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Color-tuning and Manipulation of Aggregation-Induced Emission Efficiency of *o*-Carborane-Tetraphenylethylene Dyads through Substituted *o*-Carboranes

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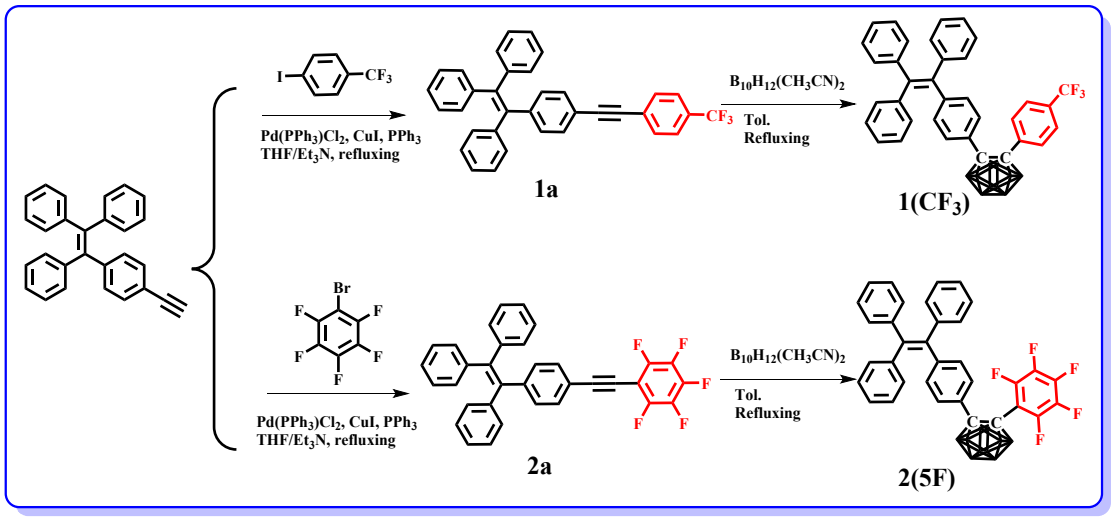
CONTENTS

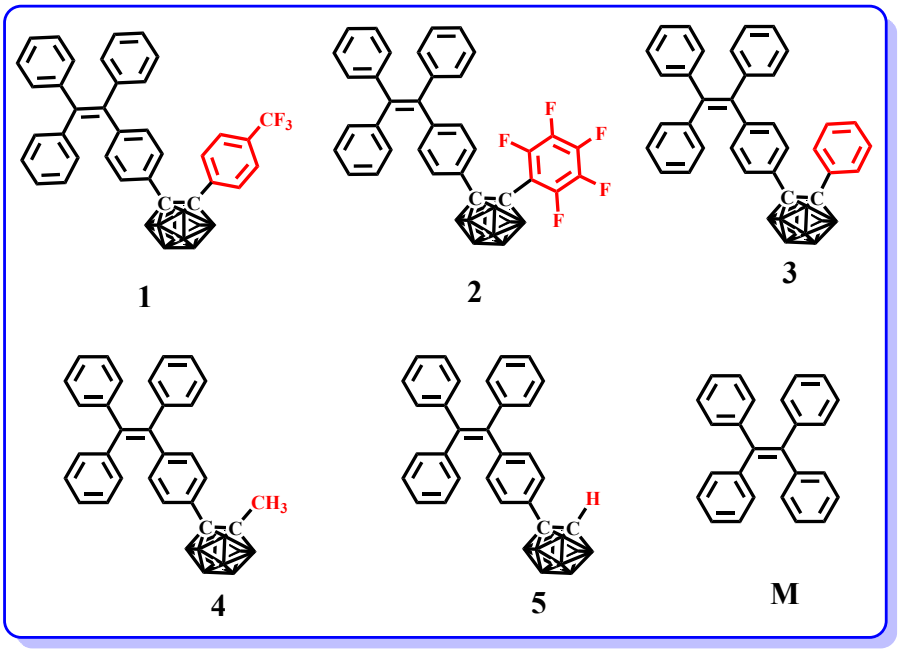
I. General method

In this work, all the synthetic steps were carried out under an inert argon atmosphere using standard Schlenk and glovebox techniques. Commercial reagents were used without any further purification after purchasing. THF and toluene were distilled on sodium / benzophenone. The compounds 1-iodo-4-(trifluoromethyl)benzene and 1-bromo-2,3,4,5,6-pentafluorobenzene were purchased from Shanghai Haohong ScientificCo.,Ltd. The (2-(4-ethynylphenyl)ethene-1,1,2-triyl)tribenzene was synthesized according to literature procedures.[S1] $B_{10}H_{12}(CH_3CN)_2$ was synthesized by a modified method according to literature reports.[S2] Model compound **M** was also synthesized according to literature procedures.[S3] NMR spectra ($^{1}H-$, $^{13}C-$, and $^{11}B-$) were recorded on DRX−500 at ambient temperature. $CDCl_3$ was used as deuterated reagent unless specified. Mass spectra were measured with EI−MS and APCI-HRMS (LCQ Fleet, Thermo Fisher Scientific). The UV-vis absorption spectra were obtained by SHIMADZU UV-2600. Photoluminescence spectra and decay curves were obtained by using Edinburgh FLS980 fluorescence spectrophotometer equipped with a 450 W xenon arc lamp, a picosecond pulsed LED (EPLED-380) and a microsecond flash-lamp (μF900). The decay curves were fitted by F980 software determined from a multi-exponential function: $R(t) = \sum B_i exp(-t/\tau_i)$. The absolute photoluminescence quantum yields of compounds were collected on FLS980 with integrating sphere and a supplied reference plug was used as a reference sample. Photoluminescence spectra and excitation-emission maps were measured on the HITACHI fluorescence spectrophotometer F-4700.

II. Synthesis



Scheme S1. Synthetic routes towards **1** and **2**.



Scheme S2. Compounds 1-5 are studied and discussed in this article.

Synthesis of (2-(4-((4-(trifluoromethyl)phenyl)ethynyl)phenyl)ethene-1,1,2-triyl)tribenzene (1a):

To a mixture of (2-(4-ethynylphenyl)ethene-1,1,2-triyl)tribenzene (970 mg, 2.8 mmol), $Pd(PPh_3)_2Cl_2$ (210 mg,0.28 mmol), PPh_3 (73.4 mg, 0.28 mmol) and copper iodide (56 mg, 0.28 mmol) was added THF (50 mL) under nitrogen and the suspension was stirred

at room temperature for 15 min. Triethylamine (25 mL) was added to the reaction mixture and stirred for 1 h at room temperature. To the reaction mixture was added 1-iodo-4-(trifluoromethyl)benzene (0.76 g, 2.8 mmol). The resulting reaction mixture was refluxed for 24h, solvent was removed in a rotary evaporator and the crude product was purified using column chromatography (silica gel, PE/DCM =4:1) to yield the (2-(4-((4-(trifluoromethyl)phenyl)ethynyl)phenyl)ethene-1,1,2-triyl)tribenzene (**1a**) (996 mg, 73%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 4H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.18 – 7.10 (m, 9H), 7.09 – 7.01 (m, 8H).^{13}C NMR (100 MHz, $CDCl_3$) δ 144.64, 143.42, 143.27, 141.94, 140.14, 131.74, 131.57 – 130.83 (m), 128.18 – 127.54 (m), 127.19, 126.72 (d, *J* = 7.9 Hz), 125.30, 120.31, 92.04, 88.21. EI-MS (m/z): calcd for $C_{35}H_{23}F_3$, 500.56; found 500.17.^{19}F NMR (377 MHz, $CDCl_3$) δ -62.73.

Synthesis of 1.

To a toluene solution (50 mL) of (2-(4-((perfluorophenyl)ethynyl)phenyl)ethene-1,1,2-triyl)tribenzene (**1a**) (683 mg, 1.4 mmol), $B_{10}H_{12}(CH_3CN)_2$ (0.57 g, 2.8 mmol) was added at room temperature. The resulting reaction mixture was refluxed for 24h. MeOH (30 mL) was then added to quench the reaction. Excessive solvent was removed under vacuum, and the resulting red solid was filtered and dissolved in toluene. Then the toluene solution was passed through an alumina column. After removal of solvent, a yellow-white solid was afforded. The crude product was purified by column chromatography using hexane / CH_2Cl_2 (V / V = 3:1) as eluent to afford **1** as a yellow solid (390 mg, 45 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.5 Hz, 2H), 7.46 (d, *J* = 8.6 Hz, 2H), 7.16 (d, *J* = 8.6 Hz, 2H), 7.07 (dq, *J* = 6.5, 3.6 Hz, 7H), 7.01 – 6.90 (m, 4H), 6.87 – 6.77 (m, 6H), 3.71−1.82 (br, 10H, B−H).^{13}C NMR (100 MHz, $CDCl_3$) δ 146.31, 142.98, 142.84, 142.37, 138.96, 134.41, 132.13, 131.80, 131.31, 131.08, 129.96, 127.89, 127.77, 127.66, 126.76 (d, *J* = 3.3 Hz), 125.31 – 124.94 (m), 85.49, 83.37.^{11}B NMR (128 MHz, $CDCl_3$) δ -1.66, -9.95.HRMS (APCI,*m*/*z*): calcd for $C_{35}H_{33}F_3B_{10}$, 618.74; found 618.35.^{19}F NMR (377 MHz, $CDCl_3$) δ -62.94.

Synthesis of (2-(4-((perfluorophenyl)ethynyl) phenyl)ethene-1,1,2-triyl)tribenzene

(2a):

To a mixture of (2-(4-ethynylphenyl)ethene-1,1,2-triyl)tribenzene (970 mg, 2.8 mmol), $Pd(PPh_3)_2Cl_2$ (210 mg,0.28 mmol), PPh_3 (73.4 mg, 0.28 mmol) and copper iodide (56 mg, 0.28 mmol) was added THF (50 mL) under nitrogen and the suspension was stirred at room temperature for 15 min. Triethylamine (25 mL) was added to the reaction mixture and stirred for 0.5 h at room temperature. To the reaction mixture was added 1-bromo-2,3,4,5,6-pentafluorobenzene (1.8 g, 7.3 mmol). The reaction mixture was refluxing under nitrogen for 24 h, solvent was removed in a rotary evaporator and the crude product was purified using column chromatography (silica gel/DCM: hexane 1:3) to yield the (2-(4-((perfluorophenyl)ethynyl)phenyl)ethene-1,1,2-triyl)tribenzene (**2a**) (776 mg, 53%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.32 (d, J = 8.1 Hz, 2H), 7.19 – 7.09 (m, 9H), 7.09 – 6.97 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.50, 143.29, 143.24, 143.12, 142.19, 139.94, 131.50, 131.32, 131.29, 131.24, 127.88, 127.81, 127.68, 126.82, 126.71, 126.69, 119.23, 101.87, and 100.36 (yne-C). EI-MS (m/z): calcd for $C_{34}H_{19}F_5$, 522.52; found 522.4. ^{19}F NMR (377 MHz, $CDCl_3$) δ -136.16, -136.18, -136.22, -136.24, -152.96, -153.01, -153.07, -161.87, -161.89, -161.93, -161.95, -161.99, -162.00.

Synthesis of 2.

To a toluene solution (50 mL) of (2-(4-((perfluorophenyl)ethynyl)phenyl)ethene-1,1,2-triyl)tribenzene (**2a**) (710 mg, 1.4 mmol), $B_{10}H_{12}(CH_3CN)_2$ (0.57 g, 2.8 mmol) was added at room temperature. The resulting reaction mixture was refluxed for 24h. MeOH (30 mL) was then added to quench the reaction. Excessive solvent was removed under vacuum, and the resulting red solid was filtered and dissolved in toluene. Then the toluene solution was passed through an alumina column. After removal of solvent, a yellow-white solid was afforded. The crude product was purified by column chromatography using hexane / CH_2Cl_2 (V / V = 3:1) as eluent to afford **2** as a yellow solid (210 mg, 25 %). ^{1}H−NMR (400 MHz, $CDCl_3$) δ (ppm): 7.25 (d, J = 6.3 Hz, 2H), 7.09 (m, 7H), 6.97 (m, 4H), 6.90 (m, 6H)., 3.25−1.70 (br, 10H, B−H).^{13}C−NMR (100 MHz, $CDCl_3$) δ (ppm): ^{13}C NMR (100 MHz, CDCl3) δ 146.78, 143.08, 142.77, 142.67,

142.59, 139.09, 131.53, 131.07, 129.49, 128.10, 127.86, 127.69, 127.48, 126.84, 126.62, 86.83 (Cb-C), and 74.62 (Cb-C). ^{11}B−NMR (128 MHz, $CDCl_3$) δ (ppm): 1.3, 0.1, -2.9, -4.1, -8.8, -9.88. HRMS (APCI, *m*/*z*): calcd for $C_{34}H_{29}F_5B_{10}$, 640.69; found 640.30. ^{19}F NMR (377 MHz, $CDCl_3$) δ -129.49, -129.50, -129.53, -129.54, -147.24, -147.26, -147.27, -147.30, -147.32, -147.33, -147.36, -147.37, -147.39, -159.37, -159.40, -159.44, -159.46, -159.50, -159.53.

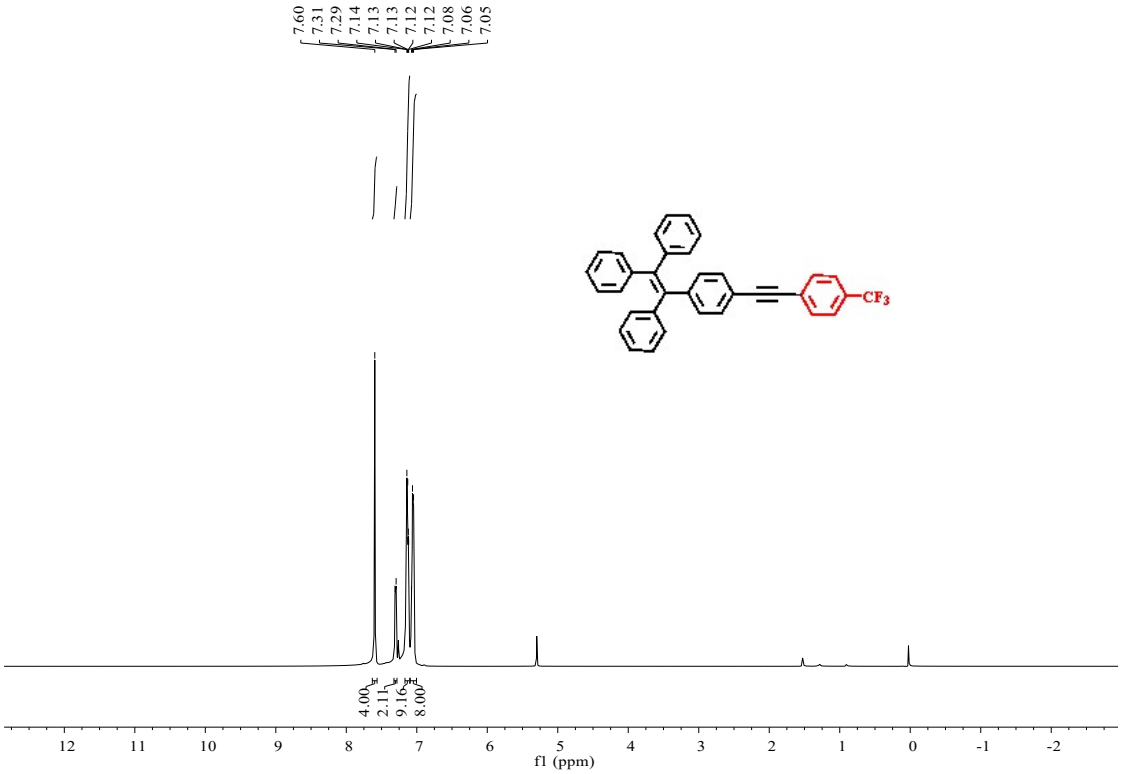


Figure.S1. The ^{1}H−NMR (400 MHz, $CDCl_3$) spectrum of compound **1a**.

