Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information for

Annihilator Dimers Enhance Triplet Fusion Upconversion

Andrew B. Pun[1], Samuel N. Sanders[2], Matthew Y. Sfeir[3,4], Luis M. Campos[1*], and Daniel N. Congreve[2*]

1) Department of Chemistry, Columbia University, New York, New York 10027, United States.
2) Rowland Institute at Harvard University, Cambridge, Massachusetts 02142, United States
3) Photonics Initiative, Advanced Science Research Center, City University of New York, New York, New York 10031, United States
4) Department of Physics, Graduate Center, City University of New York, New York, New York 10016, United States

GENERAL METHODS

All commercially obtained reagents/solvents were used as received; chemicals were purchased from Alfa Aesar®, Sigma-Aldrich®, Acros organics®, TCI America®, Mallinckrodt®, and Oakwood® Products, and were used as received without further purification. Unless stated otherwise, reactions were conducted in oven-dried glassware under argon atmosphere. Bromo-TIPS-Tetracene was synthesized according to literature procedure[1]. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker 400 MHz (100 MHz for ^{13}C) NMR and on a 500 MHz (125 MHz for ^{13}C) NMR spectrometer. Data from the ^{1}H-NMR and ^{13}C-NMR spectroscopy are reported as chemical shift (δ ppm) with the corresponding integration values. Standard abbreviations indicating multiplicity were used as follows: s (singlet), b (broad), d (doublet), t (triplet), q (quartet), m (multiplet) and virt (virtual).

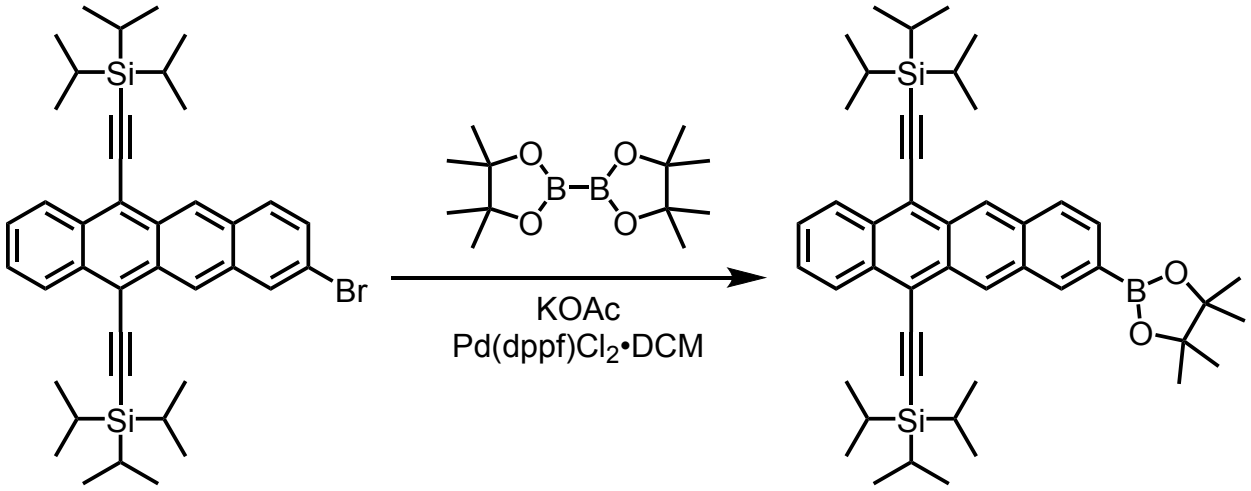
The mass spectral data for the compounds were obtained from XEVO G2-XS Waters® equipped with a QTOF detector with multiple inlet and ionization capabilities including electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), and atmospheric solids analysis probe (ASAP). The base peaks were usually obtained as $[M]^{+}$ or $[M+H]^{+}$ ions.

Absorption spectra were obtained on a Shimadzu UV 1800 UV-Vis spectrophotometer. Emission spectra were obtained on a Horiba Fluoromax-4.

Anhydrous solvents were obtained from a Schlenk manifold with purification columns packed with activated alumina and supported copper catalyst (Glass Contour, Irvine, CA).

SYNTHESIS

Synthesis of TIPS-Bpin-Tetracene



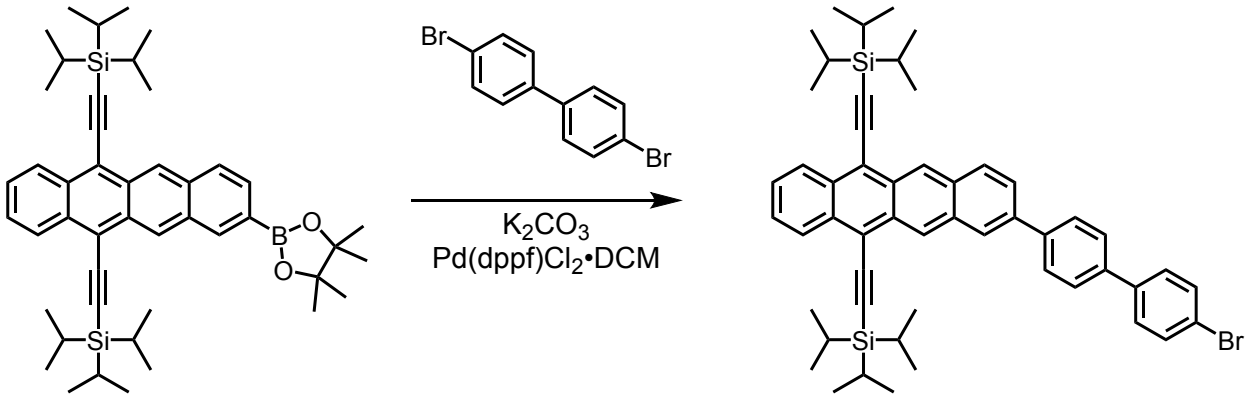
TIPS-Bromo-Tetracene (1.00 g, 1.5 mmol)**,** bis(pinacolato)diboron (571 mg, 2.25 mmol), KOAc (311 mg, 2.25 mmol) and Pd(dppf)Cl_2·DCM (61.3 mg, 0.075 mmol) were added to a reaction vial. Sequential vacuum and argon was used to degas the mixture. The solids were then dissolved in 20 mL degassed dioxane. The reaction was brought to 100 °C and allowed to stir overnight. The reaction was cooled to room temperature. The crude reaction mixture was concentrated and purified by chromatography on silica gel (25% DCM in Hexanes) to obtain **TIPS-Bpin-Tetracene** as an orange solid. (600 mg, 56% Yield).

^{1}H-NMR (400 MHz, $CDCl_3$, δ ppm): 9.30 (d, J= 22.0 Hz, 2H), 8.70-8.58 (m, 2H), 8.55 (s, 1H), 7.96 (d, J= 8.7 Hz, 1H), 7.82-7.71 (m, 1H), 7.64-7.44 (m, 2H), 1.45-1.39 (m, 12H), 1.37-1.29 (m, 42H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 137.77, 133.02, 132.85, 132.76, 131.64, 130.91, 130.30, 129.69, 127.56, 127.47, 127.41, 126.82, 126.66, 126.06, 119.01, 118.56, 106.12, 105.90, 103.91, 103.80, 84.08, 24.97, 19.01, 18.97, 11.61.

MS (ESI): Calculated $[M+H]^+$: 715.4547; Observed: 715.4487

Synthesis of TIPS-Tetracene-Ph-Ph-Br



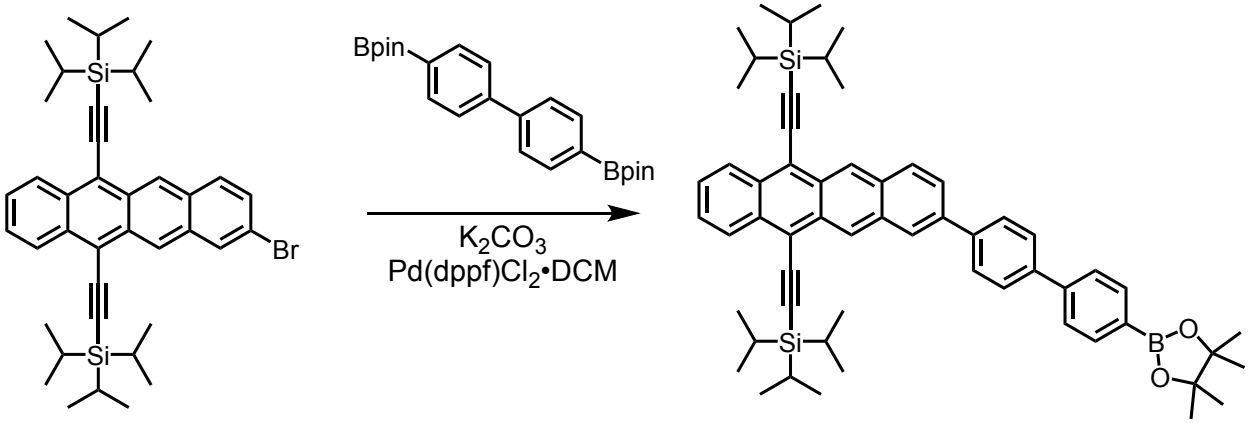
TIPS-Bpin-Tetracene (200 mg, 0.28 mmol)**,** 4,4'-dibromobiphenyl (284 mg, 0.7 mmol), K_2CO_3 (194 mg, 1.4 mmol) and $Pd(dppf)Cl_2 \cdot DCM$ (11.4 mg, 0.014 mmol) were added to a reaction vial. Sequential vacuum and argon was used to degas the mixture. The solids were then dissolved in 12 mL of a 9:1 mixture of THF: degassed water. The reaction was brought to 70 °C and allowed to stir overnight. The reaction was cooled to room temperature. The crude reaction mixture was concentrated and purified by chromatography on silica gel (10% DCM in hexanes) to obtain **TIPS-Tetracene-Ph-Ph-Br** as a red solid. (151 mg, 66% Yield).

^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.35 (d, J= 14.9 Hz, 2H), 8.82-8.54 (m, 2H), 8.21 (s, 1H), 8.11 (d, J= 8.9 Hz, 1H) 7.88 (d, J= 8.3 Hz, 2H), 7.79 (dd, J= 8.9, 1.7 Hz, 1H), 7.73 (d, J= 8.3 Hz, 2H), 7.61 (d, J= 8.5 Hz, 2H), 7.58-7.48 (m, 4H), 1.41-1.29 (m, 42H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 140.19, 139.54, 139.21, 137.64, 132.78, 132.66, 132.29, 132.00, 131.37, 130.72, 130.52, 129.38, 128.63, 127.82, 127.50, 127.42, 126.81, 126.76, 126.65, 126.18, 126.08, 125.83, 121.74, 118.72, 118.54, 106.01, 105.94, 103.92, 103.88, 18.98, 11.62.

MS (ESI): Calculated $[M]^+$: 820.3331; Observed: 820.3345

Synthesis of TIPS-Tetracene-Ph-Ph-Bpin



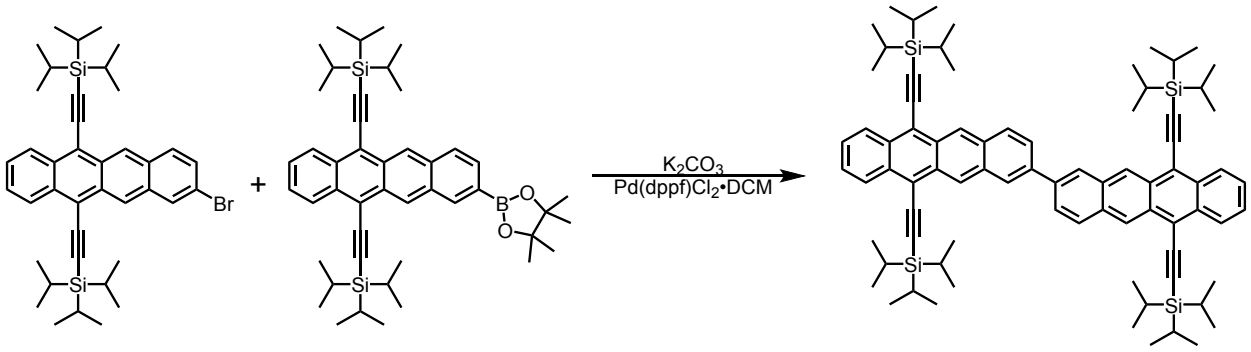
TIPS-Bromo-Tetracene (500 mg, 0.75 mmol), 4,4′-Biphenyldiboronic acid bis(pinacol) ester (762 mg, 1.88 mmol), K_2CO_3 (518 mg, 3.75 mmol) and $Pd(dppf)Cl_2$·DCM (30.6 mg, 0.0375 mmol) were added to a reaction vial. Sequential vacuum and argon was used to degas the mixture. The solids were then dissolved in 16 mL of a 9:1 mixture of THF: degassed water. The reaction was brought to 70 °C and allowed to stir overnight. The reaction was cooled to room temperature. The crude reaction mixture was concentrated and purified by chromatography on silica gel (50% DCM in hexanes) to obtain **TIPS-Tetracene-Ph-Ph-Bpin** as a red solid. (260 mg, 40% Yield).

^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.35 (d, J= 17.4 Hz, 2H), 8.80-8.51 (m, 2H), 8.23 (dd, J= 1.8, 0.9 Hz, 1H), 8.14-8.09 (m, 1H) 7.94 (d, J= 8.1 Hz, 2H), 7.89 (d, J= 8.3 Hz, 2H), 7.81 (d, J= 8.5 Hz, 3H), 7.72 (d, J= 8.1 Hz, 2H), 7.63-7.52 (m, 2H), 1.42-1.38 (m, 12H), 1.37-1.30 (m, 42H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 143.40, 140.40, 140.22, 137.93, 135.52, 132.89, 132.78, 132.46, 131.52, 130.85, 130.64, 129.46, 127.93, 127.85, 127.56, 126.91, 126.86, 126.77, 126.50, 126.31, 126.29, 125.93, 118.84, 118.69, 106.14, 106.03, 104.07, 104.04, 84.02, 25.05, 19.12, 11.75.

MS (ESI): Calculated $[M]^+$: 866.5096; Observed: 866.5104

Synthesis of BT0



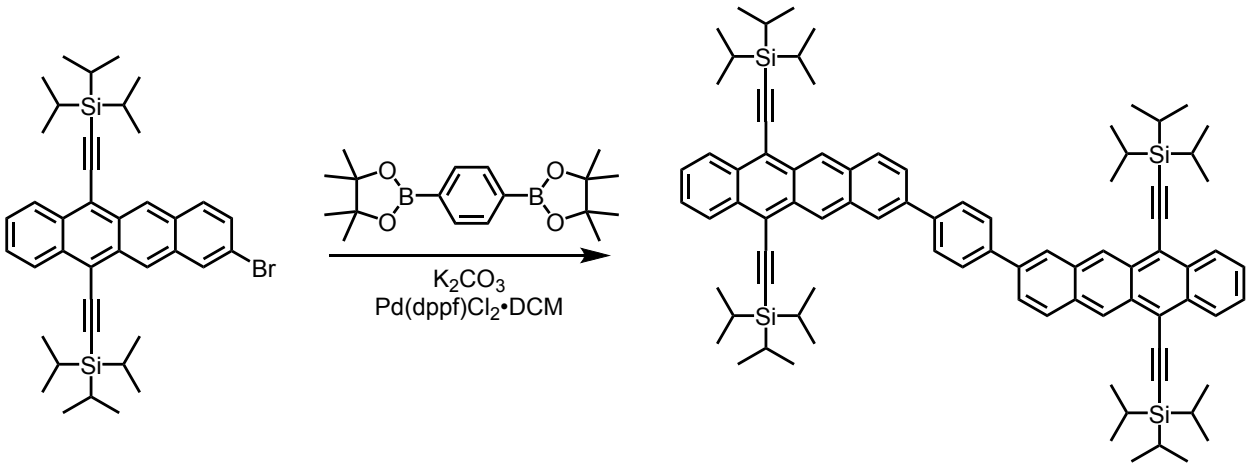
TIPS-Bromo-Tetracene (93.4 mg, 0.14 mmol)**,** TIPS-Bpin-Tetracene (100 mg, 0.14 mmol), K_2CO_3 (194 mg, 1.4 mmol) and $Pd(dppf)Cl_2 \cdot DCM$ (11.4 mg, 0.014 mmol) were added to a reaction vial. Sequential vacuum and argon was used to degas the mixture. The solids were then dissolved in 10 mL of a 9:1 mixture of THF: degassed water. The reaction was brought to 65 °C and allowed to stir overnight. The reaction was cooled to room temperature. The crude reaction mixture was concentrated and purified by chromatography on silica gel (5% chloroform in hexanes) to obtain **BT0** as a red solid. (27 mg, 16% Yield).

^{1}H-NMR (400 MHz, $CDCl_3$, δ ppm): 9.39 (d, J= 23.1 Hz, 4H), 8.65 (dd, J= 8.4, 4.0 Hz, 4H), 8.38 (s, 2H), 8.19 (d, J= 9.1 Hz, 2H), 7.97 (d, J= 9.0 Hz, 2H), 7.60-7.53 (m, 4H), 1.45-1.29 (m, 84H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 138.06, 132.97, 132.85, 132.52, 132.47, 131.60, 130.97, 130.95, 130.76, 129.69, 127.59, 126.96, 126.94, 126.37, 126.21, 118.90, 118.76, 106.21, 106.09, 104.10, 104.05, 19.14, 11.77.

MS (ESI): Calculated $[M]^+$: 1175.7085; Observed: 1175.7090.

Synthesis of BT1



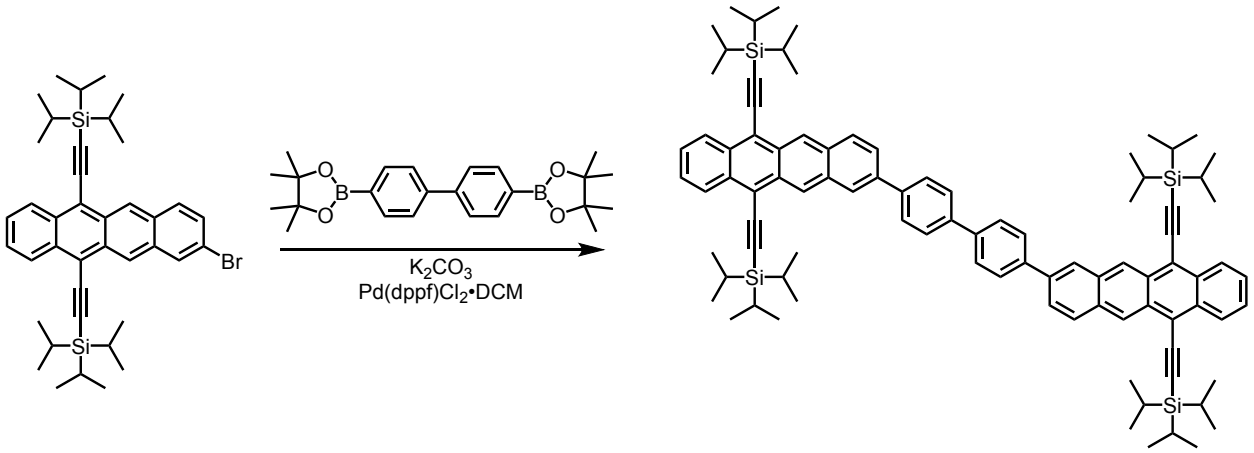
TIPS-Bromo-Tetracene (120 mg, 0.18 mmol), 1,4-Benzenedibronic acid Bis(Pinacol) Ester (25.8 mg, 0.078 mmol), K_2CO_3 (108 mg, 0.78 mmol) and $Pd(dppf)Cl_2$·DCM (6.5 mg, 0.008 mmol) were added to a reaction vial. Sequential vacuum and argon was used to degas the mixture. The solids were then dissolved in 10 mL of a 9:1 mixture of THF: degassed water. The reaction was brought to 65 °C and allowed to stir overnight. The reaction was cooled to room temperature. The crude reaction mixture was concentrated and purified by chromatography on silica gel (10% chloroform in hexanes) to obtain **BT1** as a red solid. (39 mg, 40% Yield).

