Electronic supplementary information for:

Regiocontrolled Dimerization of Asymmetric Diazaheptacene Derivatives Toward X-shaped Porous Semiconductors

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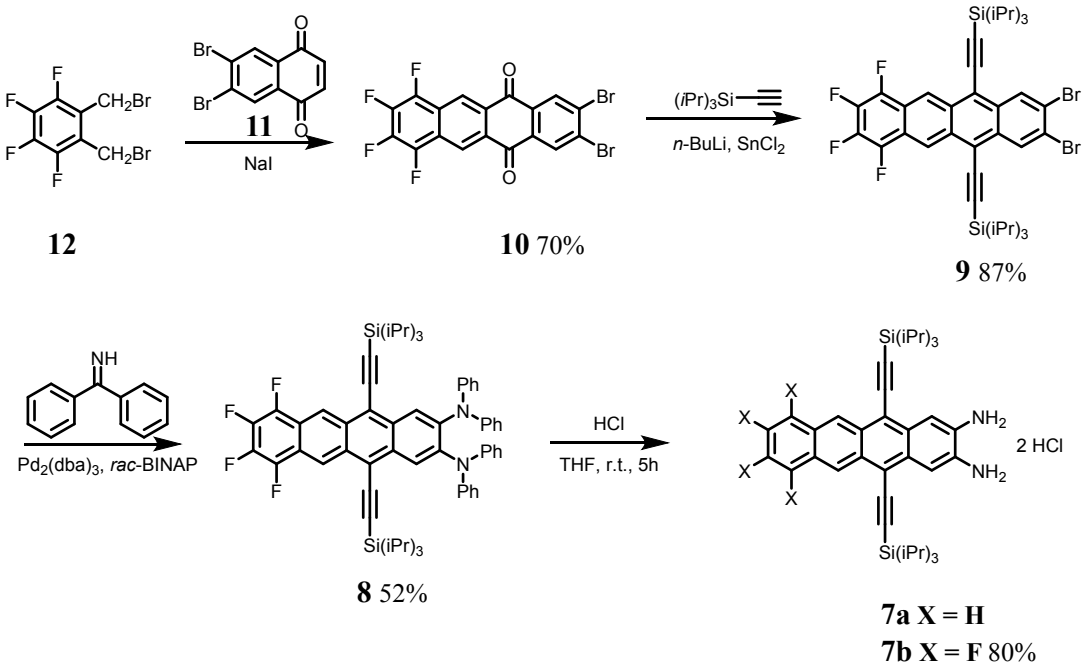
Table of contents

1. Materials and methods

Unless otherwise noted, all materials were purchased from commercial suppliers. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz spectrometer, usually in $CDCl_3$ with TMS as an internal standard, and the chemical shifts (δ) were reported in parts per million (ppm). High resolution mass spectra (HRMS) measurements were carried out on Ion Spec 9.4 Tesla Fourier Transform Mass Spectrometer.

2. Synthesis and characterization of compounds



12 **10** 70% **9** 87%

8 52%

7a X = H
7b X = F 80%

Compound **12**[1], **11**[2], **7a**[2] and tetrabrominated NDI[3]were synthesized according the literatures.

Compound 10

To a flame-dried flask was added **12** (1.00 g, 2.98 mmol), **11** (0.97 g, 2.98 mmol), and sodium iodide (3.00 g, 20.27 mmol) in anhydrous DMF (40 mL). The mixture was stirred at 110 ºC for 48 hours. The mixture was cooled to room temperature and acetone (20 mL) was added. The mixture was then filtered and the crude solid was washed by water and acetone to afford yellow solid (1.01 g, yield: 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 2H), 8.63 (s, 2H). The ^{13}C NMR spectra cannot be obtained due to the low solubility in common organic solvents. HR-MALDI-TOF (m/z): calcd. for $C_{18}H_4Br_2F_4O_2$: 485.8510, found 485.8520.

Compound 9

To a solution of triisopropylsilylacetylene (1 mL, 4.83 mmol) in dry Et_2O (28 mL), 1.24 mL of 2.5 M *n*-BuLi (2.99 mmol) was added dropwise at 0 °C under nitrogen. The solution was stirred at 0 °C for 1 h before the addition of compound **10** (0.35 g, 0.72 mmol) with THF (28 mL). The mixture was warmed to room temperature and stirred overnight. A solution of $SnCl_2{\cdot}2H_2O$ (5 g) in 10% HCl (28 mL) was added to the solution at room temperature and poured into water (100 mL), extracted with dichloromethane and dried over Na_2SO_4. The crude product was purified by silica chromatographic column (eluent: hexane) to provide a red solid **9** (0.51 g, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.48 (s, 2H), 8.96 (s, 2H), 1.31 – 1.29 (m, 42H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 131.28, 130.89, 129.21, 123.76, 119.36, 118.64, 117.46, 107.81, 17.79, 10.47. HR-MALDI-TOF

(m/z): calcd. for $C_{40}H_{46}Br_2F_4Si_2$: 816.1441, found 816.1451.

Compound 8

A mixture of tris(dibenzylideneacetone)dipalladium(0) (67.5 mg, 0.07 mmol), *rac*-BINAP (91.5 mg, 0.14 mmol), and anhydrous toluene (12 mL) was stirred at 110 °C for 0.5 h under nitrogen atmosphere. The mixture was cooled to room temperature and added with benzophenone imine (0.34 mL, 1.83 mmol), sodium *tert*-butoxide (0.18 g, 1.83 mmol), and **9** (0.5 g, 0.61 mmol). The mixture was stirred at 110 ºC overnight and toluene was evaporated. The crude product was purified by silica gel column to afford a dark red solid (315 mg, 52%). ^{1}H NMR (400 MHz, $C_2D_4Cl_2$) δ 9.22 (s, 2H), 7.78 – 7.59 (m, 4H), 7.38 (s, 2H), 7.37 – 7.20 (m, 16H), 1.16 – 1.14 (m, 42H). ^{13}C NMR (101 MHz, $C_2D_4Cl_2$) δ 168.02, 147.22, 131.61, 129.16, 128.74, 127.82, 118.89, 118.17, 116.32, 112.53, 105.80, 102.67, 18.60, 11.13. HR-MALDI-TOF (m/z): calcd. for $C_{64}H_{66}F_4N_2Si_2$: 1018.4677, found 1018.4713 (M+H+Na).

Compound 7b

1 mL 37% hydrochloric acid was added to a solution of **8** (100 mg, 0.1 mmol) in THF (10 mL). The mixture was stirred for 5 h at room temperature and THF was evaporated. The dark purple solid was washed with hexane and used in the next step without further purification (68 mg, 80%). The ^{1}H NMR and ^{13}C NMR spectra cannot be obtained due to the low stability.

General Procedure for the Synthesis of 1a and 1b

A mixture of compound tetrabrominated NDI (0.4 mmol), sodium *tert*-butoxide (1.3 mmol), and a corresponding **7a** or **7b** (0.48 mmol) in toluene (40 mL) was heated at 70 ºC for 3 h under nitrogen atmosphere. The reaction mixture was cooled to room temperature, poured into methanol (100 mL), and stirred for 0.5 h. After filtration, the crude product was purified by silica gel column (DCM/PE = 1/1 to 1/0, v/v) to afford the corresponding desired product.

1a: a dark blue solid (358 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.39 (s, 2H), 8.97 (s, 2H), 7.96 (s, 2H), 7.82 (dd, J = 6.9, 3.7 Hz, 2H), 7.40 (dd, J = 6.9, 3.7 Hz, 2H), 4.25 (t, J = 7.2 Hz, 4H), 1.82 – 1.70 (m, 4H), 1.40 – 1.30 (m, 62H), 0.90 (t, J = 6.8 Hz, 6H). ^{13}C NMR spectra cannot be obtained due to poor solubility in organic solvents. HR-MALDI-TOF (m/z): calcd. for $C_{70}H_{86}Br_2N_4O_4Si_2$: 1260.4559, found 1260.4558.

1b: a dark blue solid (424 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.47 (s, 2H), 9.28 (s, 2H), 7.99 (s, 2H), 4.24 (t, J = 8.0 Hz, 4H), 1.85 – 1.67 (m, 4H), 1.48 – 1.18 (m, 62H), 0.90 (t, J = 7.2 Hz, 6H). ^{13}C NMR spectra cannot be obtained due to the poor solubility in organic solvents. HR-MALDI-TOF (m/z): calcd. for $C_{70}H_{82}Br_2F_4N_4O_4Si_2$: 1332.4183, found 1332.4180.

General Procedure for the Synthesis of 2a and 2b

A mixture of corresponding **1a** or **1b** (0.25 mmol), isopropanol (262 mmol), and sodium *tert*-butoxide (4.4 mmol) in toluene (50 mL) was heated at 90 ºC under nitrogen atmosphere. The reaction was quenched when the starting compound completely disappeared (TLC monitoring). The reaction mixture was diluted with dichloromethane (DCM, 50 mL) and washed with water (50 mL × 3). The organic layer was separated and dried over anhydrous Na_2SO_4. The solvents were removed in vacuo and crude product was purified by column chromatography (DCM/PE=1/1, v/v) to afford the corresponding desired product.

2a: a dark blue solid (126 mg, 46%). ^{1}H NMR (400 MHz, $CDCl_3$), δ 12.85 (s, 2H), 8.99 (s, 2H), 8.20 (s, 2H), 7.95 (s, 2H), 7.89 (dd, J = 6.4, 3.2 Hz, 2H), 7.41 (dd, J = 6.4, 3.2 Hz, 2H), 4.24 (t, J = 8.0 Hz, 4H), 1.76 – 1.70 (m, 4H), 1.37 – 1.36 (m, 42H), 1.28 – 1.22 (m, 20H), 0.88 (t, J = 6.5 Hz, 6H). ^{13}C NMR (101MHz, $CDCl_3$), δ 164.53, 161.63, 137.73, 131.01, 130.47, 128.88, 127.09,

124.82, 124.36, 122.80, 121.79, 115.40, 108.76, 105.14, 102.70, 97.24, 39.23, 30.82, 28.25, 26.92, 26.12, 21.65, 17.99, 13.09, 10.74. HR-MALDI-TOF (m/z): calcd. for $C_{70}H_{88}N_4O_4Si_2$: 1104.6349, found 1104.6348.

2b: a dark blue solid (112 mg, 38%). ^{1}H NMR (400 MHz, $CDCl_3$), δ 12.68 (s, 2H), 9.13 (s, 2H), 8.21 (s, 2H), 7.77 (s, 2H), 4.21 (t, *J* = 7.2 Hz, 4H), 1.78 – 1.64 (m, 4H), 1.37 – 1.35 (m, 42H), 1.28 – 1.25 (m, 20H), 0.83 (t, *J* = 6.5 Hz, 6H). ^{13}C NMR (101MHz, $CDCl_3$), δ 164.66, 161.56, 137.65, 131.35, 129.05, 127.86, 125.25, 122.85, 122.11, 118.03, 115.69, 108.55, 106.52, 101.71, 97.74, 30.82, 28.45, 26.90, 26.10, 21.64, 17.90, 13.09, 10.63. HR-MALDI-TOF (m/z): calcd. for $C_{70}H_{84}F_4N_4O_4Si_2$: 1176.5972, found 1176.5976.

General Procedure for the synthesis of dimers

A corresponding **1** or **2** (0.08 mmol) and MnO_2 (68 mmol) were stirred in 10 mL $CHCl_3$ at room temperature for 10 min. After filtration, the crude material was purified by flash chromatography (DCM/PE = 1:1, v/v) as eluent to give the corresponding desired product.

5a: a yellow solid (92 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 4H), 7.81 (dd, *J* = 6.4, 3.3 Hz, 4H), 7.41 (dd, *J* = 6.6, 3.1 Hz, 4H), 6.57 (s, 4H), 4.34 – 4.08 (m, 8H), 1.88 – 1.71 (m, 8H), 1.50 – 1.25 (m, 124H), 0.95 – 0.91 (m, 12H).^{13}C NMR (101MHz, $CDCl_3$), δ 161.35, 159.25, 158.56, 139.32, 136.14, 135.66, 132.08, 129.79, 128.15, 126.33, 121.28, 105.73, 102.11, 52.03, 46.00, 36.35, 31.88, 29.65, 29.32, 26.48, 22.65, 19.25, 14.10, 11.75. HR-MALDI-TOF (m/z): calcd. for $C_{140}H_{168}Br_4N_8O_8Si_4$: 2516.8806, found 1258.4418.

5b: a reddish yellow solid (89 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (s, 4H), 6.57 (s, 2H), 4.31 – 4.09 (m, 8H), 1.89 – 1.72 (m, 8H), 1.51 – 1.17(m, 124H), 0.95 – 0.90 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.30, 158.50, 139.04, 137.66, 136.03, 130.32, 126.34, 121.37, 107.51, 101.01, 51.91, 46.06, 36.33, 31.89, 30.71, 29.32, 26.48, 24.60, 22.21, 19.14, 14.07, 11.65. HR-MALDI-TOF (m/z): calcd. for $C_{140}H_{160}Br_4F_8N_8O_8Si_4$: 2660.8052, found 1330.4037.

6a: a yellow solid (77 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (s, 4H), 8.70 (s, 4H), 7.78 (dd, *J* = 6.4, 3.2 Hz, 4H), 7.37 (dd, *J* = 6.6, 3.1 Hz, 4H), 6.59 (s, 2H), 4.30 – 4.02 (m, 8H), 1.82 – 1.70 (m, 8H), 1.51 – 1.43 (m, 84H), 1.35 – 1.30 (m, 40H), 0.90 (t, *J* = 6.5 Hz, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.88, 159.33, 158.89, 139.70, 136.62, 132.07, 131.62, 129.88, 128.14, 127.60, 125.68, 121.39, 105.62, 102.17, 52.12, 45.25, 36.35, 31.89, 29.64, 26.58, 22.67, 19.29, 14.09, 11.78. HR-MALDI-TOF (m/z): calcd. for $C_{140}H_{172}N_8O_8Si_4$: 2205.2386, found 1102.6194.

6b: a reddish yellow (76 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (s, 4H), 8.74 (s, 4H), 6.59 (s, 4H), 4.21 – 4.14 (m, 8H), 1.78 – 1.71 (m, 8H), 1.45 – 1.39 (m, 124H), 0.90 (t, *J* = 6.5 Hz, 12H). ^{13}C NMR (400 MHz,) δ 162.28, 158.92, 158.34, 139.40, 138.17, 131.69, 130.42, 126.94, 123.09, 121.66, 121.27, 119.84, 119.39, 105.23, 101.33, 101.07, 51.98, 41.14, 31.90, 29.37, 28.10, 22.67, 19.11, 14.12, 11.69. HR-MALDI-TOF (m/z): calcd. for $C_{140}H_{164}F_8N_8O_8Si_4$: 2349.1632, found 1174.5821.

3. CV and UV spectra of compounds

Cyclic voltammetry (CV) was recorded on a CHI620E electrochemical work station using glassy carbon discs as the working electrode, Pt wire as the counter electrode, and Ag/Ag^+ electrode as the reference electrode. The experiments were performed in nitrogen-purged DCM with tetrabutylammonium hexafluorophosphate ($TBAPF_6$, 0.1 M) as the supporting electrolyte with a scan of 100 mV/s. UV-vis absorption spectra were measured with Hitachi (model U-3010) UV-Vis spectrophotometer (chloroform solution, ~10^{-5} M).

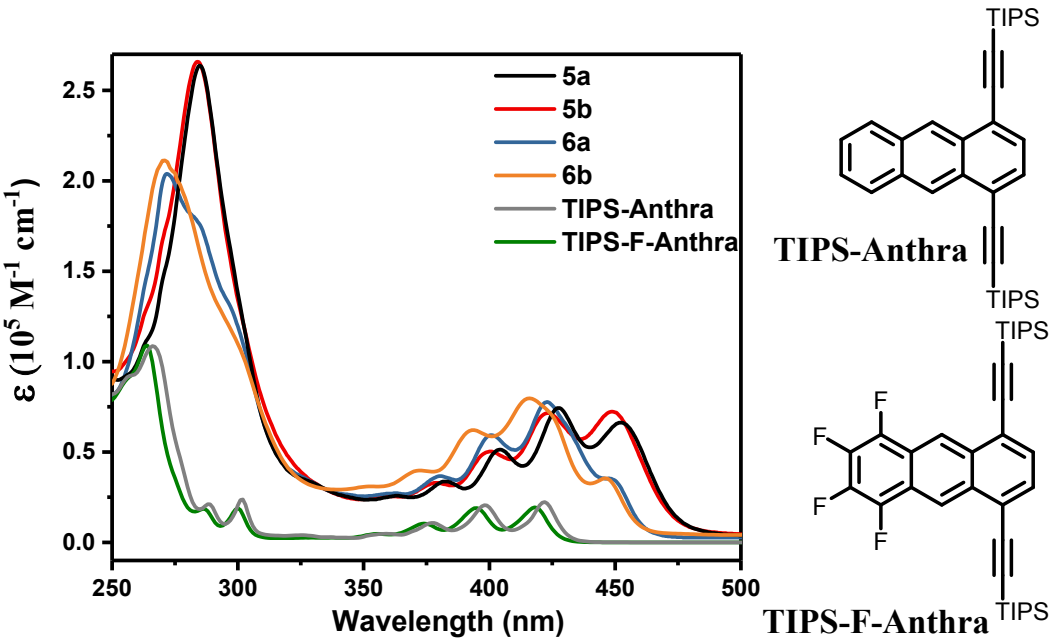


Figure S1. UV/Vis absorption of **5a**, **5b**, **6a**, **6b**, **TIPS-Anthra** and **TIPS-F-Anthra** in chloroform (~10^{-5} M).

4. X-ray crystallographic data of 2a, 5a and 5b

The measurement was made with Synchrotron Radiation (λ = 0.82653 Å). All calculations were performed using the SHELXL-97 and the crystal structure crystallographic software package.

Table S1. Crystal data and structure refinement for **2a**, **5a** and **5b**.

Identification code	**2a**	**5a**	**5b**
Empirical formula	$C_{70}H_{88}N_4O_4Si_2$	$C_{140}H_{168}Br_4N_8O_8Si_4$	$C_{140}H_{160}Br_4F_8N_8O_8Si_4$
Formula weight	1104.63	2516.88	2660.80
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	*C2/c*
Radiation type	CuK\a	CuK\a	CuK\a
Radiation wavelength(Å)	1.54184	1.54184	1.54178
T(K)	223.15	169.99(13)	169.99(13)
a(Å)	12.4231(4)	18.8621(3)	26.370(2)
b(Å)	13.9327(5)	25.0420(3)	26.4347(10)
c(Å)	21.1782(7)	34.0452(6)	24.2245(19)
α(deg)	96.811(3)	74.2830(3)	90
β(deg)	101.236(3)	77.959(2)	120.504(8)
γ(deg)	108.670(3)	68.381(2)	90
V(Å^3)	3341.0(2)	14284.1(4)	14549(2)
Z	2	4	4
ρ_{calc} (g cm^{-3})	1.145	1.259	1.302
θ, range(°)	1.573-27.484	4.238-151.442	5.128-155.69
R(int)	3.47%	5.61%	8.63%
μ(mm^{-1})	0.104	2.152	2.222
F(000)	1242	5696	5952

Crystal size (mm^3)	0.463 ×0.439× 0.035	0.04 × 0.04 × 0.02	0.32 × 0.15 × 0.1
Index ranges	-16 ≤ h ≤ 6, -18 ≤ k ≤ 18, -27 ≤ l ≤ 27	-22 ≤ h ≤ 23, -28 ≤ k ≤ 31, -39 ≤ l ≤ 42	-32 ≤ h ≤ 32, -33 ≤ k ≤ 31, -30 ≤ l ≤ 27
Reflections collected	43305	56672	83208
Independent reflections	15290	56672	14763
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F^2		
Data / restraints / parameters	15290 / 489 / 918	56672/1352/3457	14763/504/851
Goodness-of-fit on F^2	1.026	1.945	2.092
Final R indices [I>2sigma(I)]	R1 = 0.0818, wR2 = 0.2200	R1 = 0.1103, wR2 = 0.2929	R1 = 0.1345, wR2 = 0.3470
R indices (all data)	R1 = 0.1201, wR2 = 0.2446	R1 = 0.1389, wR2 = 0.3159	R1 = 0.1675, wR2 = 0.3635
Largest diff. peak and hole ($e.Å^{-3}$)	0.997 and -0.514	2.61 and -1.36	0.99 and -0.83

5. Computational study

The density functional theory (DFT) calculations were performed with the Gaussian 09 Rev. E.01 employing the B3LYP/6-31g(d,p) level. Considering the alkyl chains on the imide positions and triisopropylsilane on the acetylene positions have negligible effect on the final structural and electronic properties of these compounds, we chose methyl substituents instead of octyl on the imide positions and hydrogen substituents instead of triisopropylsilane on the acetylene positions for better view of their structures. The dimerization mechanism has been computationally analyzed by using the density functional theory within the M06-2X functional, and, since the studied systems are quite large, the economical basis set 6-31G(d) was used (denoted as M06-2X/6-31G(d)). Frequency calculations were performed at the M06-2X/6-31G(d) level for all stationary points to differentiate them as minima or saddle points. The energies reported in this paper are at the M06-2X/6-31G(d) level of theory unless otherwise stated. Where frequency calculations were performed, unscaled zero-point vibrational energies (ZPVE) at M06-2X/6-31G(d) were added to the calculated relative energies. Time-dependent DFT (TD-DFT) calculations were performed at the (U)ωB97XD/6-311G(d,p) level of theory under vacuum. Natural orbital occupation number (NOON)) calculations were done by spin unrestricted UCAM-B3LYP/6-31G(d,p) method based and the diradical character (y_0) was calculated according to Yamaguchi's scheme: $y_0 = 1-(2T/(1+T^2))$, and $T = (n\text{HOMO}–n\text{LUMO})/2$ (nHOMO is the occupation number of the HOMO, nLUMO is the occupation number of the LUMO).

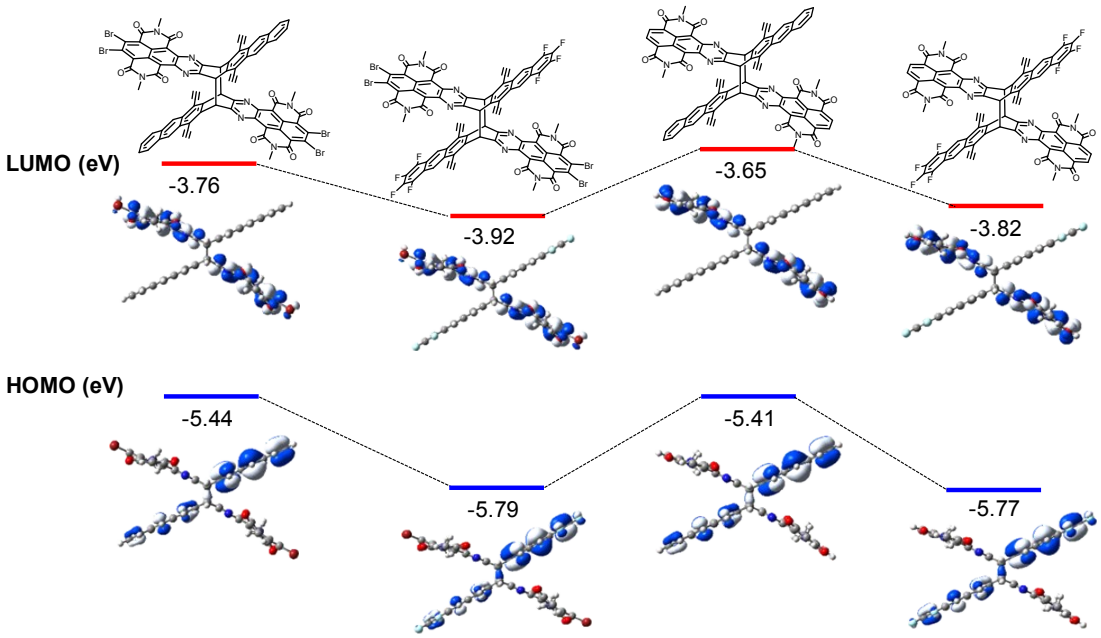


Figure S2. Calculated HOMO and LUMO of **5a**, **5b**, **6a** and **6b** at B3LYP/6-31g(d) level.

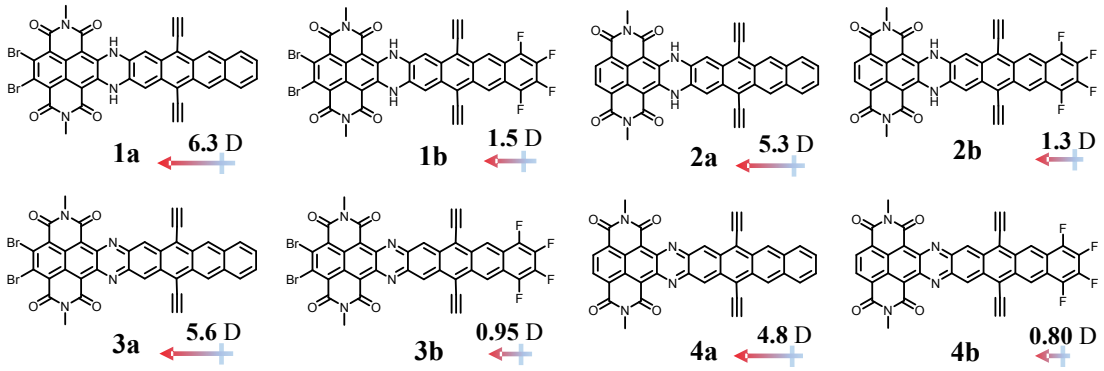


Figure S3. Calculated dipoles of compounds.

Table S2. Calculated absolute energies (E) and Gibbs free energies (G) at 298 K in Hartrees and zeropoint vibrational energies (ZPVE) in kcal/mol of the transition states, local minima, and products at (U)M06-2X/6-31G(d).

Name	(U)M06-2X/6-31G(d)		
	E (Hartrees)	ZPVE(Hartrees)	G (Hartrees)
4a	-1977.978736	-1977.511553	-1977.578688
Complex	-3956.028327	-3955.091365	-3955.192331
T1	-3955.978825	-3955.057637	-3955.143809
M1	-3956.070230	-3955.115308	-3955.217983
T2	-3956.068667	-3955.105618	-3955.212557
M2	-3956.060580	-3955.118047	-3955.222142
T3	-3956.060442	-3955.115621	-3955.218462
Dimer	-3956.051013	-3955.126853	-3955.227543

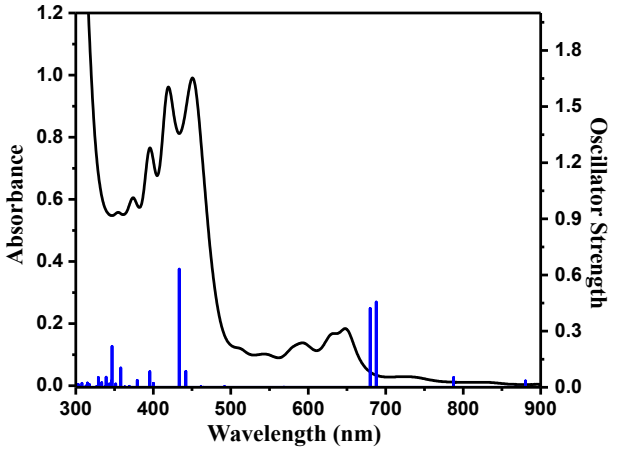


Figure S4. Calculated stick spectrum (UωB97XD/6-311G(d,p)) of **3b** along with the experimental spectrum of **5b** after 15s of irradiation.

