Electronic supplementary information (ESI)

Bodipy functionalized *ortho*-carborane dyads for low-energy photo-sensitization

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Contents

Table S1. Fluorescence maxima for compounds **1**-**6** in various solvents

Compounds	Solvent			
	acetonitrile (nm)	methylene chloride (nm)	tetrahydrofuran (nm)	*n*-hexane (nm)
1	537	542	541	540
2	537	540	539	538
3	538	543	541	539
4	538	543	540	540
5	536	544	542	541
6	539	544	542	542

Excitation wavelength is 380 nm.

Table S2. Oxidation and Reduction Potentials of compounds, **1**-**6**

Compounds	Oxidation peaks (V) [a]			Reduction peaks (V) [a]			HOMO (eV)[c]	LUMO (eV) [c]
	E_{pa} [b]	E_{pc} [b]	E_{ox}	E_{pa} [b]	E_{pc} [b]	E_{red}		
1	0.67	0.59	0.63	-1.69	-1.76	-1.73	-5.43	-3.07
2	0.66	0.58	0.62	-1.68	-1.75	-1.72	-5.42	-3.08
3	0.65	0.59	0.62	-1.68	-1.75	-1.72	-5.42	-3.08
4	0.65	0.59	0.62	-1.66	-1.73	-1.70	-5.42	-3.10
5	0.67	0.62	0.65	-1.60, -1.75	-1.70, -1.82	-1.65, -1.79	-5.45	-3.15
6	0.66	0.61	0.64	-1.50, -1.74	-1.70, -1.87	-1.60, -1.81	-5.44	-3.20

[a] Potentials calibrated with an internal ferrocene redox reference ($Fc^+|Fc$) using 0.1 M tetrabutylammonium perchlorate electrolyte in CH_2Cl_2. [b] E_{pa} = anodic peak potentials. E_{pc} = cathodic peak potentials. E_{ox} = half-wave oxidation potential between anodic and cathodic peaks. E_{red} = half-wave reduction potential between anodic and cathodic peaks. [c] HOMO (eV) = $-e(E_{ox} + 4.8)$ and LUMO (eV) = $-e\ (E_{red} + 4.8)$.

Table S3. Crystal data and structure refinement for compound **6**

Identification code	k120401
Empirical formula	C_{51} H_{59} B_{12} Cl_2 F_4 N_4
Formula weight	1004.64
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 12.955(2) Å
	b = 16.894(3) Å, β = 100.016(4)º
	c = 25.673(5) Å
Volume	5533.0(17) Å^3
Z, D_{calc}	4, 1.206 g/cm^3
μ	0.169 mm^{-1}
F(000)	2092
Crystal size	0.3 × 0.15 × 0.15 mm
θ range for data collection	1.61 to 28.41º
Limiting indices	$-17 \le h \le 17$, $-22 \le k \le 22$, $-34 \le l \le 33$
Reflections collected / unique	56353 / 13834 [R_{int} = 0.0439]
Completeness to θ = 28.41	99.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13834 / 0 / 686
Goodness-of-fit on F^2	1.005
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0814, wR_2 = 0.2338
R indices (all data)	R_1 = 0.1441, wR_2 = 0.2927
Largest diff. peak and hole	1.161 and −0.789 e.Å^{-3}

[a]$R_1 = \sum||F_o|-|F_c||$ (based on reflections with $F_o^2>2\sigma F^2$), [b]$wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0)+2F_c^2]/3$(also with $F_o^2>2\sigma F^2$)

Table S4. Important bond lengths [Å], angle [°] and torsion angles[°] for **6**. Numbering is for below crystal.

Atom1-Atom2	Distance	A1-A2-A3	Angle	A1-A2-A3-A4	Angle
C(1)-C(13)	1.428(4)	C(1)-B(3)-C(2)	59.4(2)	C(13)-C(1)-C(2)-C(39)	-3.0(4)
C(1)-C(2)	1.714(4)	C(1)-B(3)-B(9)	104.8(3)	C(2)-C(1)-C(13)-C(14)	-29(4)
C(2)-C(39)	1.504(4)	C(2)-B(3)-B(9)	105.8(2)	C(1)-C(13)-C(14)-C(15)	-18(8)
C(13)-C(14)	1.185(4)	C(1)-B(6)-C(2)	59.4(2)	C(13)-C(14)-C(15)-C(16)	143(4)
C(14)-C(15)	1.435(4)	C(13)-C(1)-C(2)	116.7(2)	C(14)-C(15)-C(16)-C(17)	-177.9(3)
		C(39)-C(2)-C(1)	117.4(2)	C(17)-C(18)-C(21)-C(30)	89.6(4)
				C(1)-C(2)-C(39)-C(40)	-125.8(3)
				C(1)-C(2)-C(39)-C(44)	51.2(4)
				C(44)-C(39)-C(40)-C(41)	-1.2(4)
				C(2)-C(39)-C(40)-C(41)	175.9(3)
				C(41)-C(42)-C(45)-C(46)	-90.9(4)
				C(43)-C(42)-C(45)-C(46)	88.9(4)

Table S5. Selected oscillator strength (> 0.001) and calculated electronic transitions of complexes.

1

No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributors
1	430	0.4745	Singlet	HOMO→LUMO (89%), H-1→LUMO (12%)
2	372	0.1826	Singlet	H-1→LUMO (88%), HOMO→LUMO (12%)
3	355	0.0332	Singlet	H-2→LUMO (99%)
4	300	0.0059	Singlet	HOMO→L+2 (99%)
5	292	0.0021	Singlet	H-4→LUMO (100%)
6	258	0.1740	Singlet	H-5→LUMO (89%)
7	240	0.0073	Singlet	H-1→L+2 (99%)
8	211	0.0569	Singlet	H-7→LUMO (64%), HOMO→L+3 (32%)
9	210	0.2272	Singlet	HOMO→L+3 (48%), H-7→LUMO (35%)
10	205	0.0015	Singlet	H-5→L+1 (95%)
11	204	0.0691	Singlet	HOMO→L+4 (79%)
12	202	0.0035	Singlet	H-3→L+1 (50%), H-4→L+2 (37%)
13	199	0.0016	Singlet	H-12→LUMO (48%), H-11→LUMO (34%)
14	197	0.0022	Singlet	H-11→LUMO (48%), H-12→LUMO (36%), HOMO→L+4 (10%)
15	194	0.0019	Singlet	H-13→LUMO (94%)
16	193	0.0134	Singlet	HOMO→L+5 (69%), H-1→L+3 (28%)
17	187	0.0154	Singlet	H-15→LUMO (79%)
18	184	0.0023	Singlet	H-17→LUMO (85%)
19	184	0.0036	Singlet	H-14→LUMO (87%)
20	183	0.0848	Singlet	H-18->LUMO (78%)
21	181	0.0026	Singlet	H-1→L+3 (36%), HOMO→L+8 (18%), HOMO→L+5 (15%), HOMO→L+6 (15%)
22	180	0.2100	Singlet	H-2→L+3 (76%), H-18→LUMO (10%)
23	178	0.2233	Singlet	H-4→L+1 (40%), H-3→L+2 (38%)
24	177	0.5860	Singlet	H-4→L+2 (45%), H-3→L+1 (27%)
25	176	0.0081	Singlet	H-19→LUMO (76%), H-20→LUMO (15%)
26	176	0.0308	Singlet	HOMO→L+7 (60%), H-1→L+4 (23%)
27	175	0.3002	Singlet	H-1→L+4 (60%), HOMO→L+7 (32%)