^{1}H-NMR (400 MHz, $CDCl_3$, δ ppm): 9.37 (d, J= 15.4 Hz, 4H), 8.70-8.60 (m, 4H), 8.28 (s, 2H), 8.15 (m, 2H), 7.99 (s, 4H), 7.86 (dd, J= 8.9, 1.7 Hz, 2H), 7.61-7.51 (m, 4H), 1.43-1.30 (m, 84H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 140.29, 137.93, 132.95, 132.82, 132.51, 131.56, 130.89, 130.68, 129.54, 128.10, 128.05, 127.58, 126.94, 126.89, 126.80, 126.34, 125.96, 118.88, 118.71, 106.17, 106.07, 104.10, 104.06, 19.13, 11.78.

MS (ESI): Calculated $[M+H]^+$: 1252.7477; Observed: 1252.7462.

Synthesis of BT2



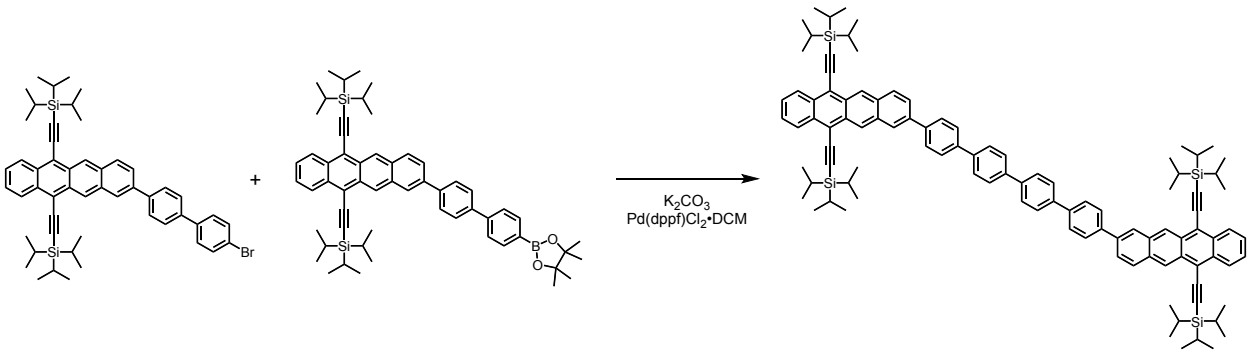
TIPS-Bromo-Tetracene (200 mg, 0.3 mmol)**,** 4,4'-Biphenyldibronic acid Bis(Pinacol) Ester (52.8 mg, 0.13 mmol), K_2CO_3 (180 mg, 1.3 mmol) and $Pd(dppf)Cl_2 \cdot DCM$ (10.6 mg, 0.013 mmol) were added to a reaction vial. Sequential vacuum and argon was used to degas the mixture. The solids were then dissolved in 10 mL of a 9:1 mixture of THF: degassed water. The reaction was brought to 65 °C and allowed to stir overnight. The reaction was cooled to room temperature. The crude reaction mixture was concentrated and purified by chromatography on silica gel (10% chloroform in hexanes) to obtain **BT2** as a red solid. (78 mg, 45% Yield).

^{1}H-NMR (400 MHz, $CDCl_3$, δ ppm): 9.36 (d, J= 15.0 Hz, 4H), 8.70-8.63 (m, 4H), 8.26 (s, 2H), 8.14 (m, 2H), 8.00-7.82 (m, 10H), 7.62-7.54 (m, 4H), 1.42-1.27 (m, 84H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 139.95, 139.85, 137.79, 132.79, 132.66, 132.36, 131.41, 130.74, 130.52, 129.36, 127.80, 127.61, 127.44, 126.80, 126.74, 126.64, 126.18, 125.77, 118.73, 118.56, 106.01, 105.91, 103.96, 103.92, 19.01, 18.99, 11.63.

MS (ESI): Calculated $[M+H]^+$: 1328.7791; Observed: 1328.7792.

Synthesis of BT4



TIPS-Tetracene-Ph-Ph-Bpin (55.5 mg, 0.064 mmol)**,** TIPS-Tetracene-Ph-Ph-Br (50 mg, 0.061 mmol), K_2CO_3 (42.2 mg, 0.3 mmol) and $Pd(dppf)Cl_2$·DCM (2.5 mg, 0.003 mmol) were added to a reaction vial. Sequential vacuum and argon was used to degas the mixture. The solids were then dissolved in 8 mL of a 9:1 mixture of THF: degassed water. The reaction was brought to 70 °C and allowed to stir overnight. The reaction was cooled to room temperature. The crude reaction mixture was concentrated and purified by chromatography on silica gel (20% chloroform in hexanes) to obtain **BT4** as a red solid. (27 mg, 16% Yield).

^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.36 (d, J= 17.9 Hz, 4H), 8.64 (dt, J=7.3, 2.9Hz 4H), 8.25 (s, 2H), 8.13 (d, J=8.9 Hz 2H), 7.95-7.89 (m, 4H), 7.89-7.74 (m, 14H), 7.59-7.51 (m, 4H), 1.40-1.25 (m, 84H).

Limited solubility prevented the acquisition of a ^{13}C NMR.

MS (ESI): Calculated $[M]^+$: 1479.8339; Observed: 1479.8326

POWER DEPENDENCE MEASUREMENTS

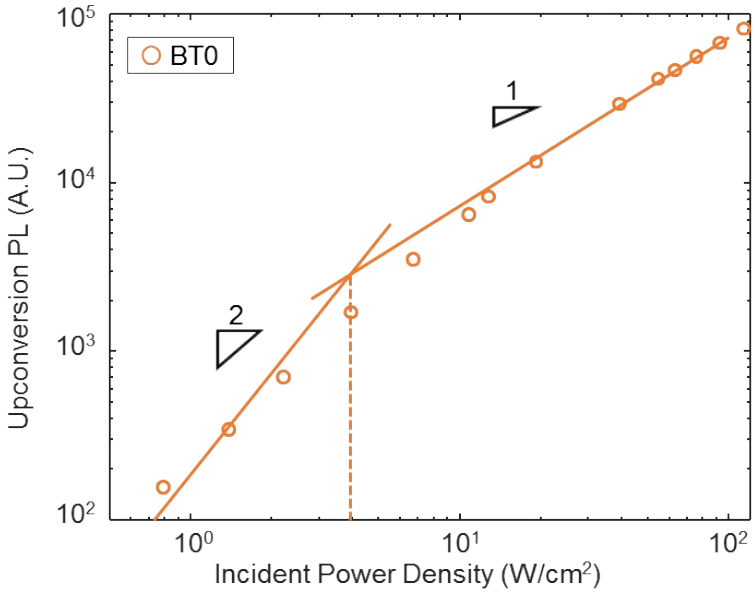


Figure S1: Dependence of upconverted PL on incident light intensity at 2.5×10^{-4} M BT0 concentration. The transition between quadratic and linear dependences occurs at 3.9 W/cm^2.

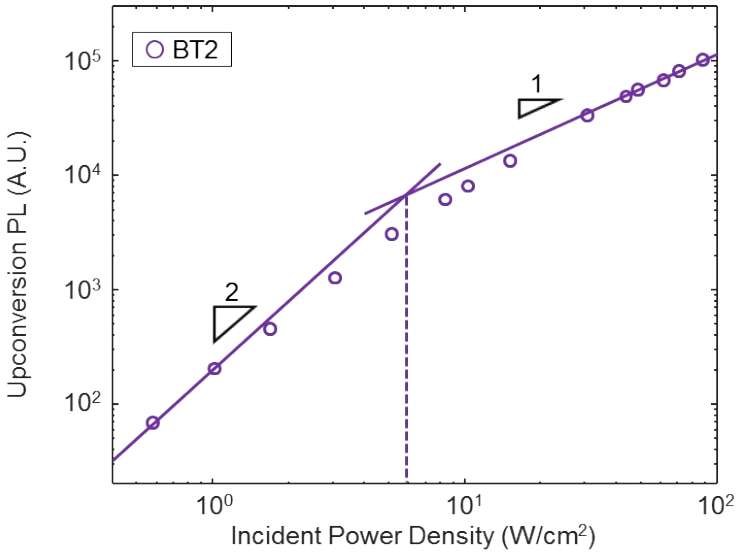


Figure S2: Dependence of upconverted PL on incident light intensity at 2.5×10^{-4} M BT2 concentration. The transition between quadratic and linear dependences occurs at 5.7 W/cm^2.

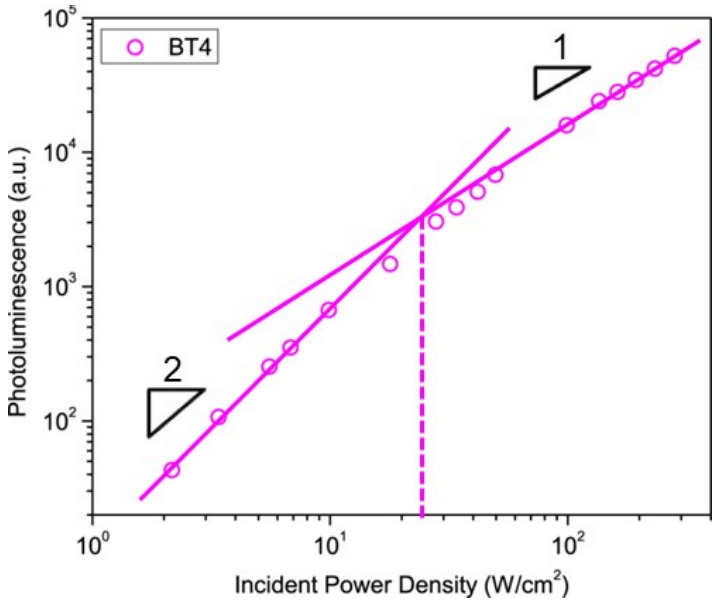


Figure S3: Dependence of upconverted PL on incident light intensity at 2.5×10^{-4} M BT4 concentration. The transition between quadratic and linear dependences occurs at 25.7 W/cm^2.

Computational Methods

Calculations were done using density functional theory (DFT) within the Gaussian 09 Suite, all geometries were optimized using the B3LYP functional and the 6-31G** basis set. To simplify the computation, the (triisopropylsilyl)acetylene groups were simplified to (trimethylsilyl)acetylene groups.

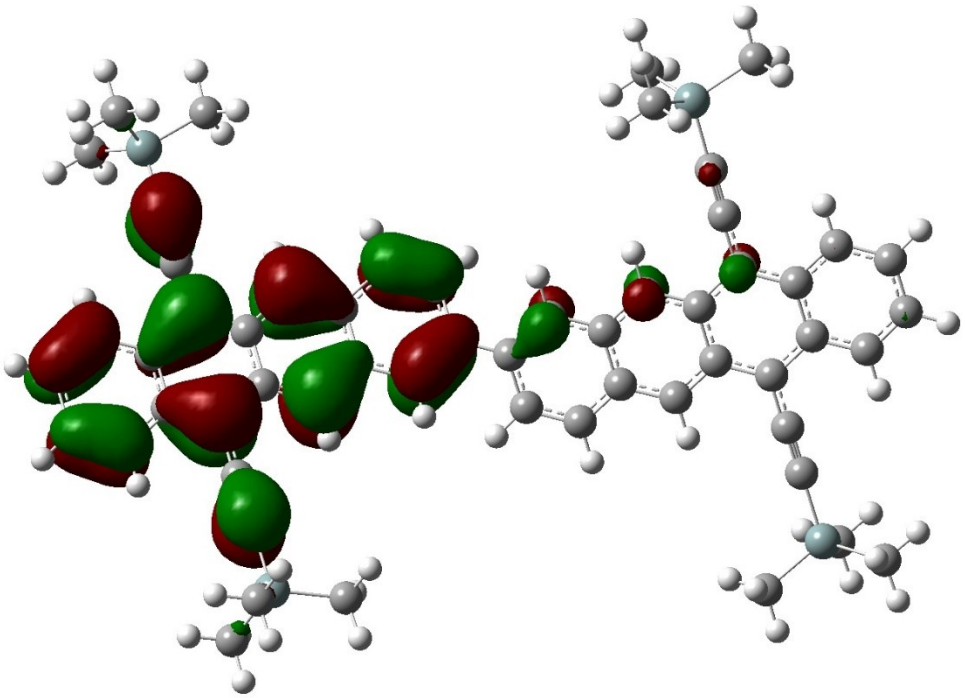


Figure S4: Zoom in of T_1 orbital of BT0

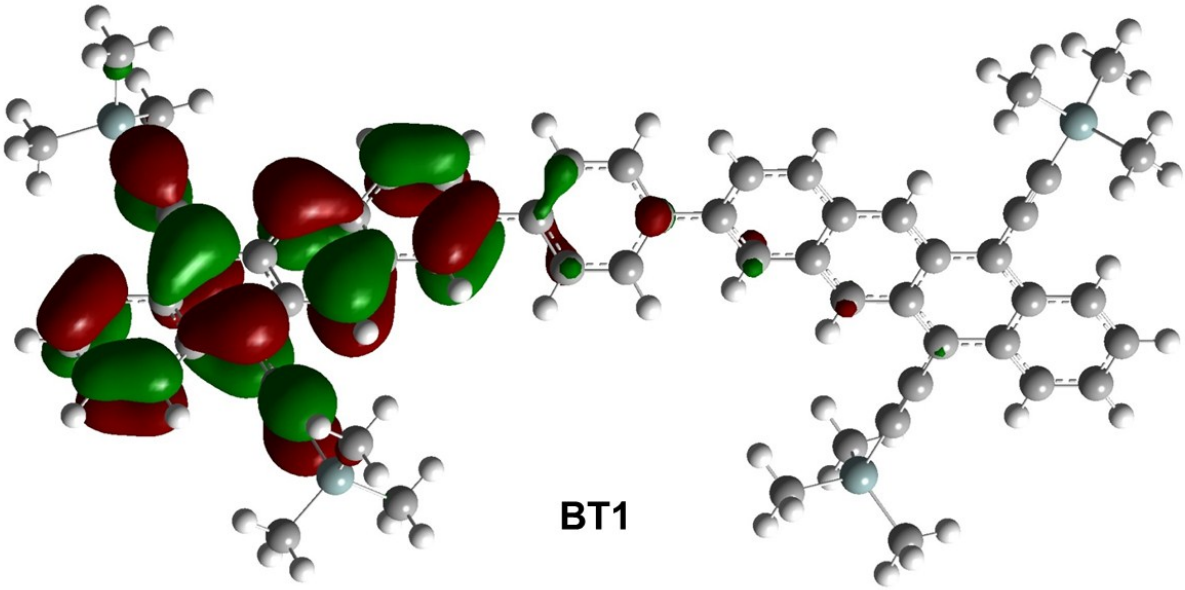


Figure S5: Zoom in of T_1 orbital of BT1

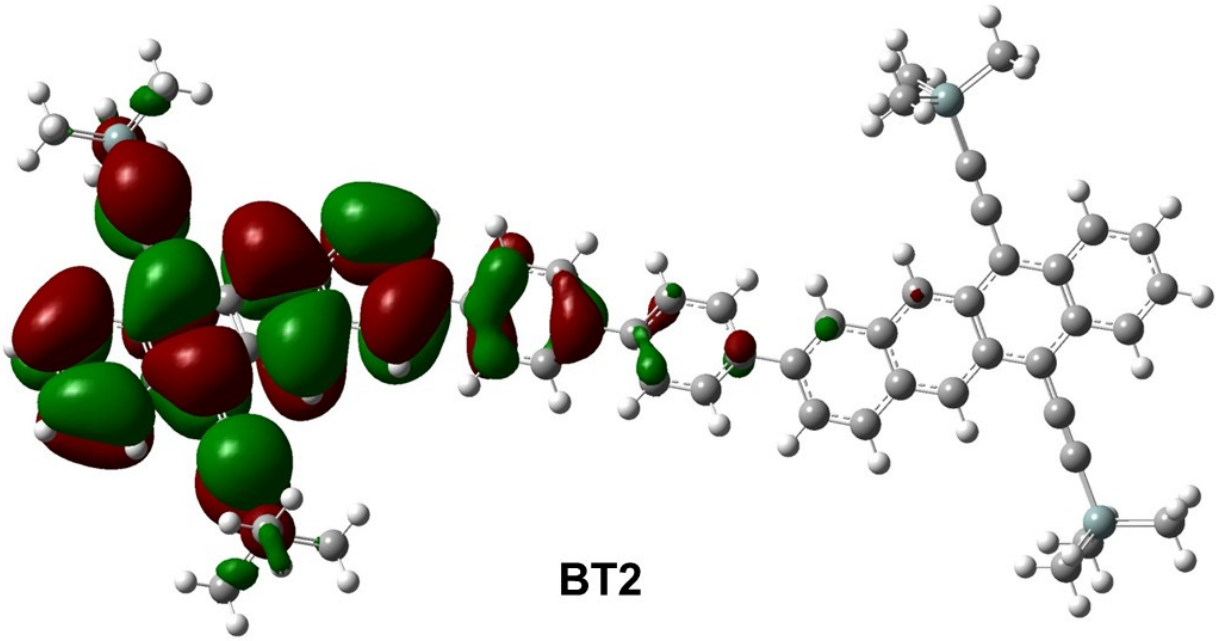


Figure S6: Zoom in of T_1 orbital of BT2

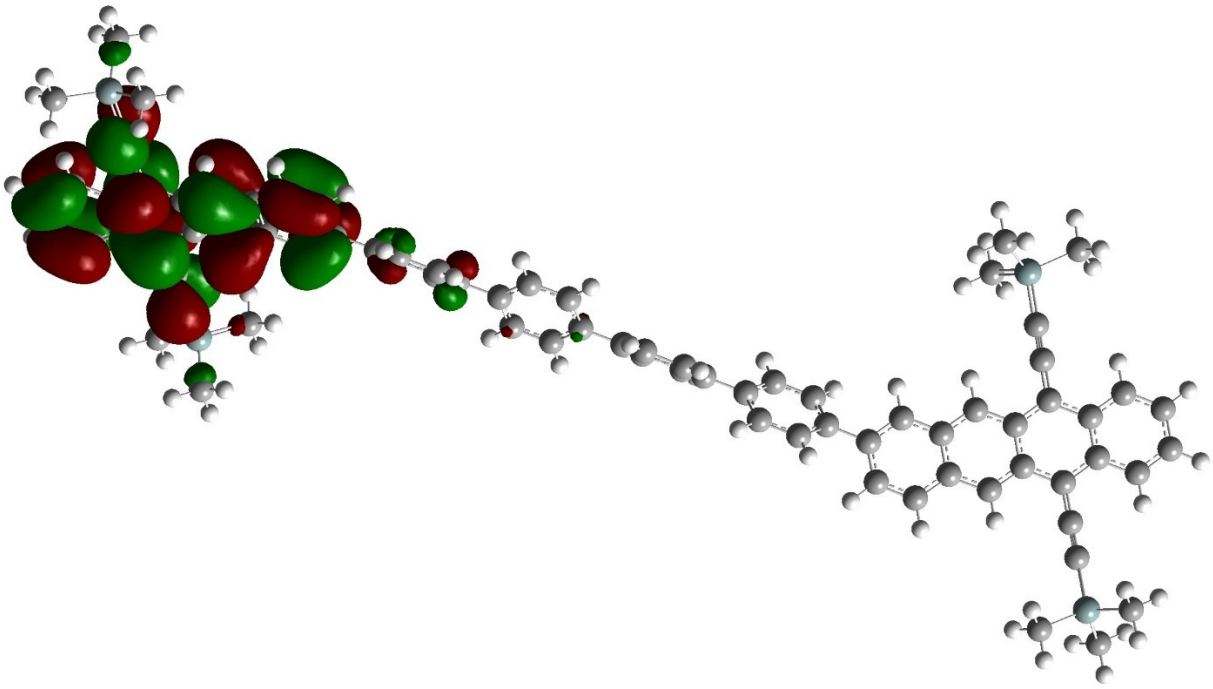


Figure S7: Zoom in of T_1 orbital of BT4

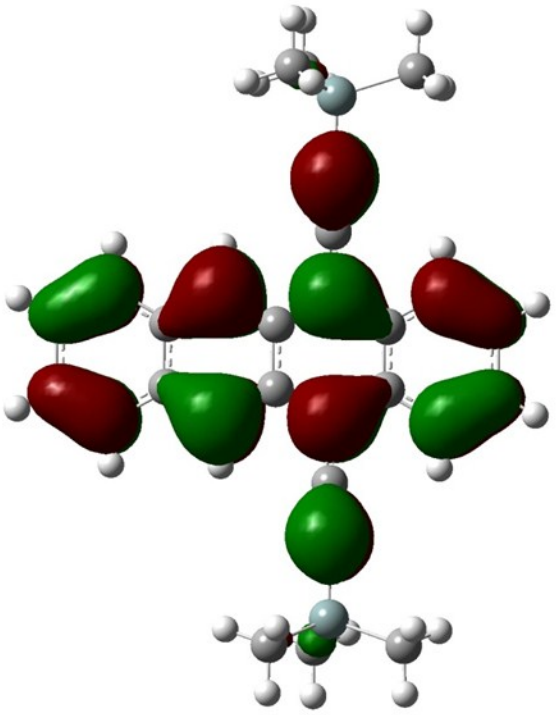


Figure S8: T_1 orbital of TIPS-Tc

Annihilator	T_1 Energy (eV)
TIPS-Tc	0.946
BT0	0.941
BT1	0.940
BT2	0.939
BT4	0.939