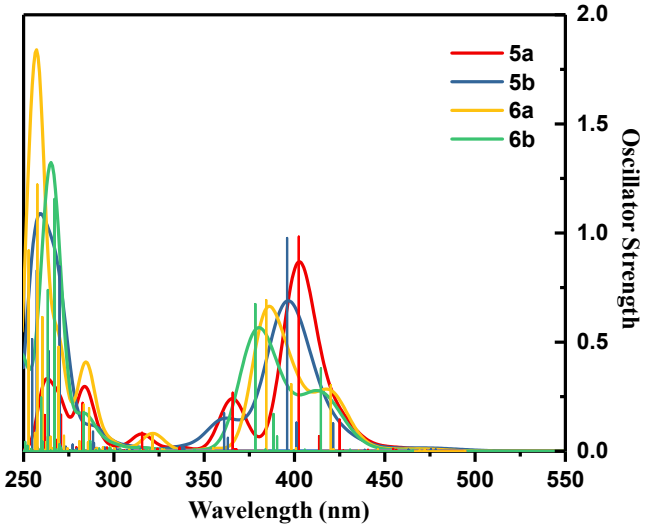


Figure S5. Computational absorption spectrum obtained from TD-ωB97XD/6-31G(d) of Compound **5a**, **5b**, **6a** and **6b**.

6. Photo-induced dissociation of the dimer

In order to prove the presence of intermediates, we used ^{1}H NMR and UV-Vis absorption spectra to detected the photodegradation process of **5b** under nitrogen atmosphere. Toluene was refluxed over sodium, and freshly distilled prior to use. In order to find the source of hydrogen in the photo-induced dissociation process of the dimer, we used toluene-d_8 and D_2O (10/1, v/v) as solvents to detect the photolysis process. The NMR tube needs to be constantly shaken during the irradiation so that the D_2O can be dissolved in toluene-d_8.

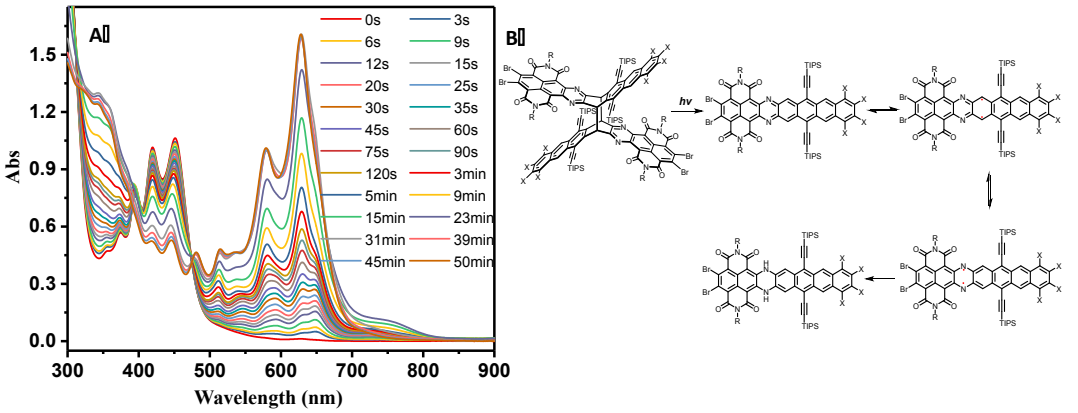


Figure S6. Photodissociation of 0.02 mM **5b** in degassed toluene at ambient temperature (A) and possible photo-induced dissociation mechanism of the dimer (B).

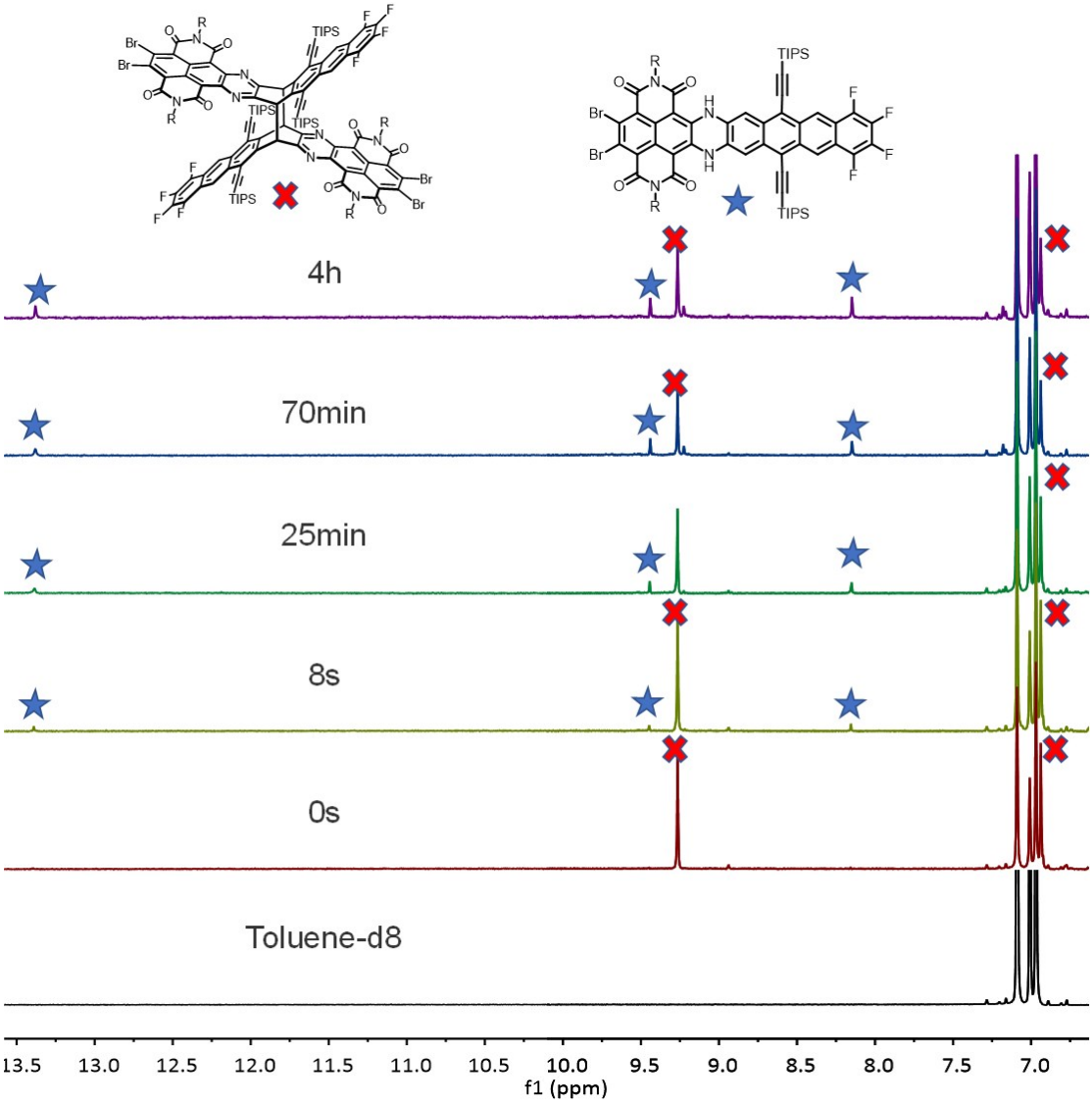


Figure S7. ^{1}H NMR spectrum of **5b** in toluene-d_8 (~2 mM) with the increase of the irradiation time under nitrogen atmosphere.

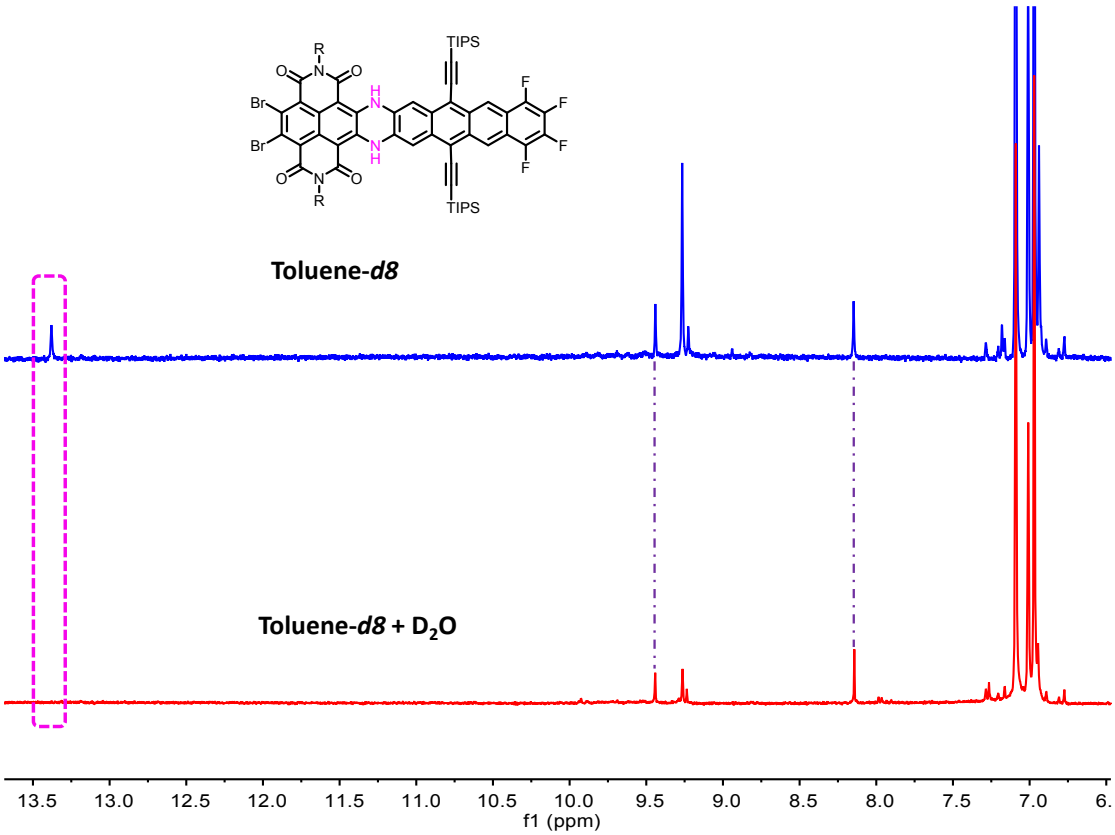


Figure S8. ^{1}H NMR spectrums of **5b** in toluene-d_8 and D_2O after 8 hours of irradiation (red) and in toluene-d_8 after 4 hours of irradiation (blue) under nitrogen atmosphere.

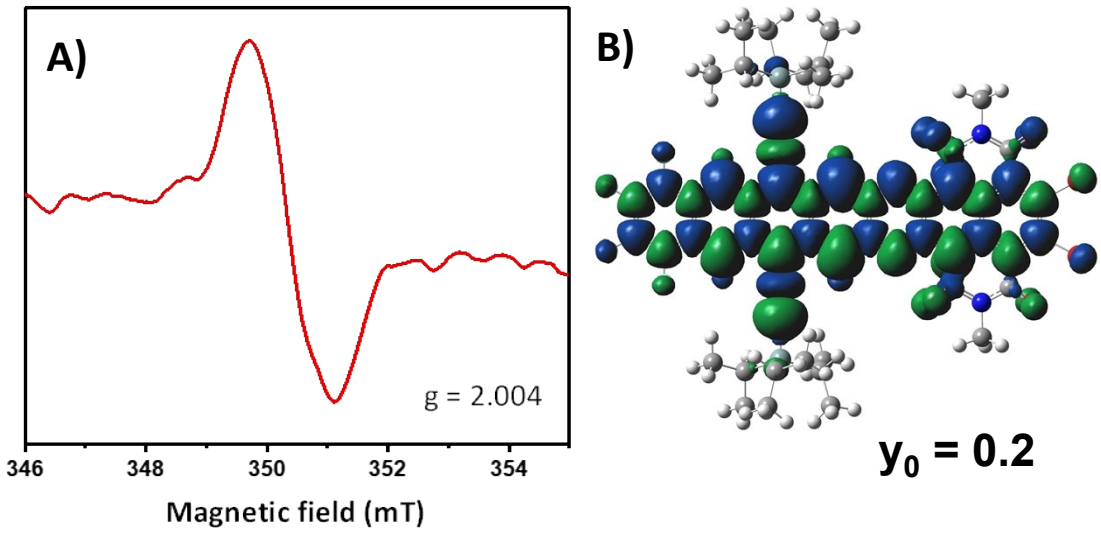


Figure S9. ESR spectrum of **5b** in degassed toluene after 10 min of irradiation at room temperature (A) and calculated spin density maps of the singlet diradicals of **3b** (B).

7. Surface areas and porosities of compound 5a.

The surface areas and porosities of **5a** was characterized by nitrogen adsorption and desorption analysis at 77.35 K with an auto-sorb computer-controlled surface analyzer (Micromeritics, ASAP 2460). The sample was degassed at 100 ºC (8h) before analyzed.

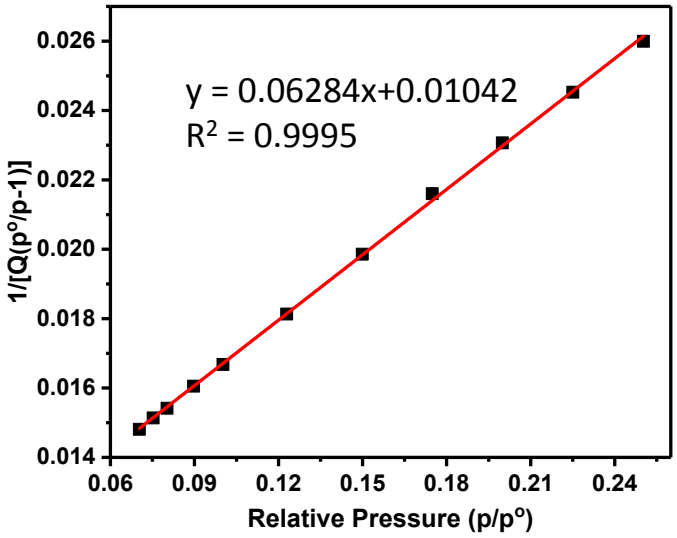


Figure S10. BET-plot of compound **5a**.

8. OFET fabrication and characterization

Thin-film devices fabrication: The SiO_2/Si wafers were cleaned with deionized water, piranha solution(H_2SO_4/H_2O_2=7:3), deionized water, isopropyl alcohol, and finally were blown with high purity nitrogen gas. Treatment of the SiO_2/Si wafers with 12-cyclohexyldodecylphosphonic acid (CDPA). $Al(NO_3)_3 \cdot 9H_2O$ (0.0375 g) was dissolved in ethanol (1 mL) and stirred for 4 hours under a nitrogen atmosphere, resulting a concentration of $Al(NO_3)_3$ in ethanol (37.5 mg/mL), which was spin-coated onto the cleaned SiO_2/Si substrate at 5000 rpm for 40 seconds. Then, the substrate was baked at 300 °C for half an hour to dehydrate the substrate completely. The bottom-gate top-contact (BGTC) devices based on thin film were fabricated with the "shadow mask" method. Firstly, films of the semiconductors were spin-coated from toluene solution (10 mg/mL, 4000 r/min) onto AlOx/SiO_2/Si substrate modified with CDPA. Secondly, silver, as the source/drain electrodes with width/length of 1000/105, were thermal evaporated (0.1 Å/s, 50 nm) on the semiconductor films through a shadow mask.

Single-crystal devices fabrication: The SiO_2/Si wafers were cleaned with deionized water, piranha solution (H_2SO_4/H_2O_2=7:3), deionized water, isopropyl alcohol, and finally were blown with high purity nitrogen gas. Treatment of the SiO_2/Si wafers with octadecyltrichlorosilane (OTS) was conducted by the vapor-deposition method. The clean wafers were dried under vacuum at 90 °C for 2 h to eliminate the moisture. When the temperature is decreased to room temperature, a small drop of OTS was dropped onto the wafers. Subsequently, this system was heated to 120 °C for 2 h under vacuum, after which the vacuum is maintained at approximately room temperature. The bottom-gate top-contact (BGTC) devices based on the micro/nanometer-sized single crystals were fabricated with the "gold strips" method.[4]

Devices characterization: All electrical characteristics of the devices were measured at room temperature using a semiconductor parameter analyzer (Keithley 4200 SCS) in nitrogen atmosphere. The mobilities of the devices were calculated in the saturation regime. The equation is listed as follows:

$$I_{DS} = (W/2L)C_{i\mu}(V_{GS}-V_T)^2$$

where W/L is the channel width/length , C_i is the insulator capacitance per unit area (10 nF/cm^2),

and V_{GS} and V_T are the gate voltage and threshold voltage, respectively. This equation defines the important characteristics of electron mobility (μ), on/off ratio ($I_{on/off}$), and threshold voltage (V_T), which could be deduced by the equation from the plot of current–voltage.

Thin film: X-ray diffraction (XRD) was measured on a D/max2500 with a CuKα source (κ = 1.541 Å). Atomic force microscopy (AFM) measurements were carried out with a Nanoscope IIIa instrument (Digital Instruments).

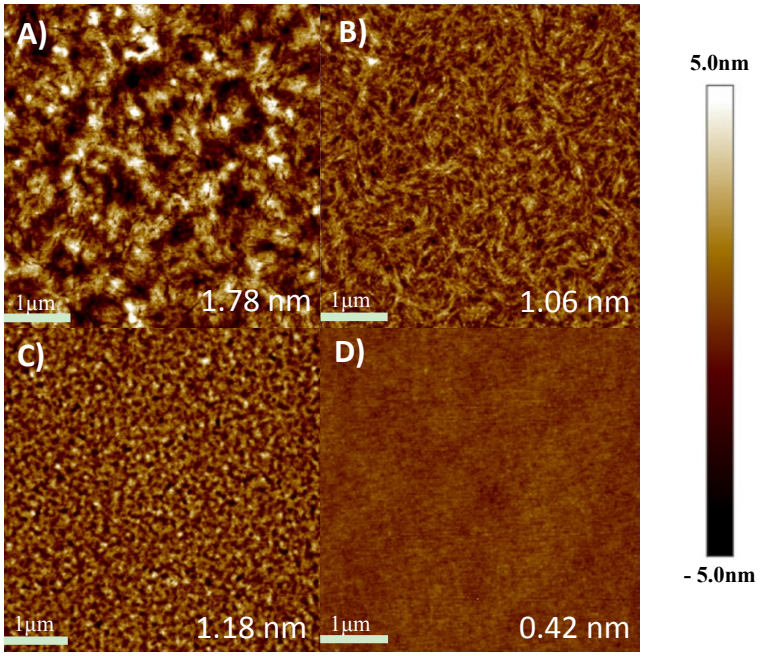


Figure S11. AFM images (5 μm×5 μm scan area) and RMS values of CDPA-modified thin films of: (A) **5a**, (B) **5b**, (C) **6a** and (D) **6b**.

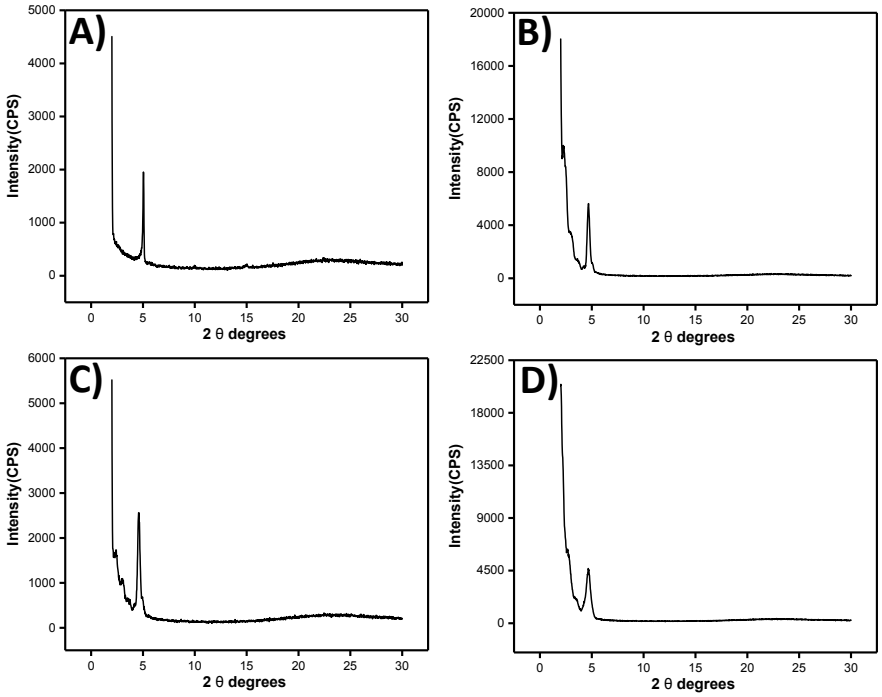


Figure S12. XRD images of (A) **5a**, (B) **5b**, (C) **6a** and (D) **6b** thin films.

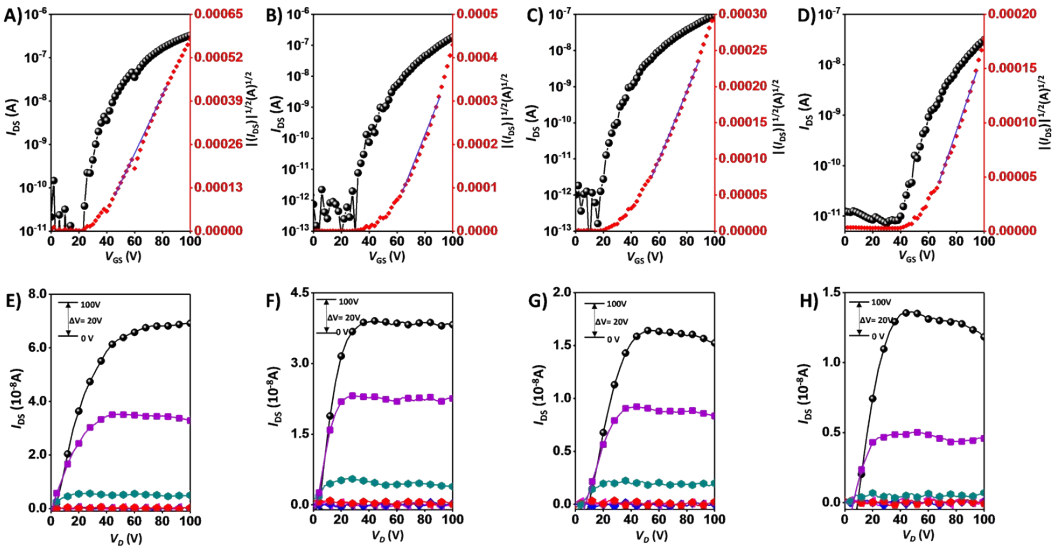


Figure S13. Representative transfer (A), (B), (C) and (D) and output curves (E), (F), (G) and (H) of OFET devices based on thin film of **5a**, **5b**, **6a** and **6b**, respectively.

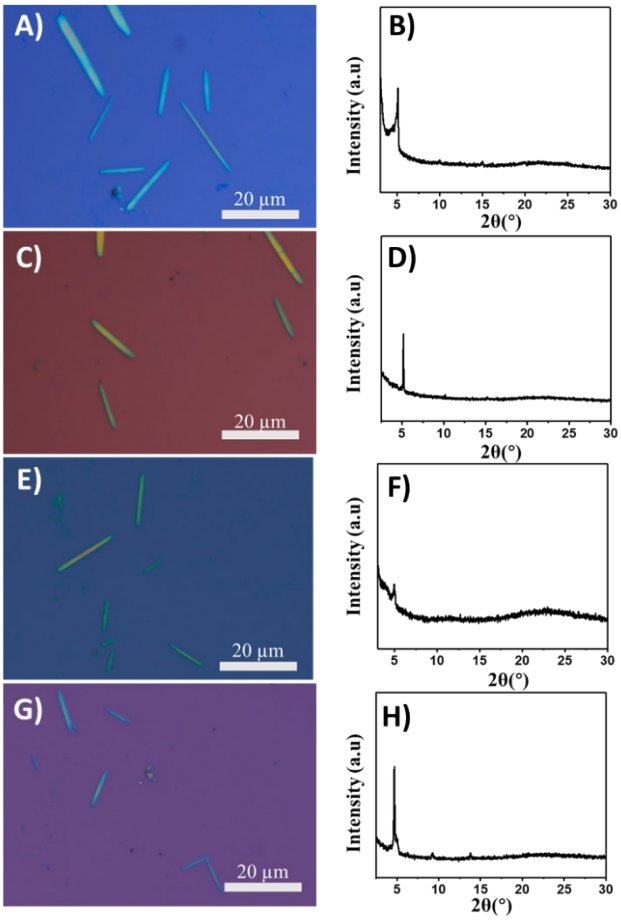


Figure S14. Optical microscopy image (A), (C), (E) and (G), and XRD image (B), (D), (F) and (H) of **5a**, **5b**, **6a** and **6b**, respectively.

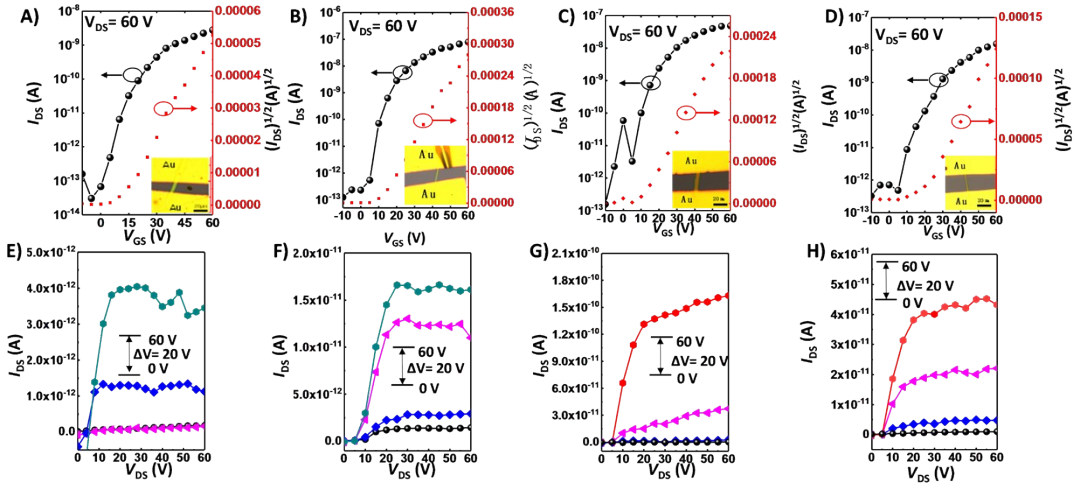


Figure S15. Representative transfer (A), (B), (C) and (D) and output curves (E), (F), (G) and (H) of OFET devices based on single-crystalline microribbons of **5a** (W/L=1/13), **5b** (W/L=1/8), **6a** (W/L=1/6) and **6b** (W/L=1/5), respectively.

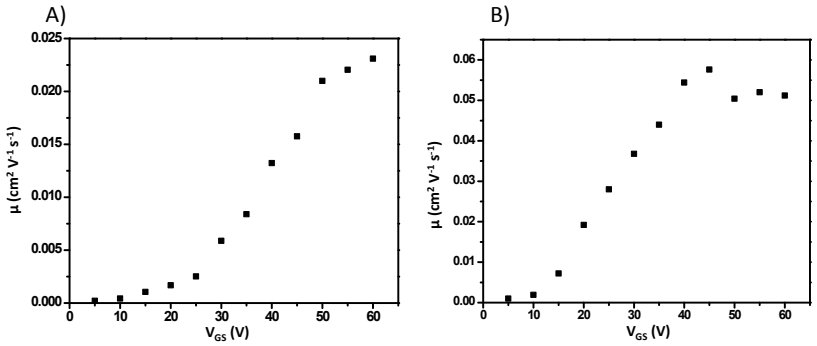


Figure S16. Plots showing dependence of mobilities on gate voltages of OFET devices based on single-crystalline microribbons of **5a** (A) and **5b** (B).

