Supplementary Information

Selective Strain-Promoted Reactivity of a Fluorene-Derived [6]Cycloparaphenyleneacetylene Carbon Nanohoop

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S1. General Information

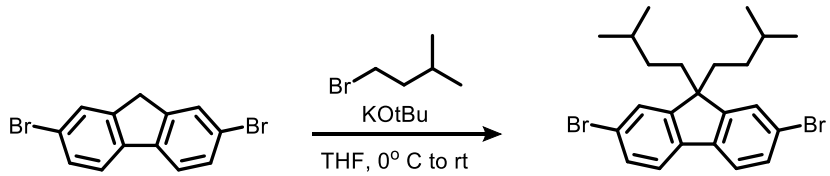
All commercially available reagents were used without purification.

^{1}H-NMR (400 MHz, 500 MHz, 700 MHz) and ^{13}C-NMR (126 MHz) were recorded on a Bruker AVIII-400 MHz Nanobay, a Bruker AVIII 500 MHz, or a Bruker Ascend™ 700 MHz at room temperature (298 K) unless otherwise specified. Chemical shifts (δ) were referenced to residual solvent peaks (chloroform, ^{1}H-NMR δ = 7.26 ppm, ^{13}C-NMR δ = 77.16 ppm; methanol, ^{1}H-NMR δ = 3.31 ppm, ^{13}C-NMR δ = 49.00 ppm).[1] Impurities are either labelled or starred. Matrix-assisted laser-desorption ionization time-of-flight/time-of-flight (MALDI-TOF/TOF) mass spectroscopy was performed by the Louisiana State University Mass Spectroscopy Facility on a Bruker rapifleX MALDI-TOF/TOF with data analyzed via flexAnalysis 3.3. Column chromatography was performed on a Biotage Isolera Flash System, using empty flash cartridges from Luknova and SiliCycle SiliaFlash® F60 silica gel (40-63 μm, 230-400 mesh).

Ultraviolet-visible (UV-Vis) spectroscopy and quantum yield calculations were performed on an Edinburgh Instruments Spectrofluorometer FS5. Absorption and emission spectra were collected with a SC-25 temperature-controlled holder. Quantum yield measurements were taken with an SC-30 integrating sphere, using a xenon lamp as a UV source. Raw data was processed via Fluoracle.

S2. Synthesis of Compounds

Synthesis of Fl-[6]CPPA



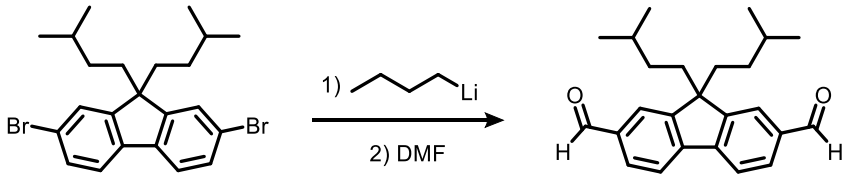
2,7-dibromo-9,9-di-*iso*-pentyl-9H-fluorene

2,7-dibromo-9H-fluorene (5.19 g, 16.00 mmol) was dissolved in THF (110 mL). The resulting solution was cooled to 0 °C. Potassium *tert*-butoxide (5.38 g, 48.00 mmol) was added to a separate vial and dissolved in minimal THF. This was added dropwise into the reaction mixture and allowed to stir for 30 minutes. Isopentyl bromide (5.00 mL, 40.00 mmol) was added in a single portion and the reaction was removed from the ice bath and stirred for 4 hours. This reaction was monitored via TLC (100% hexanes). The solvent was removed via rotary evaporation and the resulting solids were suspended in hexanes. This mixture was filtered through a bed of celite and generously washed with hexane. The filtrate was collected, dried over MgSO4, filtered, and dried via rotary evaporation. Column chromatography (24:1 hexanes:DCM) affords the product as a white crystalline solid. (6.62 g, 14.26 mmol, 89%)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.55 – 7.40 (m, 6H), 1.97 – 1.88 (m, 4H), 1.29 (dq, J = 13, 7 Hz, 4H), 0.70 (d, J = 7 Hz, 12H), 0.52 – 0.41 (m, 4H)

^{13}C NMR (126 MHz, $CDCl_3$) δ = 152.61, 139.26, 130.31, 126.25, 121.62, 121.27, 55.55, 38.17, 32.51, 28.30, 22.46.

MALDI-MS: $C_{23}H_{28}Br_2^+$, M^+, calcd. 464.0533, found 464.0546.



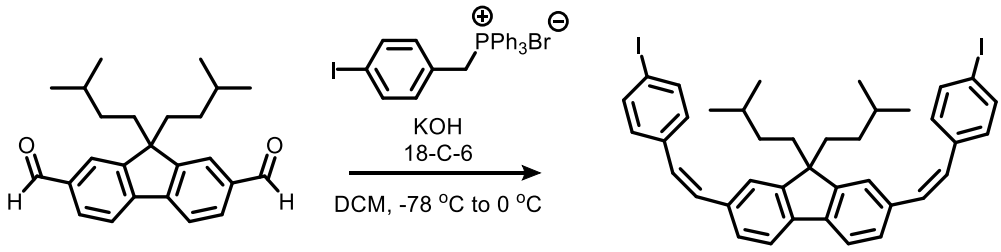
2,7-diformyl-9,9-di-*iso*-pentyl-9H-fluorene (1)

1 was synthesized in accordance with literature.[2] 2,7-dibromo-9,9'-di-*iso*-pentyl-9H-fluorene (1.00 g, 2.2 mmol) was added to an oven-dried round bottom flask and purged with nitrogen and vacuum (x3). The reaction flask was charged with nitrogen, and dry THF (20 mL) was added. The solution was cooled down to -78 °C. n-butyllithium (2.5 M in hexanes, 1.90 mL, 4.7 mmol) was added dropwise. Once added, the reaction was allowed to stir under N_2 at -78 °C for approximately 1.5 hours. Dry DMF (0.50 mL, 6.5 mmol) was added to a minimal amount of dry THF (~2 mL) and added dropwise to the reaction. The solution was allowed to slowly warm up to room temperature under N_2. This reaction was monitored via TLC (9:1 hexanes:EtOAc). When done, the reaction was quenched with 0.5 M HCl and extracted (x3) with ethyl acetate. The combined organic layers were dried with $MgSO_4$, filtered, and dried via rotary evaporation. Column chromatography (89:11 hexanes:EtOAc) affords the product as an off-white powder (697.7 mg, 1.9 mmol, 89%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.10 (s, 2H), 7.99 – 7.87 (m, 6H), 2.13 – 2.04 (m, 4H), 1.28 (hept, J = 7 Hz, 2H), 0.66 (d, J = 7 Hz, 12H), 0.47 – 0.37 (m, 4H)

^{13}C NMR (126 MHz, $CDCl_3$) δ = 192.28, 152.89, 145.79, 136.61, 130.41, 123.47, 121.46, 55.44, 37.99, 32.63, 28.24, 22.40.

MALDI-MS: $C_{25}H_{31}O_2^+$, $[M+H]^+$, calcd. 363.2319, found 363.2353.



(*Z,Z*)-distyryl fluorene (2)

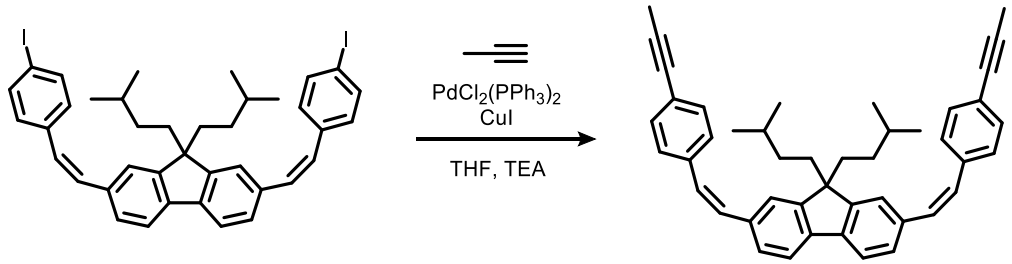
Compound **2** was synthesized via a modified literature procedure.[3] **1** (300 mg, 0.83 mmol), (4-iodophenyl)methyltriphenylphosphonium bromide (1.21 g, 2.17 mmol), and 18-crown-6 (46.6 mg, 0.17 mmol) were added to an oven-dried round bottom flask and purged with nitrogen and vacuum (x3). While purging, KOH (243 mg, 4.3 mmol) was freshly ground in a mortar and pestle, then added to a vial and placed under vacuum. The reaction flask was charged with nitrogen, and dry DCM (12 mL) was added. The solution was cooled to -78 °C under N_2. Once cooled, the powdered KOH was added in one portion, and the reaction was allowed to stir for 8 hours. After 8 hours, the acetone/dry ice -78 °C bath was swapped with a 0 °C ice bath and allowed to stir overnight. This reaction was monitored by TLC (9:1 hexanes:EtOAc). The reaction was quenched with water and extracted (x3) with DCM. The combined organic layers were

washed with brine, dried with $MgSO_4$, filtered, and dried via rotary evaporation. Column chromatography (24:1 hexanes:DCM) yielded compound **2** as a light yellow oil (341 mg, 0.45 mmol, 54%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.55 (d, J = 8 Hz, 2H), 7.52 (d, J = 8 Hz, 4H), 7.19 (d, J = 6 Hz, 2H), 7.10 (s, 2H), 7.00 (d, J = 8 Hz, 4H), 6.72 (d, J = 12 Hz, 2H), 6.50 (d, J = 12 Hz, 2H), 1.77 – 1.65 (m, 4H), 1.23 (dq, J = 13, 7 Hz, 2H), 0.68 (d, J = 7 Hz, 12H), 0.46 – 0.37 (m, 4H)

^{13}C NMR (126 MHz, $CDCl_3$) δ = 151.01, 140.16, 137.39, 137.01, 135.91, 131.91, 130.84, 128.72, 127.86, 123.06, 119.73, 92.50, 54.67, 38.05, 32.55, 28.37, 22.55.

MALDI-MS: $C_{39}H_{40}I_2$, M, calcd. 762.1214, found 762.1305.



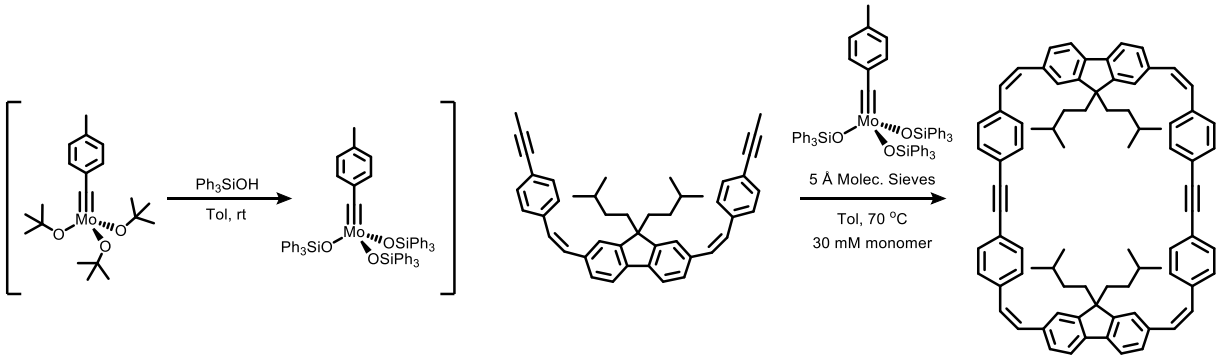
Dipropynyl (*Z,Z*)-distyryl fluorene (3)

Compound **2** (1.30 g, 1.7 mmol) was added to dry THF (15 mL) and triethylamine (6 mL) and bubbled with nitrogen for 30 minutes. Propyne (1 M in THF, 7.00 mL, 6.8 mmol) was added in a single portion, followed by dichlorobis(triphenylphosphine)palladium(II) (59 mg, 0.08 mmol) and copper(I) iodide (32 mg, 0.17 mmol). The reaction stirs at room temperature overnight under N_2. This reaction is monitored by TLC (19:1 hexanes:DCM). The reaction was quenched with a saturated NH_4Cl solution and extracted (x3) with DCM. The combined organic layers were washed with brine, dried with $MgSO_4$, filtered, and dried via rotary evaporation. Column chromatography (17:3 hexanes:DCM) affords monomer **3** as a yellow oil (938 mg, 1.6 mmol, 94%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.53 (d, J = 8 Hz, 2H), 7.25 – 7.16 (m, 10H), 7.13 (s, 2H), 6.69 (d, J = 12 Hz, 2H), 6.55 (d, J = 12 Hz, 2H), 2.03 (s, 6H), 1.76 – 1.67 (m, 4H), 1.25 (qd, J = 13, 6 Hz, 2H), 0.68 (d, J = 7 Hz, 12H), 0.48 – 0.37 (m, 4H)

^{13}C NMR (126 MHz, $CDCl_3$) δ = 151.06, 140.20, 136.92, 136.18, 131.59, 131.47, 129.41, 128.92, 127.96, 123.24, 122.76, 119.65, 86.37, 79.89, 54.73, 38.13, 32.61, 28.42, 22.54.

MALDI-MS: $C_{45}H_{46}$, [M]*, calcd. 586.3560, found 586.3557.



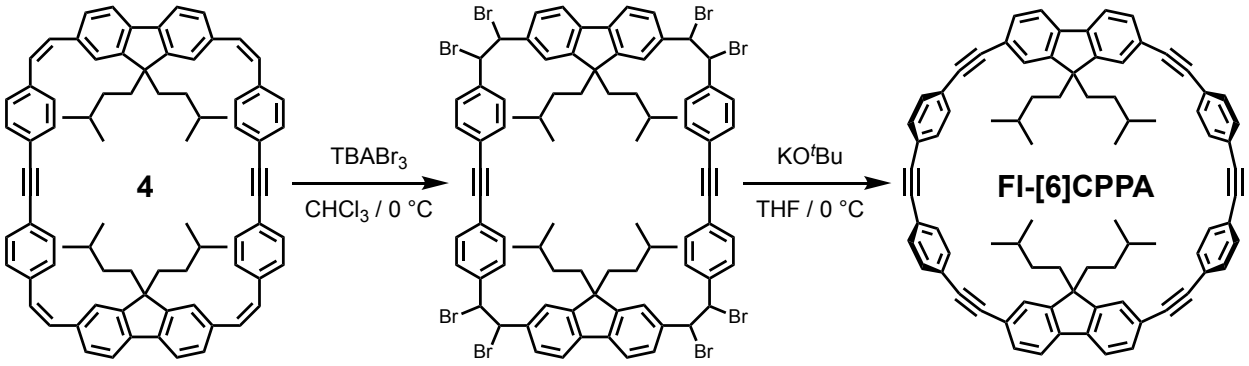
Dimeric macrocycle (4)

Metathesis was performed in similar fashion to previously reported methods.[4] Inside of a glovebox, monomer **3** (786.2 mg, 1.34 mmol) was dissolved in toluene (10 mL) and added into a round bottom flask with 5 Å molecular sieves (1.00 g). In a separate vial with a stir bar, precatalyst Mo(≡Tol)(OtBu)$_3$ (28.0 mg, 0.07 mmol) and triphenylsilanol (93.0 mg, 0.34 mmol) were added and dissolved in toluene (5 mL). This solution stirred at room temperature for approximately 20 minutes; a minor color change from brown to amber can be observed. This solution was pipetted into to the reaction flask and diluted to 30 mM of monomer with toluene (~25 mL). The reaction was allowed to stir at 70 °C overnight. This reaction is tracked via TLC by taking sacrificial aliquots out of the glovebox (7:1 hexanes:EtOAc). When finished, the reaction is removed from the glovebox and immediately quenched with MeOH. The solvents are removed via rotary evaporation. The resulting solid is suspended in DCM and filtered over a bed of celite to remove molecular sieves. The bed of celite is generously washed with DCM to ensure good extraction. The solvents are again removed via rotary evaporation, and the resulting solid is suspended in MeOH. The solids are collected via membrane filtration as a yellow solid and dried. Column chromatography (3:1 hexanes:DCM) separates dimer **4** from other byproducts as a light yellow, highly fluorescent solid (667.1 mg, 0.63 mmol, 93%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.60 (d, J = 8 Hz, 4H), 7.31 (d, J = 8 Hz, 8H), 7.24 – 7.15 (m, 16H), 6.75 (d, J = 12 Hz, 4H), 6.57 (d, J = 12 Hz, 4H), 1.76 – 1.68 (m, 8H), 1.22 (td, J = 13, 7 Hz, 8H), 0.67 (d, J = 7 Hz, 24H), 0.43 (m, 8H)

^{13}C NMR (126 MHz, $CDCl_3$) δ = 151.10, 140.28, 137.54, 136.44, 132.01, 131.54, 129.47, 129.09, 128.33, 122.68, 121.97, 119.89, 90.06, 54.84, 38.19, 32.65, 28.46, 22.59.

MALDI-MS: $C_{82}H_{80}^+$, M^+, calcd. 1064.6573, found 1064.6080.



Fl-[6]CPPA

Dimer **4** (497 mg, 0.47 mmol) was added to an oven-dried round bottom flask and dissolved in chloroform (20 mL). The flask was wrapped in aluminum foil and cooled to 0 °C. Tetrabutylammonium tribromide (1.80 g, 3.85 mmol) was dissolved in minimal chloroform and added dropwise. The reaction was allowed to stir under N_2 overnight. The reaction is tracked by TLC (2:1 hexanes:DCM). When finished, the reaction is quenched with a saturated $NaHSO_3$ solution and extracted with DCM (x3). The combined organic layers are washed with brine, dried with $MgSO_4$, filtered, and dried via rotary evaporation. Column chromatography (63:37 hexanes:DCM) yielded a mixture of octabrominated diastereomers as an off-white, faint yellow solid (556 mg, 0.33 mmol, 75%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.38 (qd, J = 10.7, 9.4, 6.2 Hz, 4H), 7.24 – 6.99 (m, 24H), 5.71 – 5.40 (m, 8H), 1.81 (dt, J = 16.6, 8.2 Hz, 8H), 1.24 – 1.13 (m, 4H), 0.75 – 0.57 (m, 24H), 0.2 (m, 8H).

Octabrominated CPPA precursor (530 mg, 0.31 mmol) was added to dry THF, cooled to 0 °C, and degassed with N_2 for 30 minutes. In a separate vial in the glovebox, KO^{t}Bu (452.2 mg, 4.03 mmol) was dissolved in minimal THF, sealed, and brought out the glovebox. This was added dropwise into the reaction mixture, resulting in a golden yellow/brown solution. This reaction was allowed to stir at 0 °C for 2 hours, monitored by TLC analysis (3:1 hexanes:DCM). When finished, the reaction is brought out of the ice bath and saturated with silica. This slurry is then dried via rotary evaporation and prepared for solid loading column chromatography (33:17 hexanes:DCM) in order to remove potassium salts. The product elutes as a yellow/blue highly fluorescent solution. The fractions are combined and concentrated via rotary evaporation to reveal **Fl-[6]CPPA** as a bright yellow powdery solid (292 mg, 0.28 mmol, 90%).

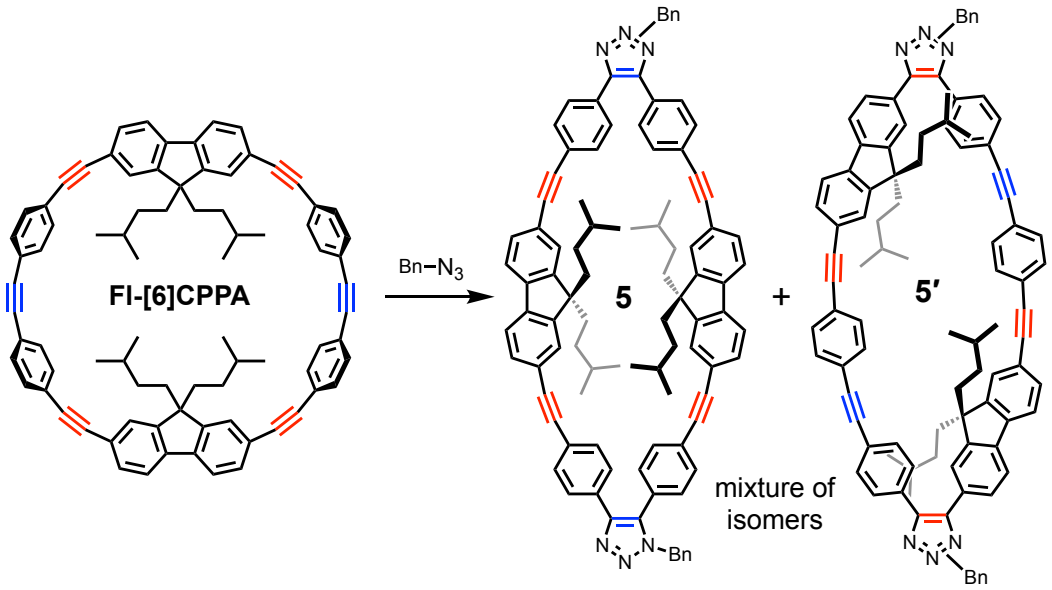
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.58 (d, J = 8 Hz, 4H), 7.42 (s, 16H), 7.38 – 7.31 (m, 8H), 1.91 – 1.83 (m, 8H), 1.17 (dq, J = 13, 7 Hz, 4H), 0.57 (d, J = 7 Hz, 24H), 0.41 (dt, J = 12, 7 Hz, 8H)

^{13}C NMR (126 MHz, $CDCl_3$) δ = 151.44, 141.33, 131.23, 131.16, 128.52, 128.30, 124.58, 123.74, 122.34, 120.52, 97.58, 96.87, 93.98, 54.81, 37.80, 32.56, 28.20, 22.40.

MALDI-MS: $C_{82}H_{72}^+$, M^+, calcd. 1056.5600, found 1056.5598.

Strain-Promoted Azide-Alkyne Cycloaddition (SPAAC)

SPAAC with Fl-[6]CPPA and benzyl azide (5)



Fl-[6]CPPA (89 mg, 0.084 mmol), benzyl azide (26 mg, 0.202 mmol), and dry $CHCl_3$ (13 mL) were added to a round bottom flask. The reaction was stirred and heated to 40 °C for 5 days, monitored by TLC (19:1 DCM:MeOH). When finished, the solution is dried via rotary evaporation and prepared for column chromatography (3:2 hexanes:EtOAc) The major product (R_f = 0.55), a light yellow powder, is a mixture of double-SPAAC regioisomers **5** and **5′** (85.8 mg, 0.065 mmol, 77%). The minor product, consisting of triple-SPAAC moieties (R_f = 0.40, 20%) can also be isolated via column chromatography (Figure S18, S32).

Peaks corresponding to **5** and **5′** (Figure S17) appear as complex, overlapped multiplets in the aromatic and aliphatic regions, owing to the five potential regioisomers this reaction can produce.

^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.13 (dd, *J* = 8.0, 1.6 Hz, Ar-*H*), 8.10 (dd, *J* = 7.9, 1.7 Hz, Ar-*H*), 7.85 (d, *J* = 7.9 Hz, Ar-*H*), 7.82 (s, Ar-*H*), 7.77-7.26 (m, Ar-*H*), 7.19-7.10 (m, Ar-*H*), 6.78 (d, *J* = 1.5 Hz, Ar-*H*), 6.76 (d, *J* = 1.5 Hz, Ar-*H*), 6.40 (d, *J* = 1.6 Hz, Ar-*H*), 6.33 (d, *J* = 1.7 Hz, Ar-*H*), 5.66 (s, -C*H*$_2$Ph), 5.60 (s, -C*H*$_2$Ph), 2.07-2.02 (m), 2.01 – 1.91 (m), 1.76-1.55 (m), 1.43 – 1.20 (m), 1.20-1.09 (m), 0.76 – 0.62 (m), 0.61 – 0.48 (m), 0.46 (dd, *J* = 7.9, 3.8 Hz), 0.43 – 0.29 (m), 0.21 (tdd, *J* = 13.6, 7.7, 5.2 Hz).

