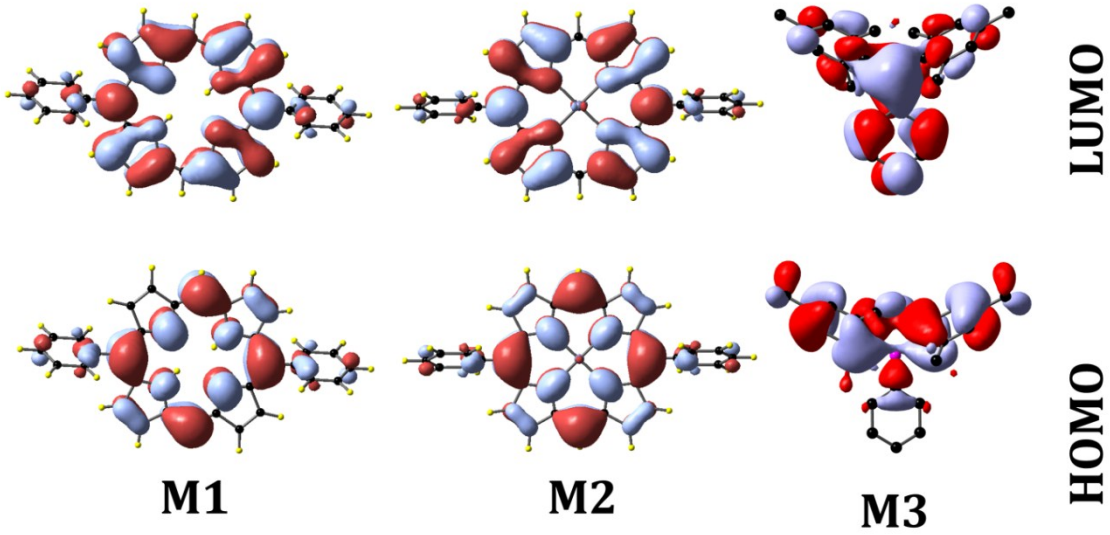


Figure S33: Molecular orbital diagrams of **M1**, **M2** and **M3**

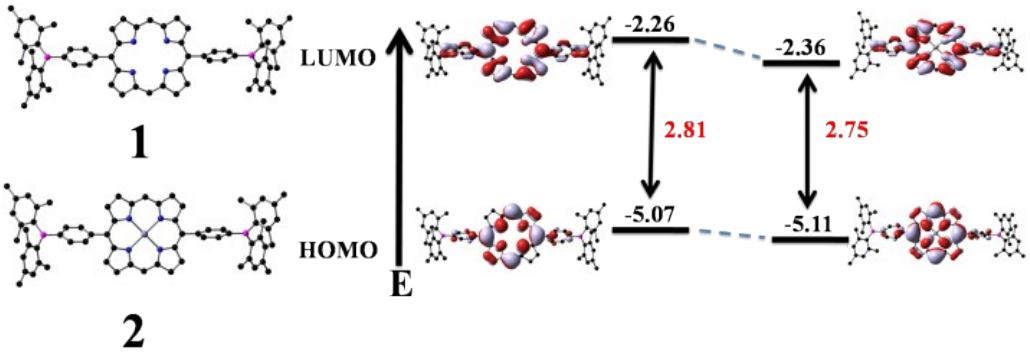


Figure S34: DFT B3LYP/6-31G(d) optimised structures of **1** and **2** and selected MOs of **1** and **2** (isovalue 0.02). Color code: C = Black, B = Magenta, N = Blue, Zn = Grey.

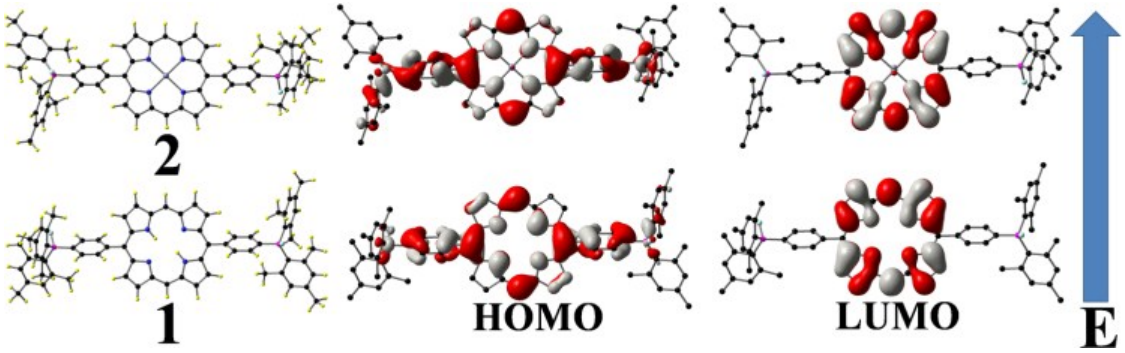
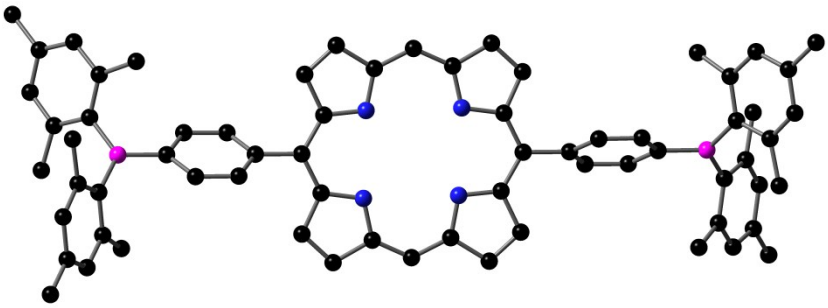


Figure S35: DFT B3LYP/6-31G(d) optimised structures of **1•2F**$^{2-}$ and **2•2F**$^{2-}$ and selected MOs of **1•2F**$^{2-}$ and **2•2F**$^{2-}$ (isovalue 0.02). Color code: C = Black, B = Magenta, N = Blue, Zn = Grey.