9. References

[1] C. R. Swartz, S. R. Parkin, J. E. Bullock, J. E. Anthony, A. C. Mayer, G. G. Malliaras, *Org. Lett*, **2005**, *7*, 3163.

[2] D. Xia, X. Guo, L. Chen, M. Baumgarten, A. Keerthi, K. Müllen, *Angew. Chem. Int. Ed*, **2016**, *55*, 941.

[3] X. Gao, W. Qiu, X. Yang, Y. Liu, Y. Wang, H. Zhang, T. Qi, Y. Liu, K. Lu, C. Du, z. Shuai, G. Yu, D. Zhu, *Org. Lett*, **2007**, *9*, 3917.

[4] Q. Tang, Y. Tong, H. Li, Y. Zhu, Q. Li, W. Hu, Y. Liu, and D. Zhu, *Adv. Mater*, **2008**, 20, 1511.

10. ^{1}H NMR, ^{13}C NMR and HRMS spectra of compounds

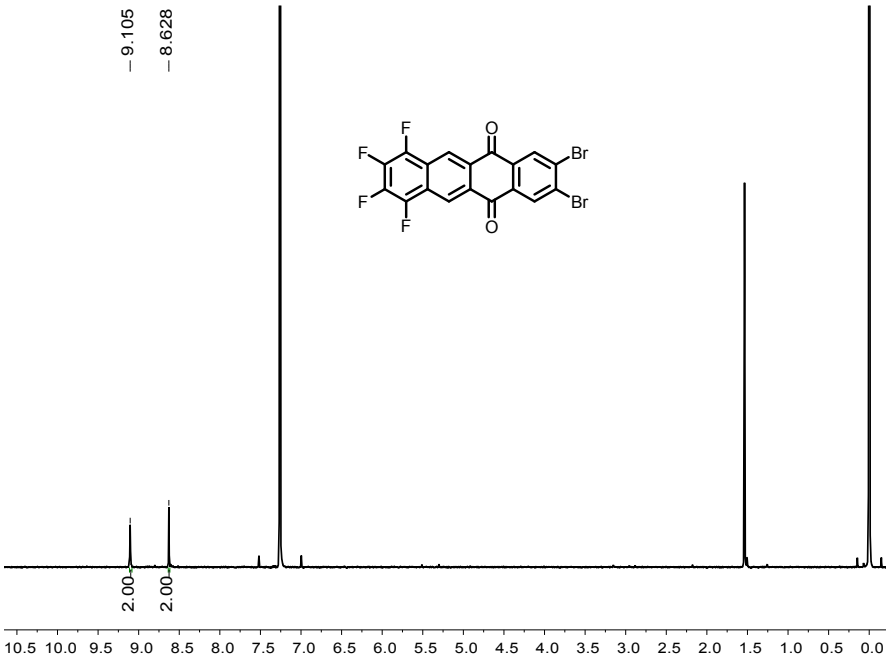


Figure S17. ^{1}H NMR spectrum of **10** in $CDCl_3$ (400 MHz, 298 K).

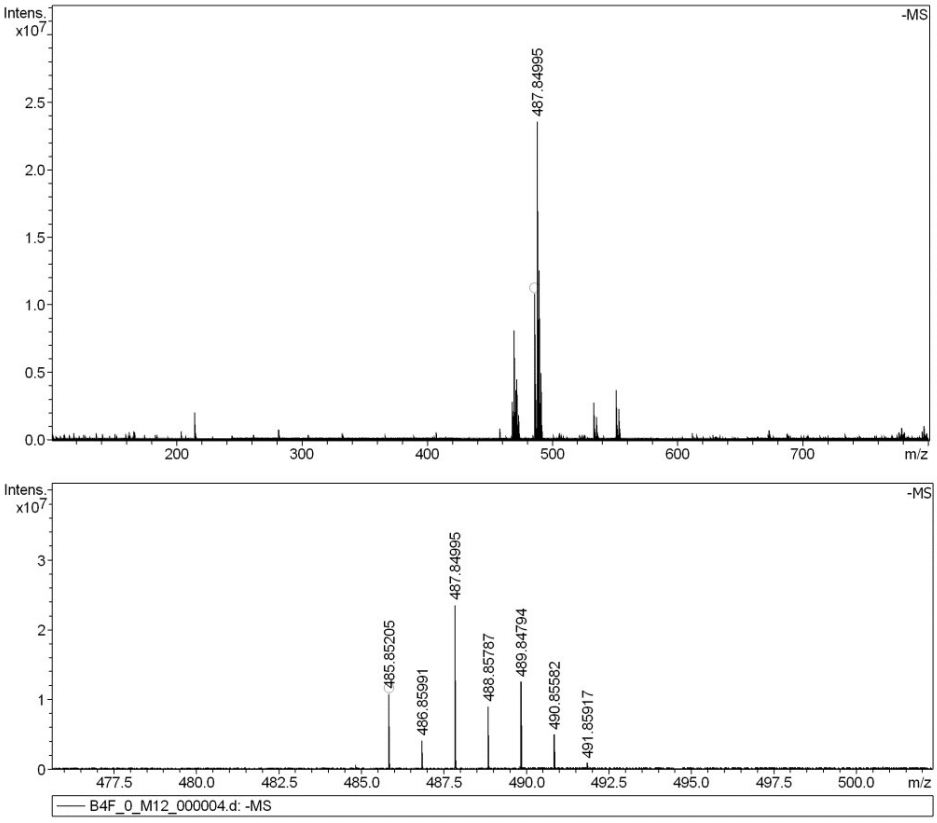


Figure S18. HR-MALDI-TOF spectra of **10**.

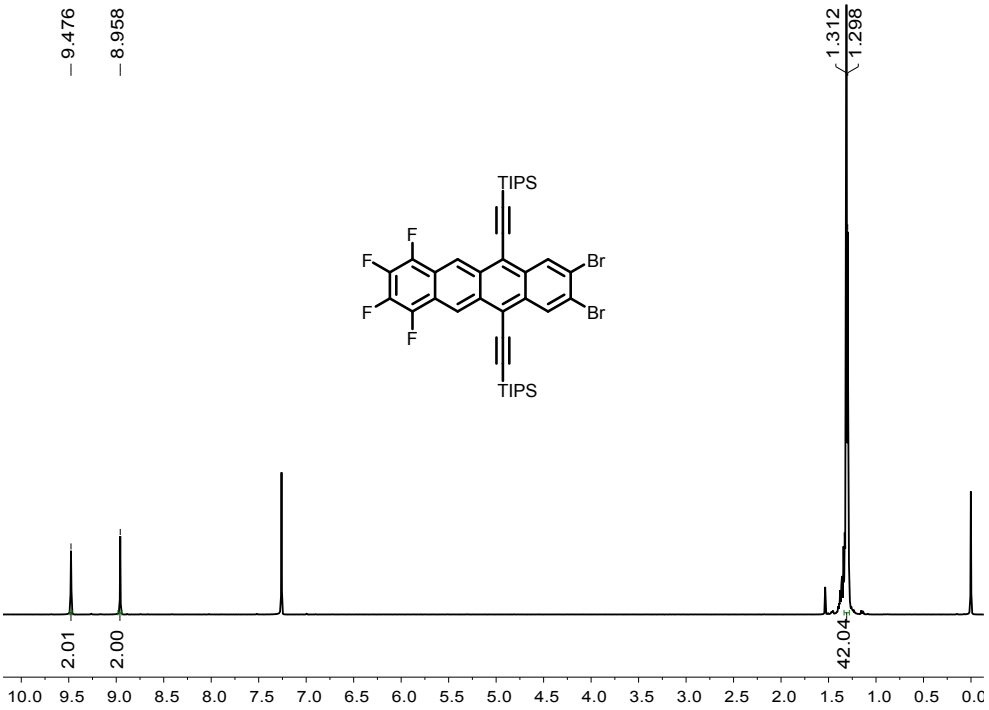


Figure S19. ^{1}H NMR spectrum of **9** in $CDCl_3$ (400 MHz, 298 K).

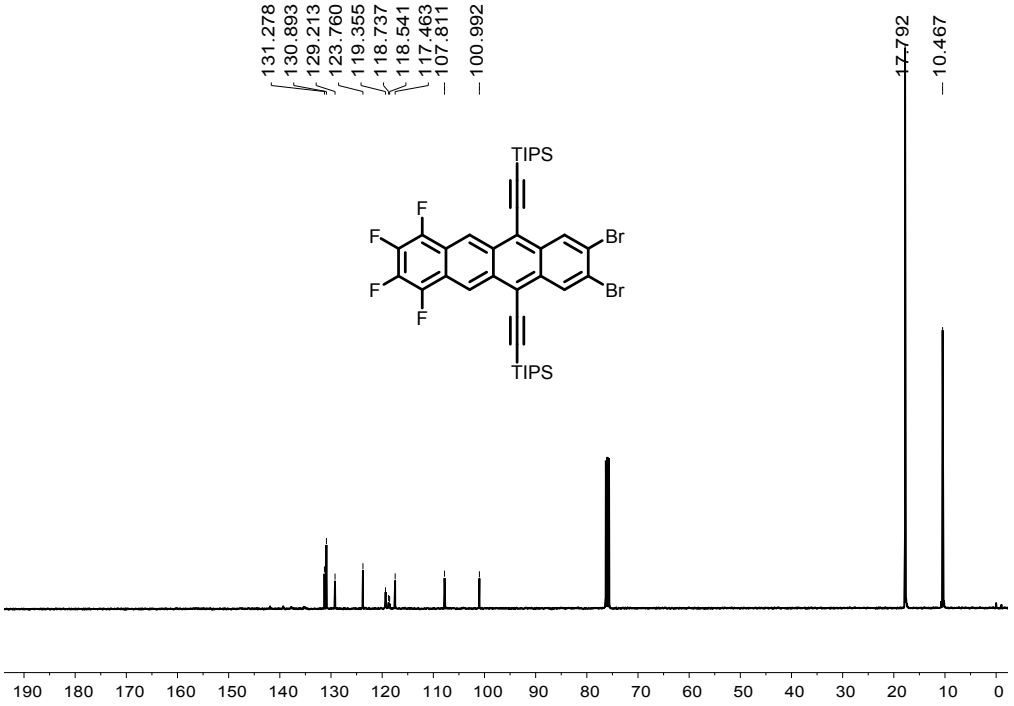


Figure S20. ^{13}C NMR spectrum of **9** in $CDCl_3$ (100 MHz, 298 K).

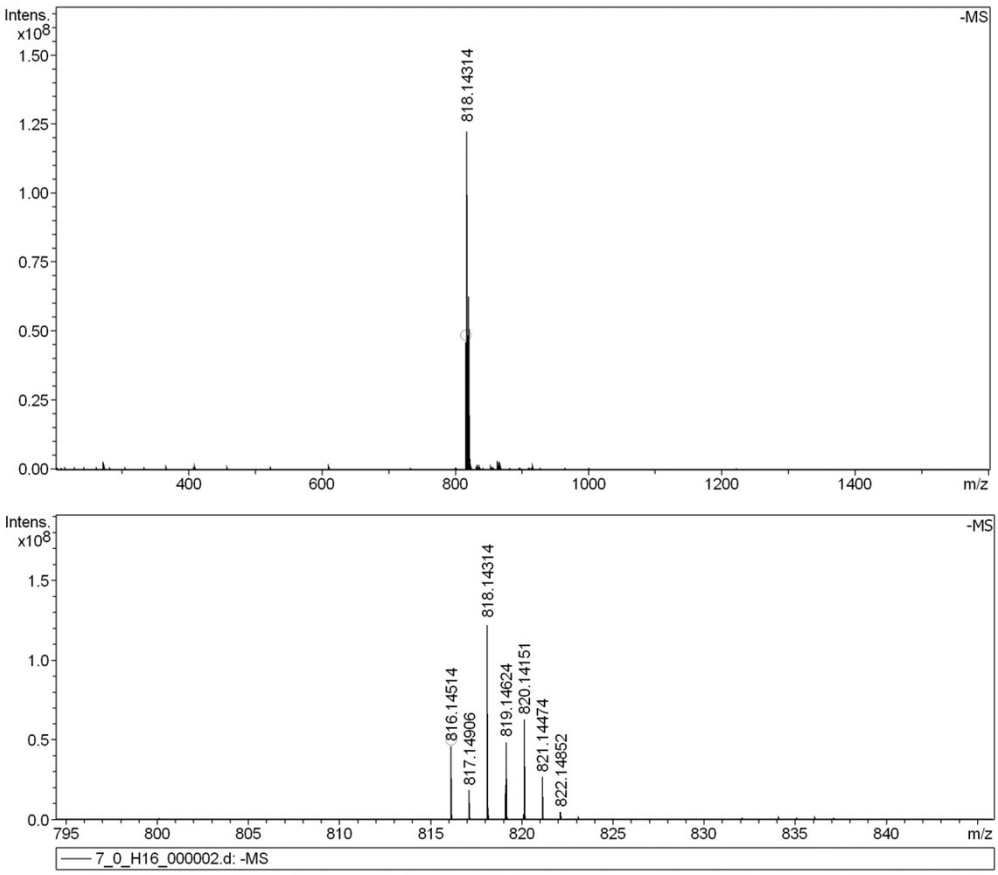


Figure S21. HR-MALDI-TOF spectra of **9**.

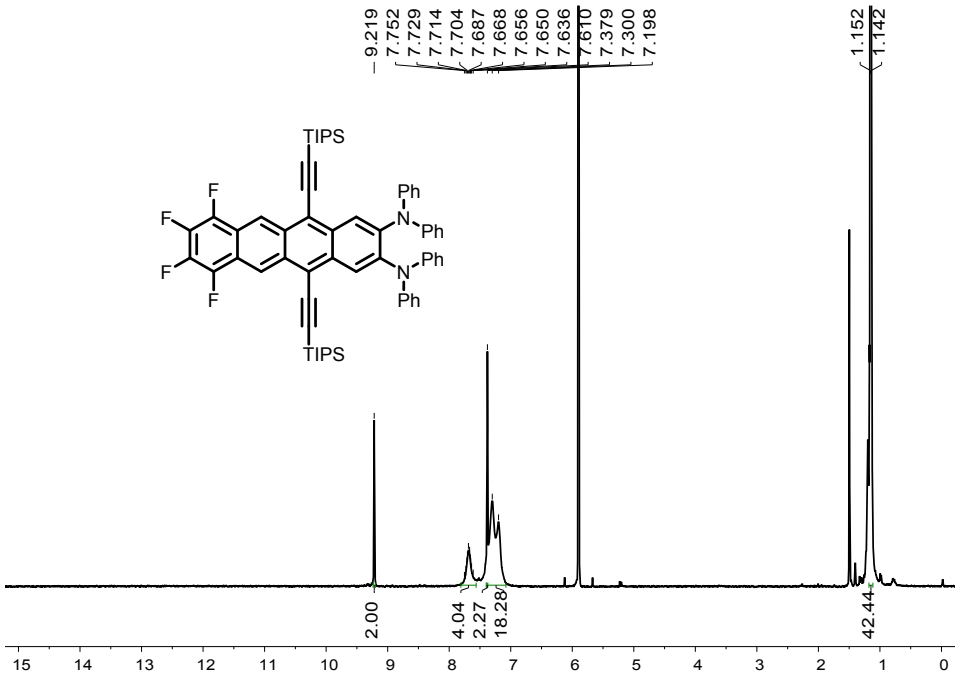


Figure S22. ^{1}H NMR spectrum of **8** in $CDCl_2CDCl_2$ (400 MHz, 298 K).

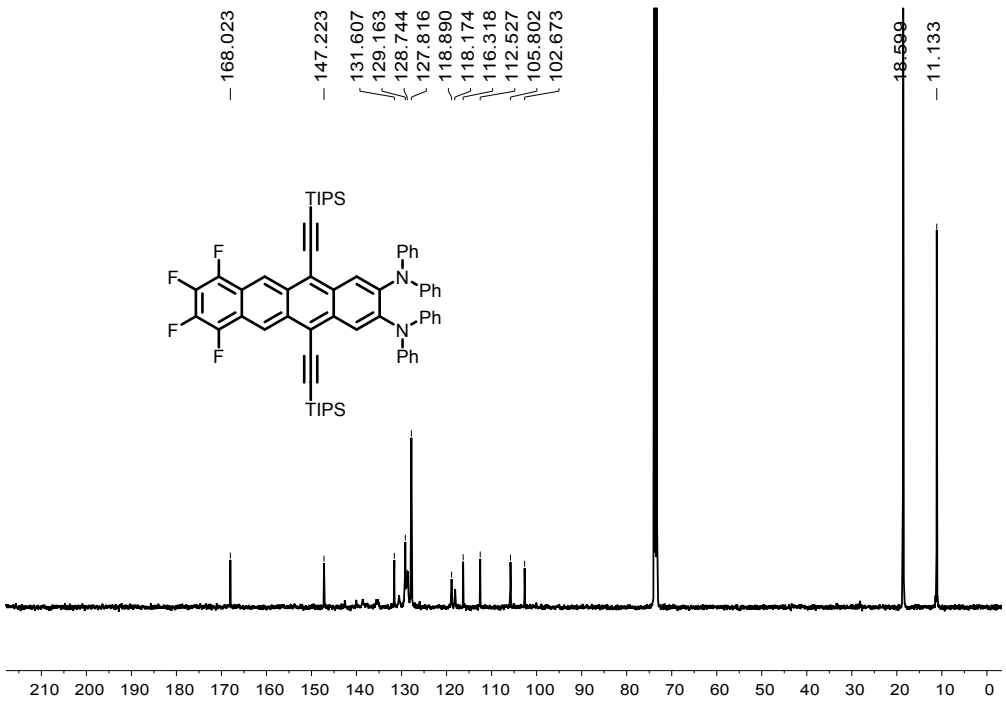


Figure S23. ^{13}C NMR spectrum of **8** in $CDCl_2CDCl_2$ (100 MHz, 298 K).

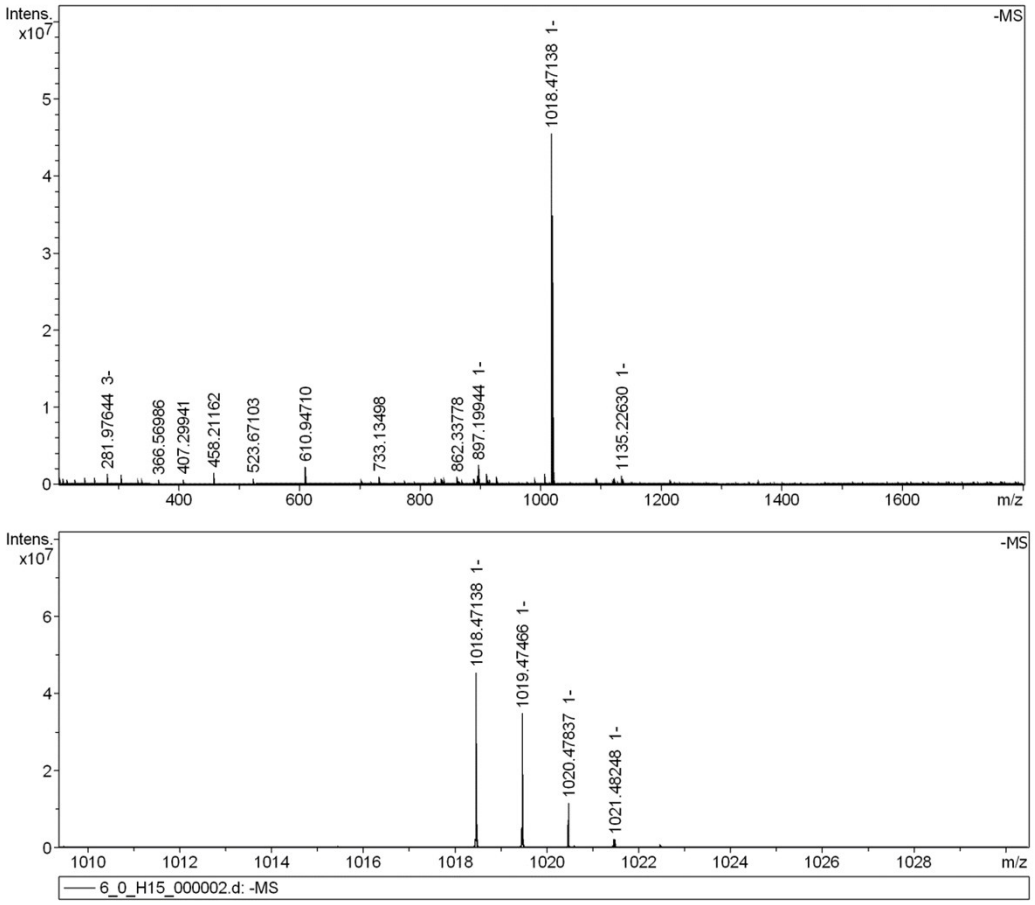


Figure S24. HR-MALDI-TOF spectra of **8**.

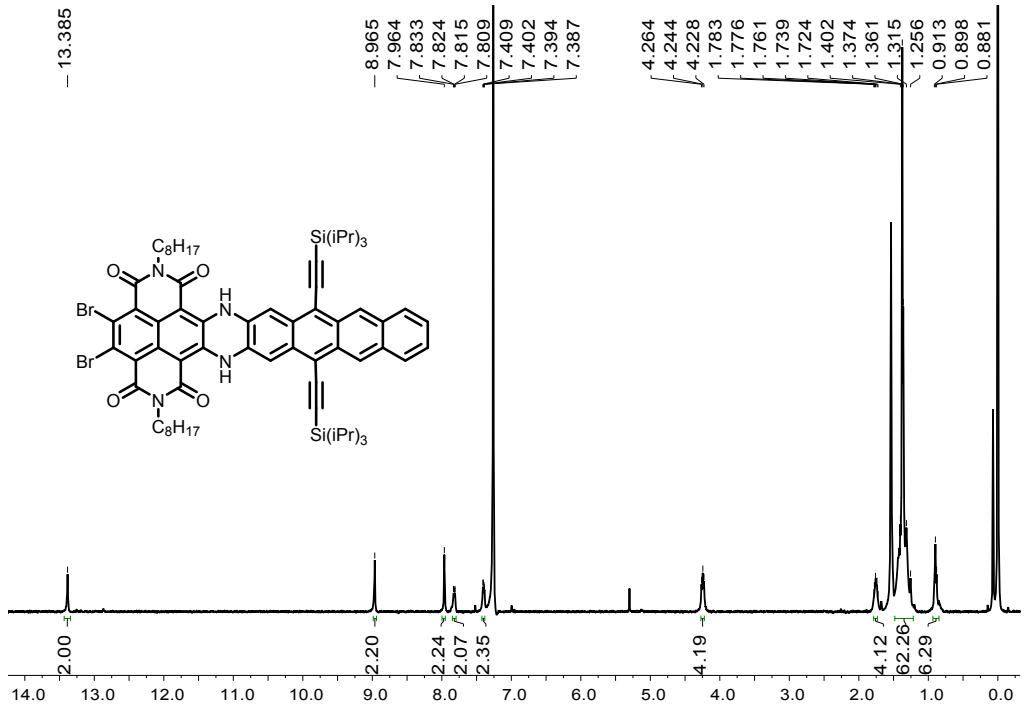


Figure S25. ^{1}H NMR spectrum of **1a** in $CDCl_3$ (400 MHz, 298 K).

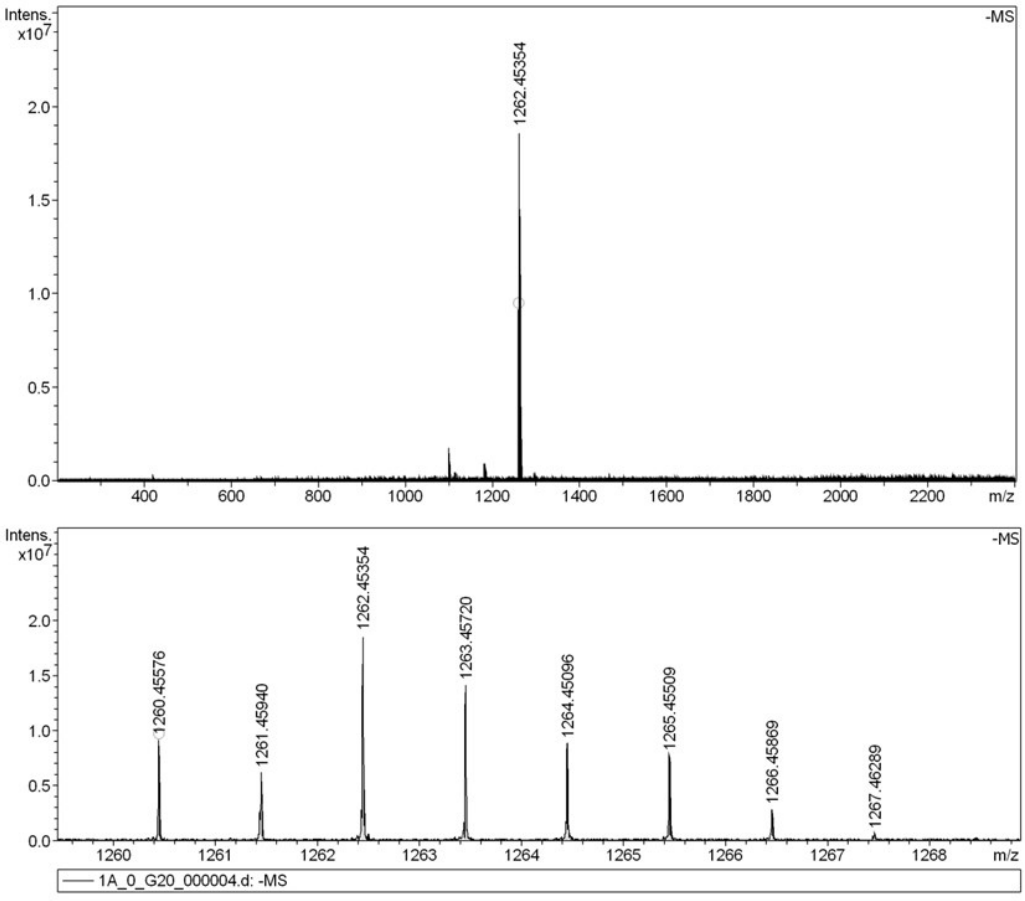


Figure S26. HR-MALDI-TOF spectra of **1a**.

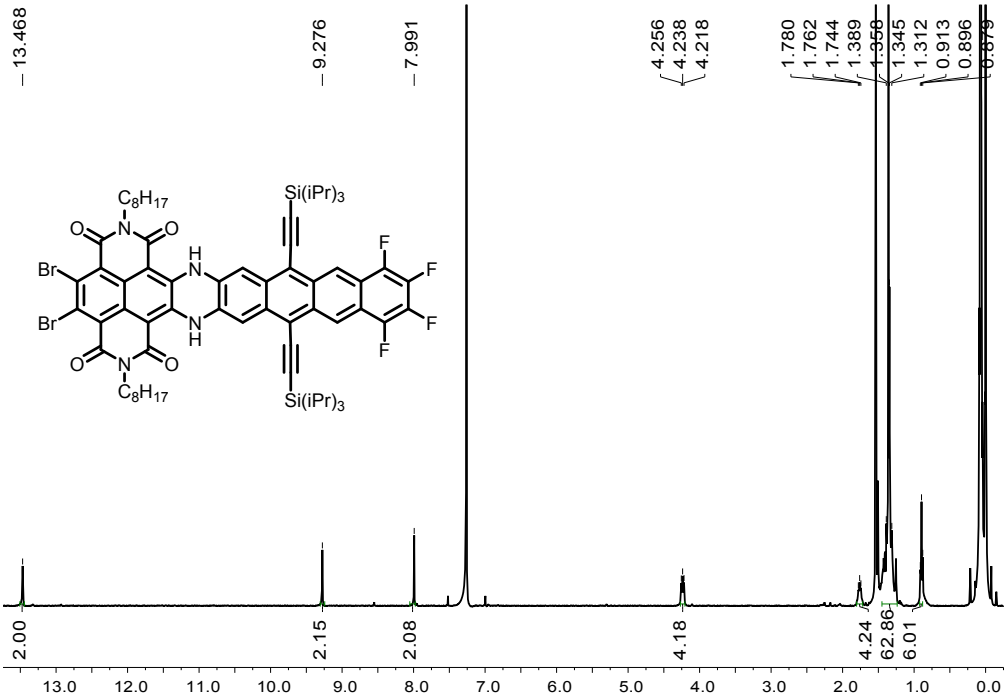


Figure S27. ^{1}H NMR spectrum of **1b** in $CDCl_3$ (400 MHz, 298 K).