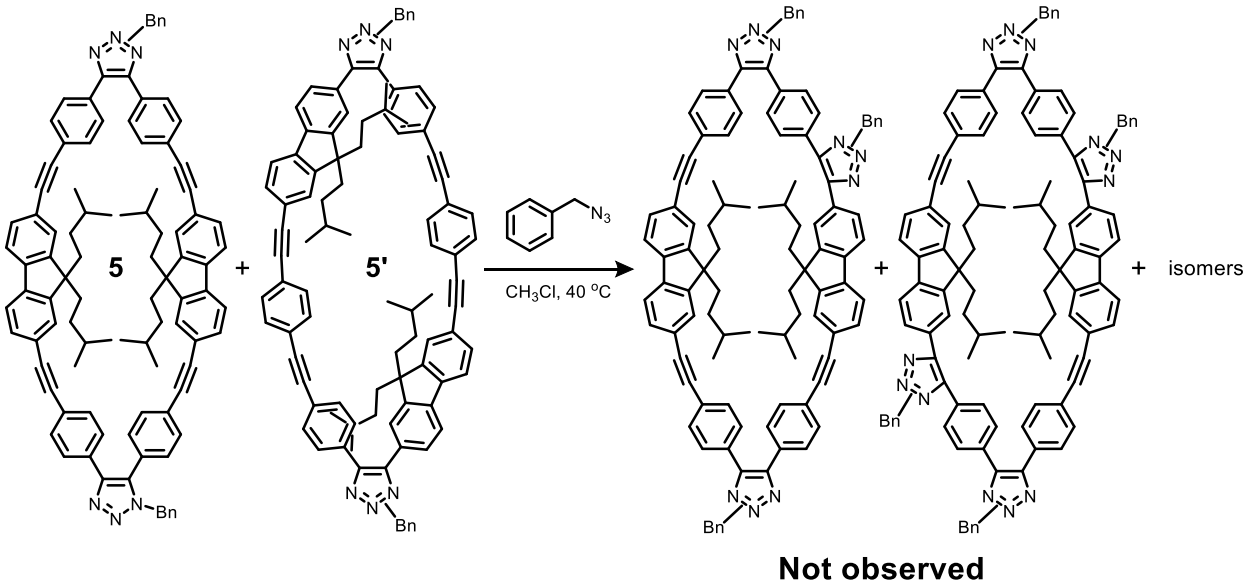
^{13}C NMR (126 MHz, $CDCl_3$) δ = 151.54, 151.22, 150.89, 141.22, 135.00, 134.80, 134.56, 132.53, 132.48, 131.92, 131.76, 131.69, 131.62, 131.48, 131.43, 130.59, 130.40, 129.10, 129.03, 128.80, 128.67, 128.41, 128.04, 127.95, 127.86, 127.78, 127.70, 127.34, 123.55, 122.29, 121.92, 121.12, 120.58, 120.22, 94.04, 93.92, 93.13, 92.49, 90.10, 54.98, 54.85, 54.67, 54.48, 54.21, 52.79, 38.04, 37.43, 32.51, 32.44, 32.38, 32.07, 29.84, 29.50, 28.22, 28.13, 28.09, 22.93, 22.88, 22.79, 22.73, 22.68, 22.64, 22.30, 22.26, 22.22, 22.15, 22.12, 14.27.

MALDI-MS: $C_{96}H_{86}N_6^+$, M^+, calcd. 1322.6900, found 1322.6432.

SPAAC with Fl-[6]CPPA and equimolar benzyl azide

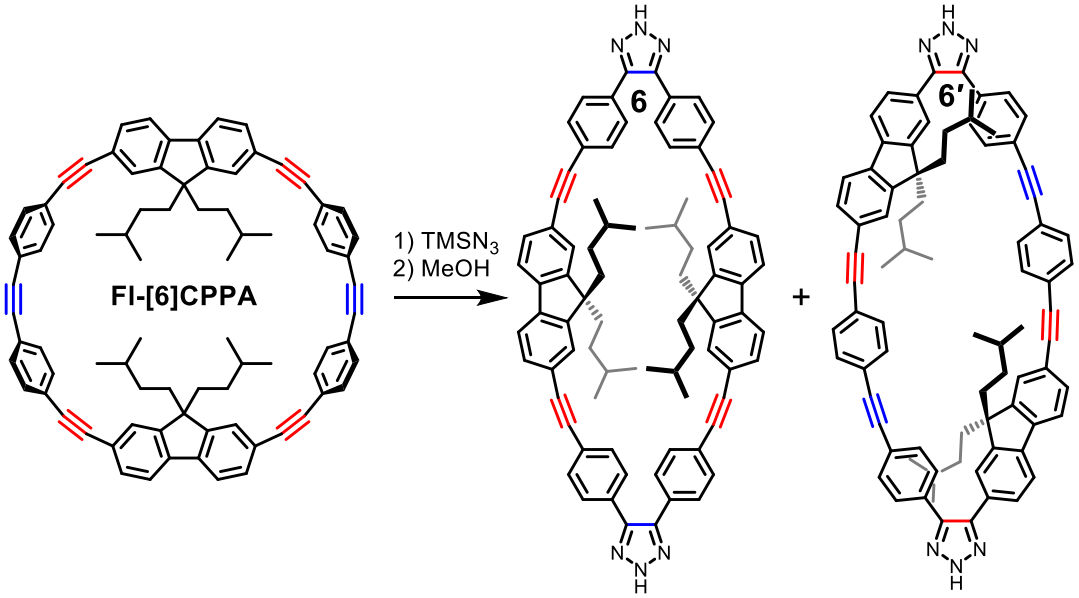
Fl-[6]CPPA (9.5 mg, 0.009 mmol), benzyl azide (1.2 mg, 0.009 mmol), and $CDCl_3$ (0.5 mL) were added to a J. Young tube and heated to 40 °C. The reaction was monitored via ^{1}H-NMR by tracking the methylene position on benzyl azide. When no more benzyl azide was detected, the solution was dried via rotary evaporation and prepared for MALDI analysis (Figure S31).

SPAAC with 5/5′ and benzyl azide (control experiment)



A mixture of **5** and **5′** (14.1 mg, 0.011 mmol) and benzyl azide (3.4 mg, 0.026 mmol) and dry chloroform (4 mL) were added to a reaction vial and stirred at 40 °C for 5 days. The reaction was monitored via TLC (1:1 hexanes EtOAc) for 5 days. Per TLC, no starting material was consumed, and no change was observed. After 5 days, the mixture was dried and prepared for ^{1}H-NMR analysis (Figure S20).

SPAAC with Fl-[6]CPPA and azidotrimethylsilane (6)



Fl-[6]CPPA (25 mg, 0.02 mmol) and azidotrimethylsilane (37.3 µL, 0.28 mmol) were added to a reaction vial with dry C_6H_6 (5 mL). This reaction was heated to 75 °C and allowed to stir for 12 days, monitoring with TLC (19:1 DCM:MeOH). When finished, the solution is removed via rotary evaporation and prepared for column chromatography (19:1 DCM:MeOH). The methanol in the column is enough to remove the trimethylsilyl groups, revealing the regioisomers **6** and **6′** as a bright yellow powder (20 mg, 0.017 mmol, 81%).

Much like **5/5′**, peaks corresponding to either **6** or **6′** overlap in both the aromatic and aliphatic regions in ^{1}H- and ^{13}C-NMR (Fig. S21-S23). In addition, this compound is poorly soluble in conventional deuterated solvents. ^{1}H- and ^{13}C- NMR were taken in a 4:1 ratio of $CDCl_3$:CD_3OD at 313 K, locking onto CD_3OD. Despite our best efforts on a 700 MHz NMR, the ^{13}C-NMR gives incomplete data due to low signal intensity, though the aliphatic region is fully visible.

^{1}H NMR (Fig. S21b) (400 MHz, CD_3OD) δ = 7.77 (s), 7.75 (s), 7.66 (m), 7.56 – 7.52 (m), 7.50 – 7.45 (m), 7.44 – 7.43 (m), 7.42 – 7.40 (m), 7.37 (s), 7.36 (d), 7.34 (s), 2.07 – 2.01 (m), 1.74 (td, J = 12.8, 4.8 Hz), 1.50 (td, J = 12.8, 4.8 Hz), 1.34-1.25 (m), 1.21 – 1.12 (m), 0.68 (d, J = 6.6 Hz), 0.57 (d, J = 6.6 Hz), 0.53 (d, J = 6.6 Hz), 0.44 – 0.33 (m), 0.32 – 0.22 (m).

^{13}C NMR (176 MHz, CD_3OD) δ = 151.25, 141.56, 132.12, 131.75, 131.69, 129.55, 129.10, 128.79, 128.57, 128.09, 125.19, 120.64, 93.92, 72.66, 61.61, 54.88, 38.75, 38.01, 35.97, 32.82, 32.80, 32.14, 29.90, 28.30, 27.44, 25.90, 22.81, 22.73, 22.11, 14.11, 1.14.

MALDI-MS: $C_{82}H_{74}N_6^+$, M^+, calcd. 1142.6000, found 1142.5907. $C_{82}H_{75}N_6$, $[M+H]^+$, calcd. 1143.6100, found 1143.6056.

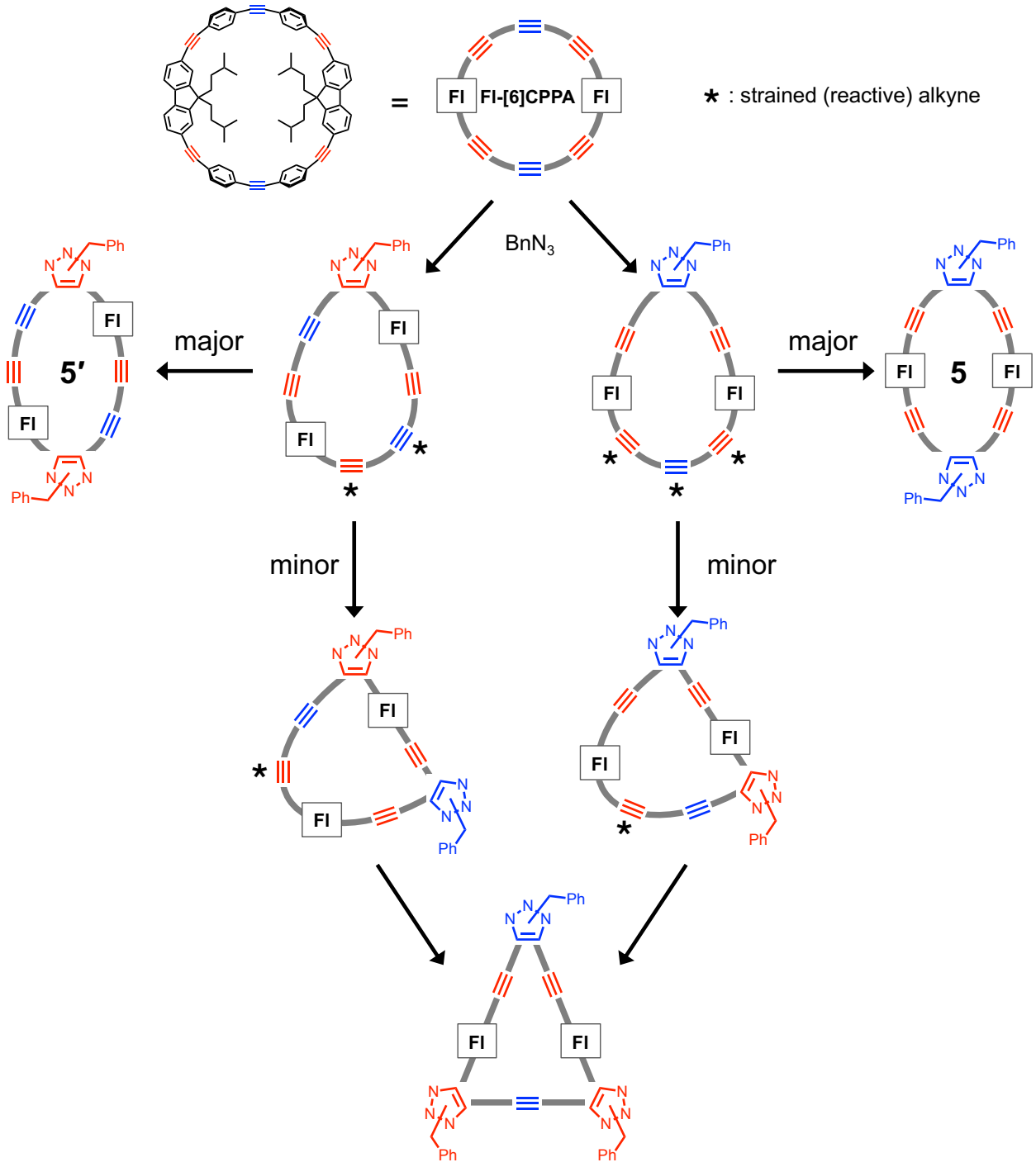


Figure S1. Proposed SPAAC reaction route of **Fl-[6]CPPA** and benzyl azide, resulting in double- and triple-SPAAC products.

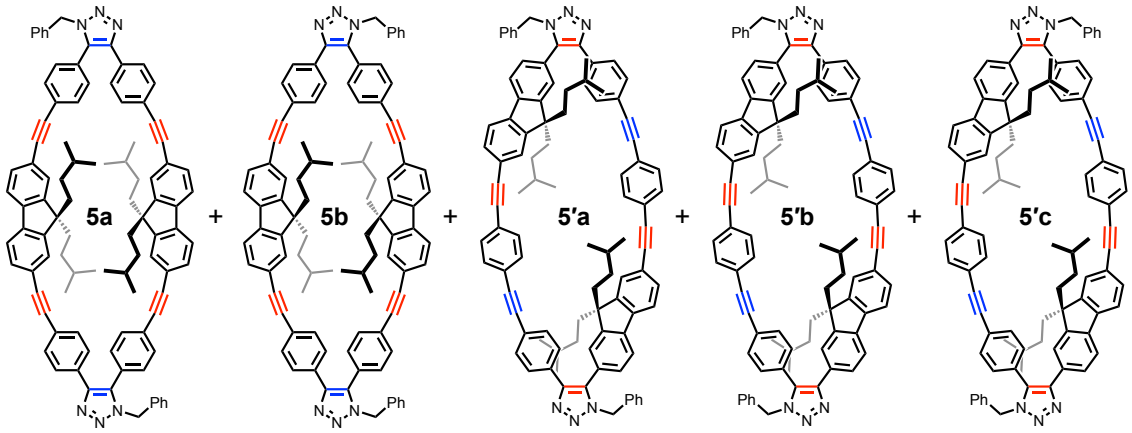


Figure S2. Proposed regioisomers of the double-SPAAC product.

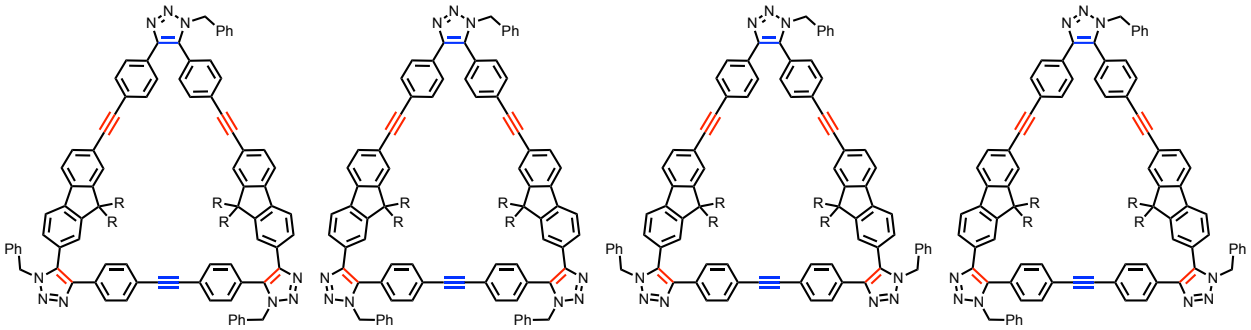


Figure S3. Proposed regioisomers of the triple-SPAAC product (R = *iso*-pentyl).

S3. ^{1}H and ^{13}C NMR & Mass Spectra of Compounds

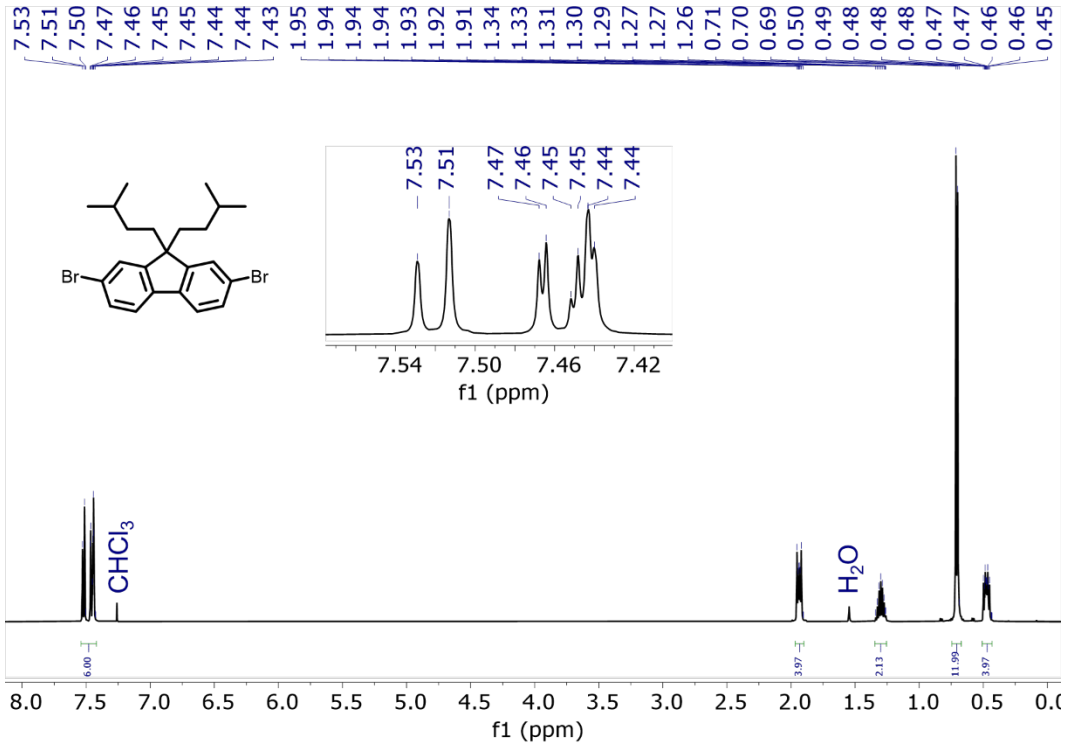


Figure S4. ^{1}H-NMR spectrum of 2,7-dibromo-9,9-di-*iso*-pentyl-9H-fluorene (400 MHz, $CDCl_3$).

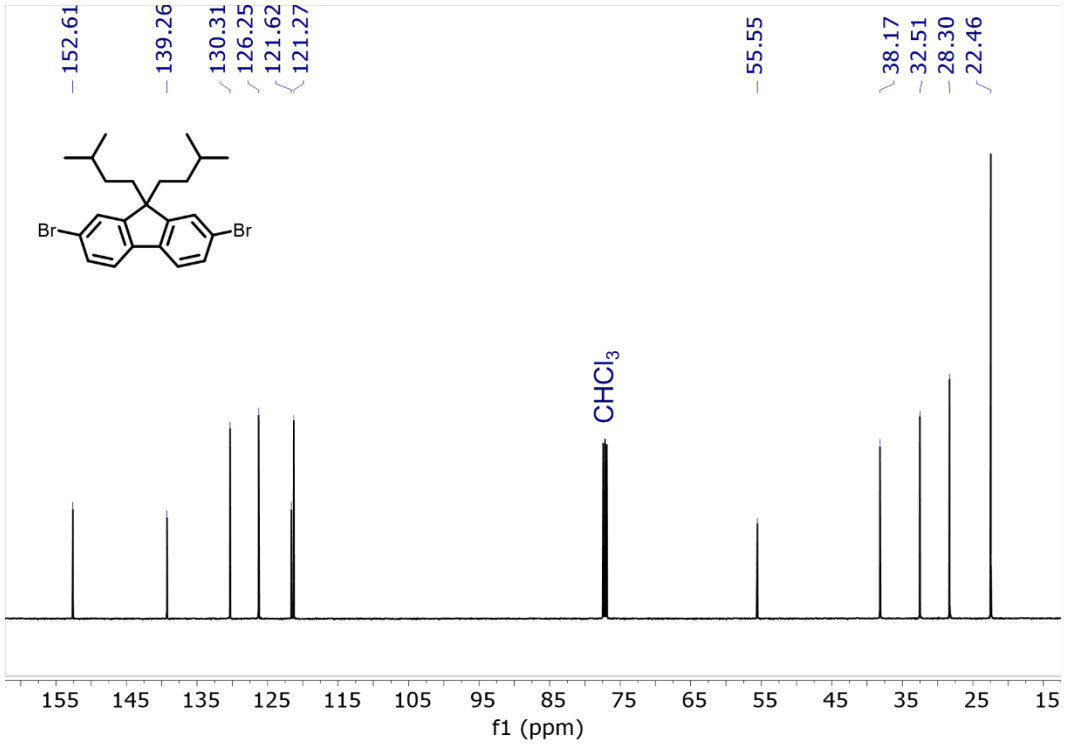


Figure S5. ^{13}C-NMR spectrum of 2,7-dibromo-9,9-di-*iso*-pentyl-9H-fluorene (126 MHz, $CDCl_3$).\

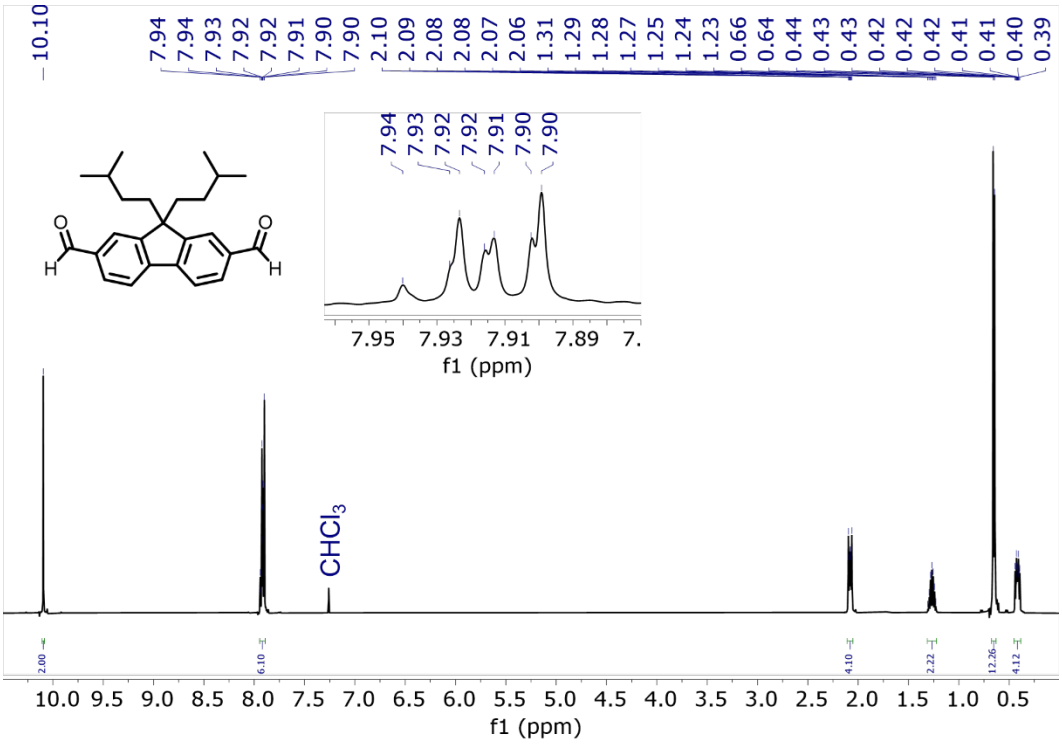


Figure S6. ^{1}H-NMR spectrum of **1** (400 MHz, $CDCl_3$).

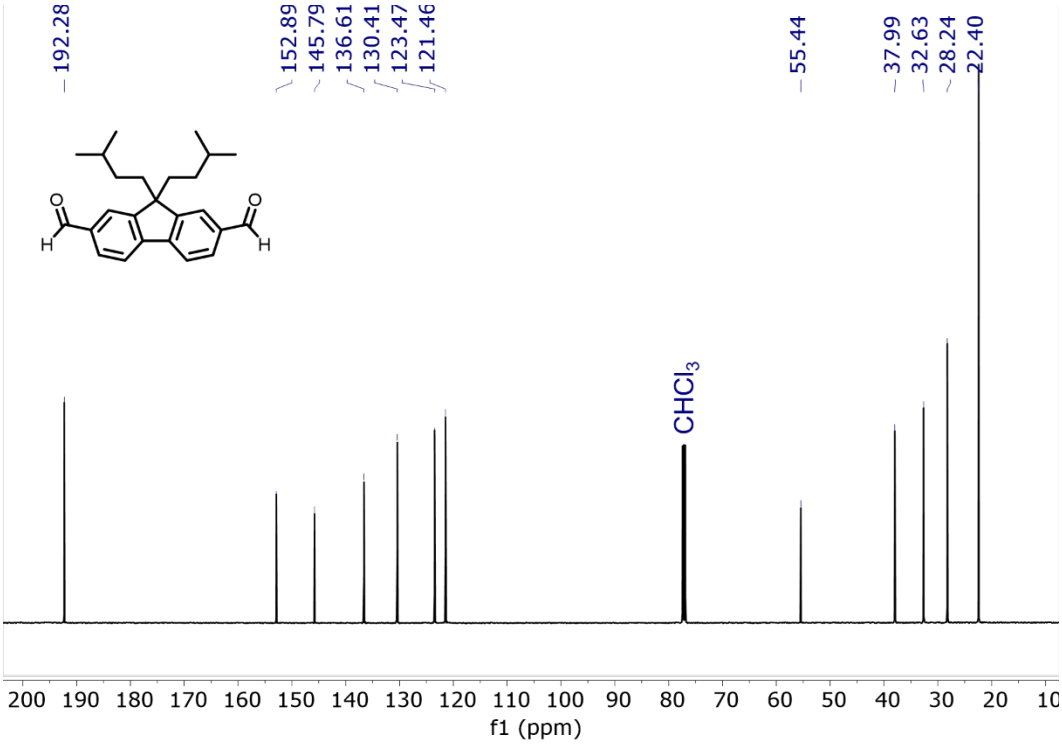


Figure S7. ^{13}C-NMR spectrum of **1** (126 MHz, $CDCl_3$).