Table S1: Calculated T_1 energies of annihilators

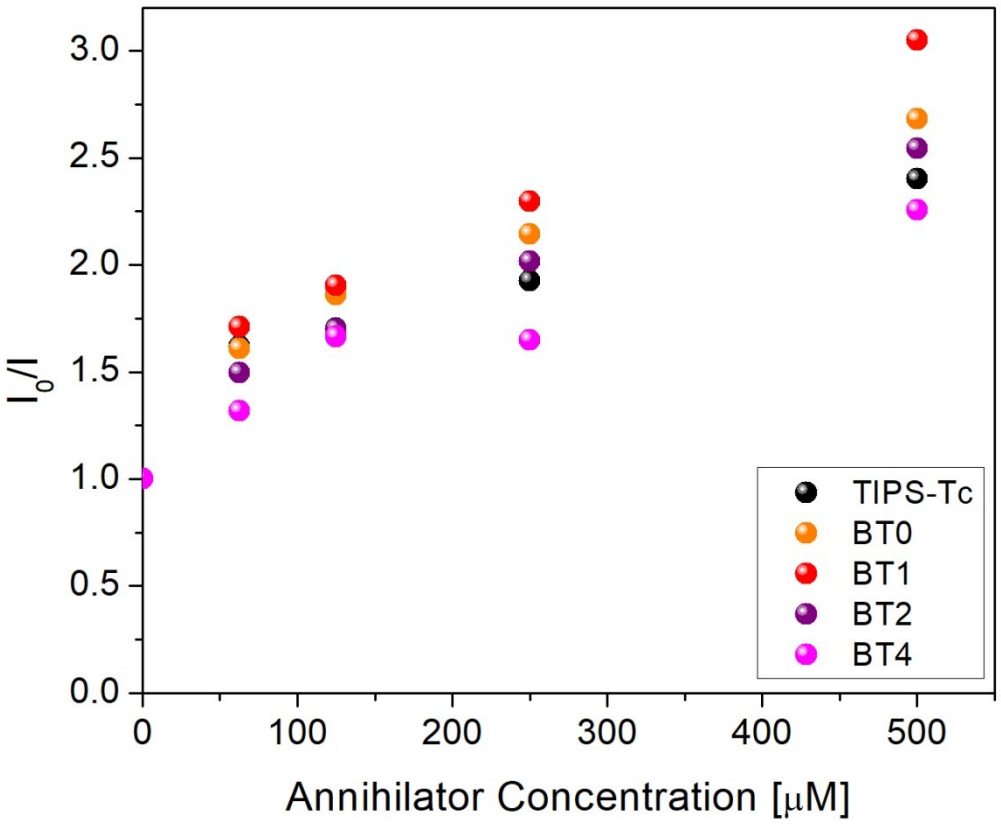


Figure S9: Stern-Volmer plot of PdPc quenching by annihilators used in this work

Annihilator	**K_{TET} ($M^{-1}*s^{-1}$)**
TIPS-Tc	$7.89*10^8$
BT0	$9.83*10^8$
BT1	$1.21*10^9$
BT2	$9.26*10^8$
BT4	$7.40*10^8$

Table S2: K_{TET} values for PdPc to annihilators studied, extracted from Stern-Volmer plot. Phosphoresence lifetime of PdPc is 3.04 μs.[2]

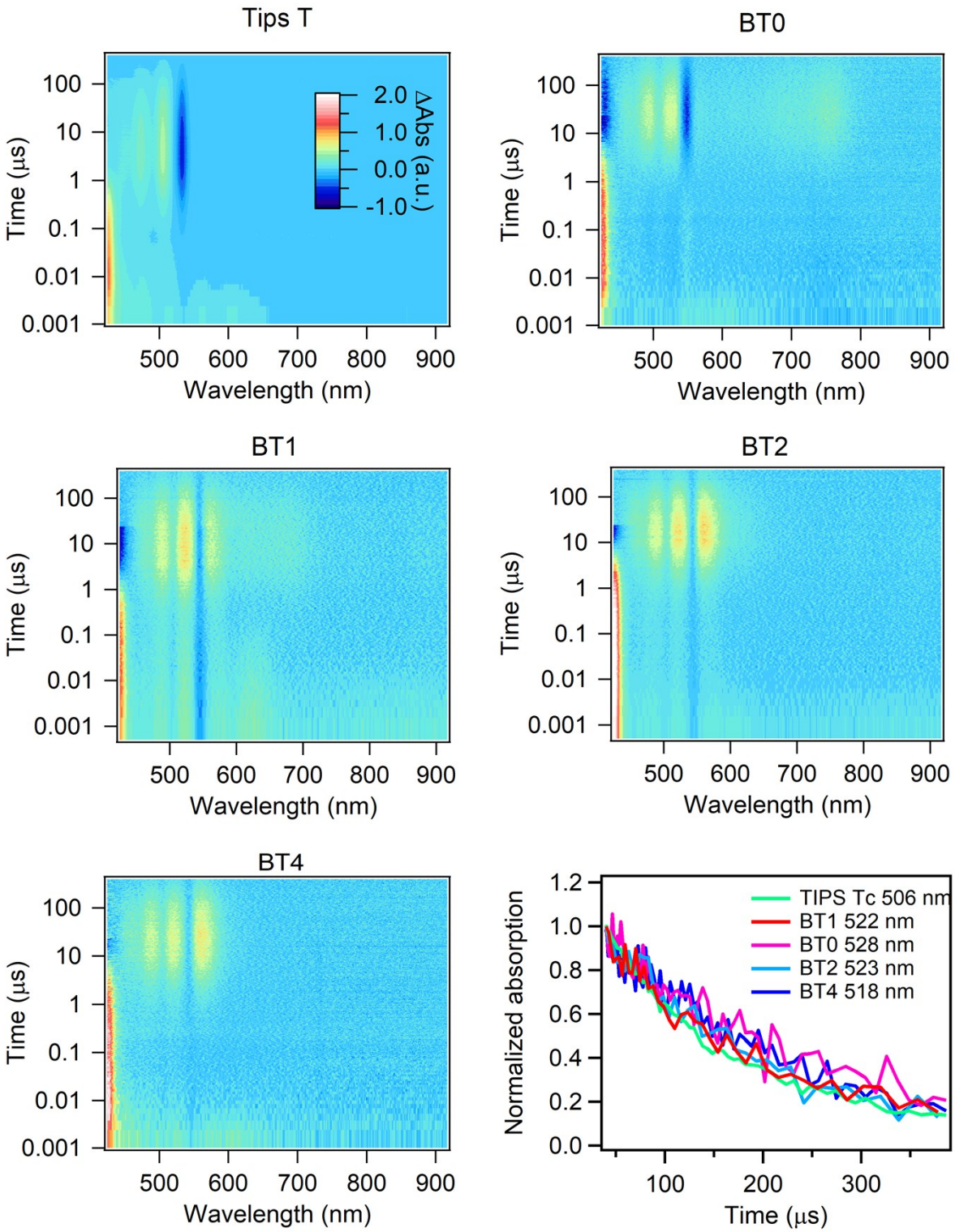


Figure S10: 2D transient absorption color plots of triplet sensitization experiments done on annihilators used in this work. Also included are kinetic traces of T1 decay, from which triplet lifetimes were extracted.

Anthracene was dissolved at ~15 mM in toluene along with the compound of interest (typically ~50 uM) and placed in a 1 mL cuvette. Argon flow was used to degas the solution, and 360 nm pump pulses (~25 μJ/cm2) were used to excite the anthracene. Anthracene undergoes intersystem crossing to produce a triplet absorption with a prominent peak near 415 nm which is quenched by transfer to the triplet state of the tetracene material. The excited state absorption was probed at the peak to extract kinetics of this state in each case. Because the kinetics at early times are convoluted by the signals from anthracene and the fact that rise of the signal via transfer occurs over several microseconds, the lifetimes of the triplet state are most clearly seen by fitting the data after anthracene decay is complete. By fitting the data after that decay is complete we obtained lifetimes for the triplet in each case. Overall these lifetimes are similar and suggest that the dynamics of an individual triplet is similar throughout these systems and not significantly altered by dimerization.

Annihilator	**T_1 Lifetime (μs)**
TIPS-Tc	119
BT0	233
BT1	118
BT2	150
BT4	250

Table S3: T_1 lifetimes of annihilators used in this work.

Annihilator	**PLQY**
TIPS-Tc	57.0%
BT0	0.3%
BT1	12.5%
BT2	10.1%
BT4	18.9%

Table S4: Photoluminescence quantum yields (PLQYs) of annihilators used in this work.

Annihilator	**Upconversion Yield**
TIPS-Tc	0.70%
BT0	N/A
BT1	4.2%
BT2	3.3%
BT4	0.33%

Table S5: Upconversion yields of annihilators used in this work.

Kinetic Modeling

To being we set the following equations:

$$\frac{d^3S^*}{dt} = 0 = {}^1S * k_\phi - k_{TET} * {}^3S^* * {}^1A - k_{Phos} * {}^3S^* - k_{TET2} * {}^3S^* * {}^3A^*$$

$$\frac{d^3A^*}{dt} = 0 = k_{TET} * {}^3S^* * {}^1A - k_{NR} * {}^3A^* - 2 * k_{TF} * ({}^3A^*)^2 - k_{TET2} * {}^3S^* * {}^3A^*$$

Where $^3S^*$ and $^3A^*$ are the concentration of the sensitizer and annihilator first excited state triplets, respectively, and ^1S and ^1A are the ground state singlets of sensitizer and annihilator respectively. Intersystem crossing of the sensitizer is assumed to be rapid. The final term $(k_{TET2})x(^3S^*)x(^3A^*)$ represents a second triplet added to a dimer which is already populated with one triplet which then proceeds to do triplet fusion, fluoresce, and return to the ground state, and is set to zero for TIPS-Tc. We can then plot the efficiency defined as:

$$eff = \frac{2 * k_{TF} * ({}^3A^*)^2 + 2 * k_{TET} * {}^3S^* * {}^3A^*}{{}^1S * k_\phi}$$

We note that this is certainly an over-simplification of the final TF process, but without a detailed spin dynamics study, we believe this to be a reasonable approximation. This leaves us with a single fit parameter k_{TF} for each material, with the following values for the remaining constants:

Rate	Value (TIPs;BT1;BT2;BT4)	Source
k_ϕ	Sets light intensity	Independent Variable
k_{TET}	(7.9; 12.1; 9.3; 7.4) *10^8 ($M^{-1}*S^{-1}$)	Stern-Volmer (Figure S9, Table S2)
k_{Phos}	3.3*10^5 (s^{-1})	Literature[2]
k_{TET2}	Same as k_{tet}	Stern-Volmer (Figure S9, Table S2)
k_{NR}	(8400; 8500; 6700; 4000) (s^{-1})	TA Measurements (Figure S10, Table S3)
k_{TF}	Fit	Fit

We assume the second triplet transfer rate to be equal to the initial triplet transfer. We can fit the data for TIPS, BT1, and BT2 as shown below. We were unable to adequately fit BT4, likely due to our simplistic iTF model approximations, and BT0 was not fit due to its ability to rapidly undergo singlet fission.

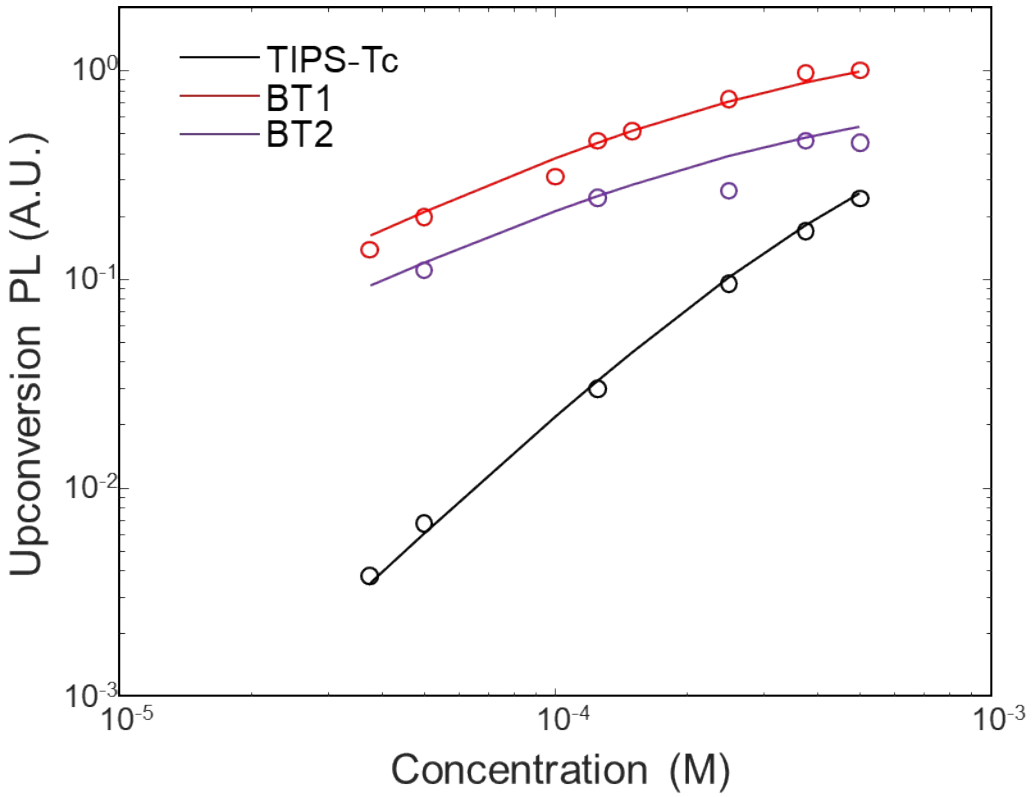


Figure S11: Kinetic modelling of our experimental data from main text Figure 4A (open circles), with solid fit lines for TIPS-Tc (black), BT1 (red) and BT2 (purple).

This fit yields the following values for k_{TF}:

Material	k_{TF} ($M^{-1}*s^{-1}$)
TIPS-Tc	$2.3*10^6$
BT1	$250*10^6$
BT2	$23*10^6$

Table S6: k_{TF} values extracted from fit lines in Figure S11

We can further model the performance of these systems using intensity dependence, observing a decent qualitative fit:

Material	Modelled Threshold (W/cm^2)	Experimental Threshold (W/cm^2)
TIPS-Tc	76.1	44.5
BT1	11.5	4.3
BT2	44.9	5.7

Table S7: Modelled threshold values from the fit in Figure S11. The threshold is defined as the power density where there is a transition between quadratic and linear dependence on UCPL.

DFT optimized coordinates

TIPS-Tc S_0

Atom	X	Y	Z
C	0.720605	-4.32611	0.001309
C	-0.70407	-4.32883	0.001223
C	-1.39736	-3.14962	0.001495
C	-0.71838	-1.89018	0.001903
C	0.725555	-1.88744	0.001794
C	1.409427	-3.14427	0.001566
C	-1.42832	-0.66668	0.002172
C	-0.72479	0.579729	0.001757
C	0.72259	0.582474	0.00178
C	1.430843	-0.66124	0.001727
C	-1.40521	1.811544	0.001103
C	-0.72926	3.030009	0.000788
C	0.717689	3.032761	0.0012
C	1.398242	1.816877	0.001621
C	-1.41778	4.286379	-5E-06
C	-0.72534	5.465513	-0.00016
C	0.704474	5.468233	0.000425
C	1.401406	4.29175	0.001041
C	2.852617	-0.65892	0.001162
C	-2.85009	-0.66928	0.002816
C	4.076389	-0.65363	0.000409
C	-4.07387	-0.66719	0.003253
Si	5.918169	-0.65515	-0.00138
Si	-5.91562	-0.66439	-0.00047
C	6.529365	0.235276	1.548758
C	6.517888	-2.44663	-0.00213
C	6.526164	0.235694	-1.55254
C	-6.53195	-0.723	1.7845
C	-6.51369	0.915514	-0.84645
C	-6.52025	-2.18188	-0.94944
H	1.259508	-5.26891	0.001101
H	-1.23936	-5.27369	0.000788
H	-2.48158	-3.1449	0.001107
H	2.493619	-3.13558	0.001547
H	-2.49029	1.804784	0.000568

H	2.483341	1.814126	0.001758
H	-2.50442	4.280984	-0.00061
H	-1.25857	6.411584	-0.00079
H	1.234103	6.416331	0.00031
H	2.48807	4.290537	0.001399
H	7.624847	0.253759	1.577851
H	6.17627	1.270978	1.580365
H	6.177923	-0.26489	2.456784
H	7.613003	-2.48747	-0.00308
H	6.162837	-2.985	-0.88676
H	6.164365	-2.98514	0.883028
H	6.172934	-0.26427	-2.45998
H	6.172895	1.271366	-1.58315
H	7.621583	0.254289	-1.58385
H	-7.62753	-0.71948	1.814788
H	-6.18526	-1.6271	2.295024
H	-6.17756	0.140177	2.356807
H	-7.60875	0.948293	-0.8757
H	-6.1489	0.976912	-1.87667
H	-6.16753	1.807769	-0.31476
H	-6.17449	-3.10891	-0.48076
H	-7.61551	-2.21004	-0.97722
H	-6.15874	-2.1742	-1.9826

TIPS-Tc T_1

Atom	X	Y	Z
C	0.693547	-4.35084	0.001314
C	-0.7004	-4.34973	0.001708
C	-1.39298	-3.13836	0.001941
C	-0.7147	-1.90962	0.001888
C	0.711723	-1.91076	0.001728
C	1.388045	-3.14057	0.00133
C	-1.43902	-0.64374	0.001761
C	-0.72572	0.60952	0.00168
C	0.726705	0.608366	0.001526
C	1.438034	-0.64604	0.001859
C	-1.39431	1.82936	0.001527
C	-0.71286	3.079324	0.001095
C	0.71775	3.078185	0.000698
C	1.397222	1.827143	0.000948
C	-1.39748	4.313818	0.000919
C	-0.69894	5.512062	0.000332
C	0.70774	5.510938	-0.00012
C	1.404356	4.311573	0.000063