2				
No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributors
1	431	0.4709	Singlet	HOMO→LUMO (89%), H-1→LUMO (12%)
2	373	0.1830	Singlet	H-1→LUMO (87%), HOMO→LUMO (-13%)
3	361	0.0024	Singlet	HOMO→L+1 (99%)
4	356	0.0350	Singlet	H-2→LUMO (99%)
5	307	0.0078	Singlet	HOMO→L+2 (99%)
6	284	0.0017	Singlet	H-4→LUMO (100%)
7	260	0.3764	Singlet	H-5→LUMO (83%)
8	251	0.0133	Singlet	H-6→LUMO (95%)
9	242	0.3313	Singlet	H-3→L+1 (74%)
10	212	0.0111	Singlet	H-9→LUMO (82%), HOMO→L+3 (-16%)
11	209	0.1891	Singlet	HOMO→L+3 (69%), H-9→LUMO (17%)
12	204	0.0332	Singlet	HOMO→L+4 (50%), HOMO→L+5 (35%)
13	204	0.0252	Singlet	HOMO→L+4 (48%), HOMO→L+5 (-30%), H-5→L+2 (-13%)
14	203	0.1253	Singlet	H-4→L+1 (41%), H-3→L+2 (32%)
15	203	0.0170	Singlet	H-5→L+2 (74%)
16	199	0.0027	Singlet	H-6→L+2 (38%), H-14→LUMO (-36%), H-13→LUMO (15%)
17	198	0.0016	Singlet	H-6→L+2 (60%), H-14→LUMO (26%)
18	197	0.0025	Singlet	H-13→LUMO (63%), H-14→LUMO (19%), HOMO→L+5 (-11%)
19	193	0.0819	Singlet	H-7→L+1 (28%), H-4→L+2 (-27%), H-8→L+1 (21%), HOMO→L+6 (-15%)
20	185	0.0015	Singlet	H-16→LUMO (89%)
21	185	0.0014	Singlet	HOMO→L+7 (95%)
22	184	0.0445	Singlet	H-7→L+1 (61%), H-8→L+1 (-23%), H-4→L+2 (12%)
23	183	0.0486	Singlet	H-17→LUMO (78%)

3				
No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributors
1	457	0.0014	Singlet	H-1→LUMO (55%), H-1→L+1 (39%)
2	434	0.0264	Singlet	H-1→L+1 (31%), HOMO→LUMO (23%), HOMO→L+1 (19%), H-1→LUMO (-14%)
3	433	0.8155	Singlet	HOMO→L+1 (31%), H-1→LUMO (23%), H-1→L+1 (-19%), HOMO→LUMO (14%)
4	408	0.0016	Singlet	HOMO→L+2 (60%), H-1→L+2 (-34%)
5	408	0.0589	Singlet	H-1→L+2 (59%), HOMO→L+2 (33%)
6	381	0.0711	Singlet	H-2→LUMO (98%)
7	374	0.0075	Singlet	H-3→LUMO (42%), H-4→L+1 (-40%)
8	373	0.3730	Singlet	H-4→LUMO (41%), H-3→L+1 (-39%)
9	357	0.0945	Singlet	H-6→LUMO (50%), H-5→L+1 (48%)
10	314	1.8056	Singlet	H-2→L+2 (90%)
11	307	0.0152	Singlet	H-1→L+4 (29%), HOMO→L+3 (29%), H-1→L+3 (-19%), HOMO→L+4 (18%)
12	306	0.0027	Singlet	H-4→L+2 (96%)
13	292	0.0048	Singlet	H-6→L+2 (98%)
14	283	0.0023	Singlet	H-9→LUMO (51%), H-8→L+1 (48%)
15	266	0.0271	Singlet	H-7→L+1 (55%), H-11→L+1 (33%)
16	257	0.1212	Singlet	H-10→LUMO (62%), H-11→L+1 (11%)
17	253	0.0069	Singlet	H-12→L+1 (54%), H-10→LUMO (21%), H-7→L+1 (20%)

4

No.	Wavelength (nm)	Osc. Strength	ymmetry	Major contributors
1	435	0.1814	Singlet	H-1→LUMO (20%), HOMO→LUMO (20%), HOMO→L+1 (16%), H-1→L+1 (-15%), HOMO→L+2 (-11%), H-1→L+2 (10%)
2	435	0.4681	Singlet	H-1→LUMO (20%), HOMO→LUMO (-19%), H-1→L+1 (-16%), HOMO→L+1 (-15%), H-1→L+2 (12%), HOMO→ +2 (11%)
3	424	0.0699	Singlet	H-1→L+2 (38%), HOMO→L+2 (-36%)
4	424	0.2011	Singlet	HOMO→L+2 (37%), H-1→L+2 (36%)
5	379	0.0568	Singlet	H-2→L+1 (95%)
6	374	0.0879	Singlet	H-4→LUMO (22%), H-3→LUMO (-22%), H-3→L+1 (22%), H-4→L+1 (21%)
7	373	0.2751	Single	H-4→L+1 (23%), H-3→LUMO (22%), H-4→LUMO (21%), H-3→L+1 (-21%)
8	357	0.1558	Singlet	H-5→LUMO (49%), H-6→L+1 (-48%)
9	347	0.8194	Singlet	H-2→L+2 (80%), H-7→L+3 (-10%)
10	346	0.0032	Singlet	HOMO→L+3 (74%), H-1→L+3 (22%)
11	346	0.0076	Singlet	H-1→L+3 (74%), HOMO→L+3 (-22%)
12	323	0.1383	Singlet	H-7→LUMO (92%)
13	316	0.001	Singlet	H-3→L+2 (92%)
14	316	0.001	Singlet	H-4→L+2 (92%)
15	310	0.024	Singlet	H-1→L+4 (34%), HOMO→L+5 (-33%), H-1→L+5 (-17%), HOMO→L+4 (-16%)
16	280	0.0015	Singlet	H-10→LUMO (44%), H-11→L+1 (43%)
17	280	0.0016	Singlet	H-11→LUMO (44%), H-10→L+1 (43%)
18	269	2.1968	Singlet	H-7→L+3 (54%), H-8→L+1 (18%), H-9→LUMO (-17%)

5				
No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributors
1	442	0.6849	Singlet	H-1→LUMO (-44%), HOMO→L+1 (47%)
2	437	0.1411	Singlet	H-1→L+1 (46%), HOMO→LUMO (-41%)
3	376	0.3052	Singlet	H-2→L+1 (35%), H-3→LUMO (32%), H-1→L+2 (-22%)
4	374	0.0688	Singlet	H-2→LUMO (35%), H-3→L+1 (31%), HOMO→L+2 (21%)
5	361	0.0284	Singlet	H-4→L+1 (52%), H-5→LUMO (-45%)
6	360	0.0391	Singlet	H-4→LUMO (54%), H-5→L+1 (-42%)
7	348	0.0074	Singlet	HOMO→L+3 (88%)
8	347	0.0112	Singlet	H-1→L+3 (89%)
9	322	0.0072	Singlet	HOMO→L+4 (41%), H-1→L+4 (-35%), HOMO→L+5 (10%)
10	322	0.0072	Singlet	H-1→L+4 (41%), HOMO→L+4 (36%), H-1→L+5 (-10%)
11	303	0.0011	Singlet	HOMO→L+5 (78%), H-1→L+4 (19%)
12	297	0.0716	Singlet	H-6→LUMO (50%), H-7→L+1 (40%)
13	296	0.0779	Singlet	H-6→L+1 (46%), H-7→LUMO (40%)
14	295	0.0052	Singlet	H-2→L+2 (93%)
15	294	0.0028	Singlet	H-3→L+2 (92%)
16	280	0.0014	Singlet	H-7→L+1 (32%), H-6→LUMO (-28%), H-11→LUMO (10%), H-8→LUMO (-10%)
17	279	0.0019	Singlet	H-7→LUMO (32%), H-6→L+1 (-29%), H-10→LUMO (11%), H-8→L+1 (-10%)
18	273	0.0049	Singlet	H-10→L+1 (23%), H-7→L+1 (-19%), H-6→LUMO (18%), H-8→LUMO (-17%), H-11→LUMO (16%)
19	272	0.0055	Singlet	H-2→L+3 (89%)
20	262	0.0125	Singlet	HOMO→L+6 (92%)
21	262	0.2042	Singlet	H-9→L+1 (37%), H-8→LUMO (28%)
22	261	0.0003	Singlet	H-4→L+3 (87%)
23	260	0.0451	Singlet	H-5→L+3 (50%), H-8→L+1 (-21%), H-9→LUMO (-12%)
24	260	0.056	Singlet	H-5→L+3 (37%), H-8→L+1 (28%), H-9→LUMO (14%)
25	259	0.0129	Singlet	H-10→L+1 (57%), H-11→LUMO (-20%), H-8→LUMO (18%)
26	259	0.165	Singlet	H-10→LUMO (46%), H-9→LUMO (-23%), H-11→L+1 (-14%)