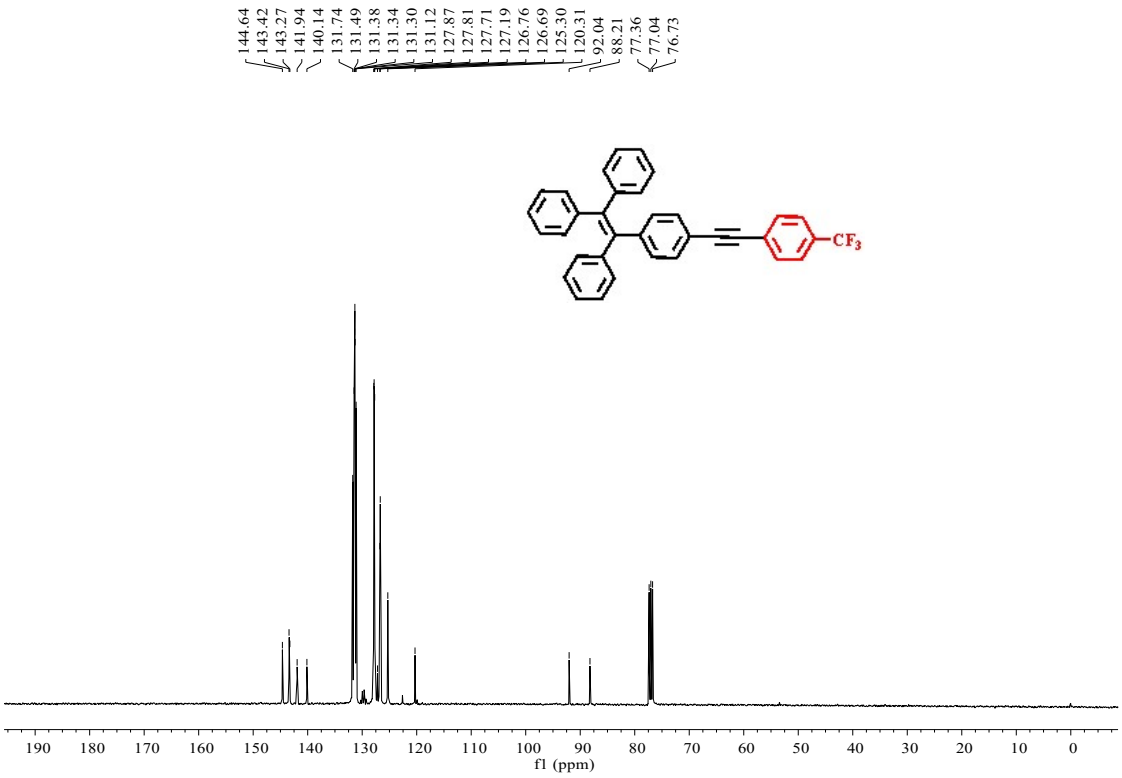


Figure.S2. The ^{13}C–NMR (100 MHz, $CDCl_3$) spectrum of compound **1a**.

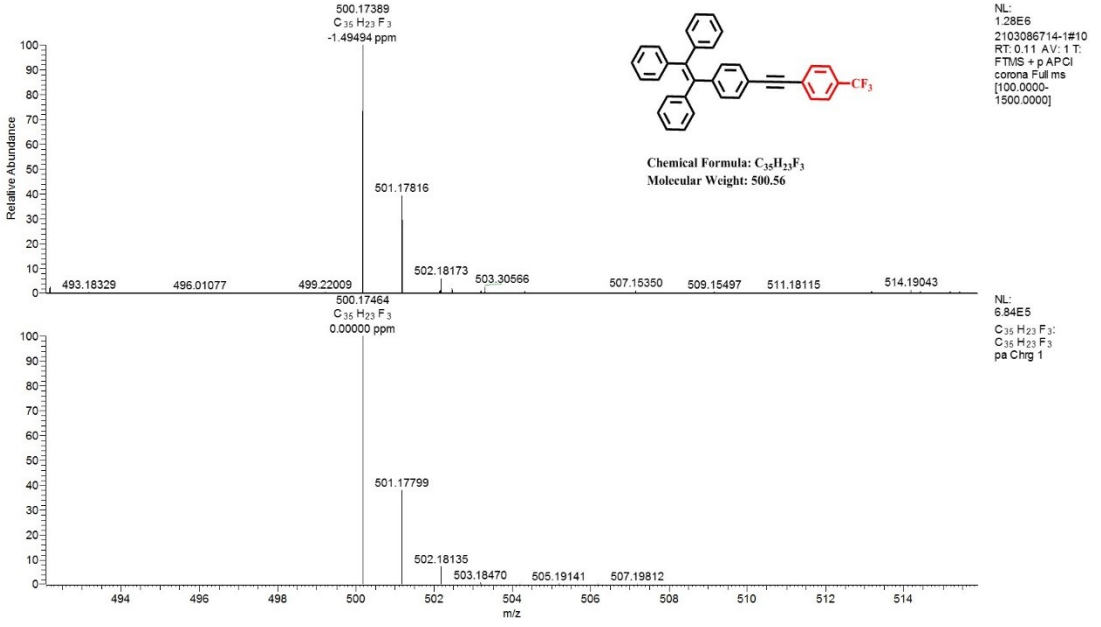


Figure.S3. The EI-MS spectrum of compound **1a**

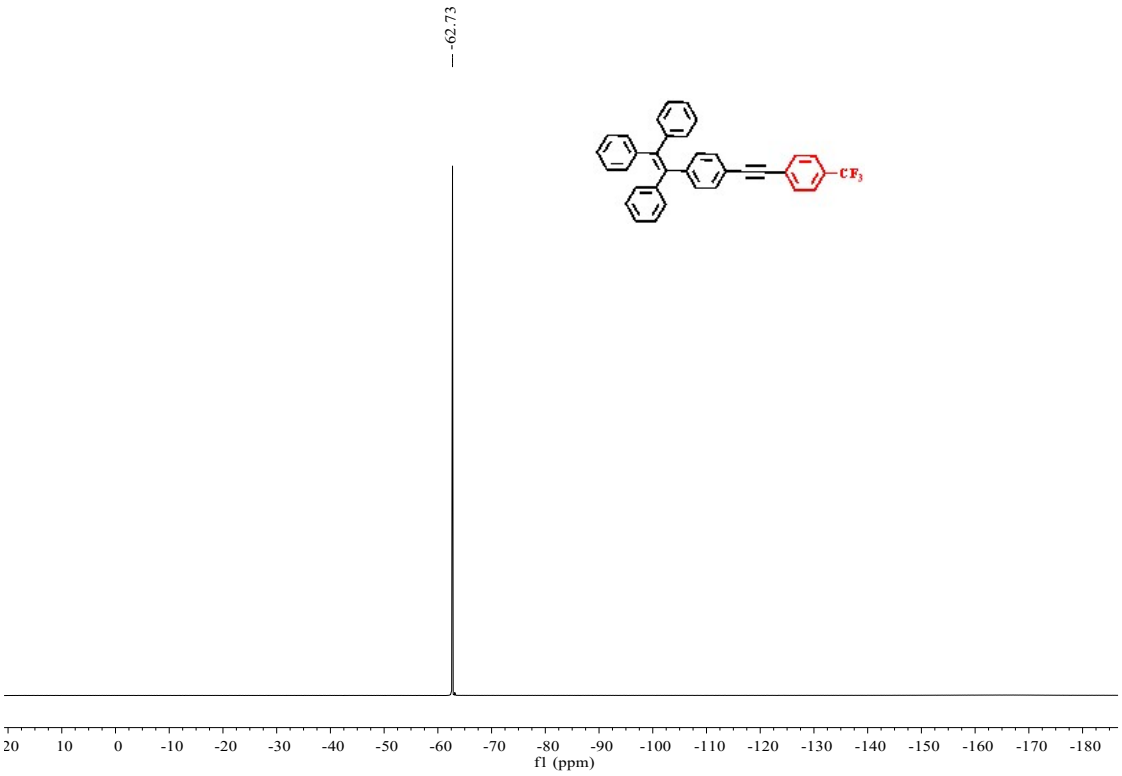


Figure.S4. The $^{19}F-NMR$ ($CDCl_3$) spectrum of compound **1a**.

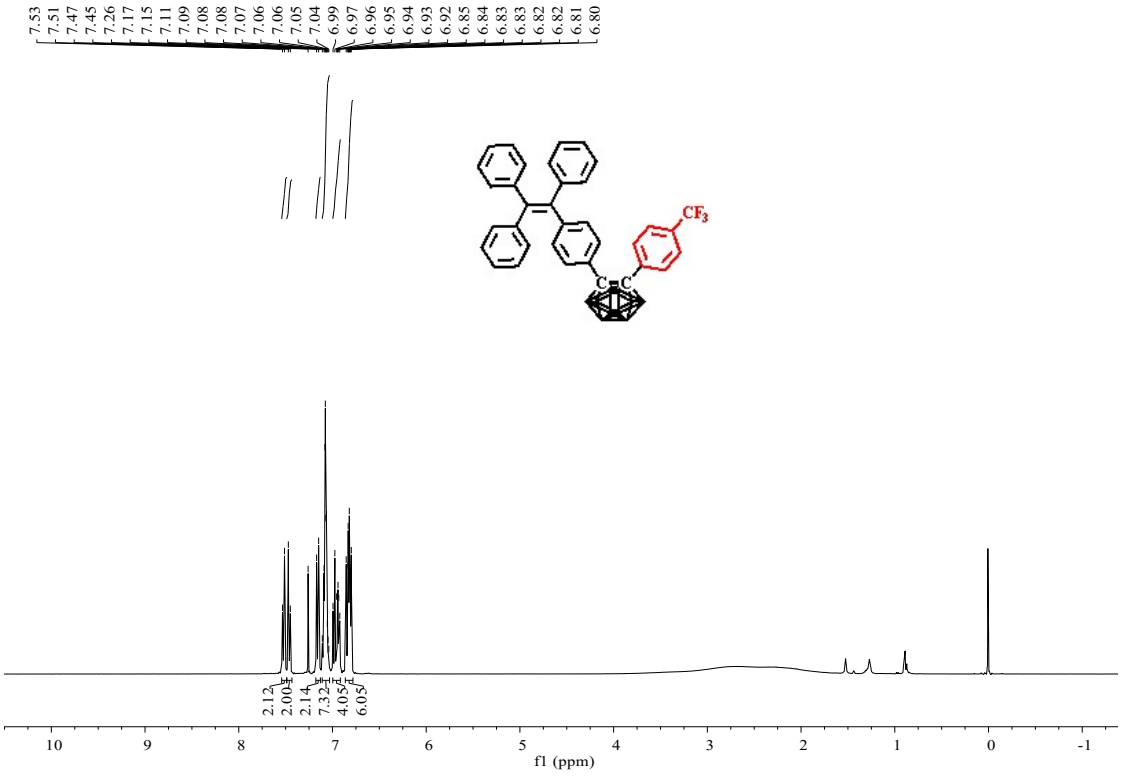


Figure.S5. The $^{1}H-NMR$ (400 MHz, $CDCl_3$) spectrum of compound **1**.

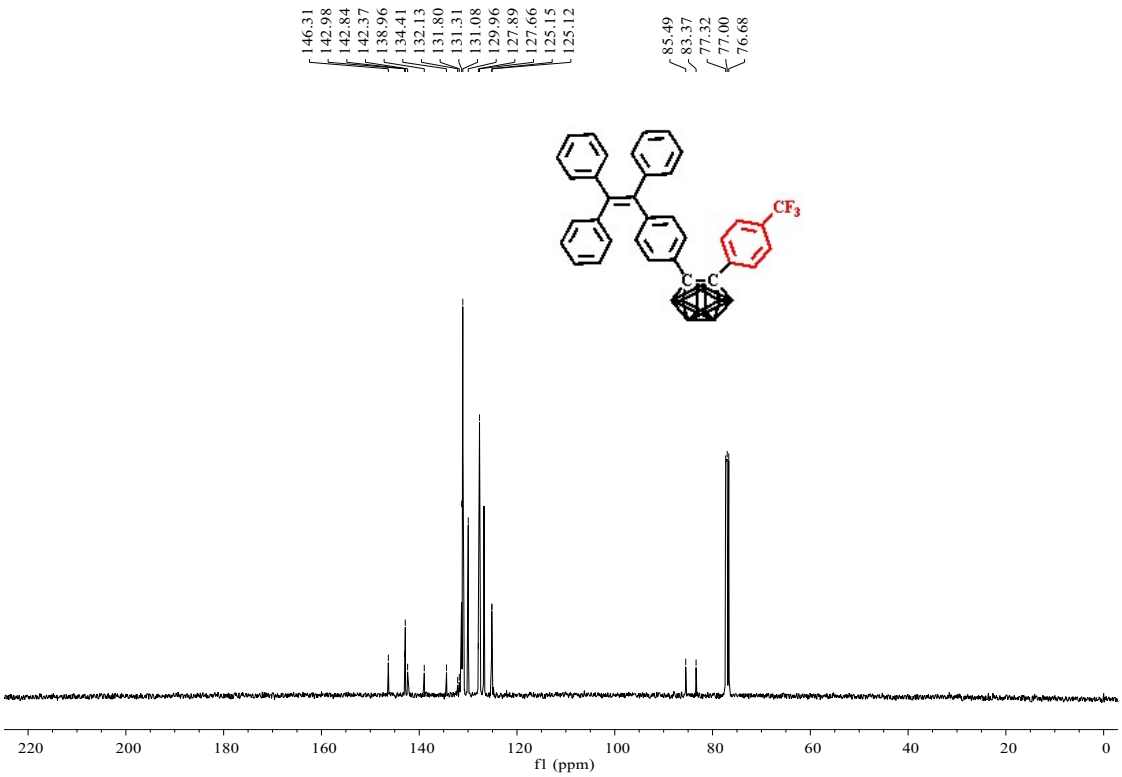


Figure.S6. The ^{13}C–NMR (100 MHz, $CDCl_3$) spectrum of compound **1**.