C	2.842064	-0.65451	0.002104
C	-2.84306	-0.65016	0.001201
C	4.071483	-0.66456	0.001904
C	-4.07248	-0.65891	0.000432
Si	5.911734	-0.68122	-0.00063
Si	-5.91274	-0.6771	-0.00148
C	6.531606	-0.21807	1.723639
C	6.498426	-2.4172	-0.46056
C	6.528938	0.572946	-1.27228
C	-6.53462	0.211809	1.545842
C	-6.53103	0.205778	-1.5537
C	-6.49683	-2.4738	0.00169
H	1.243156	-5.28725	0.000925
H	-1.25151	-5.28526	0.001734
H	-2.47759	-3.13274	0.00211
H	2.472671	-3.13664	0.0008
H	-2.47975	1.828856	0.001674
H	2.482653	1.824957	0.000463
H	-2.48422	4.312348	0.001231
H	-1.23864	6.454301	0.00019
H	1.248962	6.452308	-0.00063
H	2.491093	4.308342	-0.00034
H	7.627271	-0.21868	1.753655
H	6.188742	0.779909	2.014678
H	6.174622	-0.92669	2.477647
H	7.593241	-2.46503	-0.47184
H	6.140343	-2.70675	-1.45362
H	6.139174	-3.16265	0.256207
H	6.170135	0.328546	-2.27707
H	6.188102	1.585332	-1.03276
H	7.624436	0.587114	-1.30096
H	-7.63034	0.221733	1.571721
H	-6.18179	-0.2837	2.45585
H	-6.1898	1.250338	1.576102
H	-7.62667	0.21496	-1.58262
H	-6.17539	-0.29272	-2.46098
H	-6.18672	1.244398	-1.58666
H	-6.13882	-3.00709	0.888197
H	-7.59156	-2.52423	0.000688
H	-6.13697	-3.01117	-0.88159

BT0 S_0

Atom	X	Y	Z
C	-10.5181	-0.83024	0.553284

C	-10.1267	-2.15621	0.8962
C	-8.8078	-2.5182	0.862009
C	-7.79198	-1.58402	0.484916
C	-8.18889	-0.24021	0.137229
C	-9.57873	0.094302	0.186308
C	-6.42588	-1.95032	0.449106
C	-5.42902	-0.99546	0.070759
C	-5.82777	0.351182	-0.27964
C	-7.21133	0.710877	-0.24055
C	-4.06302	-1.33141	0.031198
C	-3.08441	-0.40779	-0.33418
C	-3.48461	0.936932	-0.68229
C	-4.83326	1.277716	-0.64939
C	-1.69613	-0.74521	-0.36592
C	-0.72962	0.172975	-0.71244
C	-1.14697	1.506433	-1.0646
C	-2.46197	1.869664	-1.05141
C	-7.60105	2.035141	-0.58163
C	-6.03413	-3.27364	0.790493
C	-7.92978	3.176878	-0.87474
C	-5.69008	-4.41129	1.08218
Si	-8.41488	4.899242	-1.31228
Si	-5.15946	-6.12098	1.515965
C	-9.76255	4.835232	-2.63441
C	-9.05931	5.762909	0.239452
C	-6.89179	5.798754	-1.97624
C	-6.13556	-7.34757	0.46154
C	-3.31144	-6.28262	1.15849
C	-5.49793	-6.41909	3.350631
C	10.49621	0.826164	0.555697
C	10.10393	2.1517	0.899149
C	8.784949	2.513222	0.863934
C	7.769897	1.578828	0.485203
C	8.167601	0.235352	0.137298
C	9.55759	-0.09863	0.187317
C	6.403646	1.944712	0.448025
C	5.407443	0.989205	0.069896
C	5.806915	-0.35737	-0.28017
C	7.190618	-0.71612	-0.2415
C	4.041294	1.324295	0.030386
C	3.063128	0.400031	-0.33439
C	3.463907	-0.94477	-0.68168
C	4.812786	-1.28465	-0.64898
C	1.674729	0.736773	-0.36625
C	0.708513	-0.18194	-0.71214

C	1.126318	-1.51561	-1.06295
C	2.441491	-1.87824	-1.04959
C	7.583504	-2.03905	-0.58418
C	6.012695	3.26871	0.787761
C	7.921303	-3.17788	-0.87829
C	5.673508	4.40812	1.078311
Si	8.450714	-4.88779	-1.31269
Si	5.170063	6.125178	1.515878
C	7.476044	-6.11399	-0.25641
C	8.108642	-5.18629	-3.14673
C	10.2992	-5.04975	-0.95864
C	3.523277	6.057322	2.438957
C	6.505099	6.881709	2.617679
C	4.9872	7.130491	-0.07349
H	-11.5682	-0.55515	0.584113
H	-10.8816	-2.88114	1.185825
H	-8.50361	-3.52585	1.122166
H	-9.86991	1.10515	-0.07625
H	-3.76951	-2.34183	0.296194
H	-5.13489	2.286304	-0.91244
H	-1.41316	-1.7516	-0.07141
H	-0.3937	2.223252	-1.37498
H	-2.75586	2.877204	-1.33309
H	-10.0735	5.846765	-2.91966
H	-9.40881	4.326124	-3.53652
H	-10.6485	4.301798	-2.27541
H	-9.35727	6.793129	0.013549
H	-8.29321	5.798439	1.020467
H	-9.93135	5.24437	0.65046
H	-6.49291	5.300352	-2.86554
H	-7.14056	6.829388	-2.25345
H	-6.09482	5.837851	-1.22665
H	-5.84623	-8.37758	0.699489
H	-7.21251	-7.25438	0.634173
H	-5.95304	-7.1857	-0.60556
H	-2.95718	-7.29082	1.401426
H	-2.72696	-5.57183	1.751525
H	-3.09426	-6.09761	0.10158
H	-4.95154	-5.70547	3.975398
H	-6.56317	-6.3179	3.581512
H	-5.18602	-7.42858	3.641915
H	11.54633	0.551401	0.587403
H	10.8582	2.876697	1.190239
H	8.480255	3.52048	1.124983
H	9.849773	-1.10917	-0.07523

H	3.747461	2.334637	0.295359
H	5.115229	-2.29324	-0.91112
H	1.391322	1.743208	-0.07232
H	0.3733	-2.23314	-1.37229
H	2.735626	-2.88602	-1.33015
H	7.765494	-7.14407	-0.49389
H	7.659783	-5.95122	0.810337
H	6.398806	-6.02148	-0.4277
H	8.419764	-6.19595	-3.43828
H	8.654149	-4.47304	-3.77271
H	7.043086	-5.08487	-3.37606
H	10.51859	-4.86381	0.097613
H	10.65284	-6.05818	-1.20158
H	10.88266	-4.33922	-1.55296
H	3.196802	7.064682	2.721237
H	2.736729	5.612798	1.820678
H	3.605383	5.462442	3.354085
H	6.23694	7.905269	2.903091
H	7.471022	6.92086	2.103861
H	6.637454	6.301684	3.53653
H	4.224034	6.700802	-0.73015
H	4.693385	8.161902	0.152765
H	5.927734	7.164262	-0.63242

BT0 T_1

Atom	X	Y	Z
C	-10.544	-0.78487	0.512154
C	-10.1619	-2.10403	0.889752
C	-8.84422	-2.47191	0.87867
C	-7.82042	-1.55075	0.491429
C	-8.20785	-0.21364	0.109127
C	-9.59663	0.127386	0.134885
C	-6.45559	-1.92356	0.477925
C	-5.45076	-0.98198	0.087225
C	-5.83992	0.358768	-0.29542
C	-7.22206	0.725025	-0.27871
C	-4.08648	-1.32569	0.065217
C	-3.10008	-0.41518	-0.31316
C	-3.49042	0.92502	-0.68968
C	-4.8375	1.273114	-0.67422
C	-1.71434	-0.76127	-0.33164
C	-0.74086	0.143769	-0.69481
C	-1.14727	1.474948	-1.06737
C	-2.46032	1.846016	-1.06733

C	-7.6026	2.042928	-0.65316
C	-6.07328	-3.23994	0.854744
C	-7.92389	3.178982	-0.97518
C	-5.73817	-4.37166	1.178268
Si	-8.39951	4.892632	-1.45533
Si	-5.22409	-6.07243	1.663892
C	-9.72581	4.803294	-2.79745
C	-9.06804	5.787745	0.06817
C	-6.86503	5.777497	-2.11258
C	-6.21205	-7.32072	0.646628
C	-3.37744	-6.2633	1.313278
C	-5.56637	-6.31125	3.506445
C	10.54079	0.836238	0.535529
C	10.15543	2.125413	0.900972
C	8.805814	2.4776	0.881447
C	7.81654	1.557446	0.499591
C	8.21096	0.238679	0.125587
C	9.574261	-0.09397	0.15232
C	6.406005	1.925096	0.479915
C	5.403521	0.965694	0.087617
C	5.806573	-0.37772	-0.29151
C	7.200565	-0.73424	-0.27416
C	4.051881	1.29287	0.062049
C	3.042902	0.361597	-0.3197
C	3.441451	-0.96242	-0.68517
C	4.822493	-1.2917	-0.66338
C	1.677037	0.700836	-0.33921
C	0.692619	-0.22489	-0.69925
C	1.10538	-1.53111	-1.06158
C	2.441302	-1.88873	-1.05453
C	7.597181	-2.03008	-0.64503
C	6.025019	3.22547	0.848841
C	7.946686	-3.16291	-0.96958
C	5.696879	4.365066	1.17282
Si	8.472305	-4.85789	-1.45803
Si	5.218524	6.073895	1.662341
C	7.062291	-6.05917	-1.08508
C	8.863841	-4.86876	-3.30681
C	10.00861	-5.325	-0.46266
C	4.28868	6.003621	3.305703
C	6.790525	7.105769	1.846391
C	4.111458	6.806289	0.31749
H	-11.5932	-0.50506	0.524754
H	-10.923	-2.81923	1.187334
H	-8.54727	-3.4746	1.165001

H	-9.88056	1.133111	-0.15395
H	-3.80036	-2.33209	0.3527
H	-5.13176	2.277763	-0.9597
H	-1.43605	-1.76271	-0.01621
H	-0.3879	2.182778	-1.38391
H	-2.7468	2.850752	-1.36615
H	-10.032	5.80921	-3.10678
H	-9.35776	4.277129	-3.68392
H	-10.6176	4.276715	-2.44265
H	-9.36231	6.813066	-0.1834
H	-8.3142	5.839274	0.860128
H	-9.94647	5.277534	0.47597
H	-6.45284	5.261452	-2.98561
H	-7.10831	6.802683	-2.4138
H	-6.07981	5.83064	-1.35155
H	-5.92914	-8.34585	0.911802
H	-7.28774	-7.21522	0.82015
H	-6.03206	-7.18947	-0.42508
H	-3.03282	-7.26579	1.591213
H	-2.78667	-5.53803	1.882044
H	-3.15788	-6.11682	0.250842
H	-5.01417	-5.58386	4.109845
H	-6.63087	-6.19366	3.73292
H	-5.26354	-7.31411	3.828601
H	11.58838	0.551056	0.547122
H	10.89892	2.857673	1.200885
H	8.50178	3.479373	1.165018
H	9.869182	-1.09806	-0.13258
H	3.753065	2.297312	0.344663
H	5.123281	-2.29589	-0.94487
H	1.38961	1.702707	-0.03338
H	0.359179	-2.25261	-1.37843
H	2.73596	-2.89298	-1.34718
H	7.34284	-7.0821	-1.36082
H	6.808946	-6.05679	-0.02019
H	6.158467	-5.79885	-1.64539
H	9.183472	-5.86659	-3.62854
H	9.667139	-4.16525	-3.54757
H	7.986974	-4.58991	-3.89974
H	9.806577	-5.30361	0.612915
H	10.34465	-6.33567	-0.72107
H	10.83661	-4.63698	-0.6616
H	3.989488	7.009205	3.622813
H	3.383121	5.39378	3.226329
H	4.912261	5.573981	4.09603

H	6.547132	8.135302	2.13261
H	7.353185	7.143529	0.908148
H	7.44951	6.692224	2.616622
H	3.20166	6.212706	0.181913
H	3.809117	7.826625	0.57962
H	4.630761	6.846942	-0.64518

BT1 S_0

Atom	X	Y	Z
C	-12.3375	1.33996	-0.77721
C	-11.724	2.352374	-1.56961
C	-10.3656	2.375912	-1.73033
C	-9.52862	1.393691	-1.11273
C	-10.1506	0.367661	-0.3096
C	-11.5741	0.381275	-0.16917
C	-8.12312	1.41169	-1.27403
C	-7.30807	0.418588	-0.64296
C	-7.9325	-0.60973	0.162165
C	-9.35442	-0.62023	0.316574
C	-5.90782	0.414356	-0.78339
C	-5.10554	-0.54684	-0.16933
C	-5.73181	-1.57534	0.630882
C	-7.11597	-1.57928	0.775424
C	-3.6833	-0.55313	-0.31047
C	-2.89508	-1.50623	0.294576
C	-3.53548	-2.52389	1.087979
C	-4.89019	-2.55515	1.249274
C	-9.96609	-1.63303	1.105275
C	-7.51068	2.420079	-2.06737
C	-10.4868	-2.50801	1.784107
C	-6.97815	3.285079	-2.74995
Si	-11.2614	-3.83181	2.803935
Si	-6.17029	4.583238	-3.77717
C	-12.0925	-3.03983	4.304299
C	-12.5392	-4.74204	1.751023
C	-9.90793	-5.02536	3.362893
C	-6.85538	6.270102	-3.27285
C	-4.30753	4.516921	-3.46904
C	-6.54486	4.243146	-5.59733
C	12.32478	1.344815	0.779835
C	11.70908	2.354744	1.573691
C	10.35048	2.376271	1.732929
C	9.515528	1.394317	1.112045
C	10.13973	0.370709	0.307563

C	11.56342	0.386357	0.168827
C	8.109814	1.410233	1.271682
C	7.296646	0.418702	0.635784
C	7.923264	-0.60738	-0.17055
C	9.345514	-0.61712	-0.3214
C	5.896126	0.413718	0.772674
C	5.095513	-0.54594	0.154175
C	5.723863	-1.57227	-0.64719
C	7.108375	-1.57545	-0.78829
C	3.672997	-0.55285	0.292045
C	2.88628	-1.50459	-0.31701
C	3.528638	-2.52005	-1.11164
C	4.88372	-2.55053	-1.27006
C	9.960961	-1.6292	-1.1081
C	7.495923	2.41442	2.069244
C	10.48845	-2.50289	-1.78337
C	6.963348	3.275371	2.756895
Si	11.29179	-3.81725	-2.79339
Si	6.165021	4.569266	3.796781
C	10.34018	-4.00359	-4.41465
C	13.07672	-3.30305	-3.13755
C	11.25702	-5.43849	-1.82369
C	4.631108	5.208395	2.897354
C	5.680261	3.804221	5.454609
C	7.397653	5.976368	4.059932
C	-1.42092	-1.50403	0.142374
C	-0.69537	-2.705	0.064114
C	0.686812	-2.70463	-0.09113
C	1.411912	-1.50326	-0.16696
C	0.68587	-0.30183	-0.08914
C	-0.69539	-0.3022	0.065937
H	-13.4168	1.332006	-0.65728
H	-12.3406	3.10799	-2.04722
H	-9.89266	3.143876	-2.33204
H	-12.0348	-0.39196	0.435374
H	-5.44466	1.187352	-1.38784
H	-7.58707	-2.3494	1.377368
H	-3.23032	0.207637	-0.93981
H	-2.9168	-3.26128	1.589516
H	-5.35271	-3.32355	1.862843
H	-12.566	-3.80346	4.932006
H	-11.3662	-2.5013	4.921273
H	-12.8672	-2.32793	4.001849
H	-13.0179	-5.54081	2.328953
H	-12.0745	-5.19676	0.870428

H	-13.3249	-4.06438	1.402125
H	-9.15004	-4.51252	3.963813
H	-10.3301	-5.83093	3.974241
H	-9.40416	-5.4849	2.506428
H	-6.39441	7.067805	-3.86642
H	-7.93818	6.323428	-3.42514
H	-6.65572	6.479047	-2.21711
H	-3.78824	5.274777	-4.06649
H	-3.89436	3.53951	-3.73842
H	-4.07246	4.702479	-2.41607
H	-7.62167	4.26629	-5.79275
H	-6.07157	4.997248	-6.23652
H	-6.17092	3.261035	-5.90346
H	13.40417	1.338631	0.660932
H	12.32417	3.110209	2.053503
H	9.875961	3.142549	2.33559
H	12.02602	-0.38463	-0.43711
H	5.431472	1.185241	1.377809
H	7.58138	-2.34355	-1.39133
H	3.218422	0.206105	0.922427
H	2.911196	-3.25632	-1.61636
H	5.347682	-3.3172	-1.88472
H	10.79033	-4.78298	-5.03993
H	9.296558	-4.28097	-4.23476
H	10.34451	-3.07023	-4.98639
H	13.58915	-4.06194	-3.73965
H	13.64055	-3.17869	-2.20739
H	13.11937	-2.35625	-3.68528
H	11.79825	-5.34455	-0.87693
H	10.23152	-5.74438	-1.59335
H	11.72601	-6.24395	-2.40041
H	4.136338	5.989525	3.48566
H	4.891601	5.635783	1.923899
H	3.904521	4.407263	2.72789
H	5.198965	4.548668	6.099118
H	6.556567	3.417723	5.984605
H	4.978948	2.974677	5.319512
H	7.7067	6.417178	3.106784
H	6.952394	6.771932	4.668151
H	8.297675	5.626211	4.575559
H	-1.22201	-3.65359	0.104309
H	1.213826	-3.65295	-0.1328
H	1.212109	0.64469	-0.16648
H	-1.22198	0.644014	0.144566

BT1 T_1

Atom	X	Y	Z
C	-12.3461	1.398926	-0.78861
C	-11.7387	2.382291	-1.56839
C	-10.3528	2.383377	-1.7271
C	-9.54704	1.410127	-1.11531
C	-10.1686	0.404053	-0.3176
C	-11.5644	0.421874	-0.17171
C	-8.09857	1.411699	-1.28073
C	-7.28577	0.4096	-0.63707
C	-7.92016	-0.61525	0.174366
C	-9.35144	-0.61732	0.327414
C	-5.90137	0.39629	-0.77228
C	-5.07725	-0.58217	-0.14438
C	-5.70458	-1.59342	0.649016
C	-7.11835	-1.57639	0.785833
C	-3.67684	-0.588	-0.28709
C	-2.87764	-1.55719	0.326329
C	-3.51551	-2.55199	1.107532
C	-4.89	-2.56838	1.26457
C	-9.97144	-1.61037	1.104104
C	-7.49303	2.398618	-2.07546
C	-10.5164	-2.47899	1.781907
C	-6.96273	3.261048	-2.77284
Si	-11.333	-3.78155	2.793922
Si	-6.16281	4.543492	-3.82341
C	-12.7348	-2.99075	3.783829
C	-12.0194	-5.11235	1.641112
C	-10.0498	-4.5284	3.962427
C	-7.26196	6.079772	-3.84831
C	-4.47445	4.961213	-3.08453
C	-5.95738	3.860563	-5.57345
C	12.32689	1.372894	0.770556
C	11.70798	2.379294	1.566382
C	10.34979	2.393028	1.730012
C	9.518515	1.406251	1.111869
C	10.14599	0.386104	0.305541
C	11.56908	0.409998	0.162091
C	8.113214	1.414308	1.27578
C	7.303748	0.417967	0.642693
C	7.933734	-0.60522	-0.1647
C	9.355455	-0.60657	-0.32049
C	5.903654	0.405523	0.783306
C	5.106656	-0.55929	0.168132