6

No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributors
1	452	0.1157	Singlet	HOMO→L+2 (64%), HOMO→L+1 (32%)
2	443	0.4286	Singlet	H-1→LUMO (88%)
3	431	0.2825	Singlet	HOMO→L+1 (57%), HOMO→L+2 (-31%), H-2→L+1 (-12%)
4	397	0.0065	Singlet	H-1→L+2 (91%)
5	387	0.0268	Singlet	H-2→LUMO (82%)
6	380	0.1401	Singlet	H-4→LUMO (72%)
7	377	0.1311	Singlet	H-2→L+1 (82%), HOMO→L+1 (12%)
8	361	0.0182	Singlet	H-5→LUMO (90%)
9	360	0.0518	Singlet	H-3→L+1 (88%)
10	355	0.0024	Singlet	HOMO→L+3 (97%)
11	349	0.0512	Singlet	H-1→L+3 (95%)
12	331	0.0129	Singlet	HOMO→L+5 (79%), HOMO→L+4 (-18%)
13	328	0.0021	Singlet	H-2→L+2 (97%)
14	320	0.0034	Singlet	H-6→LUMO (99%)
15	314	0.0298	Singlet	H-6→L+1 (96%)
16	307	0.1075	Singlet	H-7→LUMO (82%)
17	301	0.0012	Singlet	H-4→L+2 (94%)
18	286	0.0018	Singlet	H-9→LUMO (92%)
19	278	0.685	Singlet	H-6→L+2 (80%)
20	278	0.0032	Singlet	H-2→L+3 (93%)
21	277	0.0032	Singlet	H-8→LUMO (97%)
22	273	0.0065	Singlet	H-4→L+3 (90%)
23	269	0.0013	Singlet	H-10→LUMO (95%)
24	268	0.0013	Singlet	H-10→L+1 (91%)
25	268	0.0114	Singlet	H-7→L+1 (94%)
26	261	0.0063	Singlet	H-5→L+3 (80%)
27	261	0.0375	Singlet	H-12→L+2 (38%), H-5→L+3 (-17%), H-7→L+2 (11%)

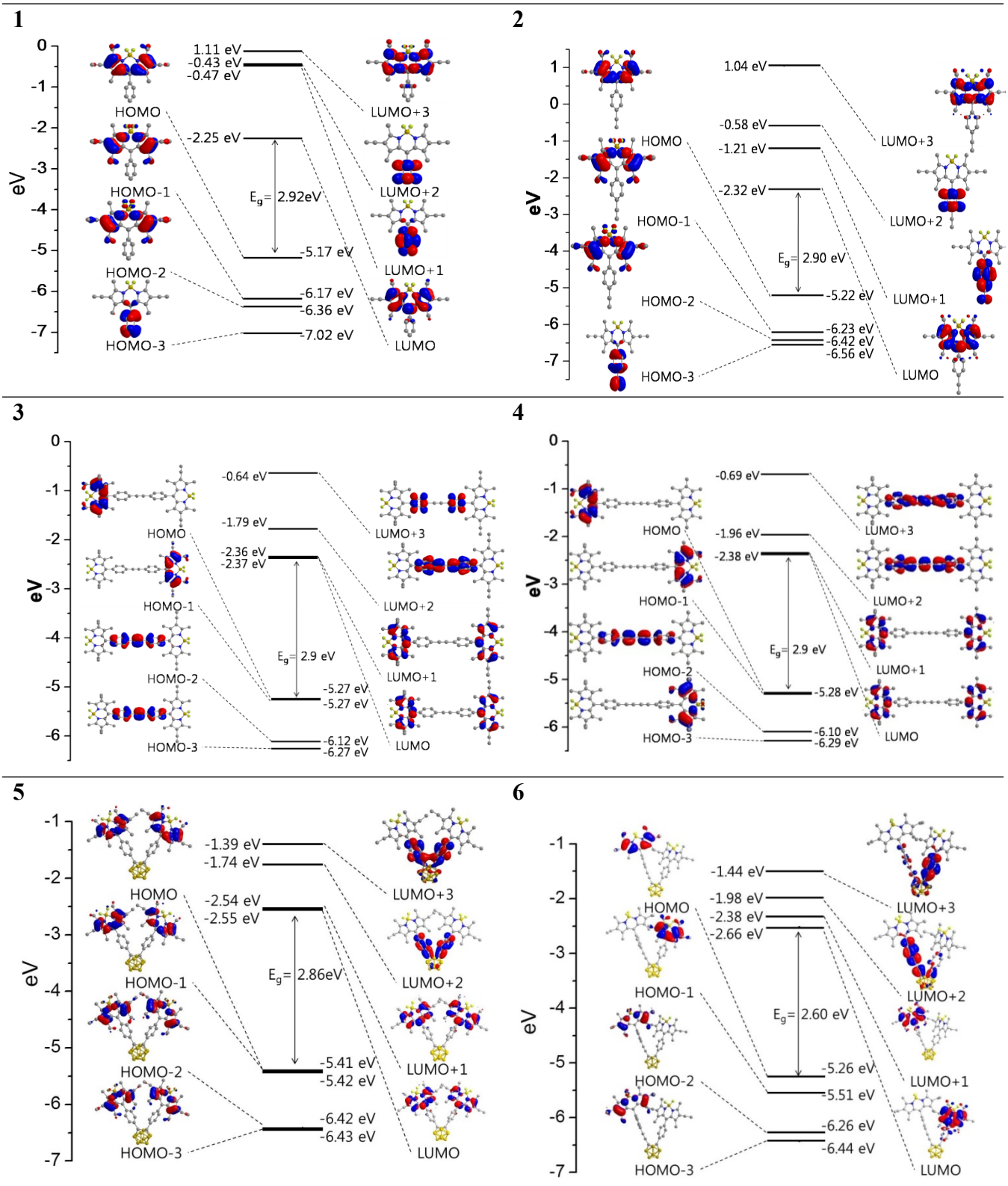


Fig. S1 Energy levels and isodensity plots for selected occupied and unoccupied molecular orbitals of the complexes.