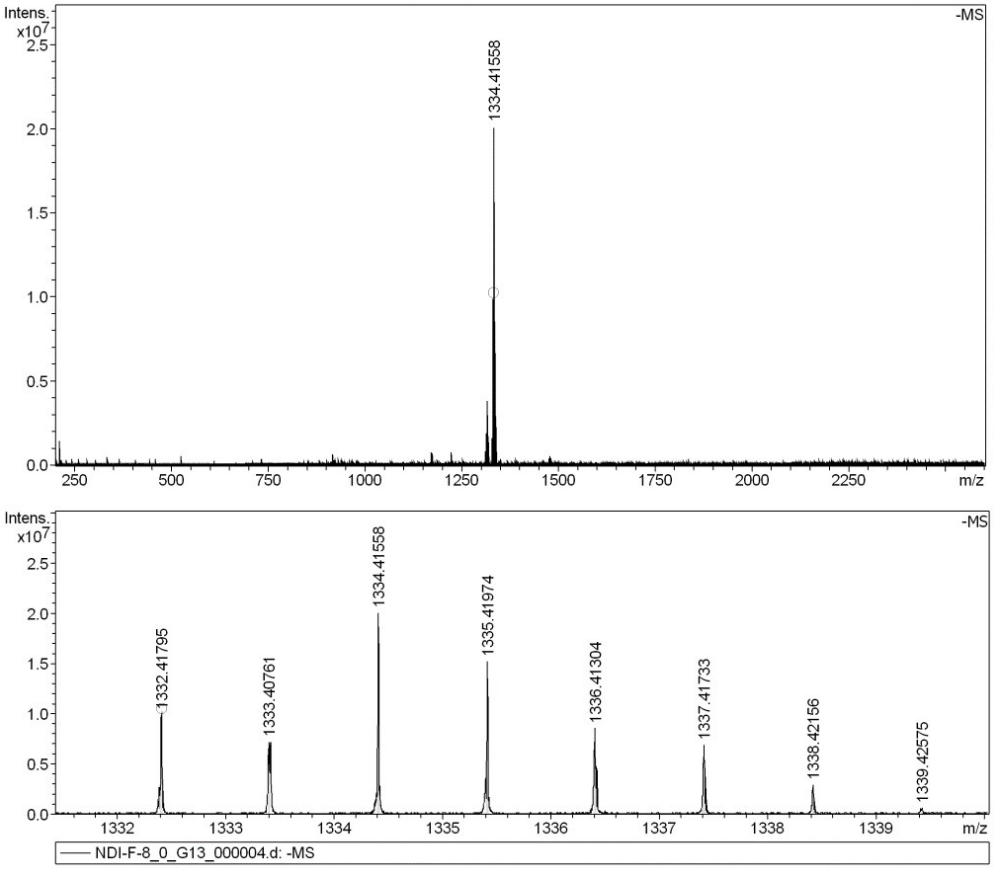


Figure S28. HR-MALDI-TOF spectra of **1b**.

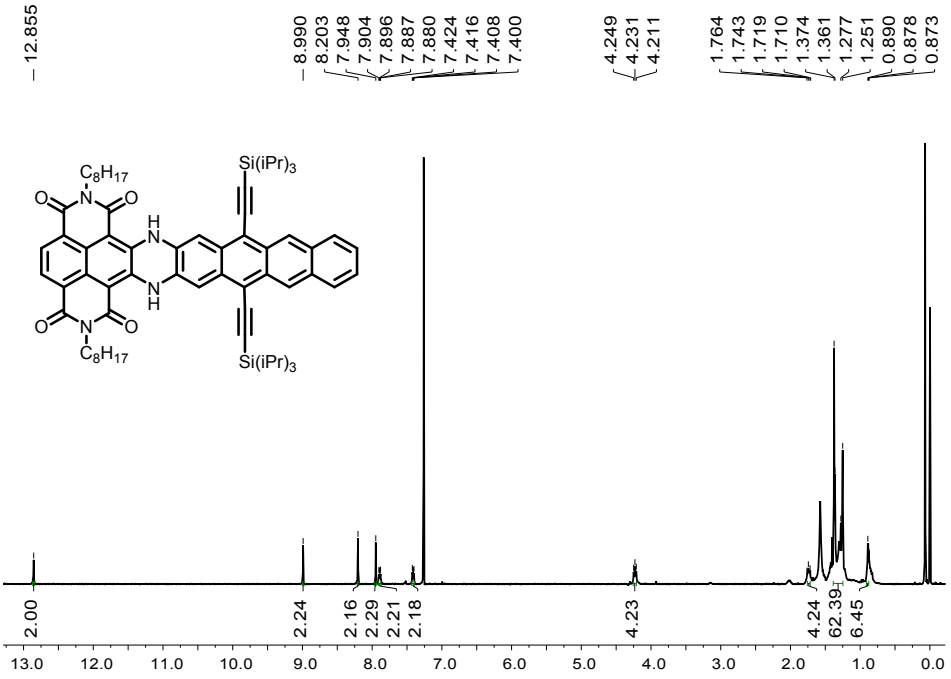


Figure S29. ^{1}H NMR spectrum of **2a** in $CDCl_3$ (400 MHz, 298 K).

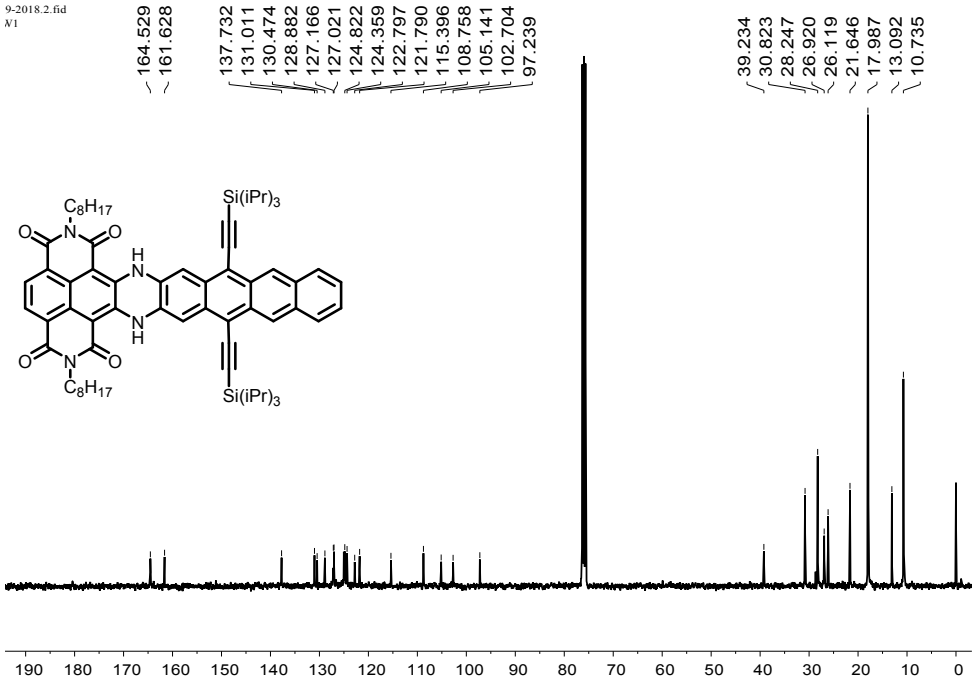


Figure S30. ^{13}C NMR spectrum of **2a** in $CDCl_3$ (100 MHz, 298 K).

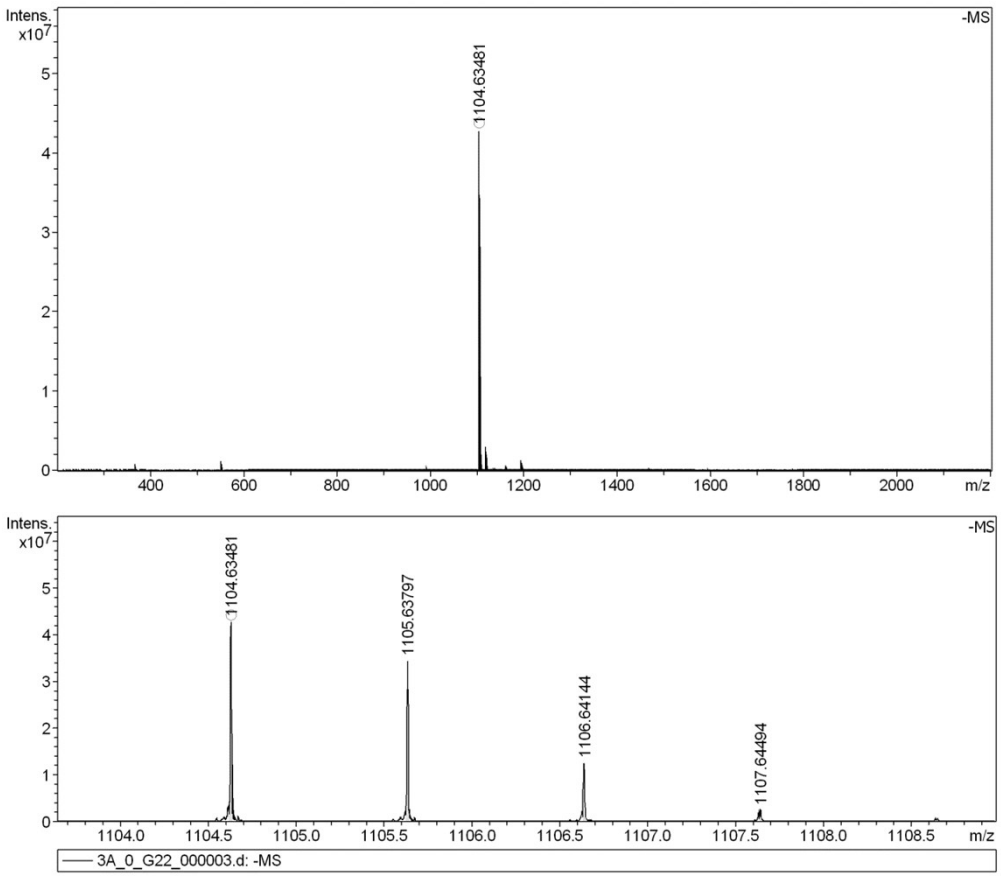


Figure S31. HR-MALDI-TOF spectra of **2a**.

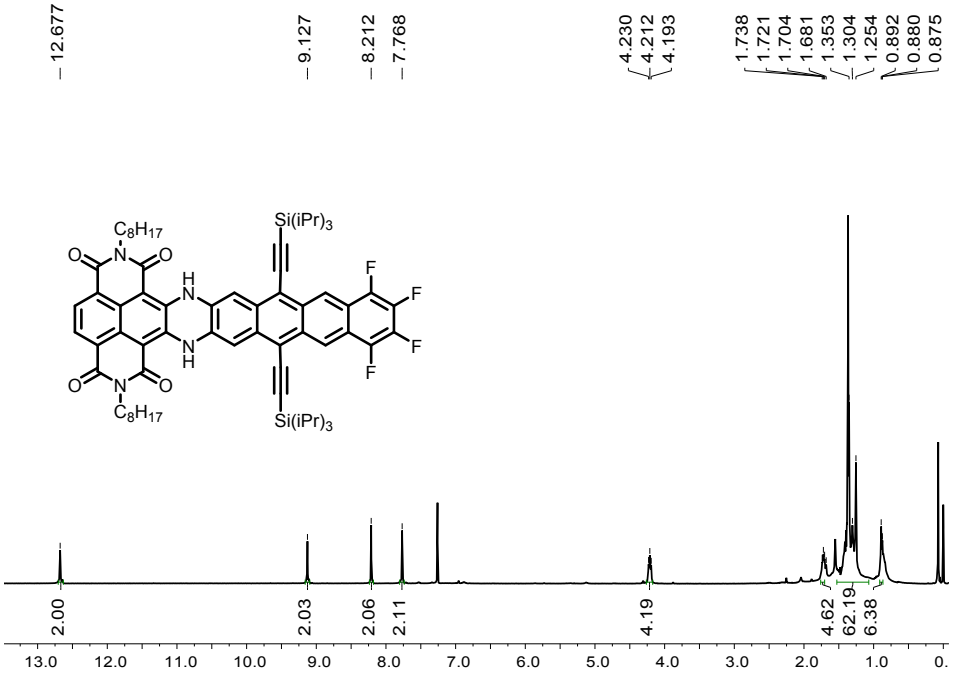


Figure S32. ^{1}H NMR spectrum of **2b** in $CDCl_3$ (400 MHz, 298 K).

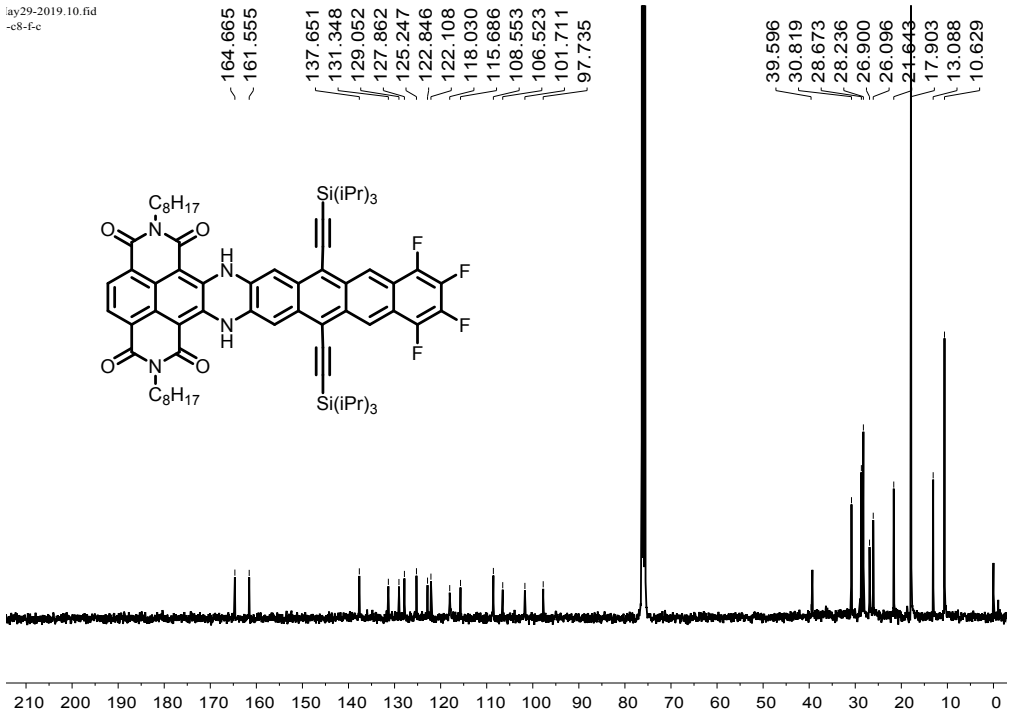


Figure S33. ^{13}C NMR spectrum of **2b** in $CDCl_3$ (100 MHz, 298 K).

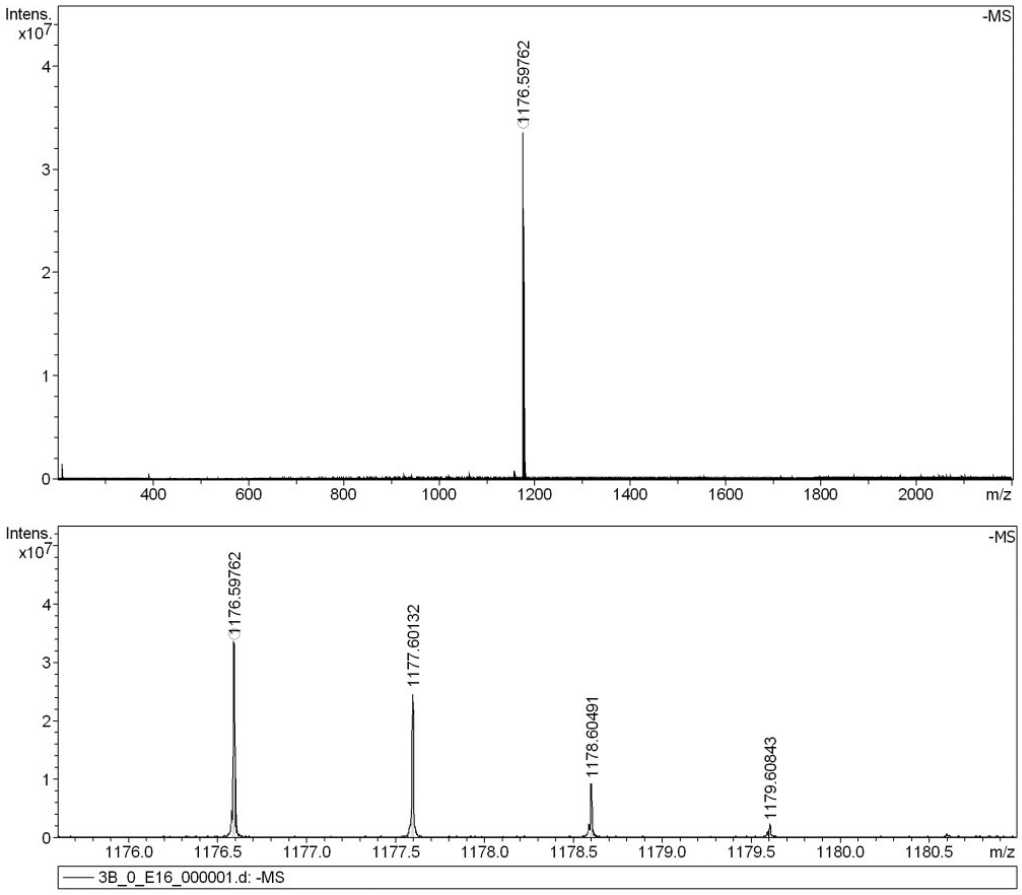


Figure S34. HR-MALDI-TOF spectra of **2b**.

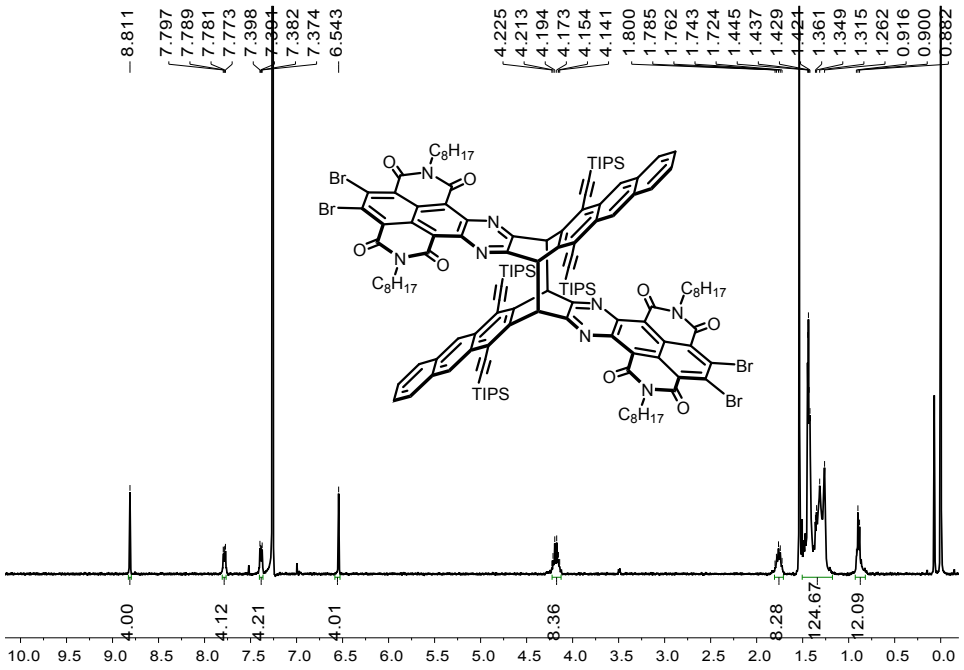


Figure S35. ^{1}H NMR spectrum of **5a** in $CDCl_3$ (400 MHz, 298 K).

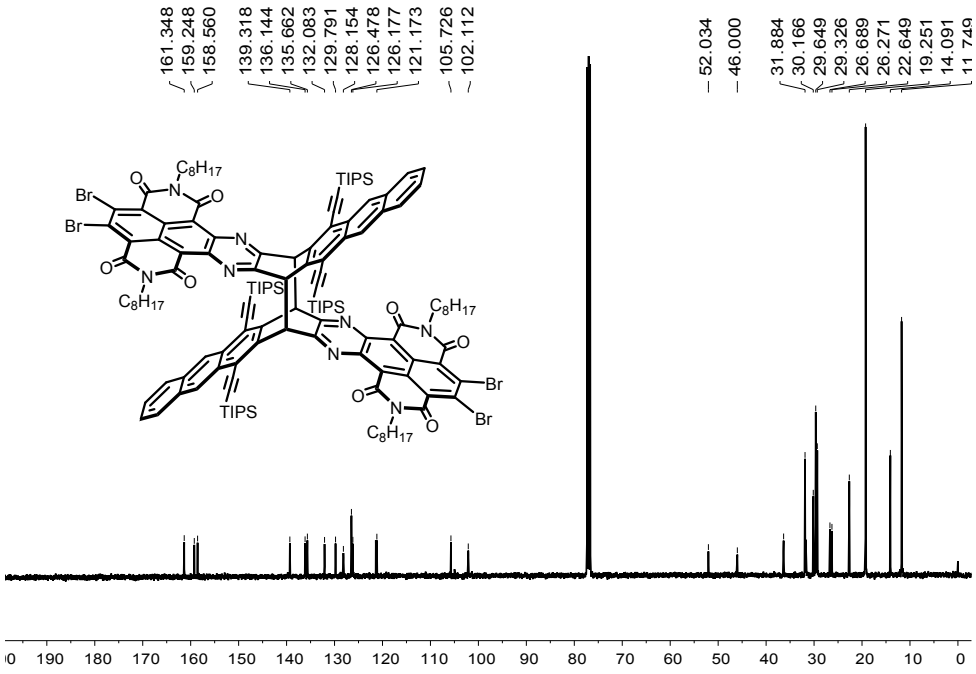


Figure S36. ^{13}C NMR spectrum of **5a** in $CDCl_3$ (100 MHz, 298 K).

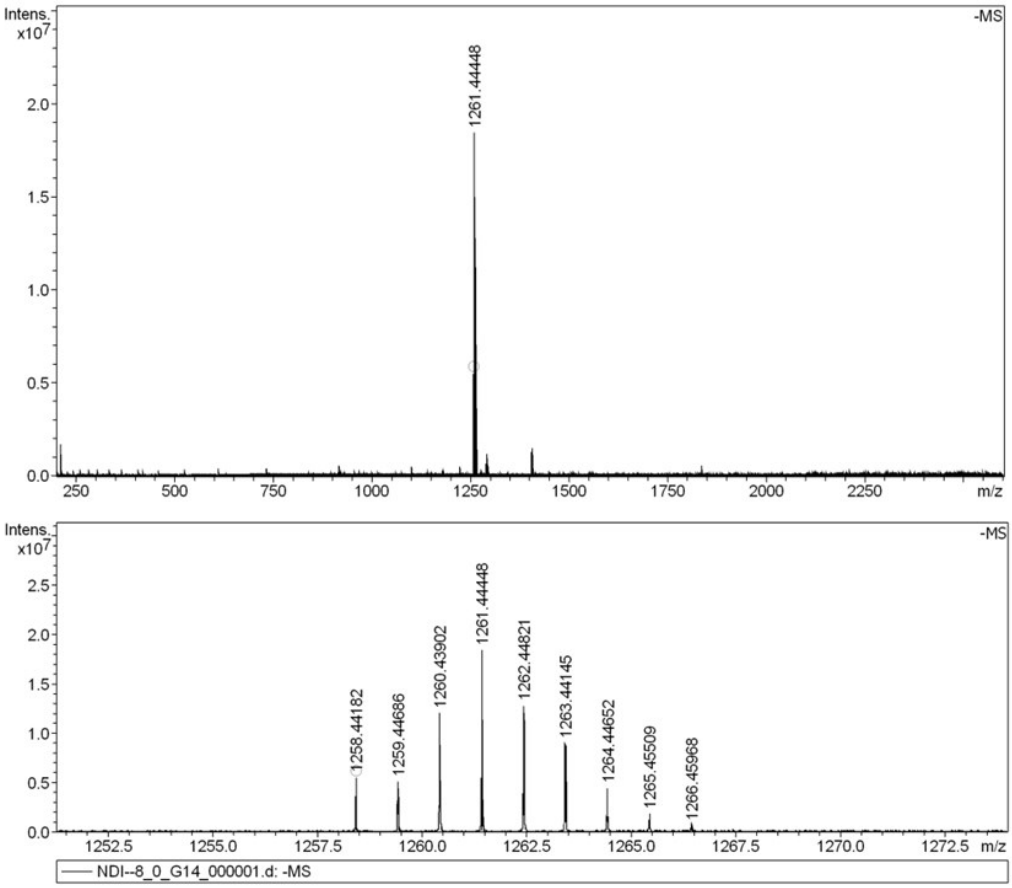


Figure S37. HR-MALDI-TOF spectra of **5a**.

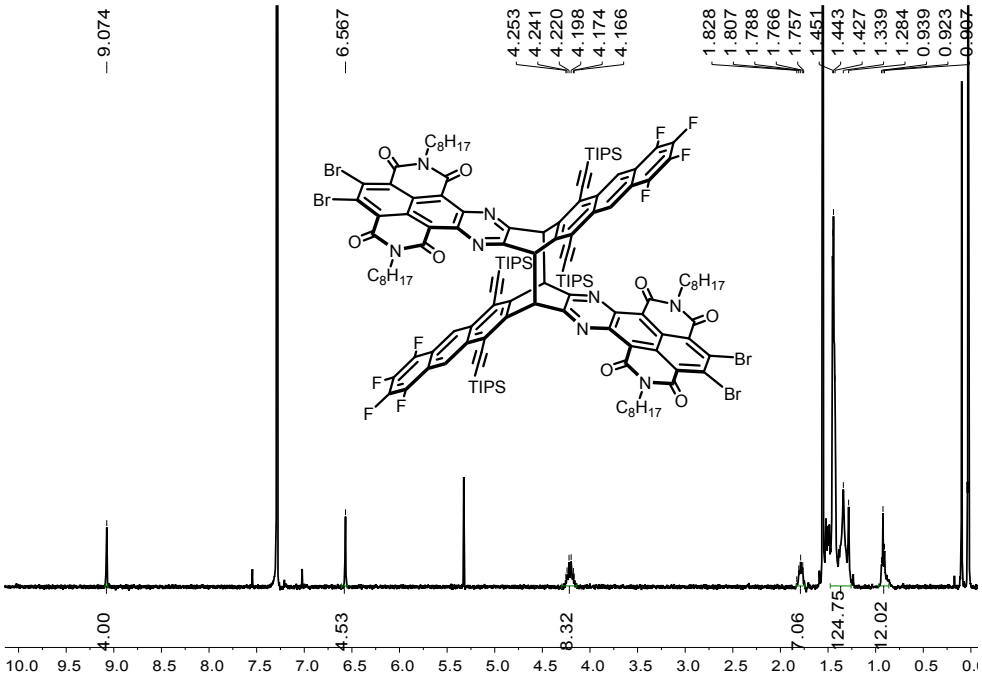


Figure S38. ^{1}H NMR spectrum of **5b** in $CDCl_3$ (400 MHz, 298 K).