C	5.738519	-1.58364	-0.63305
C	7.12256	-1.57896	-0.77846
C	3.684552	-0.57328	0.309074
C	2.901535	-1.53074	-0.29595
C	3.547433	-2.545	-1.08924
C	4.902235	-2.56818	-1.25124
C	9.974126	-1.61481	-1.10959
C	7.496119	2.415103	2.075124
C	10.50441	-2.48482	-1.78742
C	6.960792	3.272922	2.764551
Si	11.312	-3.79276	-2.80241
Si	6.158799	4.562012	3.807624
C	10.36014	-3.97679	-4.42378
C	13.09481	-3.27074	-3.14579
C	11.28376	-5.41752	-1.83844
C	4.62378	5.199961	2.909268
C	5.675002	3.791177	5.463054
C	7.388016	5.971228	4.075307
C	-1.40531	-1.54903	0.167016
C	-0.67371	-2.74704	0.093332
C	0.708178	-2.74074	-0.06094
C	1.427641	-1.53601	-0.14327
C	0.695728	-0.33781	-0.07277
C	-0.68574	-0.34396	0.080831
H	-13.424	1.388275	-0.65793
H	-12.3371	3.147717	-2.0531
H	-9.87566	3.146452	-2.33251
H	-12.0326	-0.34474	0.436084
H	-5.42898	1.16263	-1.3786
H	-7.59279	-2.34273	1.390581
H	-3.21686	0.168766	-0.91615
H	-2.91074	-3.29614	1.615934
H	-5.3573	-3.33396	1.878171
H	-13.2473	-3.74151	4.396044
H	-12.3567	-2.21214	4.453881
H	-13.4792	-2.53276	3.124597
H	-12.5148	-5.90378	2.215288
H	-11.2225	-5.57451	1.049971
H	-12.753	-4.69442	0.944379
H	-9.63138	-3.76783	4.629227
H	-10.5008	-5.30889	4.585742
H	-9.22164	-4.98172	3.408128
H	-6.81424	6.864626	-4.46849
H	-8.25215	5.855349	-4.25784
H	-7.39954	6.486074	-2.84128

H	-3.96838	5.726436	-3.68404
H	-3.82513	4.080381	-3.05138
H	-4.57179	5.34481	-2.06396
H	-6.92461	3.597133	-6.013
H	-5.48338	4.603779	-6.22486
H	-5.33208	2.962178	-5.57868
H	13.4059	1.372933	0.648127
H	12.32027	3.138303	2.044173
H	9.872809	3.156601	2.334156
H	12.03416	-0.35837	-0.44527
H	5.436396	1.175261	1.38871
H	7.598195	-2.34521	-1.38179
H	3.227217	0.184847	0.938463
H	2.932741	-3.28602	-1.59034
H	5.368897	-3.33371	-1.86528
H	10.81288	-4.75211	-5.05224
H	9.31768	-4.25878	-4.24431
H	10.36058	-3.04128	-4.99202
H	13.60979	-4.02583	-3.75047
H	13.65863	-3.14708	-2.21553
H	13.13359	-2.32213	-3.69068
H	11.82538	-5.32504	-0.89175
H	10.25954	-5.72794	-1.60845
H	11.75522	-6.2192	-2.4184
H	4.126726	5.978057	3.499666
H	4.883673	5.630937	1.937236
H	3.899307	4.397506	2.737034
H	5.191865	4.53278	6.109464
H	6.551889	3.405015	5.992331
H	4.975469	2.960562	5.325312
H	7.696501	6.415436	3.123554
H	6.940621	6.764054	4.685529
H	8.288584	5.621694	4.590403
H	-1.19716	-3.69726	0.135885
H	1.239775	-3.68665	-0.09915
H	1.217264	0.610736	-0.15673
H	-1.21587	0.60091	0.151688

BT2 S_0

Atom	X	Y	Z
C	-14.7002	-1.11635	0.461266
C	-14.1986	-2.39816	0.828158
C	-12.8509	-2.63121	0.854099
C	-11.914	-1.60406	0.516353

C	-12.4225	-0.30497	0.144202
C	-13.839	-0.10586	0.131148
C	-10.519	-1.83788	0.540132
C	-9.60282	-0.79361	0.195572
C	-10.1131	0.508522	-0.17821
C	-11.5253	0.734682	-0.19743
C	-8.21098	-0.99968	0.207806
C	-7.31075	0.008973	-0.13329
C	-7.82205	1.309809	-0.50292
C	-9.19727	1.52364	-0.5158
C	-5.89714	-0.20026	-0.12575
C	-5.01058	0.796733	-0.46559
C	-5.53667	2.087484	-0.82949
C	-6.87933	2.331368	-0.84759
C	-12.0264	2.014141	-0.5635
C	-10.0175	-3.11718	0.905074
C	-12.4556	3.116122	-0.8781
C	-9.57873	-4.21628	1.216711
Si	-13.1143	4.771948	-1.3445
Si	-8.90496	-5.86747	1.677103
C	-13.1462	4.908214	-3.22852
C	-14.8613	4.94027	-0.6456
C	-11.9887	6.10027	-0.61108
C	-9.53748	-7.14934	0.441745
C	-7.01862	-5.78075	1.616322
C	-9.48265	-6.29906	3.423243
C	14.69749	1.124745	0.433066
C	14.19566	2.407096	0.797732
C	12.84775	2.638762	0.827717
C	11.91101	1.609438	0.496167
C	12.4197	0.309772	0.126382
C	13.8364	0.112166	0.109131
C	10.51581	1.841682	0.524271
C	9.599724	0.795941	0.183824
C	10.11023	-0.50687	-0.18729
C	11.52255	-0.73214	-0.20835
C	8.207806	1.000952	0.197771
C	7.307609	-0.00904	-0.13932
C	7.819144	-1.31065	-0.50583
C	9.194478	-1.52359	-0.5202
C	5.893928	0.199489	-0.13094
C	5.007478	-0.79892	-0.46685
C	5.533765	-2.09058	-0.82716
C	6.876542	-2.33379	-0.84613
C	12.02358	-2.01343	-0.56796

C	10.01466	3.120337	0.892037
C	12.45196	-3.11773	-0.87556
C	9.577656	4.21866	1.208959
Si	13.10714	-4.7784	-1.32947
Si	8.919315	5.869716	1.691953
C	12.22205	-6.08414	-0.28977
C	12.7896	-5.07799	-3.16773
C	14.96181	-4.81061	-0.97258
C	7.791091	5.656491	3.1925
C	10.37246	6.99688	2.121851
C	7.944085	6.583935	0.239494
C	-3.54683	0.564722	-0.46307
C	-2.64752	1.578528	-0.09008
C	-1.27424	1.358302	-0.08262
C	-0.73338	0.114869	-0.45102
C	-1.63235	-0.89849	-0.826
C	-3.0049	-0.67827	-0.83433
C	0.730183	-0.11785	-0.45126
C	1.628629	0.893915	-0.83179
C	3.001207	0.673885	-0.84042
C	3.543668	-0.56731	-0.46399
C	2.644905	-1.5796	-0.08564
C	1.271583	-1.35954	-0.07781
H	-15.7722	-0.94361	0.444621
H	-14.8923	-3.19219	1.088005
H	-12.4626	-3.60456	1.132299
H	-14.2146	0.871858	-0.14901
H	-7.83366	-1.97739	0.488859
H	-9.58303	2.498817	-0.7945
H	-5.52809	-1.17377	0.184125
H	-4.8438	2.86971	-1.12295
H	-7.25602	3.308452	-1.13786
H	-13.5347	5.884672	-3.53962
H	-12.1432	4.796078	-3.6525
H	-13.7838	4.136551	-3.67133
H	-15.2864	5.91917	-0.89483
H	-14.8627	4.842588	0.444674
H	-15.5287	4.173417	-1.0518
H	-11.943	6.023226	0.479861
H	-10.9673	6.015404	-0.99561
H	-12.3579	7.10122	-0.86187
H	-9.15267	-8.1458	0.687157
H	-10.6309	-7.20227	0.446048
H	-9.21888	-6.90819	-0.57734
H	-6.57749	-6.74787	1.88292

H	-6.63161	-5.03281	2.315804
H	-6.66592	-5.51788	0.613807
H	-9.13805	-5.55634	4.149701
H	-10.5748	-6.34339	3.483131
H	-9.0903	-7.27561	3.729057
H	15.76961	0.953263	0.413071
H	14.88935	3.202769	1.052597
H	12.45958	3.612664	1.104142
H	14.21227	-0.86592	-0.16948
H	7.830585	1.979296	0.476668
H	9.580451	-2.49926	-0.79682
H	5.524603	1.173771	0.176213
H	4.840897	-2.87406	-1.11731
H	7.253408	-3.31155	-1.1339
H	12.58445	-7.08801	-0.53892
H	12.39295	-5.92136	0.779109
H	11.14107	-6.06685	-0.4616
H	13.16888	-6.06057	-3.47093
H	13.28628	-4.32175	-3.78383
H	11.71997	-5.04639	-3.39834
H	15.16529	-4.62034	0.086079
H	15.38731	-5.78858	-1.22465
H	15.49404	-4.05404	-1.55808
H	7.382504	6.622419	3.510776
H	6.94857	4.995087	2.966448
H	8.334685	5.226598	4.039748
H	10.01629	7.990667	2.415812
H	11.04565	7.122142	1.267726
H	10.95706	6.591667	2.953953
H	7.107149	5.933935	-0.03508
H	7.534164	7.567731	0.495099
H	8.577865	6.70365	-0.64488
H	-3.02978	2.541857	0.233611
H	-0.61107	2.152968	0.245698
H	-1.24701	-1.85911	-1.15427
H	-3.66799	-1.46971	-1.1699
H	1.242765	1.852911	-1.16417
H	3.663873	1.46379	-1.18042
H	3.027685	-2.54141	0.24195
H	0.608867	-2.1528	0.254766

BT2 T_1

Atom	X	Y	Z
C	-14.715	-1.09014	0.440732

C	-14.2196	-2.3738	0.809541
C	-12.8729	-2.61218	0.839717
C	-11.931	-1.58884	0.504512
C	-12.4332	-0.28788	0.130397
C	-13.8488	-0.08316	0.112964
C	-10.537	-1.82817	0.532744
C	-9.61566	-0.78801	0.189367
C	-10.1196	0.516167	-0.18585
C	-11.5308	0.748168	-0.20865
C	-8.22476	-1.00004	0.204192
C	-7.31953	0.004735	-0.1351
C	-7.82454	1.307903	-0.50522
C	-9.19881	1.5275	-0.52116
C	-5.90686	-0.2106	-0.12522
C	-5.01543	0.782901	-0.4625
C	-5.53523	2.076208	-0.82633
C	-6.8768	2.325719	-0.84721
C	-12.0257	2.029811	-0.57546
C	-10.042	-3.10869	0.902318
C	-12.4499	3.133714	-0.89028
C	-9.6099	-4.20893	1.219338
Si	-13.1018	4.792513	-1.35558
Si	-8.953	-5.86382	1.690949
C	-13.131	4.93142	-3.23944
C	-14.849	4.96607	-0.65839
C	-11.9724	6.115733	-0.61892
C	-10.0736	-7.19351	0.952829
C	-7.20233	-6.03128	1.000353
C	-8.92925	-5.99805	3.575104
C	14.72787	1.180943	0.411771
C	14.2303	2.432752	0.771412
C	12.85232	2.64698	0.806874
C	11.94597	1.624067	0.486097
C	12.45507	0.343403	0.118008
C	13.84491	0.149924	0.089365
C	10.50603	1.848378	0.522401
C	9.58981	0.788683	0.1809
C	10.10929	-0.51556	-0.19359
C	11.53189	-0.73409	-0.21987
C	8.21257	0.981969	0.19899
C	7.287497	-0.0471	-0.14109
C	7.8007	-1.33176	-0.50403
C	9.207809	-1.52651	-0.51922
C	5.895439	0.160147	-0.12597
C	4.995006	-0.85555	-0.46025

C	5.520175	-2.12264	-0.81443
C	6.884299	-2.35339	-0.83508
C	12.04071	-1.99481	-0.57407
C	10.01054	3.109214	0.89265
C	12.48903	-3.09727	-0.88159
C	9.577078	4.212592	1.218223
Si	13.1647	-4.74802	-1.33583
Si	8.923084	5.860848	1.711742
C	12.29856	-6.06689	-0.296
C	12.84834	-5.05451	-3.17367
C	15.02045	-4.75724	-0.98268
C	7.799044	5.64314	3.215313
C	10.37867	6.984808	2.141929
C	7.941917	6.584945	0.267618
C	-3.55272	0.544683	-0.45745
C	-2.65003	1.553658	-0.07953
C	-1.27773	1.327757	-0.06987
C	-0.74111	0.083298	-0.44128
C	-1.64358	-0.92527	-0.82101
C	-3.01519	-0.69946	-0.83128
C	0.721334	-0.15525	-0.44046
C	1.624746	0.855822	-0.81058
C	2.996611	0.631093	-0.81625
C	3.533588	-0.61594	-0.45036
C	2.629573	-1.62659	-0.07873
C	1.257452	-1.40174	-0.07393
H	-15.7862	-0.91319	0.42069
H	-14.9173	-3.16504	1.067343
H	-12.4894	-3.58707	1.119092
H	-14.2197	0.895935	-0.1687
H	-7.85233	-1.97951	0.485624
H	-9.57985	2.504329	-0.80056
H	-5.54249	-1.18599	0.184313
H	-4.83837	2.855706	-1.11763
H	-7.24877	3.30456	-1.13765
H	-13.5151	5.909952	-3.54959
H	-12.1281	4.815614	-3.66251
H	-13.7715	4.16311	-3.68402
H	-15.2706	5.946694	-0.90683
H	-14.8519	4.867046	0.431761
H	-15.5186	4.201942	-1.06616
H	-11.928	6.036627	0.47193
H	-10.9508	6.027996	-1.00258
H	-12.3379	7.118382	-0.86831
H	-9.70703	-8.19403	1.209108

H	-11.0979	-7.10669	1.329216
H	-10.1109	-7.11933	-0.13864
H	-6.7778	-7.00991	1.251578
H	-6.53728	-5.26415	1.410064
H	-7.19594	-5.9337	-0.08994
H	-8.29501	-5.2247	4.019903
H	-9.93434	-5.88725	3.994316
H	-8.54032	-6.97346	3.88903
H	15.79845	1.002563	0.38085
H	14.90813	3.242401	1.024235
H	12.46056	3.619155	1.085871
H	14.22783	-0.82534	-0.19107
H	7.826368	1.956686	0.479603
H	9.596305	-2.50125	-0.79685
H	5.519828	1.132414	0.179864
H	4.839597	-2.91688	-1.10427
H	7.265272	-3.33004	-1.12145
H	12.67398	-7.06543	-0.54742
H	12.4691	-5.90346	0.772821
H	11.21717	-6.06379	-0.46608
H	13.23741	-6.0339	-3.47498
H	13.33661	-4.29455	-3.79188
H	11.77819	-5.03444	-3.40317
H	15.22392	-4.56596	0.075781
H	15.45756	-5.72946	-1.23712
H	15.54188	-3.99324	-1.56826
H	7.392043	6.608465	3.537562
H	6.95542	4.983004	2.989673
H	8.344876	5.210415	4.059647
H	10.0241	7.977259	2.442272
H	11.04873	7.114105	1.285955
H	10.96613	6.575055	2.969768
H	7.103919	5.936807	-0.00811
H	7.532978	7.566874	0.531984
H	8.572147	6.711027	-0.61839
H	-3.02907	2.51755	0.24628
H	-0.61215	2.118675	0.262541
H	-1.26162	-1.88641	-1.1517
H	-3.68089	-1.48714	-1.17051
H	1.243704	1.81912	-1.13594
H	3.661906	1.422607	-1.14732
H	3.009051	-2.59062	0.24604
H	0.591057	-2.1943	0.252913

BT4 S_0

Atom	X	Y	Z
C	18.8907	-1.1159	1.062595
C	18.30392	-2.1958	1.782806
C	16.94457	-2.34578	1.817708
C	16.07968	-1.43094	1.13803
C	16.67472	-0.33681	0.407695
C	18.10026	-0.21828	0.398464
C	14.67292	-1.57897	1.169836
C	13.83008	-0.64923	0.481294
C	14.42764	0.447493	-0.25063
C	15.85076	0.587551	-0.27692
C	12.42819	-0.77188	0.49647
C	11.59916	0.130504	-0.16925
C	12.19859	1.222863	-0.90269
C	13.584	1.352728	-0.92248
C	10.17519	0.006997	-0.15758
C	9.361106	0.897242	-0.82115
C	9.975004	1.979844	-1.54653
C	11.33015	2.135587	-1.58344
C	16.43656	1.66398	-0.99812
C	14.08731	-2.65571	1.890237
C	16.93683	2.5912	-1.62067
C	13.57995	-3.58083	2.51028
Si	17.69343	3.985163	-2.55721
Si	12.81655	-4.96865	3.450422
C	16.67512	5.545773	-2.24544
C	19.46502	4.228987	-1.94868
C	17.68806	3.557263	-4.39746
C	13.48222	-4.93968	5.218384
C	10.94217	-4.73234	3.452994
C	13.26568	-6.59913	2.608597
C	-18.8861	1.095292	1.097968
C	-18.2962	2.143507	1.861106
C	-16.9362	2.28424	1.906605
C	-16.0738	1.391287	1.195263
C	-16.672	0.329331	0.421293
C	-18.0981	0.219392	0.40265
C	-14.6665	1.530581	1.237196
C	-13.8263	0.625119	0.51399
C	-14.4268	-0.44007	-0.26086
C	-15.8505	-0.57229	-0.29596
C	-12.4241	0.742361	0.534944
C	-11.5976	-0.13634	-0.16457
C	-12.1997	-1.19844	-0.93906

C	-13.5856	-1.3224	-0.96561
C	-10.1734	-0.01666	-0.14836
C	-9.36129	-0.883	-0.84515
C	-9.97766	-1.93654	-1.61025
C	-11.3332	-2.08742	-1.65309
C	-16.4396	-1.61663	-1.06034
C	-14.0779	2.574067	2.002735
C	-16.9443	-2.51493	-1.7206
C	-13.5685	3.46993	2.662794
Si	-17.7086	-3.8608	-2.71906
Si	-12.8057	4.818459	3.659011
C	-18.3732	-5.18695	-1.54935
C	-19.1154	-3.1284	-3.74591
C	-16.3877	-4.5918	-3.8549
C	-11.024	5.061949	3.080479
C	-13.8003	6.402597	3.393687
C	-12.8386	4.322091	5.481748
C	7.885526	0.760209	-0.8048
C	7.112562	1.087951	-1.932
C	5.72856	0.953242	-1.92177
C	5.049368	0.489508	-0.78242
C	5.821967	0.163869	0.345752
C	7.206002	0.297499	0.335439
C	3.573503	0.353926	-0.77261
C	2.754706	1.269876	-1.45493
C	1.370226	1.140912	-1.45315
C	0.736736	0.089338	-0.76903
C	1.555211	-0.82454	-0.08351
C	2.940097	-0.6954	-0.08519
C	-0.73893	-0.05131	-0.77406
C	-1.4965	0.273728	-1.91205
C	-2.8807	0.141468	-1.91963
C	-3.5747	-0.32453	-0.79005
C	-2.81733	-0.64972	0.34815
C	-1.43294	-0.51553	0.356226
C	-5.05007	-0.46859	-0.80125
C	-5.82004	-0.1935	0.342033
C	-7.20359	-0.33164	0.330717
C	-7.8855	-0.74718	-0.826
C	-7.11507	-1.02646	-1.96774
C	-5.73128	-0.88875	-1.9561
H	19.97101	-1.00739	1.042791
H	18.9418	-2.90195	2.306009
H	16.49231	-3.16565	2.364333
H	18.54048	0.606183	-0.1511