Table S5: Computational results of optimized structure of **1**

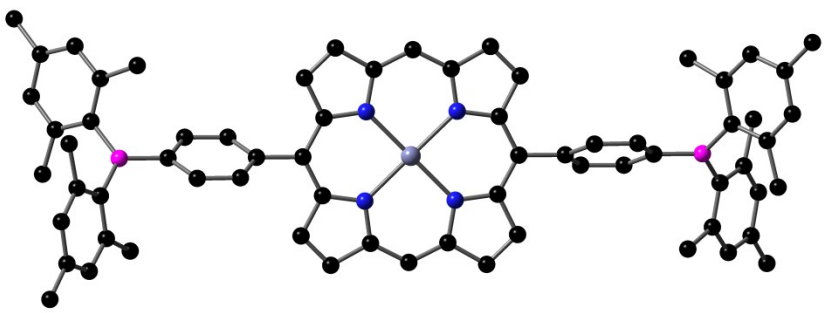


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.527955	-2.559318	0.079541
2	6	0	2.529336	-3.476036	0.081772
3	6	0	2.878514	-1.250124	0.021820
4	6	0	1.281423	-2.724248	0.037479
5	7	0	1.519154	-1.382730	0.004565
6	6	0	3.568672	-0.015910	0.019186
7	6	0	0.031017	-3.350867	0.035559
8	6	0	3.507880	2.544558	-0.026786
9	6	0	2.922242	1.233850	0.018215

10	6	0	2.489191	3.462054	-0.029547
11	6	0	1.244948	2.751073	0.001653
12	6	0	-0.028107	3.318177	-0.000479
13	7	0	-1.515993	1.349702	-0.017173
14	6	0	-2.875403	1.217166	-0.003777
15	6	0	-1.278445	2.691508	0.002924
16	6	0	-3.524919	2.526838	0.038406
17	6	0	-2.526435	3.443668	0.034991
18	6	0	-3.565763	-0.016946	0.003306
19	6	0	-1.242104	-2.783837	0.026017
20	6	0	-2.486291	-3.495136	-0.002543
21	6	0	-3.504984	-2.577677	-0.014272
22	6	0	-2.919486	-1.266587	0.018517
23	1	0	0.044506	-4.437445	0.043088
24	1	0	-0.041620	4.404772	-0.004570
25	1	0	4.593438	-2.734954	0.122299
26	1	0	2.609838	-4.555685	0.120497
27	1	0	4.569299	2.740816	-0.058866
28	1	0	2.572904	4.540506	-0.059548
29	1	0	-4.590501	2.702690	0.076393
30	1	0	-2.607100	4.523640	0.062743
31	1	0	-2.569920	-4.573858	-0.020753
32	1	0	-4.566317	-2.774177	-0.048434
33	6	0	5.061862	-0.016093	0.015413
34	6	0	5.781118	-0.567732	-1.058899
35	6	0	5.787032	0.540674	1.083092
36	6	0	7.173094	-0.570864	-1.055663
37	1	0	5.236902	-0.988509	-1.899853
38	6	0	7.178954	0.554521	1.067403
39	1	0	5.248038	0.955061	1.930731
40	6	0	7.917347	-0.004730	0.002129
41	1	0	7.702279	-1.011396	-1.896352
42	1	0	7.712440	0.998369	1.903631
43	6	0	-5.059081	-0.015431	-0.006164
44	6	0	-5.789153	-0.555938	1.066223
45	6	0	-5.773437	0.523272	-1.090553
46	6	0	-7.181317	-0.563364	1.047386
47	1	0	-5.254026	-0.962686	1.920001
48	6	0	-7.165439	0.533980	-1.089560
49	1	0	-5.225276	0.929307	-1.936202
50	6	0	-7.914493	-0.011429	-0.024743
51	1	0	-7.718801	-0.995221	1.887402
52	1	0	-7.691079	0.963576	-1.938643
53	5	0	9.490982	0.003385	-0.005841
54	6	0	10.254937	-1.044083	-0.918918
55	6	0	10.251681	1.059905	0.899863
56	6	0	10.063850	-2.442151	-0.779445
57	6	0	11.132165	-0.597796	-1.949818
58	6	0	10.044937	2.455733	0.760939
59	6	0	11.141379	0.623624	1.924286
60	6	0	10.719317	-3.335707	-1.639158
61	6	0	9.230358	-3.057183	0.328905
62	6	0	11.752424	-1.519084	-2.793689
63	6	0	11.391677	0.874517	-2.197898
64	6	0	10.697825	3.356836	1.614711
65	6	0	9.196250	3.061274	-0.341134
66	6	0	11.758719	1.552041	2.762526
67	6	0	11.417477	-0.845794	2.171477
68	1	0	10.561197	-4.404600	-1.502395
69	6	0	11.563409	-2.899318	-2.656128
70	1	0	8.609448	-3.874787	-0.055814
71	1	0	8.569638	-2.339152	0.816984
72	1	0	9.878439	-3.487848	1.104038
73	1	0	12.402898	-1.150618	-3.585437
74	1	0	12.101369	1.008973	-3.020439
75	1	0	11.803104	1.369629	-1.312755
76	1	0	10.474328	1.411475	-2.469247
77	1	0	10.527634	4.423945	1.478341
78	6	0	11.554444	2.930131	2.625324
79	1	0	8.569875	3.872570	0.048232
80	1	0	8.539455	2.335949	-0.823816
81	1	0	9.833509	3.498559	-1.121480
82	1	0	12.419070	1.190974	3.549486
83	1	0	12.136672	-0.972464	2.986962
84	1	0	11.824511	-1.338064	1.282738

85	1	0	10.508015	-1.391044	2.452671
86	6	0	12.257102	-3.871613	-3.580664
87	6	0	12.245580	3.910453	3.543298
88	1	0	11.981227	-4.906323	-3.353682
89	1	0	13.348608	-3.791212	-3.499434
90	1	0	12.000352	-3.678637	-4.629837
91	1	0	11.954401	4.941784	3.320010
92	1	0	13.337103	3.843918	3.450446
93	1	0	12.002453	3.713588	4.594971
94	5	0	-9.486847	-0.003756	-0.029886
95	6	0	-10.254563	-1.063233	0.866505
96	6	0	-10.244028	1.072810	-0.913180
97	6	0	-10.064635	-2.458541	0.699345
98	6	0	-11.132137	-0.636663	1.905503
99	6	0	-9.990421	2.460720	-0.762262
100	6	0	-11.194241	0.677455	-1.896920
101	6	0	-10.720161	-3.368738	1.540963
102	6	0	-9.234925	-3.050014	-0.424445
103	6	0	-11.754022	-1.574959	2.729855
104	6	0	-11.389001	0.830041	2.187681
105	6	0	-10.673557	3.393097	-1.554171
106	6	0	-9.007563	3.015663	0.254038
107	6	0	-11.831060	1.636956	-2.686007
108	6	0	-11.523749	-0.779652	-2.152622
109	1	0	-10.562731	-4.434811	1.382952
110	6	0	-11.565164	-2.952090	2.565665
111	1	0	-8.630025	-3.890555	-0.064430
112	1	0	-8.559805	-2.326732	-0.884672
113	1	0	-9.885368	-3.443548	-1.217320
114	1	0	-12.405541	-1.222021	3.527791
115	1	0	-12.137312	0.946359	2.978099
116	1	0	-11.748022	1.360906	1.301118
117	1	0	-10.480806	1.345737	2.525061
118	1	0	-10.479161	4.453598	-1.401585
119	6	0	-11.591026	3.005891	-2.528992
120	1	0	-8.008398	3.137726	-0.182343
121	1	0	-8.890512	2.375424	1.131279
122	1	0	-9.333485	4.002104	0.601867
123	1	0	-12.542318	1.307451	-3.441814
124	1	0	-12.270496	-0.873589	-2.947503
125	1	0	-11.919204	-1.270045	-1.257706
126	1	0	-10.640546	-1.349093	-2.466921
127	6	0	-12.261274	-3.942263	3.469232
128	6	0	-12.309258	4.021744	-3.385436
129	1	0	-11.973599	-4.971542	3.232327
130	1	0	-13.352437	-3.870592	3.375409
131	1	0	-12.019319	-3.760528	4.523842
132	1	0	-12.018059	5.043924	-3.123593
133	1	0	-13.397815	3.943776	-3.271236
134	1	0	-12.088854	3.873607	-4.450196
135	1	0	-0.904964	-0.667074	0.034998
136	1	0	0.907710	0.634497	0.032991
137	7	0	-1.556711	-1.447982	0.039108
138	7	0	1.559441	1.415430	0.030994