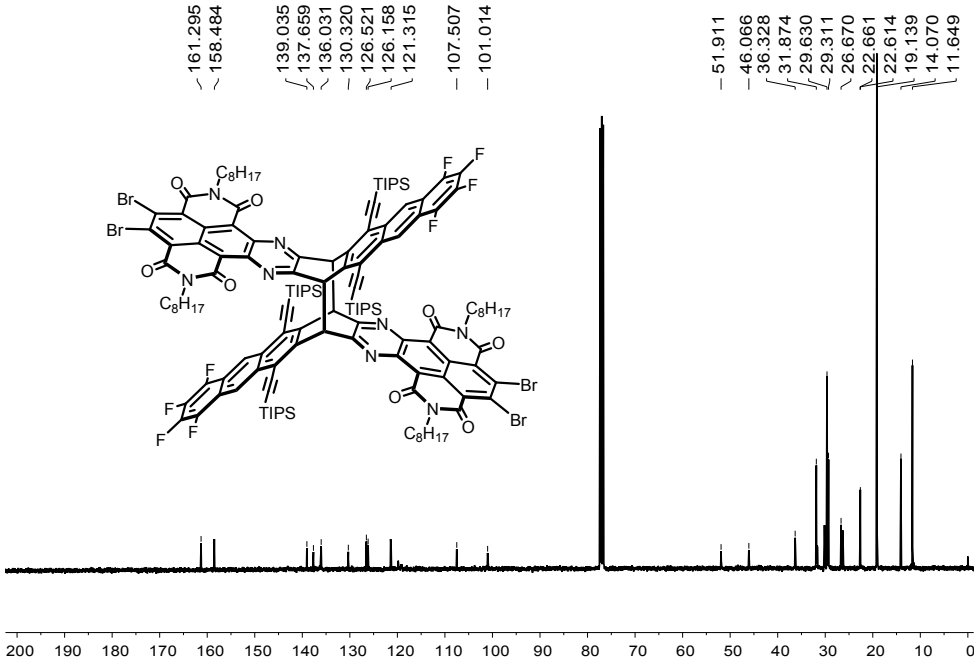


Figure S39. ^{13}C NMR spectrum of **5b** in $CDCl_3$ (100 MHz, 298 K).

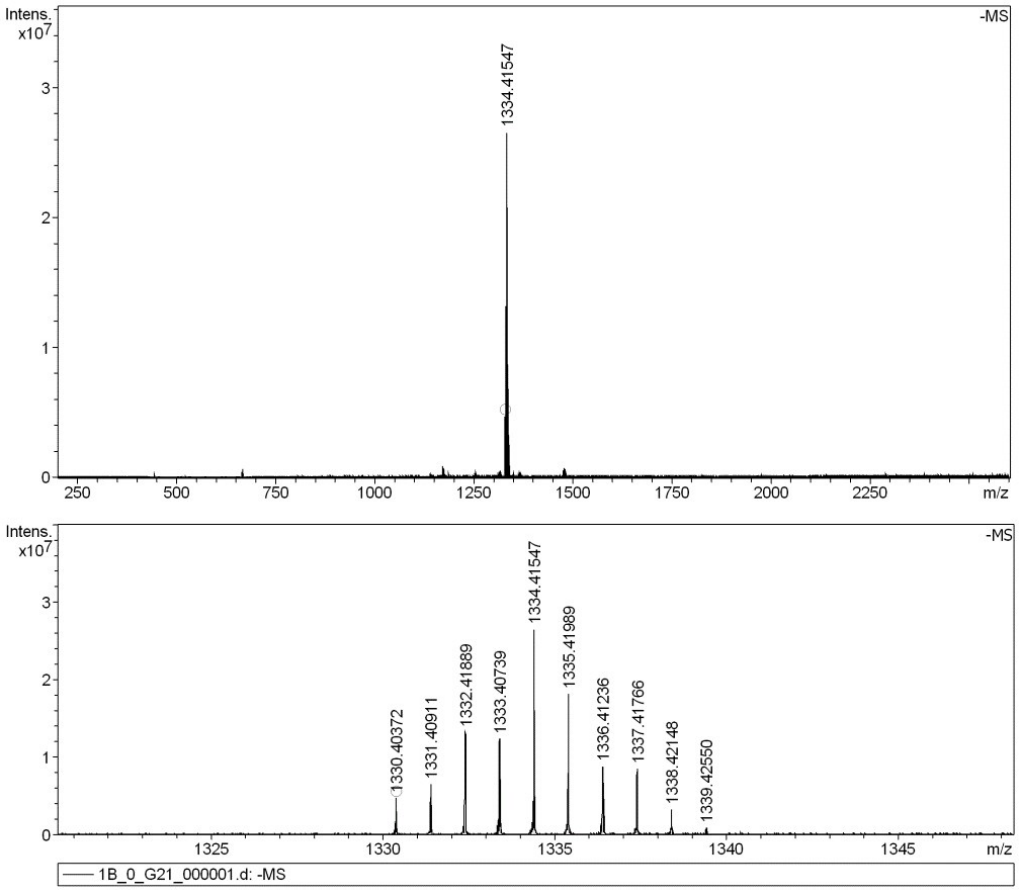


Figure S40. HR-MALDI-TOF spectra of **5b**.

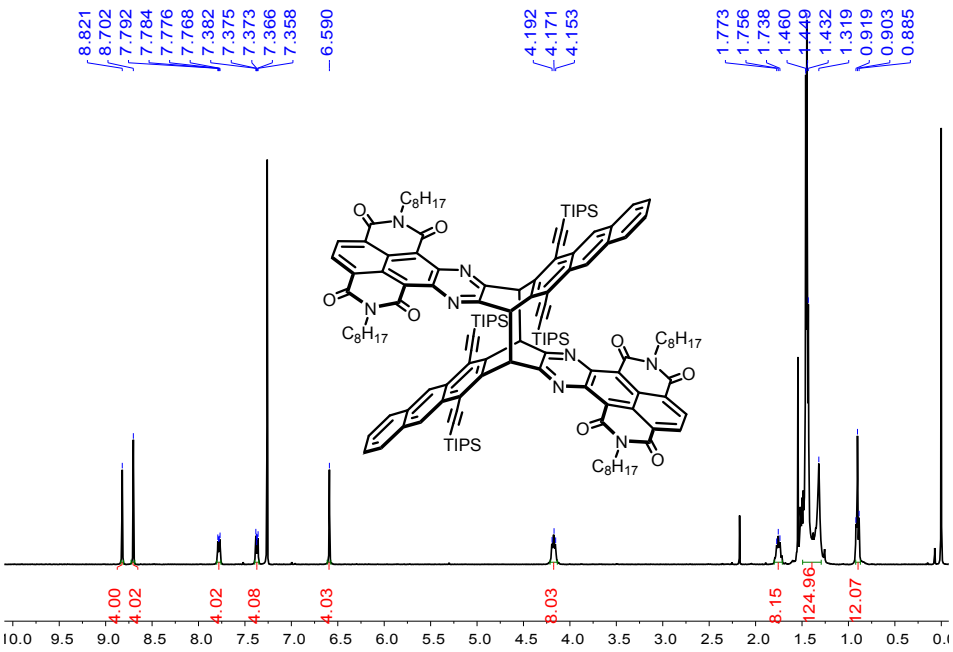


Figure S41. ^{1}H NMR spectrum of **6a** in $CDCl_3$ (400 MHz, 298 K).

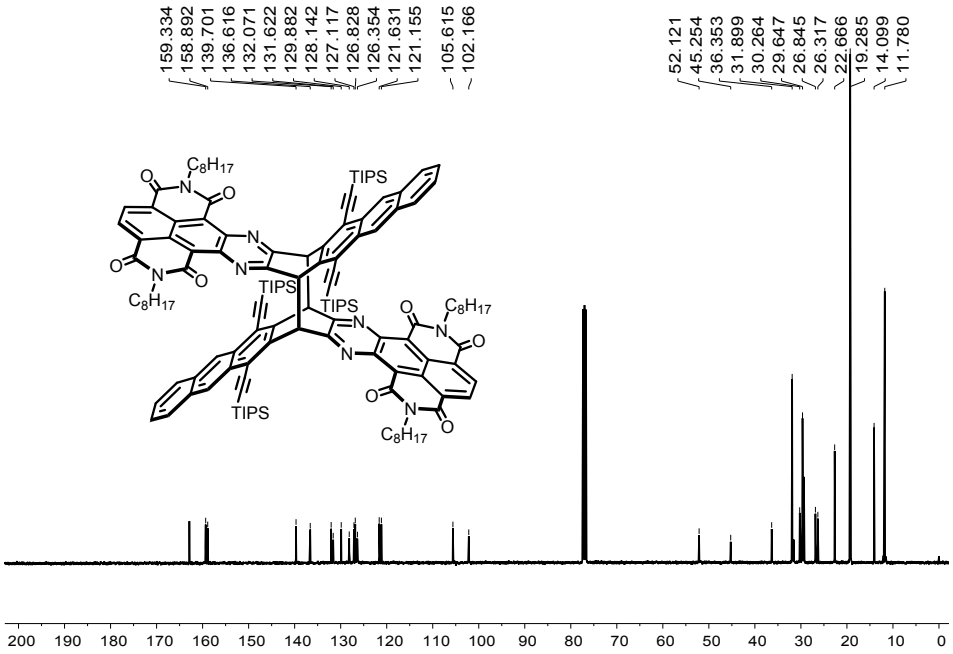


Figure S42. ^{13}C NMR spectrum of **6a** in $CDCl_3$ (100 MHz, 298 K).

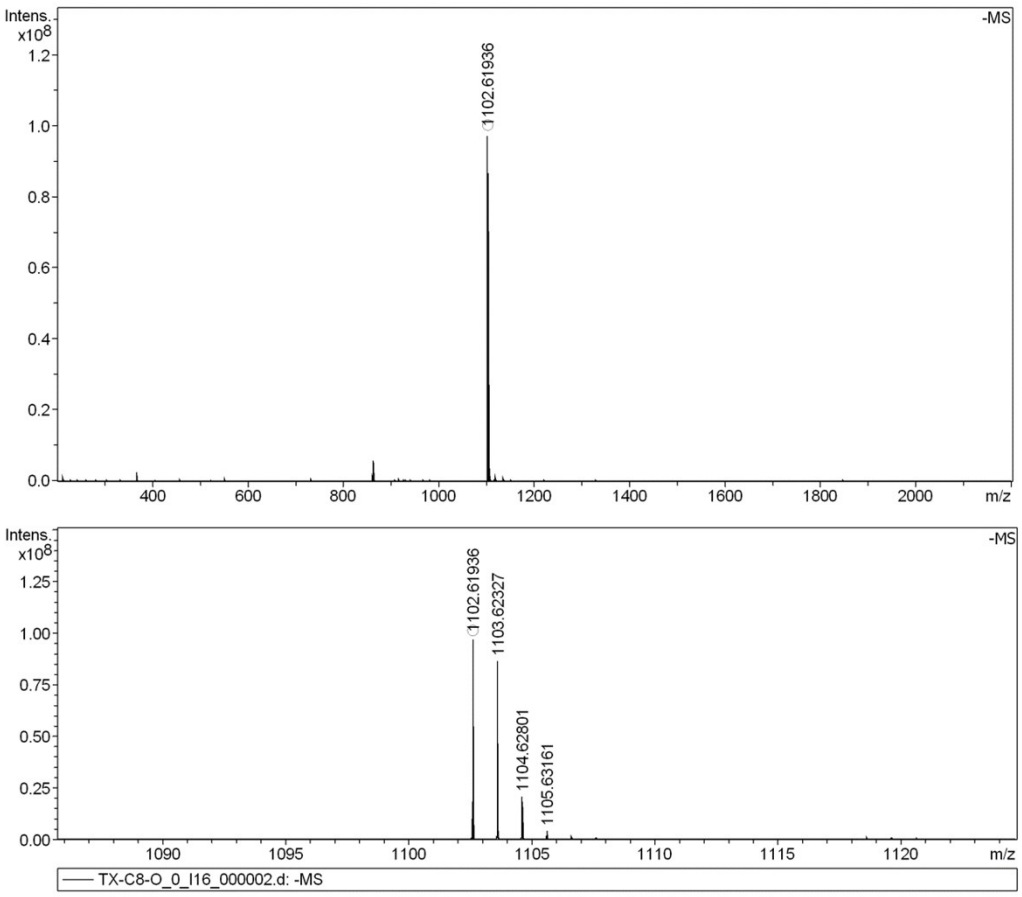


Figure S43. HR-MALDI-TOF spectra of **6a**.

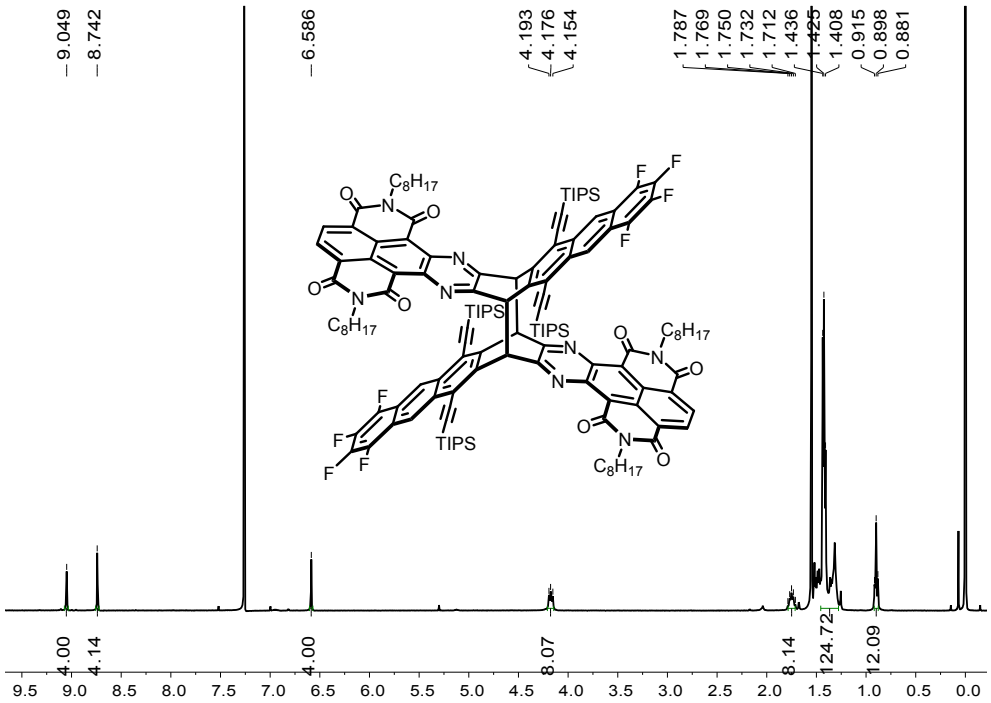


Figure S44. ^{1}H NMR spectrum of **6b** in $CDCl_3$ (400 MHz, 298 K).

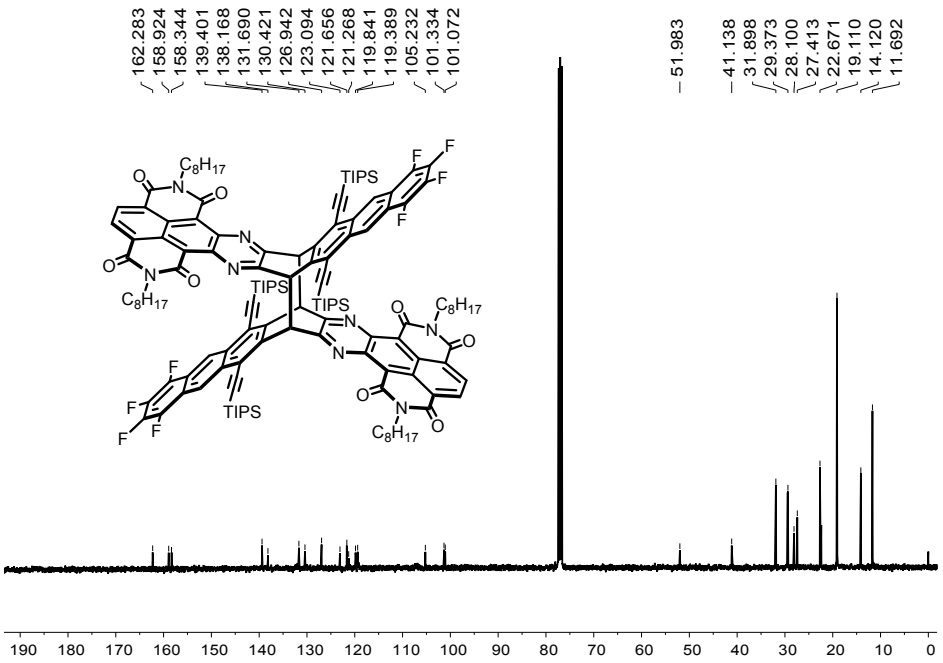


Figure S45. ^{13}C NMR spectrum of **6b** in $CDCl_3$ (100 MHz, 298 K).

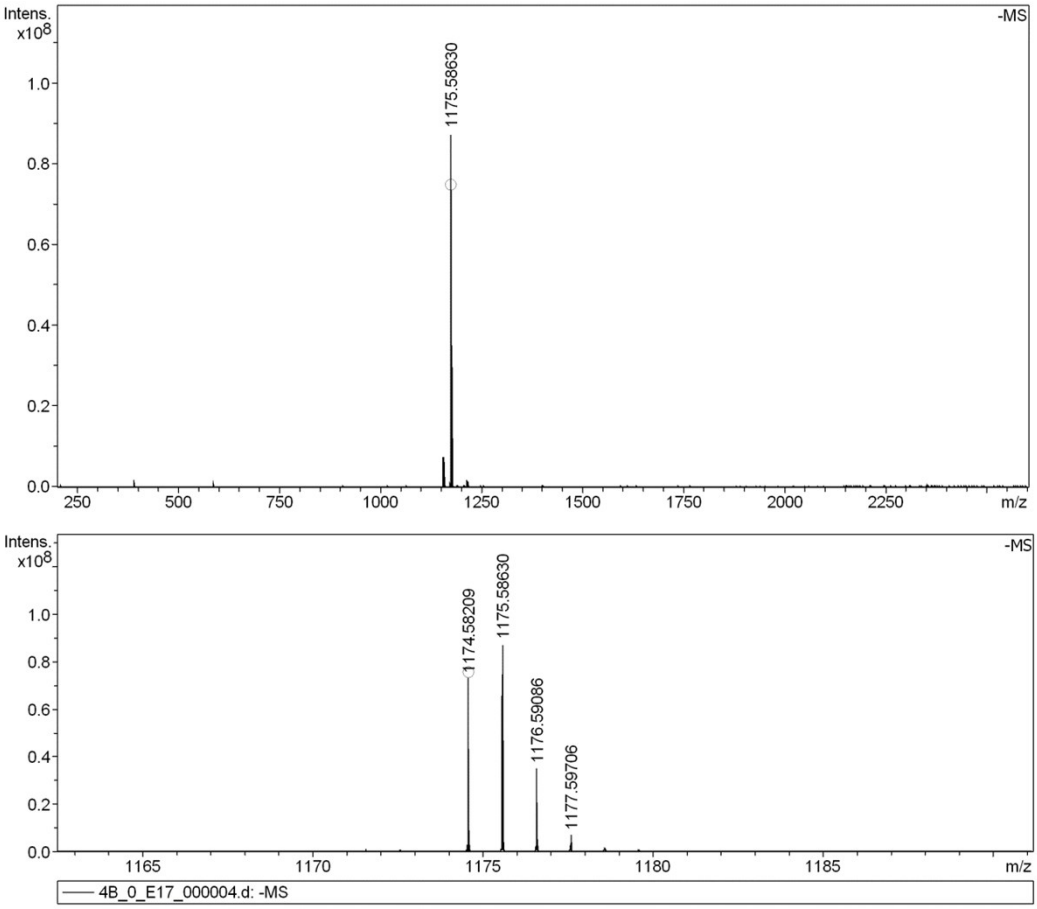


Figure S46. HR-MALDI-TOF spectra of **6b**.

11. Supplementary data of DFT calculations

Table S3. Selected wavelengths, oscillator strengths and comparison of major electronic transitions of the compounds.

Name	Transition	Energy (eV)	Wavelength (nm)	*f*	Electronic Configuration
5a	$S_0 \rightarrow S_1$	2.5154	492.89	0.0006	HOMO-1 → LUMO+1 (3%)
					HOMO → LUMO (75%)
					HOMO → LUMO+1 (18%)
	$S_0 \rightarrow S_2$	2.6256	472.22	0.0041	HOMO-1 → LUMO (30%)
					HOMO-1 → LUMO+1 (16%)
					HOMO → LUMO (9%)
					HOMO → LUMO+1 (41%)
	$S_0 \rightarrow S_3$	2.7188	456.02	0.0061	HOMO-9 → LUMO (18%)
					HOMO-8 → LUMO+1 (25%)
					HOMO-8 → LUMO+1 (11%)
					HOMO-2 → LUMO (13%)
					HOMO-2 → LUMO+1 (9%)
	$S_0 \rightarrow S_4$	2.7289	454.34	0.0107	HOMO-9 → LUMO (16%)
					HOMO-8 → LUMO (15%)
					HOMO-6 → LUMO (25%)
					HOMO-6 → LUMO+1 (8%)
					HOMO-2 → LUMO+1 (10%)
	$S_0 \rightarrow S_5$	2.8153	440.40	0.0067	HOMO-1 → LUMO (34%)
					HOMO-1 → LUMO+1 (16%)
					HOMO → LUMO (9%)
					HOMO → LUMO+1 (32%)
					HOMO → LUMO+3 (4%)
	$S_0 \rightarrow S_6$	2.9057	426.69	0.0034	HOMO-1 → LUMO (30%)
					HOMO-1 → LUMO+1 (54%)
					HOMO-1 → LUMO+2 (7%)
					HOMO → LUMO (3%)
	$S_0 \rightarrow S_8$	2.9192	424.71	0.1450	HOMO-4 → LUMO (35%)
					HOMO-3 → LUMO+1 (34%)
	$S_0 \rightarrow S_9$	2.9966	413.75	0.0101	HOMO-11 → LUMO (27%)
					HOMO-11 → LUMO+1 (21%)
					HOMO-10 → LUMO (7%)
					HOMO-10 → LUMO+1 (4%)
					HOMO-4 → LUMO+1 (8%)
					HOMO-4 → LUMO+1 (9%)
	$S_0 \rightarrow S_{10}$	2.9996	413.33	0.0688	HOMO-10 → LUMO+1 (29%)
					HOMO-10 → LUMO (21%)

					HOMO-4 → LUMO (9%)
					HOMO-3 → LUMO+1 (12%)
	$S_0 \rightarrow S_{11}$	3.0833	402.10	0.9837	HOMO-13 → LUMO (3%)
					HOMO-13 → LUMO+1 (28%)
					HOMO-12 → LUMO (20%)
					HOMO-9 → LUMO (3%)
					HOMO-8 → LUMO (18%)
					HOMO-6 → LUMO (3%)
					HOMO-3 → LUMO+5 (2%)
					HOMO-2 → LUMO (14%)
	$S_0 \rightarrow S_{12}$	3.3734	367.53	0.0094	HOMO-1 → LUMO+1 (5%)
					HOMO-1 → LUMO+2 (19%)
					HOMO-1 → LUMO+3 (5%)
					HOMO → LUMO+2 (11%)
					HOMO → LUMO+3 (48%)
	$S_0 \rightarrow S_{13}$	3.3803	366.79	0.0089	HOMO-13 → LUMO (31%)
					HOMO-12 → LUMO+1 (19%)
					HOMO-8 → LUMO+1 (14%)
					HOMO-2 → LUMO+1 (13%)
	$S_0 \rightarrow S_{14}$	3.3919	365.53	0.2684	HOMO-1 → LUMO+2 (45%)
					HOMO-1 → LUMO+3 (5%)
					HOMO → LUMO+1 (3%)
					HOMO → LUMO+2 (10%)
					HOMO → LUMO+3 (25%)
					HOMO → LUMO+6 (3%)
5b	$S_0 \rightarrow S_1$	2.5807	480.43	0.0013	HOMO-1 → LUMO+1 (3%)
					HOMO → LUMO (71%)
					HOMO → LUMO+1 (21%)
	$S_0 \rightarrow S_2$	2.5943	477.89	0.0078	HOMO-4 → LUMO (18%)
					HOMO-4 → LUMO+1 (11%)
					HOMO-8 → LUMO (19%)
					HOMO-8 → LUMO+1 (31%)
	$S_0 \rightarrow S_3$	2.6091	475.20	0.0091	HOMO-8 → LUMO (10%)
					HOMO-6 → LUMO (31%)
					HOMO-6 → LUMO+1 (18%)
					HOMO-4 → LUMO+1 (11%)
	$S_0 \rightarrow S_4$	2.6790	462.80	0.0072	HOMO-1 → LUMO (23%)
					HOMO-1 → LUMO+1 (16%)
					HOMO → LUMO (12%)
					HOMO → LUMO+1 (42%)
	$S_0 \rightarrow S_5$	2.8267	438.62	0.0066	HOMO-1 → LUMO (31%)

					HOMO-1 → LUMO+1 (23%)
					HOMO → LUMO (9%)
					HOMO → LUMO+1 (23%)
	$S_0 \rightarrow S_7$	3.1219	422.14	0.0014	HOMO-2 → LUMO (32%)
					HOMO-3 → LUMO+1 (27%)
					HOMO-10 → LUMO (10%)
	$S_0 \rightarrow S_8$	2.9440	421.14	0.1279	HOMO-10 → LUMO (8%)
					HOMO-10 → LUMO+1 (4%)
					HOMO-9 → LUMO (7%)
					HOMO-9 → LUMO+1 (11%)
					HOMO-3 → LUMO (26%)
					HOMO-2 → LUMO+1 (27%)
	$S_0 \rightarrow S_{10}$	3.0933	400.17	0.1313	HOMO-10 → LUMO (24%)
					HOMO-10 → LUMO+1 (14%)
					HOMO-9 → LUMO (5%)
					HOMO-9 → LUMO+1 (8%)
					HOMO-3 → LUMO (20%)
					HOMO-2 → LUMO+1 (17%)
	$S_0 \rightarrow S_{11}$	3.1337	395.65	0.9772	HOMO-13 → LUMO (6%)
					HOMO-13 → LUMO+1 (10%)
					HOMO-12→ LUMO+1 (19%)
					HOMO-11→ LUMO (9%)
					HOMO-8→ LUMO (9%)
					HOMO-6→ LUMO (23%)
					HOMO-4→ LUMO (10%)
					HOMO-2→ LUMO+5 (2%)
	$S_0 \rightarrow S_{13}$	3.4165	362.90	0.0616	HOMO→ LUMO+3 (54%)
					HOMO-6→ LUMO+2 (15%)
					HOMO-1→ LUMO+1 (7%)
					HOMO-1→ LUMO+3 (9%)
	$S_0 \rightarrow S_{14}$	3.4363	360.74	0.1749	HOMO-1→ LUMO (4%)
					HOMO-1→ LUMO+1 (8%)
					HOMO-1→ LUMO+2 (59%)
					HOMO→ LUMO+1 (3%)
					HOMO→ LUMO+2 (9%)
					HOMO→ LUMO+3 (11%)
6a	$S_0 \rightarrow S_1$	2.5092	489.12	0.0005	HOMO-1 → LUMO+1 (5%)
					HOMO → LUMO (79%)
					HOMO → LUMO+1 (12%)
	$S_0 \rightarrow S_2$	2.6274	471.88	0.0047	HOMO-1 → LUMO (30%)
					HOMO-1 → LUMO+1 (11%)