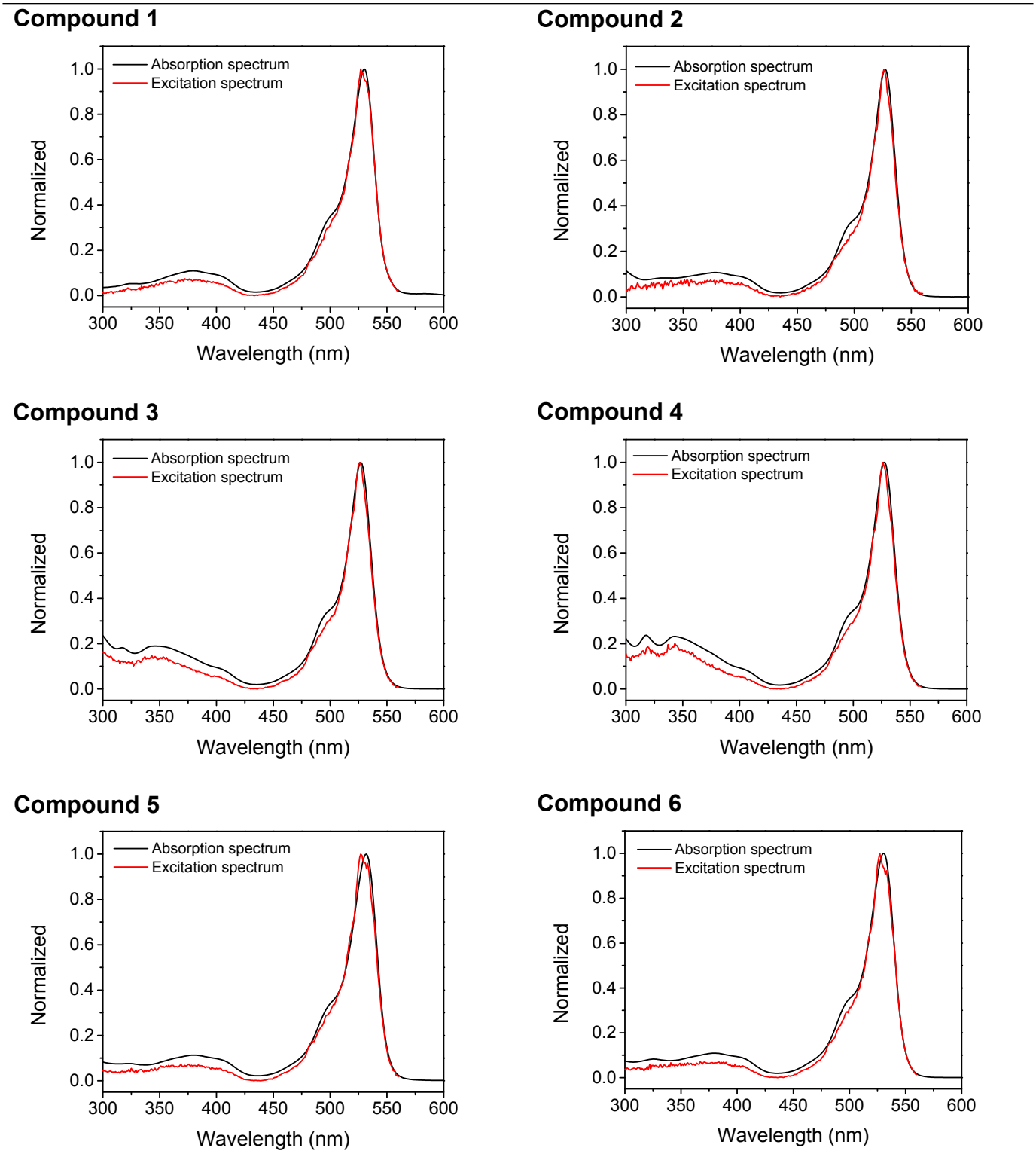


Fig. S2 Absorption (black lines) and excitation (red lines) spectra of **1**–**6** in CH_2Cl_2 at room temperature.

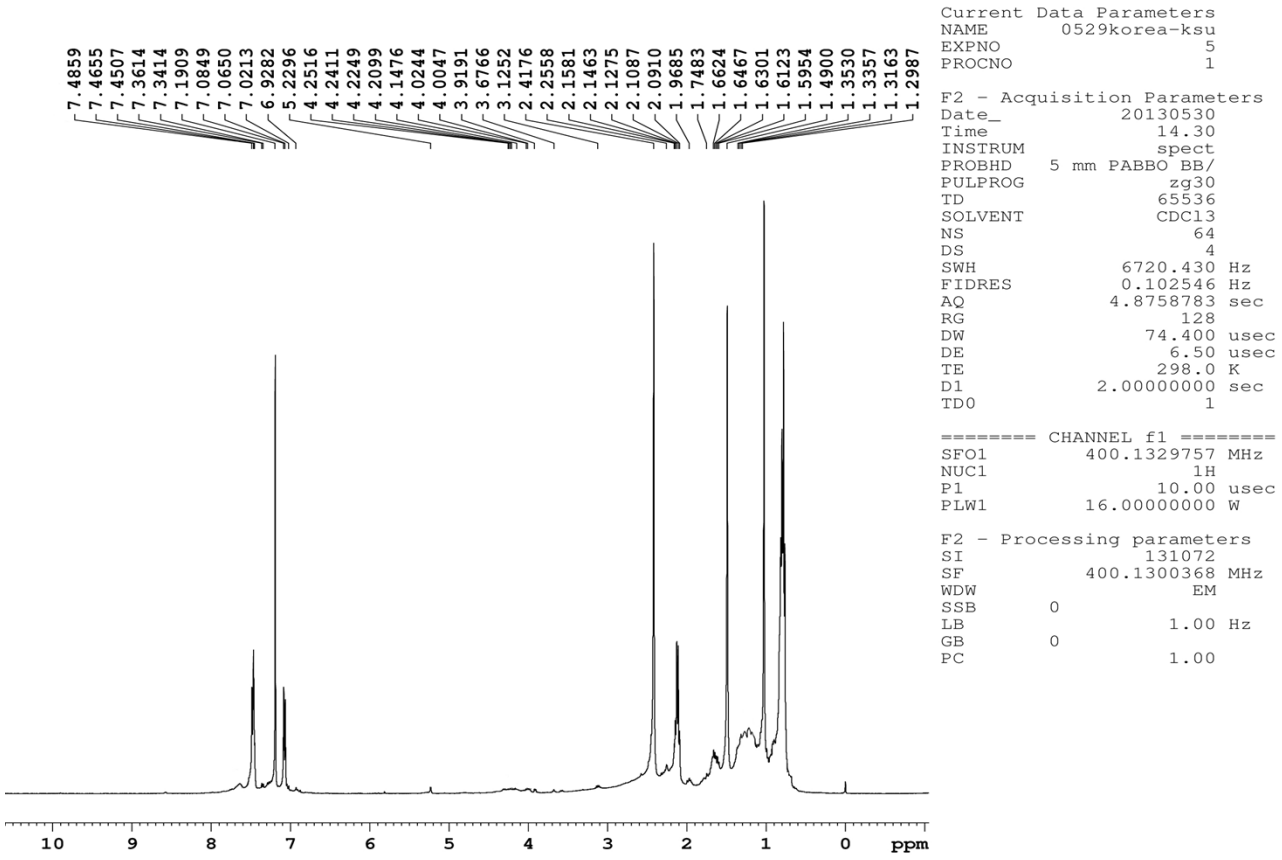


Fig. S3 ^{1}H-NMR spectrum of compound **5**.