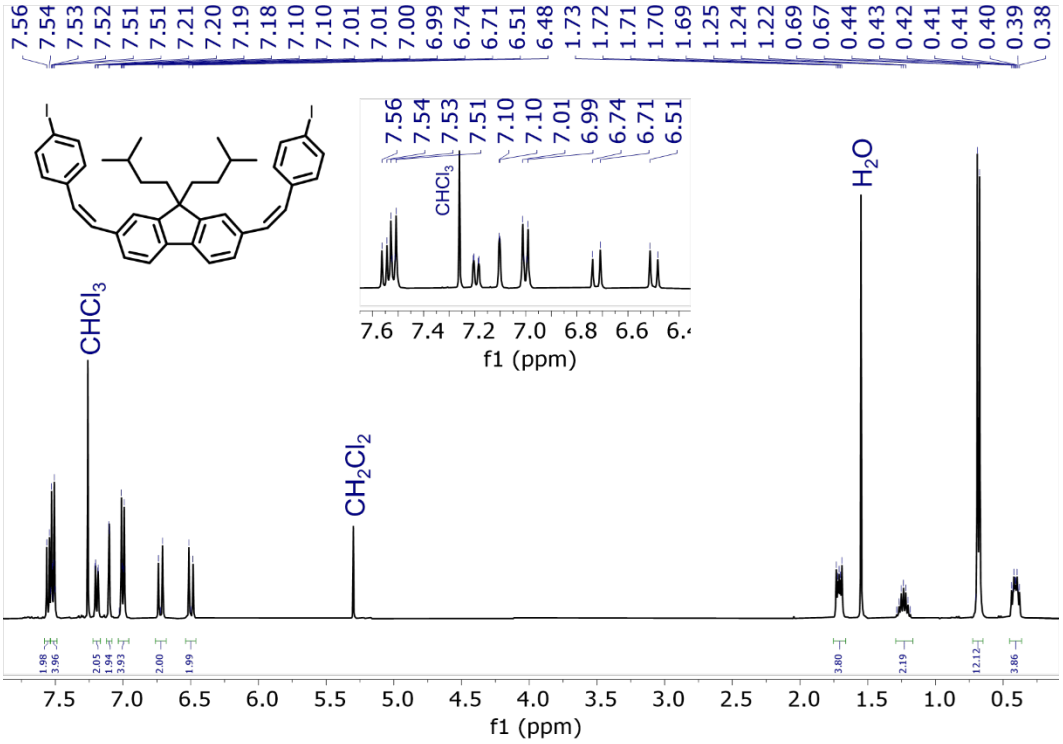


Figure S8. ^{1}H-NMR spectrum of **2** (400 MHz, $CDCl_3$).

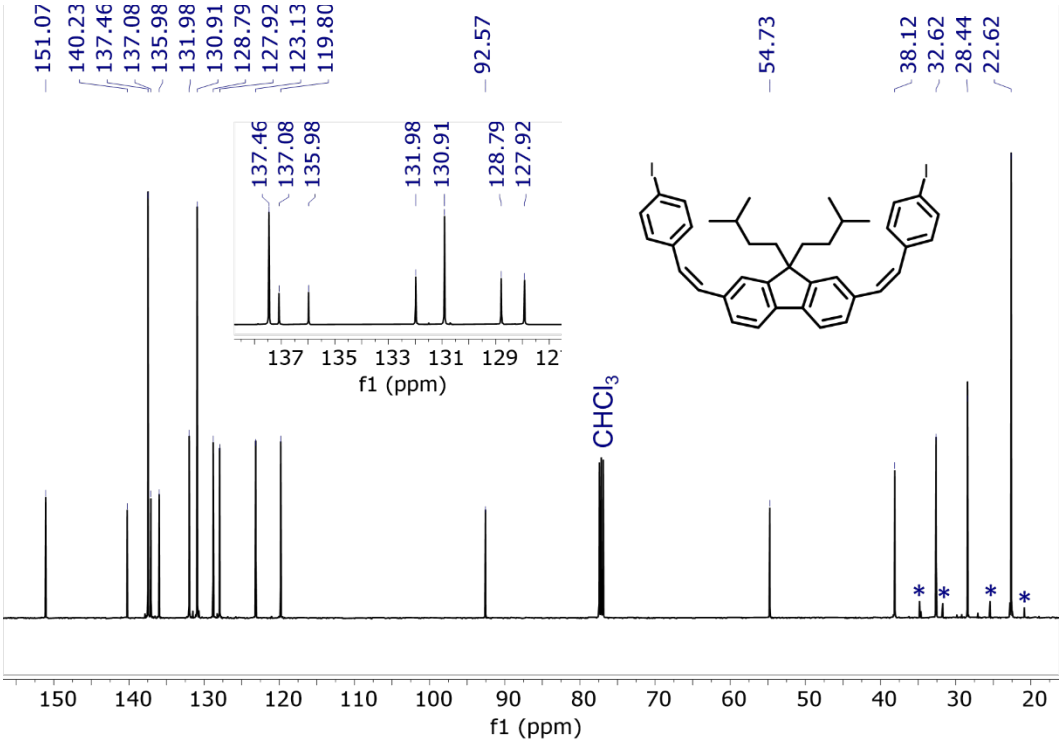


Figure S9. ^{13}C-NMR spectrum of **2** (126 MHz, $CDCl_3$).

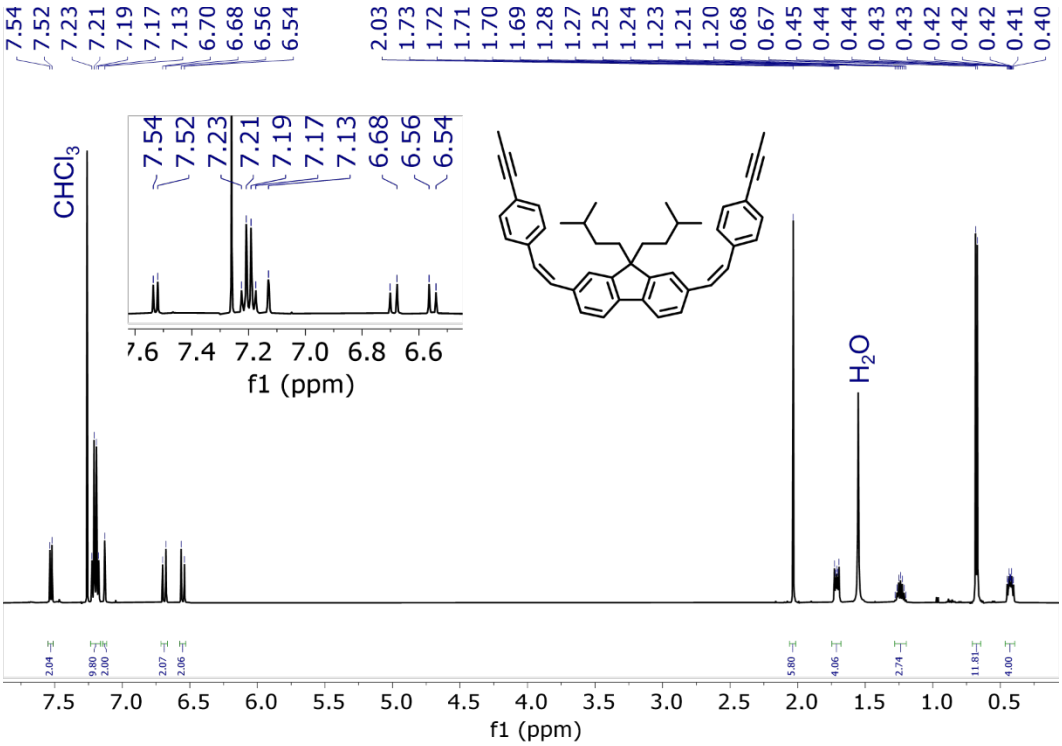


Figure S10. ^{1}H-NMR spectrum of **3** (400 MHz, $CDCl_3$).

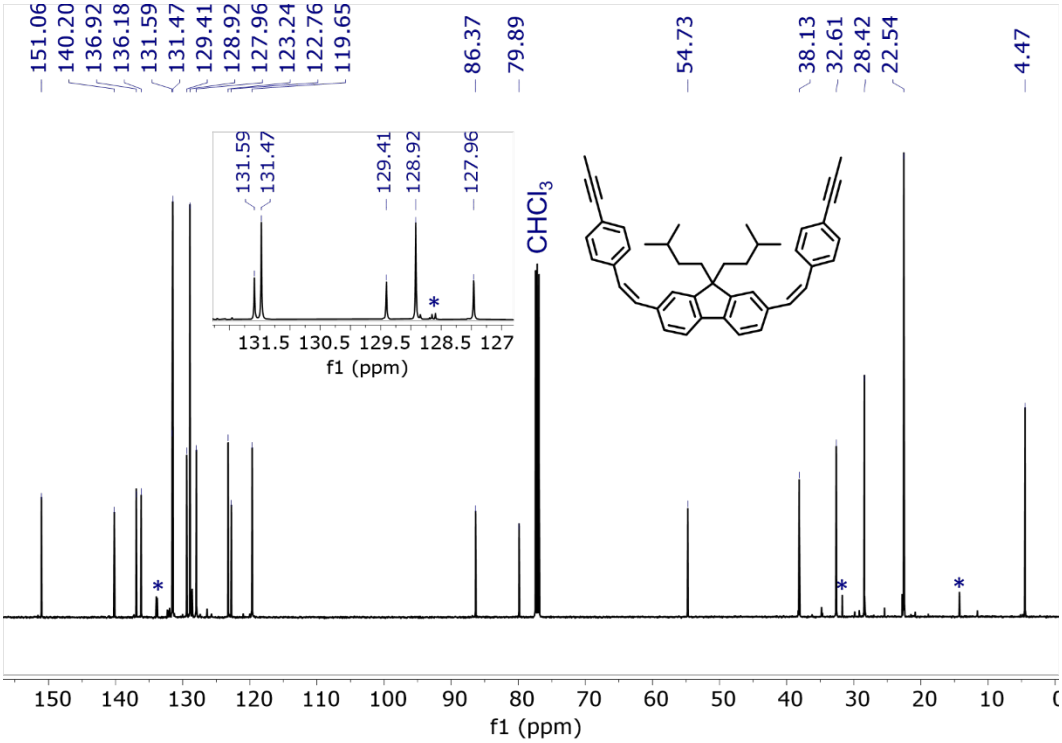


Figure S11. ^{13}C-NMR spectrum of **3** (126 MHz, $CDCl_3$).

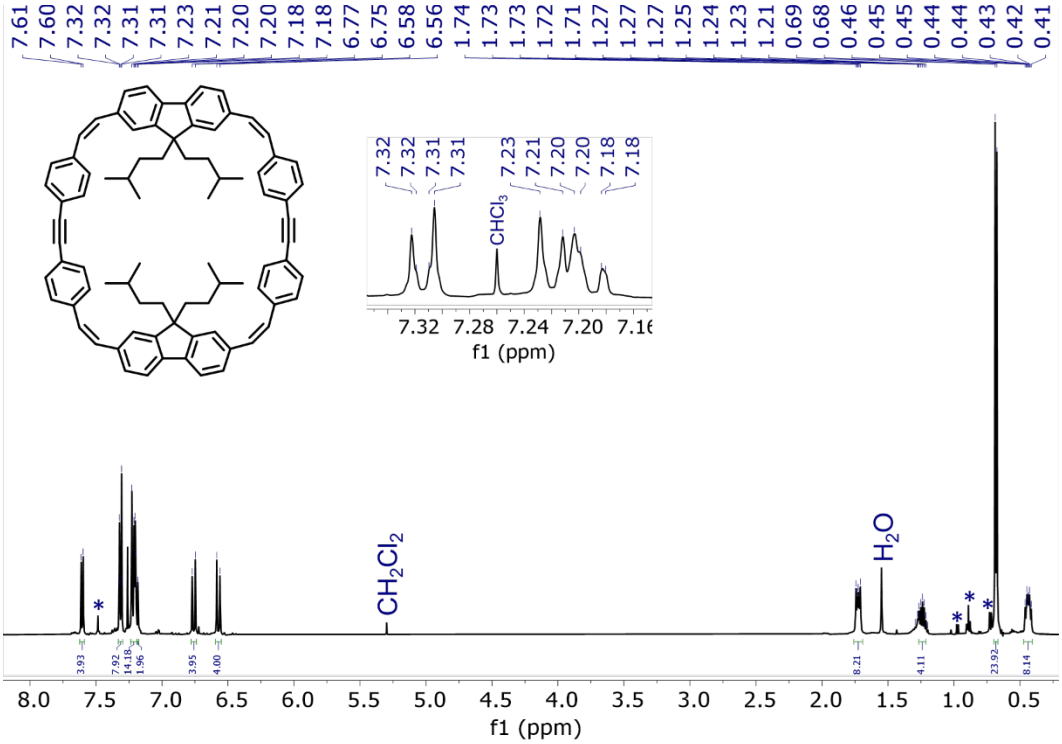


Figure S12. ^{1}H-NMR spectrum of dimer **4** (400 MHz, $CDCl_3$).

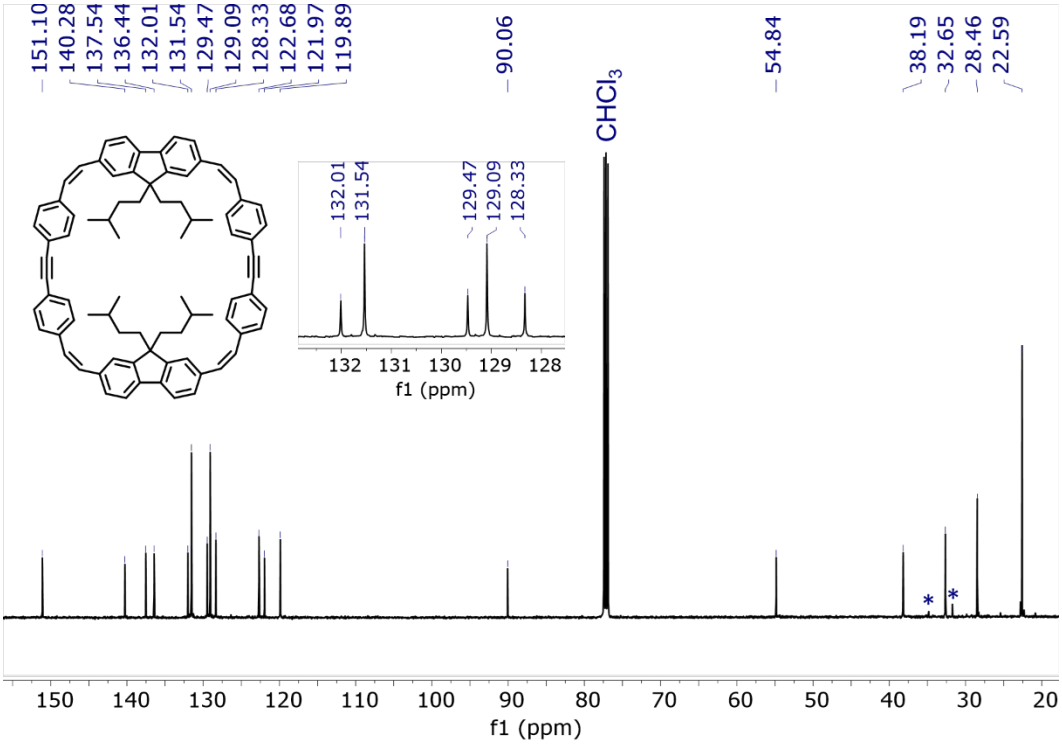


Figure S13. ^{13}C-NMR spectrum of dimer **4** (126 MHz, $CDCl_3$).

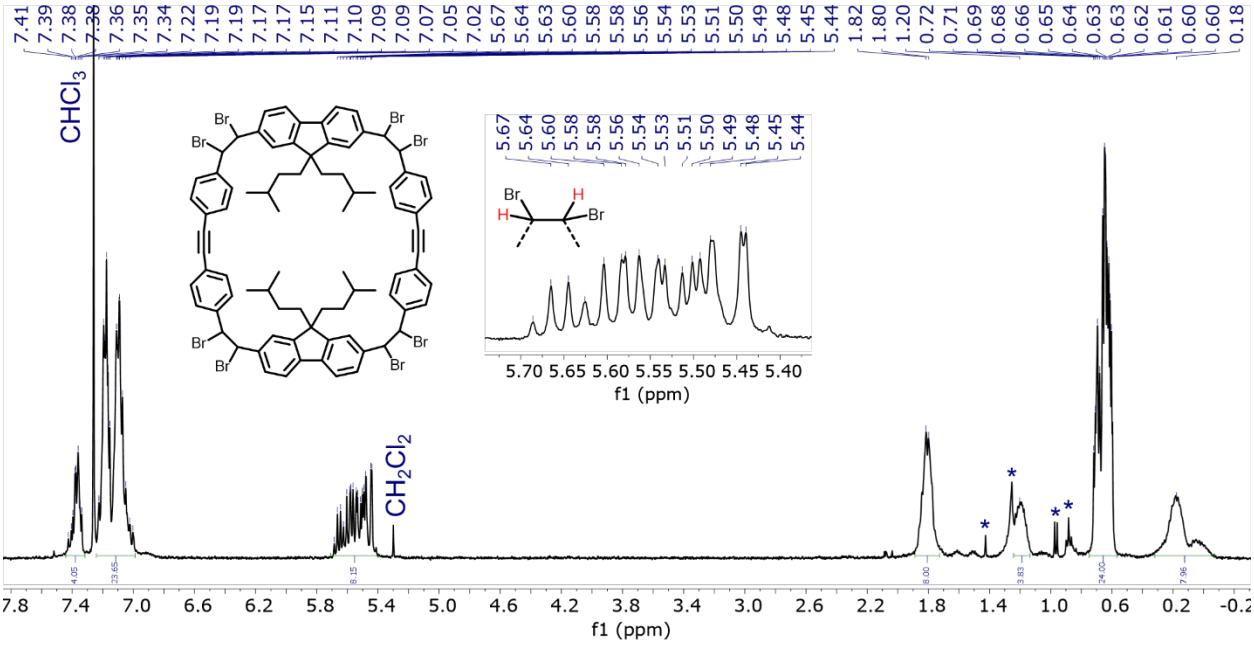


Figure S14. ^{1}H-NMR spectrum of octabrominated dimer (400 MHz, $CDCl_3$). The spectrum shows a complex mix of diastereomers.

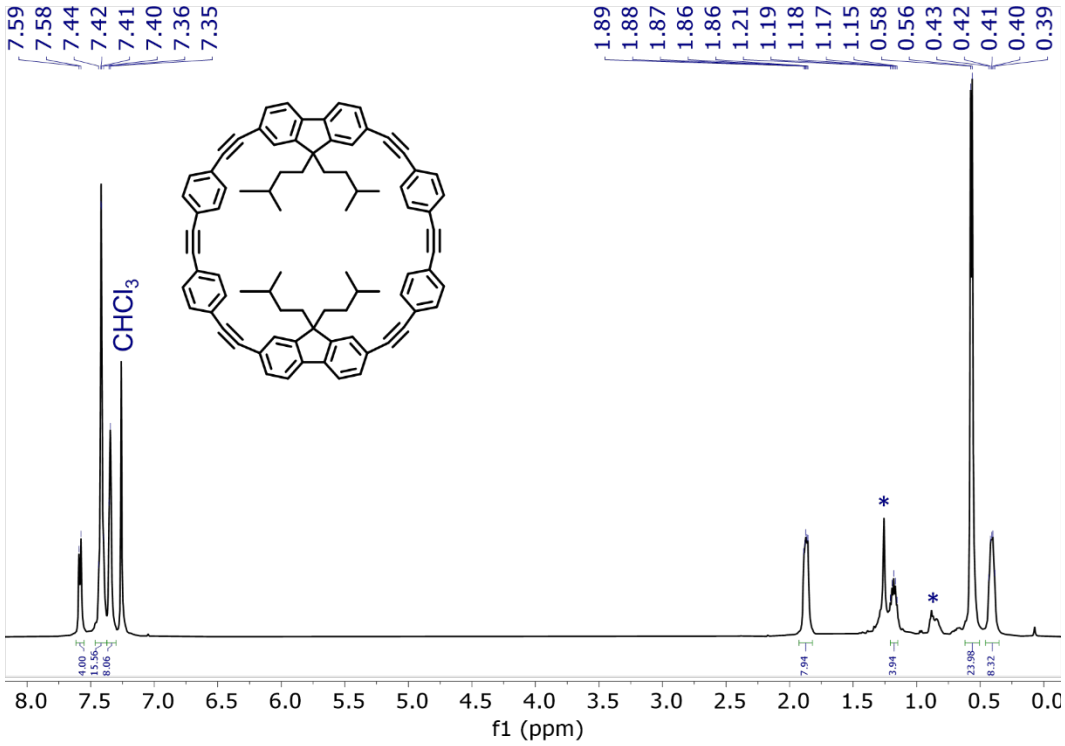


Figure S15. ^{1}H-NMR spectrum of **Fl-[6]CPPA** (400 MHz, $CDCl_3$).

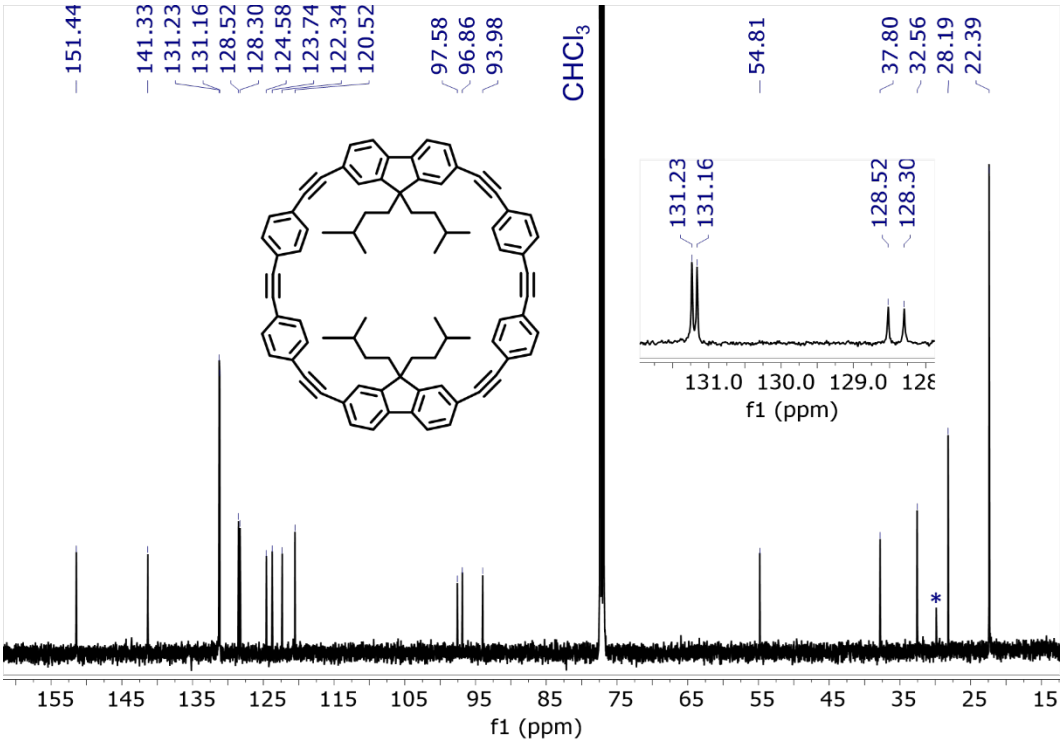


Figure S16. ^{13}C-NMR spectrum of **Fl-[6]CPPA** (126 MHz, $CDCl_3$).