Table S6: Computational results of optimized structure of **2**

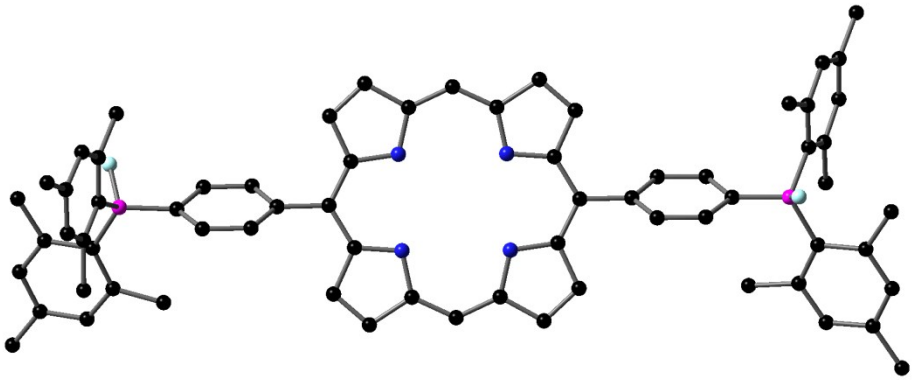


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.485438	-2.534126	0.039525
2	6	0	2.508197	-3.482633	0.035509
3	6	0	2.825885	-1.245181	-0.005267
4	6	0	1.247869	-2.784570	0.000242
5	7	0	1.461755	-1.427295	-0.023755
6	6	0	3.484297	-0.000031	0.000040
7	6	0	0.000052	-3.405120	0.000185
8	6	0	3.485397	2.534060	-0.039343
9	6	0	2.825858	1.245100	0.005372
10	6	0	2.508144	3.482552	-0.035279
11	7	0	1.461727	1.427195	0.023787
12	6	0	1.247824	2.784464	-0.000100
13	6	0	-0.000005	3.404990	-0.000017
14	7	0	-1.461698	1.427195	-0.023830
15	6	0	-2.825836	1.245049	-0.005289
16	6	0	-1.247837	2.784472	0.000104
17	6	0	-3.485397	2.533985	0.039462
18	6	0	-2.508169	3.482511	0.035370
19	6	0	-3.484246	-0.000096	0.000096
20	6	0	-1.247797	-2.784636	0.000090
21	6	0	-2.508115	-3.482699	-0.035074
22	7	0	-1.461692	-1.427361	0.023935
23	6	0	-3.485363	-2.534193	-0.039198
24	6	0	-2.825833	-1.245241	0.005489
25	1	0	0.000085	-4.491549	0.000248
26	1	0	0.000002	4.491418	0.000003
27	1	0	4.554301	-2.685651	0.078311
28	1	0	2.621760	-4.559120	0.064889
29	1	0	4.554258	2.685597	-0.078142
30	1	0	2.621690	4.559042	-0.064615
31	1	0	-4.554261	2.685497	0.078273
32	1	0	-2.621751	4.558997	0.064697
33	1	0	-2.621681	-4.559188	-0.064367
34	1	0	-4.554223	-2.685732	-0.078006
35	30	0	-0.000113	-0.000101	0.000421
36	6	0	4.980682	-0.000020	0.000032
37	6	0	5.702533	-0.492815	-1.100221
38	6	0	5.702556	0.492800	1.100259
39	6	0	7.094983	-0.503683	-1.090083
40	1	0	5.160510	-0.866128	-1.964915
41	6	0	7.095004	0.503692	1.090083
42	1	0	5.160551	0.866132	1.964956
43	6	0	7.835636	0.000005	-0.000008
44	1	0	7.626877	-0.900555	-1.951280
45	1	0	7.626919	0.900602	1.951250
46	6	0	-4.980635	-0.000085	0.000079
47	6	0	-5.702530	-0.492791	1.100344
48	6	0	-5.702462	0.492670	-1.100205
49	6	0	-7.094979	-0.503653	1.090152
50	1	0	-5.160542	-0.866064	1.965077
51	6	0	-7.094913	0.503583	-1.090076
52	1	0	-5.160422	0.865940	-1.964907
53	6	0	-7.835588	-0.000029	0.000017
54	1	0	-7.626910	-0.900474	1.951352
55	1	0	-7.626788	0.900439	-1.951293
56	5	0	9.406628	0.000021	-0.000024
57	6	0	10.169304	-1.066889	-0.890063
58	6	0	10.169294	1.066968	0.889999
59	6	0	9.920119	-2.456766	-0.737762
60	6	0	11.119778	-0.668927	-1.870614
61	6	0	9.920174	2.456859	0.737675
62	6	0	11.119811	0.668976	1.870477
63	6	0	10.606792	-3.387062	-1.526484
64	6	0	8.940439	-3.008978	0.282917
65	6	0	11.761394	-1.628662	-2.658244
66	6	0	11.451997	0.788043	-2.124891
67	6	0	10.606956	3.387131	1.526308
68	6	0	8.940466	3.009028	-0.282992
69	6	0	11.761533	1.628700	2.658054
70	6	0	11.452121	-0.787997	2.124632
71	1	0	10.419011	-4.448288	-1.370235
72	6	0	11.523090	-2.996740	-2.503233
73	1	0	7.926527	-3.074784	-0.130420
74	1	0	8.871480	-2.395198	1.184750
75	1	0	9.235187	-4.018644	0.588846