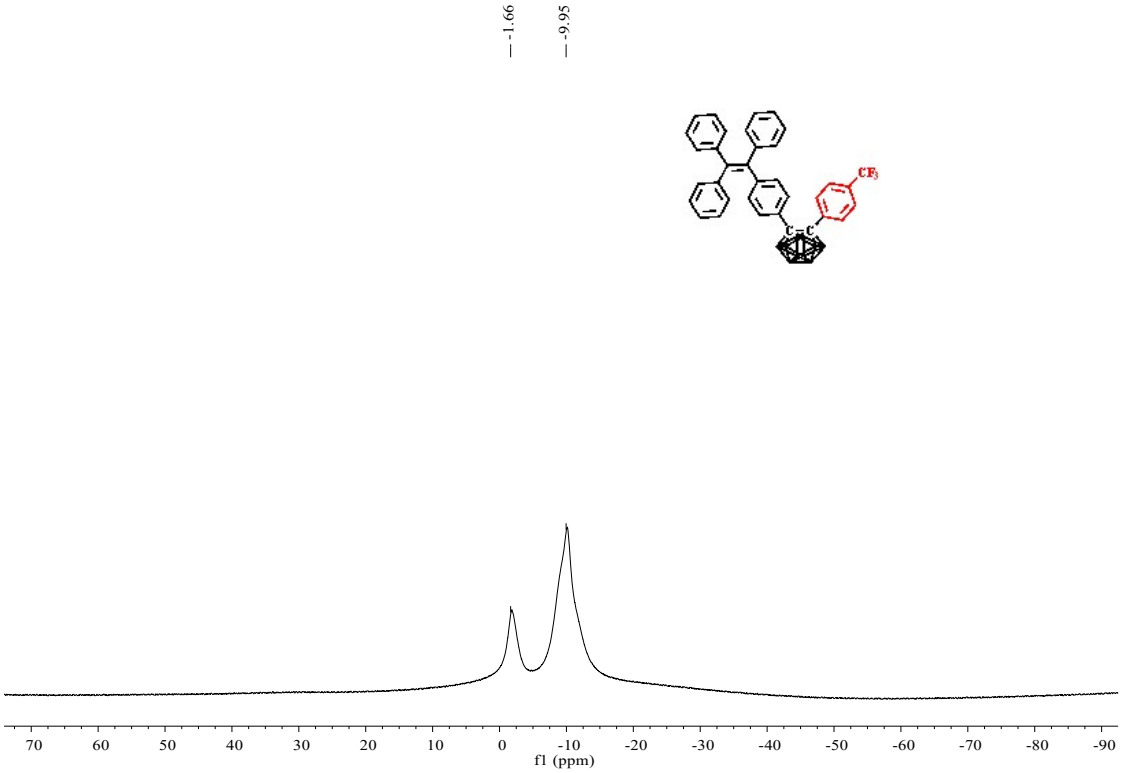


Figure.S7. The ^{11}B–NMR (128 MHz, $CDCl_3$) spectrum of compound **1.**

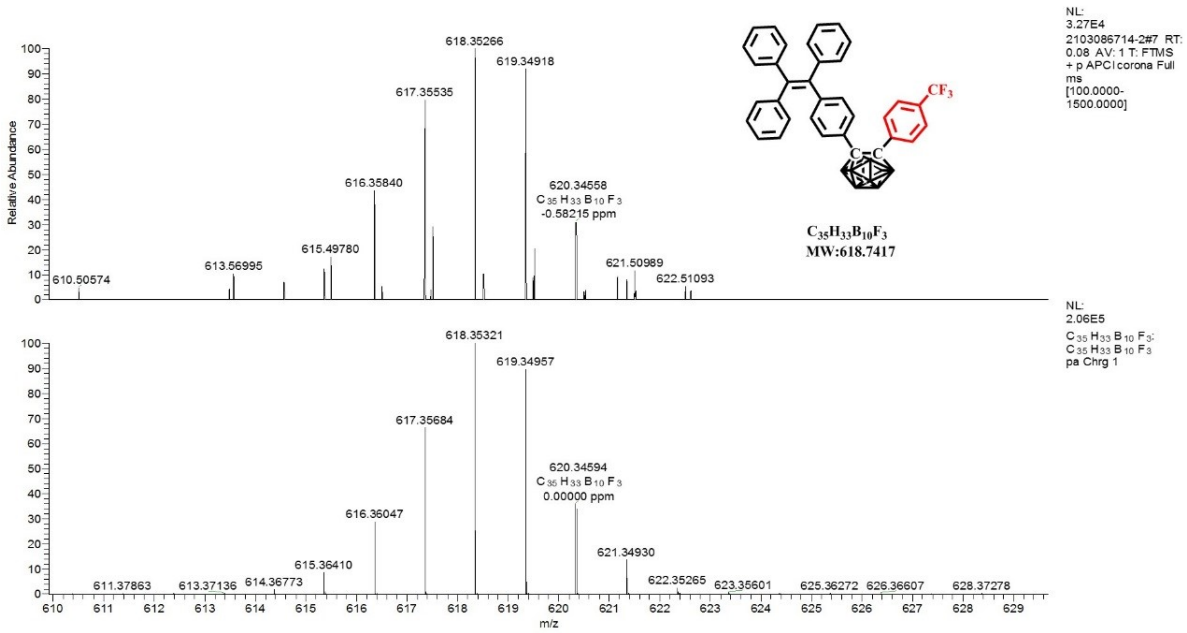


Figure.S8. The HRMS (APCI) spectrum of compound **1.**

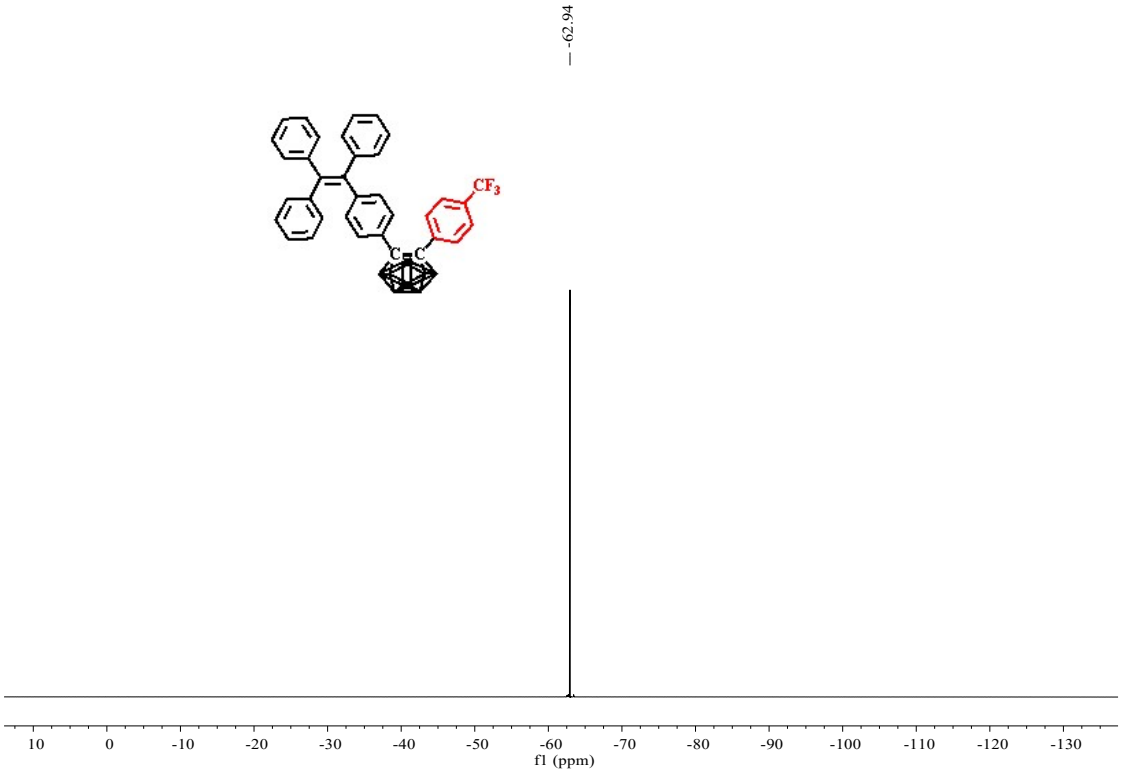


Figure.S9. The $^{19}F-NMR$ ($CDCl_3$) spectrum of compound **1**.

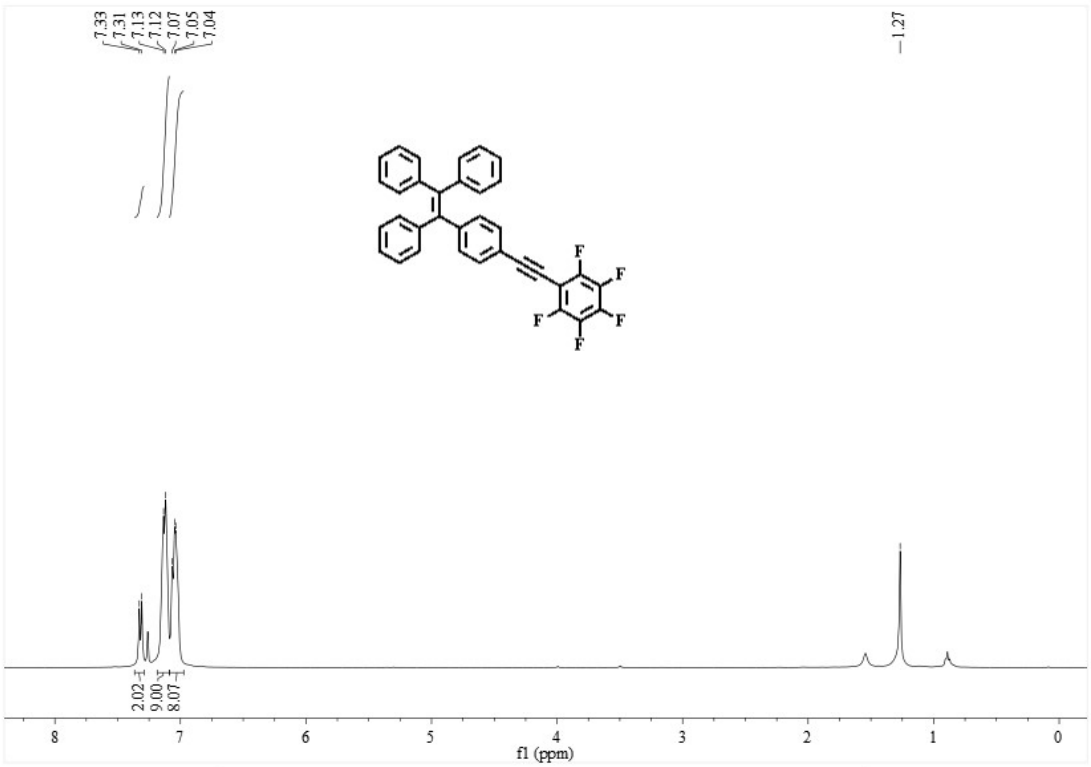


Figure.S10. The $^{1}H-NMR$ (400 MHz, $CDCl_3$) spectrum of compound **2a**.

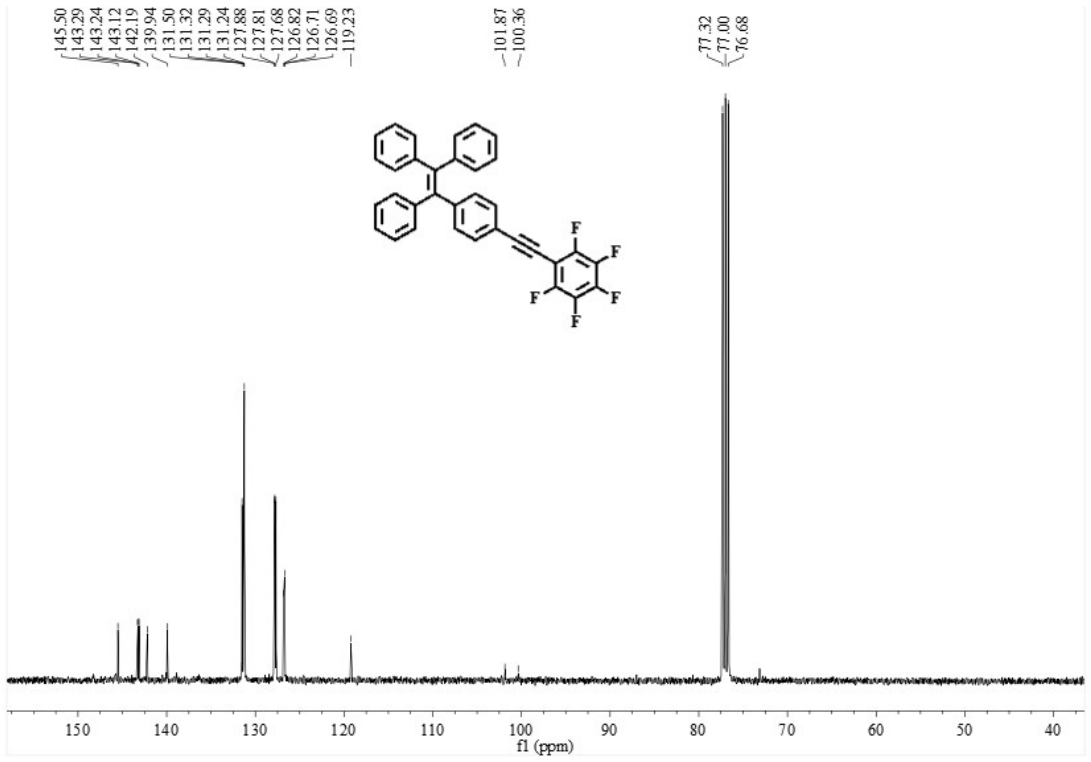


Figure.S11. The $^{13}C-NMR$ (100 MHz, $CDCl_3$) spectrum of compound **2a**.