H	11.98557	-1.59596	1.046393
H	14.03477	2.173645	-1.47046
H	9.74069	-0.83597	0.372237
H	9.336738	2.700368	-2.04808
H	11.77293	2.966824	-2.12554
H	17.10139	6.400327	-2.78315
H	15.64084	5.421829	-2.58233
H	16.6517	5.797441	-1.18044
H	19.94889	5.052424	-2.48612
H	20.06731	3.328413	-2.10618
H	19.48967	4.466161	-0.88032
H	18.26245	2.64672	-4.59535
H	16.66986	3.395796	-4.76548
H	18.13238	4.369103	-4.98461
H	13.04799	-5.75373	5.809955
H	14.57043	-5.05764	5.235244
H	13.24075	-3.99598	5.717584
H	10.45105	-5.53977	4.007843
H	10.5402	-4.73473	2.434661
H	10.66139	-3.78452	3.923331
H	12.89531	-6.62874	1.579002
H	14.3498	-6.74767	2.578046
H	12.82626	-7.44587	3.148229
H	-19.9669	0.993855	1.069962
H	-18.9322	2.832841	2.408496
H	-16.4813	3.080134	2.485573
H	-18.5408	-0.58041	-0.18033
H	-11.9792	1.5434	1.116166
H	-14.0386	-2.11947	-1.54603
H	-9.73716	0.805317	0.412065
H	-9.34111	-2.63917	-2.13865
H	-11.778	-2.89634	-2.22643
H	-18.8368	-6.00391	-2.11411
H	-17.5721	-5.61357	-0.93757
H	-19.129	-4.77701	-0.87185
H	-19.594	-3.90399	-4.35464
H	-18.748	-2.34988	-4.42199
H	-19.885	-2.6818	-3.10821
H	-15.9788	-3.83098	-4.52743
H	-15.5568	-5.01489	-3.28104
H	-16.8087	-5.393	-4.47279
H	-10.5375	5.86093	3.651477
H	-10.4335	4.149771	3.214316
H	-10.9834	5.335244	2.021277
H	-13.371	7.230558	3.96919

H	-14.8406	6.279076	3.711616
H	-13.8058	6.694721	2.338814
H	-12.2796	3.396433	5.651718
H	-12.39	5.104723	6.104241
H	-13.8634	4.161815	5.83148
H	7.604764	1.41745	-2.84193
H	5.166861	1.179874	-2.82293
H	5.327238	-0.16069	1.256214
H	7.768593	0.075487	1.237136
H	3.208189	2.114643	-1.96455
H	0.767701	1.887948	-1.96097
H	1.101894	-1.66931	0.426307
H	3.542883	-1.44199	0.423129
H	-0.99177	0.61789	-2.80966
H	-3.4352	0.420135	-2.81058
H	-3.31889	-1.0296	1.233153
H	-0.88132	-0.75917	1.259263
H	-5.32826	0.147755	1.248002
H	-7.76574	-0.13094	1.237688
H	-7.60761	-1.33792	-2.88382
H	-5.16699	-1.13022	-2.85174

BT4 T_1

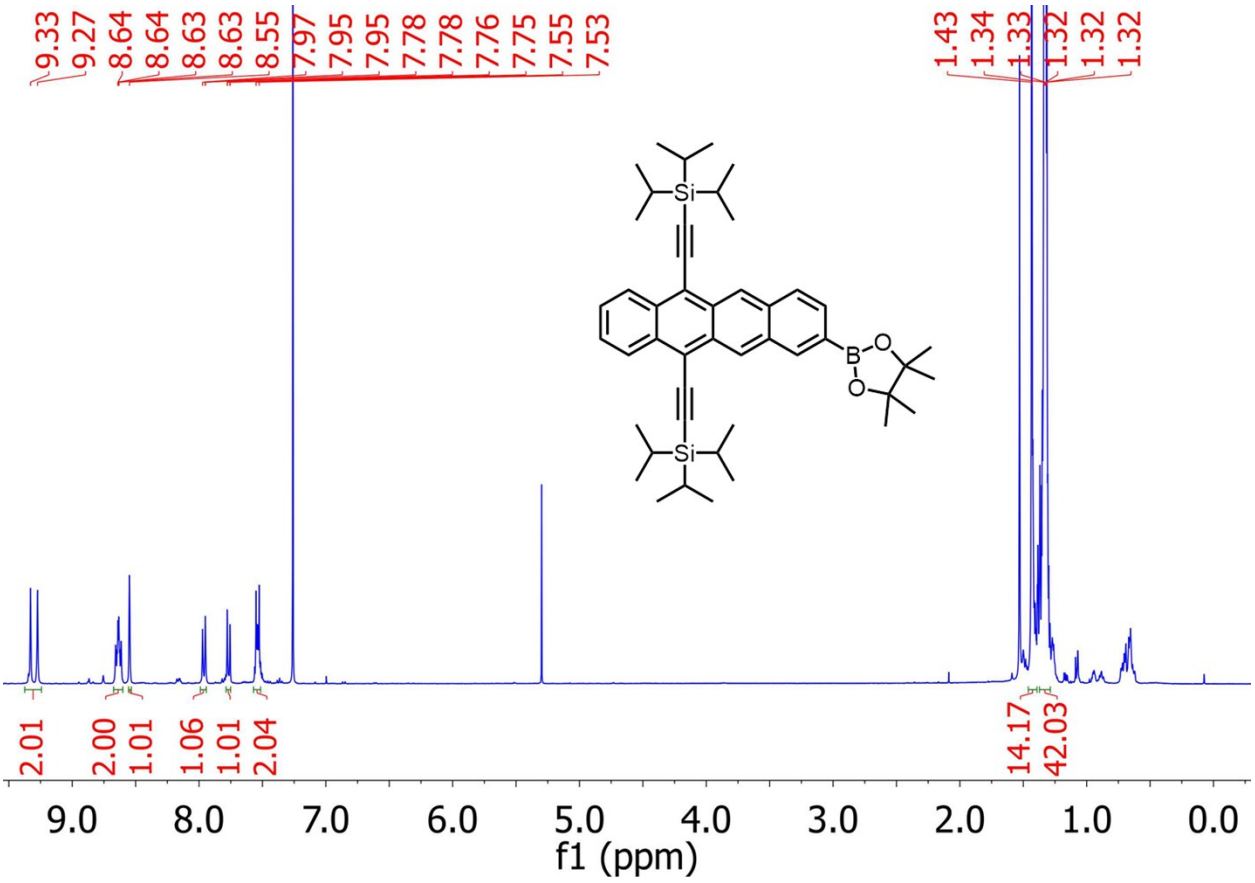
Atom	X	Y	Z
C	18.88389	-1.14043	1.106666
C	18.2889	-2.22112	1.81892
C	16.9289	-2.3671	1.843929
C	16.07162	-1.44696	1.161685
C	16.67488	-0.35173	0.43978
C	18.1008	-0.23782	0.440596
C	14.66431	-1.59106	1.183002
C	13.82902	-0.65587	0.49267
C	14.43474	0.441415	-0.23171
C	15.85838	0.577801	-0.24688
C	12.42676	-0.77365	0.498789
C	11.60496	0.133378	-0.16943
C	12.21247	1.225081	-0.89716
C	13.59845	1.350651	-0.90749
C	10.18058	0.015302	-0.16555
C	9.373395	0.909665	-0.8319
C	9.995148	1.99056	-1.55302
C	11.3511	2.141514	-1.58202
C	16.45235	1.656428	-0.95801
C	14.07094	-2.6704	1.893102

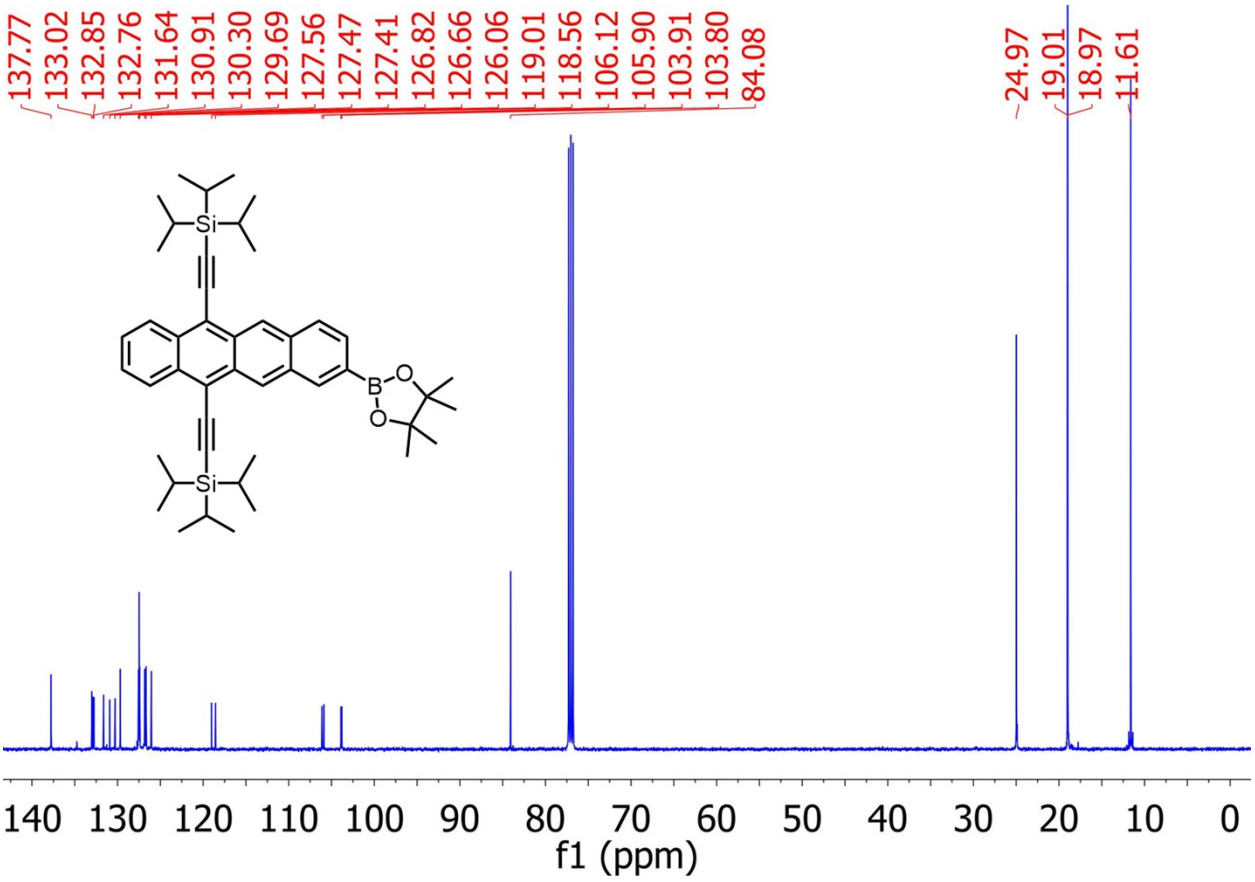
C	16.96041	2.585918	-1.57078
C	13.55714	-3.59871	2.502996
Si	17.72934	3.981513	-2.49494
Si	12.79075	-4.99677	3.42538
C	16.57745	4.475428	-3.90853
C	17.97617	5.434637	-1.31302
C	19.39365	3.407084	-3.17985
C	14.08136	-5.72144	4.598968
C	11.31443	-4.33852	4.403877
C	12.22132	-6.30598	2.188086
C	-18.9051	1.080376	1.185793
C	-18.3247	2.11294	1.921187
C	-16.9371	2.255986	1.939811
C	-16.1029	1.377986	1.229837
C	-16.6969	0.322027	0.476949
C	-18.0948	0.19657	0.472582
C	-14.6527	1.527253	1.249581
C	-13.8113	0.615325	0.514955
C	-14.4177	-0.45985	-0.25148
C	-15.8501	-0.60126	-0.26971
C	-12.4256	0.73708	0.519214
C	-11.5736	-0.15323	-0.19658
C	-12.1732	-1.20855	-0.95311
C	-13.5885	-1.33047	-0.95484
C	-10.172	-0.02121	-0.18858
C	-9.34556	-0.89482	-0.90124
C	-9.95616	-1.93434	-1.64509
C	-11.3311	-2.0866	-1.66916
C	-16.4426	-1.63468	-1.01449
C	-14.0747	2.569339	1.992691
C	-16.9633	-2.53646	-1.66762
C	-13.5724	3.482756	2.644427
Si	-17.7438	-3.88106	-2.65265
Si	-12.8278	4.854573	3.620142
C	-19.1616	-3.14823	-3.66437
C	-16.4387	-4.61981	-3.80205
C	-18.4005	-5.20401	-1.47409
C	-11.681	4.120254	4.930584
C	-11.8517	5.973527	2.451237
C	-14.2194	5.828136	4.447197
C	7.897287	0.777947	-0.82183
C	7.129825	1.105236	-1.95288
C	5.745445	0.973249	-1.94823
C	5.060527	0.513216	-0.81079
C	5.82766	0.189374	0.321641

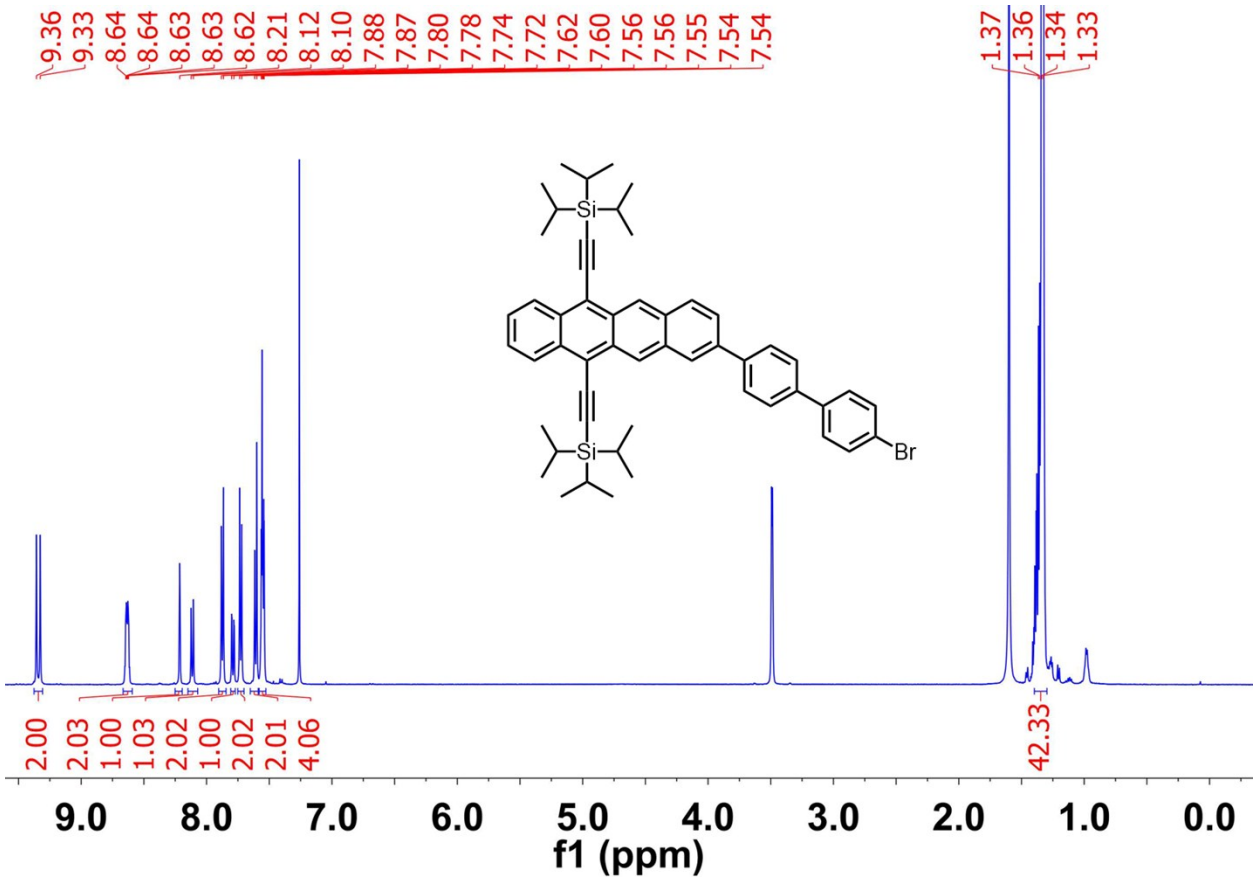
C	7.211947	0.319945	0.31682
C	3.584547	0.378495	-0.80658
C	2.768347	1.291481	-1.49595
C	1.383767	1.162808	-1.49838
C	0.747753	0.114732	-0.81127
C	1.563637	-0.7964	-0.11908
C	2.94849	-0.66776	-0.11688
C	-0.72788	-0.02584	-0.81949
C	-1.48261	0.290625	-1.96177
C	-2.86665	0.156493	-1.97234
C	-3.56318	-0.30237	-0.84136
C	-2.80867	-0.61799	0.30147
C	-1.42452	-0.48236	0.312339
C	-5.03795	-0.45068	-0.85532
C	-5.81175	-0.16777	0.283362
C	-7.19487	-0.31029	0.269838
C	-7.87243	-0.7419	-0.8839
C	-7.09812	-1.02447	-2.02264
C	-5.7152	-0.88215	-2.00871
H	19.96466	-1.03543	1.094312
H	18.92101	-2.93112	2.343908
H	16.47044	-3.18755	2.384521
H	18.54733	0.586943	-0.1034
H	11.97809	-1.59763	1.043896
H	14.05547	2.171007	-1.45115
H	9.739921	-0.8267	0.360692
H	9.362197	2.713686	-2.05759
H	11.79994	2.971618	-2.12085
H	17.00419	5.304947	-4.4837
H	16.41343	3.640028	-4.59651
H	15.60083	4.797675	-3.53307
H	18.43485	6.283251	-1.83339
H	18.62939	5.160226	-0.47864
H	17.02332	5.773118	-0.89386
H	20.07362	3.108497	-2.37547
H	19.27255	2.551073	-3.85121
H	19.87781	4.211397	-3.74533
H	13.65814	-6.55169	5.175683
H	14.94825	-6.10393	4.050572
H	14.43854	-4.96874	5.308981
H	10.83703	-5.1441	4.973364
H	10.55846	-3.90539	3.740944
H	11.62171	-3.56306	5.112653
H	11.48268	-5.89857	1.490465
H	13.061	-6.68898	1.599537