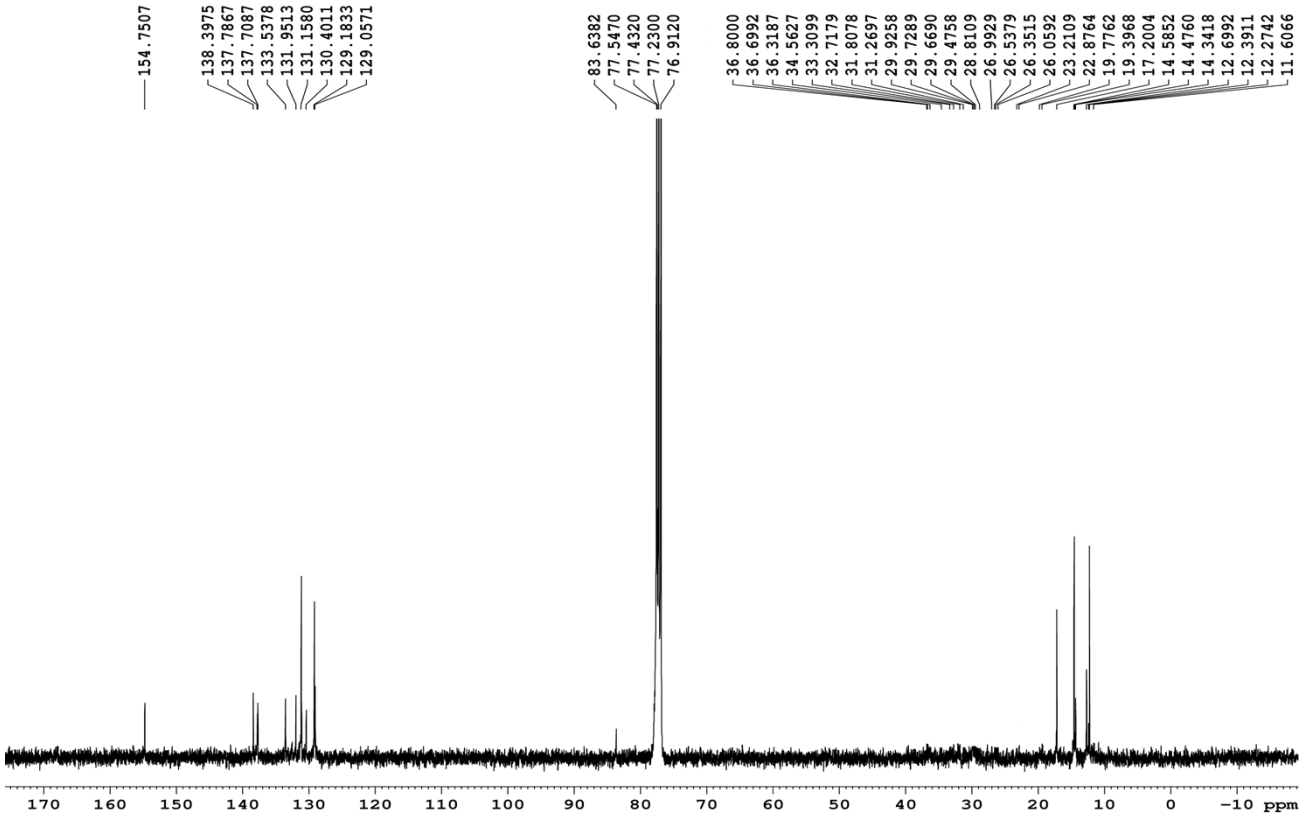
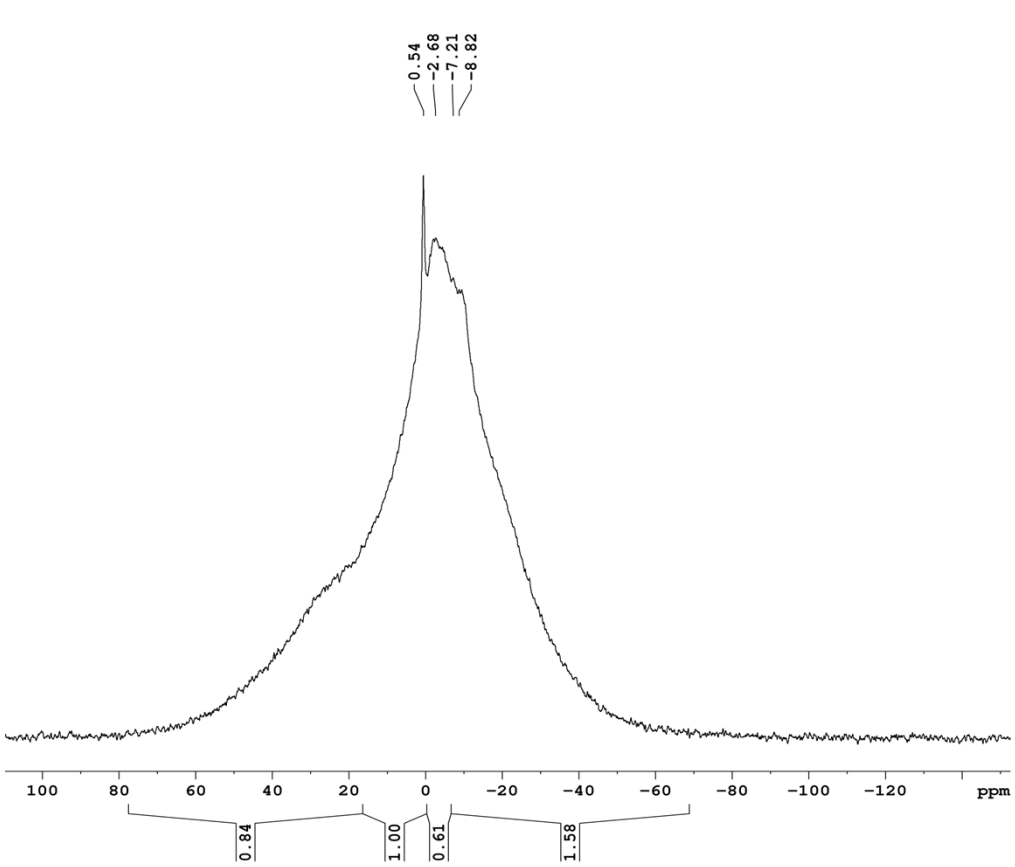


Fig. S4 ^{13}C-NMR spectrum of compound **5**.

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PROCNO                  1

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DS                    4
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RG                  812
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DE                6.50 usec
TE                298.0 K
D1           5.00000000 sec
D11          0.03000000 sec
TD0                   1

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P1                5.00 usec
PLW1        60.00000000 W