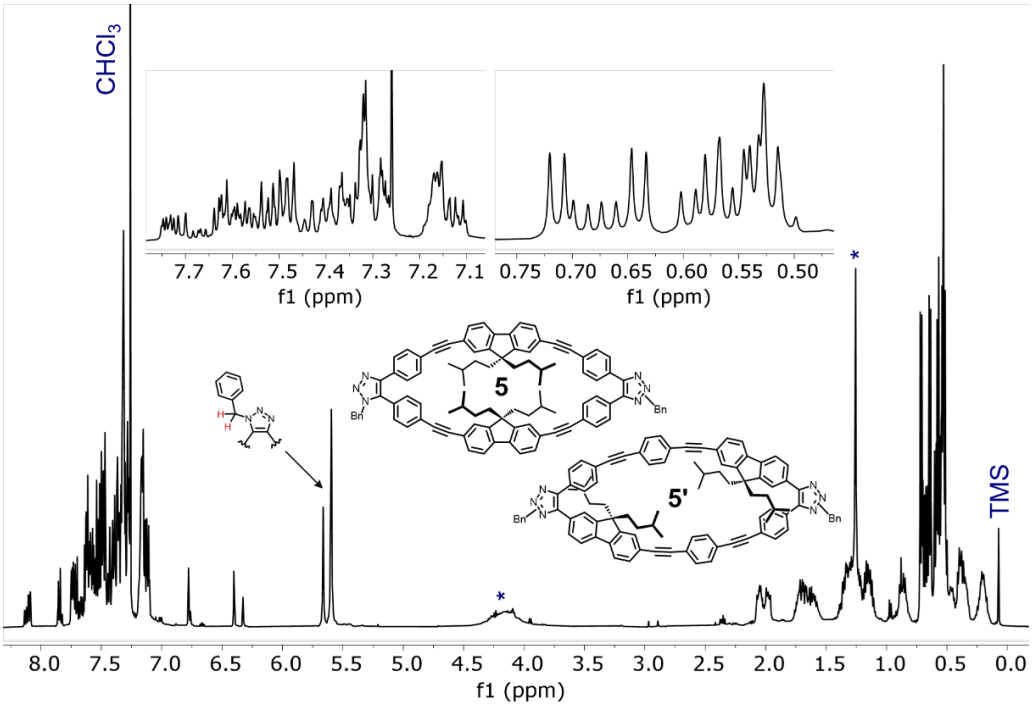


Figure S17. ^{1}H-NMR spectrum of **5** and **5′** (500 MHz, $CDCl_3$). Peaks are reported on page S7. Singlets at 5.60 and 5.66 ppm correspond to benzyl methylene (CH_2) after SPAAC.

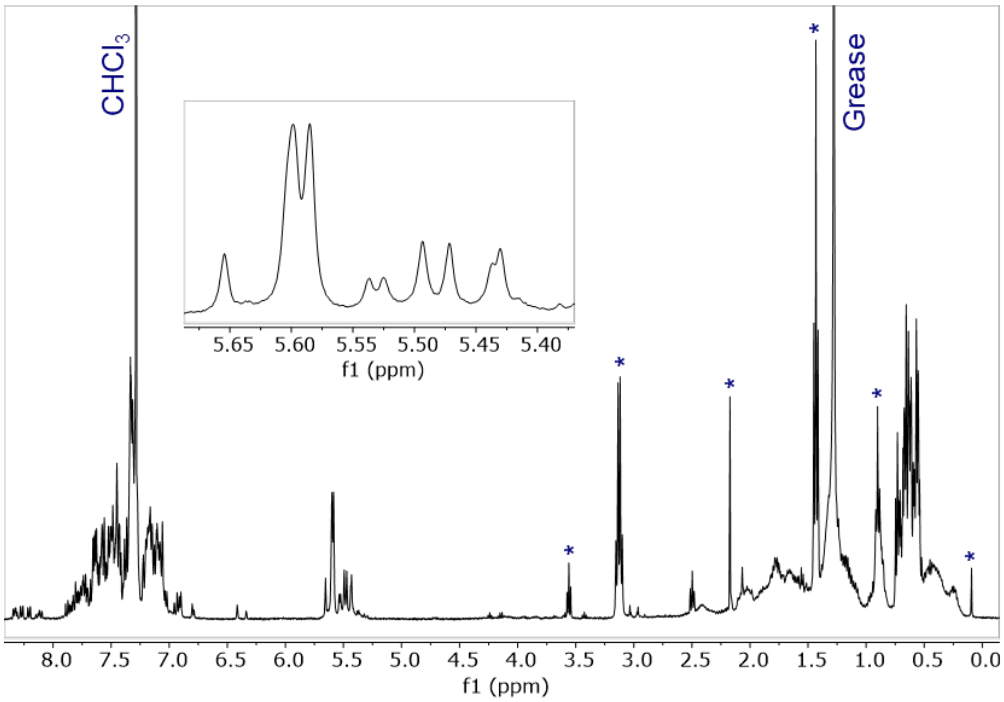


Figure S18. ^{1}H-NMR spectrum of the minor products of SPAAC with **Fl-[6]CPPA** and benzyl azide (400 MHz, $CDCl_3$), showing triple-SPAAC moieties. Impurities are labelled or otherwise starred.

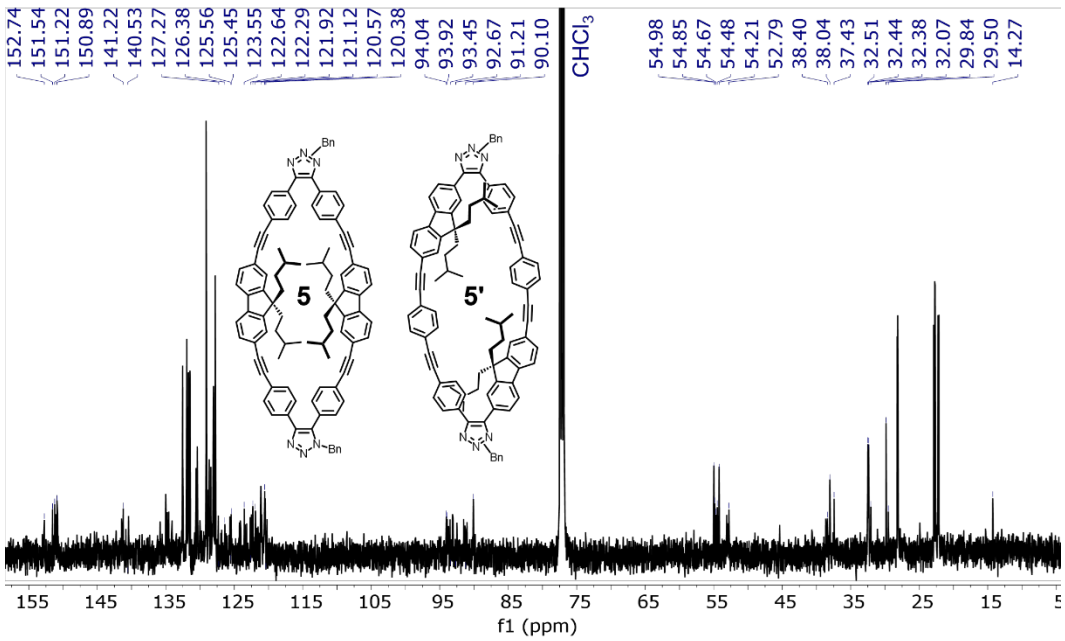


Figure S19. ^{13}C-NMR spectrum of **5** and **5′** (126 MHz, $CDCl_3$).

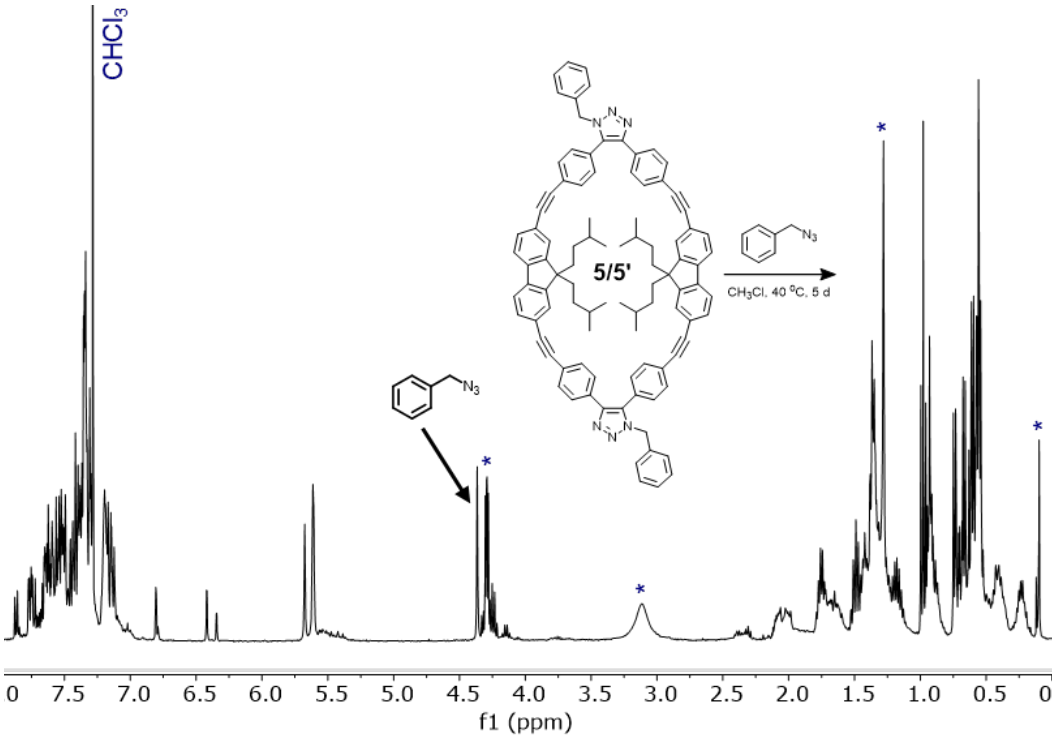


Figure S20. Crude ^{1}H-NMR spectrum of SPAAC with **5**/**5′** and benzyl azide (page S8) after 5 days of heating at 40 °C (400 MHz, $CDCl_3$). Unreacted benzyl azide (≈4.35 ppm) can be observed. **5** and **5′** still dominate the reaction mixture.

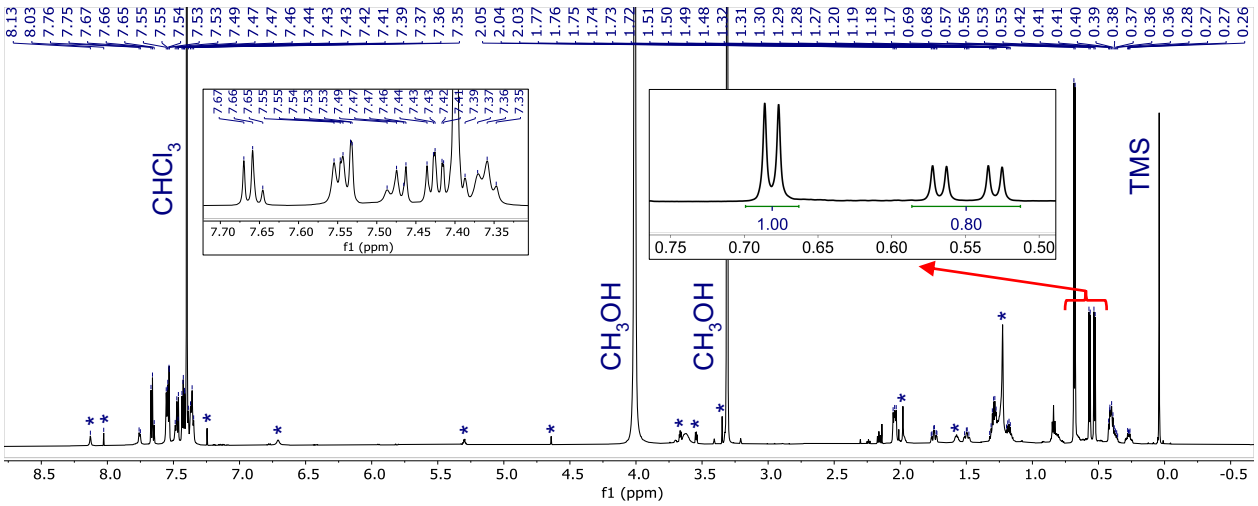


Figure S21. ^{1}H-NMR spectrum of **6** and ***6′*** (700 MHz, 4:1 $CDCl_3$:CD_3OD). The sample was prepared by precipitating **6**/**6'** in hexanes, then isolating the solid via membrane filtration. Impurities (solvents, grease, etc.) are labelled or otherwise starred. These isomers contain overlapping peaks and express poor solubility in conventional deuterated solvents, causing low signal strength and resolution of peaks.

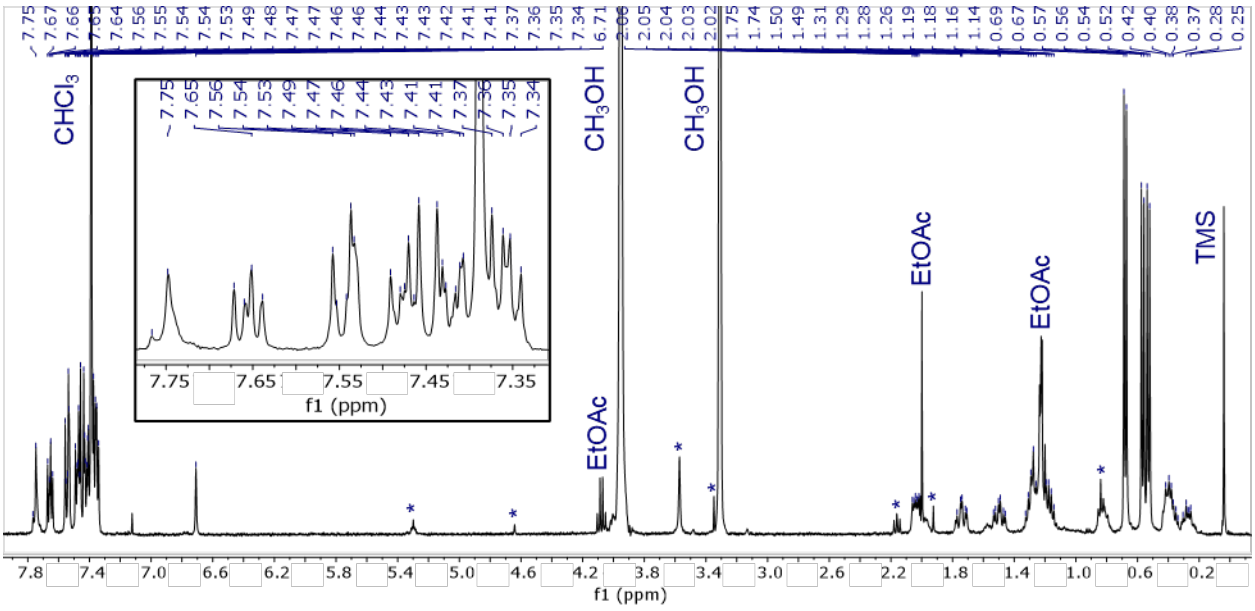


Figure S22. ^{1}H-NMR spectrum of a purified sample of **6** and ***6′*** (400 MHz, 4:1 $CDCl_3$:CD_3OD). The sample was prepared by dissolving **6**/**6'** in hot ethyl acetate and allowing the sample to cool and precipitate over the course of two days. Ethyl acetate was removed via syringe and the sample was washed with hexanes (x2). As a result of this method, the ratio of **6** to **6'** in the sample changed, with **6'** being the dominant compound in this mixture (1.6:1). Impurities (solvents, grease, etc.) are labelled or otherwise starred.

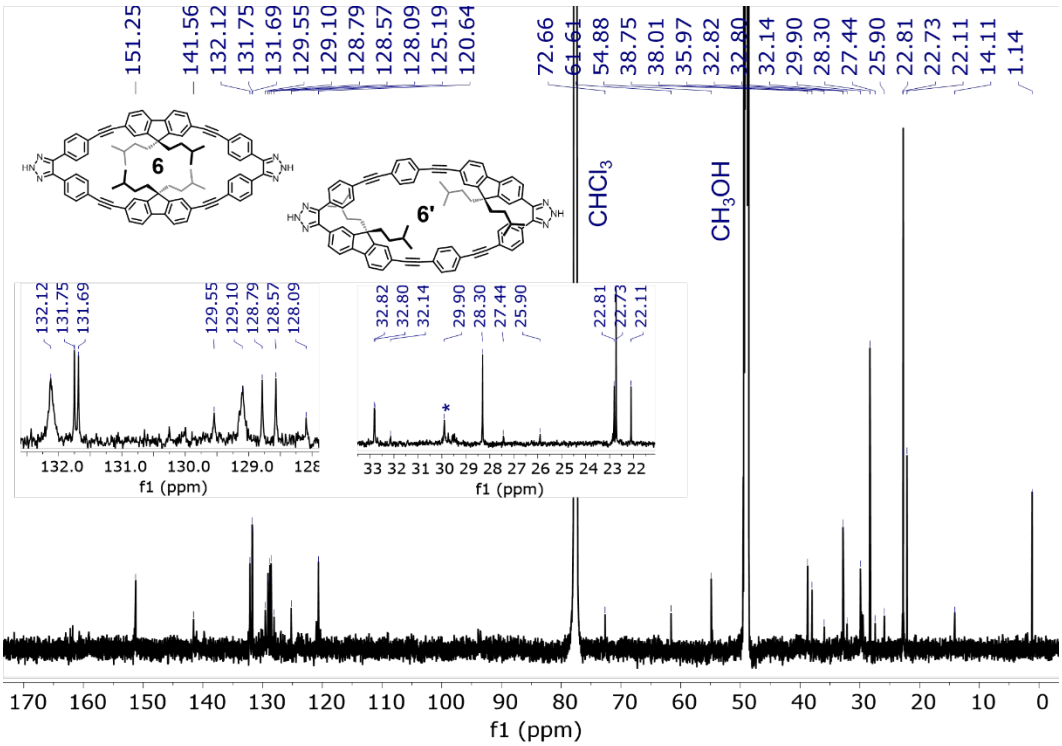


Figure S23. ^{13}C-NMR spectrum of **6** and ***6′*** (176 MHz, 4:1 $CDCl_3$:CD_3OD).

S4. 2D NMR Analysis of Double-SPAAC Products 6 and 6′

Note: Due to the limited solubility of the double-SPAAC compounds **6** and **6′** in common organic solvents ($CDCl_3$, CD_2Cl_2, DMSO-d_6, acetone-d_6, CD_3CN, CD_3OD, C_6D_6), a 4:1 mixture of $CDCl_3$:CD_3OD was used to collect all 2D NMR spectra (at 40 °C). Spectra were referenced to CHD_2OD (δ = 3.31 ppm). Also, considering the complex overlapping ^1H and ^{13}C NMR peaks in the aromatic region, we mainly focused on the aliphatic region, which clearly indicates two different compounds in two different spin systems.

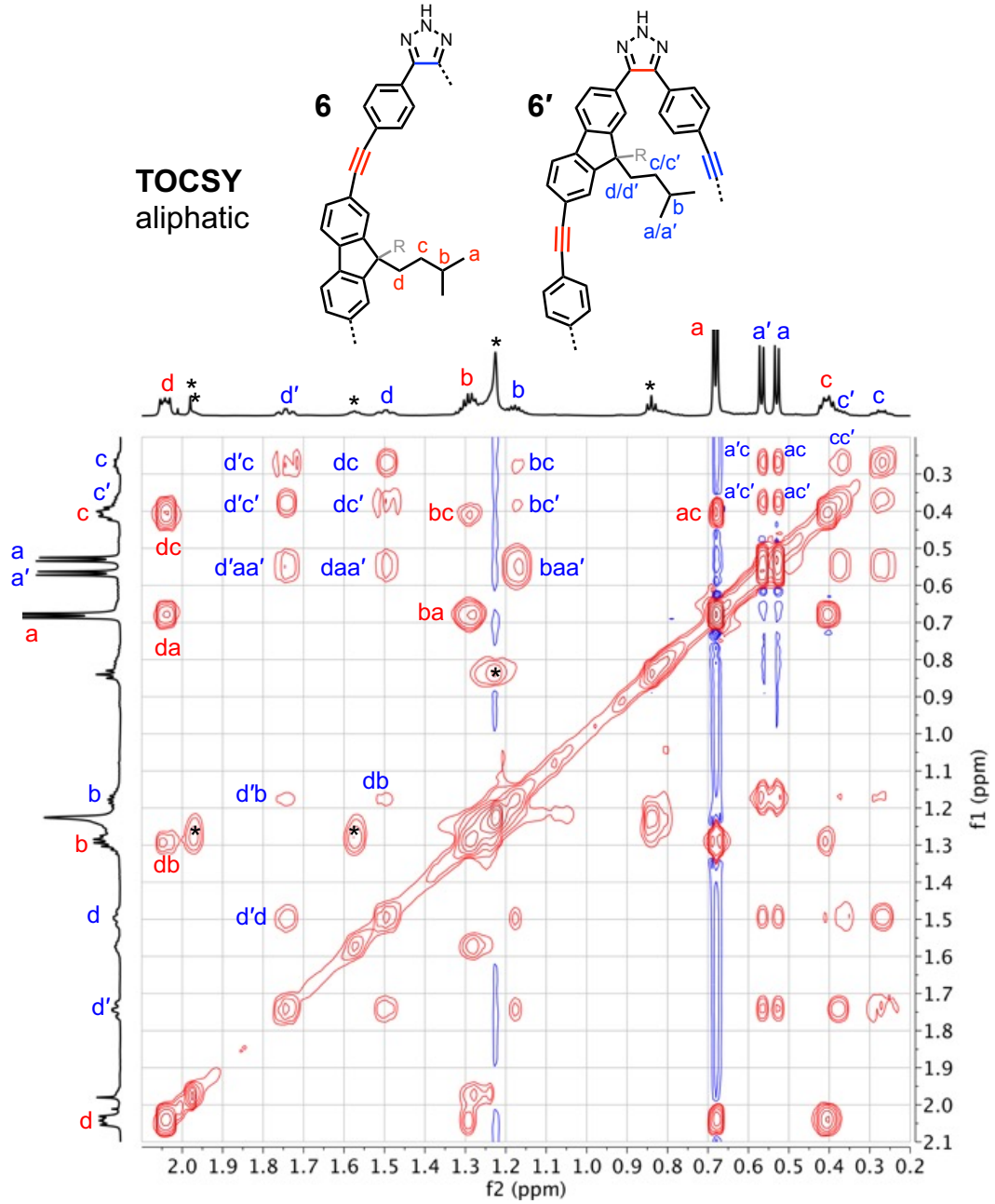


Figure S24. Total correlational spectroscopy (TOCSY) NMR spectra of the aliphatic region of **6** and **6′** (700 MHz, 4:1 $CDCl_3$:CD_3OD). Spectra were referenced to CD_3OD (δ = 3.31 ppm). Proton peaks correlating to **6** are labeled in red, and **6′** in blue. Impurities are labeled*

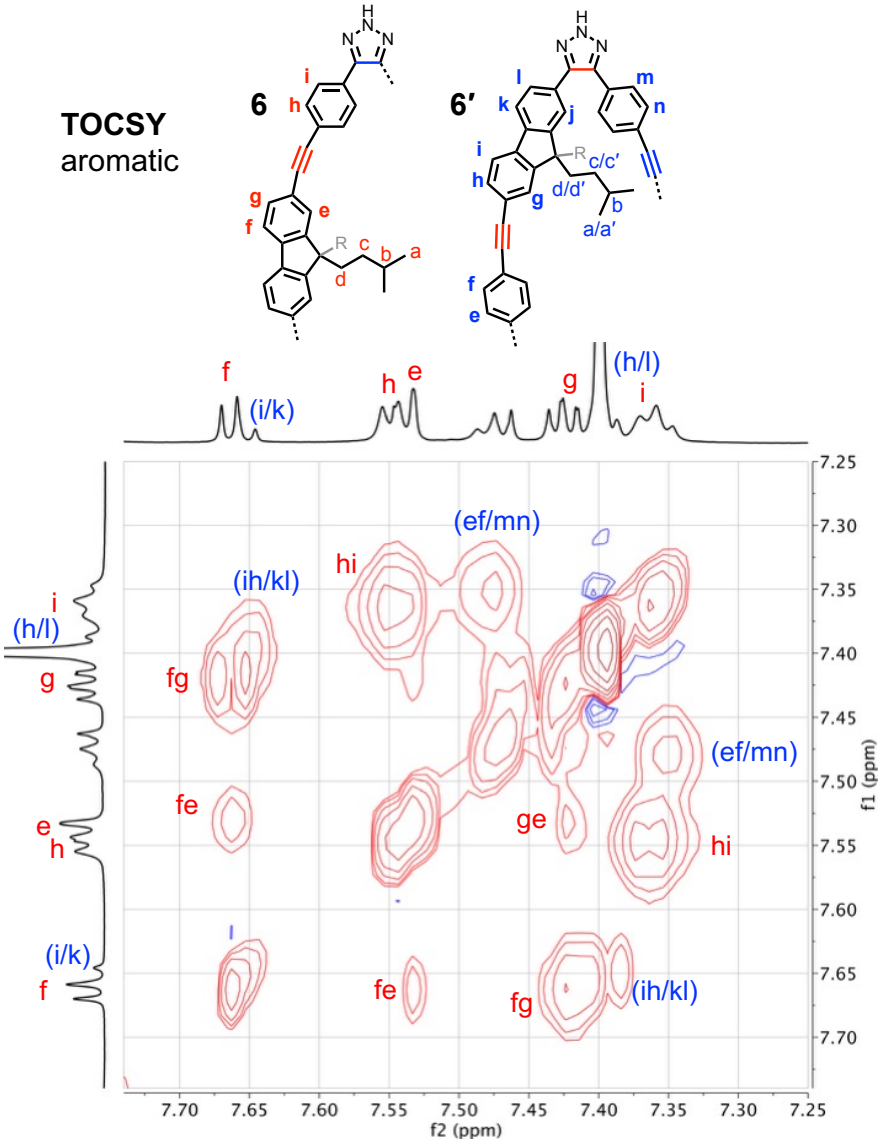


Figure S25. Total correlational spectroscopy (TOCSY) NMR spectra of the aromatic region of **6** and **6′** (700 MHz, 4:1 $CDCl_3$:CD_3OD). Spectra were referenced to CD_3OD (δ = 3.31 ppm). Proton peaks correlating to **6** are labeled in red, and **6′** in blue. We note that the proton peaks of the less symmetric product **6′** were predominantly overlapping with the more symmetric **6**, making it difficult to analyze and assign. The cross peaks labeled in parentheses are speculative assignments based on HSQC and HMBC. Impurities are labeled*