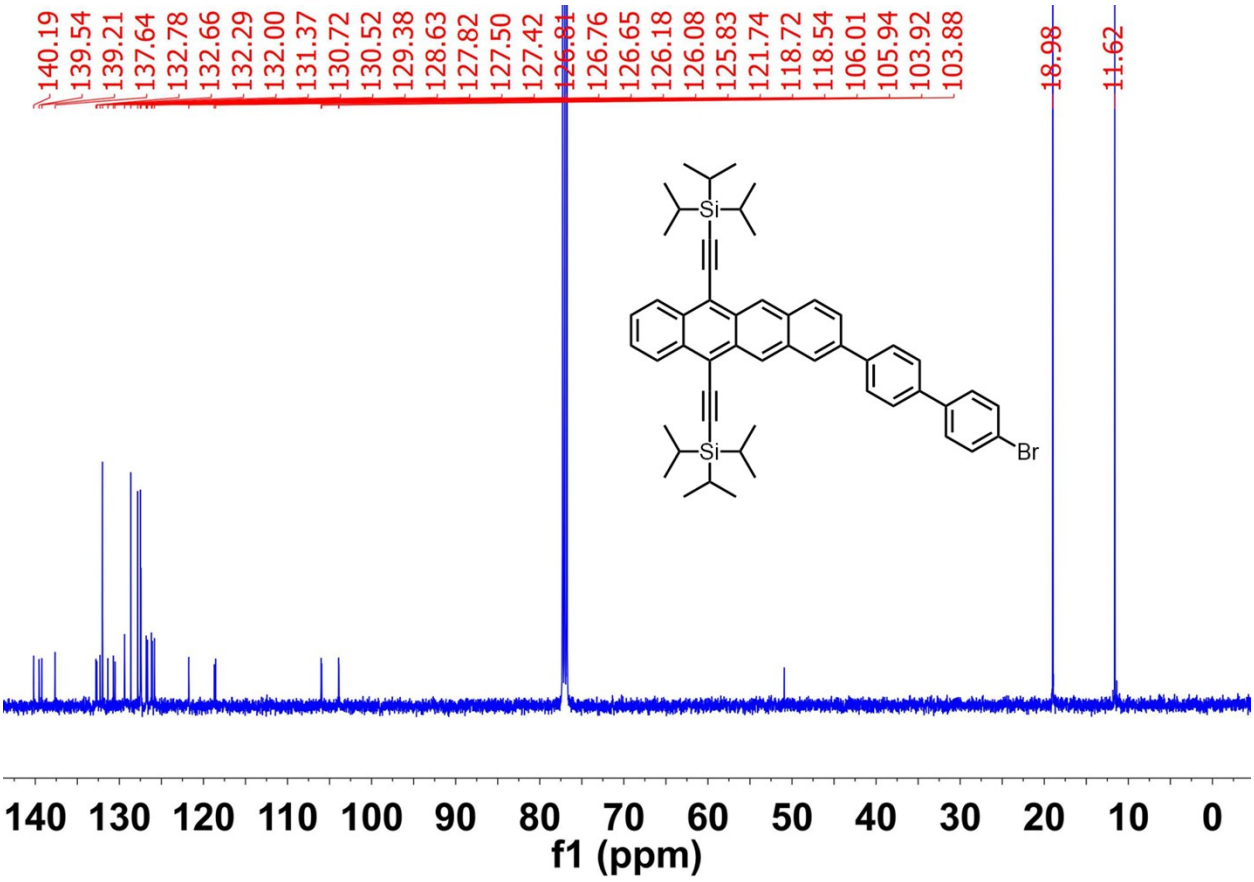
H	11.76036	-7.1539	2.707456
H	-19.9839	0.959274	1.164118
H	-18.9453	2.806907	2.47988
H	-16.4814	3.057709	2.510752
H	-18.5419	-0.60796	-0.10117
H	-11.9746	1.541476	1.091591
H	-14.0416	-2.13282	-1.52841
H	-9.73198	0.802293	0.366555
H	-9.33095	-2.64107	-2.1814
H	-11.7776	-2.89785	-2.23792
H	-19.6515	-3.92518	-4.26243
H	-19.9207	-2.69569	-3.01827
H	-18.801	-2.37442	-4.34936
H	-16.8695	-5.42158	-4.41249
H	-15.6026	-5.04385	-3.23657
H	-16.0354	-3.86234	-4.48163
H	-17.5943	-5.63473	-0.87196
H	-19.1462	-4.79033	-0.78773
H	-18.8749	-6.01845	-2.03358
H	-11.2178	4.91468	5.526862
H	-12.2293	3.464158	5.614021
H	-10.878	3.532278	4.474769
H	-11.3922	6.80237	3.001837
H	-12.4997	6.401538	1.679793
H	-11.0514	5.422472	1.947193
H	-14.802	5.192145	5.121311
H	-13.8131	6.657199	5.037574
H	-14.9056	6.250204	3.706065
H	7.626634	1.431772	-2.8614
H	5.18812	1.198815	-2.85237
H	5.328432	-0.13159	1.230908
H	7.770329	0.099144	1.221428
H	3.223757	2.13383	-2.00784
H	0.78308	1.907509	-2.01181
H	1.108292	-1.63869	0.393012
H	3.549314	-1.41239	0.396578
H	-0.97565	0.629053	-2.86032
H	-3.41899	0.427846	-2.8669
H	-3.31231	-0.99208	1.18775
H	-0.87506	-0.71898	1.218548
H	-5.32348	0.184073	1.187172
H	-7.75865	-0.10204	1.174115
H	-7.58867	-1.34245	-2.93751
H	-5.148	-1.12729	-2.90151

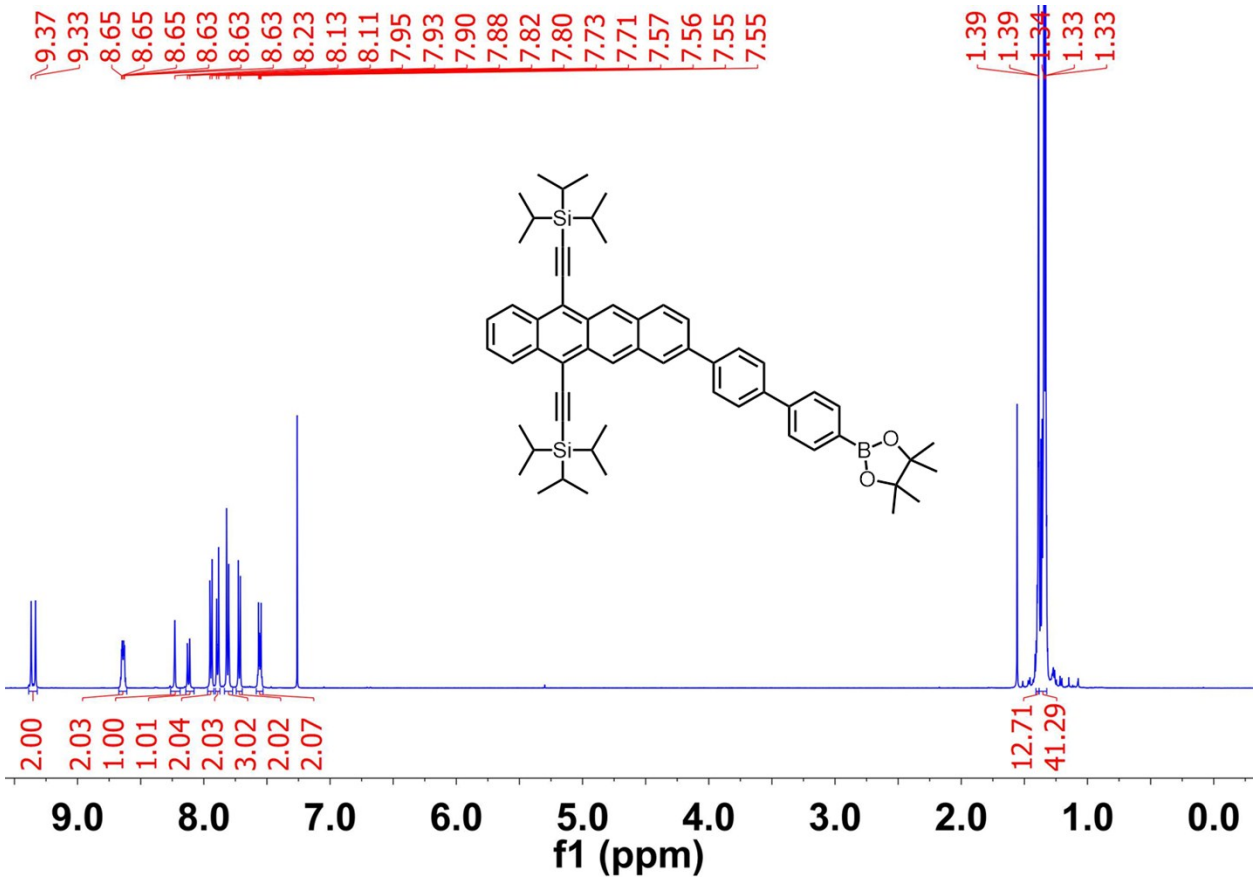
NMR SPECTRA

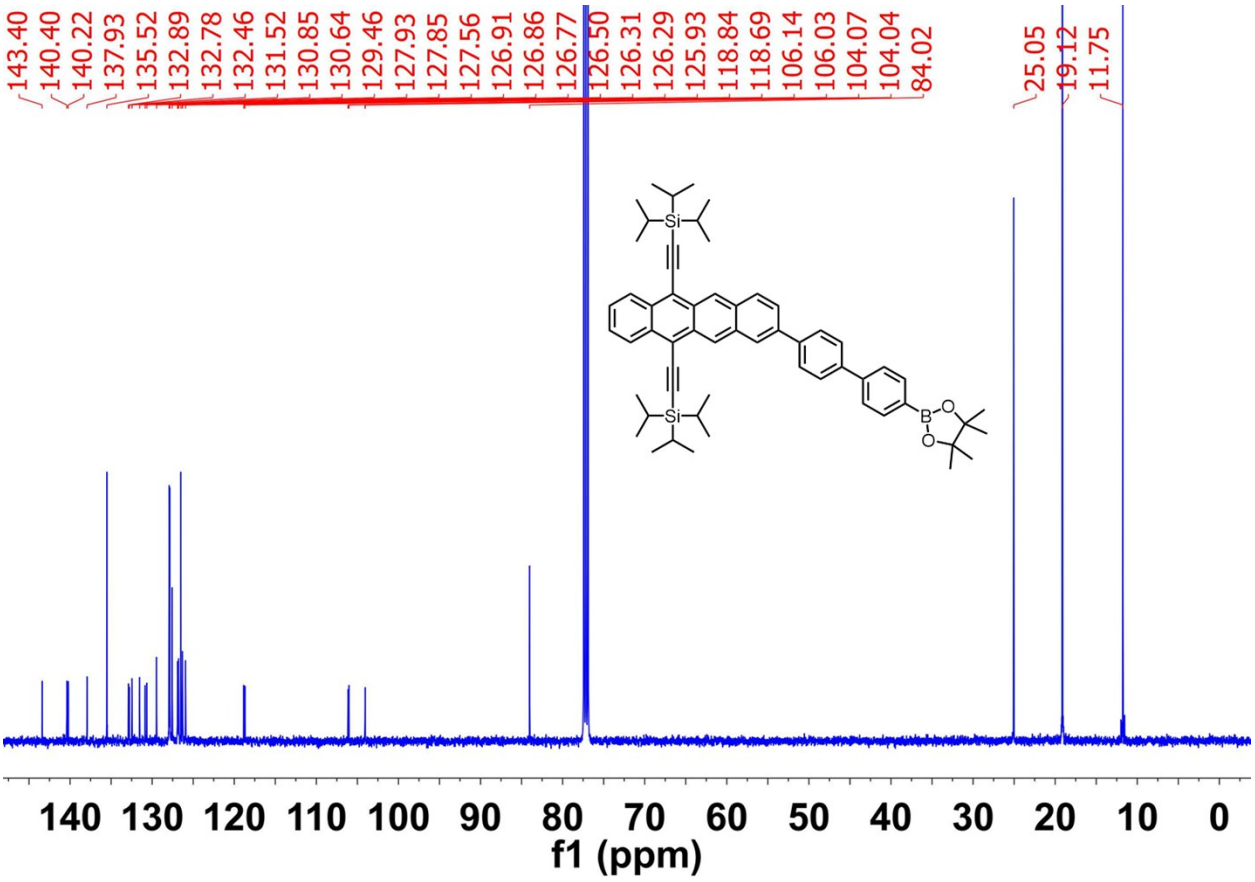

9.33
9.27
8.64
8.64
8.63
8.63
8.55
7.97
7.95
7.95
7.78
7.78
7.76
7.75
7.55
7.53
1.43
1.34
1.33
1.32
1.32
1.32
Si
Si
B
O
O
2.01
2.00
1.01
1.06
1.01
2.04
14.17
42.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

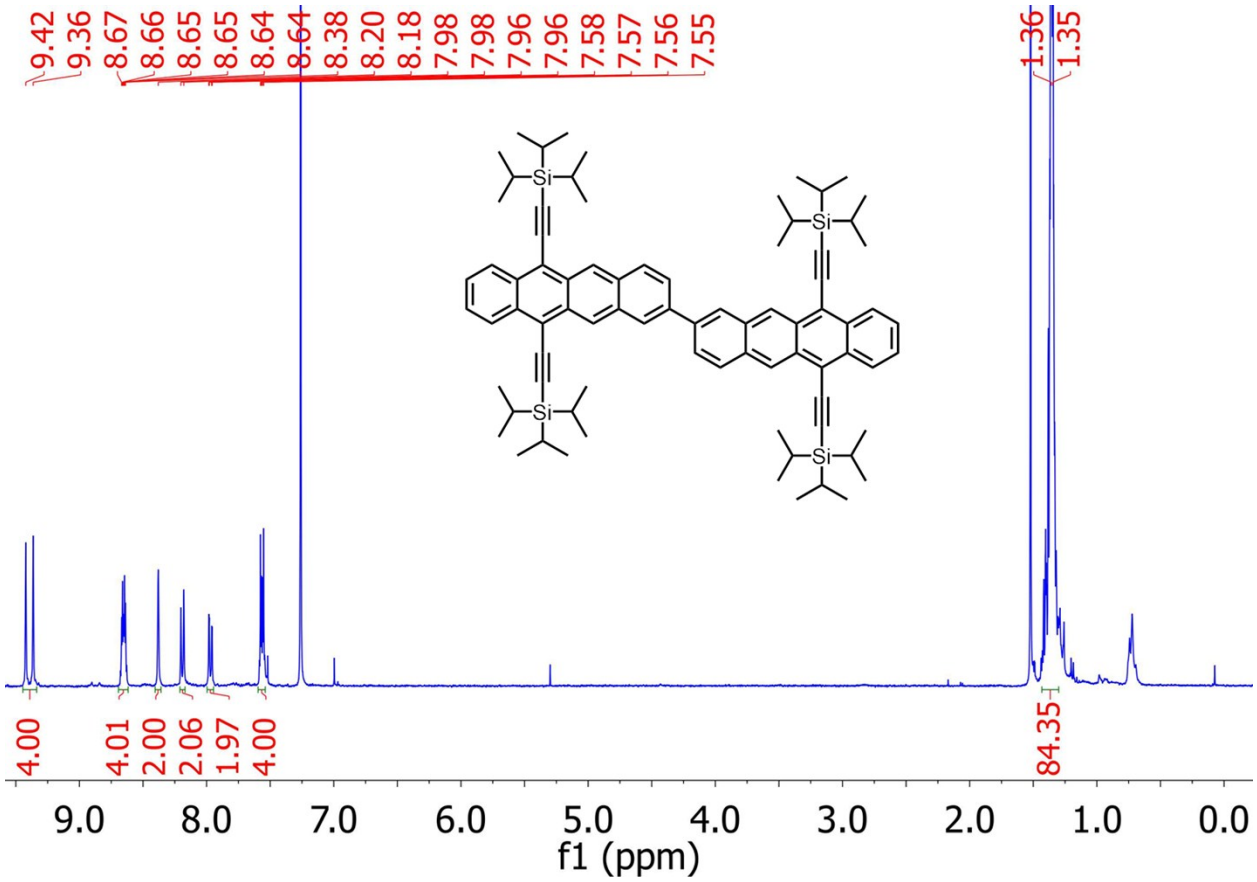

137.77
133.02
132.85
132.76
131.64
130.91
130.30
129.69
127.56
127.47
127.41
126.82
126.66
126.06
119.01
118.56
106.12
105.90
103.91
103.80
84.08
24.97
19.01
18.97
11.61
Si
Si
B
O
O
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

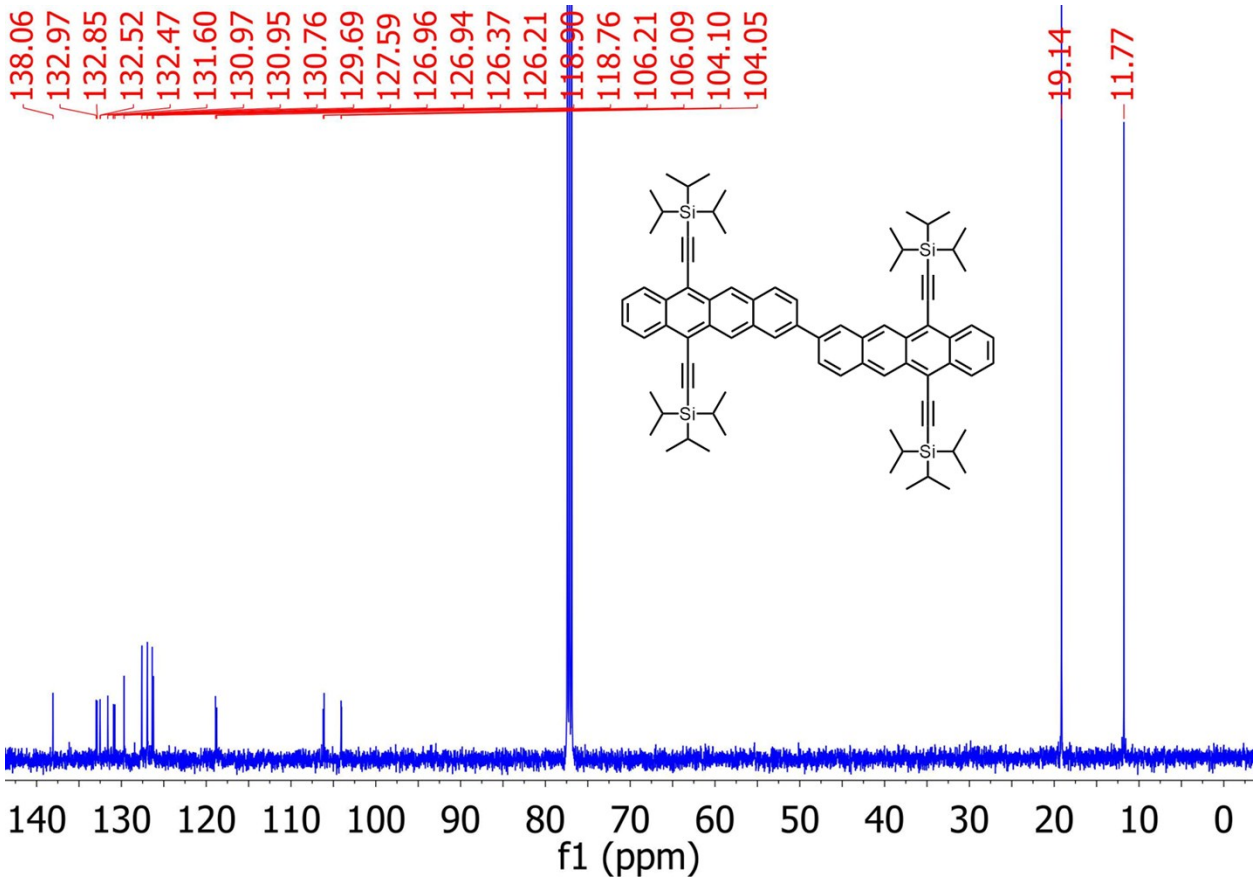

9.36
9.33
8.64
8.64
8.63
8.63
8.62
8.21
8.12
8.10
7.88
7.87
7.80
7.78
7.74
7.72
7.62
7.60
7.56
7.56
7.55
7.54
7.54
1.37
1.36
1.34
1.33
Si
Si
Br
2.00
2.03
1.00
1.03
2.02
1.00
2.02
2.01
4.06
42.33
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

