Supplementary Material (ESI) for Chemical Communications

Supplementary information

Cation recognition and pseudorotaxane formation of tris-dipyrrin BF_2 macrocycles

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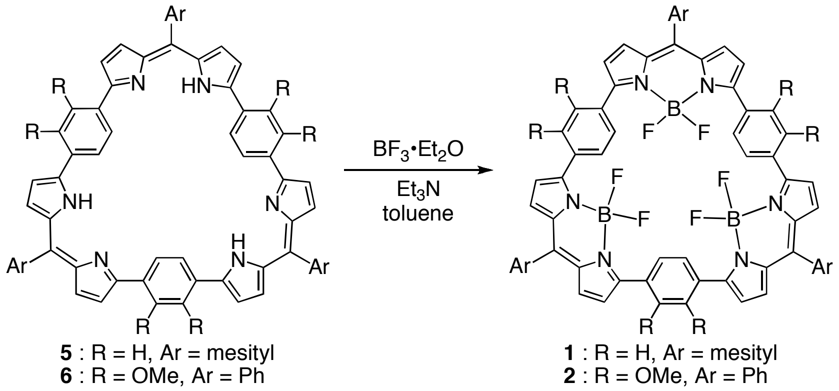
Contents

1. General

All chemicals were reagent grade, and used without further purification. All reactions were performed under nitrogen atmosphere. Tris-dipyrrin macrocycles were prepared as previously described. Column chromatography was performed with Kanto Chemical silica gel 60 N (spherical, neutral) or Wako Chemical alumina (activated, about 200 mesh). ^{1}H NMR spectra were recorded on a Bruker ARX400 spectrometer at 400 MHz, or a Bruker AC300 spectrometer at 300 MHz. ^{13}C NMR spectra were recorded on a Bruker ARX400 spectrometer at 100 MHz. In both NMR measurements, tetramethylsilane was used as an internal standard (0 ppm). ^{11}B NMR spectra were recorded on a Bruker ARX400 spectrometer at 128 MHz, boron trifluoride-diethyl etherate was used as an internal standard (0 ppm). ^{19}F NMR spectra were recorded on a Bruker AVANCE500 spectrometer at 470 MHz, hexafluorobenzene was used as an internal standard (-162 ppm). UV-Vis spectra were recorded on JASCO V-660 spectrophotometer. Fluorescence spectra and absolute quantum yields were measured on a Hitachi F-4500 spectrometer and a Hamamatsu Photonics absolute PL quantum yield measurement system C9920-02, respectively. Mass spectra (ESI-TOF, positive mode) were recorded on an Applied Biosystems QStar Pulsar *i* spectrometer. Elemental analyses were performed at Chemical Analysis Center, University of Tsukuba. Geometry optimizations and surface potential calculations were performed with Spartan08 programs.[1] X-ray crystallographic analysis: Intensities of reflections were collected on a Rigaku Mercury CCD diffractometer with a graphite monochromated Mo-Kα radiation (λ = 0.71070) using CrystalClear (Rigaku Corp.). The structure was solved by direct methods. The structure refinement was performed with SHELXL-97.

2. Synthesis of 1 and 2



1: To a stirred solution containing **5** (14.94 mg, 0.015 mmol) and trietylamine (0.5 mL, 3.6 mmol) in toluene (30 mL) was added boron trifluoride-diethyl etherate (0.5 mL, 4.0 mmol). After stirred for 48 h at 80 °C, the reaction mixture was washed with water (2 × 30 mL). The organic phase was dried over Na_2SO_4, filtered, evaporated to dryness. The obtained residue was purified by column chromatography on silica gel using chloroform as the eluent, and recrystallized from CH_2Cl_2/hexane to give **1** (5.0 mg, >29%).
green powder, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.22 (s, 18H), 2.36 (s, 9H), 6.44 (d, J = 4.4 Hz, 6H), 6.47 (d, J = 4.4 Hz, 6H), 6.95 (s, 6H), 8.38 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.1, 21.1, 121.7, 128.1, 129.0, 130.1, 130.3, 133.7, 136.8, 137.8, 138.5, 143.5, 158.1. MS(MALDI-TOF) observed *m/z* 1153.08 ($[M+H]^+$), calcd for $C_{72}H_{58}B_3F_6N_6$ *m/z* 1153.49. Anal. Calcd for $C_{72}H_{57}B_3F_6N_6$•$2H_2O$: C, 72.75; H, 5.17; N, 7.07. Found: C, 72.54; H, 5.18; N, 6.82.

2: To a stirred solution containing **6** (40.3 mg, 0.038 mmol) and trietylamine (0.5 mL, 3.6 mmol) in toluene (40 mL) was added boron trifluoride-diethyl etherate (0.5 mL, 4.0 mmol). After stirred for 10h at 80 °C, the reaction mixture was added water (80 mL) and the organic layer separated. The aqueous phase was extracted with dichloromethane (3 × 80 mL). The combined organic phase was dried over Na_2SO_4, filtered, evaporated to dryness. The obtained residue was purified by column chromatography on silica gel using dichloromethane as the eluent, and recrystallized from CH_2Cl_2/hexane to give **2** (45.3 mg, >99%).
Green powder, mp > 300 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80 (s, 18H), 6.67 (d, J = 4.0 Hz, 6H), 6.88 (d, J = 4.0 Hz, 6H), 7.50-7.65 (m, 15H), 7.84 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 62.3, 123.2, 126.3, 128.3, 128.5, 130.0, 130.1, 130.6, 134.4, 136.1, 143.6, 152.0, 154.6. MS(ESI) observed *m/z* 1229.42 ($[M+Na]^+$), calcd for $C_{69}H_{51}B_3F_6N_6NaO_6$ *m/z* 1229.40. Anal. Calcd for $C_{69}H_{51}B_3F_6N_6O_6$•$1.5H_2O$•$1/4C_6H_{14}$: C, 67.46; H, 4.62; N, 6.70. Found: C, 67.58; H, 4.70; N, 6.32.

3. Absorption spectral changes of 1 upon addition of K^+ and Rb^+

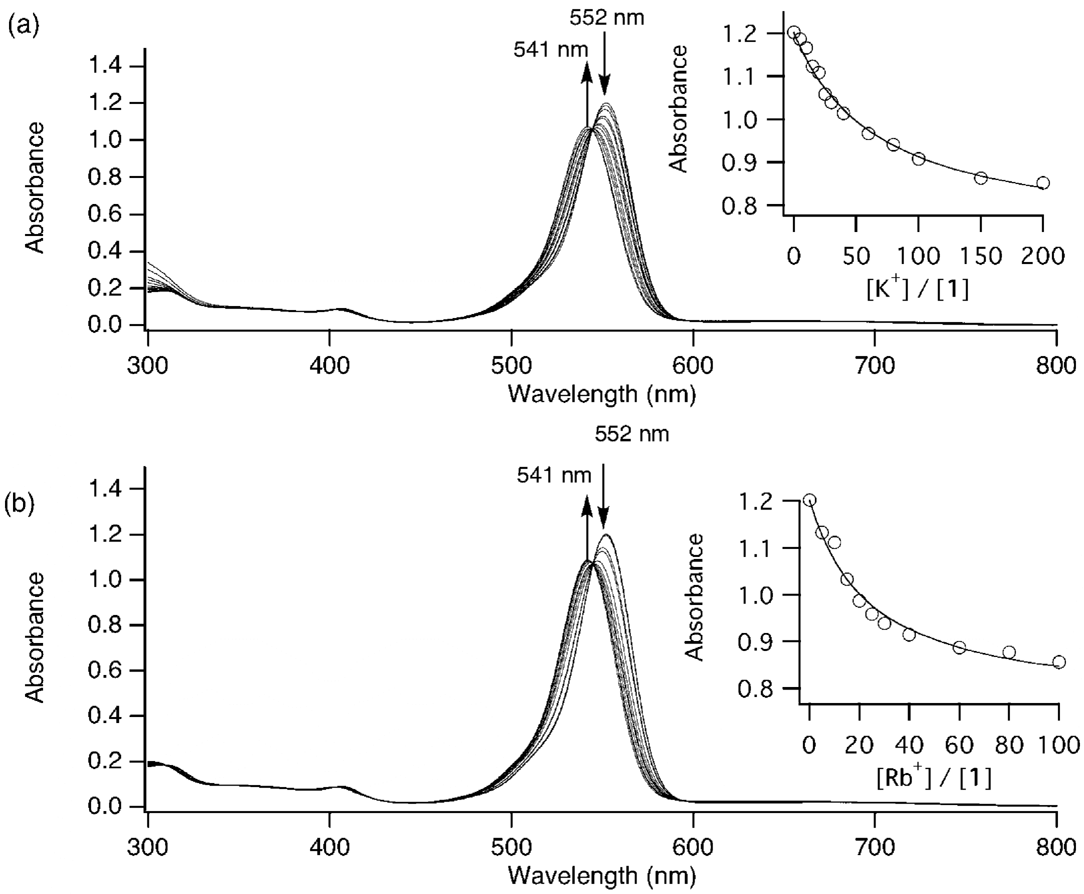


Figure S1. Absorption spectral changes of **1** (4.0 μM) upon addition of (a) KTFPB (0–0.8 mM) and (b) RbTFPB (0–0.4 mM) in $CHCl_3$-CH_3OH (10:1). Inset shows the binding isotherm at 552 nm analyzed by a nonlinear least-square regression (calculated lines are shown in solid lines).