					HOMO → LUMO (6%)
					HOMO → LUMO+1 (48%)
	$S_0 \rightarrow S_3$	2.6298	471.46	0.0032	HOMO-9 → LUMO (2%)
					HOMO-8 → LUMO+1 (14%)
					HOMO-8 → LUMO+1 (28%)
					HOMO-2 → LUMO (16%)
	$S_0 \rightarrow S_4$	2.6439	468.95	0.0041	HOMO-9 → LUMO (16%)
					HOMO-8 → LUMO (4%)
					HOMO-7 → LUMO (22%)
					HOMO-7 → LUMO+1 (30%)
					HOMO-2 → LUMO+1 (14%)
	$S_0 \rightarrow S_5$	2.7806	445.89	0.0086	HOMO-1 → LUMO (42%)
					HOMO-1 → LUMO+1 (12%)
					HOMO → LUMO (6%)
					HOMO → LUMO+1 (31%)
					HOMO → LUMO+3 (4%)
	$S_0 \rightarrow S_6$	2.9057	426.69	0.0034	HOMO-1 → LUMO (21%)
					HOMO-1 → LUMO+1 (61%)
					HOMO-1 → LUMO+2 (5%)
					HOMO → LUMO (4%)
					HOMO → LUMO+2 (3%)
	$S_0 \rightarrow S_8$	2.9535	419.79	0.303	HOMO-4→ LUMO (51%)
					HOMO-4→ LUMO+1 (3%)
					HOMO-3→ LUMO+1 (40%)
	$S_0 \rightarrow S_9$	3.0954	400.54	0.0135	HOMO→ LUMO+3 (34%)
					HOMO→ LUMO+2 (28%)
					HOMO-1→ LUMO+3 (14%)
	$S_0 \rightarrow S_{10}$	3.1154	397.98	0.3076	HOMO-1→ LUMO+2 (51%)
					HOMO→ LUMO+1 (3%)
					HOMO→ LUMO+2 (5%)
					HOMO→ LUMO+3 (29%)
	$S_0 \rightarrow S_{11}$	3.2282	384.07	0.6925	HOMO-11→ LUMO+1 (24%)
					HOMO-10→ LUMO (31%)
					HOMO-8→ LUMO (13%)
					HOMO-4→ LUMO+7 (2%)
					HOMO-3→ LUMO+6 (2%)
					HOMO-2→ LUMO (18%)
	$S_0 \rightarrow S_{14}$	3.4959	354.66	0.0152	HOMO-11→ LUMO (27%)
					HOMO-10→ LUMO+1 (25%)
					HOMO-2→ LUMO+1 (18%)
6b	$S_0 \rightarrow S_1$	2.6540	467.15	0.0033	HOMO-1 → LUMO+1 (12%)

					HOMO → LUMO (35%)
					HOMO → LUMO+1 (34%)
	$S_0 \rightarrow S_2$	2.6611	465.91	0.0023	HOMO-4 → LUMO (2%)
					HOMO-4 → LUMO+1 (28%)
					HOMO-6 → LUMO (44%)
					HOMO-8 → LUMO+1 10%)
	$S_0 \rightarrow S_3$	2.6810	462.45	0.0005	HOMO-1 → LUMO+1 (5%)
					HOMO → LUMO (70%)
					HOMO→ LUMO+1 (19%)
	$S_0 \rightarrow S_4$	2.6925	460.47	0.0066	HOMO-1 → LUMO (22%)
					HOMO-1 → LUMO+1 (13%)
					HOMO → LUMO (12%)
					HOMO → LUMO+1 (46%)
	$S_0 \rightarrow S_5$	2.8472	435.46	0.0054	HOMO-1 → LUMO (32%)
					HOMO-1 → LUMO+1 (23%)
					HOMO → LUMO (8%)
					HOMO → LUMO+1 (19%)
	$S_0 \rightarrow S_7$	2.9778	416.35	0.0018	HOMO-3 → LUMO+1 (40%)
					HOMO-2 → LUMO+1 (27%)
					HOMO-2 → LUMO (3%)
	$S_0 \rightarrow S_8$	2.9925	414.30	0.3796	HOMO-3→ LUMO (49%)
					HOMO-2→ LUMO+1 (43%)
					HOMO→ LUMO+1 (2%)
	$S_0 \rightarrow S_{10}$	3.1946	388.1	0.1711	HOMO-12→ LUMO (3%)
					HOMO-1→ LUMO (3%)
					HOMO-1→ LUMO+1 (8%)
					HOMO-1→ LUMO+2 (50%)
					HOMO→ LUMO+2 (9%)
					HOMO→ LUMO+3 (12%)
	$S_0 \rightarrow S_{11}$	3.2813	377.85	0.6365	HOMO-11→ LUMO+1 (27%)
					HOMO-10→ LUMO (25%)
					HOMO-8→ LUMO (9%)
					HOMO-3→ LUMO+6 (5%)
					HOMO-2→ LUMO (16%)
	$S_0 \rightarrow S_{14}$	3.6004	344.36	0.0069	HOMO-13→ LUMO (30%)
					HOMO-10→ LUMO+1 (24%)
					HOMO-8→ LUMO+6 (23%)
					HOMO-4→ LUMO+1 (5%)

Table S4. Cartesian coordinates of the ground state optimized geometry for compound **5a**. The calculated absolute energy value for this molecule is -36535556.93 kJ/mol

C	-0.52388900	2.03639200	-0.71538600
C	-0.52388400	2.03658500	0.71480200
C	-1.26499900	2.96727200	-1.42750100
C	-2.05668800	3.95207400	-0.72125400
C	-2.05668600	3.95226500	0.72016400
C	-1.26499200	2.96765600	1.42667100
C	-2.82312800	4.90282700	-1.40161700
C	-3.59237300	5.85613900	-0.72162100
C	-3.59237200	5.85633000	0.72002900
C	-2.82312600	4.90319800	1.40027600
C	-1.26115800	2.96074900	-2.85388500
C	-1.25875700	2.95902500	-4.06452400
C	-1.26114700	2.96151800	2.85305700
C	-1.25874700	2.96010600	4.06369800
C	-4.38090800	6.82951700	-1.40908300
C	-5.12473400	7.74692200	-0.71392700
C	-5.12473400	7.74711000	0.71183600
C	-4.38090700	6.82988900	1.40723400
C	8.82858200	0.59028000	0.71862100
C	8.82856700	0.58995600	-0.71890300
C	7.63473100	0.61824400	-1.42615700
C	6.40042300	0.79053000	-0.71793500
C	6.40043600	0.79082700	0.71762100
C	7.63476200	0.61886400	1.42588900
C	5.19373500	0.98362400	-1.42051900
C	3.96669100	0.99644300	-0.71974800
C	3.96670100	0.99670300	0.71938500
C	5.19375500	0.98417900	1.42014500
C	7.57704800	0.40480700	-2.91337200
N	6.39881900	0.80738500	-3.54299400
C	5.23320100	1.22966600	-2.88963700
C	5.23322900	1.23080200	2.88916500
N	6.39888600	0.80886500	3.54267400
C	7.57712700	0.40608600	2.91320000
O	8.48981100	-0.08326200	-3.55738500
O	4.33937600	1.75143900	-3.53037700
O	4.33941400	1.75284700	3.52969700
O	8.48994600	-0.08162000	3.55741000
C	6.36283400	0.84143500	-5.01079700
C	6.36294100	0.84356700	5.01046300

N	2.78496200	0.98529500	-1.41675300
C	1.68303300	0.98883900	-0.72050500
C	1.68304400	0.98905600	0.72017700
N	2.78498300	0.98575800	1.41641000
C	-8.80928500	-1.28995100	-0.71844000
C	-8.80926300	-1.28976000	0.71901300
C	-7.61816000	-1.20132000	1.42616600
C	-6.39439100	-0.96489800	0.71798500
C	-6.39441200	-0.96509400	-0.71757900
C	-7.61820500	-1.20170200	-1.42565600
C	-5.19909300	-0.70966300	1.42082900
C	-3.97542700	-0.62319200	0.71973900
C	-3.97544700	-0.62339100	-0.71949600
C	-5.19913400	-0.71005600	-1.42052800
C	-7.55012700	-1.41465200	2.91287100
N	-6.39083000	-0.96183500	3.54337000
C	-5.24924700	-0.47599700	2.89183500
C	-5.24932700	-0.47680600	-2.89160000
N	-6.39094300	-0.96279500	-3.54296500
C	-7.55022900	-1.41541900	-2.91230700
O	-8.43937500	-1.94534600	3.55605400
O	-4.38116000	0.08349700	3.53609500
O	-4.38128500	0.08256000	-3.53603300
O	-8.43952600	-1.94623300	-3.55532300
C	-6.35430200	-0.93763300	5.01144100
C	-6.35447300	-0.93896600	-5.01104300
N	-2.79383400	-0.57321300	1.41610900
C	-1.69547200	-0.48055100	0.72073900
C	-1.69549100	-0.48074600	-0.72059500
N	-2.79387200	-0.57360200	-1.41591000
C	0.51025200	-1.53322800	0.71539700
C	0.51023100	-1.53342600	-0.71503000
C	1.25112200	-2.46504200	1.42639000
C	2.04083000	-3.45255200	0.72113700
C	2.04081000	-3.45275000	-0.72028900
C	1.25108100	-2.46543400	-1.42578900
C	2.80479000	-4.40545200	1.40122300
C	3.57255900	-5.36035200	0.72146000
C	3.57254000	-5.36054900	-0.72013200
C	2.80475100	-4.40583600	-1.40013500
C	1.24825500	-2.45818000	2.85342900
C	1.24801000	-2.45709100	4.06432800
C	1.24817000	-2.45896100	-2.85283000
C	1.24787600	-2.45820900	-4.06373000

C	4.35944700	-6.33482900	1.40903400
C	5.10208600	-7.25309400	0.71373400
C	5.10206700	-7.25328800	-0.71193000
C	4.35940900	-6.33521300	-1.40746000
C	0.33428300	0.98440100	-1.40320500
C	0.33430600	0.98479000	1.40289900
C	-0.34672800	-0.47993400	-1.40319900
C	-0.34669000	-0.47955100	1.40330500
H	-2.82209800	4.89813900	-2.48723200
H	-2.82209600	4.89879800	2.48589200
H	-1.26206300	2.93830200	-5.13083400
H	-1.26194700	2.93953000	5.13001200
H	-4.37853800	6.82637900	-2.49627100
H	-5.72087300	8.48242800	-1.24706700
H	-5.72087300	8.48275700	1.24478300
H	-4.37853700	6.82703800	2.49442300
H	6.26396700	1.87429000	-5.35372200
H	7.28657300	0.40060100	-5.37697400
H	5.49893800	0.27637400	-5.36722900
H	5.49909000	0.27861000	5.36716900
H	7.28671800	0.40295600	5.37681000
H	6.26401700	1.87656900	5.35292900
H	-5.45222700	-1.44394600	5.36094700
H	-6.32768200	0.09653400	5.36402900
H	-7.24449900	-1.44450500	5.37517500
H	-6.32785700	0.09511000	-5.36389700
H	-5.45241600	-1.44537700	-5.36045400
H	-7.24468900	-1.44592300	-5.37461200
H	2.80277500	-4.40248700	2.48690200
H	2.80270900	-4.40316700	-2.48581500
H	1.24392700	-2.44079200	5.13084800
H	1.24376500	-2.44218200	-5.13025300
H	4.35761000	-6.33167200	2.49619700
H	5.69780200	-7.98889300	1.24678800
H	5.69777000	-7.98923300	-1.24479900
H	4.35754400	-6.33235300	-2.49462500
H	0.48843500	1.25406500	-2.44736400
H	0.48847200	1.25474300	2.44698100
H	-0.50297900	-0.75032300	-2.44677300
H	-0.50290900	-0.74966100	2.44695500
Br	10.50038600	0.57503200	1.60699700
Br	10.50035400	0.57428700	-1.60730400
Br	-10.47829000	-1.39058800	1.60681100
Br	-10.47834000	-1.39102300	-1.60615700

Cartesian coordinates and calculated energy for 5b.

Table S5. Cartesian coordinates of the ground state optimized geometry for compound **5b**. The calculated absolute energy value for this molecule is -38572280.08 kJ/mol

C	0.72443000	1.90913600	0.71554900
C	0.72443900	1.90934100	-0.71496100
C	1.55545800	2.75968700	1.42874700
C	2.43855500	3.66180100	0.72079200
C	2.43856900	3.66200200	-0.71967900
C	1.55548200	2.76009100	-1.42790500
C	3.29013400	4.53313700	1.40699700
C	4.14098100	5.40586600	0.72120300
C	4.14099500	5.40606600	-0.71957200
C	3.29016100	4.53352800	-1.40562500
C	1.55558600	2.75403500	2.85451400
C	1.56012500	2.75448100	4.06495800
C	1.55563700	2.75483900	-2.85367300
C	1.56018800	2.75561900	-4.06411700
C	5.01545000	6.30139000	1.40052100
C	5.84117600	7.14750100	0.71260000
C	5.84119000	7.14769700	-0.71045400
C	5.01547800	6.30177700	-1.39862400
C	-8.72274400	1.56219300	-0.71895300
C	-8.72275600	1.56196200	0.71931400
C	-7.53493100	1.43901900	1.42619100
C	-6.28845200	1.45560700	0.71815900
C	-6.28844100	1.45584100	-0.71778900
C	-7.53490700	1.43948200	-1.42584900
C	-5.06784600	1.49826300	1.42141400
C	-3.84788700	1.36673800	0.71981400
C	-3.84787800	1.36696600	-0.71943100
C	-5.06782400	1.49872000	-1.42100900
C	-7.50529600	1.21867700	2.91314200
N	-6.28583100	1.46870500	3.54396900
C	-5.07667400	1.74243000	2.89213900
C	-5.07662400	1.74336400	-2.89165400
N	-6.28576500	1.46983500	-3.54359600
C	-7.50524600	1.21962500	-2.91287200
O	-8.47235400	0.84842400	3.55581500
O	-4.12347200	2.14398800	3.53409000
O	-4.12341400	2.14514300	-3.53345400
O	-8.47229800	0.84959900	-3.55568600
C	-6.24680900	1.49416400	5.01214000

C	-6.24671700	1.49576900	-5.01175800
N	-2.67486100	1.21975100	1.41612000
C	-1.57940600	1.10223900	0.71995800
C	-1.57939800	1.10245400	-0.71963100
N	-2.67484400	1.22018500	-1.41576900
C	8.63425400	-2.18454400	0.71892000
C	8.63425500	-2.18435100	-0.71950200
C	7.45643300	-1.98701700	-1.42656800
C	6.25934100	-1.63982200	-0.71812300
C	6.25933700	-1.64002100	0.71768100
C	7.45642900	-1.98740600	1.42603600
C	5.09345600	-1.27482500	-1.42111800
C	3.88320600	-1.07394700	-0.71971800
C	3.88320200	-1.07415100	0.71941700
C	5.09344700	-1.27522300	1.42077000
C	7.36930100	-2.19120900	-2.91367100
N	6.25522800	-1.63482000	-3.54404000
C	5.16529300	-1.04476400	-2.89215500
C	5.16527100	-1.04557500	2.89187200
N	6.25521200	-1.63579700	3.54359900
C	7.36929500	-2.19199900	2.91308400
O	8.20695400	-2.79855400	-3.55768100
O	4.35287200	-0.40424300	-3.53390600
O	4.35283700	-0.40524800	3.53380000
O	8.20695500	-2.79950400	3.55693300
C	6.22252600	-1.60544400	-5.01241200
C	6.22249800	-1.60682500	5.01197900
N	2.71164400	-0.91191600	-1.41587400
C	1.62753300	-0.71432000	-0.72021200
C	1.62752900	-0.71452600	0.71999900
N	2.71163500	-0.91232100	1.41561100
C	-0.67627000	-1.53161700	-0.71557000
C	-0.67627100	-1.53182500	0.71511500
C	-1.50670200	-2.38355000	-1.42765800
C	-2.38727900	-3.28933400	-0.72073800
C	-2.38728100	-3.28954200	0.71976700
C	-1.50670500	-2.38396500	1.42695300
C	-3.23487800	-4.16466400	-1.40666100
C	-4.08229700	-5.04111700	-0.72104200
C	-4.08230000	-5.04132300	0.71956100
C	-3.23488300	-4.16506800	1.40543500
C	-1.50688500	-2.37839900	-2.85413500
C	-1.51215600	-2.38017200	-4.06482500
C	-1.50689100	-2.37922500	2.85343200

C	-1.51214900	-2.38134400	4.06412100
C	-4.95205300	-5.94087500	-1.40047800
C	-5.77354500	-6.79127200	-0.71255300
C	-5.77354900	-6.79147500	0.71056200
C	-4.95206000	-5.94127600	1.39873500
C	-0.23850400	0.95259000	1.40363500
C	-0.23849200	0.95300400	-1.40334000
C	0.28561400	-0.57421700	1.40336400
C	0.28561800	-0.57380600	-1.40353600
H	3.29269000	4.53304200	2.49036700
H	3.29273900	4.53373500	-2.48899400
H	1.56882000	2.73856800	5.13154600
H	1.56870700	2.73999600	-5.13071000
H	-6.01508700	2.50466000	5.35745200
H	-7.22011200	1.17590400	5.37690600
H	-5.46407300	0.82067900	5.36762800
H	-5.46388200	0.82250200	-5.36743700
H	-7.21997100	1.17749900	-5.37664400
H	-6.01512400	2.50640500	-5.35675000
H	5.26811900	-2.00433300	-5.36138200
H	6.31606900	-0.57509000	-5.36522100
H	7.04882000	-2.21086900	-5.37622100
H	6.31591800	-0.57655600	5.36506600
H	5.26813600	-2.00592100	5.36084000
H	7.04885800	-2.21225700	5.37562700
H	-3.23643800	-4.16666300	-2.49006400
H	-3.23644800	-4.16737800	2.48883700
H	-1.51322800	-2.36994000	-5.13165700
H	-1.51316200	-2.37142300	5.13095700
H	-0.36278300	1.23769200	2.44766000
H	-0.36276300	1.23842500	-2.44727900
H	0.41216900	-0.86043000	2.44675500
H	0.41216500	-0.85970500	-2.44701400
Br	-10.38255100	1.75823900	-1.60646800
Br	-10.38257400	1.75773000	1.60687000
Br	10.28671000	-2.43666300	-1.60628500
Br	10.28670900	-2.43708500	1.60563600
F	-6.59063000	-7.63790600	1.34425200
F	-4.96196800	-5.95196200	2.74207400
F	-6.59062200	-7.63752500	-1.34648700
F	-4.96195400	-5.95117700	-2.74382100
F	6.66339200	7.98956600	1.34670100
F	6.66342000	7.98993400	-1.34430700
F	5.02624400	6.31264300	-2.74204700

F	5.02618900	6.31188500	2.74394700

Cartesian coordinates and calculated energy for 6a.

Table S6. Cartesian coordinates of the ground state optimized geometry for compound **6a**. The calculated absolute energy value for this molecule is -10150908.72 kJ/mol

C	0.76563500	1.82157500	0.71538900
C	0.76555100	1.82180600	-0.71506800
C	1.62079300	2.64962400	1.42706500
C	2.52906500	3.52785600	0.72091300
C	2.52892300	3.52812700	-0.72032000
C	1.62054600	2.65013200	-1.42661800
C	3.40636700	4.37761000	1.40123700
C	4.28509000	5.23103700	0.72122000
C	4.28494300	5.23131400	-0.72033500
C	3.40608300	4.37814700	-1.40049800
C	1.61916200	2.64111400	2.85354900
C	1.62012600	2.63614700	4.06421300
C	1.61862400	2.64211900	-2.85310200
C	1.61932600	2.63757500	-4.06377100
C	5.18422600	6.10320100	1.40871400
C	6.03150700	6.92600000	0.71349200
C	6.03136500	6.92626900	-0.71230600
C	5.18394500	6.10373800	-1.40767300
C	-8.68919300	1.56271500	-0.70398000
C	-8.68916500	1.56272400	0.70466300
C	-7.50057400	1.56490700	1.40415100
C	-6.24972000	1.55982300	0.71856700
C	-6.24975100	1.55986000	-0.71796900
C	-7.50062700	1.56491900	-1.40350800
C	-5.03797000	1.54422100	1.43487300
C	-3.82315500	1.39489400	0.72400600
C	-3.82318400	1.39498800	-0.72353300
C	-5.03803200	1.54435600	-1.43432200
C	-7.55749200	1.54193700	2.88859400
N	-6.33029200	1.58824900	3.54648000
C	-5.06977100	1.71049900	2.92245300
C	-5.06989500	1.71077200	-2.92188600
N	-6.33042200	1.58847100	-3.54587800
C	-7.55758900	1.54192000	-2.88795200
O	-8.61842700	1.49839000	3.49739600
O	-4.09685200	1.95011700	3.61295800
O	-4.09701100	1.95057600	-3.61237600
O	-8.61853500	1.49820900	-3.49672200

C	-6.32809300	1.65984200	5.01234200
C	-6.32829600	1.66013700	-5.01173800
N	-2.65035800	1.22296200	1.41494600
C	-1.55871600	1.07240900	0.72002800
C	-1.55874400	1.07254300	-0.71968100
N	-2.65041600	1.22319800	-1.41456100
C	8.52347300	-2.60252900	0.70402700
C	8.52361200	-2.60195600	-0.70431200
C	7.39318200	-2.23421500	-1.40361500
C	6.20113300	-1.85424100	-0.71839600
C	6.20101300	-1.85476700	0.71825300
C	7.39292100	-2.23530900	1.40340400
C	5.04315200	-1.49668300	-1.43530300
C	3.84382900	-1.25404100	-0.72393800
C	3.84373700	-1.25444200	0.72384600
C	5.04294400	-1.49762000	1.43522000
C	7.44158300	-2.27388000	-2.88788700
N	6.28626700	-1.85952100	-3.54663500
C	5.12117900	-1.36055800	-2.92466500
C	5.12078900	-1.36245600	2.92468100
N	6.28561200	-1.86222800	3.54650600
C	7.44102500	-2.27617100	2.88765700
O	8.43976100	-2.63763100	-3.49565900
O	4.26236600	-0.84991100	-3.61927000
O	4.26204900	-0.85197100	3.61948700
O	8.43903600	-2.64054000	3.49532900
C	6.30344200	-1.80021900	-5.01305100
C	6.30252500	-1.80395400	5.01296900
N	2.67467600	-1.05458100	-1.41422200
C	1.59574700	-0.82851000	-0.72015700
C	1.59568000	-0.82875600	0.72002600
N	2.67453000	-1.05520900	1.41411500
C	-0.72804700	-1.58170700	-0.71560900
C	-0.72813700	-1.58186800	0.71504100
C	-1.58236900	-2.41104400	-1.42662200
C	-2.48956200	-3.29130500	-0.72119300
C	-2.48968900	-3.29142600	0.72001100
C	-1.58259200	-2.41133000	1.42575700
C	-3.36489400	-4.14313300	-1.40141400
C	-4.24255900	-4.99802200	-0.72164500
C	-4.24271100	-4.99811700	0.71985500
C	-3.36516900	-4.14334400	1.39992600
C	-1.58003300	-2.40369000	-2.85357500
C	-1.58074100	-2.40074800	-4.06442300

C	-1.58044400	-2.40427700	2.85270400
C	-1.58131800	-2.40155000	4.06355200
C	-5.14004300	-5.87168400	-1.40926700
C	-5.98627400	-6.69560000	-0.71405600
C	-5.98643300	-6.69568300	0.71167900
C	-5.14035200	-5.87185400	1.40717400
C	-0.22227600	0.89089400	1.40378800
C	-0.22236100	0.89122200	-1.40357700
C	0.25888700	-0.64990600	1.40376200
C	0.25900000	-0.64949800	-1.40397200
H	3.40475200	4.37373400	2.48687700
H	3.40424300	4.37467500	-2.48613800
H	1.62160800	2.61086800	5.13044700
H	1.62062400	2.61259500	-5.13001400
H	5.18141900	6.10052800	2.49590400
H	6.71078700	7.58562400	1.24649200
H	6.71054600	7.58609000	-1.24518900
H	5.18092600	6.10147300	-2.49486300
H	-9.61773800	1.55083500	-1.26422900
H	-9.61768900	1.55088600	1.26494900
H	-6.03650500	2.66084800	5.34216200
H	-7.33404900	1.42912600	5.35529600
H	-5.60533800	0.94398300	5.40732400
H	-5.60515400	0.94469600	-5.40675500
H	-7.33413600	1.42889800	-5.35468400
H	-6.03727600	2.66132200	-5.34152800
H	9.40320900	-2.89949600	1.26444500
H	9.40346600	-2.89844100	-1.26480000
H	5.40302500	-2.27672800	-5.40439200
H	6.31622300	-0.75974300	-5.34905800
H	7.19782200	-2.31686200	-5.35347800
H	6.31476500	-0.76370900	5.34969000
H	5.40227000	-2.28115700	5.40385800
H	7.19707300	-2.32045600	5.35316300
H	-3.36247300	-4.14059900	-2.48709700
H	-3.36296200	-4.14097800	2.48561000
H	-1.57576800	-2.38066000	-5.13084600
H	-1.57649000	-2.38164800	5.12997900
H	-5.13718700	-5.86924100	-2.49645100
H	-6.66460500	-7.35612100	-1.24707100
H	-6.66489000	-7.35626000	1.24446600
H	-5.13773500	-5.86953900	2.49435900
H	-0.33994300	1.17894500	2.44773900
H	-0.34018100	1.17951000	-2.44743600

H	0.37794300	-0.93914200	2.44717300
H	0.37820400	-0.93842300	-2.44746900

Cartesian coordinates and calculated energy for 6b.