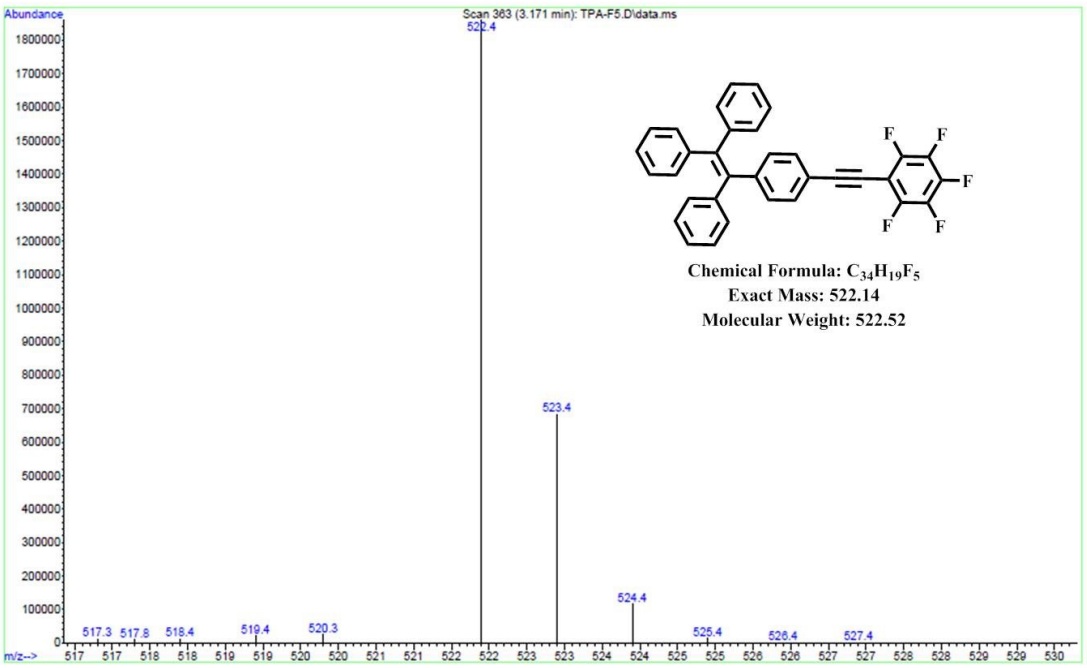


Figure.S12. The EI-MS spectrum of compound **2a**

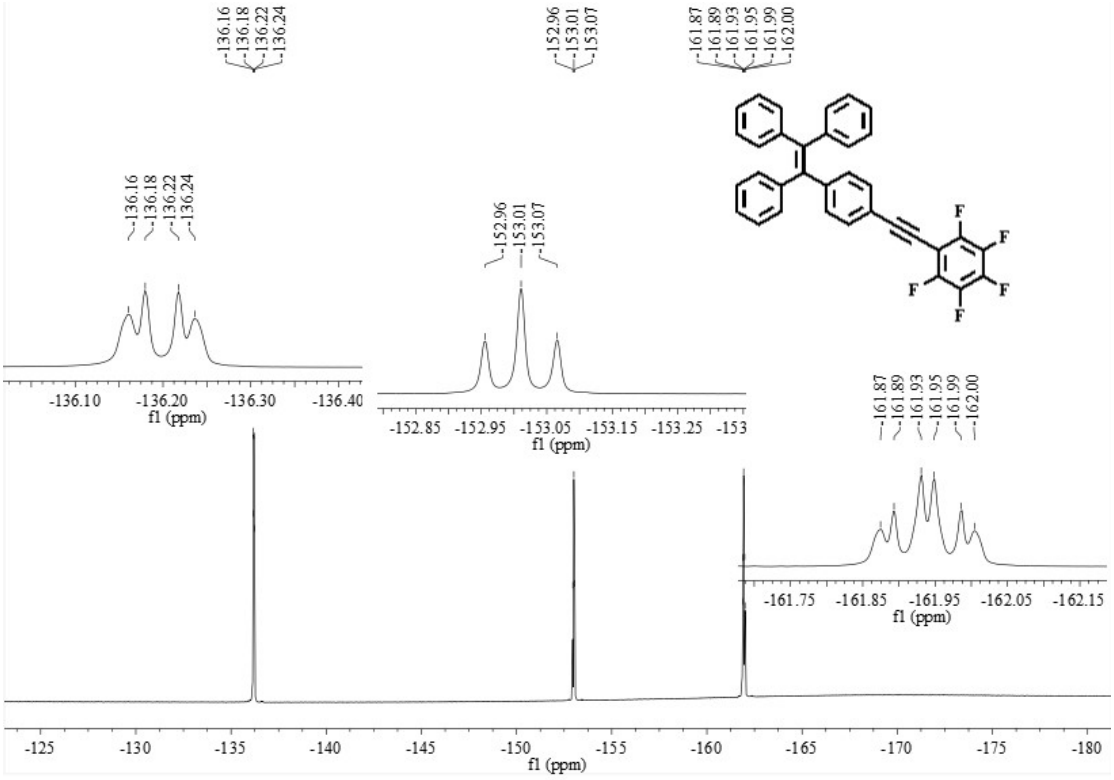


Figure.S13. The $^{19}F-NMR$ ($CDCl_3$) spectrum of compound **2a**.

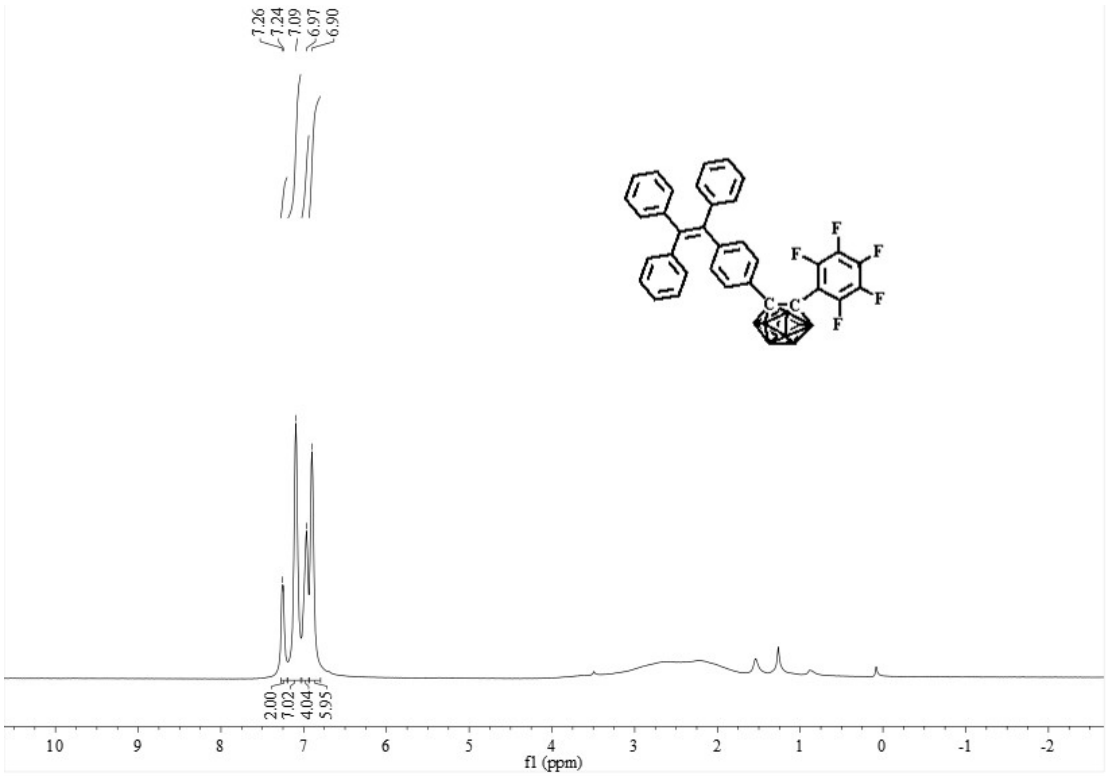


Figure.S14. The $^{1}H-NMR$ (400 MHz, $CDCl_3$) spectrum of compound **2**.

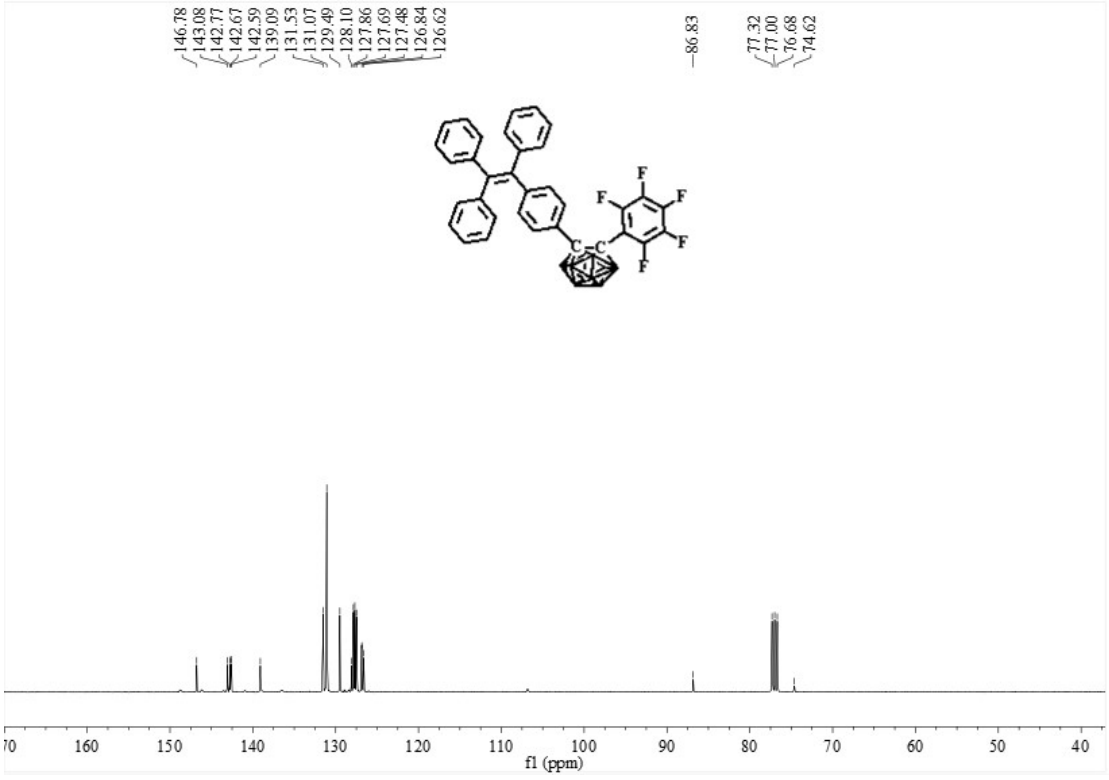


Figure.S15. The $^{13}C-NMR$ (100 MHz, $CDCl_3$) spectrum of compound **2**.

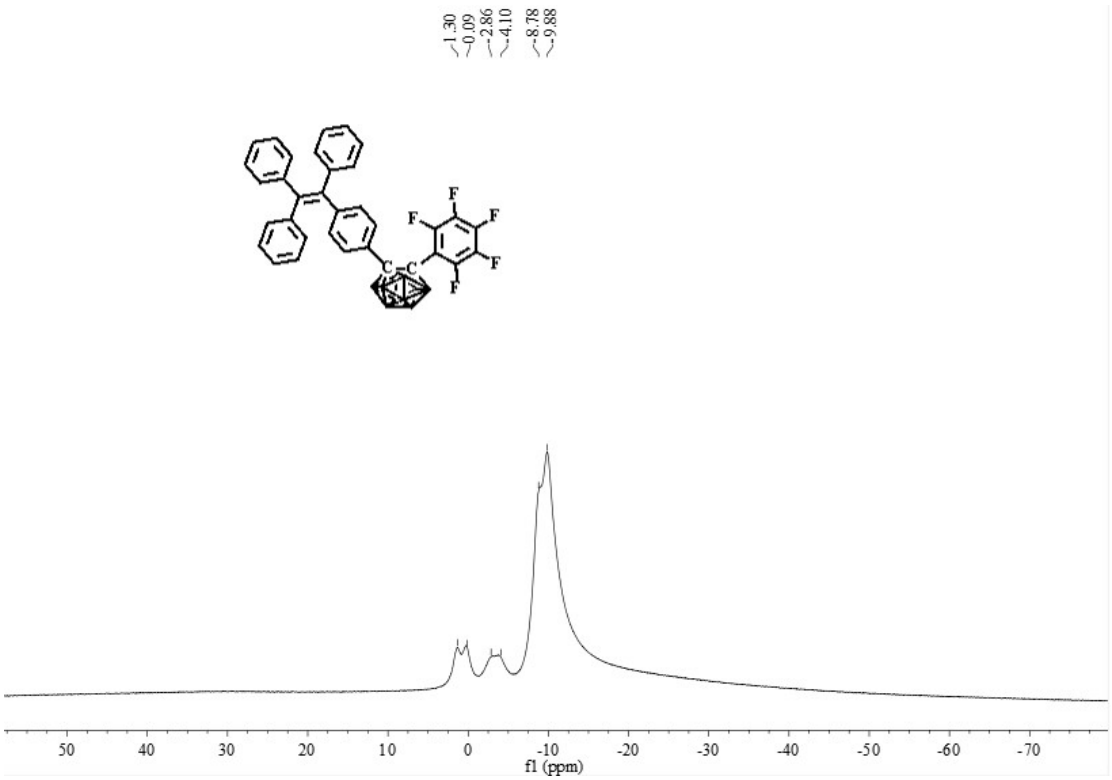


Figure.S16. The $^{11}B-NMR$ (128 MHz, $CDCl_3$) spectrum of compound **2**.

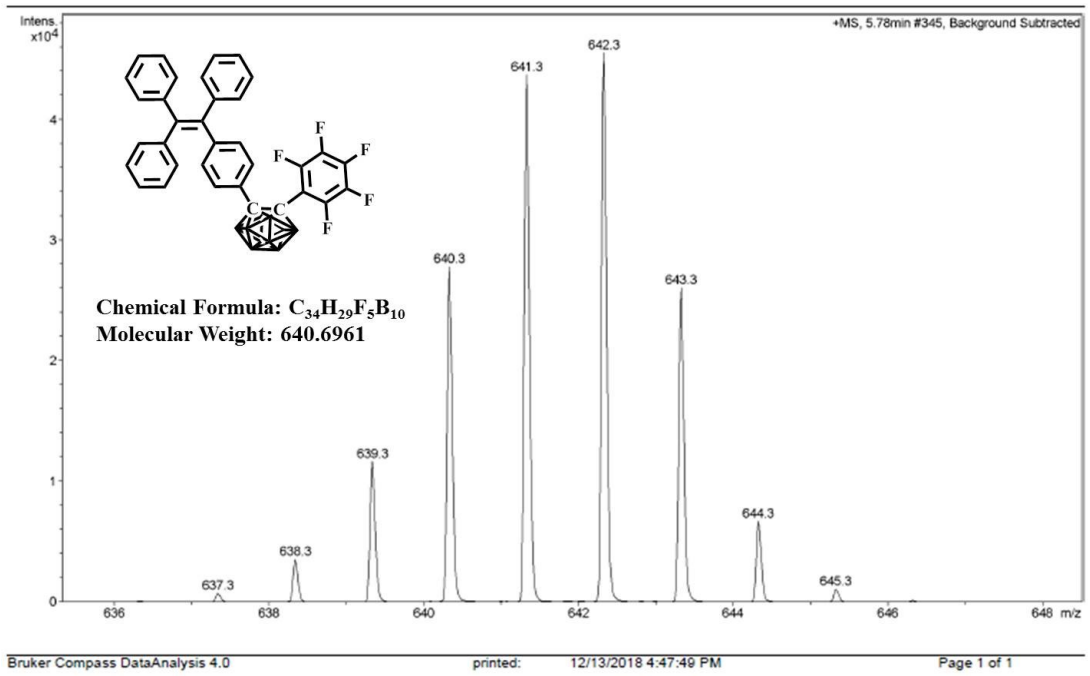


Figure.S17. The HRMS (APCI) spectrum of compound **2**.