4. Absorption spectral changes of 2 upon addition of K^+, Rb^+, and Cs^+

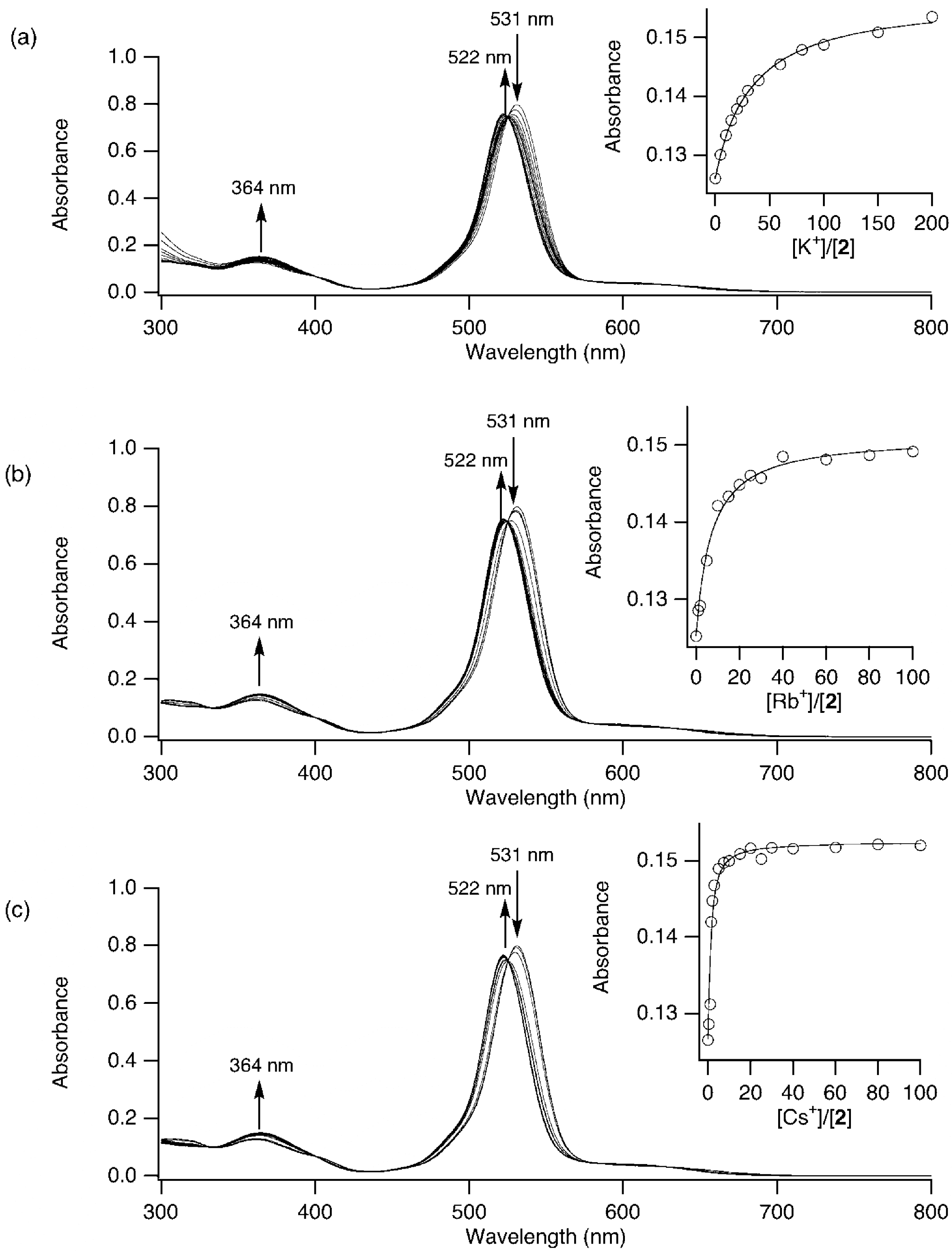


Figure S2. Absorption spectral changes of **2** upon (a) K^+, (b) Rb^+, and (c) Cs^+ in $CHCl_3$-CH_3OH (10:1). Inset shows the binding isotherm at 364 nm analyzed by a nonlinear least-square regression (calculated lines are shown in solid lines).

5. Absorption spectral changes of 2 upon addition of 3.

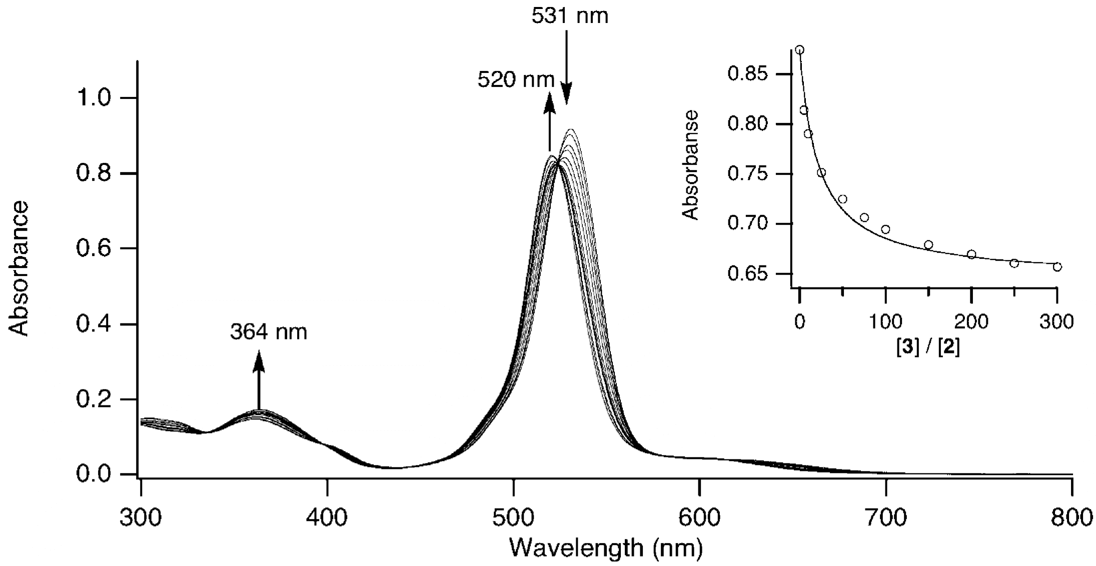


Figure S3. Absorption spectral changes of **2** upon **3** in $CHCl_3$-CH_3OH (10:1). Inset shows the binding isotherm at 531 nm analyzed by a nonlinear least-square regression (calculated lines are shown in solid lines).

6. ^{1}H NMR spectral changes of 2 upon addition of Cs^+.