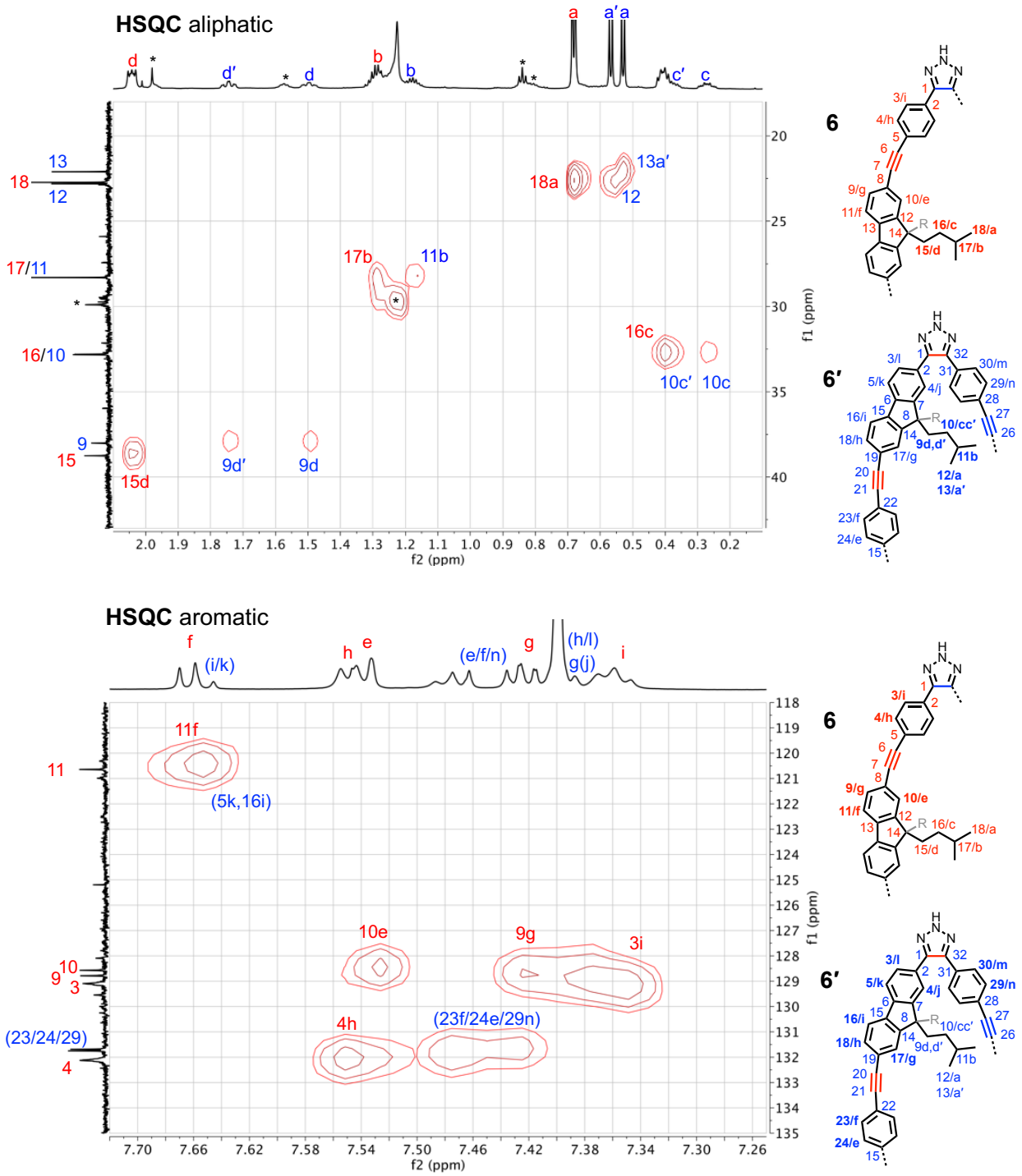


Figure S26. Heteronuclear single quantum coherence (HSQC) NMR spectra of the (top) aliphatic and (bottom) aromatic regions of **6** and **6′** (^{1}H-NMR, 700 MHz; ^{13}C-NMR, 176 MHz; 4:1 $CDCl_3$:CD_3OD). Spectra were referenced to CD_3OD (δ = 3.31 ppm). Carbons are numbered, and relevant hydrogens are lettered. Peaks correlating to **6** are labeled in red, and **6′** in blue. We note that the proton peaks of the less symmetric product **6′** were predominantly overlapping with the more symmetric **6**, making it difficult to analyze and assign. The cross peaks labeled in parentheses are speculative assignments. Impurities are labeled*

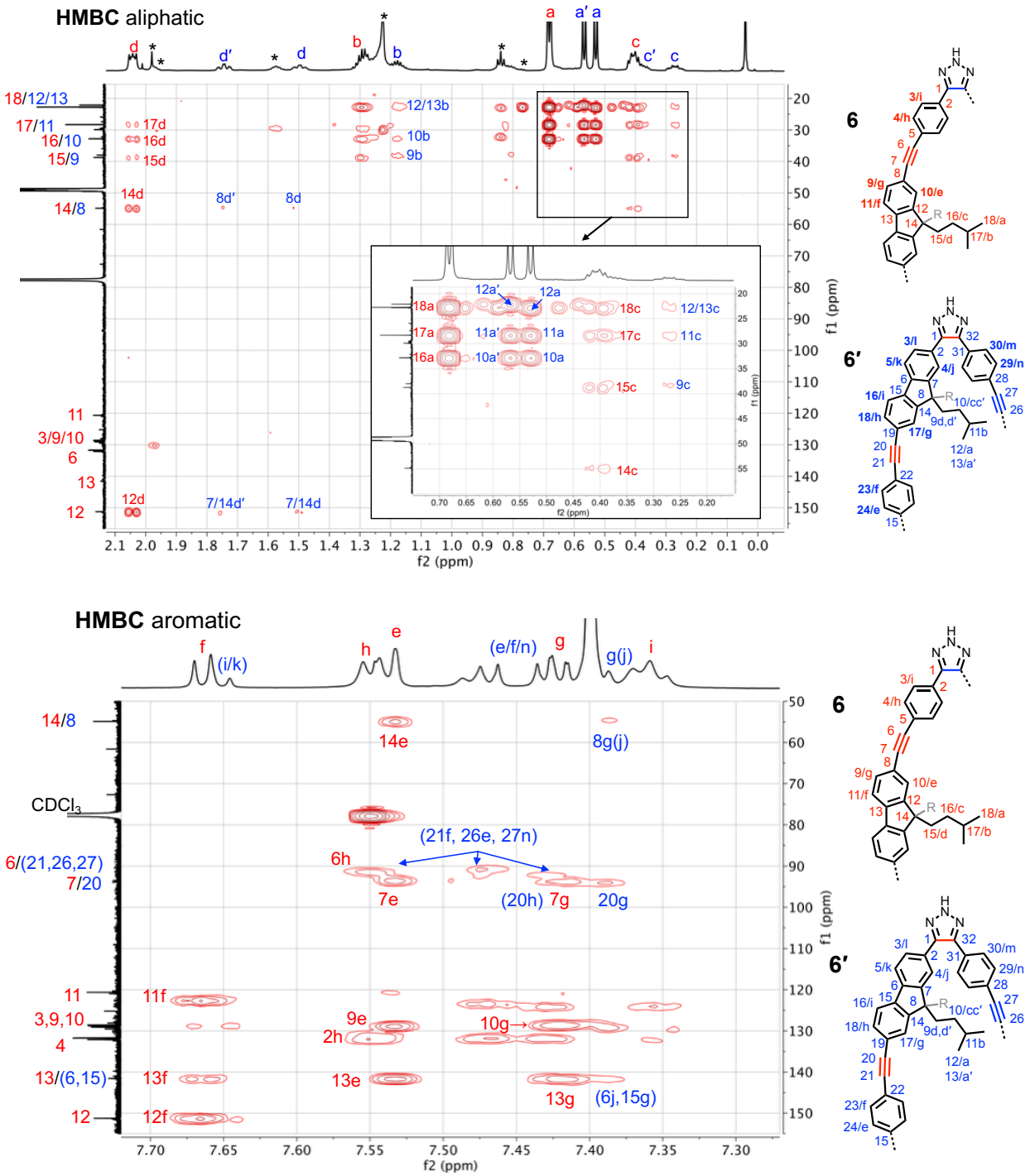


Figure S27. Heteronuclear multiple bond correlation (HMBC) NMR spectra of the (top) aliphatic and (bottom) aromatic regions of **6** and **6′** (^{1}H-NMR, 700 MHz; ^{13}C-NMR, 176 MHz; 4:1 $CDCl_3$:CD_3OD). Spectra were referenced to CD_3OD (δ = 3.31 ppm). Carbons are numbered, and relevant hydrogens are lettered. Peaks correlating to **6** are labeled in red, and **6′** in blue. We note that the proton peaks of the less symmetric product **6′** were predominantly overlapping with the more symmetric **6**, making it difficult to analyze and assign. The cross peaks labeled in parentheses are speculative assignments. Impurities are labeled*

S5. Mass Spectrometry Analysis of Compounds

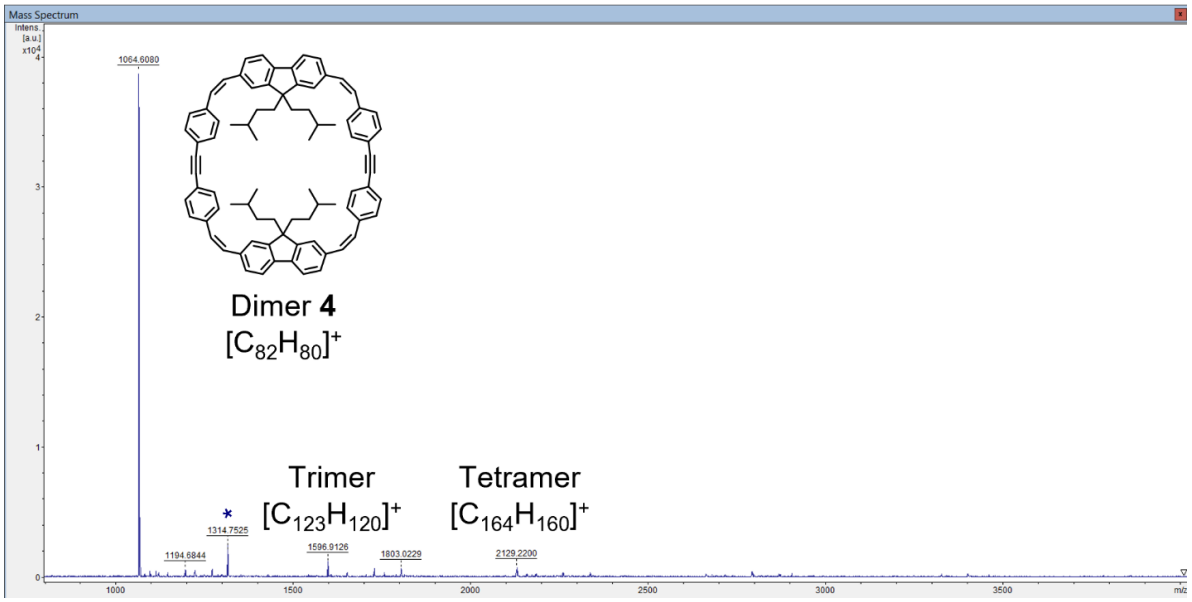


Figure S28. MALDI-TOF spectrum of a crude mixture of dimer **4** post-metathesis, showing trace amounts of trimer and tetramer. The starred impurity detected at 1314.7525 g/mol corresponds with the addition of a *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) matrix molecule (250.15 g/mol) to the dimer.

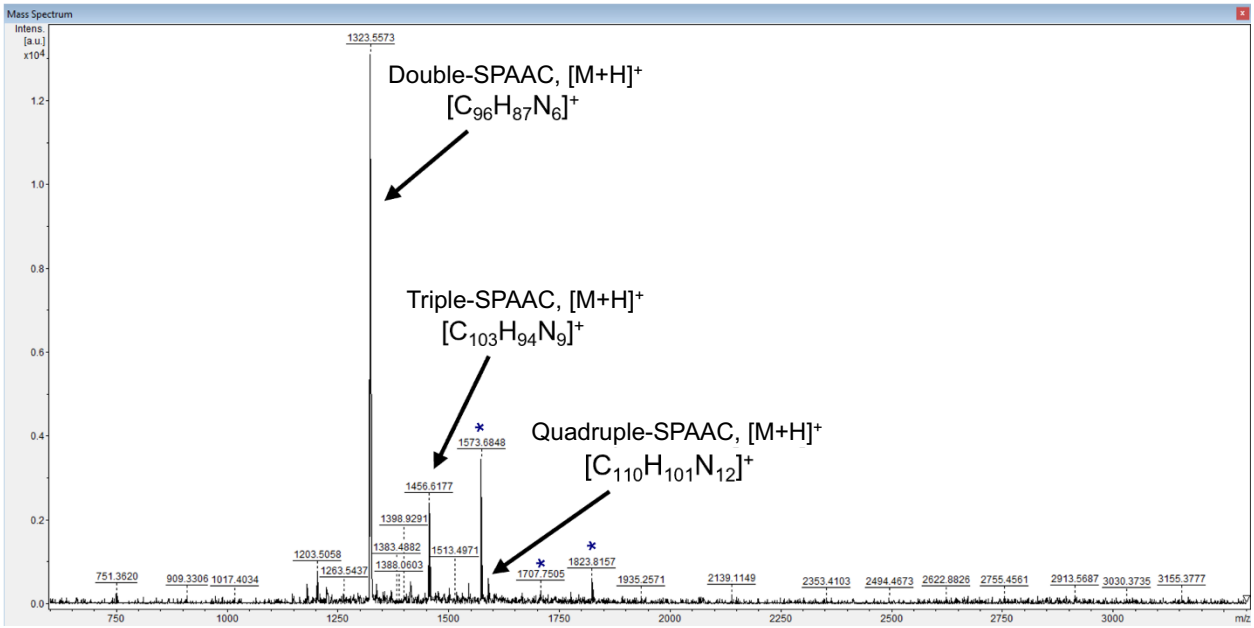


Figure S29. MALDI-TOF spectrum of a crude reaction mixture of SPAAC with approximately 2.4 equivalents of benzyl azide, showing triple- and quadruple-SPAAC products. The major product, double-SPAAC **5**/**5′**, can be isolated via column chromatography. Notably, the single-SPAAC intermediate ($C_{89}H_{79}N_3$, 1189.63 g/mol) was not detected. The starred peaks correspond to the addition of one or two DCTB matrix molecules to the products.

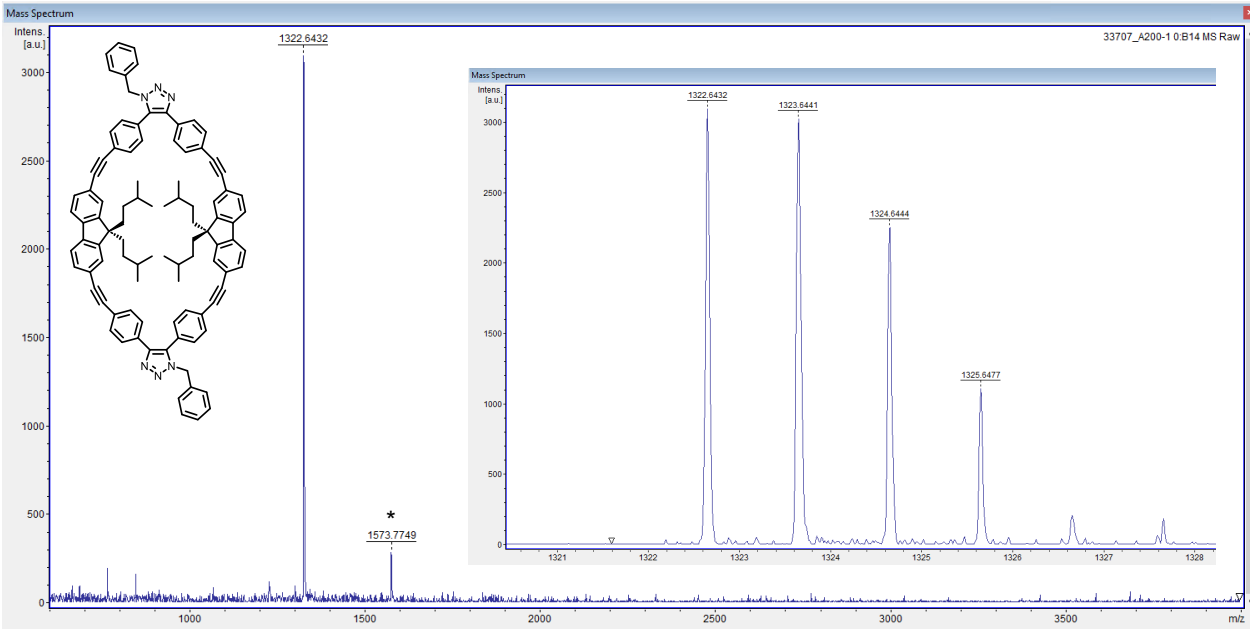


Figure S30. MALDI-TOF spectrum of a mixture of **5**/**5′** purified via column chromatography. Starred peaks correspond to the addition of one DCTB matrix molecule to the regioisomers.

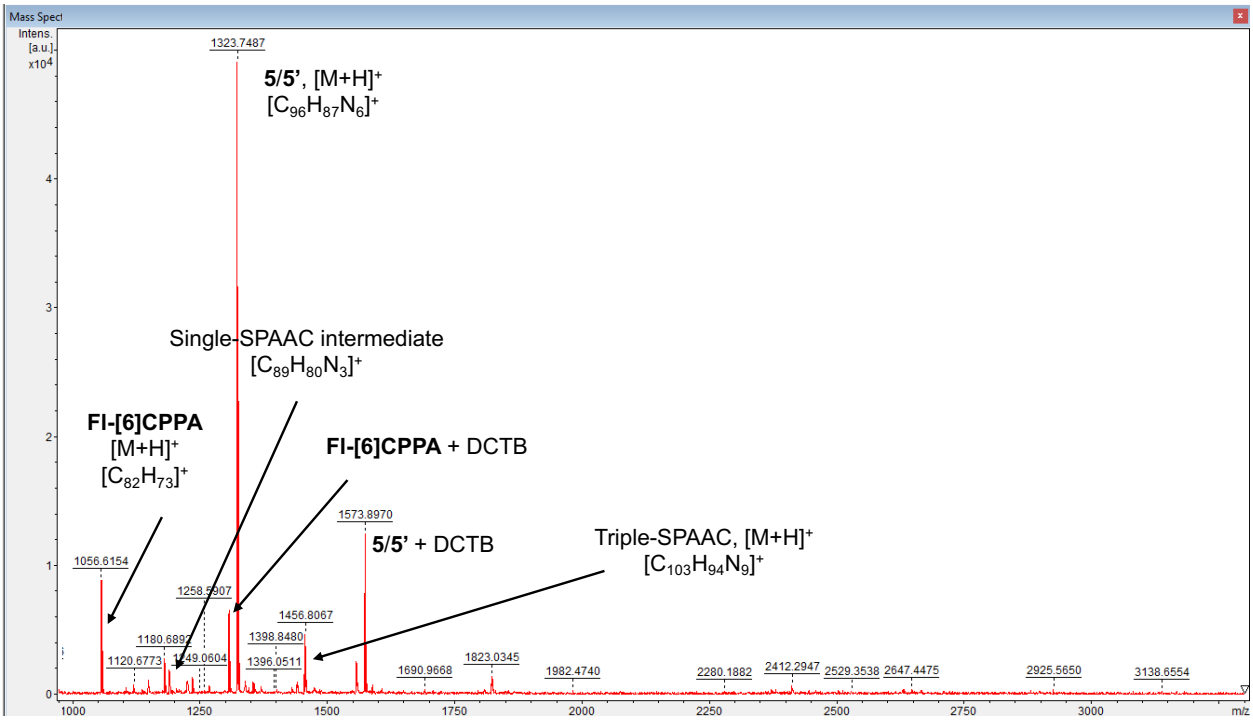


Figure S31. MALDI-TOF spectrum of a crude mixture SPAAC with equimolar **Fl-[6]CPPA** and benzyl azide (page S8). Unreacted **Fl-[6]CPPA** and double-SPAAC **5**/**5′** dominate the mixture as major products, with trace amounts of triple-SPAAC product and single-SPAAC intermediate also detected.

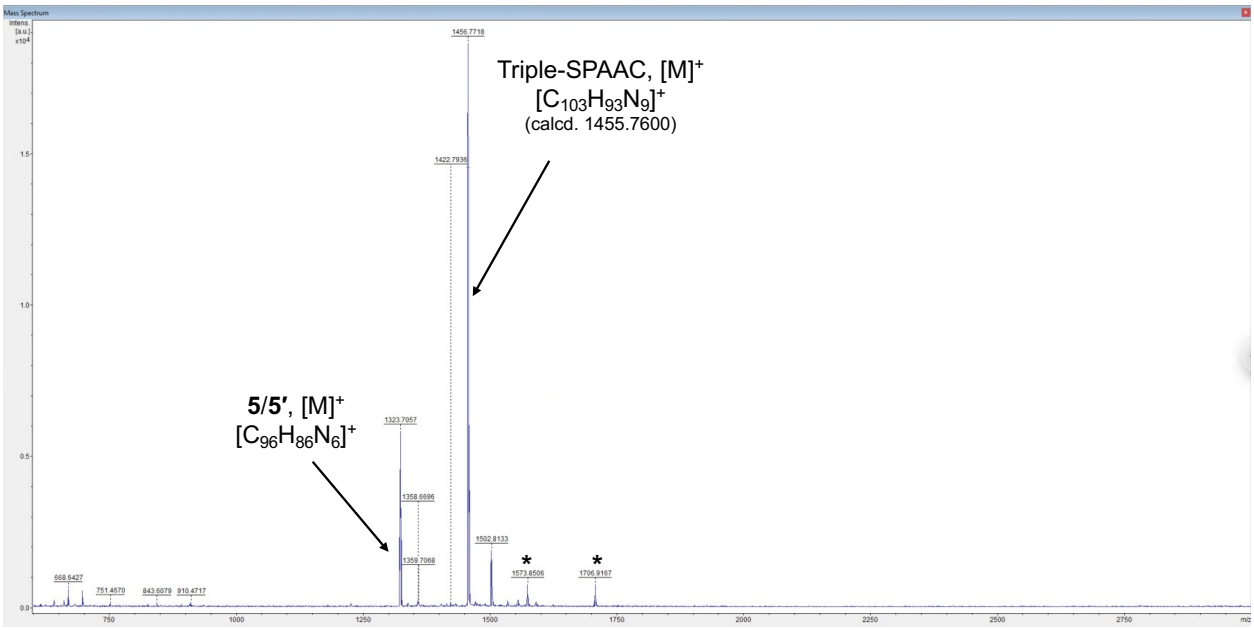


Figure S32. MALDI-TOF spectrum of the minor product of SPAAC with **Fl-[6]CPPA** and 2.4 equivalents of benzyl azide (Page S7), isolated via column chromatography. The spectrum primarily shows triple-SPAAC species, which were obtained in 20% yield. Starred peaks correspond to the addition of one DCTB matrix molecule to the products.

S6. X-ray Crystallography

Data for **Fl-[6]CPPA**, **5a**, and **6** were collected at 100K on a Bruker D8 Venture DUO diffractometer with a Photon III C14 detector and CuKα and AgKα microfocus X-ray sources. Images, distances, strain angles, and dihedral angles of solid-state **Fl-[6]CPPA**, **5** (**5a**), and **6** were processed and rendered via Mercury 2023.3.0.

Single crystals of **Fl-[6]CPPA** suitable for X-ray diffraction (XRD) were grown by slowly diffusing pentane into a concentrated solution in tetrahydrofuran. **Fl-[6]CPPA** used AgKα radiation and crystallized with two independent molecules, both on inversion centers. One isopropyl group was disordered and disordered solvent contribution was removed using SQUEEZE; R=0.078 for 9065 observed (of 15087 independent) data, CCDC 2392291.

Single crystals of **5** (**5a**) suitable for XRD were grown by slowly diffusing pentane into a concentrated solution in chloroform. **5** (**5a**) used CuKα radiation and crystallized with the molecule on an inversion center as the bis chloroform solvate. Some restraints were necessary to control the displacement parameters of the benzyl group; R=0.143 for 2934 observed (of 6087 independent) data, CCDC 2392290.

Single crystals of **6** suitable for XRD were grown by slowly evaporating a solution of **6** in ethyl acetate. **6** used CuKα radiation and crystallized with the molecule on an inversion center as the bis ethyl acetate solvate. Many displacement parameter restraints were necessary to control the refinement; R=0.135 for 1353 observed (of 3779 independent) data, CCDC 2392289.