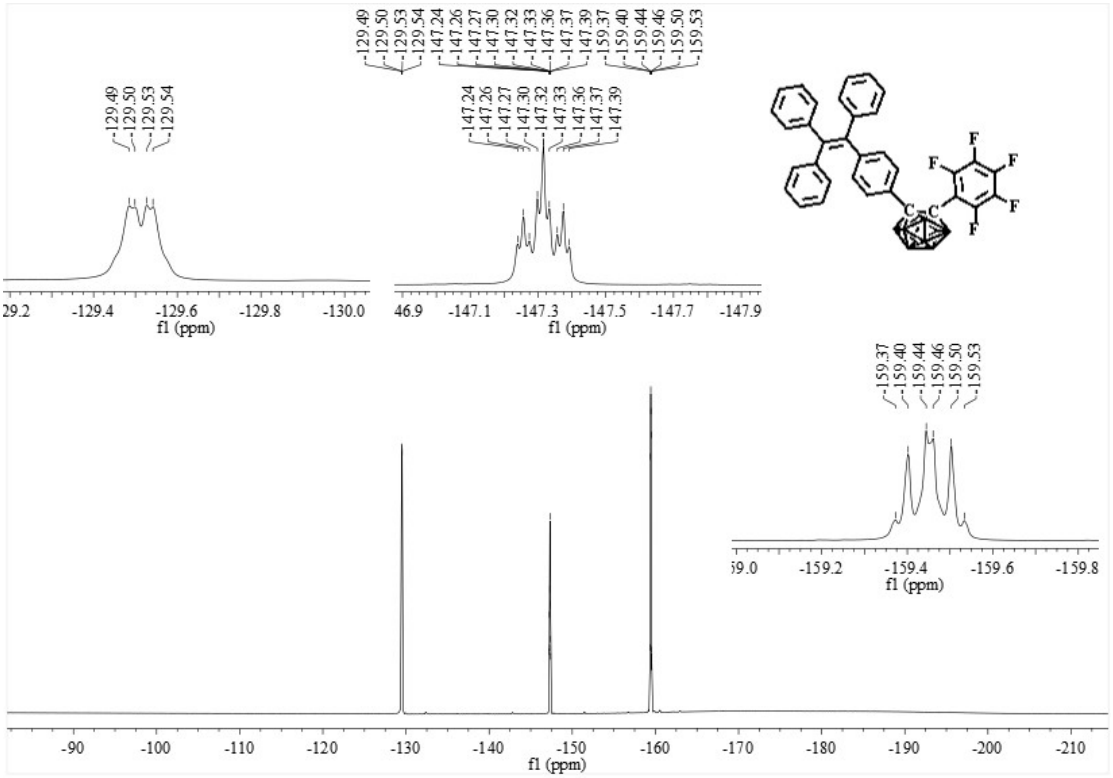
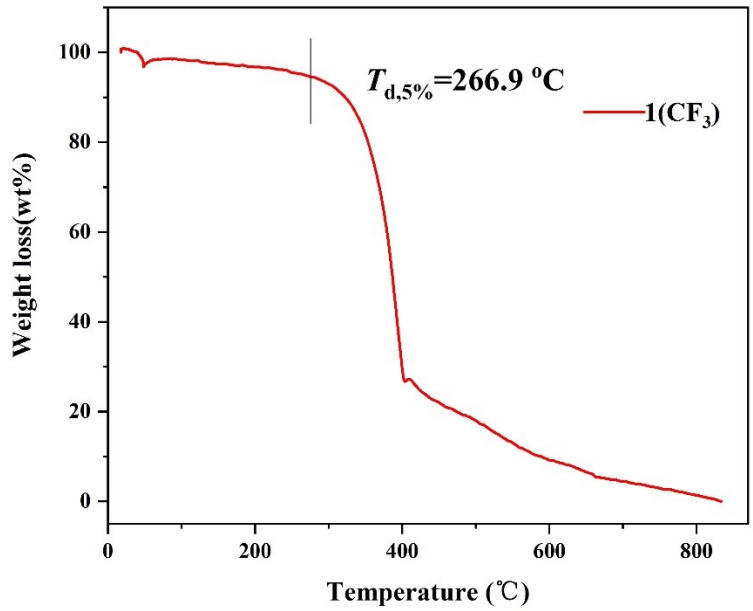


Figure.S18. The $^{19}F-NMR$ ($CDCl_3$) spectrum of compound **2**.



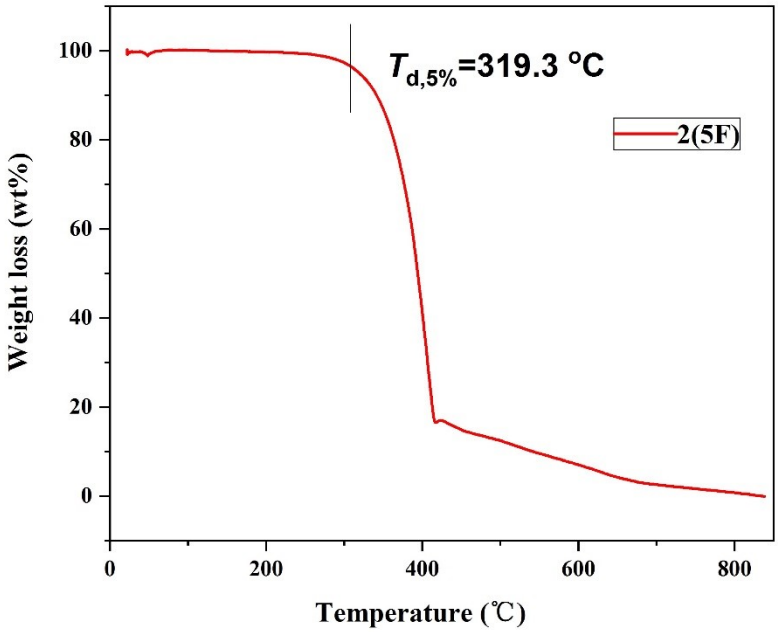


Figure S19. TGA curves of compound 1 and 2. (T_d, corresponding to 5% weight loss)

III. Quantum yields determination Absolute quantum yields of all compounds in THF/water or in solid state were measured by employing an integrating sphere.

The Principle of Absolute Quantum Yield Measurements

The absolute fluorescence quantum yield, η, is, by definition, the ratio of the number of photons emitted to the number of photons absorbed:

$$\eta = \frac{N^{em}}{N^{abs}} \quad (1)$$

There are two different methods for the measurement of the absolute fluorescence quantum yield: "Direct Excitation" measurements and "Direct & Indirect Excitation" measurements.

With "Direct Excitation" measurements one records the scatter and the emission of the sample being directly exited by the radiation from the excitation monochromator only, whereas with "Direct and Indirect Excitation" one also records the emission of the sample while it is in a position where it is only indirectly excited by excitation radiation bouncing within the sphere.

"Direct Excitation" Method

This method only requires two experimental setups, see figure 1.

Note that with the "Direct Excitation" method the emission measurement actually contains the information of both direct and indirect excitation, as photons that pass the sample in the direct excitation beam may still be absorbed after scattering in the sphere.

Figure 1. Two different measurement configurations required for Direct Excitation measurements: (A) reference sample (solvent only) in sample position (1); (B) test sample in position 1 (position 2 remains empty for both measurements.)

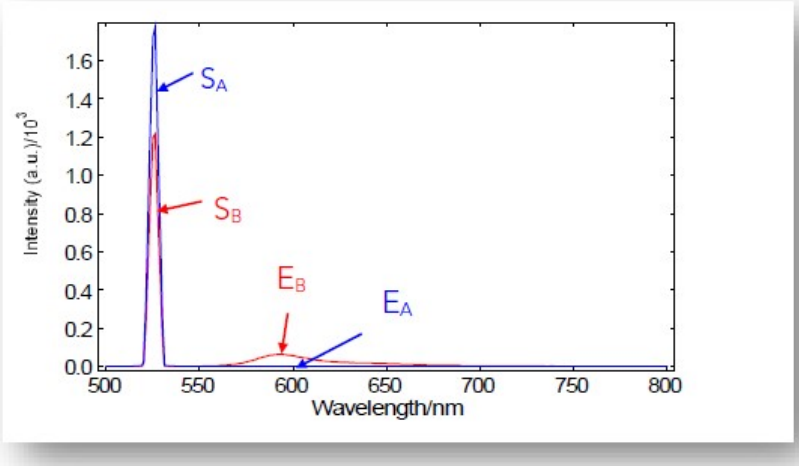


Figure 2. Spectral scans of the excitation scatter region or S-region (peaks on the left) and the emission region (E-region) of the sample and the solvent. The indices "A" and "B" refer to the experimental setup illustrated in Figure 1. Note that the quantities S_A, S_B, E_A, and E_B refer to the integral of the scans.

The absolute fluorescence quantum yield, calculated with the "Direct Excitation" method is calculated as follows:

$$\eta_{DExc} = \frac{E_B - E_A}{S_A - S_B} \qquad (2)$$

$E_A(\lambda)$ and $S_A(\lambda)$, as well as $E_B(\lambda)$ and $S_B(\lambda)$ may be measured in four individual scans. However, it is often convenient to measure these spectra in two scans only. For the calculation of the integrals, the selection of the integral regions, and the final calculation of η_{DExc} use the quantum yield wizard that is supplied with the F980 software.

If the sphere background, $E_A(\lambda)$, is sufficiently low the measurement of this region may be omitted to save measurement time. In this case the equation degrades to:

$$\eta_{DExc} = \frac{E_B}{S_A - S_B} \quad (3)$$

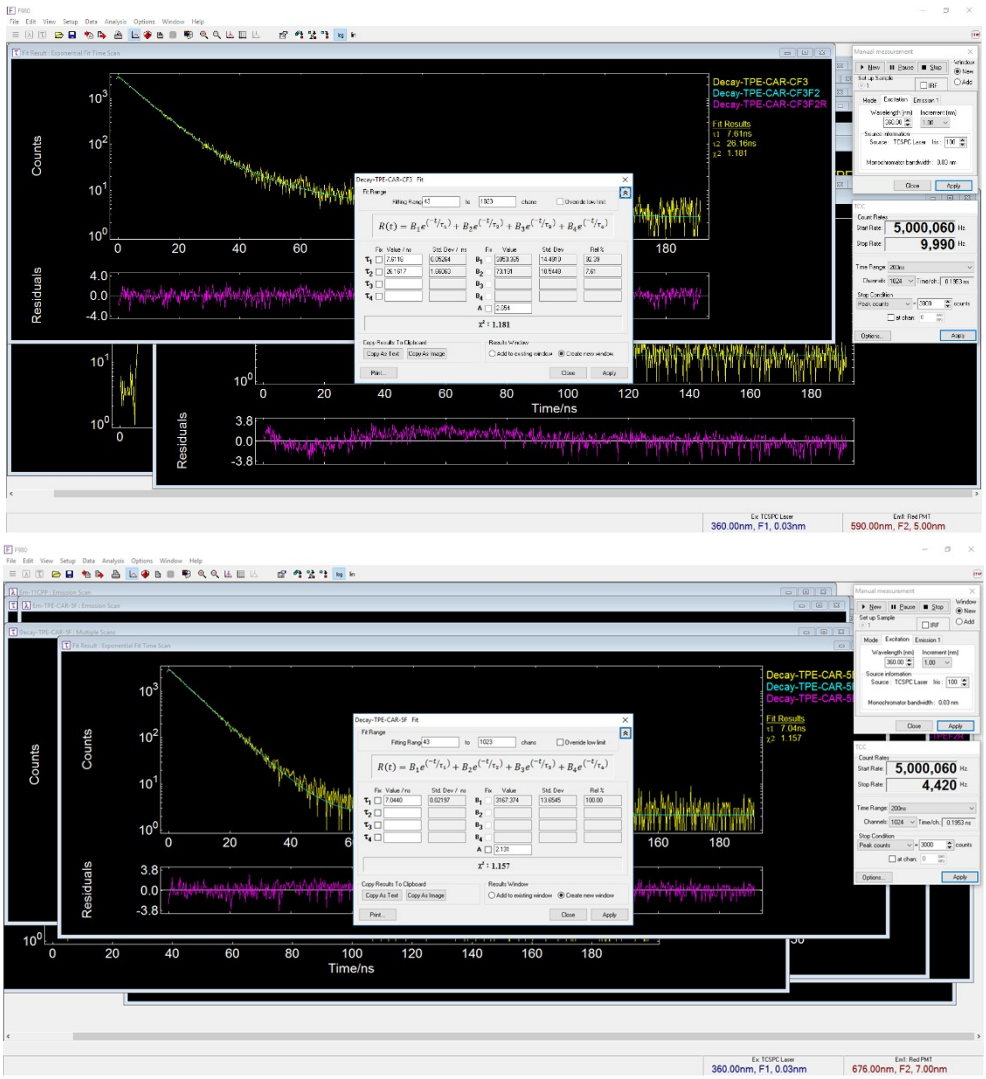


Figure S20. The lifetime measurement of compounds 1 and 2

IV. PL Spectra data: UV−vis absorption spectra were recorded with Shimadzu UV−3600 spectrophotometers. FL and PL spectra were recorded on a Hitachi F−7000 fluorescence spectrophotometer.

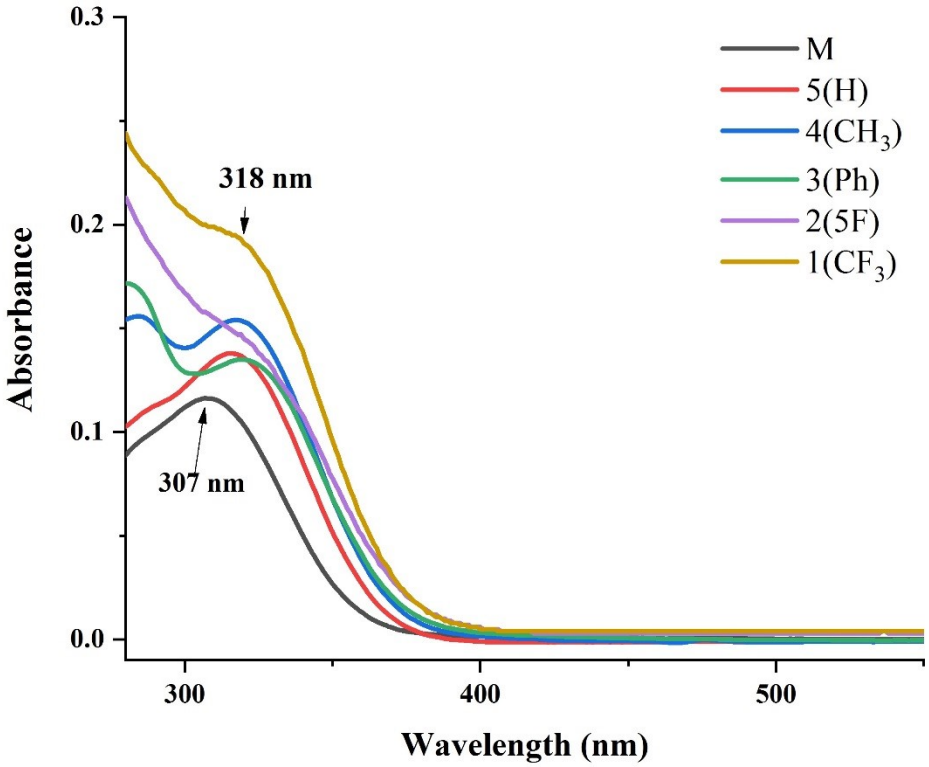


Figure S21. The absorption spectra of **1-5** in THF (1.0×10^{-5} M) at room temperature.