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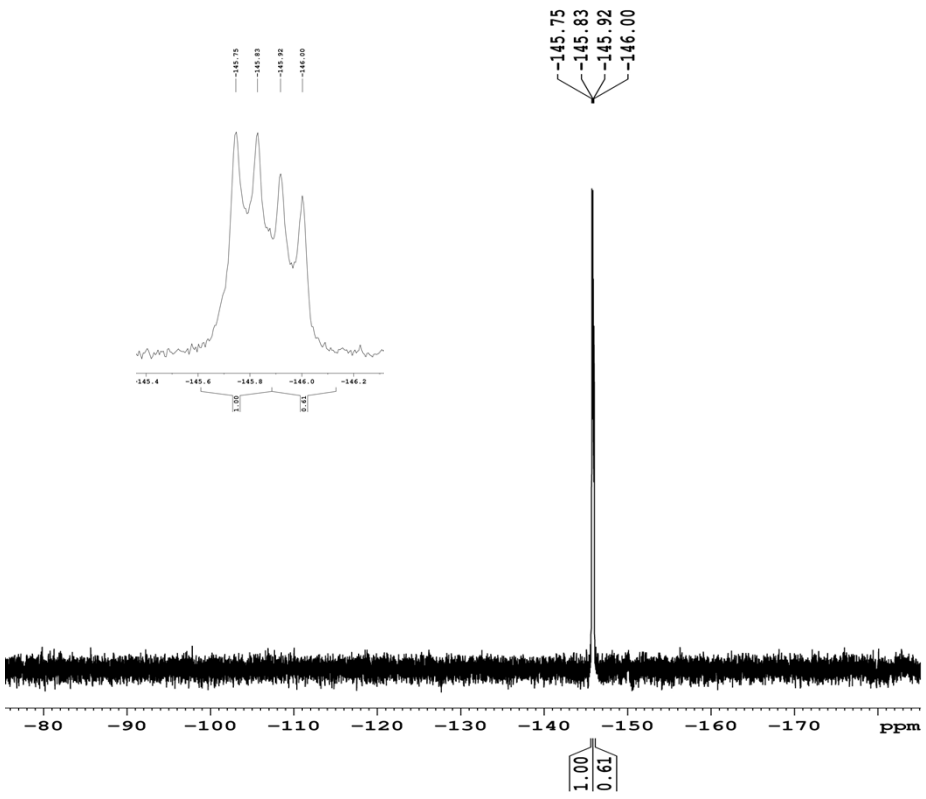
Fig. S5 $^{11}B\{^{1}H\}$-NMR spectrum of compound **5**.

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PROCNO                  1

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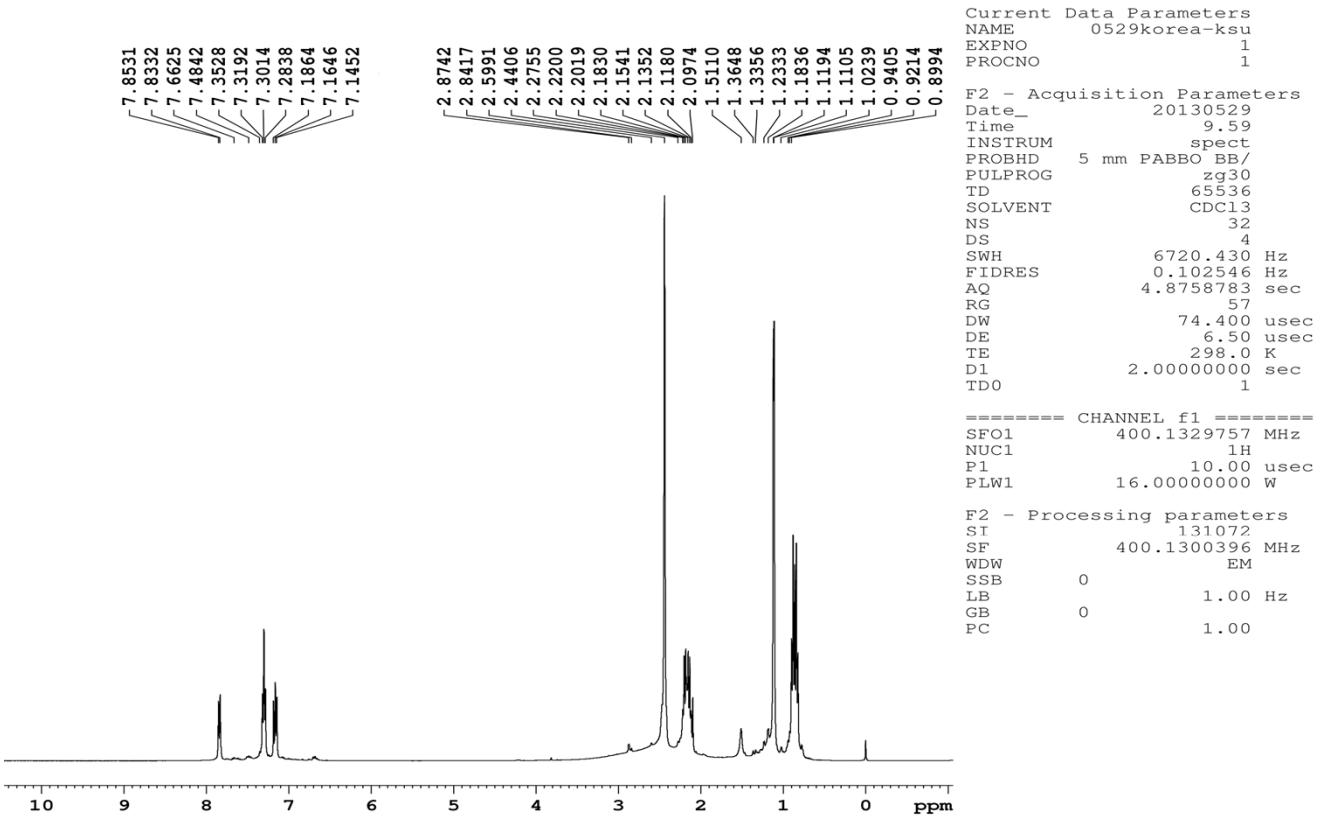
RG                  812
DW               7.800 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

========= CHANNEL f1 =========
SFO1        376.4607162 MHz
NUC1               19F
P1               14.00 usec
PLW1        27.00000000 W

========= CHANNEL f2 =========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        16.00000000 W
PLW12        0.19753000 W
PLW13        0.16000000 W

F2 - Processing parameters
SI                32768
SF           376.4983660 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

Fig. S6 ^{19}F-NMR spectrum of compound **5**.



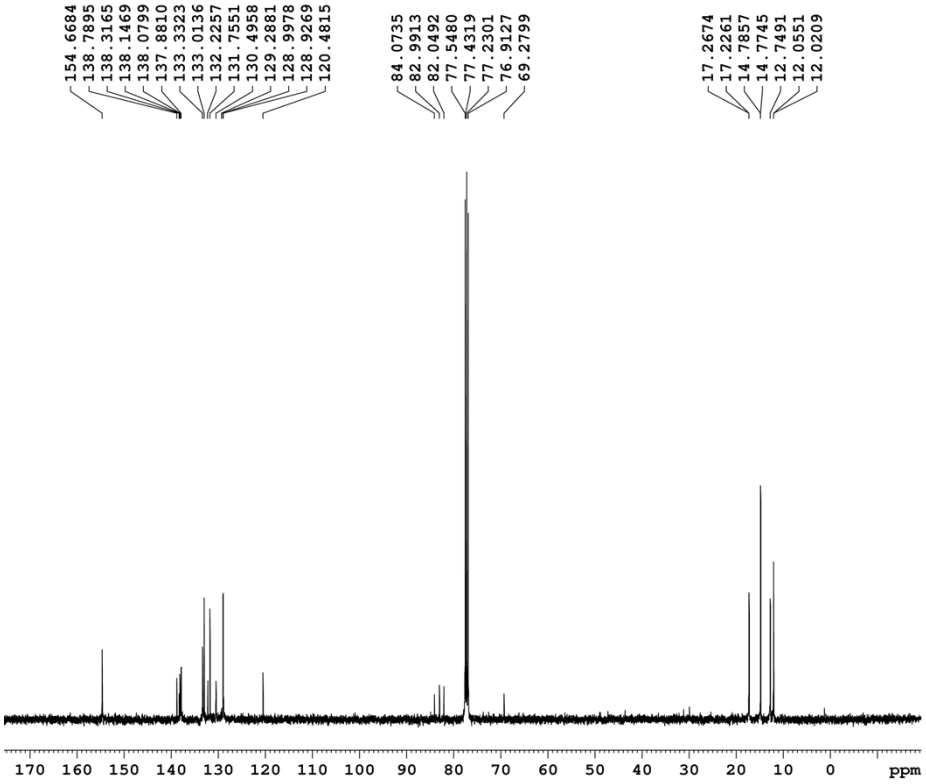

```
Current Data Parameters
NAME       0529korea-ksu
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130529
Time                9.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH             6720.430 Hz
FIDRES          0.102546 Hz
AQ             4.8758783 sec
RG                    57
DW               74.400 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1329757 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         16.00000000 W

F2 - Processing parameters
SI                131072
SF           400.1300396 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

Fig. S7 [1]H-NMR spectrum of compound **6**.