Fl-[6]CPPA (CCDC 2392291)

Crystal data

$C_{82}H_{72}$·2.33(C_4H_8O)	Z = 2
M_r = 1225.03	F(000) = 1314
Triclinic, P-1	D_x = 1.142 Mg m^{-3}
a = 10.825 (4) Å	Ag $K\alpha$ radiation, λ = 0.56086 Å
b = 18.566 (6) Å	Cell parameters from 3280 reflections
c = 19.147 (6) Å	θ = 2.2–19.8°
α = 107.809 (12)°	μ = 0.04 mm^{-1}
β = 100.919 (11)°	T = 100 K
γ = 93.994 (11)°	Needle, colourless
V = 3564 (2) Å^3	0.30 × 0.11 × 0.07 mm

Data collection

Bruker D8 Venture DUO with Photon III C14 diffractometer	7943 reflections with $I > 2\sigma(I)$
Radiation source: IμS 3.0 microfocus	R_{int} = 0.237
ϕ and ω scans	θ_{max} = 19.9°, θ_{min} = 1.9°

Absorption correction: multi-scan *SADABS* (Krause *et al.*, 2015)	h = -13 – 13
T_{min} = 0.938, T_{max} = 0.997	k = -22 – 22
95656 measured reflections	l = -23 – 23
13128 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.082	$w = 1/[\sigma^2(F_o^2) + (0.1265P)^2 + 0.5313P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.247	$(\Delta/\sigma)_{max} < 0.001$
S = 1.01	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
13128 reflections	$\Delta\rho_{min}$ = -0.41 e Å^{-3}
740 parameters	Extinction correction: *SHELXL2019*/1 (Sheldrick 2019), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
0 restraints	Extinction coefficient: 0.036 (3)

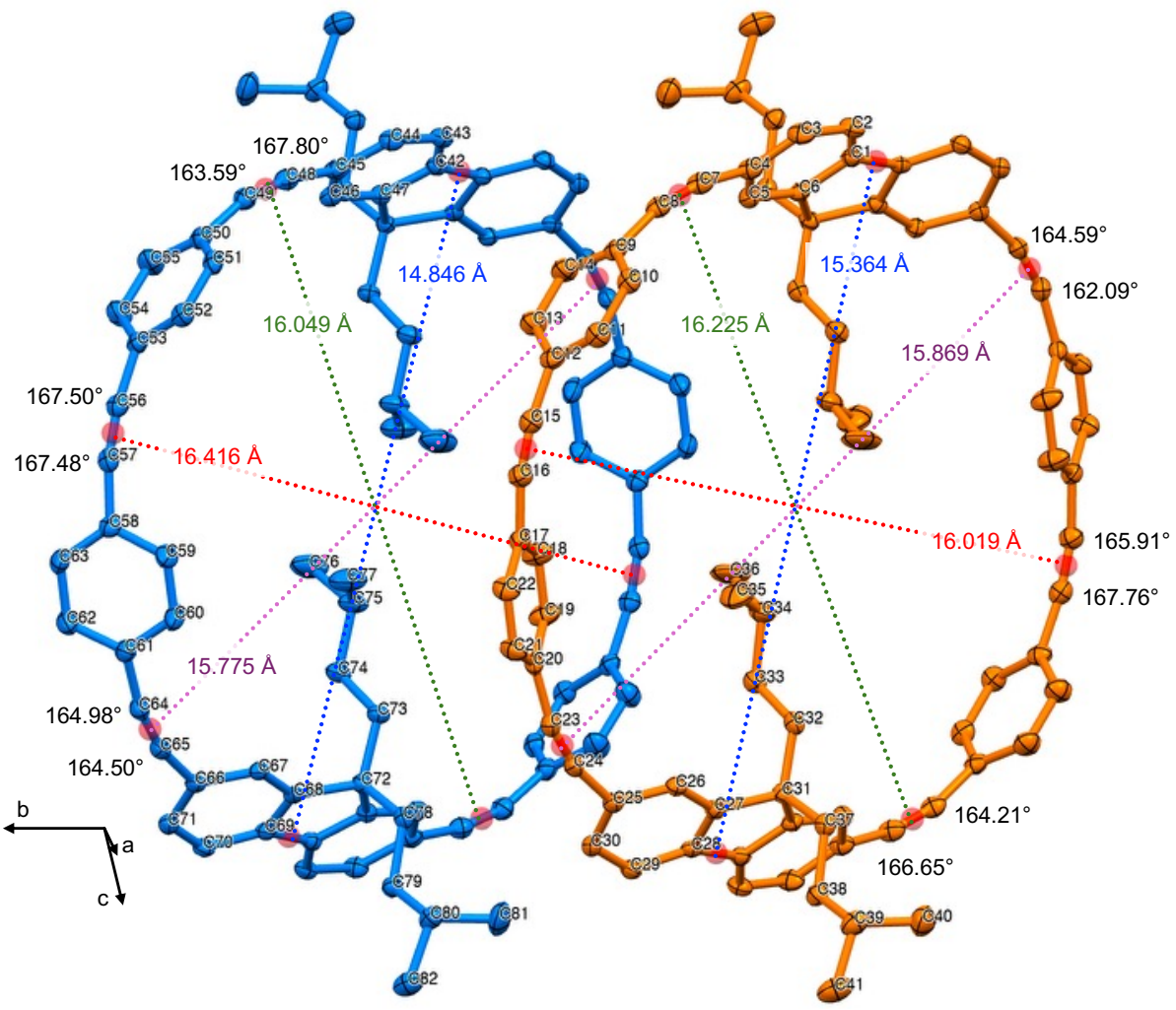


Figure S33. Alternating conformations **Fl-[6]CPPA** in solid state. The diameters and alkyne angles (∠C-C≡C) are labeled. Hydrogen atoms are omitted for clarity. Ellipsoids are drawn at 50% probability.

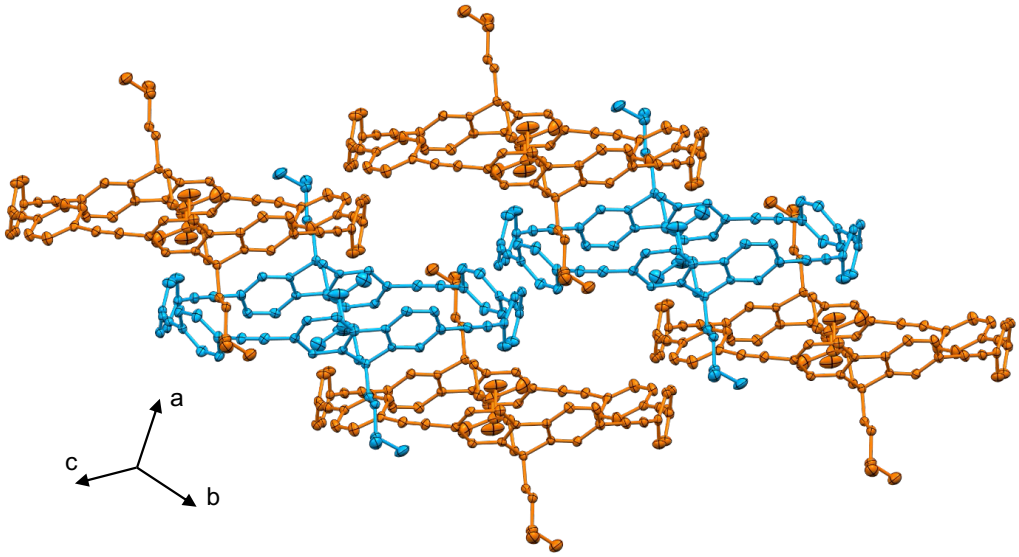


Figure S34. Solid-state packing of **Fl-[6]CPPA**, drawn at 50% ellipsoid probability.

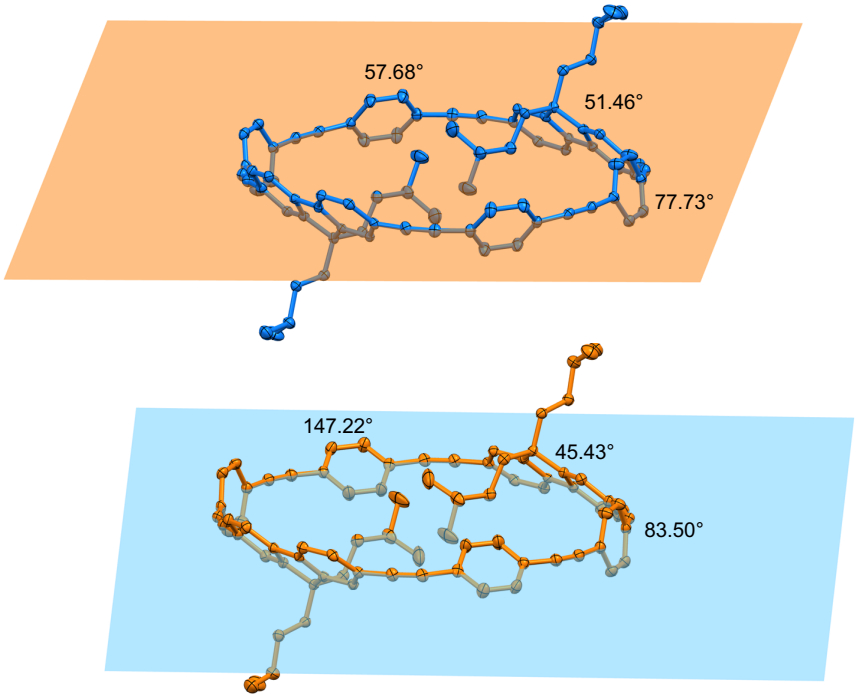


Figure S35. Angle of phenylene and fluorenyl groups against the horizontal plane of **Fl-[6]CPPA**. The horizontal planes of **Fl-[6]CPPA** were determined by the mean of twelve alkyne carbon atoms for both conformations. The fluorenyl planes were based solely on their central five-membered rings. The angles measure the degree to which the arene units are leaning either into (<90°) or away (>90°) from the inner cavity.

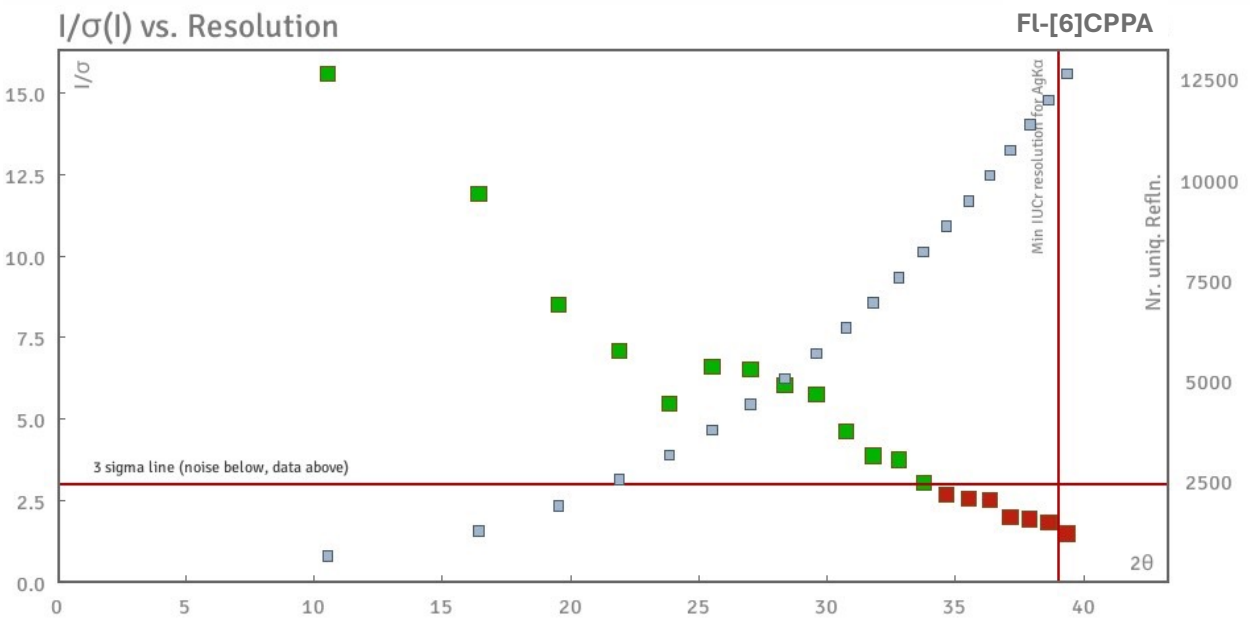


Figure S36. I/σ(I) versus resolution of solid-state Fl-[6]CPPA. The resolution scattering limit of datasets was 0.83 Å. Data was processed via Olex2-1.5.

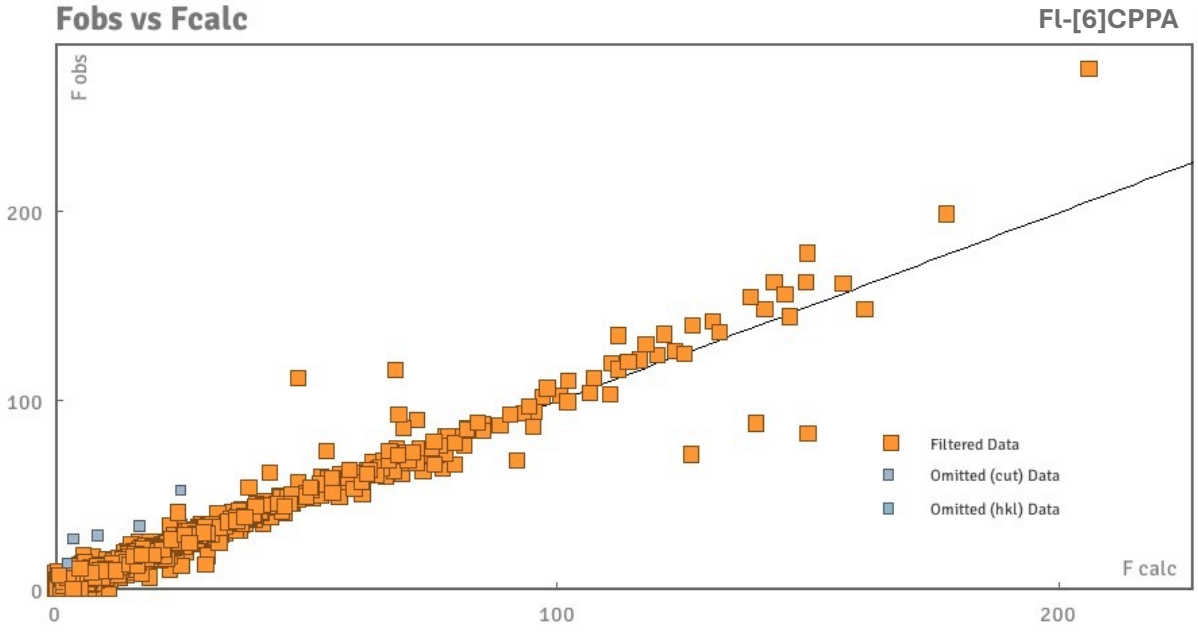


Figure S37. F_{obs} versus F_{calc} of solid-state **Fl-[6]CPPA**. Data was processed via Olex2-1.5.

5 (5a) (CCDC 2392290)

Crystal data

$C_{96}H_{86}N_6 \cdot 2(CHCl_3)$	$F(000) = 1640$
$M_r = 1562.44$	$D_x = 1.214$ Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
$a = 18.272$ (4) Å	Cell parameters from 5896 reflections
$b = 25.467$ (7) Å	$\theta = 3.0–52.8°$
$c = 9.441$ (3) Å	$\mu = 2.22$ mm^{-1}
$\beta = 103.359$ (15)°	$T = 100$ K
$V = 4274.5$ (19) Å^3	Lath, colourless
$Z = 2$	0.27 × 0.08 × 0.01 mm

Data collection

Bruker D8 Venture DUO with Photon III C14 diffractometer	2934 reflections with $I > 2\sigma(I)$
Radiation source: IμS 3.0 microfocus	$R_{int} = 0.250$
ϕ and ω scans	$\theta_{max} = 58.9°$, $\theta_{min} = 2.5°$
Absorption correction: multi-scan *SADABS* (Krause *et al.*, 2015)	$h = -20 – 19$
$T_{min} = 0.566$, $T_{max} = 0.978$	$k = -28 – 28$
41962 measured reflections	$l = -10 – 10$
6087 independent reflections	

Refinement

Refinement on F^2	30 restraints
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.143$	H-atom parameters constrained
$wR(F^2) = 0.406$	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.24$	$(\Delta/\sigma)_{max} < 0.001$
6087 reflections	$\Delta\rho_{max} = 0.74$ e Å^{-3}
500 parameters	$\Delta\rho_{min} = -0.84$ e Å^{-3}

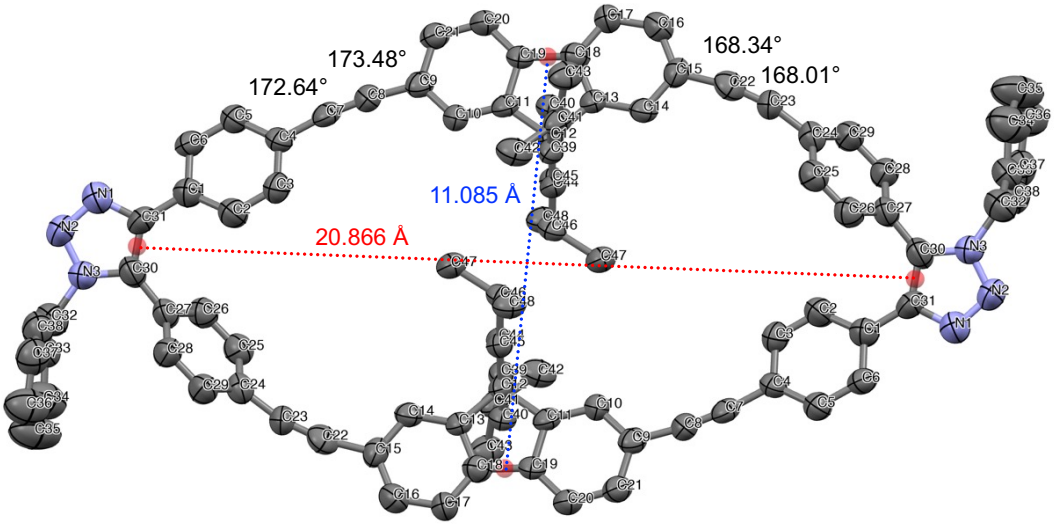


Figure S38. Solid-state structure of **5a** (Fig. S2). Alkyne angles (∠C-C≡C) are labeled. The major axis length was calculated by the distance between the centroids of C30 and C31. The minor axis length was calculated by measuring the centroidal distance between C18 and C19. Ellipsoids are drawn at 35% probability. Hydrogens are omitted for clarity.

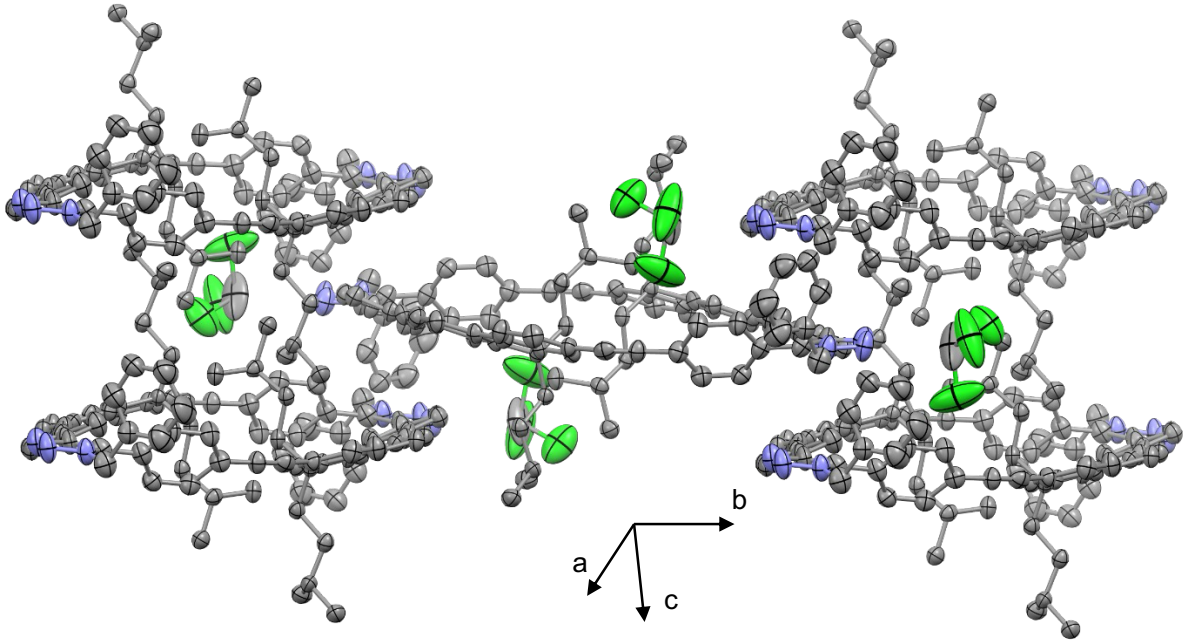


Figure S39. Solid-state packing of **5a** (Fig. S2) with chloroform, drawn at 50% ellipsoid probability.

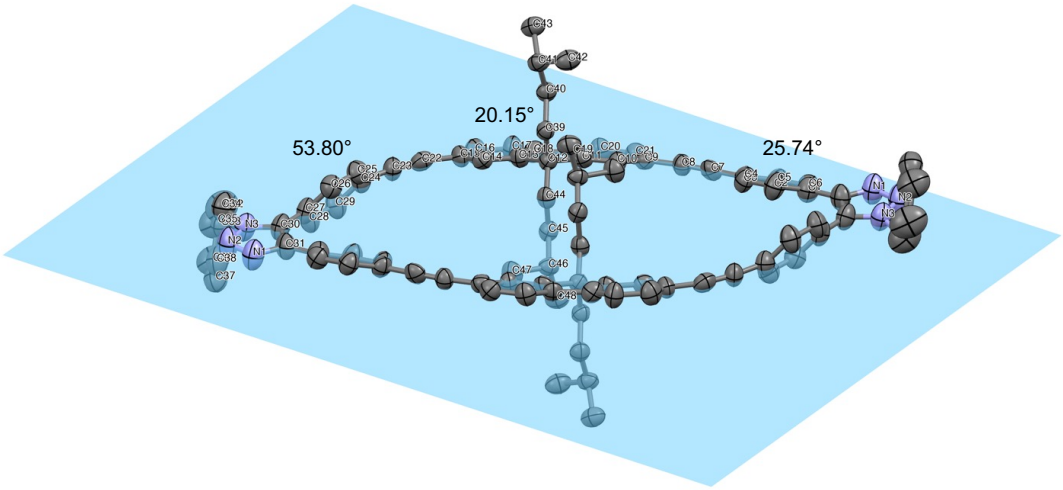


Figure S40. Angle of phenylene and fluorenyl groups against the horizontal plane of **5a**. The plane of the macrocycle was defined by the least square plane of fourteen carbons (C1, C4, C7, C8, C9, C15, C18, C19, C22, C23, C24, C27, C30, C31). The fluorenyl planes were based solely on their central five-membered rings. The angles measure the degree to which the arene units are leaning either into (<90°) or away (>90°) from the inner cavity.6 (CCDC 2392289)

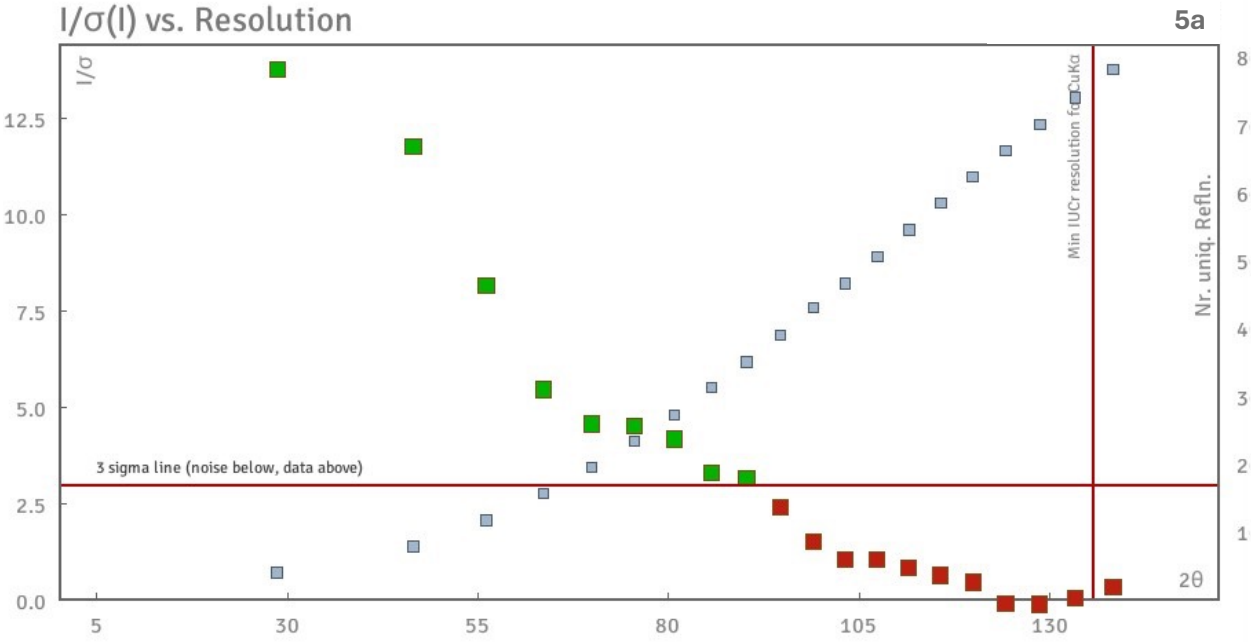


Figure S41. I/σ(I) versus resolution of solid-state **5a**. The resolution scattering limit of datasets was 0.90 Å. Data was processed via Olex2-1.5.