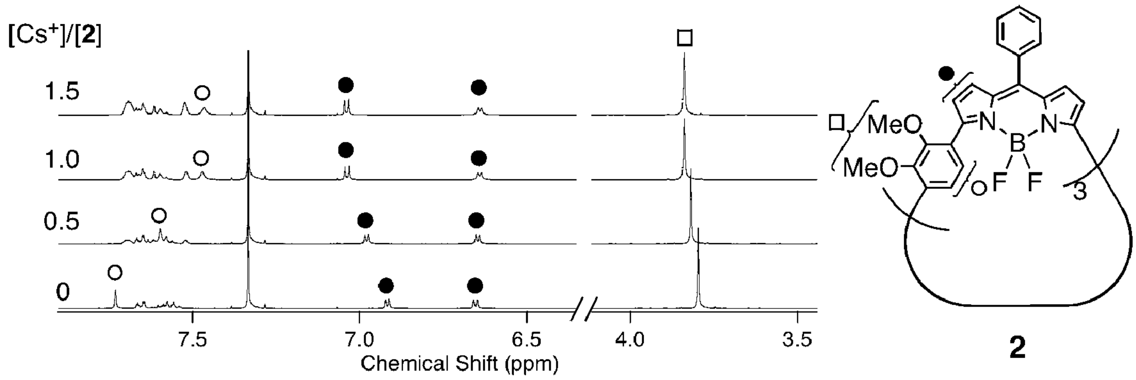


Figure S4. ^{1}H NMR spectral changes of **2** (1 mM) upon addition of CsTFPB in $CDCl_3$-CD_3OD (10:1).

7. ^{19}F NMR spectral change of 1 upon addition of Cs^+.

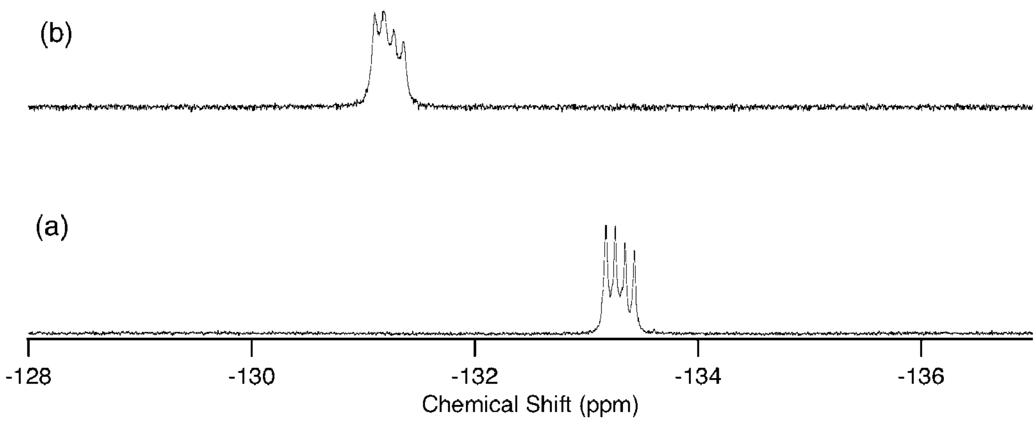


Figure S5. ^{19}F NMR spectra of **1** (0.5 mM) in the (a) absence and (b) presence of CsTFPB (2.5 mM) in $CDCl_3$-CD_3OD (10:1).

8. ^{11}B NMR spectral change of 1 upon addition of Cs^+.

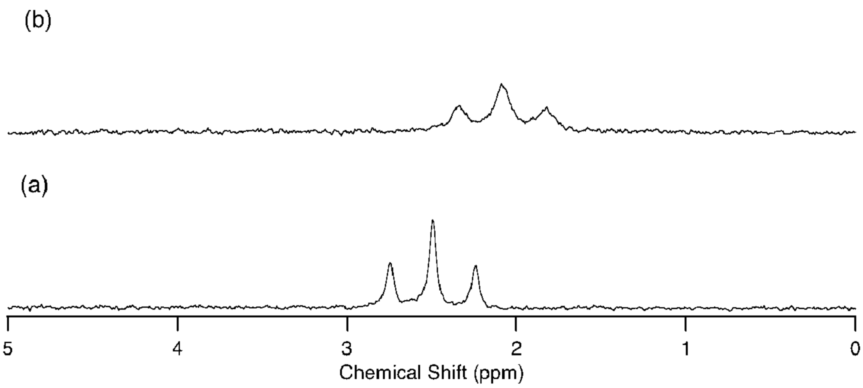


Figure S6. ^{11}B NMR spectra of **1** (0.5 mM) in the (a) absence and (b) presence of CsTFPB (2.5 mM) in $CDCl_3$-CD_3OD (10:1).

9. ^{1}H NMR spectral change of 2 upon addition of 3.

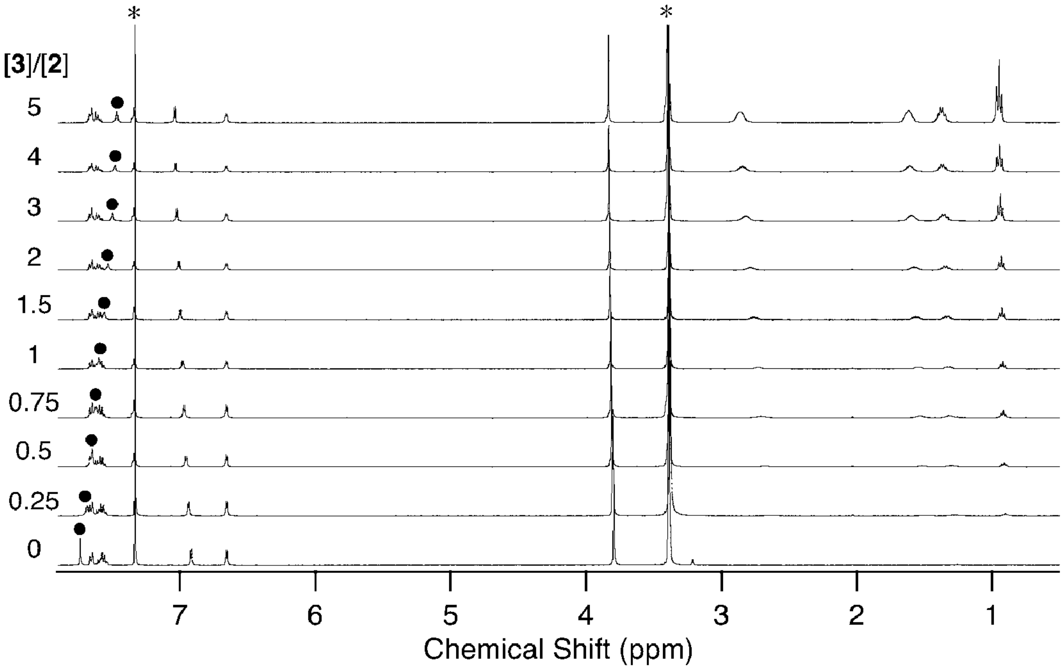


Figure S7. ^{1}H NMR spectral changes of **2** (1.0 mM) upon addition of **3** in $CDCl_3$-CD_3OD (10:1). Asterisk denotes the residual solvent peaks. Phenylene protons are indicated with filled circles.