76	1	0	12.476543	-1.298375	-3.409833
77	1	0	12.214707	0.879904	-2.904703
78	1	0	11.826799	1.284815	-1.225041
79	1	0	10.575191	1.355066	-2.461662
80	1	0	10.419248	4.448364	1.370028
81	6	0	11.523307	2.996779	2.503011
82	1	0	7.926488	3.074448	0.130234
83	1	0	8.871803	2.395415	-1.184968
84	1	0	9.234955	4.018846	-0.588671
85	1	0	12.476692	1.298389	3.409622
86	1	0	12.214235	-0.879904	2.905019
87	1	0	11.827760	-1.284422	1.224933
88	1	0	10.575193	-1.355337	2.460520
89	6	0	12.221784	-4.013196	-3.374871
90	6	0	12.222134	4.013241	3.374538
91	1	0	12.265080	-4.994705	-2.891085
92	1	0	13.246542	-3.704308	-3.609506
93	1	0	11.697534	-4.144015	-4.331310
94	1	0	12.265914	4.994589	2.890469
95	1	0	13.246718	3.704052	3.609536
96	1	0	11.697673	4.144547	4.330797
97	5	0	-9.406586	0.000017	-0.000034
98	6	0	-10.169326	-1.066990	0.889828
99	6	0	-10.169166	1.067085	-0.889954
100	6	0	-9.920099	-2.456874	0.737520
101	6	0	-11.120080	-0.669072	1.870099
102	6	0	-9.919848	2.456936	-0.737562
103	6	0	-11.119763	0.669276	-1.870433
104	6	0	-10.606961	-3.387190	1.526022
105	6	0	-8.940227	-3.008992	-0.283024
106	6	0	-11.761887	-1.628847	2.657552
107	6	0	-11.452668	0.787872	2.124087
108	6	0	-10.606523	3.387340	-1.526133
109	6	0	-8.940030	3.008985	0.283074
110	6	0	-11.761385	1.629129	-2.657930
111	6	0	-11.452187	-0.787647	-2.124733
112	1	0	-10.419162	-4.448412	1.369777
113	6	0	-11.523517	-2.996901	2.502568
114	1	0	-7.926278	-3.074328	0.130296
115	1	0	-8.871515	-2.395386	-1.184994
116	1	0	-9.234625	-4.018833	-0.588705
117	1	0	-12.477234	-1.298585	3.408962
118	1	0	-12.214343	0.879739	2.904908
119	1	0	-11.829005	1.283944	1.224483
120	1	0	-10.575721	1.355585	2.459281
121	1	0	-10.418659	4.448542	-1.369819
122	6	0	-11.522958	2.997166	-2.502830
123	1	0	-7.926162	3.074815	-0.130383
124	1	0	-8.870956	2.395078	1.184802
125	1	0	-9.234712	4.018621	0.589164
126	1	0	-12.476627	1.298952	-3.409479
127	1	0	-12.214456	-0.879410	-2.904988
128	1	0	-11.827641	-1.284225	-1.225051
129	1	0	-10.575320	-1.354935	-2.460903
130	6	0	-12.222378	-4.013416	3.374004
131	6	0	-12.221629	4.013764	-3.374320
132	1	0	-12.265661	-4.994870	2.890100
133	1	0	-13.247153	-3.704505	3.608536
134	1	0	-11.698259	-4.144371	4.330494
135	1	0	-12.264728	4.995252	-2.890471
136	1	0	-13.246463	3.705031	-3.608833
137	1	0	-11.697491	4.144565	-4.330820

Table S7: Computational results of optimized structure of **1+2F^{2-}**



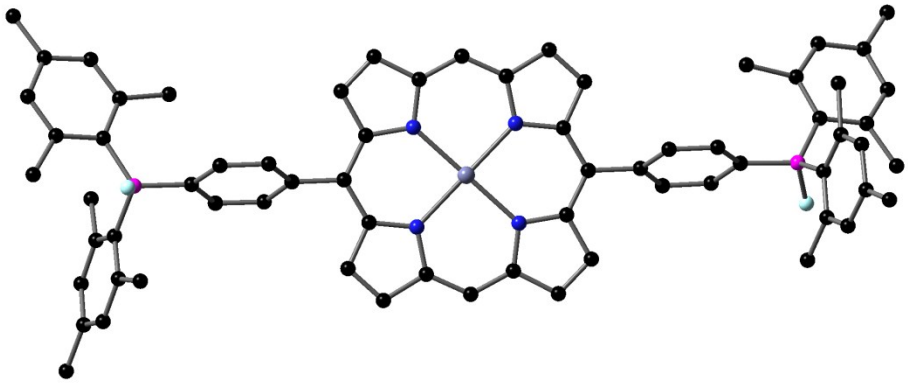
N	-1.53032194	1.57122834	-0.44033995
C	-2.91959217	-0.95344333	0.23593299
C	-1.34675906	-2.37591726	0.73080277
N	-1.56625427	-1.07363579	0.39507375
C	-1.17196051	2.86353373	-0.73283830
C	-2.90048935	1.42940952	-0.43544900
C	-3.59163483	0.23625667	-0.14001757
C	-0.10887859	-2.98270714	0.97172405
H	-0.14541139	-4.03862946	1.22891913
C	-3.58231867	-2.23398328	0.47124881
H	-4.64446523	-2.41317705	0.38638171
C	-2.39392470	3.58458998	-0.93710109
H	-2.44329317	4.63815766	-1.18119964
C	-2.60073605	-3.11554517	0.78855211
H	-2.69641791	-4.16920449	1.02451435
C	-3.44279516	2.72007149	-0.74954594
H	-4.49902821	2.93689196	-0.80753985
N	1.53736898	-1.15894397	0.60996228
C	2.92756424	1.36165013	-0.07956817
C	7.96173371	0.05386950	0.50199970
C	5.88276780	0.45678236	-0.74913748
H	5.39735854	0.71859218	-1.68710994
C	7.14779152	-0.21460582	1.62059146
H	7.63386824	-0.44489716	2.56524895
C	5.75482243	-0.18145870	1.56270588
H	5.16743437	-0.38911954	2.45531537
C	1.35418231	2.78787705	-0.56145701
N	1.57323915	1.48498838	-0.22795293
C	1.17874126	-2.44961816	0.90933619
C	2.90764207	-1.01887324	0.59929291
C	5.08818836	0.14914672	0.36887300
C	3.59930813	0.17125352	0.29353913
C	7.27563059	0.41372502	-0.67276893
H	7.84871902	0.67198472	-1.56138222
C	0.11582745	3.39665354	-0.79498593
H	0.15227060	4.45331210	-1.04914862
C	3.59181892	2.64032331	-0.32101045