```
Current Data Parameters
NAME       0529korea-ksu
EXPNO                  2
PROCNO                 1

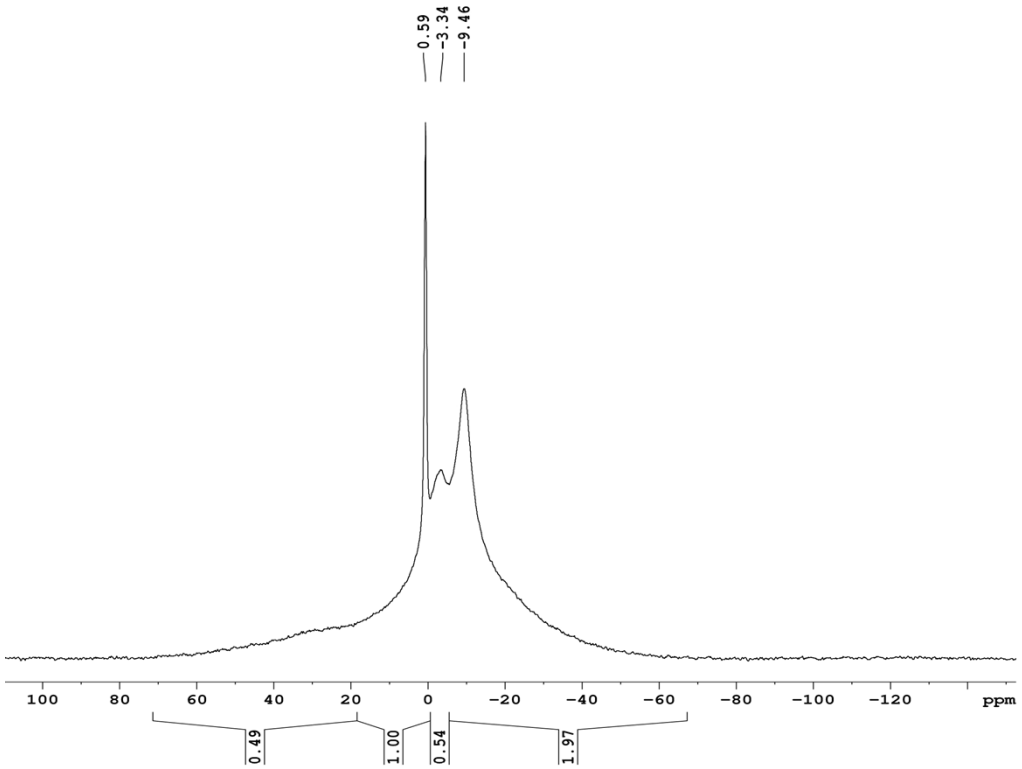
F2 - Acquisition Parameters
Date_           20130529
Time               10.09
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   526
DS                     8
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                  2050
DW               20.800 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                  13C
P1                 10.00 usec
PLW1         75.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
PLW13         0.16000000 W

F2 - Processing parameters
SI                 32768
SF           100.6127493 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Fig. S8 [13]C-NMR spectrum of compound **6**.




```
Current Data Parameters
NAME       0529korea-ksu
EXPNO                  4
PROCNO                 1

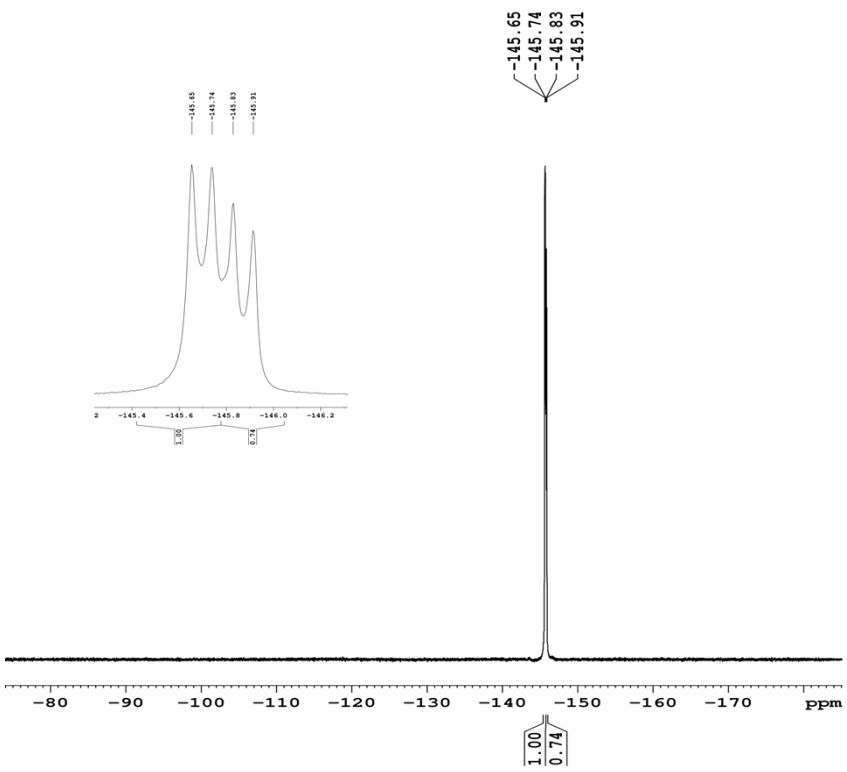
F2 - Acquisition Parameters
Date_           20130529
Time               11.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           38461.539 Hz
FIDRES         0.586877 Hz
AQ            0.8519680 sec
RG                  812
DW               13.000 usec
DE                6.50 usec
TE                298.0 K
D1           5.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        128.3772674 MHz
NUC1                  11B
P1                   5.00 usec
PLW1        60.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2        16.00000000 W
PLW12        0.19753000 W
PLW13        0.16000000 W

F2 - Processing parameters
SI                 32768
SF          128.3776250 MHz
WDW                   EM
SSB       0
LB                30.00 Hz
GB        0
PC                 0.50
```