10. ^{1}H NMR spectra of 2+3 at low temperature

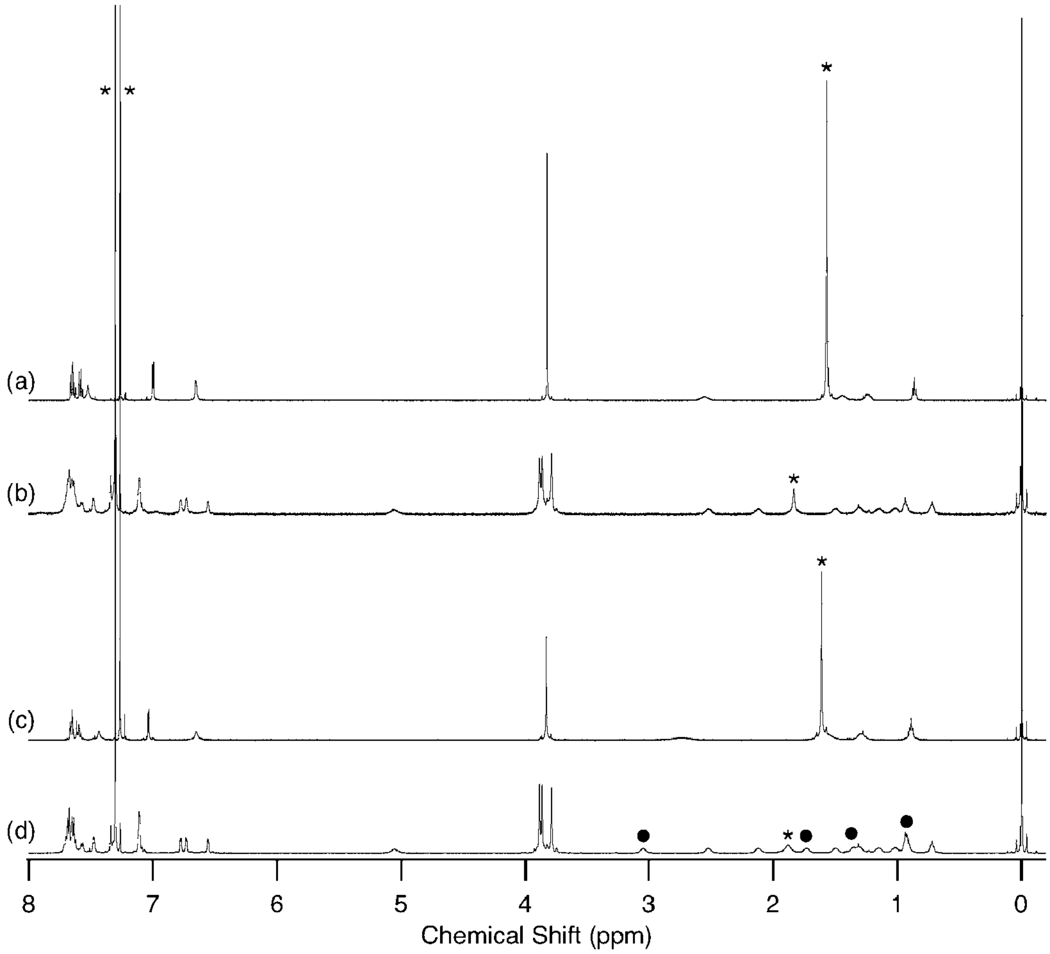


Figure S8. ^{1}H NMR spectra of **2** in the presence of (a), (b) 1 equiv or (c), (d) 2 equiv of **3** in $CDCl_3$ recorded at (a), (c) 298 K and (b), (d) 218 K. Filled circles in (d) denotes the free **3**. Asterisks denotes the solvent peaks and residual H_2O.

11. Fluorescence spectral changes of 2 upon addition of 3

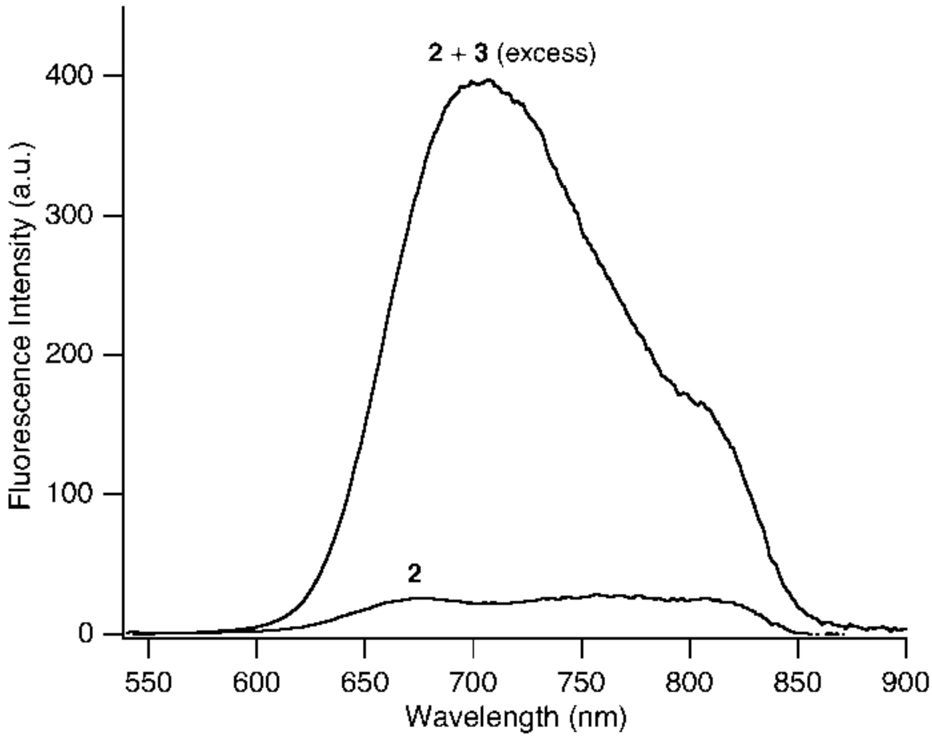


Figure S9. Fluorescence spectra of **2** in $CHCl_3$-CH_3OH (10:1).

12. Geometry optimized structures of 1 and 2

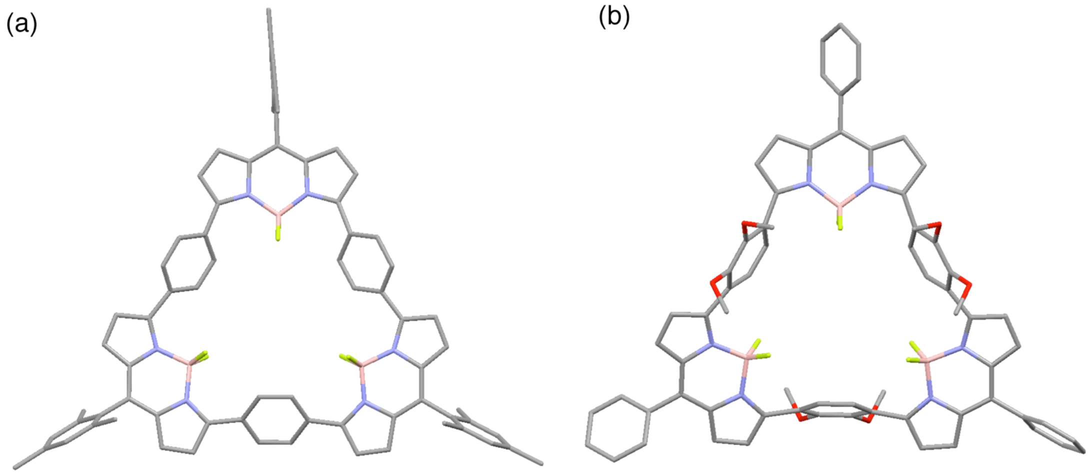


Figure S10. Geometry optimized structure of (a) **1** and (b) **2** by DFT calculation at the B3LYP/6-31G* level. Hydrogen atoms were omitted for clarity.

Geometries (Z matrices) of **1**

1	C1	1.41714661	-5.208704801	-0.135657823
2	C2	1.629210412	-6.601694667	-0.174692851
3	H3	0.963939507	-7.274868222	-0.240296268
4	C4	2.979109892	-6.797809148	-0.100374277
5	H5	3.419410452	-7.639691206	-0.084863724
6	C6	3.597837095	-5.548064635	-0.050582301
7	C7	4.939726378	-5.240590341	0.002713716
8	C8	5.381604093	-3.933297732	0.065631904
9	C9	6.693593418	-3.396988331	0.238161821
10	H10	7.505410245	-3.889543029	0.259297455
11	C11	6.565003137	-2.058074016	0.364312867
12	H12	7.282315372	-1.451958163	0.506967755
13	C13	5.20886374	-1.699313222	0.25507969
14	N14	2.611337251	-4.554971544	-0.057132752
15	N15	4.4780473	-2.842301507	0.042935113
16	B16	2.947559462	-3.057555127	-0.12887905
17	F17	2.322888432	-2.342348463	0.905821549
18	F18	2.510961221	-2.573588284	-1.352938138
19	C19	5.967996547	-6.333234955	-0.03330363
20	C20	6.256452082	-7.056301603	1.119549529
21	C21	7.164239746	-8.105645933	1.034103849
22	H22	7.369981024	-8.607834543	1.813611861
23	C23	7.780725978	-8.430792194	-0.180214295
24	C24	7.477866339	-7.704338797	-1.291212217
25	H25	7.89519152	-7.930385761	-2.114397169
26	C26	6.579246835	-6.644373788	-1.261816129
27	C27	5.632667262	-6.738642442	2.427019079
28	H28	4.67386304	-6.939781607	2.38889639
29	H29	5.760473143	-5.789042305	2.627108821
30	H30	6.051440694	-7.281774771	3.128374574
31	C31	8.764691315	-9.596089316	-0.28162939
32	H32	8.462926249	-10.21549133	-0.978804027
33	H33	8.803401955	-10.06405702	0.576700523
34	H34	9.654348624	-9.252797103	-0.51029294
35	C35	6.230515599	-5.900194504	-2.503934468
36	H36	6.668205133	-6.324402687	-3.27195768
37	H37	6.536473299	-4.972223438	-2.424523533
38	H38	5.258998916	-5.914252649	-2.630731619
39	C39	4.699862241	-0.331895399	0.332000569
40	C40	3.592892518	0.156085571	-0.390771879
41	H41	3.06553744	-0.438551174	-0.910705522
42	C42	3.281611402	1.490136366	-0.338460277
43	H43	2.524720255	1.80302543	-0.820717561
44	C44	4.029546066	2.399668409	0.390709962
45	C45	5.105463343	1.919322982	1.128991522
46	H46	5.619243244	2.520414564	1.657623998
47	C47	5.434608154	0.581844535	1.104241976
48	H48	6.171155866	0.271355368	1.617399181
49	C49	3.845086272	3.863664152	0.333763985
50	C50	4.930702226	4.75796312	0.336634345