H	4.65540174	2.81646069	-0.24687604
C	2.40051981	-3.17059035	1.11491468
H	2.44962539	-4.22288743	1.36447754
C	2.60961894	3.52460624	-0.62873614
H	2.70608385	4.57794604	-0.86575079
C	3.44954953	-2.30819810	0.91929571
H	4.50567981	-2.52584971	0.97485278
C	-5.07928204	0.25044826	-0.23229334
C	-5.73411435	0.60504271	-1.42577826
C	-5.88538802	-0.06960999	0.87412869
C	-7.12644314	0.62057951	-1.50267089
H	-5.13786748	0.85357996	-2.30183505
C	-7.27741746	-0.04433012	0.77893028
H	-5.40952401	-0.31160751	1.82226233
C	-7.95229975	0.27828431	-0.41313079
H	-7.60193265	0.90927818	-2.43661767
H	-7.85884747	-0.26641035	1.67181621
B	9.60640527	0.01690041	0.66892404
C	10.24303868	1.22367756	-0.30148185
C	10.24563879	2.57432169	0.15801129
C	10.73181283	1.01832771	-1.62021697
C	10.75488532	3.61070146	-0.63581903
C	11.22906190	2.08209860	-2.39054410
C	11.26756383	3.38970846	-1.91410460
H	10.73620299	4.62845279	-0.24324377
H	11.59181555	1.87544985	-3.39842070
C	10.36466536	-1.47127782	0.51783004
C	9.78813125	-2.68872098	0.06896922
C	11.72046007	-1.55648510	0.96095040
C	10.52558621	-3.88596360	0.05861296
C	12.42761519	-2.76409892	0.92848783
C	11.84962224	-3.95233628	0.47939657
H	10.04015869	-4.79614647	-0.29555380
H	13.46388723	-2.77430549	1.27015561
C	-10.38847183	-0.95401653	-1.22734737
C	-9.84164806	-2.23906466	-1.48553931
C	-11.74315209	-0.76446128	-1.64036148
C	-10.60593590	-3.24820310	-2.09743691
C	-12.47650593	-1.79419716	-2.24186883
C	-11.92849590	-3.05474503	-2.48228097
H	-10.14320701	-4.21937744	-2.27608036
H	-13.50958740	-1.60113105	-2.53519585
C	-10.22057966	0.91544942	0.87438882
C	-10.18965057	2.30744906	1.18530702
C	-10.73355562	0.06559321	1.89144502
C	-10.69206452	2.79139554	2.40026973
C	-11.22426951	0.58515744	3.10059279
C	-11.23059032	1.95005436	3.37413573
H	-10.64795966	3.86394024	2.59532570
H	-11.60778104	-0.10653821	3.85191702

C	-8.41892406	-2.63502032	-1.12909280
H	-8.25249935	-3.69515691	-1.35698382
H	-7.67622766	-2.05265952	-1.68214005
H	-8.19354578	-2.48500759	-0.06851846
C	-12.47063984	0.55622708	-1.46115303
H	-11.99801994	1.34417606	-2.05153598
H	-13.52145356	0.46247408	-1.76364515
H	-12.44302647	0.89502231	-0.42078902
C	-12.74292323	-4.16195489	-3.11258059
H	-12.10134588	-4.98013063	-3.46097229
H	-13.46615163	-4.59517086	-2.40570487
H	-13.32077431	-3.80137275	-3.97396455
C	-10.78246530	-1.44699680	1.75557088
H	-11.55528914	-1.77354773	1.05225457
H	-9.83853554	-1.86169391	1.39148254
H	-10.99557117	-1.90841472	2.72839295
C	-11.79722718	2.49846037	4.66423282
H	-12.82940323	2.85913982	4.54010741
H	-11.81631641	1.73380287	5.45033167
H	-11.20768589	3.34618900	5.03620419
C	-9.59281881	3.34568354	0.25020833
H	-8.60063247	3.04749163	-0.09998203
H	-10.20007960	3.48552807	-0.64771750
H	-9.50185414	4.31025077	0.76642295
C	12.47743453	-0.35569705	1.50062261
H	13.53888170	-0.59908368	1.63773800
H	12.40605180	0.50461304	0.82888035
H	12.06174924	-0.03090739	2.45764791
C	8.35990985	-2.80701399	-0.43459432
H	8.17287363	-3.82112702	-0.80898449
H	7.62711731	-2.59843960	0.35101166
H	8.13904698	-2.10796977	-1.24675569
C	12.63253559	-5.24535489	0.43958762
H	11.98216918	-6.09660007	0.20587140
H	13.42645101	-5.22226852	-0.32119179
H	13.12255663	-5.45552406	1.40010582
C	9.68052226	2.98458167	1.50716689
H	8.67776768	2.57710518	1.66407766
H	10.28953590	2.61398072	2.33542800
H	9.62256238	4.07870380	1.57521840
C	10.74747097	-0.34469440	-2.29150293
H	11.51098621	-1.00482899	-1.86762259
H	9.79392087	-0.86977687	-2.18857450
H	10.95336955	-0.23696047	-3.36417843
C	11.84282845	4.51765817	-2.74042452
H	11.29866786	5.45644631	-2.57646613
H	12.89711156	4.71327546	-2.49301563
H	11.80207508	4.29026271	-3.81275061
F	-9.79220665	1.40352718	-1.59809865
B	-9.59477295	0.37454832	-0.58045096

F	9.83504064	0.35758567	2.07018050
H	0.91881824	-0.38621256	0.37242205
H	-0.91160340	0.79811610	-0.20453667

Table S8: Computational results of optimized structure of **2**+**2F**$^{2-}$



N	-1.42169192	1.60460549	-0.36159073
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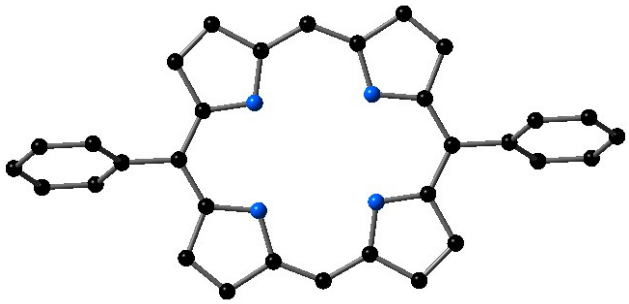
C	-1.32944437	-2.45535419	0.74995409
N	-1.50747229	-1.13257290	0.42119616
C	-1.16858716	2.92249008	-0.65928577
C	-2.79234294	1.45575863	-0.36662668
C	-3.49602609	0.26434349	-0.09338716
C	-0.09935485	-3.07467163	0.96644295
H	-0.12930464	-4.13216547	1.21647277
C	-3.55378555	-2.19609781	0.49808440
H	-4.62247283	-2.33317264	0.42244301
C	-2.40888880	3.62890057	-0.85606838
H	-2.49215804	4.68263681	-1.09382574
C	-2.60444994	-3.12392999	0.80653841
H	-2.74584674	-4.17301740	1.03723847
C	-3.41386182	2.72744039	-0.66916535
H	-4.47985626	2.89506304	-0.71859219
N	1.42054525	-1.18063588	0.57040035
C	2.86353902	1.36755651	-0.06057368
C	7.86269062	0.03809555	0.49039714
C	5.78332323	0.38966087	-0.77552726
H	5.29799932	0.61875460	-1.72236407
C	7.04841135	-0.18983601	1.61757011
H	7.53411526	-0.38628634	2.56998343
C	5.65495917	-0.15842963	1.55827072
H	5.06685845	-0.33768517	2.45660473
C	1.32685507	2.88356221	-0.52364278
N	1.50567102	1.55812897	-0.20614237
C	1.16628125	-2.49722245	0.87304381
C	2.79182820	-1.03705838	0.55718941
C	4.98936554	0.12542056	0.35314047
C	3.49632448	0.15351992	0.27967398
C	7.17659374	0.35188454	-0.69739155
H	7.74923385	0.57870642	-1.59485117
C	0.09651196	3.50311927	-0.73965218