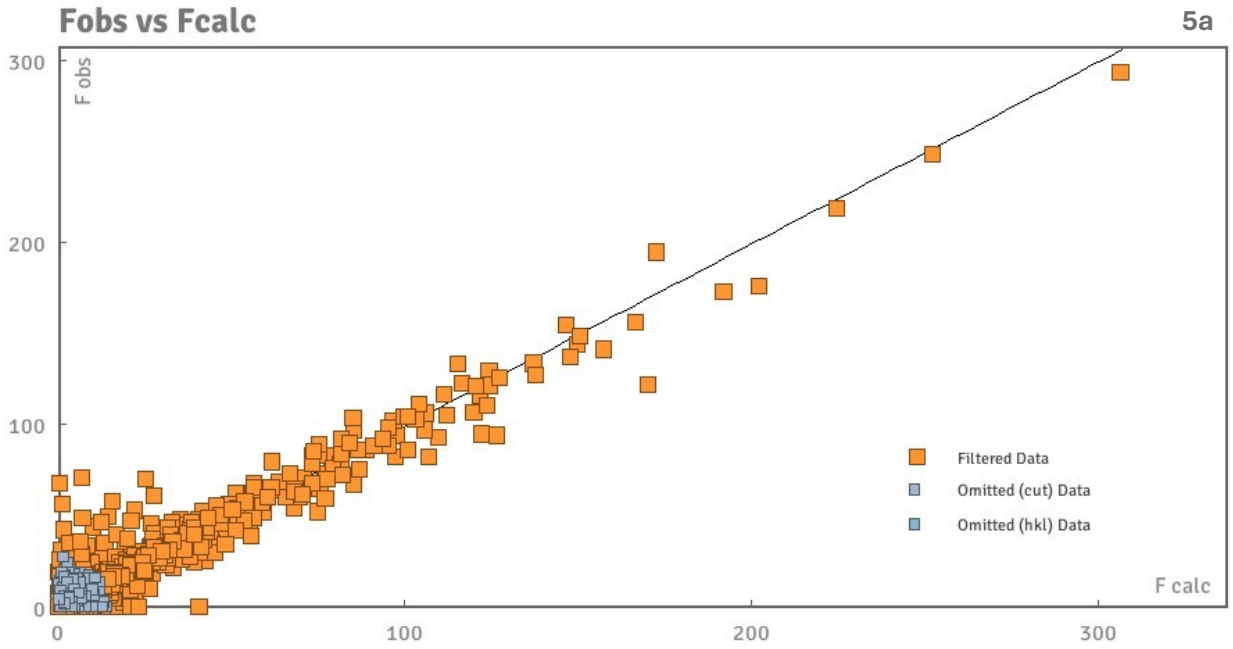


Figure S42. F_{obs} versus F_{calc} of solid-state **5a**. Data was processed via Olex2-1.5.

6 (CCDC 2392291)

Crystal data

$C_{82}H_{74}N_6 \cdot 2(C_4H_8O_2)$	$Z = 1$
$M_r = 1319.67$	$F(000) = 704$
Triclinic, P-1	$D_x = 1.194$ Mg m^{-3}
$a = 9.708$ (2) Å	Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
$b = 14.094$ (3) Å	Cell parameters from 1107 reflections
$c = 14.845$ (3) Å	$\theta = 3.1$–$41.9°$
$\alpha = 73.353$ (12)°	$\mu = 0.57$ mm^{-1}
$\beta = 84.160$ (12)°	$T = 100$ K
$\gamma = 70.601$ (12)°	Lath, colourless
$V = 1835.6$ (7) Å^3	0.25 × 0.06 × 0.01 mm

Data collection

Bruker D8 Venture DUO with Photon III C14 diffractometer	1353 reflections with $I > 2\sigma(I)$
Radiation source: IμS 3.0 microfocus	$R_{int} = 0.230$

ϕ and ω scans	θ_{max} = 50.9°, θ_{min} = 3.1°
Absorption correction: multi-scan *SADABS* (Krause *et al.*, 2015)	h = -9 – 9
T_{min} = 0.735, T_{max} = 0.994	k = -14 – 12
13305 measured reflections	l = -14 – 13
3779 independent reflections	

Refinement

Refinement on F^2	16 restraints
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.128	H-atom parameters constrained
$wR(F^2)$ = 0.388	$w = 1/[\sigma^2(F_o^2) + (0.1935P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
3779 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
450 parameters	$\Delta\rho_{min}$ = -0.23 e Å^{-3}

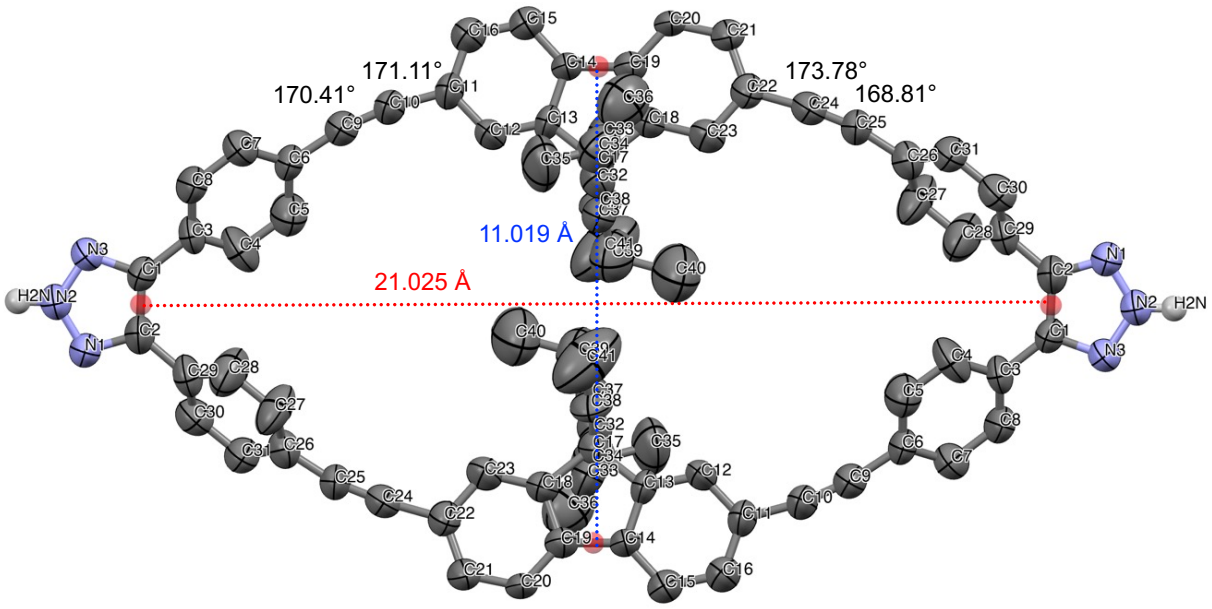


Figure S43. Solid-state structure of **6**. Alkyne angles (left to right, ∠C6, C9, C10; ∠C9, C10, C11; ∠C22, C24, C25; ∠C24, C25, C26) are displayed in black. The major axis length was calculated by measuring the centroidal distance C1 and C2. The minor axis length was calculated by measuring the centroidal distance between C14 and C19. Ellipsoids are drawn at 50% probability. Nonrelevant hydrogens are omitted for clarity.

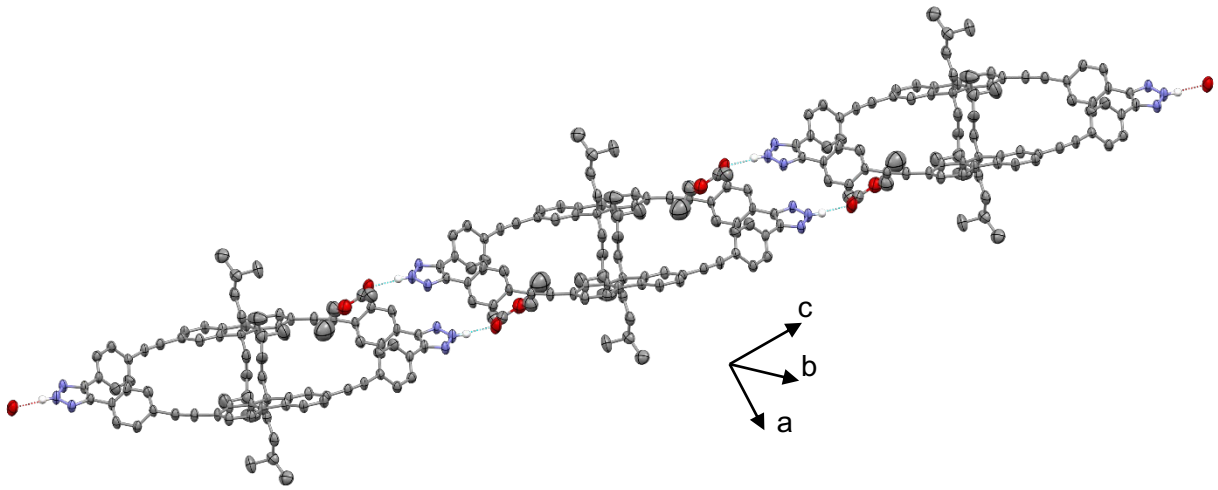


Figure S44. Solid-state packing of **6** with ethyl acetate along the *c* axis, drawn at 50% ellipsoid probability. The carbonyl oxygen on each ethyl acetate molecule forms one hydrogen bond with a *2H*-1,2,3-triazole ring.

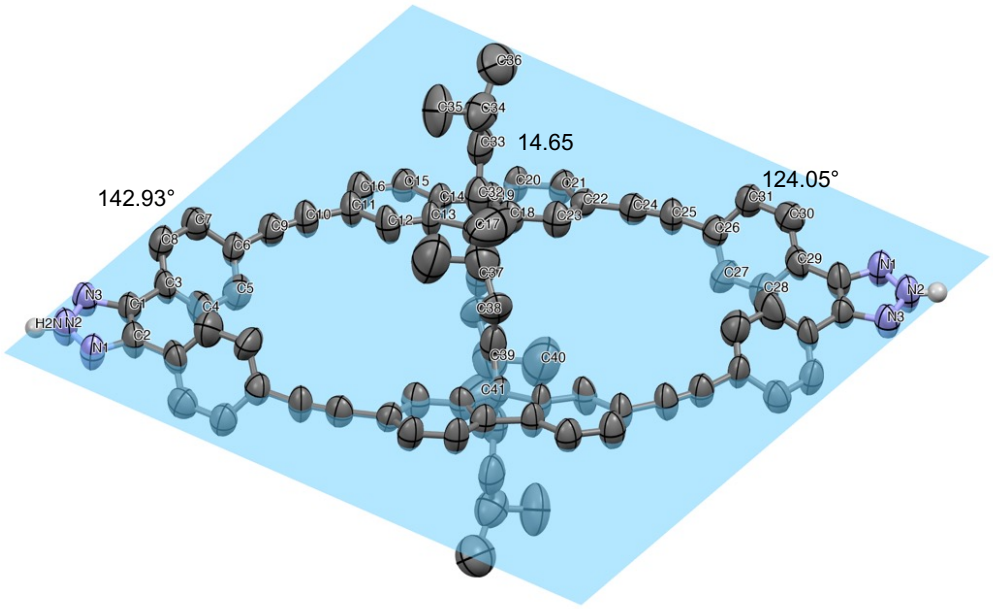


Figure S45. Angle of phenylene and fluorenyl groups against the horizontal plane of **5a**. The plane of the macrocycle was defined by the least square plane of fourteen carbons (C1, C2, C3, C6, C9, C10, C11, C14, C19, C22, C24, C25, C26, C29). The fluorenyl planes were based solely on their central five-membered rings. The angles measure the degree to which the arene units are leaning either into (<90°) or away (>90°) from the inner cavity.

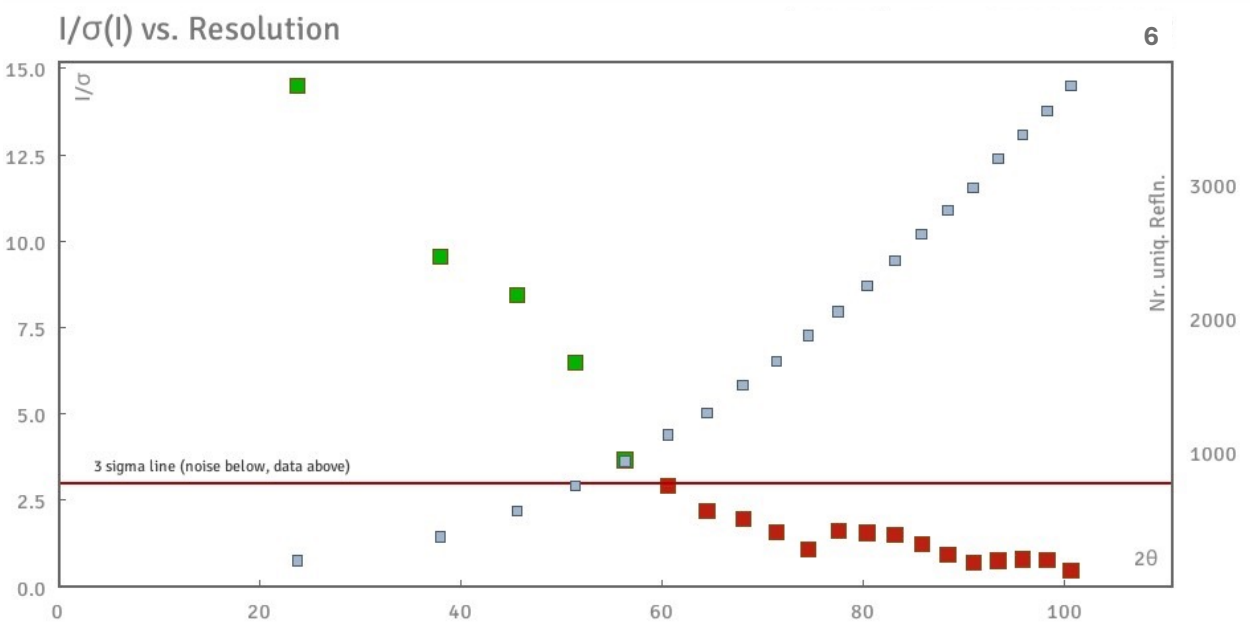


Figure S46. I/σ(I) versus resolution of solid-state 6. The resolution scattering limit of datasets was 0.99 Å. Data was processed via Olex2-1.5.

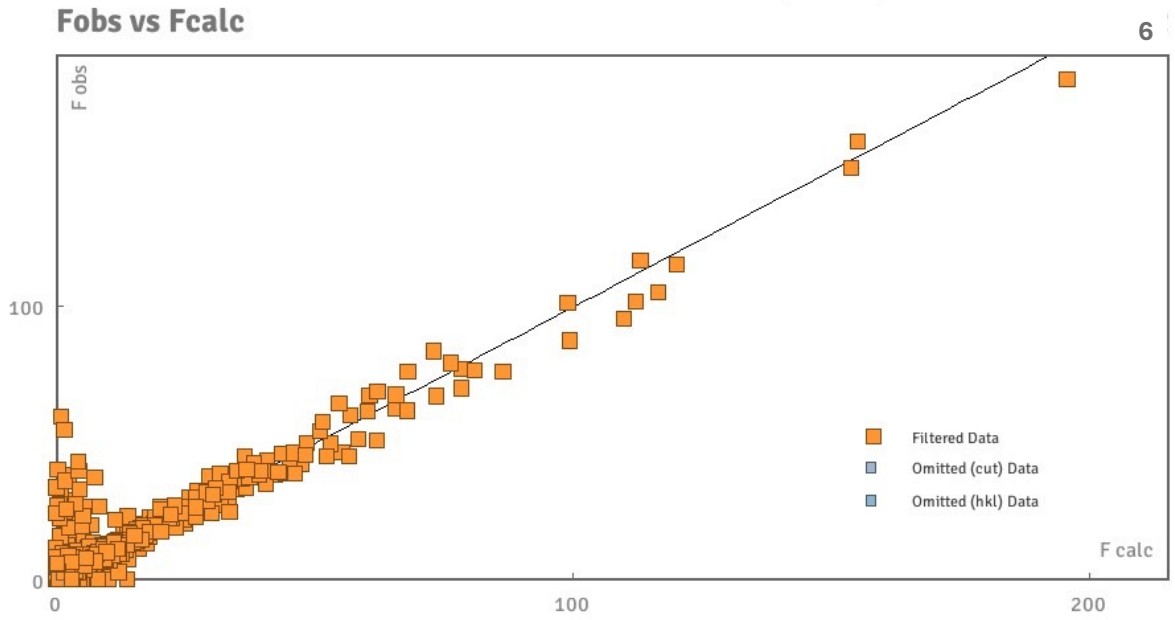
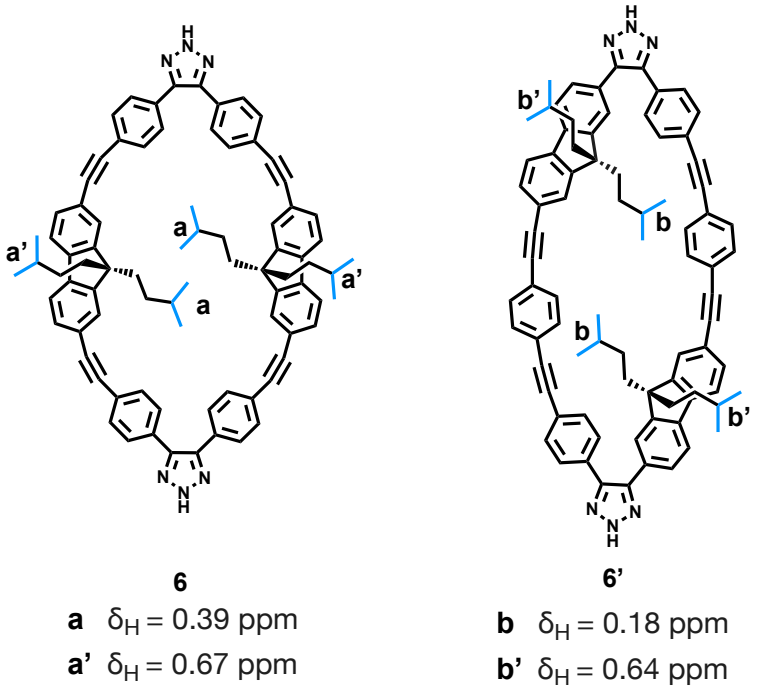


Figure S47. F_{obs} versus F_{calc} of solid-state **6**. Data was processed via Olex2-1.5.

S7. Computational Studies

Computational NMR Analysis

NMR calculations were performed at the B97-2[5]/6-311+G(d,p)[6, 7]//ωB97X-D/def2-SVP level. The B97-2 functional has been benchmarked for a broad range of organic compounds in previous works,[8] showing standard deviations of 0.21 ppm for ^{1}H chemical shifts. Proton chemical shifts were calculated using benzene as secondary reference. $\delta_H = (\sigma_{benzeneH} - \sigma_H) + \delta_{benzeneH}$, where δ_H is the predicted proton chemical shift, $\sigma_{benzeneH}$ is the computed proton shielding of benzene (24.3 ppm, geometry based on microwave data),[9] σ_H is the computed proton shielding of the compound, and $\delta_{benzeneH}$ is the experimental proton chemical shift of benzene (7.34 ppm, in $CDCl_3$).[10]



6

a δ_H = 0.39 ppm

a' δ_H = 0.67 ppm

6'

b δ_H = 0.18 ppm

b' δ_H = 0.64 ppm

Figure S48. Computed averaged proton chemical shifts for the six equivalent protons of the terminal methyl groups (colored blue) on isopentyl solubilizing chains of **6** and **6′**.

Conformation Analysis of Fl-[6]CPPA

Geometry optimizations were performed at ωB97X-D[11]/def2-SVP.[12] Harmonic vibrational frequencies verified the nature of the stationary points. Relative Gibbs free energies were computed at ωB97X-D/def2-SVP. All calculations were performed using Gaussian16 version C.01 (ref 15).

To compare the reactivity of the two distinct alkyne positions in **Fl-[6]CPPA**, we performed a conformational sampling at GFN2-xTB[1] using the CREST software.[2] An energy cutoff of 3.19 kcal/mol was used to capture 99% of the conformers accessible at 75 °C. A total of 2870 conformers were considered.

We used ellipticity (ε), defined as the ratio between the major and the minor axes of the macrocycle, to evaluate distortion of the macrocycle. The major axis was measured as the distance between the centroids of the alkynes clamped between two phenyl groups, and the minor axis was the average distance between the centroids of diagonal alkynes clamped between a fluorenyl and a phenyl group (Fig. S43). The

distribution of the ellipticity values (Fig. S41) showed that: 18.8% (538 conformers) exhibited oblong shapes (ε > 1.05) distorted along the major axis; 41.7% (1198 conformers) have moderately distorted oblong shapes (ε = 1.03–1.05) distorted along the major axis; 37.3% (1071 conformers) maintain a shape similar to the macrocycle (ε = 1.00–1.03); and 2.2% (63 conformers) adopted oblong shapes (ε < 1.00) distorted along the minor axis. These results suggest that, at 75°C, oblong conformations distorted along the major axis may occur, and that representations of these conformers can increase the reactivity of alkyne positions clamped between two phenyl groups.

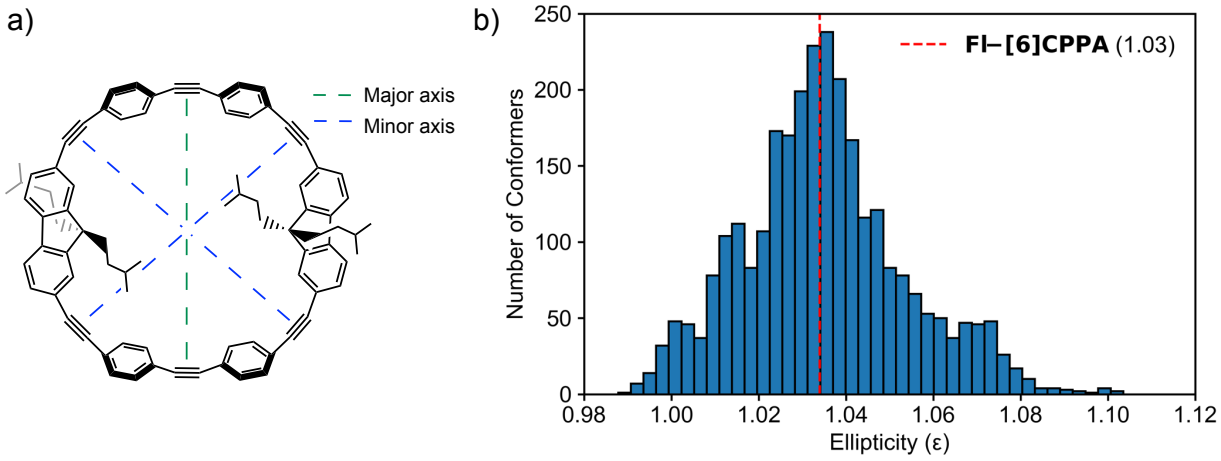


Figure S49. (a) Major and minor axes in **Fl-[6]CPPA** used to calculate ellipticity (ε) and (b) distribution of **Fl-[6]CPPA** conformers according to ε values.

<u>Calculated Free Energy of the Double-SPAAC Reaction for 8'</u>

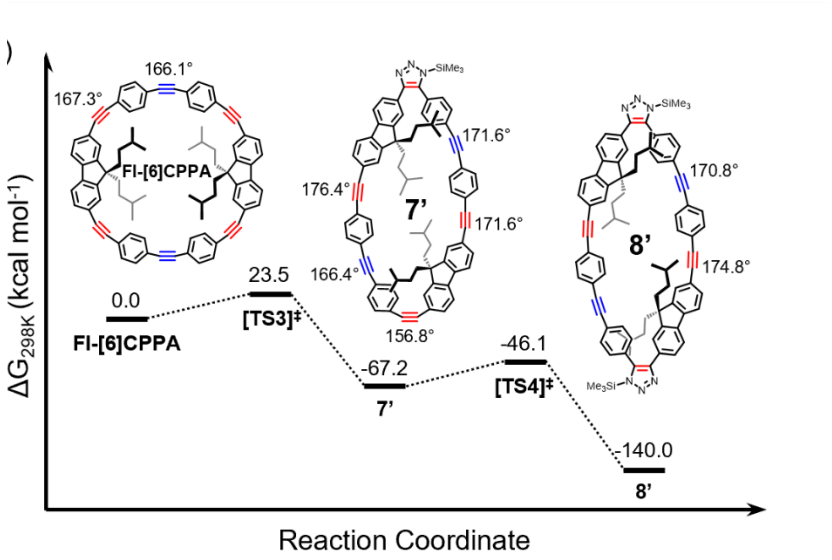


Figure S50. Computed free energy profiles for **Fl-[6]CPPA** reacting with two equivalents of $TMSN_3$ at the fluorene-benzene flanked alkyne positions.