51	H51		5.848789876	4.522752078	0.399687069
52	C52		4.426099824	6.03255343	0.227098722
53	H53		4.929132227	6.83856773	0.210398706
54	C54		3.023023686	5.913112731	0.148214052
55	C55		2.079397415	6.926644888	0.09231966
56	C56		0.711624052	6.58237056	0.129773528
57	C57	-	0.404003461	7.44686374	0.034381531
58	H58	-	0.384980071	8.395782752	-0.018878193
59	C59	-	1.520392068	6.651164832	0.034674478
60	H60	-	2.424345241	6.944931851	-0.025142538
61	C61	-	1.077532145	5.311639063	0.14029041
62	N62		2.698817563	4.546485758	0.203479235
63	N63		0.270935997	5.295102695	0.232007722
64	B64		1.224751309	4.058752222	0.220540042
65	F65		0.940375811	3.331988793	-0.937319634
66	F66		1.043459964	3.270705574	1.337759584
67	C67		2.522895415	8.321641355	-0.110562275
68	C68		2.533853924	9.243429131	0.929238082
69	C69		2.982462711	10.52825128	0.678925685
70	H70		3.006825588	11.14993444	1.395806581
71	C71		3.401022258	10.94235	-0.578631462
72	C72		3.344893911	10.01579804	-1.616385135
73	H73		3.610132708	10.28359319	-2.489446664
74	C74		2.907833354	8.716938372	-1.413546954
75	C75		2.098636548	8.88000842	2.348327051
76	H76		2.132168381	9.678036893	2.915103473
77	H77		2.702366612	8.196541092	2.709526645
78	H78		1.182955038	8.529344666	2.329377908
79	C79		3.893066076	12.34636614	-0.775992162
80	H80		3.943695073	12.54395451	-1.735070078
81	H81		4.78220733	12.44100292	-0.375132233
82	H82		3.273829964	12.97311603	-0.346368893
83	C83		2.907634776	7.766186132	-2.596312534
84	H84		3.521399695	7.02345426	-2.418487052
85	H85		3.197599589	8.245546746	-3.400303215
86	H86		2.00172763	7.417313878	-2.734105833
87	C87	-	2.005073601	4.152736919	0.080226625
88	C88	-	1.917580716	3.009619889	0.869796476
89	H89	-	1.17384883	2.899332581	1.448653705
90	C90	-	2.894612286	2.030822284	0.829331257
91	H91	-	2.801171113	1.248430702	1.358643093
92	C92	-	4.011059153	2.186400911	0.023483779
93	C93	-	4.091303156	3.310472467	-0.822345295
94	H94	-	4.821870972	3.411098398	-1.419323604
95	C95	-	3.095692983	4.252162888	-0.769524478
96	H96	-	3.157732815	5.008694971	-1.342264123
97	C97	-	5.187458469	1.337891612	0.04619664
98	C98	-	6.505332729	1.842936312	-0.052251872
99	H99	-	6.740390042	2.760678745	-0.148839283
100	C100	-	7.390045813	0.803070721	0.014163368
101	H101	-	8.337600785	0.862883074	-0.008408248
102	C102	-	6.628173883	-0.372917592	0.119684316
103	C103	-	7.033983409	-1.687827168	0.100361524
104	C104	-	6.109912204	-2.723867499	0.050537516
105	C105	-	6.307233105	-4.109799958	-0.114116127
106	H106	-	7.143535533	-4.557303803	-0.158892376
107	C107	-	5.081467363	-4.681808953	-0.195956758
108	H108	-	4.910059305	-5.609525283	-0.307462778
109	C109	-	4.096509645	-3.662847605	-0.087279191
110	N110	-	5.27049935	-0.013791942	0.137945262
111	N111	-	4.739402324	-2.477833773	0.052781739
112	B112	-	4.123418658	-1.065928503	0.316498128
113	F113	-	3.113534803	-0.792724113	-0.59467507
114	F114	-	3.670110091	-0.993080361	1.625677471
115	C115	-	8.510535933	-1.974847913	-0.004018633
116	C116	-	9.255329566	-2.07850619	1.20046314
117	C117	-1	0.635316073	-2.298704006	1.080913025
118	H118	-1	1.150173194	-2.383363737	1.873605662
119	C119	-1	1.270227833	-2.397435781	-0.120767979
120	C120	-1	0.503684885	-2.2804714	-1.266127811
121	H121	-1	0.930448564	-2.333032795	-2.112514629
122	C122	-	9.12003479	-2.086910459	-1.219776993
123	C123	-	8.594346623	-1.925053311	2.53266339
124	H124	-	7.8939179	-2.602472571	2.627697596
125	H125	-	9.260102049	-2.042849176	3.242412382
126	H126	-	8.199335205	-1.031798572	2.60110361
127	C127	-1	2.75122523	-2.620427651	-0.203165443
128	H128	-1	2.937025557	-3.58208804	-0.183046026

129	H129	-1	3.095024479	-2.238040265	-1.038144297
130	H130	-1	3.189579346	-2.186661727	0.558680512
131	C131	-	8.367182318	-1.966360077	-2.545501026
132	H132	-	7.850465172	-1.133819488	-2.553233265
133	H133	-	9.007401609	-1.959873647	-3.285825663
134	H134	-	7.757685357	-2.727619613	-2.645749179
135	C135	-	2.638831049	-3.878490224	-0.165218741
136	C136	-	1.690387722	-3.167537389	0.570360434
137	H137	-	1.963769627	-2.427807187	1.100340971
138	C138	-	0.372216896	-3.523530503	0.538875263
139	H139		0.257277342	-3.023879472	1.045265256
140	C140		0.070473304	-4.609222871	-0.221896652
141	C141	-	0.874573481	-5.280459663	-0.990974804
142	H142	-	0.591442875	-5.999571835	-1.543932805
143	C143	-	2.216041613	-4.932045131	-0.972214021
144	H144	-	2.84203234	-5.407174181	-1.506257686