H	0.12636530	4.56183638	-0.98448379
C	3.55243207	2.62061997	-0.28506397
H	4.62170861	2.75661971	-0.21516525
C	2.40592430	-3.20834989	1.05412726
H	2.48829271	-4.26223921	1.29146832
C	2.60191755	3.55213637	-0.57885259
H	2.74308068	4.60308281	-0.80103408
C	3.41181617	-2.31169663	0.85045613
H	4.47731857	-2.48548258	0.88242095
C	-4.98762441	0.28073126	-0.19861670
C	-5.62624786	0.53871605	-1.42386363
C	-5.80506818	0.04471821	0.91916141
C	-7.01789708	0.53769852	-1.52034461
H	-5.01823864	0.72932898	-2.30645922
C	-7.19652917	0.05289258	0.80432505
H	-5.33989502	-0.12650943	1.88820824
C	-7.85590567	0.27271424	-0.41887409
H	-7.48275575	0.74904707	-2.48002516
H	-7.78963368	-0.10621217	1.70308591
B	9.50760629	0.01247140	0.65914353
C	10.13473208	1.20541664	-0.33452805
C	10.12721501	2.56461661	0.09930684
C	10.62348447	0.97902476	-1.64979446
C	10.62732000	3.58979935	-0.71446329
C	11.11142717	2.03209259	-2.44064295
C	11.14029141	3.34869741	-1.98901831
H	10.60125490	4.61459394	-0.34106246
H	11.47489442	1.80950317	-3.44484836
C	10.27847842	-1.47195166	0.53495289
C	9.70896406	-2.70483699	0.11678537
C	11.63591189	-1.53669156	0.97265388
C	10.45539233	-3.89545577	0.12789091
C	12.35289393	-2.73996124	0.96282925
C	11.78358055	-3.94123872	0.54106196
H	9.97426411	-4.81739398	-0.20109017
H	13.39007991	-2.73552366	1.30152526
C	-10.24112206	-1.07098062	-1.18950707
C	-9.66240514	-2.36028828	-1.32616788
C	-11.58205567	-0.94196644	-1.66649654
C	-10.38185468	-3.42748036	-1.89290853
C	-12.27061269	-2.02766657	-2.22000960
C	-11.68879506	-3.28996569	-2.34797581
H	-9.89554359	-4.40018037	-1.97577586
H	-13.29541905	-1.87845080	-2.56406435
C	-10.16618124	0.95122752	0.77769347
C	-10.15582244	2.36210987	0.99119126
C	-10.69902019	0.16966078	1.83836861
C	-10.69239558	2.92502731	2.15638245
C	-11.22351295	0.76779192	2.99609198
C	-11.24716405	2.14821716	3.17378779

H	-10.66280981	4.00905724	2.27596360
H	-11.62107191	0.12660890	3.78401428
C	-8.25305891	-2.70155495	-0.87332993
H	-8.06853681	-3.77690054	-0.98852574
H	-7.49177208	-2.16673622	-1.44913852
H	-8.07665312	-2.44468793	0.17554221
C	-12.34338229	0.37073451	-1.60752473
H	-11.88905256	1.11506028	-2.26534041
H	-13.38997323	0.22288869	-1.90328110
H	-12.32924341	0.80232956	-0.60198005
C	-12.45075108	-4.45354381	-2.94125130
H	-11.80470377	-5.33118995	-3.06178448
H	-13.29870010	-4.75529116	-2.30926458
H	-12.86560938	-4.20923378	-3.92889951
C	-10.73612694	-1.34895217	1.80714452
H	-11.47367424	-1.72939639	1.09328102
H	-9.77459664	-1.78235374	1.51796024
H	-10.99274494	-1.74261142	2.79905199
C	-11.84975115	2.77904465	4.40872591
H	-12.87889914	3.12679561	4.23320053
H	-11.88861313	2.06810641	5.24304828
H	-11.27237151	3.65187842	4.73959157
C	-9.54704730	3.33784199	-0.00132199
H	-8.53842933	3.03391813	-0.29590542
H	-10.12694714	3.39454522	-0.92565293
H	-9.48972687	4.34078986	0.44129728
C	12.38576060	-0.31947960	1.48483229
H	13.44800725	-0.55424349	1.63057330
H	12.31236488	0.52363603	0.79170669
H	11.96582581	0.02693954	2.43233228
C	8.27728702	-2.84503760	-0.37049263
H	8.09185188	-3.87064506	-0.71295129
H	7.55050795	-2.61616785	0.41505093
H	8.04657103	-2.17115286	-1.20094393
C	12.58082619	-5.22571356	0.50840597
H	11.92782612	-6.10466860	0.57335474
H	13.16352749	-5.32631184	-0.41967276
H	13.29586260	-5.27783323	1.33940749
C	9.55990567	2.99548872	1.44107990
H	8.55783521	2.58810893	1.60336575
H	10.16866954	2.63933280	2.27568137
H	9.49915602	4.09044745	1.49127898
C	10.64994683	-0.39633918	-2.29561279
H	11.42008298	-1.04170922	-1.86104516
H	9.70144069	-0.92835085	-2.18136810
H	10.85312015	-0.30666629	-3.37049074
C	11.70604936	4.46530214	-2.83704931
H	11.15245005	5.40189660	-2.69316959
H	12.75787460	4.67634481	-2.59182932
H	11.66958339	4.21585510	-3.90461496

F	-9.69653104	1.26675353	-1.71591478
B	-9.49619935	0.32108047	-0.62092025
F	9.73476272	0.38069250	2.05374913
Zn	-0.00077439	0.21234527	0.10598050