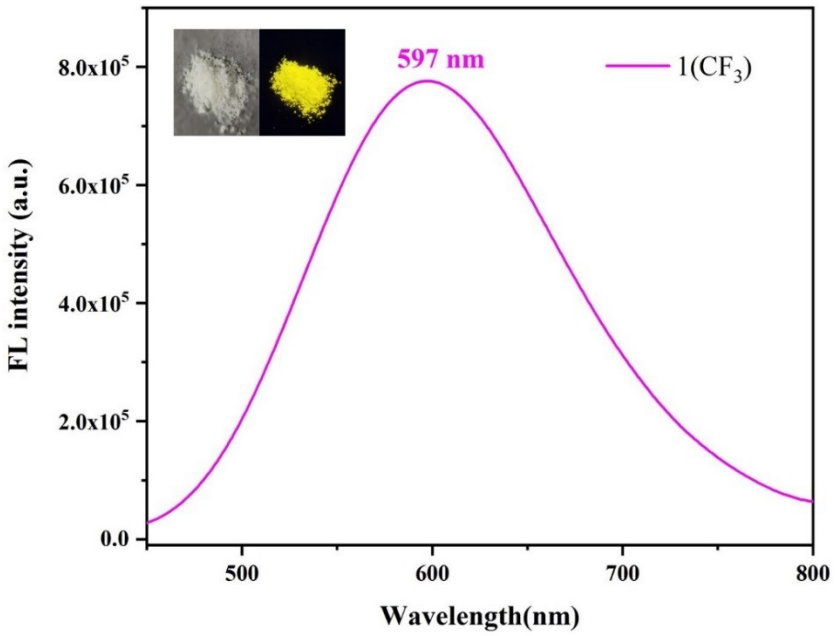


Figure S22. Normalized PL spectra of compounds **1** in solid state at room temperature (λ_{ex} = 360 nm).

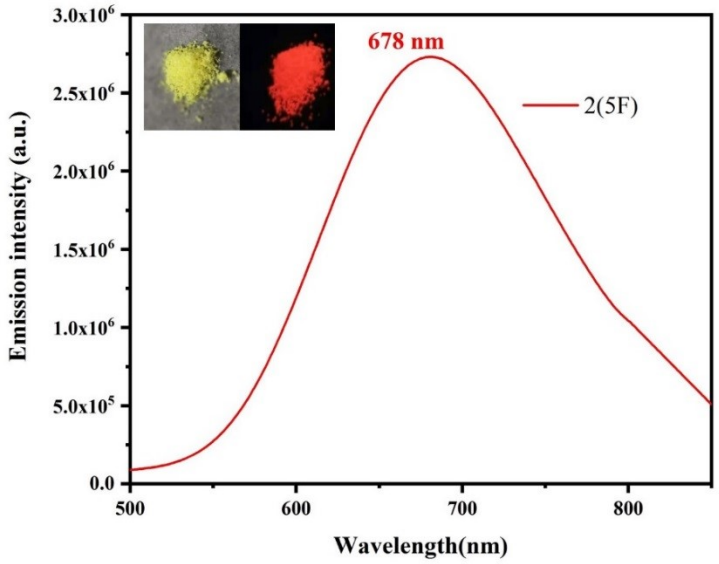


Figure S23. Normalized PL spectra of compounds **2** in solid state at room temperature (λ_{ex} = 360 nm).

V. Quantum chemical calculations: Geometries of all complexes were optimized using density functional theory (DFT) method. The electronic transition energies including electron correlation effects were computed by TD−DFT method using B3LYP functional (TD−B3LYP). The 6−31G(d, p) basis set was used to treat all atoms. All calculations described here were performed by using Gaussian 16 program.[S4]

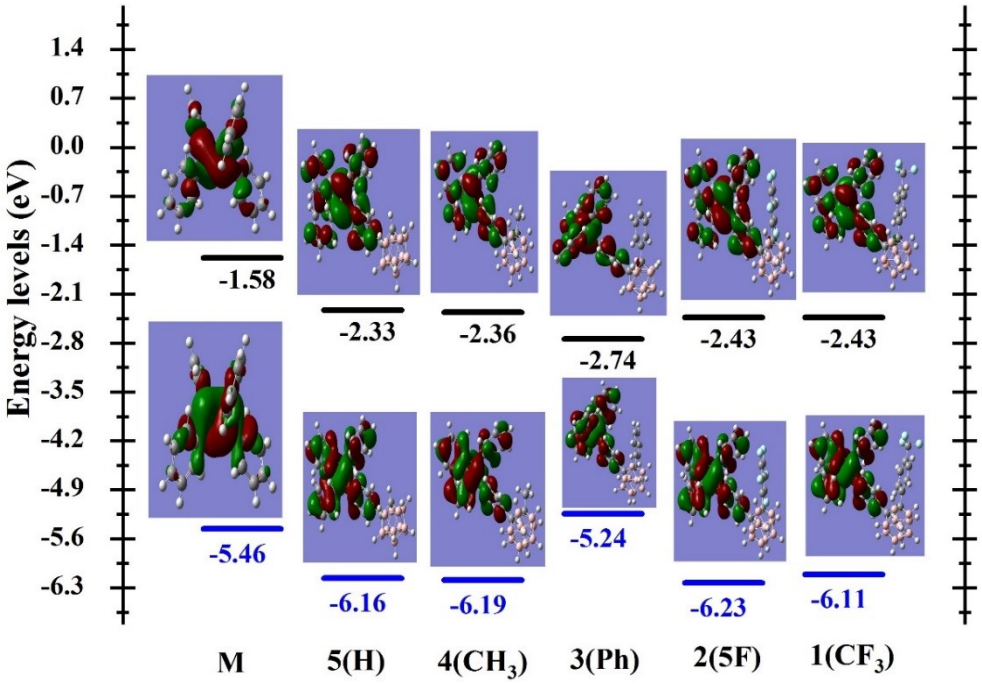


Figure S24. Optimized structures and electronic transitions of **1-5** at S_1 states.

Table S1. Coordinates of the optimized structures of carboranes in the ground and first excited states

Compound **1**(CF_3) at S_0

C	7.602	6.8329	2.9471
C	7.2457	5.1281	4.7541
C	8.4801	7.4015	1.8738
C	4.3911	8.3637	4.2909
H	3.9806	8.5077	5.1133
C	5.7212	3.849	6.7458
C	4.9291	3.1865	7.8379
C	6.2468	7.4559	3.0343
C	5.2329	3.9909	5.4537
H	4.3894	3.6623	5.2443
C	3.7721	8.8032	3.1296
C	4.4016	8.5515	1.9229
H	4.0056	8.8331	1.1302
C	3.6138	5.5719	8.3776
C	9.5214	5.4908	3.7733
C	7.0096	4.2885	7.0024
H	7.376	4.1616	7.8469
C	5.9843	4.615	4.4727
H	5.6391	4.6929	3.6116
C	8.0677	5.8589	3.7547
C	5.6099	7.8858	1.882
H	6.0076	7.7226	1.0579
C	7.7529	4.9073	6.03
H	8.6167	5.1868	6.2278
C	5.6086	7.7172	4.2435
H	6.0113	7.4495	5.037
C	9.0436	6.5694	0.9137

H	8.8703	5.6562	0.9386
C	9.9285	4.1797	3.6315
H	9.2944	3.5151	3.4864
C	4.6557	6.4957	8.4183
C	8.7475	8.7627	1.8142
H	8.3641	9.3388	2.4364
C	3.8118	4.1306	8.7509
C	2.3525	6.0168	8.0111
C	9.5877	9.2652	0.8244
H	9.781	10.1751	0.7978
C	2.1298	7.3535	7.7448
C	10.488	6.4637	3.994
H	10.2331	7.3535	4.0906
C	3.1608	8.2517	7.8107
C	11.2707	3.8415	3.7041
H	11.5327	2.954	3.6135
C	11.8326	6.1202	4.0711
H	12.4735	6.7763	4.2295
C	10.132	8.4203	-0.115
H	10.6879	8.7606	-0.7782
C	4.4312	7.8186	8.1236
C	9.8583	7.0814	-0.0768
H	10.2219	6.5149	-0.7196
C	12.2121	4.8145	3.9088
H	13.1124	4.5883	3.9401
B	5.3045	3.6357	9.4698
H	6.1068	4.3408	9.7319
B	3.7783	3.5834	10.3814
H	3.5902	4.2416	11.2434
B	4.3676	1.581	7.702

H	4.5607	0.9356	6.8321
B	2.4936	3.1439	9.2358
H	1.4649	3.514	9.3584
B	5.6539	2.0163	8.8482
H	6.6853	1.6567	8.7209
B	4.9246	2.2232	10.4569
H	5.4824	1.9896	11.3763
B	3.2337	2.9518	7.6295
H	2.6976	3.2175	6.705
B	3.1809	1.9149	10.3107
H	2.6033	1.4754	11.1358
B	2.8292	1.5287	8.5919
H	2.0181	0.8449	8.2986
B	4.3296	0.9527	9.3662
H	4.494	-0.1131	9.5813
H	2.83645	9.32103	3.16575
H	5.64082	6.17162	8.68176
H	5.24425	8.51407	8.13702
H	1.14716	7.68855	7.48585
H	1.54525	5.31872	7.93401
C	2.90132	9.74452	7.53548
F	4.0718	10.36377	7.27279
F	2.32703	10.30871	8.61917
F	2.07766	9.86974	6.47321

Compound **1**(CF_3) at S_1

C	3.35040800	0.38873100	-0.25606000
C	1.38219000	-1.14222400	0.00030100
C	4.81305000	0.63493600	-0.43199700
C	0.75112700	3.11329500	0.29060600

H	0.03871400	3.41233200	1.05222200
C	-1.36221900	-1.85180900	-0.21541100
C	-2.79935600	-2.28624000	-0.32913600
C	2.47984900	1.58258900	-0.48080700
C	-0.68759500	-1.24139800	-1.28284700
H	-1.20240900	-1.05258400	-2.21624600
C	0.88092700	3.86811700	-0.87632200
C	1.82121400	3.49278900	-1.83850300
H	1.93516800	4.07844600	-2.74631900
C	-3.73230400	0.34277600	0.11384600
C	3.68611100	-1.95256500	0.60195000
C	-0.63681400	-2.11415600	0.95781100
H	-1.11997100	-2.60263600	1.79551600
C	0.65369900	-0.88937300	-1.17297500
H	1.14982700	-0.42090400	-2.01577000
C	2.83991700	-0.82912900	0.09528800
C	2.62249600	2.37036400	-1.63644200
H	3.36268800	2.09214600	-2.38079700
C	0.70895900	-1.77905100	1.05642300
H	1.24944700	-2.01515500	1.96748700
C	1.53956300	1.98035000	0.48386600
H	1.43579500	1.39717100	1.39325600
C	5.61063700	-0.22870100	-1.20216800
H	5.15926300	-1.10541000	-1.65441500
C	3.53322400	-3.25234000	0.08812500
H	2.81066100	-3.43066200	-0.70268900
C	-3.53943600	0.83046200	1.41481500
C	5.41529900	1.77765400	0.12342400
H	4.81058300	2.46747200	0.70412800
C	-4.08271600	-1.10389600	-0.12889300

C	-3.64833900	1.24425200	-0.95711200
C	6.77405300	2.02972300	-0.05674400
H	7.22164500	2.91168400	0.39236400
C	-3.35565600	2.58739300	-0.73953800
C	4.61159300	-1.75345300	1.64041100
H	4.73089600	-0.76023900	2.06046200
C	-3.14683000	3.05369300	0.55813700
C	4.30064700	-4.30940300	0.57422200
H	4.17471100	-5.30317300	0.15422700
C	5.37140000	-2.81246700	2.13370600
H	6.07754100	-2.63665000	2.94010000
C	7.55542800	1.15734800	-0.81667600
H	8.61255000	1.35776300	-0.96445200
C	-3.24791200	2.17264300	1.63637600
C	6.96630300	0.03063600	-1.39335700
H	7.56250300	-0.64701600	-1.99762800
C	5.22308400	-4.09380100	1.59971600
H	5.81613700	-4.91846100	1.98396000
B	-3.76225400	-2.26076100	1.10547600
H	-3.25690900	-1.90114200	2.10614300
B	-5.42294300	-1.83570400	0.63726700
H	-6.05082500	-1.15240700	1.37065900
B	-3.30783200	-3.48217700	-1.44233100
H	-2.47139300	-3.94454500	-2.13852900
B	-5.40900200	-1.53169500	-1.11218100
H	-6.03037000	-0.64170900	-1.58186600
B	-3.32109800	-3.78397400	0.30594800
H	-2.49869500	-4.46471200	0.81334600
B	-4.97221000	-3.53103400	0.90773700
H	-5.37022200	-4.12184900	1.85492900

B	-3.74292800	-1.77933300	-1.67947700
H	-3.24953600	-1.09863200	-2.50244400
B	-5.99806500	-3.08724600	-0.48712900
H	-7.15034800	-3.35932700	-0.54328700
B	-4.95439400	-3.03706300	-1.93724200
H	-5.34272300	-3.26761700	-3.03297400
B	-4.70405400	-4.28816900	-0.68859300
H	-4.91195200	-5.43800700	-0.88779400
H	0.25407200	4.74120800	-1.02771300
H	-3.62124400	0.16295000	2.26266900
H	-3.09142500	2.53188500	2.64761400
H	-3.28151900	3.26855100	-1.57940100
H	-3.81721000	0.90093600	-1.96961900
C	-2.86274900	4.51017800	0.80863200
F	-2.00347600	4.67681500	1.84389400
F	-3.98310600	5.19718100	1.11798100
F	-2.31309200	5.11250600	-0.27082200

Compound **2**(5F) at S_0

C	7.60200000	6.83290000	2.94710000
C	7.24570000	5.12810000	4.75410000
C	8.48010000	7.40150000	1.87380000
C	4.39110000	8.36370000	4.29090000
H	3.98060000	8.50770000	5.11330000
C	5.72120000	3.84900000	6.74580000
C	4.92910000	3.18650000	7.83790000
C	6.24680000	7.45590000	3.03430000
C	5.23290000	3.99090000	5.45370000
H	4.38940000	3.66230000	5.24430000
C	3.77210000	8.80320000	3.12960000

C	4.40160000	8.55150000	1.92290000
H	4.00560000	8.83310000	1.13020000
C	3.61380000	5.57190000	8.37760000
C	9.52140000	5.49080000	3.77330000
C	7.00960000	4.28850000	7.00240000
H	7.37600000	4.16160000	7.84690000
C	5.98430000	4.61500000	4.47270000
H	5.63910000	4.69290000	3.61160000
C	8.06770000	5.85890000	3.75470000
C	5.60990000	7.88580000	1.88200000
H	6.00760000	7.72260000	1.05790000
C	7.75290000	4.90730000	6.03000000
H	8.61670000	5.18680000	6.22780000
C	5.60860000	7.71720000	4.24350000
H	6.01130000	7.44950000	5.03700000
C	9.04360000	6.56940000	0.91370000
H	8.87030000	5.65620000	0.93860000
C	9.92850000	4.17970000	3.63150000
H	9.29440000	3.51510000	3.48640000
C	4.65570000	6.49570000	8.41830000
C	8.74750000	8.76270000	1.81420000
H	8.36410000	9.33880000	2.43640000
C	3.81180000	4.13060000	8.75090000
C	2.35250000	6.01680000	8.01110000
C	9.58770000	9.26520000	0.82440000
H	9.78100000	10.17510000	0.79780000
C	2.12980000	7.35350000	7.74480000
C	10.48800000	6.46370000	3.99400000
H	10.23310000	7.35350000	4.09060000
C	3.16080000	8.25170000	7.81070000