Geometries (Z matrices) of **2**

1	B1	2.611648729	3.304987706	0.053345381
2	F2	2.203923037	2.867334673	1.314176154
3	F3	2.085270388	2.527098257	-0.965329287
4	B4	-4.125596609	0.556383895	0.385864703
5	F5	-3.599283938	0.482025742	-0.902663194
6	F6	-3.144042914	0.420879974	1.356812897
7	B7	1.666694344	-3.867393212	-0.00780843
8	F8	1.364507924	-3.231320394	1.193888295
9	F9	1.402729797	-3.065483731	-1.109308083
10	N10	4.183773693	3.285756197	0.038934251
11	N11	2.170124819	4.793604095	-0.191513866
12	N12	-4.866269886	1.928222296	0.557894166
13	N13	-5.211052727	-0.56068531	0.565710427
14	N14	0.841526899	-5.194562777	-0.164127475
15	N15	3.181009261	-4.276394591	0.041040163
16	C16	4.976355742	2.227820035	0.351754906
17	C17	6.304711352	2.683012693	0.555644264
18	H18	7.136657343	2.04538764	0.816041153
19	C19	6.31207575	4.048813132	0.352476862
20	H20	7.153287947	4.722335118	0.430675305
21	C21	4.982323641	4.429643562	0.03467046
22	C22	4.439015922	5.704012165	-0.186175952
23	C23	3.053276517	5.86342192	-0.338087957
24	C24	2.310916012	7.006087787	-0.734678178
25	H25	2.72678251	7.982933394	-0.935359612
26	C26	0.990635801	6.617185555	-0.833461765
27	H27	0.140788282	7.219371889	-1.11772676
28	C28	0.920651508	5.241532158	-0.485977741
29	C29	-0.333419822	4.47749307	-0.380892132
30	C30	-1.324059169	4.650549083	-1.373720367
31	O31	-1.05343276	5.335168546	-2.534234579
32	C32	-0.207079184	4.63802177	-3.456314918
33	H33	0.686647957	4.237533632	-2.96505525
34	H34	0.084259319	5.366507625	-4.216355703
35	H35	-0.75143298	3.811517783	-3.93156857
36	C36	-2.623245855	4.167414081	-1.171964227
37	O37	-3.591322418	4.423141353	-2.112029017
38	C38	-3.844952879	3.342154241	-3.017714553
39	H39	-3.958784778	2.391916765	-2.485004873
40	H40	-3.030567098	3.249334902	-3.748262928
41	H41	-4.771021202	3.592052893	-3.540720661
42	C42	-2.944916519	3.462018864	0.004402223
43	C43	-1.926693081	3.190925879	0.930591728
44	H44	-2.156623609	2.609206578	1.814998845
45	C45	-0.645518574	3.69893654	0.746489409
46	H46	0.118091298	3.520689724	1.492338831
47	C47	-4.360120659	3.156609016	0.291677335
48	C48	-5.394943322	4.120964934	0.388224885
49	H49	-5.263467973	5.17914891	0.213922342
50	C50	-6.552963206	3.452325612	0.736516222
51	H51	-7.537276823	3.87231768	0.886420583
52	C52	-6.225356181	2.074101419	0.835028976
53	C53	-7.061552257	0.962554283	1.023554103
54	C54	-6.551989626	-0.336970759	0.880325575
55	C55	-7.20624306	-1.595389278	0.948217238
56	H56	-8.2453211	-1.74803594	1.201872888
57	C57	-6.266674797	-2.558481893	0.633287018
58	H58	-6.40425108	-3.628686812	0.573016986
59	C59	-5.033765625	-1.894115039	0.415455487

60	C60	-3.75101232	-2.570144107	0.131906204
61	C61	-3.642227604	-3.362583596	-1.026499555
62	O62	-4.661344241	-3.372484233	-1.947463701
63	C63	-4.586118926	-2.331045323	-2.928798
64	H64	-4.405937227	-1.355921393	-2.462889719
65	H65	-5.548782431	-2.327068875	-3.445239508
66	H66	-3.788395552	-2.53725581	-3.65351368
67	C67	-2.517738439	-4.174969088	-1.223798278
68	O68	-2.446573764	-4.935052842	-2.36645716
69	C69	-1.450148607	-4.513168913	-3.306157928
70	H70	-0.476996179	-4.362269329	-2.826953388
71	H71	-1.75184792	-3.577930059	-3.795445883
72	H72	-1.377727295	-5.3076787	-4.052177587
73	C73	-1.505128986	-4.241997663	-0.241112885
74	C74	-1.588580569	-3.38645133	0.868855293
75	H75	-0.797424283	-3.399811356	1.60630059
76	C76	-2.689653441	-2.555983966	1.047416123
77	H77	-2.749266818	-1.916504095	1.919687359
78	C78	-0.499369677	-5.315544652	-0.338970572
79	C79	-0.81803197	-6.681160408	-0.563913554
80	H80	-1.817584297	-7.056739286	-0.72568508
81	C81	0.358981664	-7.399250475	-0.504514759
82	H82	0.484717983	-8.468071543	-0.601257152
83	C83	1.404637163	-6.466348467	-0.280605841
84	C84	2.787849801	-6.672929695	-0.182812026
85	C85	3.655636579	-5.586959747	-0.003279733
86	C86	5.062772674	-5.55816585	0.183137947
87	H87	5.713370131	-6.420804425	0.167796047
88	C88	5.417188441	-4.238341473	0.382045685
89	H89	6.402437485	-3.834509835	0.564575396
90	C90	4.236029076	-3.458480469	0.277869467
91	C91	4.194914404	-1.98662354	0.364439279
92	C92	4.788300789	-1.361264387	1.481282471
93	O93	5.23471604	-2.110014334	2.542362103
94	C94	4.20359968	-2.575351315	3.422778167
95	H95	3.358246196	-2.994697893	2.866559588
96	H96	3.84077164	-1.757538636	4.059193521
97	H97	4.658611941	-3.346115343	4.048862187
98	C98	4.967549178	0.027443066	1.503334388
99	O99	5.582972663	0.601710339	2.587950649
100	C100	4.701366956	1.298133571	3.479298451
101	H101	4.018904313	1.961556426	2.937252025
102	H102	5.339168754	1.883169437	4.145672103
103	H103	4.112059097	0.586607363	4.072182594
104	C104	4.559632559	0.816311562	0.406048995
105	C105	3.888493139	0.194075876	-0.658441077
106	H106	3.535789578	0.796405194	-1.485632571
107	C107	3.708749228	-1.184683949	-0.679139994
108	H108	3.217068705	-1.652854514	-1.522526209
109	C109	5.332849004	6.886287088	-0.264162301
110	C110	5.102383372	8.011715172	0.545376537
111	H111	4.270761661	8.001972124	1.243419897
112	C112	5.946987488	9.118806109	0.476531614
113	H113	5.762352712	9.976207578	1.117900065
114	C114	7.02739531	9.124271291	-0.407866559
115	H115	7.683112924	9.989038374	-0.462747189
116	C116	7.261332132	8.014494092	-1.222063107
117	H117	8.095150827	8.014989402	-1.918922645
118	C118	6.424630851	6.901941837	-1.148855755
119	H119	6.600426625	6.045515272	-1.792687684
120	C120	-8.498558012	1.172106047	1.334244345
121	C121	-9.501898242	0.611025336	0.526298118
122	H122	-9.220163031	0.031694316	-0.347691144
123	C123	-10.84830964	0.819062965	0.822364236
124	H124	-11.61197809	0.387773497	0.180953081
125	C125	-11.2138885	1.582245315	1.9327094
126	H126	-12.26361268	1.740503635	2.164417169
127	C127	-10.22482054	2.143544047	2.742838957
128	H128	-10.5013105	2.734544108	3.611755582
129	C129	-8.877444564	1.945689106	2.444478646
130	H130	-8.109424583	2.372901318	3.082197469
131	C131	3.337218872	-8.052689982	-0.264979668
132	C132	3.146105434	-8.830650024	-1.418524566
133	H133	2.604965012	-8.411421769	-2.26151681
134	C134	3.667509512	-10.12187238	-1.494758969
135	H135	3.521117616	-10.70773795	-2.39820053
136	C136	4.377561645	-10.6581846	-0.419086223
137	H137	4.77994773	-11.66574432	-0.479280583

138	C138	4.567814217	-9.894770307	0.734044224
139	H139	5.112753389	-10.30756562	1.578671836
140	C140	4.055706509	-8.599876093	0.810383616
141	H141	4.193597229	-8.011828257	1.712944097