Table S9: Computational results of optimized structure of **M1**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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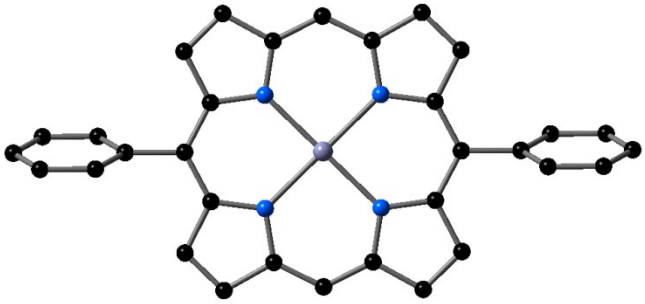
3	6	0	5.787249	0.571438	1.057474
4	1	0	5.249545	1.008021	1.894477
5	6	0	7.167880	-0.579335	-1.072688
6	1	0	7.700241	-1.024893	-1.908976
7	6	0	5.772899	-0.579694	-1.063282
8	1	0	5.223341	-1.018975	-1.890938
9	6	0	1.245654	2.765732	-0.090801
10	7	0	1.558208	1.431930	-0.006254
11	6	0	1.277593	-2.707745	0.104476
12	6	0	2.875080	-1.234916	0.048864
13	6	0	5.060901	-0.004687	0.002317
14	6	0	3.566491	-0.002365	0.009748
15	6	0	7.182468	0.571792	1.048052
16	1	0	7.726031	1.016633	1.877507
17	6	0	-0.026745	3.333257	-0.126823
18	1	0	-0.039211	4.417778	-0.194392
19	6	0	3.507978	2.553571	-0.128988
20	1	0	4.569418	2.745532	-0.181131
21	6	0	2.525004	-3.457410	0.185213
22	1	0	2.604862	-4.534961	0.264092
23	6	0	2.490820	3.472355	-0.160737
24	1	0	2.575951	4.548366	-0.238145
25	6	0	3.523815	-2.541254	0.156484
26	1	0	4.588980	-2.714461	0.214871
27	7	0	-1.515686	1.368379	-0.024263
28	6	0	-2.920747	-1.246881	0.027936
29	6	0	-7.877543	0.003540	0.017178
30	6	0	-5.787272	-0.571363	-1.057538
31	1	0	-5.249587	-1.007914	-1.894570
32	6	0	-7.167854	0.579347	1.072693
33	1	0	-7.700197	1.024882	1.909004
34	6	0	-5.772873	0.579671	1.063274
35	1	0	-5.223295	1.018909	1.890938
36	6	0	-1.245647	-2.765736	0.090737
37	7	0	-1.558226	-1.431951	0.006101
38	6	0	-1.277585	2.707723	-0.104412
39	6	0	-2.875072	1.234884	-0.048833
40	6	0	-5.060903	0.004688	-0.002357
41	6	0	-3.566492	0.002341	-0.009809
42	6	0	-7.182492	-0.571685	-1.048100
43	1	0	-7.726076	-1.016470	-1.877571
44	6	0	0.026745	-3.333268	0.126802
45	1	0	0.039195	-4.417790	0.194368
46	6	0	-3.507987	-2.553617	0.128866
47	1	0	-4.569426	-2.745589	0.180985
48	6	0	-2.525001	3.457387	-0.185019
49	1	0	-2.604862	4.534939	-0.263875
50	6	0	-2.490813	-3.472377	0.160655

51	*1*	*0*	*-2.575923*	*-4.548389*	*0.238070*
52	*6*	*0*	*-3.523810*	*2.541231*	*-0.156265*
53	*1*	*0*	*-4.588979*	*2.714436*	*-0.214600*
54	*1*	*0*	*-8.964222*	*0.003479*	*0.024672*
55	*6*	*0*	*7.877545*	*-0.003467*	*-0.017191*
56	*1*	*0*	*8.964224*	*-0.003379*	*-0.024673*
57	*1*	*0*	*-0.904698*	*-0.653851*	*-0.035545*
58	*1*	*0*	*0.904596*	*0.653909*	*0.035288*

Table S10: Computational results of optimized structure of **M2**



Atomic Type	Coordinates (Angstroms) X	Y	Z
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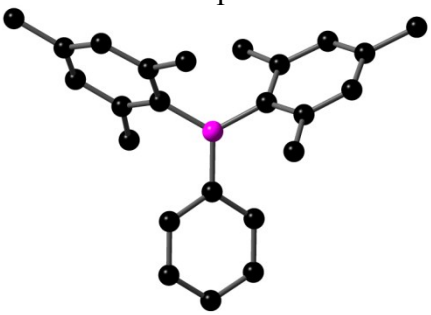
C	5.69930147	-0.49578086	-1.09970518
H	5.15518599	-0.87524005	-1.96019082
C	7.09480490	0.49556495	1.09996601
H	7.63281020	0.87891955	1.96308171
C	5.69939889	0.49572337	1.09956149
H	5.15529916	0.87504459	1.96010438
C	1.24785637	-2.78356031	0.09016419
N	1.46098142	-1.42770566	0.02267714
C	1.24780587	2.78356164	-0.08970642
C	2.82514254	1.24411551	-0.03705013
C	4.98106204	-0.00001980	-0.00003919
C	3.48333536	0.00000725	0.00009584
C	7.09464985	-0.49545403	-1.10024717
H	7.63274358	-0.87879522	-1.96329555
C	0.00003426	-3.40394080	0.11397421
H	0.00003389	-4.48902528	0.16879669
C	3.48567649	-2.53028258	0.12376295
H	4.55490876	-2.67886695	0.16771557
C	2.50880561	3.47913861	-0.14980164
H	2.62297180	4.55412549	-0.21401539
C	2.50888527	-3.47909801	0.15040742
H	2.62309003	-4.55406052	0.21495580
C	3.48564003	2.53036740	-0.12323009
H	4.55485541	2.67903580	-0.16715783
Zn	-0.00000664	-0.00002453	-0.00003606
N	-1.46095430	-1.42771728	0.02242682
C	-2.82515405	1.24406588	-0.03727882
C	-7.79704824	0.00011667	0.00027730
C	-5.69923569	0.49570906	1.09976844
H	-5.15503761	0.87498657	1.96027503
C	-7.09486025	-0.49540516	-1.09991988
H	-7.63299726	-0.87870445	-1.96299963
C	-5.69947308	-0.49571944	-1.09955647
H	-5.15545897	-0.87506924	-1.96014956
C	-1.24784952	2.78352874	-0.09016048
N	-1.46100266	1.42766927	-0.02270902
C	-1.24779258	-2.78359616	0.08969575
C	-2.82511210	-1.24413298	0.03701313
C	-4.98107579	-0.00003409	0.00004143
C	-3.48334601	-0.00004673	-0.00008539
C	-7.09462323	0.49554701	1.10036599
H	-7.63257540	0.87888765	1.96354436
C	-0.00002714	3.40389733	-0.11398104

H	-0.00002832	4.48898136	-0.16882636
C	-3.48567499	2.53029008	-0.12374174
H	-4.55489641	2.67892202	-0.16766727
C	-2.50880050	-3.47916214	0.14981297
H	-2.62297791	-4.55414607	0.21405688
C	-2.50886127	3.47907706	-0.15049012
H	-2.62304583	4.55403789	-0.21510557
C	-3.48562100	-2.53037751	0.12324316
H	-4.55483968	-2.67902394	0.16722675
H	-8.88377918	0.00023113	0.00034161
C	7.79705422	0.00012948	-0.00019957
H	8.88377548	0.00006525	-0.00046436