Table S7. Cartesian coordinates of the ground state optimized geometry for compound **6b**. The calculated absolute energy value for this molecule is -12187638.65 kJ/mol

C	1.16232500	-1.53551900	-0.71559700
C	1.16238400	-1.53572300	0.71506800
C	2.19282800	-2.12912800	-1.42838400
C	3.28648100	-2.76055200	-0.72076500
C	3.28653800	-2.76075900	0.71972000
C	2.19294200	-2.12953600	1.42760500
C	4.34192700	-3.36914700	-1.40678800
C	5.39764300	-3.97860800	-0.72119400
C	5.39769900	-3.97881500	0.71963600
C	4.34203600	-3.36955000	1.40548600
C	2.19401100	-2.11879400	-2.85423600
C	2.20138800	-2.11178200	-4.06468800
C	2.19423800	-2.11960500	2.85346100
C	2.20172800	-2.11293400	4.06391400
C	6.48262000	-4.60283800	-1.40042600
C	7.50756400	-5.19206300	-0.71250000
C	7.50761900	-5.19226700	0.71043300
C	6.48272800	-4.60324000	1.39860700
C	-8.03358500	-3.70546000	0.70428300
C	-8.03366000	-3.70524300	-0.70458100
C	-6.88777400	-3.39063300	-1.40400500
C	-5.68303600	-3.05218400	-0.71872100
C	-5.68295900	-3.05241300	0.71837000
C	-6.88762300	-3.39107100	1.40368000
C	-4.51935600	-2.71622500	-1.43596000
C	-3.38417500	-2.25908500	-0.72398000
C	-3.38410100	-2.25931200	0.72363200
C	-4.51920100	-2.71668600	1.43558800
C	-6.94918700	-3.38704800	-2.88853500
N	-5.75468700	-3.10381300	-3.54750300
C	-4.50887300	-2.87638400	-2.92558100
C	-4.50855000	-2.87733500	2.92515500
N	-5.75429700	-3.10493700	3.54714500
C	-6.94887600	-3.38793700	2.88821900
O	-7.98302400	-3.63100900	-3.49581300
O	-3.50927500	-2.83290100	-3.61835400
O	-3.50887400	-2.83406500	3.61782900

O	-7.98265200	-3.63206500	3.49553300
C	-5.73435500	-3.17181600	-5.01388200
C	-5.73380300	-3.17340100	5.01350000
N	-2.29278800	-1.79531000	-1.41410300
C	-1.27341200	-1.37653900	-0.71944400
C	-1.27334700	-1.37674900	0.71916100
N	-2.29265300	-1.79573400	1.41379100
C	7.70028800	4.48595100	-0.70404600
C	7.70034900	4.48574900	0.70466100
C	6.67313700	3.88810300	1.40393300
C	5.58874300	3.26357900	0.71877100
C	5.58868400	3.26378000	-0.71832000
C	6.67301700	3.88850100	-1.40339900
C	4.53538800	2.66548000	1.43609300
C	3.41989400	2.16284000	0.72401100
C	3.41983600	2.16304300	-0.72369100
C	4.53527300	2.66587700	-1.43572300
C	6.71266100	3.93684600	2.88832700
N	5.67193600	3.28622600	3.54769800
C	4.63949800	2.55202400	2.92654800
C	4.63927200	2.55282100	-2.92621400
N	5.67162800	3.28723600	-3.54724800
C	6.71240700	3.93767400	-2.88778200
O	7.61089300	4.50412900	3.49529200
O	3.90674700	1.87231100	3.62093900
O	3.90643500	1.87333600	-3.62073700
O	7.61057600	4.50514600	-3.49466400
C	5.70191900	3.23235200	5.01443100
C	5.70147200	3.23379600	-5.01399900
N	2.32624500	1.70297100	1.41371400
C	1.32913400	1.23323000	0.71960500
C	1.32907700	1.23343200	-0.71937900
N	2.32613300	1.70336800	-1.41343600
C	-1.10940800	1.40299100	0.71560800
C	-1.10946200	1.40320000	-0.71513900
C	-2.13885800	1.99914200	1.42766700
C	-3.23165300	2.63316200	0.72073400
C	-3.23170300	2.63337500	-0.71975300
C	-2.13896100	1.99956100	-1.42695100
C	-4.28525500	3.24503700	1.40657400
C	-5.33956900	3.85728000	0.72109800
C	-5.33961800	3.85749300	-0.71961100
C	-4.28535200	3.24545300	-1.40534000
C	-2.13850400	1.99222100	2.85404700

C	-2.14451100	1.98987900	4.06469000
C	-2.13871200	1.99305400	-2.85333200
C	-2.14480300	1.99104500	-4.06397500
C	-6.42255100	4.48470600	1.40037200
C	-7.44578300	5.07708100	0.71247400
C	-7.44583100	5.07729200	-0.71048400
C	-6.42264500	4.48512100	-1.39862600
C	-0.02220300	-0.87282500	-1.40396200
C	-0.02208600	-0.87321900	1.40371500
C	0.07414700	0.73930000	-1.40366900
C	0.07425900	0.73890400	1.40385900
H	4.34395900	-3.36862200	-2.49017000
H	4.34415400	-3.36933300	2.48886900
H	2.20538700	-2.08770800	-5.13117700
H	2.20603100	-2.08915100	5.13040800
H	-5.16146400	-4.04292200	-5.34302100
H	-6.76435300	-3.24675500	-5.35458900
H	-5.25523600	-2.27525700	-5.41105700
H	-5.25465000	-2.27696100	5.41090600
H	-6.76376200	-3.24845700	5.35429700
H	-5.16086500	-4.04460300	5.34230100
H	4.72206500	3.51032900	5.40633900
H	5.93225400	2.21761400	5.35026600
H	6.46860100	3.92470400	5.35427600
H	5.93178400	2.21915800	-5.35015600
H	4.72157900	3.51188000	-5.40573400
H	6.46811400	3.92625500	-5.35371200
H	-4.28702500	3.24594800	2.48997300
H	-4.28719800	3.24668100	-2.48873800
H	-2.14300100	1.97459500	5.13143700
H	-2.14328700	1.97582000	-5.13072300
H	-0.06581900	-1.18056800	-2.44803200
H	-0.06561800	-1.18125300	2.44770400
H	0.11952700	1.04847000	-2.44719100
H	0.11972400	1.04778700	2.44746200
F	-8.46439300	5.66653400	-1.34430800
F	-6.43569000	4.49272600	-2.74214100
F	-8.46430100	5.66613500	1.34654200
F	-6.43550700	4.49191400	2.74388900
F	8.52823800	-5.77801100	-1.34661600
F	8.52834300	-5.77839700	1.34430200
F	6.49618800	-4.61091000	2.74213400
F	6.49597800	-4.61012400	-2.74395600
H	-8.93145200	-3.94274100	1.26439900

H	-8.93158500	-3.94235600	-1.26467500
H	8.49822600	4.96073600	1.26496400
H	8.49811500	4.96109900	-1.26428200

Table S8. Cartesian coordinates of the ground state optimized geometry for compound **4a**.

C	-6.93256200	-0.71257200	-0.25871000
C	-6.93257000	0.71253300	-0.25869000
C	-5.76540200	1.40400800	-0.13951200
C	-4.50456300	0.72437700	-0.02013300
C	-4.50455900	-0.72438500	-0.02013200
C	-5.76538600	-1.40403300	-0.13953800
C	-3.32735000	1.43706500	0.09839900
C	-2.07213200	0.73334300	0.10247100
C	-2.07212900	-0.73333600	0.10247700
C	-3.32734200	-1.43706300	0.09841100
C	-5.82679900	2.89081100	-0.16597600
N	-4.61772100	3.54572400	-0.00070900
C	-3.37993200	2.92635600	0.25100000
C	-3.37991800	-2.92635000	0.25104800
N	-4.61766800	-3.54573800	-0.00080400
C	-5.82675700	-2.89083800	-0.16605200
O	-6.87541700	3.48724700	-0.31213400
O	-2.44161600	3.61404500	0.57798200
O	-2.44163000	-3.61401300	0.57816000
O	-6.87536200	-3.48728800	-0.31224400
N	-0.93968400	1.41596100	0.05945600
C	0.21403800	0.72277600	0.04800600
C	0.21404000	-0.72277400	0.04800500
N	-0.93968200	-1.41595800	0.05945900
C	1.42860900	1.41542600	0.01953800
C	2.64358900	0.72773300	0.00154000
C	2.64359100	-0.72773000	0.00154000
C	1.42861100	-1.41542400	0.01953500
C	3.88732800	1.42454400	-0.01662200
C	5.10580700	0.72511000	-0.03344000
C	5.10580900	-0.72509400	-0.03343700
C	3.88733500	-1.42453400	-0.01662400
C	6.34939600	1.40465300	-0.04976500
C	7.54809400	0.72482700	-0.06477300
C	7.54809500	-0.72480800	-0.06476800
C	6.34939900	-1.40463600	-0.04975800
C	3.88436100	2.85237900	-0.01600400
C	3.87262900	4.06004500	-0.01534800

C	3.88438500	-2.85236900	-0.01601900
C	3.87275800	-4.06003800	-0.01510900
C	8.81322600	1.41191200	-0.08070100
C	9.97962800	0.71959600	-0.09530800
C	9.97962900	-0.71957500	-0.09530200
C	8.81322800	-1.41189200	-0.08068900
C	-4.61827600	5.00617900	0.06823000
C	-4.61820700	-5.00619400	0.06811900
H	-7.85730200	-1.27070800	-0.36239400
H	-7.85731800	1.27066100	-0.36234700
H	1.40166200	2.49958000	0.02085500
H	1.40166300	-2.49957700	0.02085300
H	6.34554100	2.49060600	-0.04961100
H	6.34554300	-2.49058900	-0.04959900
H	3.85700600	5.12733300	-0.01322600
H	3.85728900	-5.12732900	-0.01310400
H	8.80670000	2.49839900	-0.08056200
H	10.92827600	1.24702300	-0.10734100
H	10.92827700	-1.24700000	-0.10732800
H	8.80670300	-2.49837800	-0.08054100
H	-3.82428800	5.39258200	-0.57130700
H	-5.59248800	5.35397000	-0.26512200
H	-4.42670800	5.33196100	1.09309000
H	-5.59236900	-5.35399900	-0.26536900
H	-3.82412600	-5.39257100	-0.57131700
H	-4.42677400	-5.33199000	1.09300000

Table S9. Cartesian coordinates of the ground state optimized geometry for compound **Complex**.

C	0.50350600	-2.10468700	1.29542300
C	-0.69958700	-1.39346300	1.36980800
C	-0.67229300	0.03433700	1.58534700
C	0.55355100	0.69487200	1.72197300
C	1.75405500	-0.01492300	1.66854100
C	1.72926300	-1.45333600	1.44983600
C	0.69936600	1.39349000	-1.36976700
C	-0.50385700	2.10437900	-1.29515700
C	0.67241200	-0.03426600	-1.58551100
C	-1.72949000	1.45272700	-1.44966500
H	-0.45975400	3.17341900	-1.11869900
C	-0.55320800	-0.69510100	-1.72229600
C	-1.75392700	0.01439800	-1.66876600
H	-0.54361500	-1.76977200	-1.87196900

H	0.45910200	-3.17375800	1.11923100
H	0.54422000	1.76957600	1.87142200
C	3.00775700	0.64908600	1.81962800
C	2.96360800	-2.16670000	1.38650200
C	4.19056700	-1.50448500	1.56840200
C	4.21170000	-0.07193800	1.79169800
C	-3.00743200	-0.64985100	-1.82002400
C	-2.96399500	2.16569500	-1.38592600
C	-4.19080400	1.50342100	-1.56878000
C	-4.21156200	0.07094500	-1.79243900
C	2.98686300	1.34724300	-1.30682700
C	-2.98704200	-1.34667000	1.30693900
C	2.95726700	-0.10326700	-1.52632100
C	-2.95712200	0.10381200	1.52638400
C	4.19290000	-0.83961100	-1.59281600
C	4.25800300	2.00513700	-1.14216500
C	5.42735300	-2.19750300	1.51075200
H	5.41430600	-3.26889400	1.32816900
C	5.46188200	0.57632100	1.95892200
H	5.46916300	1.65118800	2.12374500
C	-4.25823800	-2.00433900	1.14231800
C	-4.19256900	0.84037100	1.59296700
C	-5.42770200	2.19623400	-1.51159700
H	-5.41508200	3.26760100	-1.32882500
C	-5.46152500	-0.57753500	-1.96019000
H	-5.46855200	-1.65239400	-2.12506700
C	-6.65154400	0.11484200	-1.91074800
C	-6.63372100	1.54592300	-1.67264700
C	5.38899600	-0.17447100	-1.40703900
C	5.41924600	1.25570100	-1.17049300
C	6.63355200	-1.54737900	1.67097000
C	6.65174000	-0.11627400	1.90902600
C	-5.41934000	-1.25464000	1.17020700
C	-5.38876500	0.17552900	1.40654600
C	6.63908300	-0.88566600	-1.43717600
C	6.69885900	1.87208200	-0.94642300
C	7.82823200	-0.24214100	-1.28144400
H	8.74181700	-0.82664400	-1.30153300
C	7.89116700	-2.24171900	1.57281400
H	7.87647400	-3.30714200	1.36279400
C	7.92184600	0.54468500	2.05899100
H	7.92766100	1.61936300	2.22476000
C	9.06408200	-1.57253400	1.70909800
H	10.00660200	-2.10395500	1.62274000

C	-6.69901900	-1.87081700	0.94610200
C	-6.63862700	0.88707400	1.43592800
C	-7.85609000	-1.15681900	1.02321700
H	-8.79412700	-1.66900100	0.83647700
C	-7.89148500	2.24005200	-1.57514400
H	-7.87709200	3.30547300	-1.36512100
C	-7.92144500	-0.54637600	-2.06120100
H	-7.92698400	-1.62105800	-2.22694600
C	-9.08054200	0.15374200	-1.96574200
H	-10.03487700	-0.35265100	-2.07322400
C	7.85607900	1.15840400	-1.02403400
H	8.79402500	1.67075200	-0.83728000
C	9.08076300	-0.15565700	1.96300700
H	10.03524300	0.35054400	2.07012900
C	-7.82792300	0.24382000	1.28000900
H	-8.74135200	0.82858000	1.29952000
C	-9.06422200	1.57062900	-1.71194100
H	-10.00687300	2.10189800	-1.62605300
C	-6.79160300	-3.29894500	0.55201900
C	-6.66408700	2.36764500	1.57275600
C	6.79123700	3.30010300	-0.55194800
C	6.66495800	-2.36620800	-1.57432500
N	5.59830400	4.00135200	-0.55625800
N	-5.43476300	2.97834100	1.73719500
N	-5.59868500	-4.00024400	0.55598300
N	5.43559400	-2.97733200	-1.73630500
C	4.34214000	3.48519100	-0.93488900
C	-4.19707300	2.31808400	1.85391500
C	4.19755900	-2.31758100	-1.85222200
C	-4.34269700	-3.48445900	0.93580600
O	-7.84951100	-3.81425200	0.24007800
O	-3.42093300	-4.25724000	1.05630900
O	-3.22482900	2.97138200	2.14979600
O	3.41987700	4.25764500	-1.05385600
O	7.84906300	3.81543000	-0.23976200
O	7.70421100	-2.99837900	-1.53229600
O	3.22510600	-2.97162300	-2.14577200
O	-7.70307300	3.00013800	1.52904500
C	-5.62587800	-5.42855000	0.25156100
H	-4.90414300	-5.64348700	-0.53849300
H	-5.34528000	-6.00245300	1.13669000
H	-6.63369800	-5.68112100	-0.06735800
C	-5.38783600	4.42981700	1.89799200
H	-5.06581400	4.68241100	2.91044600

H	-4.66409500	4.83815200	1.19062100
H	-6.38546600	4.81693600	1.70731200
C	5.62524900	5.42959800	-0.25150100
H	5.34133700	6.00333600	-1.13565400
H	4.90587500	5.64388600	0.54090800
H	6.63385800	5.68290700	0.06431800
C	5.38834900	-4.42931500	-1.89271900
H	4.66291900	-4.83375400	-1.18491500
H	5.06801200	-4.68536400	-2.90483200
H	6.38541500	-4.81634200	-1.69887300
N	-1.80879000	0.74949400	1.64912300
N	-1.86777400	-2.04741800	1.22403700
N	1.80912400	-0.74914400	-1.64933100
N	1.86746900	2.04771600	-1.22399700
C	3.02721200	2.06992400	1.95906100
C	2.94418200	-3.57389300	1.14826000
C	-3.02664400	-2.07070500	-1.95929200
C	-2.94503000	3.57251800	-1.14571300
C	-3.01945300	-3.27681600	-2.03001300
H	-2.98862000	-4.34344700	-2.07068200
C	-2.91790500	4.76418000	-0.94851100
H	-2.87623800	5.81703600	-0.77662900
C	3.02015900	3.27602600	2.02992900
H	2.98934400	4.34265500	2.07075600
C	2.91645300	-4.76596500	0.95353000
H	2.87418900	-5.81918800	0.78403900

Table S10. Cartesian coordinates of the ground state optimized geometry for **T1**

C	-0.13104000	-1.78711600	0.54707500
C	-1.38159800	-1.21426800	0.94323100
C	-1.36014100	0.16811300	1.40366600
C	-0.10431100	0.77629800	1.64653400
C	1.11290800	0.05299200	1.61194600
C	1.08330000	-1.32900500	1.15081300
C	1.41301100	1.32902600	-1.32869600
C	0.20393600	2.05158300	-1.30965800
C	1.37178800	-0.11878800	-1.51003400
C	-1.04641300	1.44348800	-1.53582900
H	0.24230300	3.12969000	-1.16945600
C	0.09120300	-0.78375500	-1.53785000
C	-1.10920700	-0.00332200	-1.71899200
H	0.07676500	-1.79863400	-1.92724000
H	-0.14983900	-2.81945600	0.19970100

H	-0.08116700	1.82105800	1.94917300
C	2.33976900	0.61397800	1.94361200
C	2.22937500	-2.08352000	1.17240100
C	3.47725800	-1.55080900	1.61443100
C	3.54211800	-0.14720000	1.94326300
C	-2.33416000	-0.58446500	-1.95878700
C	-2.21479200	2.19158500	-1.57520200
C	-3.48248800	1.59708800	-1.79025100
C	-3.54577600	0.17167000	-1.99984000
C	3.86101200	1.25531500	-1.17173300
C	-3.82945900	-1.21067600	0.99902600
C	3.82665300	-0.17145500	-1.37885500
C	-3.81853300	0.19544900	1.32329300
C	5.01927200	-0.88723600	-1.33855900
C	5.08788900	1.88673100	-0.96203300
C	4.63570800	-2.31804900	1.66070000
H	4.57987300	-3.37895400	1.42214800
C	4.78344700	0.41722100	2.23903300
H	4.84560100	1.48241300	2.45354200
C	-5.04514400	-1.86739000	0.84529900
C	-5.03437800	0.87427000	1.41202900
C	-4.66361900	2.34057900	-1.78338500
H	-4.61177200	3.41740200	-1.63405500
C	-4.78924500	-0.43072000	-2.16481500
H	-4.84469500	-1.50986600	-2.29485500
C	-5.97891500	0.31193600	-2.13431100
C	-5.91360400	1.73258200	-1.94734300
C	6.25050300	-0.25726000	-1.10408600
C	6.28621800	1.16477400	-0.91968300
C	5.87847100	-1.75732000	1.99444800
C	5.95599400	-0.35155400	2.26516800
C	-6.26907500	-1.19181500	0.97120400
C	-6.26068100	0.21717700	1.23605600
C	7.46981300	-0.99040200	-1.01760700
C	7.54492000	1.79498300	-0.68479900
C	8.65590200	-0.35397500	-0.78235700
H	9.57518900	-0.92650000	-0.70388400
C	7.07055900	-2.53605700	2.05718600
H	7.00283700	-3.60358400	1.86168900
C	7.22956500	0.21957400	2.55761600
H	7.28802500	1.29012400	2.73687800
C	8.27164800	-1.95589400	2.35714400
H	9.17294600	-2.55991600	2.40380300
C	-7.52159100	-1.85673900	0.82796000

C	-7.50700100	0.90563300	1.31612300
C	-8.69718200	-1.16592000	0.92762600
H	-9.64544500	-1.68383000	0.81844100
C	-7.13028700	2.47800900	-1.92100200
H	-7.07465300	3.55577900	-1.78949200
C	-7.25789700	-0.30490900	-2.25841800
H	-7.30288800	-1.38548000	-2.36809000
C	-8.40278500	0.44001300	-2.21956500
H	-9.37109900	-0.04464300	-2.30023700
C	8.69451100	1.05998500	-0.62034500
H	9.64595600	1.55019600	-0.43665400
C	8.35321400	-0.55702400	2.60241800
H	9.31733600	-0.10846500	2.82236500
C	-8.68914700	0.23638400	1.16665100
H	-9.63090200	0.77368400	1.22595900
C	-8.33732100	1.85271100	-2.05518300
H	-9.25675300	2.43000100	-2.02912400
C	7.41709900	-2.52174400	-1.17192100
C	7.57728500	3.32381400	-0.50251600
C	-7.49077900	2.42539800	1.56441900
C	-7.52069500	-3.37311900	0.55928100
C	-2.42273000	-2.10774400	-2.16705400
C	-2.49181500	-3.29590200	-2.32950200
H	-2.55335500	-4.35428500	-2.47420700
C	-2.13560700	3.71653400	-1.37554700
C	-2.07384300	4.90599400	-1.21981700
H	-2.01882500	5.96553600	-1.08109600
C	2.18337500	-3.54644300	0.69350700
C	2.14749500	-4.68752300	0.31996900
H	2.11553300	-5.70397000	-0.01276900
C	2.40897000	2.09939200	2.34405600
C	2.46294600	3.25801500	2.65640300
H	2.51102700	4.29008900	2.93463300
N	-6.24601300	-4.09807500	0.45669200
N	-6.20903800	3.12976300	1.71243900
N	6.12862400	-3.19078400	-1.40239100
N	6.32867300	4.09643800	-0.57265600
N	2.56068900	-0.81227700	-1.54650200
N	2.63551400	1.96585200	-1.16670400
N	-2.57984200	-1.85965800	0.76738200
N	-2.56809400	0.84244400	1.53024800
C	-5.04972700	-3.37136500	0.51418300
C	-5.03233000	2.38550700	1.70827100
C	4.98616600	-2.41630800	-1.51867500

C	5.12113600	3.41227400	-0.75415600
O	-8.60741500	-3.99374700	0.42725100
O	-8.57099700	3.06635800	1.64103300
O	-4.00073100	3.06012200	1.96178100
O	-4.01472500	-4.04528000	0.27297800
O	3.94862400	-3.07999200	-1.77674700
O	8.47324300	-3.20230000	-1.10139900
O	4.09623600	4.14206600	-0.73063700
O	8.66894300	3.91395000	-0.29372900
C	-6.17039600	4.59162700	1.86196700
H	-5.86045100	4.84047100	2.85540100
H	-5.47765000	5.00393200	1.15840000
H	-7.14496200	4.99455600	1.68094100
C	-6.22697000	-5.55921500	0.29666400
H	-5.89598400	-5.80560500	-0.69057400
H	-5.55894300	-5.98792300	1.01419300
H	-7.21212400	-5.94766500	0.44989100
C	6.05397900	-4.65511700	-1.50753900
H	5.37012300	-5.03087700	-0.77538800
H	5.71384600	-4.92561500	-2.48531200
H	7.02363400	-5.07473400	-1.33845400
C	6.34790100	5.56153800	-0.45428500
H	5.83945900	5.99365200	-1.29074500
H	5.85700500	5.85271700	0.45077700
H	7.36123500	5.90468000	-0.43672500

Table S11. Cartesian coordinates of the ground state optimized geometry for **M1**

C	-0.08278300	1.28707700	0.81784700
C	1.16801700	0.66497600	1.36389200
C	1.24969900	-0.77141700	1.28747000
C	0.02732800	-1.51700900	0.82511300
C	-1.23415000	-0.89368200	1.36292200
C	-1.31752200	0.53576800	1.28455900
C	-1.24970700	-0.77126100	-1.28751600
C	-0.02731800	-1.51690300	-0.82526400
C	-1.16801800	0.66513800	-1.36381500
C	1.23416500	-0.89350100	-1.36299300
H	-0.12340800	-2.56210600	-1.12011900
C	0.08276800	1.28718500	-0.81770000
C	1.31750300	0.53594600	-1.28451400
H	0.13162600	2.33371600	-1.11914900
H	-0.13165200	2.33357100	1.11942200
H	0.12342300	-2.56224800	1.11984200

C	-2.34258400	-1.65001400	1.66357000
C	-2.52240400	1.17186700	1.48550600
C	-3.71463300	0.41134700	1.78875400
C	-3.62151800	-1.01607600	1.88870500
C	2.52235500	1.17210200	-1.48543900
C	2.34263700	-1.64977200	-1.66366400
C	3.62155200	-1.01577300	-1.88875700
C	3.71460900	0.41164900	-1.78874500
C	-3.50789200	-0.64029300	-1.53272200
C	3.40955500	0.78337700	1.70109000
C	-3.40954700	0.78359500	-1.70100400
C	3.50787800	-0.64050000	1.53270800
C	-4.57633700	1.57195500	-1.72735300
C	-4.76758100	-1.24773200	-1.35201600
C	-4.95772400	1.02644600	1.93482700
H	-5.02623400	2.10852900	1.85295700
C	-4.77760700	-1.76082000	2.11457800
H	-4.70544400	-2.84394100	2.17502500
C	4.57636600	1.57170900	1.72747600
C	4.76754800	-1.24795000	1.35192400
C	4.77767800	-1.76045500	-2.11464000
H	4.70556800	-2.84357700	-2.17512000
C	4.95766900	1.02681300	-1.93478800
H	5.02613000	2.10889600	-1.85287100
C	6.11755400	0.28265600	-2.17848200
C	6.02620200	-1.14552400	-2.26071700
C	-5.80418100	0.97661900	-1.42337000
C	-5.90260600	-0.43649800	-1.23701400
C	-6.11757100	0.28222800	2.17851700
C	-6.02615400	-1.14595200	2.26071000
C	5.80419300	0.97636900	1.42342300
C	5.90258500	-0.43673600	1.23695300
C	-6.97020100	1.77553300	-1.22850000
C	-7.17213300	-0.99397000	-0.90010900
C	-8.17158200	1.20364400	-0.90714900
H	-9.02744900	1.85143000	-0.74688400
C	-7.39394300	0.90265400	2.34363600
H	-7.45685000	1.98636300	2.28091900
C	-7.21971800	-1.90081200	2.47546500
H	-7.14983200	-2.98534200	2.50796600
C	-8.51057600	0.14734300	2.56285800
H	-9.47686000	0.62692400	2.68691700
C	6.97023100	1.77526500	1.22858900
C	7.17208800	-0.99421800	0.89996800

C	8.17159100	1.20336800	0.90717000
H	9.02747200	1.85114400	0.74694200
C	7.21980800	-1.90032100	-2.47546100
H	7.14996900	-2.98485300	-2.50800200
C	7.39390100	0.90314800	-2.34355600
H	7.45675600	1.98685700	-2.28080400
C	8.51057300	0.14789500	-2.56277600
H	9.47683800	0.62752500	-2.68680100
C	-8.27674400	-0.19951300	-0.75276200
H	-9.21644900	-0.66695600	-0.47758800
C	-8.42389200	-1.27454900	2.61868900
H	-9.32608500	-1.85923400	2.76735300
C	8.27671800	-0.19978200	0.75267000
H	9.21641000	-0.66722500	0.47744800
C	8.42395700	-1.27400000	-2.61864300
H	9.32618000	-1.85863900	-2.76730200
N	-2.19076900	1.41034900	-1.63937000
N	-2.37561800	-1.40262300	-1.40150400
N	2.19078000	1.41015200	1.63950800
N	2.37559900	-1.40280300	1.40141200
C	-6.89359900	3.25889100	-1.30322200
C	-7.31617800	-2.45081700	-0.63901000
C	7.31607200	-2.45105000	0.63874800
C	6.89367000	3.25861800	1.30343100
C	2.63551500	2.58258700	-1.26641200
C	2.27341500	-3.07945300	-1.62710100
C	2.22449500	-4.28465900	-1.58155100
H	2.17011000	-5.34932500	-1.52653400
C	2.73417900	3.76340600	-1.03412900
H	2.80175900	4.80779000	-0.82317100
C	-2.27330100	-3.07968900	1.62696400
C	-2.22435400	-4.28489300	1.58137700
H	-2.16989700	-5.34955600	1.52638700
C	-2.63561800	2.58236100	1.26655700
C	-2.73433500	3.76318800	1.03434100
H	-2.80198100	4.80757200	0.82340400
N	-6.14791500	-3.19536100	-0.71405100
N	-5.66070700	3.78700700	-1.66158700
N	5.66080500	3.78673600	1.66188900
N	6.14775700	-3.19553100	0.71358700
C	4.90929500	-2.73082600	1.19473300
C	4.52000500	3.03899300	2.00401900
C	-4.51993900	3.03925700	-2.00379900
C	-4.90936200	-2.73061300	-1.19492300