13. Electrostatic potential surface of 1, 2, and tetramethyl-BODIPY

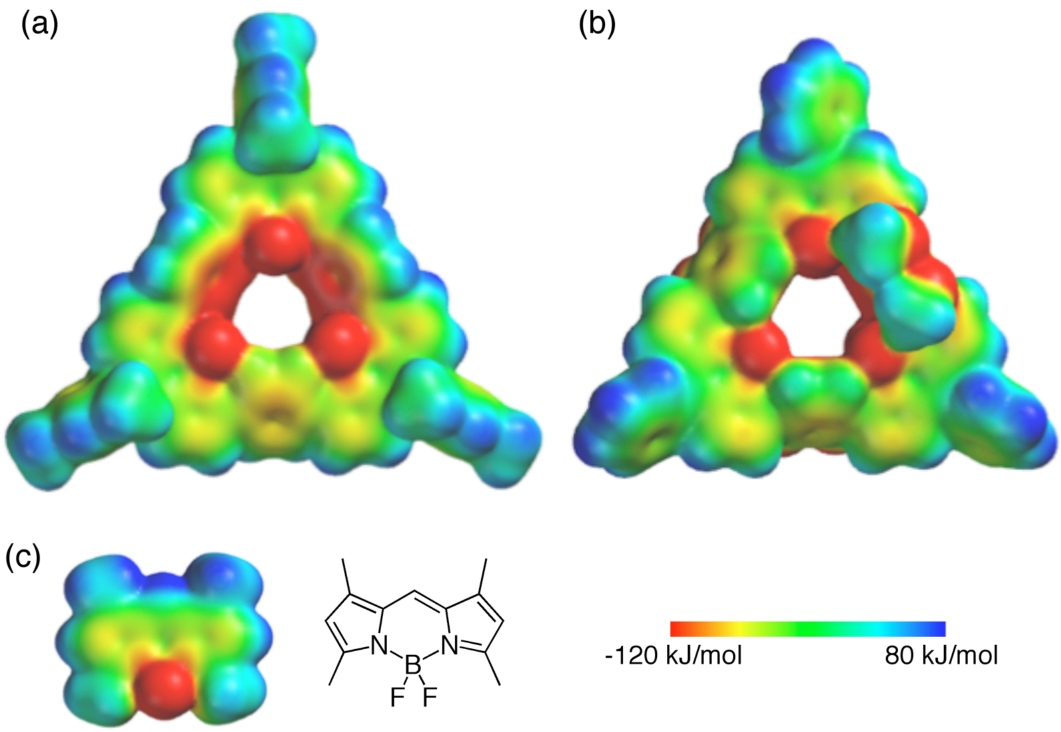
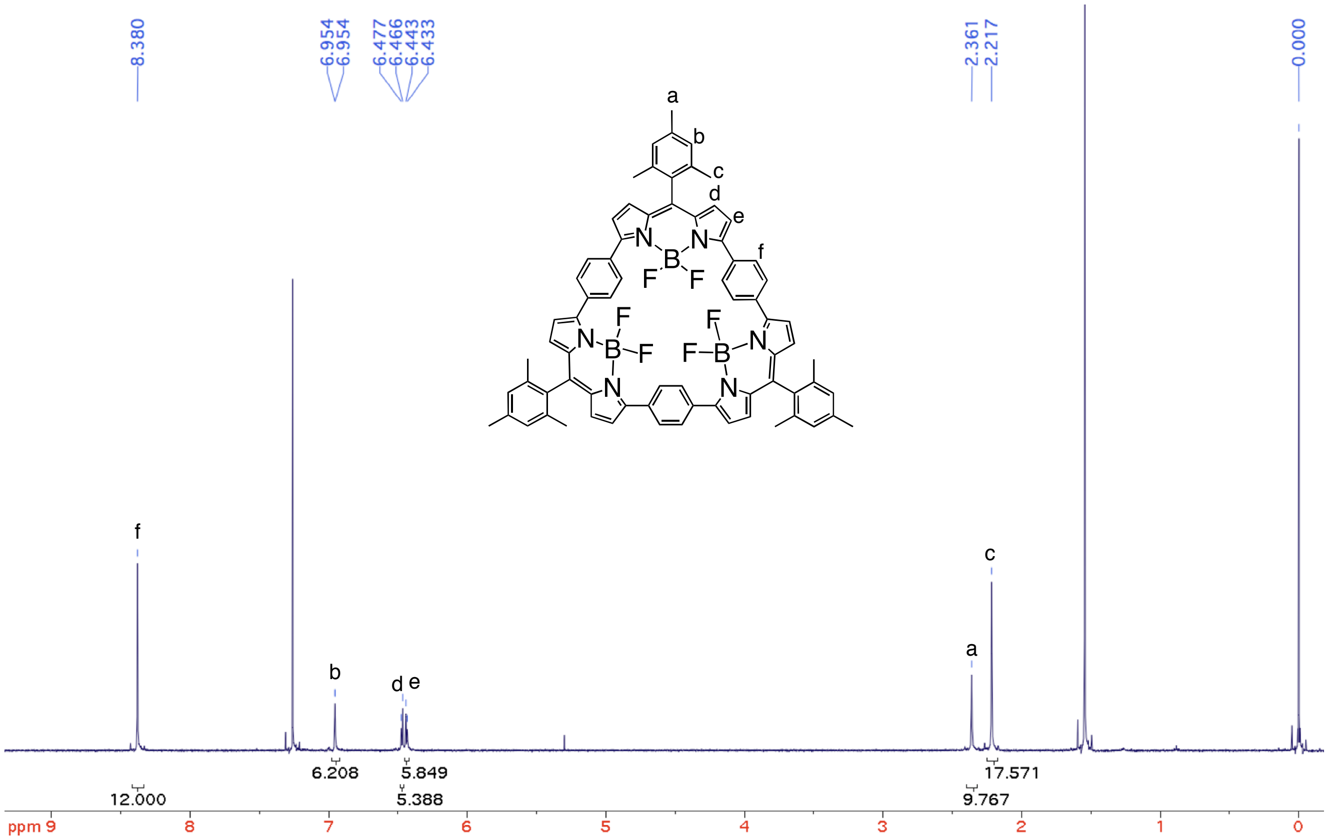


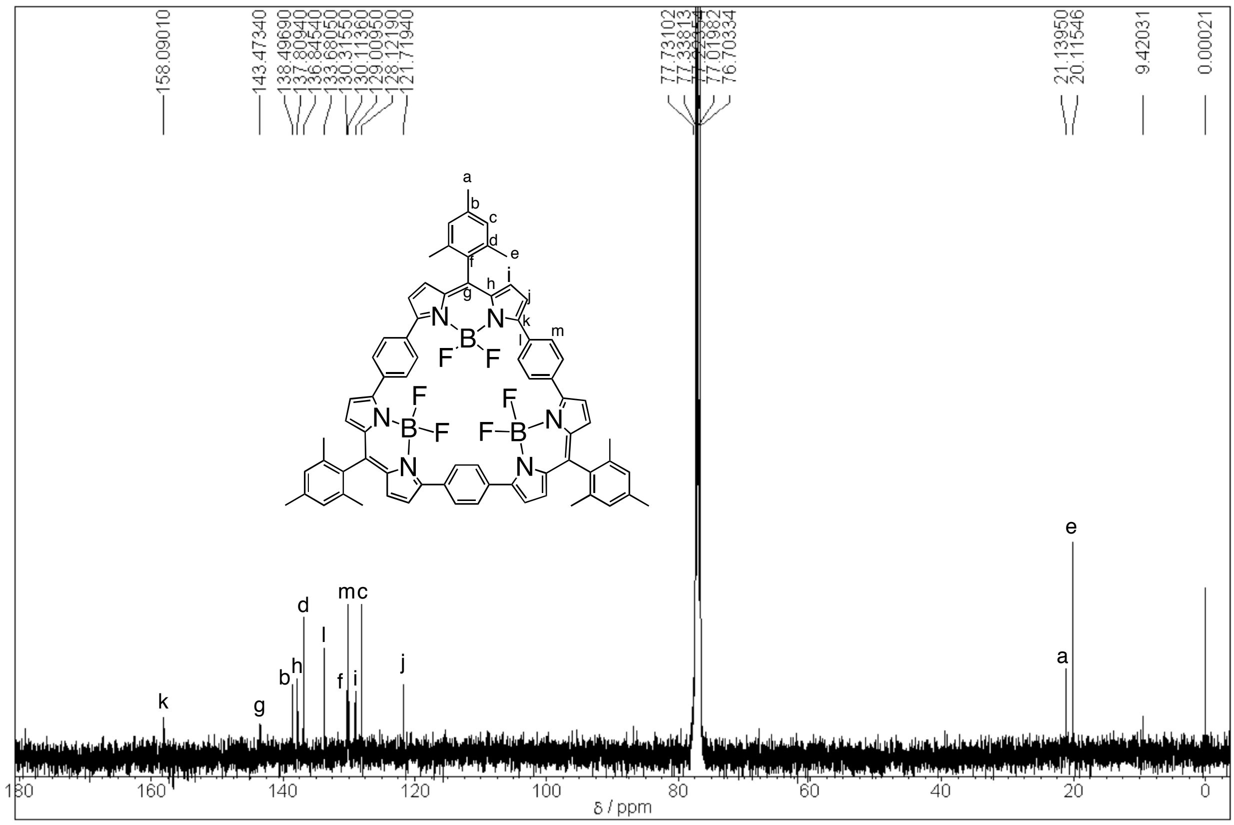
Figure S11. Electrostatic potential surfaces of (a) **1**, (b) **2** and (c) tetramethyl-BODIPY by DFT calculation at the B3LYP/6-31G* level.