Table S11: Computational results of optimized structure of **M3**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	*6*	*0*	*-0.029212*	*4.775898*	*0.011141*
2	*6*	*0*	*1.058507*	*4.084881*	*0.551691*
3	*6*	*0*	*-1.107550*	*4.066585*	*-0.523392*
4	*6*	*0*	*1.070279*	*2.691219*	*0.540605*
5	*1*	*0*	*1.896651*	*4.633826*	*0.973762*
6	*6*	*0*	*-1.100029*	*2.672804*	*-0.504694*
7	*1*	*0*	*-1.954600*	*4.601204*	*-0.946034*
8	*6*	*0*	*-0.008763*	*1.945333*	*0.017935*
9	*1*	*0*	*1.926676*	*2.161609*	*0.950434*
10	*1*	*0*	*-1.951165*	*2.129564*	*-0.906623*
11	*5*	*0*	*0.003114*	*0.373214*	*0.019419*
12	*6*	*0*	*1.395568*	*-0.383418*	*0.071958*
13	*6*	*0*	*-1.380603*	*-0.399406*	*-0.047709*
14	*6*	*0*	*1.677694*	*-1.326808*	*1.098881*
15	*6*	*0*	*2.408847*	*-0.133131*	*-0.890320*
16	*6*	*0*	*-2.389146*	*-0.206621*	*0.930087*
17	*6*	*0*	*-1.667846*	*-1.287009*	*-1.125326*
18	*6*	*0*	*2.920134*	*-1.963323*	*1.148709*
19	*6*	*0*	*0.674120*	*-1.649900*	*2.187976*
20	*6*	*0*	*3.629633*	*-0.816024*	*-0.822286*
21	*6*	*0*	*2.235371*	*0.851675*	*-2.033372*
22	*6*	*0*	*-3.620011*	*-0.869272*	*0.818385*
23	*6*	*0*	*-2.182820*	*0.634194*	*2.175934*
24	*6*	*0*	*-2.910818*	*-1.915559*	*-1.206889*
25	*6*	*0*	*-0.669970*	*-1.549389*	*-2.235339*
26	*6*	*0*	*3.911637*	*-1.731276*	*0.191175*
27	*1*	*0*	*3.117633*	*-2.667100*	*1.955705*
28	*1*	*0*	*-0.248822*	*-2.071435*	*1.777396*
29	*1*	*0*	*1.090447*	*-2.374505*	*2.895195*
30	*1*	*0*	*0.391563*	*-0.759517*	*2.762494*
31	*1*	*0*	*4.382285*	*-0.621665*	*-1.584978*
32	*1*	*0*	*2.555468*	*1.860056*	*-1.744412*
33	*1*	*0*	*2.842470*	*0.549516*	*-2.893791*
34	*1*	*0*	*1.199730*	*0.938029*	*-2.370938*
35	*6*	*0*	*-3.907205*	*-1.723177*	*-0.242703*
36	*1*	*0*	*-4.371725*	*-0.710096*	*1.590372*
37	*1*	*0*	*-2.035474*	*-0.009487*	*3.053757*
38	*1*	*0*	*-1.319463*	*1.297482*	*2.106967*
39	*1*	*0*	*-3.063519*	*1.254064*	*2.380981*
40	*1*	*0*	*-3.109941*	*-2.576207*	*-2.049389*
41	*1*	*0*	*-0.459700*	*-0.643160*	*-2.817584*
42	*1*	*0*	*0.287463*	*-1.909888*	*-1.847800*
43	*1*	*0*	*-1.056257*	*-2.298418*	*-2.934047*
44	*6*	*0*	*5.229467*	*-2.467643*	*0.241494*

45	*6*	*0*	*-5.243407*	*-2.417651*	*-0.359621*
46	*1*	*0*	*5.125566*	*-3.496551*	*-0.128521*
47	*1*	*0*	*5.988429*	*-1.973571*	*-0.373973*
48	*1*	*0*	*5.613564*	*-2.533044*	*1.266026*
49	*1*	*0*	*-5.123530*	*-3.504534*	*-0.448425*
50	*1*	*0*	*-5.874587*	*-2.220053*	*0.512687*
51	*1*	*0*	*-5.791369*	*-2.083248*	*-1.250014*
52	*1*	*0*	*-0.036624*	*5.863168*	*0.007735*

References:

(1) (a) X. Y.Liu, D. R.Bai, S.Wang, *Angew. Chem., Int. Ed.*2006, **45**, 5475. (b) Y.Sun, N.Ross, S.-B.Zhao, K.Huszarik, W.-L.Jia, R.-Y.Wang, D.Macartney, S.Wang, *J. Am. Chem. Soc.* 2007, **129**, 7510.

2. (a) A. D.Becke, *J. Chem. Phys.,* 1993, **98**, 5648. (b) M. J.Frisch, G. W.Trucks, H. B.Schlegel, G. E.Scuseria, M. A.Robb, J. R.Cheeseman, G.Scalmani, V.Barone, B.Mennucci, G. A.Petersson, H.Nakatsuji, M.Caricato, X.Li, H. P.Hratchian, A. F.Izmaylov, J.Bloino, G.Zheng, J. L.Sonnenberg, M.Hada, M.Ehara, K.Toyota, R.Fukuda, J.Hasegawa, M.Ishida, T.Nakajima, Y.Honda, O.Kitao, H.Nakai, T.Vreven, J. A.Montgomery, Jr., J. E.Peralta, F.Ogliaro, M.Bearpark, J. J.Heyd, E.Brothers, K. N.Kudin, V. N.Staroverov, R.Kobayashi, J.Normand, K.Raghavachari, A.Rendell, J. C.Burant, S. S.Iyengar, J.Tomasi, M.Cossi, N.Rega, J. M.Millam, M.Klene, J. E.Knox, J. B.Cross, V.Bakken, C.Adamo, J.Jaramillo, R.Gomperts, R. E.Stratmann, O.Yazyev, A. J.Austin, R.Cammi, C.Pomelli, J. W.Ochterski, R. L.Martin, K.Morokuma, V. G.Zakrzewski, G. A.Voth, P.Salvador, J. J.Dannenberg, S.Dapprich, A. D.Daniels, O.Farkas, J. B.Foresman, J. V.Ortiz, J.Cioslowski, D. J.Fox, GAUSSIAN 09 (Revision A.02), Gaussian, Inc., Wallingford, CT, 2009. (c) A. D.Becke, *Phys. Rev. A: At., Mol., Opt. Phys.,* 1988, **38**, 3098. (d) C.Lee, W.Yang, R. G.Parr, *Phys. Rev. B*., 1988, **37**, 785.