C	11.27070000	3.84150000	3.70410000
H	11.53270000	2.95400000	3.61350000
C	11.83260000	6.12020000	4.07110000
H	12.47350000	6.77630000	4.22950000
C	10.13200000	8.42030000	-0.11500000
H	10.68790000	8.76060000	-0.77820000
C	4.43120000	7.81860000	8.12360000
C	9.85830000	7.08140000	-0.07680000
H	10.22190000	6.51490000	-0.71960000
C	12.21210000	4.81450000	3.90880000
H	13.11240000	4.58830000	3.94010000
B	5.30450000	3.63570000	9.46980000
H	6.10680000	4.34080000	9.73190000
B	3.77830000	3.58340000	10.38140000
H	3.59020000	4.24160000	11.24340000
B	4.36760000	1.58100000	7.70200000
H	4.56070000	0.93560000	6.83210000
B	2.49360000	3.14390000	9.23580000
H	1.46490000	3.51400000	9.35840000
B	5.65390000	2.01630000	8.84820000
H	6.68530000	1.65670000	8.72090000
B	4.92460000	2.22320000	10.45690000
H	5.48240000	1.98960000	11.37630000
B	3.23370000	2.95180000	7.62950000
H	2.69760000	3.21750000	6.70500000
B	3.18090000	1.91490000	10.31070000
H	2.60330000	1.47540000	11.13580000
B	2.82920000	1.52870000	8.59190000
H	2.01810000	0.84490000	8.29860000
B	4.32960000	0.95270000	9.36620000

H	4.49400000	-0.11310000	9.58130000
H	2.83644601	9.32102722	3.16574680
F	0.88989106	7.77638766	7.41877569
F	1.33363927	5.13639275	7.91463294
F	2.93281843	9.56056365	7.57111632
F	5.45843908	8.69440762	8.13912027
F	5.89866107	6.08646600	8.75007600

Compound **2**(5F) at S_1

C	3.46306800	0.34712700	-0.28724400
C	1.39560400	-1.05992400	-0.10613700
C	4.94467900	0.50386200	-0.39472200
C	1.05357800	3.27021900	0.10250500
H	0.35204200	3.65477300	0.83640600
C	-1.38461000	-1.57116800	-0.41824000
C	-2.85233300	-1.85820300	-0.58165200
C	2.68203000	1.59065700	-0.57077900
C	-0.63620200	-0.98375000	-1.45034500
H	-1.11027900	-0.73193400	-2.39047000
C	1.26209700	3.96799400	-1.08827700
C	2.19396400	3.49078400	-2.01245100
H	2.36927200	4.03173600	-2.93786000
C	-3.51581700	0.77332600	0.28170100
C	3.62048300	-1.99969400	0.60035700
C	-0.71122600	-1.92752000	0.76134500
H	-1.24934900	-2.40984600	1.56810400
C	0.72243600	-0.73167100	-1.29429500
H	1.27367800	-0.27924900	-2.11089300
C	2.86350900	-0.83384100	0.04896800
C	2.90810200	2.32358200	-1.74884400

H	3.64416200	1.96614900	-2.46285700
C	0.65033100	-1.68558500	0.90799600
H	1.14596200	-1.98531000	1.82566500
C	1.75145100	2.08940300	0.35566900
H	1.58567800	1.54818700	1.28197700
C	5.72556500	-0.41518700	-1.11645400
H	5.24555900	-1.27007000	-1.58070400
C	3.42907400	-3.29017200	0.07648200
H	2.74299500	-3.43184900	-0.75332600
C	-3.48021400	1.09570000	1.65527800
C	5.58611000	1.61709500	0.17650000
H	4.99644600	2.34908500	0.71990300
C	-4.02336700	-0.55957000	-0.20980100
C	-3.08286100	1.80423000	-0.57667100
C	6.96434100	1.78702600	0.05935900
H	7.44128900	2.64737100	0.51998400
C	-2.56623000	3.01031400	-0.10914700
C	4.49646100	-1.84679700	1.68807700
H	4.64388300	-0.86028000	2.11505500
C	-2.49928900	3.25896900	1.25433200
C	4.11311400	-4.38477600	0.60243000
H	3.95961000	-5.37125700	0.17456400
C	5.17229600	-2.94302900	2.22095200
H	5.84126000	-2.80290200	3.06511100
C	7.72806300	0.86037600	-0.65270200
H	8.80093800	0.99680600	-0.75163600
C	-2.96795300	2.29708300	2.13886900
C	7.10161300	-0.23770600	-1.24505800
H	7.68480700	-0.95688500	-1.81288200
C	4.98755900	-4.21557400	1.67752500

H	5.51528800	-5.06922500	2.09244600
B	-3.82465000	-1.92662200	0.84052500
H	-3.29324600	-1.78175600	1.87480500
B	-5.43575600	-1.25823700	0.43839700
H	-6.01303700	-0.63494100	1.25845300
B	-3.47325500	-2.82354200	-1.84420600
H	-2.68370000	-3.26472800	-2.60599900
B	-5.36084800	-0.71269600	-1.25244400
H	-5.87920900	0.29164600	-1.60064400
B	-3.54215900	-3.36163200	-0.15988300
H	-2.80276200	-4.18414900	0.25842600
B	-5.16515000	-3.01276400	0.47214600
H	-5.63952500	-3.67791500	1.33048700
B	-3.71764000	-1.06893000	-1.84704000
H	-3.13556100	-0.37993300	-2.58949500
B	-6.11809900	-2.27237300	-0.84749900
H	-7.29192900	-2.40953000	-0.93847300
B	-5.05381700	-2.13574100	-2.27327000
H	-5.44553300	-2.16742300	-3.39118700
B	-4.96096600	-3.56850000	-1.21251100
H	-5.28905200	-4.64946400	-1.57158700
H	0.70815600	4.87972800	-1.28903100
F	-2.13906100	3.93209100	-0.97650900
F	-3.15148000	1.69786800	-1.90717500
F	-1.97501100	4.39944000	1.70713700
F	-2.94117400	2.52682900	3.45417000
F	-3.95201800	0.26564600	2.59142400

Compound **3**(Ph) at S_0

B	0.2409	11.537	4.8819

H	1.0179	12.0512	5.4664
B	-0.9337	12.4226	3.8926
H	-0.9353	13.522	3.8425
B	-1.3129	11.434	2.4723
H	-1.5642	11.8843	1.5011
B	-0.3591	9.9432	2.5934
H	0.0287	9.4309	1.7001
B	-0.8905	9.0481	4.0314
H	-0.8651	7.9488	4.0709
B	-2.0708	9.9355	3.0305
H	-2.8219	9.4115	2.4224
B	-2.1807	10.	4.81
H	-3.0052	9.5189	5.3559
B	-0.5242	10.0409	5.4637
H	-0.2652	9.5916	6.4344
B	-1.4648	11.5547	5.3423
H	-1.8201	12.087	6.2379
B	-2.4252	11.477	3.8523
H	-3.4129	11.957	3.7835
C	0.5031	10.0242	4.0881
C	0.2563	11.4504	3.1573
C	1.4399	12.0712	2.4639
C	1.9966	13.2521	2.957
H	1.6518	13.6417	3.727
C	3.0722	13.8505	2.2939
H	3.4376	14.6376	2.6288
C	3.5932	13.2907	1.1596
H	4.3073	13.6929	0.7198
C	3.0536	12.1423	0.6867
H	3.4086	11.7564	-0.0811

C	1.9863	11.5292	1.3188
H	1.6333	10.7441	0.968
C	1.8772	9.4132	4.1157
C	2.8817	9.9121	4.9301
H	2.7154	10.6551	5.464
C	4.132	9.3127	4.9559
H	4.7923	9.6581	5.5131
C	4.4195	8.2013	4.1623
C	3.3936	7.6931	3.3666
H	3.5516	6.9406	2.8425
C	2.1483	8.2863	3.3415
H	1.4813	7.9294	2.8008
C	5.7761	7.5864	4.2066
C	6.4525	7.2277	3.0909
C	5.9723	7.5187	1.7146
C	5.705	8.8106	1.2935
H	5.8159	9.5261	1.877
C	5.2677	9.0297	-0.0115
H	5.1037	9.8976	-0.3046
C	5.0756	7.9693	-0.8729
H	4.7679	8.1238	-1.737
C	5.3392	6.6776	-0.4572
H	5.2011	5.9611	-1.0343
C	5.8065	6.4606	0.8169
H	6.0164	5.5957	1.0859
C	6.3584	7.4176	5.5679
C	5.663	6.7127	6.5504
H	4.8285	6.3511	6.3558
C	6.2107	6.5476	7.8166
H	5.7462	6.0604	8.4588

C	7.4314	7.0972	8.1294
H	7.792	6.9857	8.9797
C	8.1213	7.8198	7.1675
H	8.9409	8.2067	7.3778
C	7.5955	7.9695	5.8966
H	8.0726	8.4432	5.2551
C	7.7611	6.5068	3.1523
C	7.9184	5.3106	3.8449
H	7.1909	4.9345	4.2847
C	9.1433	4.6762	3.8857
H	9.2336	3.8741	4.3486
C	10.2351	5.2262	3.245
H	11.0622	4.8035	3.2848
C	10.0926	6.4135	2.5428
H	10.8247	6.7891	2.1079
C	8.8608	7.0373	2.4885
H	8.7666	7.8239	1.9998

Compound **3**(Ph) at S_1

B	-4.33091800	-1.49560700	0.77145100
H	-3.82565200	-1.66151100	1.82103000
B	-5.89054000	-0.66521700	0.58257900
H	-6.42905100	-0.26297200	1.55562900
B	-5.78313400	0.32952300	-0.88327000
H	-6.24539400	1.41757100	-0.91985800
B	-4.15892200	0.08672000	-1.56010700
H	-3.52467600	0.95058000	-2.04659400
B	-4.00227100	-1.61052100	-2.06049900
H	-3.23323700	-1.87029900	-2.92035300
B	-5.54130600	-0.75160000	-2.26940200
H	-5.92641700	-0.45074600	-3.34942800

B	-5.52487500	-2.43131200	-1.65897000
H	-5.90267500	-3.34745700	-2.30985300
B	-4.10947700	-2.60571800	-0.59610800
H	-3.41071300	-3.54736300	-0.44180800
B	-5.71928200	-2.36963500	0.11482800
H	-6.23394800	-3.22702700	0.75133200
B	-6.62206800	-1.23798000	-0.93266300
H	-7.80083500	-1.28442100	-1.05053800
C	-3.34579900	-1.07661100	-0.57703300
C	-4.43435300	0.10692600	0.14019800
C	-3.87106500	1.24037500	0.95988100
C	-3.77758700	1.13176500	2.35603800
H	-4.08841700	0.21932100	2.84964300
C	-3.30483400	2.19444900	3.12333000
H	-3.24369300	2.08825500	4.20209500
C	-2.92154300	3.38821000	2.51195400
H	-2.55832400	4.21789100	3.11108700
C	-3.02192000	3.51149400	1.12627600
H	-2.74100800	4.43930000	0.63735000
C	-3.49364700	2.44912400	0.35678800
H	-3.57775500	2.56970900	-0.71567600
C	-1.85934200	-0.92912900	-0.39223700
C	-1.20928800	-1.41088700	0.75329900
H	-1.77831800	-1.88150800	1.54495100
C	0.17177000	-1.31098000	0.88562500
H	0.64786400	-1.70343800	1.77830800
C	0.96167700	-0.71510700	-0.11151200
C	0.30802400	-0.25796700	-1.26771700
H	0.88980100	0.17995600	-2.07110100
C	-1.07125500	-0.36173100	-1.40571400

H	-1.53490200	-0.01339400	-2.32067300
C	2.44651000	-0.64565100	0.03211000
C	3.16460200	0.48113600	-0.25653800
C	2.52257100	1.81110400	-0.48388400
C	1.56812900	2.32334800	0.41099900
H	1.27983300	1.73295400	1.27441700
C	0.99231000	3.57564400	0.20413900
H	0.25492800	3.94800200	0.90922200
C	1.35956000	4.34413400	-0.90185700
H	0.91078700	5.31981500	-1.06433500
C	2.31606200	3.85417900	-1.79346400
H	2.61207400	4.44636100	-2.65464800
C	2.89916500	2.60653400	-1.58072900
H	3.65007700	2.23651600	-2.27220500
C	3.08436900	-1.90606600	0.52342100
C	2.75905600	-3.14534900	-0.05533400
H	2.05703100	-3.17839400	-0.88317400
C	3.33017600	-4.32680500	0.41430800
H	3.07406300	-5.27197000	-0.05570300
C	4.22325400	-4.29696400	1.48701300
H	4.66310300	-5.21803200	1.85801000
C	4.53989400	-3.07597800	2.08499100
H	5.22401000	-3.04331200	2.92806700
C	3.97700500	-1.89342200	1.60827900
H	4.22685600	-0.94762700	2.07755700
C	4.65514000	0.47822200	-0.36594800
C	5.32554400	-0.47162700	-1.15518500
H	4.75029000	-1.23204800	-1.67263000
C	6.71307000	-0.44437100	-1.28222500
H	7.21010100	-1.18463700	-1.90253300

C	7.46103000	0.53106000	-0.62058400
H	8.54254700	0.55038100	-0.71797200
C	6.80833800	1.48748100	0.15956300
H	7.38090300	2.25350600	0.67467000
C	5.41964900	1.46838000	0.27569300
H	4.91708300	2.22325400	0.87286800

Compound **4**(CH_3) at S_0

C	3.8824	1.7271	6.802
C	2.9155	3.4387	8.9321
C	5.6631	0.9969	5.4408
C	4.4672	0.8187	5.7274
C	6.2448	0.3434	4.2201
C	2.6763	1.921	8.8274
H	2.1864	1.5181	9.5075
C	2.446	4.3592	10.0842
C	6.4854	1.8888	6.318
C	3.143	1.0892	7.7778
H	2.9639	0.1769	7.7501
C	4.0808	-1.6981	4.6965
H	4.9157	-1.9571	5.0168
C	4.0588	3.2625	6.8795
H	4.5203	3.6717	6.1819
C	3.5845	4.0949	7.9076
H	3.7104	5.0163	7.9025
C	6.505	1.7032	7.7063
H	6.0296	1.0023	8.0917
C	3.6828	-0.2638	5.0003
C	7.2678	2.9249	5.7606
H	7.2939	3.0281	4.8373

C	3.3666	-2.6907	4.0001
H	3.6897	-3.5505	3.8468
C	2.5065	0.1081	4.6144
H	2.1628	0.9564	4.7808
C	7.3032	-0.4635	4.3258
H	7.6848	-0.6191	5.1593
C	8.0035	3.7995	6.5673
H	8.5007	4.4857	6.1843
C	7.9843	3.6357	7.9357
H	8.4579	4.2204	8.4801
C	7.2437	2.5761	8.5091
H	7.2481	2.4598	9.4313
C	5.764	0.5716	2.942
H	5.0367	1.1415	2.839
C	7.3411	-0.8369	1.9389
H	7.7129	-1.2447	1.1897
C	1.7954	-0.8844	3.922
H	0.9471	-0.6436	3.6231
C	3.2619	4.561	11.484
C	2.2248	-2.2797	3.6027
H	1.6641	-2.843	3.1192
C	7.8442	-1.0776	3.1829
H	8.5612	-1.6606	3.2765
B	1.5697	6.3526	12.6658
H	1.2924	6.9815	13.5239
C	6.3084	-0.0082	1.8157
H	5.9558	0.1801	0.9758
B	0.9073	4.6232	12.2684
H	0.1077	4.1974	12.8922
B	2.0138	3.4965	11.5406