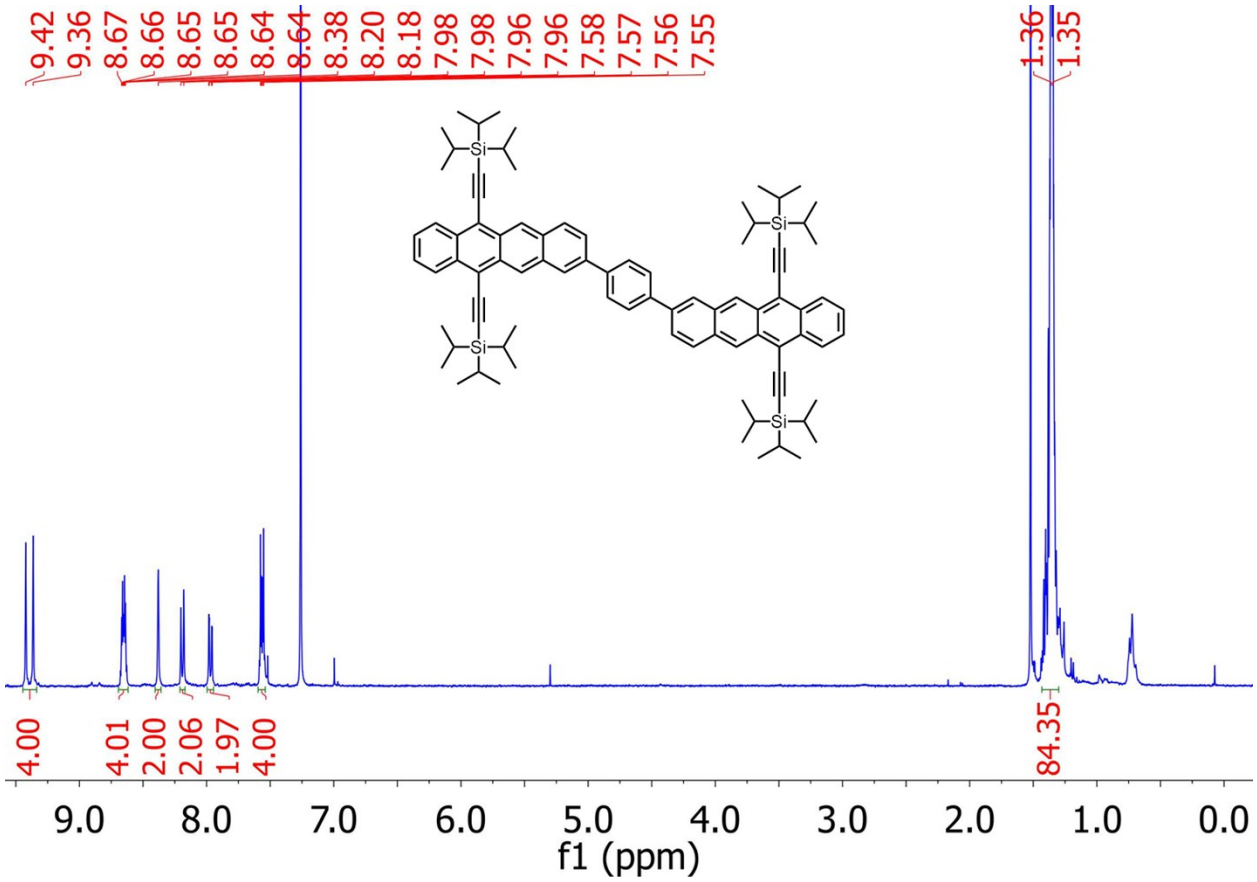

140.19
139.54
139.21
137.64
132.78
132.66
132.29
132.00
131.37
130.72
130.52
129.38
128.63
127.82
127.50
127.42
126.81
126.76
126.65
126.18
126.08
125.83
121.74
118.72
118.54
106.01
105.94
103.92
103.88
18.98
11.62
Si
Si
Br
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

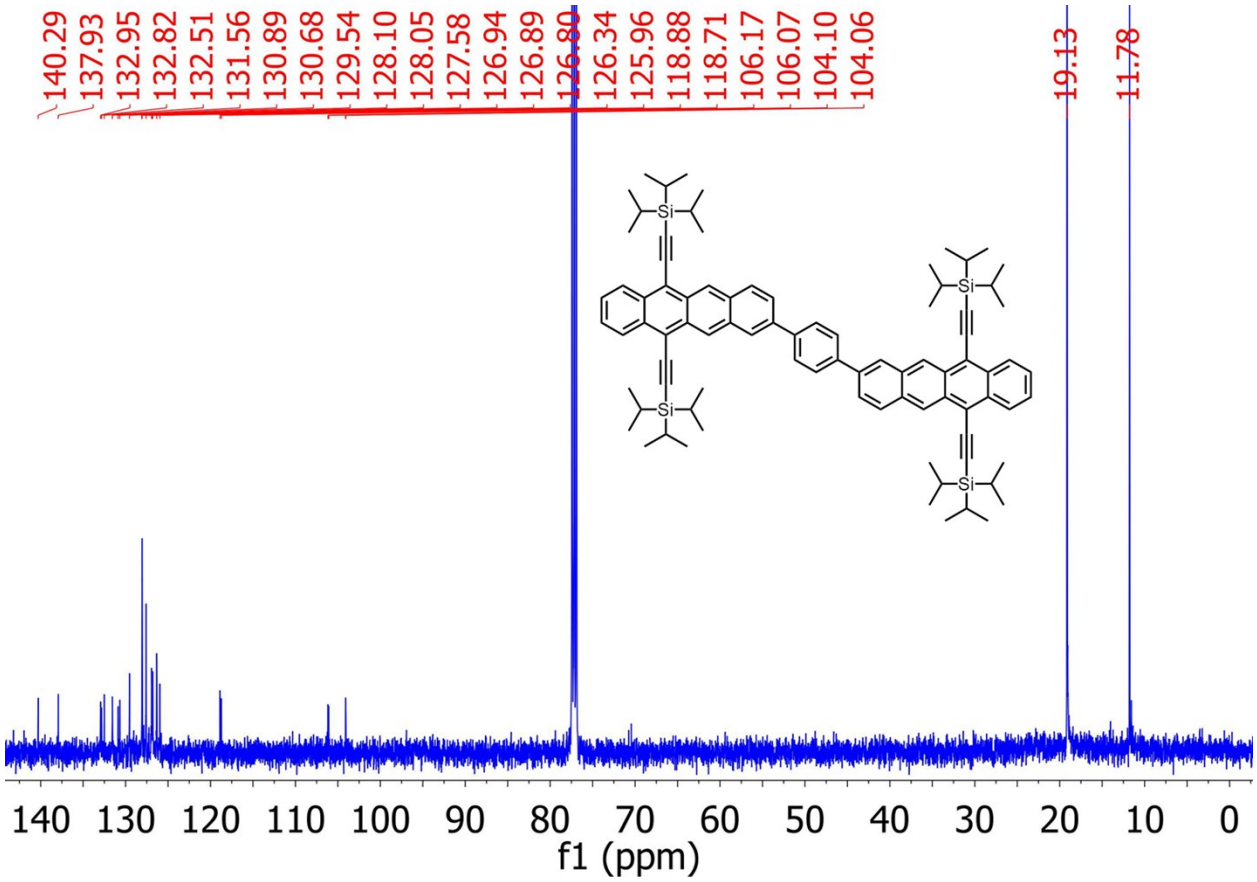

9.37
9.33
8.65
8.65
8.65
8.63
8.63
8.63
8.23
8.13
8.11
7.95
7.93
7.90
7.88
7.82
7.80
7.73
7.71
7.57
7.56
7.55
7.55
1.39
1.39
1.34
1.33
1.33
Si
Si
B
O
O
2.00
2.03
1.00
1.01
2.04
2.03
3.02
2.02
2.07
12.71
41.29
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

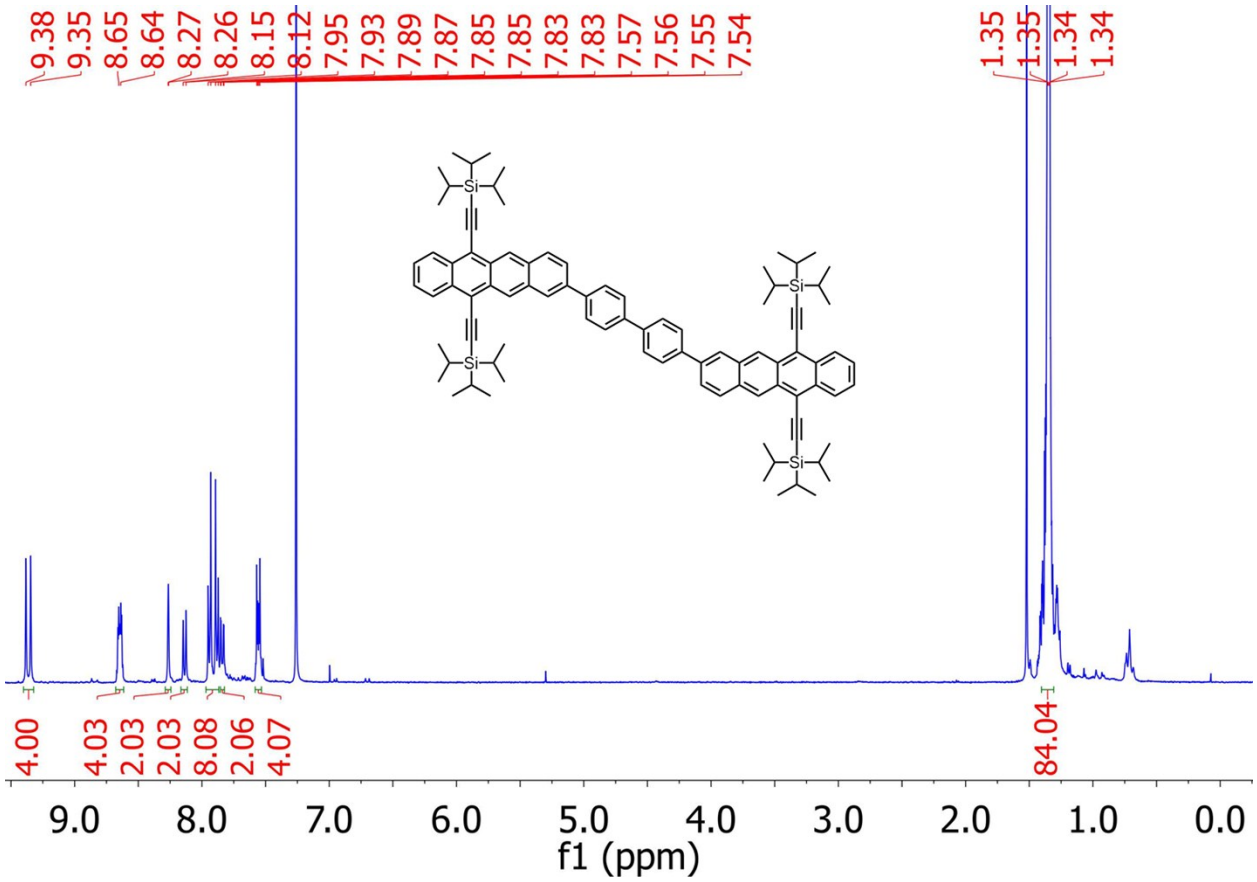

143.40
140.40
140.22
137.93
135.52
132.89
132.78
132.46
131.52
130.85
130.64
129.46
127.93
127.85
127.56
126.91
126.86
126.77
126.50
126.31
126.29
125.93
118.84
118.69
106.14
106.03
104.07
104.04
84.02
25.05
19.12
11.75
Si
Si
B
O
O
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

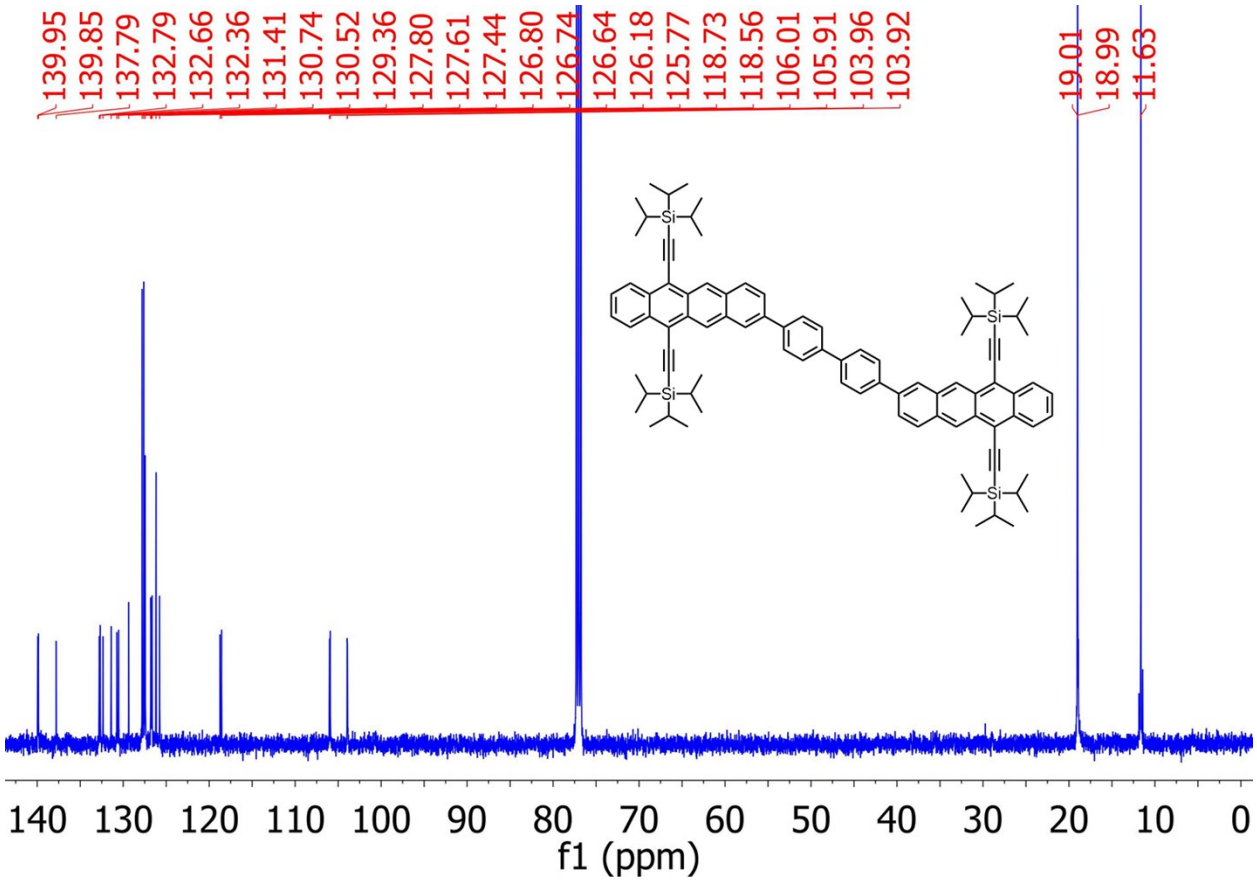

9.42
9.36
8.67
8.66
8.65
8.65
8.64
8.64
8.38
8.20
8.18
7.98
7.98
7.96
7.96
7.58
7.57
7.56
7.55
1.36
1.35
Si
Si
Si
Si
4.00
4.01
2.00
2.06
1.97
4.00
84.35
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

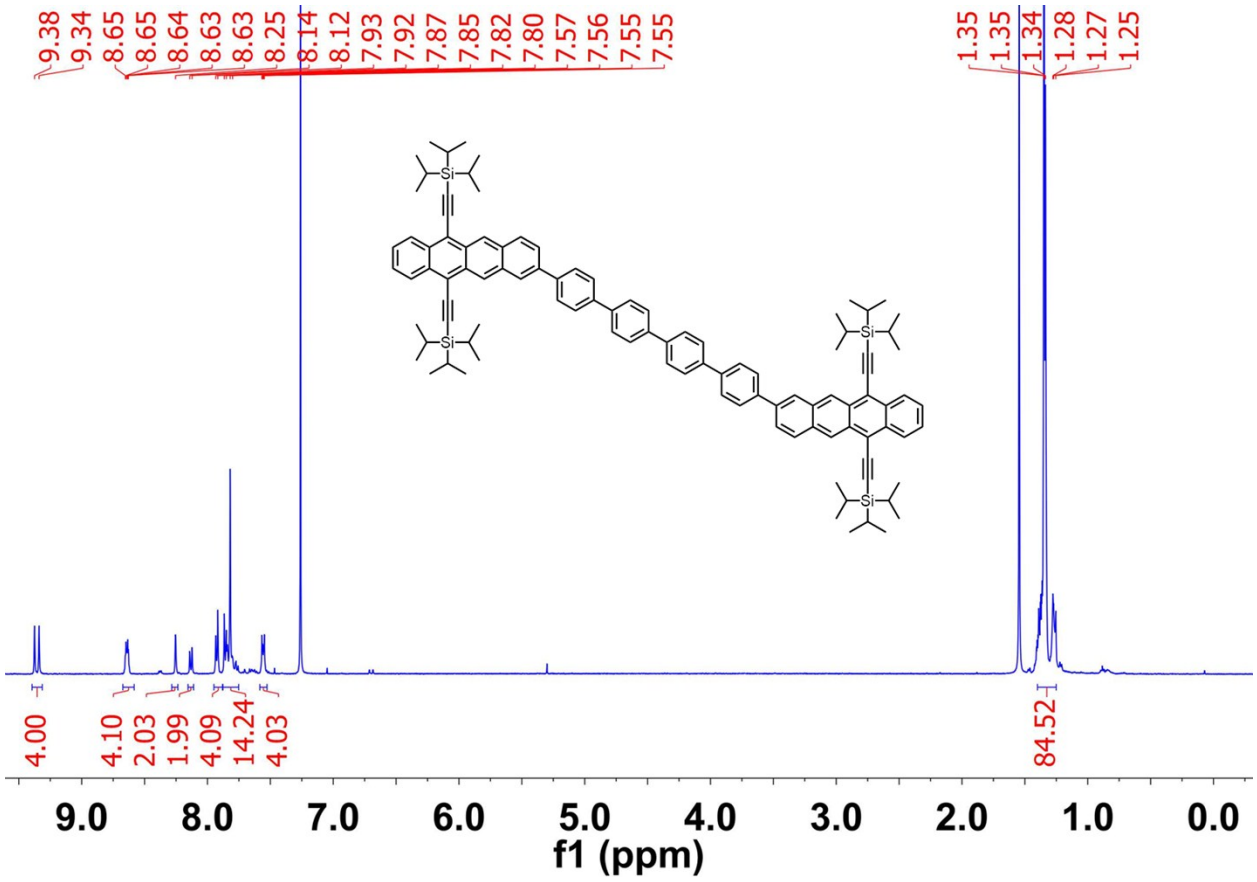

138.06
132.97
132.85
132.52
132.47
131.60
130.97
130.95
130.76
129.69
127.59
126.96
126.94
126.37
126.21
118.90
118.76
106.21
106.09
104.10
104.05
19.14
11.77
Si
Si
Si
Si
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.42
9.36
8.67
8.66
8.65
8.65
8.64
8.64
8.38
8.20
8.18
7.98
7.98
7.96
7.96
7.58
7.57
7.56
7.55
1.36
1.35
Si
Si
Si
Si
4.00
4.01
2.00
2.06
1.97
4.00
84.35
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


140.29
137.93
132.95
132.82
132.51
131.56
130.89
130.68
129.54
128.10
128.05
127.58
126.94
126.89
126.80
126.34
125.96
118.88
118.71
106.17
106.07
104.10
104.06
19.13
11.78
Si
Si
Si
Si
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.38
9.35
8.65
8.64
8.27
8.26
8.15
8.12
7.95
7.93
7.89
7.87
7.85
7.85
7.83
7.83
7.57
7.56
7.55
7.54
1.35
1.35
1.34
1.34
Si
Si
Si
Si
4.00
4.03
2.03
2.03
8.08
2.06
4.07
84.04
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


139.95
139.85
137.79
132.79
132.66
132.36
131.41
130.74
130.52
129.36
127.80
127.61
127.44
126.80
126.74
126.64
126.18
125.77
118.73
118.56
106.01
105.91
103.96
103.92
19.01
18.99
11.63
Si
Si
Si
Si
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.38
9.34
8.65
8.65
8.64
8.63
8.63
8.25
8.14
8.12
7.93
7.92
7.87
7.85
7.82
7.80
7.57
7.56
7.55
7.55
1.35
1.35
1.34
1.28
1.27
1.25
Si
Si
Si
Si
4.00
4.10
2.03
1.99
4.09
14.24
4.03
84.52
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

REFERENCES

(1) Sanders, S. N.; Kumarasamy, E.; Pun, A. B.; Steigerwald, M. L.; Sfeir, M. Y.; Campos, L. M. *Angew. Chem. Int. Ed.* **2016**, *55* (10), 3373.

(2) Soldatova, A. V; Kim, J.; Rizzoli, C.; Kenney, M. E.; Rodgers, M. A. J.; Rosa, A.; Ricciardi, G. *Inorg. Chem.* **2011**, *50* (3), 1135.