O	4.04600500	-3.53640400	1.45130900
O	8.38623800	-2.95686100	0.36204100
O	7.85498900	3.96462500	1.06729800
O	3.57604700	3.60442200	2.50477000
O	-3.57597800	3.60469000	-2.50453900
O	-7.85489500	3.96490900	-1.06703500
O	-4.04598600	-3.53617600	-1.45127100
O	-8.38638000	-2.95659400	-0.36237500
C	-6.22129000	-4.63152500	-0.45887300
H	-6.15367800	-5.18835200	-1.39646900
H	-5.37925500	-4.91715500	0.17384600
H	-7.17074400	-4.83463700	0.03049700
C	-5.55047800	5.23078100	-1.85635100
H	-4.67034000	5.59721200	-1.32612000
H	-5.42958100	5.45659600	-2.91811800
H	-6.45700100	5.68901100	-1.46977100
C	5.55061100	5.23049500	1.85678500
H	4.67062600	5.59704800	1.32638000
H	5.42946200	5.45618700	2.91854700
H	6.45725200	5.68871500	1.47047000
C	6.22111600	-4.63166200	0.45823400
H	6.15437000	-5.18861900	1.39582100
H	5.37859500	-4.91730300	-0.17381800
H	7.17020400	-4.83462300	-0.03191600

Table S12. Cartesian coordinates of the ground state optimized geometry for **T2**

C	-0.02126500	-1.51071700	0.81805600
C	-1.29858500	-0.87965700	1.31350400
C	-1.35934100	0.55237300	1.27269000
C	-0.10322000	1.29681500	0.85613200
C	1.12621200	0.64862900	1.42342700
C	1.18577900	-0.78955800	1.34958500
C	1.36022200	0.60602500	-1.21973600
C	0.10387700	1.32969100	-0.77263500
C	1.30640400	-0.82436300	-1.30150500
C	-1.12069400	0.69877300	-1.36676800
H	0.14338000	2.38177300	-1.05452700
C	0.02986600	-1.47798600	-0.82860200
C	-1.18058400	-0.74101000	-1.33410400
H	-0.03257800	-2.51753800	-1.15069000
H	0.04533600	-2.56142500	1.10015600
H	-0.14710200	2.33716700	1.17855400
C	3.43461900	-0.70079300	1.65455000

C	3.36460200	0.72880300	1.78616100
C	-3.35498800	0.79296000	-1.74780200
C	-3.43016100	-0.63807000	-1.63948300
C	2.43731100	-1.55440600	-1.58728600
C	2.55380500	1.26776900	-1.40380000
C	-2.55957100	1.20029600	1.46396100
C	-2.42454800	-1.62576500	1.57439100
C	3.75975300	0.53736900	-1.72248700
C	-3.69409500	-0.97839400	1.81583800
C	3.69926300	-0.89090600	-1.82800000
C	-3.76446800	0.45199200	1.74618100
C	4.86791600	-1.60503900	-2.09351000
C	4.98489500	1.18374000	-1.88727400
H	5.02839800	2.26631500	-1.79567600
C	4.68039200	-1.33650200	1.48564800
C	4.54678400	1.49451900	1.77838800
C	-4.86072800	-1.70929200	2.03803900
H	-4.80681200	-2.79435000	2.07500700
C	-4.99761800	1.08346000	1.90744400
H	-5.04930400	2.16763500	1.84427300
C	-4.53423300	1.56310500	-1.74085300
C	-4.67971500	-1.27102200	-1.48839700
C	-5.82452000	-0.48392700	-1.32141700
C	-5.75054100	0.93630200	-1.45146100
C	6.09542100	-0.95754400	-2.27391600
C	6.15487100	0.47164200	-2.16993400
C	5.82199300	-0.54900800	1.30207100
C	5.75620700	0.86916000	1.45674100
C	-6.09727400	-1.07728000	2.21007900
C	-6.16681200	0.35366900	2.14719700
C	7.29984700	-1.67861400	-2.54476200
H	7.25784400	-2.76314100	-2.59475100
C	7.41213900	1.12661200	-2.35379600
H	7.45162100	2.20954900	-2.26400400
C	8.48217900	-1.01904300	-2.71306900
H	9.39148800	-1.57802700	-2.90932000
C	7.05536900	-1.13771200	0.89526600
C	6.92851000	1.63918000	1.19892400
C	8.16571500	-0.36917000	0.67267100
H	9.07370000	-0.85510900	0.33196600
C	-7.30093300	-1.81595100	2.43046700
H	-7.24918300	-2.90133600	2.45059400
C	-7.43306400	0.99216000	2.32524300
H	-7.47989100	2.07710800	2.27006600

C	-8.49303600	-1.17200600	2.59124900
H	-9.40190500	-1.74420000	2.74708300
C	-6.92401900	1.70755100	-1.20239300
C	-7.07420700	-1.07447400	-0.96686300
C	-8.18756400	-0.30418200	-0.76575700
H	-9.11003800	-0.79362000	-0.47215300
C	8.53841700	0.40392800	-2.62290100
H	9.48924400	0.90940300	-2.76185800
C	8.10065200	1.03635000	0.82764000
H	8.96016000	1.66266600	0.61313300
C	-8.55904500	0.25236900	2.54606700
H	-9.51691000	0.74577500	2.68000300
C	-8.10977400	1.10490700	-0.87948500
H	-8.97086500	1.73181800	-0.67237800
H	4.82125300	-2.68874900	-2.16386400
C	-6.85644200	3.19129700	-1.19645500
C	-7.17654800	-2.53782000	-0.72054000
C	7.13191400	-2.59389900	0.60711600
C	6.88001100	3.12452700	1.23566200
N	-5.63319400	3.75546000	-1.52479700
N	5.66887500	3.68486600	1.61955200
N	5.99082500	-3.33551800	0.87254700
N	-6.00364800	-3.26231900	-0.87916100
N	2.15815500	1.37751000	1.71095600
N	2.29216900	-1.44391000	1.50861600
N	-2.14830400	1.43663500	-1.64498100
N	-2.28968800	-1.38786800	-1.50730000
C	-2.37950400	-3.05463100	1.48854100
C	-2.34897800	-4.25784000	1.39444000
H	-2.30750900	-5.32022000	1.29784700
C	-2.65466800	2.61437500	1.25810000
C	-2.74294000	3.79740100	1.03213300
H	-2.80448500	4.84309800	0.82503400
C	2.40898400	-2.98484000	-1.52556500
C	2.40099700	-4.18920500	-1.44306300
H	2.38216700	-5.25285300	-1.35439300
C	2.63793400	2.67676600	-1.16220700
C	2.71014800	3.85562300	-0.91048400
H	2.75329100	4.89790200	-0.68320200
C	4.52379100	2.96971800	2.01320200
C	4.79037500	-2.82842800	1.40860600
C	-4.49593600	3.04290900	-1.95167800
C	-4.79827700	-2.76083600	-1.40396100
O	-3.56938800	3.62752300	-2.46120100

O	-7.81407700	3.88756000	-0.91768400
O	-8.21934000	-3.06616000	-0.38611800
O	-3.94202800	-3.53925600	-1.75122500
O	3.92968600	-3.58819400	1.78395500
O	8.13728400	-3.11641400	0.16441100
O	7.84364000	3.80723400	0.94542100
O	3.60293400	3.56647700	2.52054300
C	5.58968800	5.13522800	1.77406200
H	4.70025500	5.50169900	1.25998900
H	5.50541400	5.39451900	2.83159800
H	6.49128800	5.56554500	1.34629500
C	6.07180600	-4.77807200	0.65197000
H	7.09048200	-5.10424800	0.85319800
H	5.36223500	-5.26524100	1.31593100
H	5.82121100	-5.01129500	-0.38737900
C	-6.04379600	-4.70753800	-0.67203200
H	-5.17220300	-4.99975500	-0.08421700
H	-6.96766400	-4.94356200	-0.15000900
H	-6.00683500	-5.23007600	-1.63059100
C	-5.59346000	5.21424600	-1.59298200
H	-4.55445800	5.51929200	-1.68795800
H	-6.16181700	5.57076400	-2.45579400
H	-6.04632500	5.61815500	-0.68768100

Table S13. Cartesian coordinates of the ground state optimized geometry for **M2**

C	0.05436400	-1.51554100	1.20223100
C	-1.12391000	-0.88715800	1.90088500
C	-1.19469600	0.54216500	1.86363600
C	-0.01409900	1.29060500	1.27704200
C	1.28089000	0.63762700	1.66598000
C	1.33102300	-0.79803800	1.55038000
C	1.12534000	0.59182200	-0.97868700
C	-0.04183300	1.33627700	-0.34793300
C	1.02614100	-0.83562900	-1.07861200
C	-1.33575500	0.73424200	-0.81116900
H	-0.02060600	2.38810900	-0.63368700
C	-0.17346000	-1.47095800	-0.41425500
C	-1.42282700	-0.70724000	-0.77752900
H	-0.30655800	-2.50446300	-0.73516500
H	0.16610000	-2.56790000	1.46466800
H	-0.01191800	2.32683800	1.61571200
C	3.60237800	-0.70321400	1.54367400
C	3.54760500	0.71757500	1.75350500

C	-3.52022600	0.86296700	-1.43015800
C	-3.62617800	-0.57038600	-1.33588000
C	2.08666900	-1.58662600	-1.52868600
C	2.30119900	1.22931200	-1.30610900
C	-2.34207400	1.19142400	2.25751900
C	-2.16835300	-1.63394900	2.39098100
C	3.44384200	0.47411600	-1.76993100
C	-3.35571200	-0.98169500	2.89287400
C	3.33122100	-0.94997200	-1.89637400
C	-3.45061000	0.44623600	2.80846700
C	4.44482900	-1.68923700	-2.29151800
C	4.66313800	1.09036300	-2.04794500
H	4.74734400	2.16911200	-1.94131100
C	4.81923200	-1.32248000	1.19485600
C	4.72464900	1.48636900	1.66632000
C	-4.42572200	-1.70691800	3.41193100
H	-4.35306800	-2.78956800	3.46553600
C	-4.61198200	1.08085900	3.24428800
H	-4.68015500	2.16315800	3.17501700
C	-4.64168000	1.63356000	-1.79319700
C	-4.86055000	-1.20294900	-1.56908300
C	-5.94456500	-0.43910300	-2.02261400
C	-5.83371700	0.97995400	-2.14040000
C	5.66760200	-1.07227200	-2.57815600
C	5.77917700	0.35198900	-2.45644600
C	5.94423900	-0.52452600	0.95707500
C	5.89717400	0.88207300	1.20096800
C	-5.58888700	-1.07184800	3.85663700
C	-5.68477200	0.35555600	3.77018700
C	6.81841600	-1.82070600	-2.97371500
H	6.73775000	-2.90288200	-3.03993200
C	7.02992800	0.97469900	-2.75393200
H	7.10772900	2.05502900	-2.65827000
C	7.99959200	-1.19230700	-3.24304700
H	8.87048300	-1.77365100	-3.52808200
C	7.14660200	-1.08966500	0.43648900
C	7.04875500	1.66753100	0.89675800
C	8.24019400	-0.30807900	0.17959700
H	9.12722000	-0.77735000	-0.23279900
C	-6.69284600	-1.80506100	4.39255100
H	-6.61315500	-2.88701100	4.45556600
C	-6.88063300	0.99441300	4.22358500
H	-6.94655800	2.07707000	4.15612300
C	-7.81794700	-1.16037800	4.81482900

H	-8.65117700	-1.72540200	5.22108200
C	-6.95969400	1.71156500	-2.61720700
C	-7.17165500	-1.06353100	-2.39014800
C	-8.23123800	-0.32703700	-2.85036200
H	-9.14024600	-0.84796600	-3.13186300
C	8.10440400	0.22612600	-3.14096600
H	9.05160600	0.70801300	-3.36393600
C	8.18774900	1.08810000	0.40553100
H	9.03259300	1.72599200	0.16736900
C	-7.91341400	0.26092900	4.72881400
H	-8.81776100	0.75470800	5.07066900
C	-8.12422100	1.07728100	-2.96318500
H	-8.94953900	1.67715000	-3.33199000
H	4.36079000	-2.77000700	-2.37480600
C	-6.89217600	3.18783100	-2.77837400
C	-7.32494600	-2.54167400	-2.31389200
C	7.22322100	-2.53708400	0.10367400
C	7.01826300	3.14702100	1.04494700
N	-5.70322000	3.78658000	-2.38595100
N	5.84347900	3.68330100	1.55388000
N	6.06426000	-3.26829900	0.32035000
N	-6.23575100	-3.24070900	-1.81391700
N	2.34000600	1.36239500	1.84395900
N	2.45166000	-1.44782700	1.52709300
N	-2.32745500	1.48764800	-1.16099900
N	-2.52330200	-1.33535600	-1.04120400
C	-2.11059100	-3.06419100	2.35798500
C	-2.05881500	-4.26937200	2.32736600
H	-2.01644800	-5.33484900	2.28447100
C	-2.48335300	2.59426600	2.01511700
C	-2.60974900	3.75809700	1.72099900
H	-2.73007500	4.77373000	1.41535900
C	2.01779100	-3.01682200	-1.51313400
C	1.97206400	-4.22265800	-1.48204400
H	1.92180000	-5.28797800	-1.43669700
C	2.44909400	2.63335100	-1.06657600
C	2.58395100	3.80747900	-0.81931100
H	2.68524400	4.84544700	-0.59103700
C	4.72908200	2.94465500	1.99138600
C	4.91637300	-2.80280100	0.98945400
C	-4.61128700	3.13340500	-1.78648900
C	-5.06078000	-2.66399700	-1.29994700
O	-3.72764900	3.80580200	-1.30755600
O	-7.82438500	3.83070400	-3.21880200

O	-8.34692200	-3.09998900	-2.66043900
O	-4.29428400	-3.35659800	-0.67334700
O	4.09011900	-3.60473800	1.35553800
O	8.23260700	-3.04612800	-0.34337800
O	7.96712900	3.84341400	0.73958400
O	3.85499200	3.51004800	2.60618800
C	5.78808600	5.12009600	1.81267800
H	4.85278700	5.51813100	1.41735700
H	5.81286000	5.30825400	2.88843600
H	6.64453000	5.58019100	1.32680100
C	6.07603900	-4.69731400	0.01937500
H	6.13084900	-5.28017900	0.94184000
H	5.14848300	-4.95290200	-0.49578700
H	6.94289900	-4.89992700	-0.60491100
C	-6.36580900	-4.68496100	-1.62883300
H	-5.45312500	-5.16965400	-1.97552900
H	-6.50271100	-4.91768200	-0.57010000
H	-7.22778100	-5.01624000	-2.20211400
C	-5.60821100	5.24371200	-2.45601500
H	-5.67031600	5.67387300	-1.45356700
H	-4.64702900	5.51678900	-2.89180500
H	-6.43147600	5.60014500	-3.06965800

Table S14. Cartesian coordinates of the ground state optimized geometry for **T3**

C	-0.13744500	-1.54058600	-0.22011800
C	1.07821800	-1.01547800	-0.94951600
C	1.16912300	0.40935900	-1.08585800
C	-0.01858400	1.23900800	-0.62102200
C	-1.29890200	0.55712400	-1.00410800
C	-1.37249800	-0.86446700	-0.76364600
C	-1.22954400	0.82230100	1.66491700
C	-0.03879000	1.47199500	0.98897100
C	-1.15212000	-0.58033000	1.94204500
C	1.24797600	0.90600700	1.51571000
C	0.04539300	-1.30614900	1.38392300
C	1.31016800	-0.52823100	1.64081500
C	-3.55445000	-0.84468900	-1.42345400
C	-3.49442300	0.58341100	-1.60204100
C	3.51100300	1.02316700	1.63397400
C	3.58131200	-0.41207300	1.66943600
C	-2.19640200	-1.23801000	2.54749000
C	-2.38622000	1.51990900	1.92597800
C	2.35045700	0.99342700	-1.48693300

C	2.15413500	-1.82217000	-1.23739200
C	-3.49860700	0.87103400	2.58018900
C	3.40282400	-1.24532300	-1.68098600
C	-3.39395100	-0.51855000	2.91663800
C	3.50536700	0.18019300	-1.79745100
C	-4.46428700	-1.14912100	3.54770100
H	-4.38313700	-2.20301900	3.79908900
C	-4.67173100	1.56047200	2.87997300
H	-4.74698800	2.61262200	2.61890000
C	-4.75855600	-1.53387500	-1.65579000
C	-4.65385200	1.30860400	-1.94372600
C	4.52808500	-2.03222100	-1.92057700
H	4.45155600	-3.11162800	-1.81604900
C	4.72610900	0.74909100	-2.15907900
H	4.80358000	1.83066800	-2.23976200
C	4.67913600	1.78101800	1.42359800
C	4.81136200	-1.06669800	1.45573300
C	5.93170400	-0.30686600	1.09895100
C	5.86245700	1.11973900	1.08131400
C	-5.63944600	-0.45771200	3.85617600
C	-5.74685700	0.92942000	3.51225600
C	-5.91840200	-0.80299400	-1.94954500
C	-5.86673900	0.61808300	-2.09412500
C	5.75206300	-1.46389300	-2.28944500
C	5.85207200	-0.03979800	-2.41948200
C	-6.74487500	-1.09474600	4.50098800
H	-6.65713700	-2.14649800	4.75985100
C	-6.95508200	1.62591600	3.82606500
H	-7.02905300	2.67784700	3.56351000
C	-7.88253400	-0.39762400	4.78283700
H	-8.71684900	-0.89019600	5.27223700
C	-7.17688600	-1.46011300	-2.08076900
C	-7.07482600	1.31098200	-2.39823100
C	-8.31835400	-0.75708000	-2.36175000
H	-9.25487400	-1.29882900	-2.44102100
C	6.91430200	-2.25992200	-2.52728900
H	6.84190600	-3.33711000	-2.39934800
C	7.10206400	0.53180400	-2.80934800
H	7.17088400	1.61265200	-2.90695200
C	8.09490300	-1.67840400	-2.88888100
H	8.97425100	-2.29240500	-3.05538700
C	7.00259100	1.85420600	0.63913900
C	7.15000100	-0.93640600	0.70434000
C	8.23392400	-0.19743700	0.31430200

H	9.13067100	-0.72173100	0.00085600
C	-7.98933300	0.98359300	4.44017700
H	-8.90323100	1.52046200	4.67416800
C	-8.26406100	0.64375500	-2.53231500
H	-9.15542900	1.21786200	-2.76161200
C	8.18755100	-0.26366600	-3.04176600
H	9.13382500	0.17914800	-3.33802200
C	8.15654500	1.21551700	0.27366100
H	8.99134400	1.81349000	-0.07748500
H	-0.25436100	-2.61487600	-0.36509900
H	0.00563300	2.22836900	-1.07844000
H	-0.05236600	2.55065200	1.14666700
H	0.15690700	-2.29709400	1.82470600
C	-7.08409800	2.78677400	-2.57094800
C	-7.29379600	-2.93014000	-1.88262400
C	6.92951500	3.33019300	0.48816000
C	7.24983500	-2.41851100	0.63724200
C	2.49105600	2.41835800	-1.46948100
C	2.62149300	3.61694600	-1.40037800
H	2.72064600	4.67783700	-1.32948900
C	2.09362300	-3.22892200	-0.97820300
C	2.05726800	-4.41181700	-0.74060600
H	2.01274700	-5.45447400	-0.51618600
C	-2.52882400	2.86139300	1.45011500
C	-2.65406600	3.95971800	0.96471000
H	-2.76660400	4.91185300	0.49488300
C	-2.12699300	-2.65085700	2.77282700
C	-2.06788200	-3.84191700	2.95861700
H	-2.00973900	-4.89603200	3.11573800
N	6.09586600	-3.11734200	0.96127900
N	5.74483800	3.93386600	0.88007900
N	-5.86114300	3.42099300	-2.41400200
N	-6.10986700	-3.60434000	-1.62421100
C	4.92696000	-2.55859900	1.51178800
C	4.65537800	3.27534300	1.48308300
C	-4.63483300	2.80084900	-2.11244600
C	-4.82591300	-3.03201800	-1.63214300
O	8.27277000	-2.98435900	0.30322800
O	4.09791600	-3.29591700	1.99048000
O	7.85215400	3.98849600	0.04696000
O	3.77948000	3.91381200	2.01686200
O	-3.65375800	3.50063400	-2.00740700
O	-8.10159100	3.39744700	-2.83292300
O	-3.86223000	-3.76088600	-1.63136300

O	-8.36263800	-3.50389500	-1.95071300
C	6.12910400	-4.57636000	0.90742900
H	6.19312200	-4.99480200	1.91475400
H	5.20607400	-4.92886000	0.44413700
H	6.99973300	-4.86807900	0.32518200
C	5.71263500	5.39251100	0.80376900
H	6.41666900	5.82370000	1.51960900
H	6.00924400	5.69890400	-0.19987200
H	4.70207200	5.71882300	1.03575100
C	-5.80616500	4.87354400	-2.56946500
H	-5.47583800	5.32984400	-1.63410300
H	-5.08806400	5.12942100	-3.35007400
H	-6.80324200	5.21680600	-2.83166100
C	-6.15192000	-5.06081700	-1.50512700
H	-5.54133000	-5.36397400	-0.65459600
H	-7.18965700	-5.35262700	-1.36597600
H	-5.74535100	-5.52364800	-2.40734600
N	2.43534000	-1.16111300	1.75068700
N	2.29737500	1.66112900	1.59272200
N	-2.45405000	-1.54093600	-0.98201500
N	-2.31082000	1.25077200	-1.41260000

Table S15. Cartesian coordinates of the ground state optimized geometry for **Dimer**

C	3.02114400	-2.83494700	-0.42331700
C	1.94607100	-2.24797500	-1.18974700
C	0.93741800	-1.55914600	-0.55742200
C	0.94922700	-1.38985600	0.86493600
C	1.98396600	-1.88889700	1.62076100
C	3.04364000	-2.64700700	0.99752200
C	-0.16510400	-0.85615300	-1.32412500
C	-0.15485300	-0.55003900	1.47321100
C	-1.46478700	-0.92288300	0.83271400
C	-1.46803300	-1.08927300	-0.60173000
C	-3.69668600	-1.55666800	-0.53218600
C	-3.70915600	-1.31151500	0.88705800
H	-0.26138300	-1.27685400	-2.32540300
H	-0.23479100	-0.73923200	2.54389700
H	0.24206900	0.90040900	-2.57046900
C	0.14339300	0.71417700	-1.50070100
C	1.44768800	1.08644400	-0.84411100
C	-0.95846800	1.56831100	-0.91128700
C	1.43878300	1.24019000	0.59200500
C	-0.97789800	1.71122700	0.51353600

C	-1.95669500	2.11164600	-1.68546500
C	3.69657500	1.43774200	-0.86286000
C	0.12413500	1.02500400	1.29462300
C	-2.01302700	2.36881100	1.13631600
C	-3.03079900	2.85758000	-1.07160300
C	3.69498700	1.54475700	0.57317700
H	0.20270300	1.44790900	2.29650600
C	-3.06276500	2.98181100	0.35605700
C	4.09038700	-3.18716400	1.74166300
C	5.11684800	-3.91547100	1.13400900
C	5.09341800	-4.10584900	-0.28627100
C	-4.91968800	-1.36657000	1.60690200
C	-6.10651500	-1.66754100	0.91977300
C	-6.08745700	-1.93938700	-0.48334000
C	-4.10884400	3.67958800	0.95720600
C	-5.12489400	4.26622700	0.19793900
C	-5.09230700	4.14278100	-1.22954800
C	4.90759400	1.69840600	1.27170600
C	6.11484300	1.65947700	0.55919200
C	6.11351900	1.58357300	-0.86709800
C	-4.04500100	3.43851600	-1.83011100
C	-4.88219100	-1.91668800	-1.19869300
C	4.04551500	-3.55835500	-1.03151500
C	4.90590100	1.53017800	-1.57582900
H	-4.01794700	3.34031100	-2.91177400
H	-4.13059600	3.76896700	2.03979500
H	4.10386400	-3.04018500	2.81809000
H	4.02615400	-3.69820900	-2.10878500
C	-7.32075100	-2.20979800	-1.14563800
C	-8.50474600	-2.23740900	-0.45769200
H	-9.41861600	-2.43841000	-1.00649000
C	-8.52083300	-2.00221900	0.93468000
C	-6.20122600	4.98731500	0.80276700
C	-7.18057900	5.54769500	0.03710700
C	-7.14809900	5.42462400	-1.38442900
C	6.19379500	-4.47787300	1.88726600
C	7.18283900	-5.18291800	1.26757700
C	7.16032800	-5.37173800	-0.14681700
C	7.36744000	1.68359500	1.23803400
C	8.54973000	1.63662000	0.54697000
C	8.54760700	1.56268800	-0.86431400
C	-7.35720200	-1.72203500	1.60165800
C	6.14893000	-4.85085900	-0.89872800
C	7.36258600	1.53783800	-1.55149600

C	-6.13737800	4.74469500	-1.99713700
H	-9.44578600	-2.03021100	1.50071700
H	-6.21980900	5.07795400	1.88551300
H	-7.99423600	6.09242500	0.50570700
H	-7.93737200	5.87906200	-1.97516000
H	-6.10618500	4.64763200	-3.07901900
H	6.20475800	-4.33036300	2.96379800
H	7.99679200	-5.60685000	1.84740300
H	7.95802400	-5.93479100	-0.62117100
H	6.12578400	-4.99175000	-1.97599200
H	9.47766400	1.64391300	1.10890400
H	9.47371400	1.51041800	-1.42691500
C	-7.36323000	-2.44179000	-2.61465300
C	-7.43872900	-1.47644600	3.06535000
C	7.42488200	1.72628200	2.72367300
C	4.93494400	1.59514800	-3.07269400
C	1.96523400	-2.34757800	-2.61827000
C	1.98300000	-2.41704900	-3.82304400
H	1.99207500	-2.46910800	-4.88908100
C	2.05223500	-1.60191800	3.02200600
C	2.11553700	-1.32574500	4.19529400
H	2.16647800	-1.06627500	5.22949100
C	-1.96119200	1.90969200	-3.10326100
C	-1.96565200	1.72923300	-4.29654800
H	-1.96377800	1.56011400	-5.35037800
C	-2.09258000	2.39047400	2.56528600
C	-2.16993000	2.36797800	3.76938900
H	-2.24169800	2.32450200	4.83345500
N	-2.53800900	-1.40734400	-1.25534900
N	-2.53909900	-1.02394300	1.54591400
N	2.53038600	1.19119900	-1.54500500
N	2.51750700	1.45353100	1.27376500
N	6.18794400	1.42135200	-3.68585200
N	6.20255300	1.79592400	3.37576900
N	-6.23978500	-1.18563200	3.69696100
C	-4.97915000	-1.08069500	3.08054500
C	-4.88321400	-2.31615200	-2.64497500
C	4.94430500	1.90628300	2.75646500
C	7.41316000	1.42386400	-3.03431200
O	8.46554200	1.34692100	-3.63672300
O	3.96768200	1.79865800	-3.76793700
O	8.47947300	1.70750700	3.32711900
O	3.98142700	2.16166900	3.44048400
O	-3.89119800	-2.55109100	-3.29362000

O	-8.40820700	-2.63395900	-3.20412500
O	-8.49293600	-1.52927100	3.66781700
O	-4.03271300	-0.76985000	3.76508600
C	6.19916400	1.91208000	4.83287000
H	5.91062600	2.92340700	5.12797900
H	5.47191800	1.21116600	5.24361800
H	7.20203200	1.68625700	5.18575000
C	6.17801100	1.40505600	-5.14750000
H	5.89928900	2.38912600	-5.53135800
H	7.17594200	1.13629300	-5.48387400
H	5.43999700	0.67931900	-5.48998900
C	-6.11033700	-2.73358900	-4.69593600
H	-5.46453800	-2.01272700	-5.19796200
H	-5.70391300	-3.73428200	-4.85928300
H	-7.12933300	-2.67249300	-5.06890500
C	-6.25584900	-0.92156400	5.13484500
H	-5.56505800	-1.60150000	5.63585100
H	-5.92873500	0.10276300	5.32391300
H	-7.27251400	-1.07140500	5.48806400
N	-6.13917500	-2.43152200	-3.26583400