H	2.0389	2.4025	11.6583
B	0.9589	4.3448	10.5323
H	0.2213	3.7372	9.9893
B	3.0834	6.0464	10.3907
H	3.8697	6.4918	9.7632
B	1.5904	5.8875	9.8315
H	1.2983	6.2331	8.8291
B	2.3561	4.6936	12.8563
H	2.6098	4.299	13.8508
B	0.6462	6.0677	11.2331
H	-0.3482	6.5344	11.1667
B	3.0583	6.297	12.1401
H	3.8328	6.8849	12.6538
B	1.9356	7.1387	11.1205
H	1.8825	8.2262	10.9676
C	4.4908	3.7618	11.5084
H	4.2813	2.8611	11.7689
H	5.1075	4.1417	12.1376
H	4.8877	3.7585	10.6333

Compound **4**(CH_3) at S_1

B	4.59928600	0.74170500	1.21764700
H	3.94741700	1.53185000	1.80136600
B	6.11718500	1.19414300	0.42238400
H	6.46833000	2.32055900	0.51825400
B	6.17957100	0.35408900	-1.13493200
H	6.57322300	0.90549700	-2.10571000
B	4.69835000	-0.60722700	-1.28534100
H	4.09482200	-0.68212900	-2.29639900
B	4.70331500	-1.84520200	-0.01023300

H	4.08229300	-2.83681400	-0.18178200
B	6.21202700	-1.39388300	-0.82745100
H	6.74339200	-2.13937200	-1.58055000
B	7.09994200	-0.27343700	0.24736600
H	8.28390800	-0.21382300	0.26242800
B	6.11184600	-0.02276100	1.71665600
H	6.57181000	0.21624500	2.78268600
B	4.63905700	-1.00187000	1.55623300
H	3.97262900	-1.42078000	2.43897100
B	6.18686700	-1.63179500	0.94411800
H	6.70543400	-2.56196200	1.46512300
C	3.92697800	2.04761400	-1.13156600
H	4.20521800	2.14121800	-2.18285700
H	4.15132000	2.98783900	-0.62462400
H	2.85054100	1.87129800	-1.07127800
C	4.70207500	0.91064000	-0.48725500
C	3.81326300	-0.39902200	0.18594400
C	2.30752300	-0.40318300	0.11089900
C	1.52447600	0.25357600	1.07249300
H	1.99832400	0.78476200	1.88825500
C	0.13538300	0.22207600	1.00657000
H	-0.44381700	0.74218500	1.76163400
C	-0.53115700	-0.47570700	-0.01280200
C	0.25608600	-1.17001300	-0.94635500
H	-0.22826000	-1.74908800	-1.72619600
C	1.64519700	-1.12491100	-0.89518500
H	2.21735600	-1.66841200	-1.63713800
C	-2.02255700	-0.54015200	-0.06541400
C	-2.58343000	-1.91736500	-0.21471600
C	-2.11037800	-2.97158700	0.58635000

H	-1.34955300	-2.77149300	1.33488100
C	-2.61056400	-4.26393200	0.43737800
H	-2.24003600	-5.06098400	1.07549500
C	-3.57917300	-4.53438900	-0.53092200
H	-3.96405300	-5.54261200	-0.65245000
C	-4.04279800	-3.50175300	-1.34809900
H	-4.78693100	-3.70455200	-2.11291300
C	-3.55077400	-2.20736500	-1.19177600
H	-3.91433700	-1.40960900	-1.83084900
C	-2.80206300	0.57894500	0.01507700
C	-4.27947400	0.52416900	0.23060400
C	-4.83802900	-0.26209500	1.25267000
H	-4.18481500	-0.86310800	1.87645200
C	-6.21387800	-0.27415900	1.47363700
H	-6.62386000	-0.88389800	2.27358400
C	-7.06155200	0.49614200	0.67544800
H	-8.13390500	0.48460200	0.84697500
C	-6.52051700	1.28845400	-0.33880600
H	-7.17118300	1.89457800	-0.96263000
C	-5.14327800	1.31161900	-0.55070800
H	-4.72739700	1.94120700	-1.33146900
C	-2.23735500	1.95765000	-0.11035200
C	-2.56905200	2.95408300	0.82407600
H	-3.22647700	2.70681600	1.65212300
C	-2.06076600	4.24602300	0.70292300
H	-2.31826800	4.99720200	1.44404100
C	-1.23070900	4.57704800	-0.37020600
H	-0.84294900	5.58656500	-0.47015000
C	-0.91326900	3.60461100	-1.31993100
H	-0.28424700	3.85714800	-2.16895100

C	-1.40997400	2.30835700	-1.19053600
H	-1.16456400	1.55802700	-1.93520200

Compound **5**(H) at S_0

C	28.8109	7.9081	11.9533
C	27.4716	8.0134	11.2982
C	27.0292	7.0802	10.4382
C	25.4086	8.3983	9.0561
H	26.0283	9.0899	9.0265
C	25.732	7.2366	9.7133
C	24.1837	8.5647	8.438
H	23.9896	9.3645	8.0048
C	26.67	9.2011	11.6744
C	23.246	7.5493	8.4591
C	21.897	7.7327	7.822
C	29.9674	7.7588	11.2253
H	29.9294	7.7758	10.2966
C	28.9017	7.9392	13.3406
H	28.1375	8.0775	13.852
C	24.8181	6.1932	9.6626
H	25.0415	5.3703	10.0345
C	23.5868	6.3596	9.0699
H	22.9757	5.66	9.0804
C	28.2744	5.0205	11.1524
H	28.0832	5.228	12.0378
C	27.1276	10.475	11.4102
H	27.9613	10.5903	11.0108
C	27.8051	5.8354	10.1434
C	30.1132	7.7678	13.9545
H	30.1626	7.7778	14.8833

C	25.4297	9.0758	12.2745
H	25.093	8.2269	12.451
C	28.08	5.4866	8.8533
H	27.7362	6.0028	8.1601
C	25.1518	11.4352	12.3358
H	24.6457	12.183	12.5566
C	29.0269	3.8969	10.8576
H	29.3276	3.3457	11.5434
C	26.3637	11.5876	11.7304
H	26.679	12.4395	11.5328
C	31.1817	7.5844	11.8529
H	31.9546	7.4681	11.3489
C	31.2489	7.5824	13.2181
H	32.0657	7.4541	13.6439
B	20.5738	8.0475	8.8871
H	20.6416	8.0515	9.9849
C	29.326	3.6013	9.5591
H	29.8535	2.8616	9.3594
C	24.6799	10.1864	12.6169
H	23.8568	10.0821	13.0384
B	21.8455	8.6338	6.3724
H	22.7372	9.0127	5.8515
C	28.8513	4.3911	8.5542
H	29.0484	4.1886	7.6677
B	19.0071	8.4253	6.515
H	18.0309	8.6659	6.0702
B	19.6569	6.8327	6.4791
H	19.099	6.0138	6.0036
B	20.6437	6.5791	7.9287
H	20.7554	5.5938	8.4042

B	19.1475	7.4872	8.0164
H	18.2694	7.1023	8.5553
B	21.4283	6.953	6.403
H	22.0513	6.2052	5.8905
B	20.4233	8.0815	5.5186
H	20.3759	8.0825	4.4198
B	20.3629	9.5459	6.4463
H	20.281	10.5342	5.9708
B	19.5569	9.1871	7.9921
H	18.9499	9.9378	8.5194
C	21.2732	9.2272	7.8421
H	21.83718	10.01867	8.28976

Compound **5**(H) at S_1

C	-4.15244800	0.52122000	0.22384000
C	-2.67903300	0.59782200	-0.01358200
C	-1.88317700	-0.51123200	-0.07621900
C	0.29102800	0.33723500	0.90268600
H	-0.27461800	0.90954300	1.62940200
C	-0.39190700	-0.43256000	-0.05230500
C	1.68100300	0.37250300	0.94162100
H	2.16283600	0.96022100	1.71542500
C	-2.14429200	1.98389900	-0.18061900
C	2.44679400	-0.35554500	0.01995900
C	3.95631800	-0.31619600	0.04475400
C	-4.68230300	-0.24186900	1.27808300
H	-4.00938400	-0.80836600	1.91313400
C	-5.04190500	1.26393800	-0.57229100
H	-4.64877700	1.87555900	-1.37874600
C	0.38262400	-1.18408200	-0.95149300
H	-0.11271700	-1.80990000	-1.68681200

C	1.77299500	-1.13735800	-0.92760100
H	2.33471800	-1.71667300	-1.64967800
C	-3.39912400	-2.22635800	-1.14602800
H	-3.77234500	-1.45120600	-1.80698800
C	-2.49409500	2.99787700	0.72837200
H	-3.14272400	2.75885300	1.56573000
C	-2.43208600	-1.89820000	-0.18107900
C	-6.41580100	1.21867200	-0.34306400
H	-7.08638800	1.78966400	-0.97882200
C	-1.32873400	2.32326000	-1.27329000
H	-1.06702200	1.55844700	-1.99727300
C	-1.94712000	-2.92360700	0.64963000
H	-1.18614300	-2.69401300	1.38956200
C	-1.19674400	4.61678000	-0.51537900
H	-0.83141500	5.63135400	-0.64442300
C	-3.87880000	-3.52963200	-1.26294700
H	-4.62276800	-3.76204600	-2.01943900
C	-2.01537900	4.29705800	0.56990600
H	-2.28718900	5.06227300	1.29135800
C	-6.05501600	-0.27578000	1.51605700
H	-6.44249600	-0.86739000	2.34047700
C	-6.92821300	0.44915700	0.70315200
H	-7.99808100	0.42031800	0.88762600
B	4.73791400	0.67143300	-1.16228500
H	4.03369400	1.25448600	-1.90803500
C	4.67982100	1.09391000	0.49589400
C	-3.40277400	-4.53321500	-0.41733100
H	-3.77764300	-5.54839600	-0.50839100
C	-0.86100800	3.62588000	-1.43944800
H	-0.23799400	3.86784500	-2.29575400

B	4.72187500	-0.21880000	1.60130900
H	4.02040700	-0.17848600	2.54803100
C	-2.43470000	-4.22469100	0.54013500
H	-2.05482500	-4.99897100	1.20043900
B	7.20758500	0.08092300	0.19168100
H	8.38034900	0.24219000	0.25184300
B	6.46451700	-1.46095400	-0.30550100
H	7.09747700	-2.41549400	-0.61152200
B	4.93737500	-1.09159200	-1.13030300
H	4.41883900	-1.73545500	-1.97372100
B	6.34204900	-0.02800800	-1.37196400
H	6.88045400	0.04359500	-2.42531800
B	4.92356000	-1.64138000	0.56240300
H	4.35787900	-2.63623200	0.86008900
B	6.32591300	-0.91482200	1.38926100
H	6.85202100	-1.46210100	2.29933700
B	6.11749200	0.85202000	1.36452300
H	6.37561000	1.61449900	2.23153700
B	6.13404800	1.39566700	-0.33124800
H	6.39955500	2.51971500	-0.58736400
H	4.00150300	1.90042900	0.74044500

Compound **M**(TPE) at S_0

C	3.6304	2.8571	7.1091
C	4.8126	2.5771	7.7137
C	5.0044	2.7388	9.1864
C	5.6125	1.7279	9.9253
H	5.9927	0.9582	9.4405
C	5.766	1.8471	11.3005
H	6.1781	1.1467	11.7924
C	5.322	2.9791	11.9533

H	5.4176	3.0558	12.8962
C	4.7377	3.9983	11.2288
H	4.4383	4.7819	11.6756
C	4.5835	3.8902	9.8648
H	4.1884	4.6044	9.378
C	2.405	3.1703	7.9156
C	1.9412	2.274	8.8769
H	2.3957	1.4507	9.0142
C	0.8185	2.5753	9.6352
H	0.5054	1.9571	10.286
C	0.1504	3.7756	9.4456
H	-0.6101	3.989	9.9734
C	0.6042	4.6654	8.4762
H	0.1516	5.4897	8.3419
C	1.7044	4.3559	7.7117
H	1.9901	4.9593	7.0363
C	3.4111	2.8562	5.6395
C	2.2473	2.2805	5.124
H	1.6225	1.8795	5.7174
C	1.9885	2.2833	3.7621
H	1.2014	1.8675	3.4311
C	2.8496	2.8756	2.9002
H	2.6579	2.8931	1.9697
C	4.0057	3.4522	3.3788
H	4.6133	3.8569	2.7721
C	4.2958	3.4503	4.7408
H	5.0967	3.8523	5.0564
C	5.9927	2.044	6.9779
C	5.8699	0.9943	6.0679
H	5.0137	0.6246	5.8875

C	6.9789	0.4907	5.4284
H	6.8784	-0.2218	4.8084
C	8.2372	1.0072	5.6774
H	8.9959	0.657	5.2255
C	8.3816	2.0384	6.5905
H	9.244	2.3932	6.7729
C	7.2746	2.5494	7.2331
H	7.3829	3.2554	7.8592

Compound **M** (TPE) at S_1

C	0.00001100	0.68308900	0.00009200
C	1.49776200	2.56994700	-0.73530700
C	-0.00007500	-0.68303900	0.00001300
C	1.25167100	1.49056400	0.13141100
C	3.32948100	2.01485000	1.28734200
C	2.64996600	3.34342100	-0.60755900
C	2.18306800	-1.23379400	-1.15130300
C	1.49710700	-2.57043100	0.73506300
C	-1.25152300	1.49078200	-0.13126900
C	-1.49778500	-2.56987100	-0.73555600
C	1.25143400	-1.49069100	-0.13133500
C	-2.64962400	3.34373600	0.60782200
C	3.32932800	-2.01504600	-1.28704800
C	-3.57072900	3.07009900	-0.40516900
C	3.57072900	-3.06989300	-0.40516200
C	-2.18301100	-1.23403200	1.15164300
C	2.64918300	-3.34410900	0.60727300
C	-2.64991500	-3.34347400	-0.60777500
C	-2.18274100	1.23442900	-1.15175800
C	2.18307700	1.23378800	1.15162200

C	-1.25174000	-1.49056300	0.13125400
C	-1.49758900	2.57000400	0.73564500
C	3.57126300	3.06935400	0.40515400
C	-3.32895800	2.01574700	-1.28755100
C	-3.32932400	-2.01521200	1.28739500
C	-3.57111500	-3.06962200	0.40508800
H	4.03321800	1.80098400	2.08678000
H	2.82600600	4.16453600	-1.29675600
H	2.00133300	-0.41553900	-1.84014800
H	0.77795000	-2.79763000	1.51622800
H	-0.77889200	-2.79677200	-1.51705200
H	-2.82566000	4.16471800	1.29717700
H	4.03325900	-1.80106100	-2.08628200
H	-4.46497600	3.67753000	-0.51032600
H	4.46502400	-3.67725600	-0.51028800
H	-2.00095000	-0.41611200	1.84080200
H	2.82490400	-4.16548900	1.29623300
H	-2.82596000	-4.16450900	-1.29706500
H	-2.00071400	0.41655400	-1.84097900
H	2.00102800	0.41581000	1.84071400
H	-0.77879400	2.79673100	1.51728100
H	4.46565600	3.67658000	0.51024100
H	-4.03255400	1.80221500	-2.08720000
H	-4.03297600	-1.80153900	2.08695600
H	-4.46542800	-3.67695700	0.51023100
H	0.77882600	2.79701100	-1.51670600

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