14. NMR spectra of 1 and 2

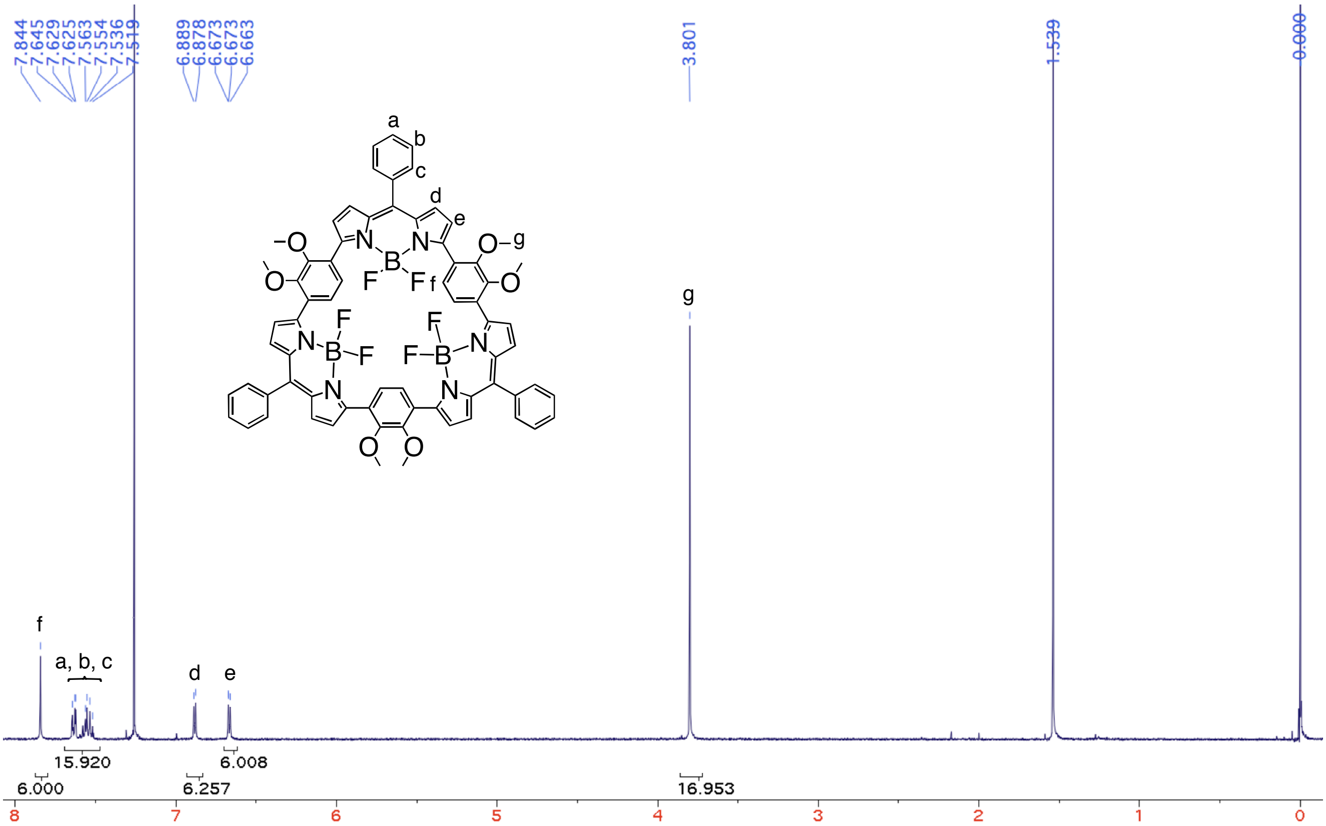
[1]H NMR spectrum of **1**



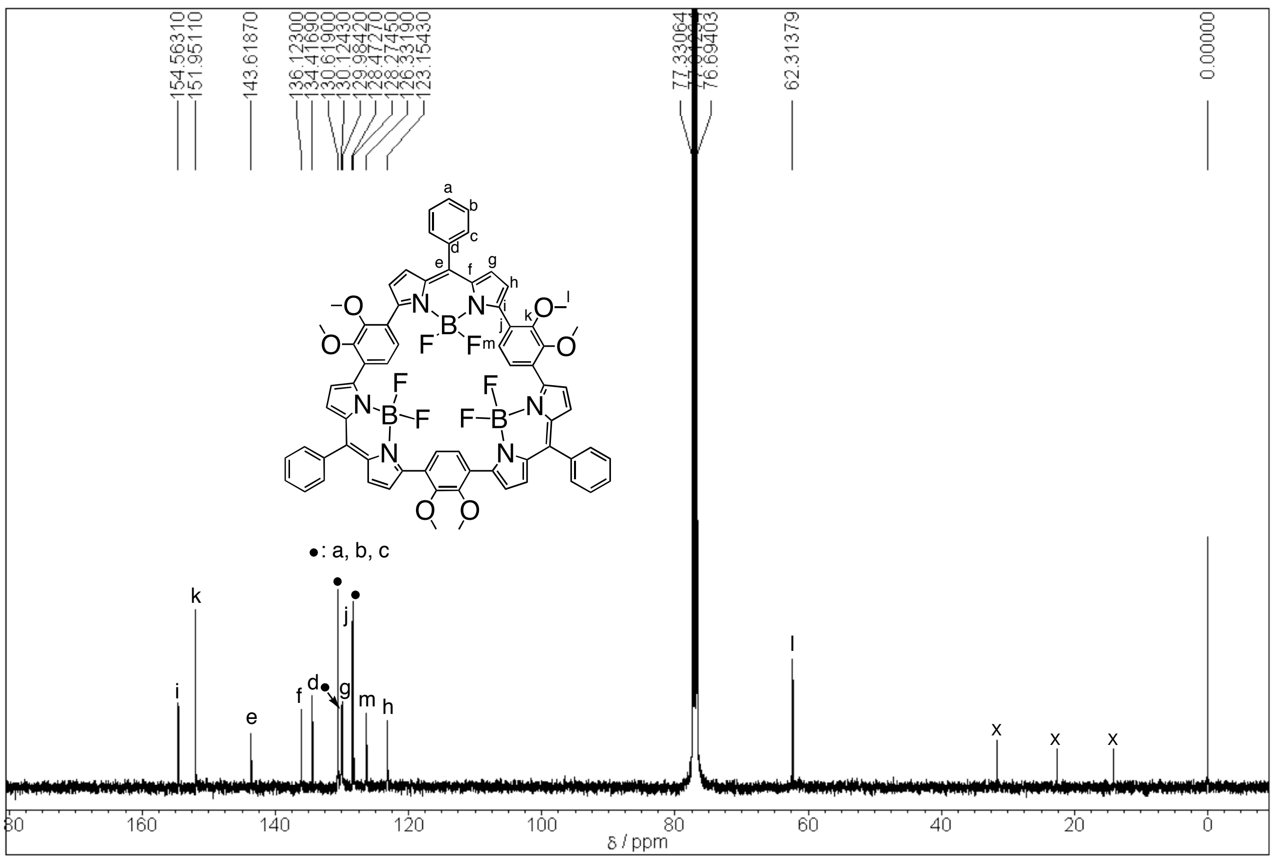
[13]C NMR spectrum of **1**



^{1}H NMR spectrum of **2**



^{13}C NMR spectrum of **2**



Reference

1 Spartan08 for Windows; Wavefunction, Inc.: Irvine, CA.