Fig. S9 $^{11}B\{^{1}H\}$-NMR spectrum of compound **6**.




```
Current Data Parameters
NAME       0529korea-ksu
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130529
Time               10.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    8
SWH           64102.562 Hz
FIDRES         0.978127 Hz
AQ            0.5111808 sec
RG                  812
DW               7.800 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        376.4607162 MHz
NUC1                  19F
P1                  14.00 usec
PLW1        27.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2        16.00000000 W
PLW12        0.19753000 W
PLW13        0.16000000 W

F2 - Processing parameters
SI                 32768
SF          376.4983660 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Fig. S10 ^{19}F-NMR spectrum of compound **6**.

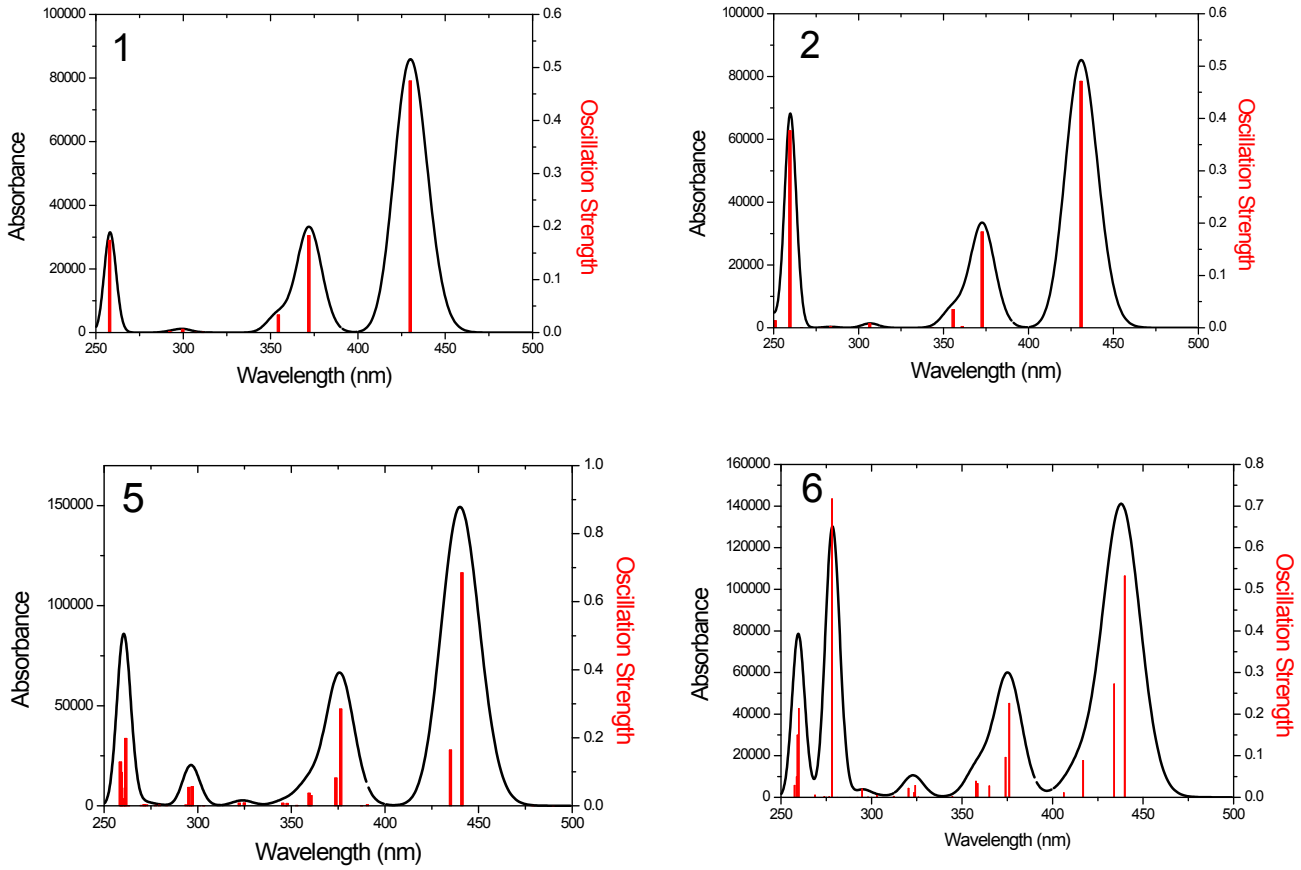


Fig. S11 Simulated absorption spectra of references (**1** and **2**) and dyads (**5** and **6**) calculated by TD-DFT.

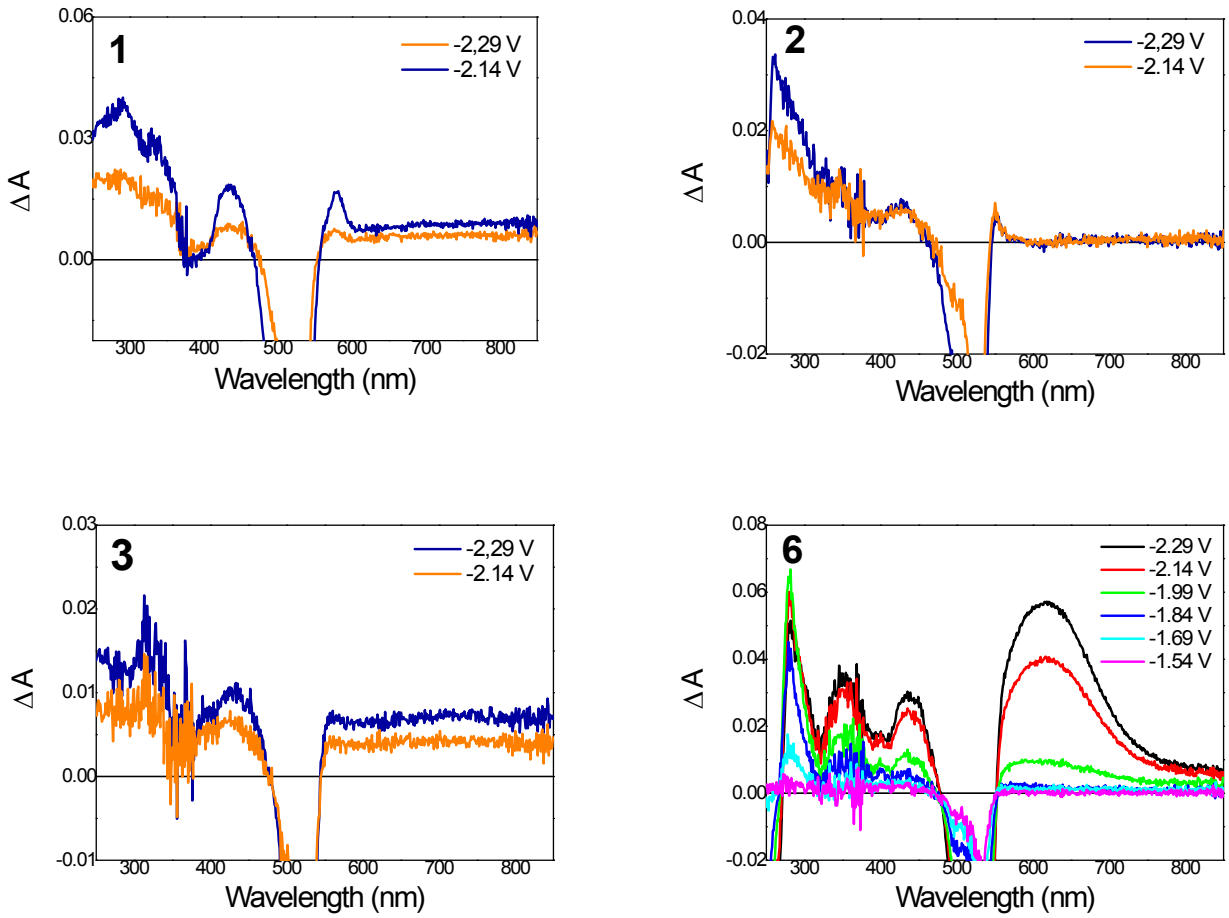


Fig. S12 Spectroelectrochemical spectra for **1**, **2**, **3** and **6** under various voltages.