Calculated HOMO and LUMO Energy of Compounds

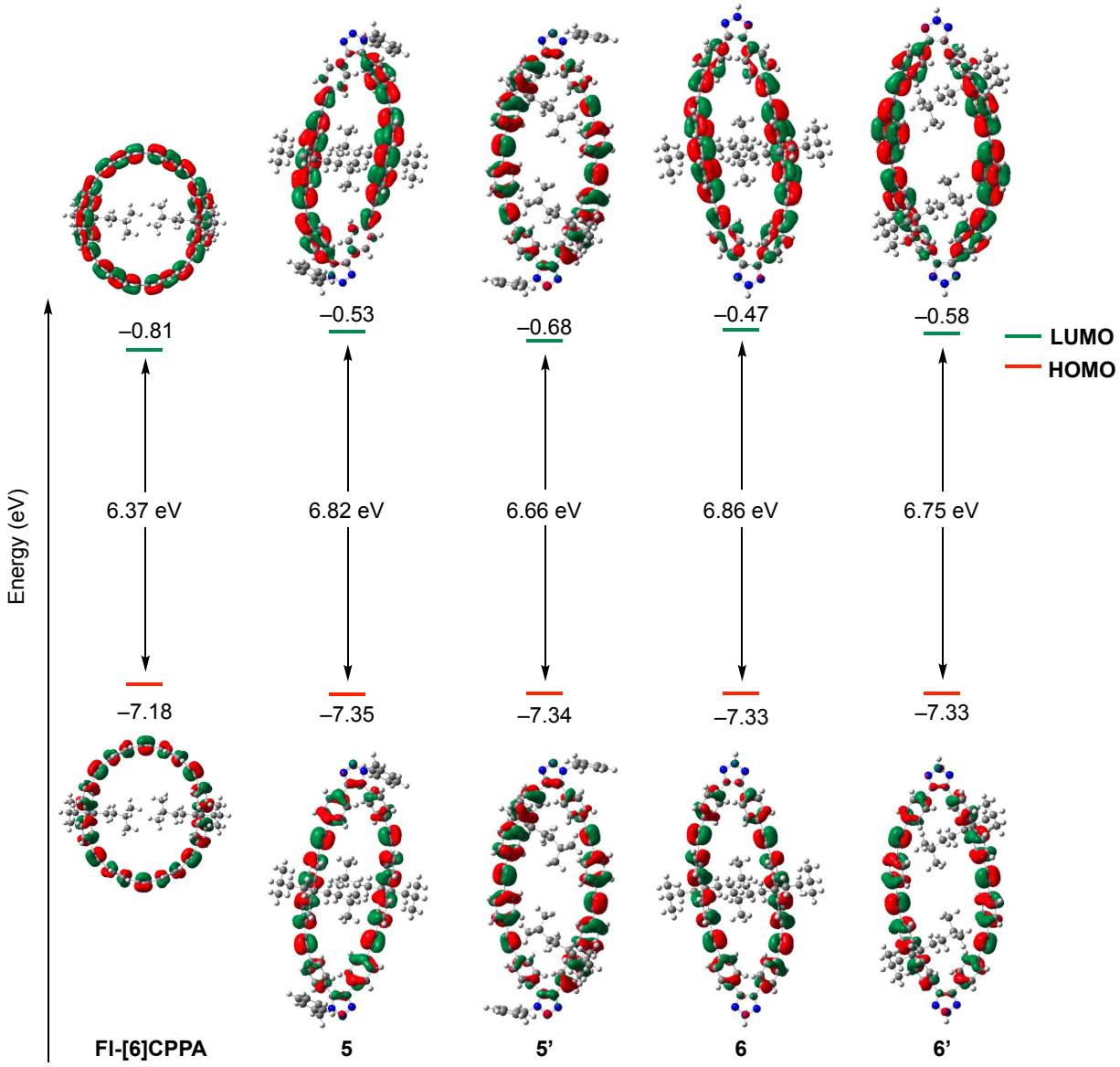


Figure S51. HOMO-LUMO energy gaps of **Fl-[6]CPPA**, **5**, **5′**, **6** and **6′** computed at the ωB97X-D/def2-SVP level of theory.

S6. Cartesian Coordinates of Calculated Structures

Fl-[6]CPPA

	X	Y	Z
H	-8.168364	1.472201	3.443180
C	-7.648413	1.786493	2.535580
C	-6.289955	2.605726	0.212999
C	-7.254808	0.852285	1.576985
C	-7.322093	3.129044	2.351767
C	-6.613234	3.545809	1.210899
C	-6.598113	1.272430	0.407666
H	-7.577322	3.864126	3.116977
H	-5.737933	2.932414	-0.671099
C	-7.294462	-0.618308	1.573476
C	-6.777852	-3.337790	1.202397
C	-7.728916	-1.534919	2.531479
C	-6.663937	-1.066879	0.400501
C	-6.417564	-2.412522	0.203398
C	-7.464719	-2.890876	2.345211
H	-8.228922	-1.198230	3.442256
H	-5.880857	-2.763095	-0.680914
H	-7.749136	-3.614084	3.111450
C	-6.232185	0.094363	-0.478748
C	-7.015791	0.121170	-1.812251
H	-6.712263	-0.765770	-2.393613
H	-6.668198	0.997682	-2.384535
C	-4.719174	0.043074	-0.784167
H	-4.535117	-0.859337	-1.390838
H	-4.473455	0.896345	-1.438359
C	-6.265815	-4.671952	1.079134
C	-6.051581	4.859820	1.087311
C	-5.350015	5.840742	0.932055
C	-5.594920	-5.674024	0.923094
C	-4.286371	6.779660	0.727665
C	-1.819230	8.065218	0.308678
C	-3.547389	7.275148	1.815643
C	-3.837499	7.054602	-0.576000
C	-2.621794	7.689747	-0.782907
C	-2.329270	7.908255	1.608939
H	-3.901932	7.091322	2.831280
H	-4.420969	6.700637	-1.427713
H	-2.246185	7.834285	-1.797338
H	-1.725766	8.222557	2.462226
C	-4.559818	-6.643716	0.716207
C	-2.132499	-8.002786	0.296642
C	-3.842723	-7.173122	1.802816
C	-4.112417	-6.918948	-0.587948
C	-2.916539	-7.590351	-0.795107
C	-2.644124	-7.842521	1.595827
H	-4.196822	-6.988544	2.818472
H	-4.679532	-6.537602	-1.438874
H	-2.540060	-7.736334	-1.808997
H	-2.055610	-8.184536	2.448928
C	-0.762575	-8.367966	0.088864
C	-0.438750	8.387118	0.099187

H	8.229401	1.198245	-3.441899
C	7.729237	1.534925	-2.531206
C	6.417477	2.412515	-0.203353
C	7.294605	0.618308	-1.573294
C	7.465023	2.890887	-2.344969
C	6.777959	3.337794	-1.202278
C	6.663876	1.066874	-0.400423
H	7.749597	3.614097	-3.111148
H	5.880615	2.763085	0.680865
C	7.254964	-0.852285	-1.576806
C	6.613386	-3.545823	-1.210801
C	7.648751	-1.786495	-2.535321
C	6.598079	-1.272433	-0.407592
C	6.289911	-2.605732	-0.212967
C	7.322429	-3.129053	-2.351549
H	8.168845	-1.472204	-3.442839
H	5.737739	-2.932423	0.671036
H	7.577811	-3.864135	-3.116708
C	6.232015	-0.094370	0.478767
C	7.015483	-0.121166	1.812360
H	6.667837	-0.997680	2.384607
H	6.711882	0.765775	2.393683
C	4.718977	-0.043103	0.784026
H	4.473198	-0.896396	1.438166
H	4.534847	0.859287	1.390705
C	6.051744	-4.859844	-1.087265
C	6.265926	4.671964	-1.079058
C	5.595028	5.674038	-0.923049
C	5.350172	-5.840768	-0.932048
C	4.559939	6.643772	-0.716279
C	2.132611	8.002863	-0.296818
C	3.842631	7.172737	-1.802969
C	4.112743	6.919470	0.587842
C	2.916857	7.590883	0.794950
C	2.644033	7.842146	-1.596031
H	4.196569	6.987790	-2.818615
H	4.680016	6.538473	1.438819
H	2.540541	7.737218	1.808850
H	2.055354	8.183803	-2.449160
C	4.286516	-6.779688	-0.727718
C	1.819348	-8.065219	-0.308807
C	3.547514	-7.275075	-1.815727
C	3.837648	-7.054723	0.575930
C	2.621931	-7.689857	0.782799
C	2.329381	-7.908167	-1.609060
H	3.902053	-7.091179	-2.831353
H	4.421136	-6.700839	1.427665
H	2.246330	-7.834469	1.797223
H	1.725863	-8.222393	-2.462365
C	0.438859	-8.387103	-0.099342
C	0.762684	8.368017	-0.089027
C	-3.809110	0.046841	0.443367
H	-3.878033	1.030103	0.937766
H	-4.183501	-0.688941	1.174756
C	-2.330060	-0.266064	0.158345
H	-1.807642	-0.158309	1.125859

C	-2.116802	-1.708259	-0.307622
H	-2.549483	-1.882128	-1.306178
H	-2.577790	-2.427748	0.387024
H	-1.043676	-1.944711	-0.375138
C	-1.694782	0.729857	-0.813424
H	-2.126321	0.639848	-1.823431
H	-0.612171	0.553065	-0.907611
H	-1.838844	1.768796	-0.476971
C	-8.534808	0.158646	-1.667279
H	-8.817317	1.042697	-1.071077
H	-8.862041	-0.719104	-1.084833
C	-9.320494	0.189191	-2.988784
H	-10.386710	0.214065	-2.702659
C	-9.108866	-1.072772	-3.827679
H	-9.786803	-1.087651	-4.694964
H	-9.297149	-1.982978	-3.236986
H	-8.080257	-1.132764	-4.218670
C	-9.044564	1.451925	-3.807601
H	-9.720936	1.515313	-4.673904
H	-8.014270	1.465389	-4.198534
H	-9.185890	2.361017	-3.202271
C	3.809052	-0.046845	-0.443612
H	3.878091	-1.030075	-0.938061
H	4.183483	0.689002	-1.174915
C	2.329947	0.265945	-0.158738
H	1.807631	0.158154	-1.126304
C	1.694646	-0.730034	0.812956
H	0.612014	-0.553310	0.907045
H	2.126083	-0.640015	1.823005
H	1.838801	-1.768958	0.476499
C	2.116525	1.708122	0.307216
H	1.043375	1.944508	0.374578
H	2.577569	2.427652	-0.387349
H	2.549043	1.882002	1.305841
C	8.534516	-0.158631	1.667564
H	8.861811	0.719111	1.085140
H	8.817103	-1.042691	1.071413
C	9.320040	-0.189145	2.989163
H	10.386291	-0.214034	2.703168
C	9.044002	-1.451855	3.807982
H	8.013663	-1.465296	4.198796
H	9.720273	-1.515228	4.674365
H	9.185387	-2.360963	3.202691
C	9.108320	1.072843	3.827998
H	8.079665	1.132854	4.218864
H	9.296681	1.983031	3.237301
H	9.786154	1.087740	4.695363

Total Electronic Energy = -3164.5615294999993 a.u.

N_{im}= 0

TS1

	X	Y	Z
H	2.481281	6.896232	3.711251
C	2.656265	6.379339	2.765168
C	3.107581	5.023280	0.341162
C	1.698697	6.399852	1.750964
C	3.824662	5.643269	2.580972
C	4.047157	4.934154	1.386495
C	1.941227	5.740837	0.533860
H	4.561944	5.576401	3.382840
H	3.282371	4.470074	-0.584314
C	0.326777	6.927783	1.718673
C	-2.383407	7.396073	1.240140
C	-0.438258	7.571550	2.691468
C	-0.244796	6.579695	0.483030
C	-1.583211	6.820507	0.233736
C	-1.791633	7.799545	2.450628
H	-0.000315	7.856070	3.650705
H	-2.046904	6.507309	-0.704308
H	-2.416319	8.253254	3.221963
C	0.755872	5.864098	-0.409137
C	1.109225	6.710588	-1.655444
H	0.203896	6.772636	-2.282505
H	1.851536	6.143690	-2.242181
C	0.237584	4.484591	-0.869924
H	-0.629987	4.654896	-1.529340
H	1.013639	4.031301	-1.509018
C	-3.804852	7.383342	1.051549
C	5.126398	4.000211	1.249555
C	5.885161	3.063636	1.093037
C	-4.973445	7.116088	0.847659
C	6.577301	1.825777	0.886869
C	7.486790	-0.805857	0.452526
C	6.897051	0.990813	1.971121
C	6.803192	1.352853	-0.417513
C	7.252814	0.056977	-0.630433
C	7.344225	-0.306625	1.756445
H	6.741186	1.353892	2.988517
H	6.571800	1.998157	-1.266852
H	7.375678	-0.320170	-1.647559
H	7.550393	-0.962312	2.604362
C	-6.237982	6.491534	0.592944
C	-8.337533	4.687762	0.092907
C	-7.017765	5.994956	1.651660
C	-6.611906	6.180512	-0.726176
C	-7.648335	5.292288	-0.973098
C	-8.053167	5.103731	1.405001
H	-6.753405	6.254269	2.678242
H	-6.031530	6.587221	-1.556163
H	-7.882927	4.997147	-1.997245
H	-8.602864	4.661618	2.237753
C	-9.130515	3.518493	-0.146618
H	-2.283369	-7.576547	-3.398130
C	-1.878971	-7.202981	-2.454808
C	-0.819900	-6.219698	-0.040933
C	-2.702837	-6.569436	-1.524186

C	-0.514503	-7.308508	-2.193656
C	0.033331	-6.788638	-1.006393
C	-2.171736	-6.106370	-0.308486
H	0.151429	-7.756991	-2.932835
H	-0.392516	-5.819129	0.881028
C	-4.113030	-6.157778	-1.591805
C	-6.571359	-4.861148	-1.322471
C	-5.061974	-6.271756	-2.607982
C	-4.417594	-5.453187	-0.414445
C	-5.637848	-4.820616	-0.268060
C	-6.285864	-5.618941	-2.472130
H	-4.839293	-6.826398	-3.522122
H	-5.862840	-4.230200	0.622941
H	-7.017463	-5.653370	-3.281245
C	-3.236250	-5.432453	0.540783
C	-3.534331	-6.246369	1.823281
H	-4.328001	-5.715694	2.375745
H	-2.634594	-6.203990	2.459965
C	-2.834138	-3.997354	0.941830
H	-3.650977	-3.575193	1.550906
H	-1.966380	-4.072101	1.618252
C	-7.698771	-3.978182	-1.243469
C	1.447964	-6.682154	-0.804484
C	2.611111	-6.383142	-0.616242
C	-8.466560	-3.043119	-1.121089
C	3.897243	-5.797758	-0.379033
C	6.269156	-4.308598	-0.063339
C	4.016769	-4.851861	0.655597
C	5.008249	-6.039813	-1.202624
C	6.181985	-5.310061	-1.040755
C	5.181359	-4.118381	0.807427
H	3.164003	-4.668553	1.311743
H	4.934075	-6.784551	-1.997073
H	7.034075	-5.485674	-1.698863
H	5.248881	-3.353706	1.583540
C	-9.084573	-1.761710	-0.946405
C	-9.624890	0.971205	-0.558796
C	-9.302444	-0.915605	-2.047389
C	-9.279938	-1.250178	0.348513
C	-9.547817	0.097336	0.539884
C	-9.567611	0.433624	-1.856139
H	-9.182329	-1.310664	-3.057597
H	-9.144862	-1.907966	1.208866
H	-9.621416	0.501744	1.550874
H	-9.655866	1.099749	-2.716148
C	-9.523122	2.385109	-0.348987
C	-0.139187	3.523331	0.255102
H	0.744232	3.354140	0.893282
H	-0.895371	4.001218	0.900403
C	-0.679236	2.158758	-0.205806
H	-0.874069	1.585994	0.718526
C	-2.010600	2.272860	-0.950618
H	-1.889890	2.775049	-1.924165
H	-2.750126	2.843242	-0.366815
H	-2.436234	1.277273	-1.150008
C	0.345570	1.365578	-1.018770

H	0.540333	1.836330	-1.995904
H	-0.014007	0.344471	-1.217581
H	1.306129	1.285110	-0.485721
C	1.636974	8.111322	-1.356759
H	2.533456	8.029394	-0.719286
H	0.887716	8.658638	-0.760301
C	1.990848	8.957017	-2.591331
H	2.352497	9.923534	-2.198413
C	0.773065	9.255015	-3.468440
H	1.025989	9.974337	-4.262560
H	-0.051961	9.682086	-2.877040
H	0.396100	8.345090	-3.962815
C	3.130334	8.350202	-3.412589
H	3.457186	9.041893	-4.204264
H	2.821486	7.414534	-3.906199
H	4.003508	8.124026	-2.780694
C	-2.511749	-3.061792	-0.221238
H	-3.408801	-2.950555	-0.853132
H	-1.744413	-3.530930	-0.859616
C	-2.018085	-1.663136	0.187173
H	-1.850944	-1.115087	-0.757470
C	-3.063426	-0.879304	0.982824
H	-2.738876	0.160243	1.143332
H	-3.233405	-1.323774	1.976797
H	-4.030499	-0.851085	0.456401
C	-0.677286	-1.707485	0.923245
H	-0.283887	-0.692747	1.087669
H	0.076234	-2.271076	0.350628
H	-0.772685	-2.181601	1.913453
C	-3.940675	-7.698741	1.588371
H	-3.137684	-8.211179	1.032289
H	-4.828413	-7.723085	0.934046
C	-4.248355	-8.507711	2.859390
H	-4.516082	-9.521073	2.511907
C	-5.454632	-7.961634	3.626115
H	-5.239855	-6.977831	4.073913
H	-5.737712	-8.637110	4.448089
H	-6.329698	-7.846787	2.967398
C	-3.029656	-8.652065	3.773155
H	-2.744369	-7.687896	4.224289
H	-2.157405	-9.034987	3.220582
H	-3.237234	-9.348556	4.600101
C	7.745607	-2.204735	0.215996
C	7.372194	-3.376257	0.017865
N	9.901147	-2.318525	-0.071005
N	9.885876	-3.506056	-0.386627
N	9.217936	-4.442304	-0.502967
Si	11.138680	-1.073065	-0.419618
C	10.827511	0.299017	0.805427
H	11.611090	1.068140	0.713745
H	10.840129	-0.081564	1.838003
H	9.854281	0.782433	0.631961
C	12.821837	-1.859291	-0.186530
H	13.619895	-1.123782	-0.376152
H	12.967434	-2.701894	-0.880181
H	12.943025	-2.236934	0.840256

C	10.899642	-0.482848	-2.180339
H	11.642949	0.288368	-2.438755
H	9.898384	-0.043699	-2.307152
H	11.005460	-1.311056	-2.898038

Total Electronic Energy = -3737.63797116 a.u.

N_{im}= 1

ν = 443.8*i* cm^{-1}

7

	X	Y	Z
H	1.587617	6.466706	3.677515
C	1.782248	6.033884	2.693906
C	2.283001	4.889065	0.170470
C	0.826259	6.100891	1.680307
C	2.976077	5.358359	2.455076
C	3.225231	4.755104	1.208123
C	1.092307	5.549820	0.415338
H	3.716726	5.257037	3.250177
H	2.478529	4.419396	-0.796122
C	-0.565386	6.573906	1.689716
C	-3.300403	6.927460	1.264793
C	-1.353865	7.097001	2.714827
C	-1.126722	6.301572	0.431022
C	-2.478866	6.488373	0.208222
C	-2.719549	7.267899	2.500188
H	-0.923496	7.324119	3.692613
H	-2.933804	6.224232	-0.749010
H	-3.361655	7.618150	3.310134
C	-0.098925	5.704426	-0.516362
C	0.217489	6.662700	-1.689118
H	-0.690385	6.736799	-2.311073
H	0.982416	6.176738	-2.317988
C	-0.560105	4.345859	-1.084960
H	-1.426883	4.529371	-1.741804
H	0.239740	3.969751	-1.744496
C	-4.720917	6.819429	1.101546
C	4.363521	3.907474	1.010711
C	5.239441	3.084745	0.832291
C	-5.868483	6.457444	0.924973
C	6.181404	2.027569	0.615170
C	7.892272	-0.172325	0.207836
C	6.976755	1.537570	1.664354
C	6.269061	1.410899	-0.645316
C	7.112464	0.325977	-0.842989
C	7.815462	0.447130	1.461103
H	6.910589	2.003654	2.648866
H	5.653944	1.784111	-1.465716
H	7.163218	-0.156499	-1.821172
H	8.403149	0.051543	2.292235
C	-7.074849	5.715827	0.704101
C	-8.985805	3.699529	0.264246
C	-7.769060	5.144443	1.784587
C	-7.453257	5.365549	-0.603850
C	-8.396986	4.372262	-0.820993
C	-8.711342	4.148426	1.567602
H	-7.503772	5.432291	2.803305

H	-6.942585	5.828125	-1.450248
H	-8.627829	4.050925	-1.838091
H	-9.186850	3.652866	2.415778
C	-9.647225	2.446639	0.048401
H	-1.305393	-7.110837	-3.556264
C	-0.956247	-6.733192	-2.592724
C	-0.043527	-5.730441	-0.125927
C	-1.861651	-6.351149	-1.602897
C	0.408067	-6.578604	-2.359544
C	0.876525	-6.046165	-1.143684
C	-1.398678	-5.879161	-0.363235
H	1.129035	-6.830558	-3.139118
H	0.322454	-5.321186	0.818360
C	-3.326390	-6.225554	-1.621732
C	-5.975048	-5.431482	-1.240656
C	-4.258345	-6.443432	-2.636715
C	-3.732926	-5.683171	-0.390874
C	-5.046501	-5.301833	-0.189103
C	-5.578393	-6.040678	-2.444717
H	-3.954609	-6.876675	-3.592182
H	-5.357980	-4.827712	0.744344
H	-6.306183	-6.147523	-3.250953
C	-2.553448	-5.501232	0.550153
C	-2.647997	-6.452967	1.766926
H	-3.517801	-6.137454	2.367450
H	-1.758954	-6.277005	2.395698
C	-2.431987	-4.049378	1.056302
H	-3.288406	-3.845508	1.720744
H	-1.537639	-3.996118	1.699222
C	-7.232325	-4.754381	-1.107759
C	2.258626	-5.710624	-0.962718
C	3.389733	-5.294665	-0.808255
C	-8.135200	-3.954299	-0.952878
C	4.675103	-4.685563	-0.627910
C	7.153769	-3.365595	-0.345239
C	4.771394	-3.483825	0.093685
C	5.844485	-5.232073	-1.181464
C	7.063702	-4.581698	-1.038536
C	5.991322	-2.836052	0.233211
H	3.872063	-3.056462	0.540860
H	5.786861	-6.170587	-1.735748
H	7.971149	-5.006053	-1.471186
H	6.036555	-1.907787	0.804614
C	-8.928858	-2.777267	-0.754965
C	-9.827844	-0.143523	-0.347959
C	-9.298746	-1.973900	-1.847584
C	-9.153579	-2.293847	0.545993
C	-9.598169	-0.995230	0.746902
C	-9.740851	-0.673380	-1.646862
H	-9.157323	-2.352044	-2.861502
H	-8.900981	-2.923164	1.401146
H	-9.693621	-0.601077	1.760126
H	-9.947055	-0.028857	-2.503135
C	-9.903577	1.272584	-0.141065
C	-0.911370	3.295409	-0.034721
H	-0.050581	3.160831	0.641673

H	-1.735685	3.674183	0.592387
C	-1.310227	1.920444	-0.592726
H	-1.527188	1.294606	0.289209
C	-2.589607	1.970211	-1.429236
H	-2.437167	2.516564	-2.374190
H	-3.407438	2.464427	-0.881590
H	-2.927770	0.955728	-1.692185
C	-0.169240	1.243721	-1.354395
H	0.057950	1.767330	-2.297051
H	-0.428592	0.206267	-1.615661
H	0.752938	1.216251	-0.752626
C	0.684914	8.056024	-1.276749
H	1.576709	7.961398	-0.634380
H	-0.092990	8.525253	-0.651108
C	1.018759	9.007301	-2.437876
H	1.327346	9.957314	-1.967182
C	-0.196647	9.313176	-3.315466
H	0.034591	10.102056	-4.047679
H	-1.051868	9.654307	-2.711267
H	-0.519684	8.426540	-3.884676
C	2.199825	8.516966	-3.278052
H	2.505821	9.279815	-4.010451
H	1.945256	7.606805	-3.844890
H	3.072402	8.286384	-2.646941
C	-2.356436	-2.988779	-0.039521
H	-3.314239	-2.966680	-0.585439
H	-1.591672	-3.284144	-0.777339
C	-2.032823	-1.569230	0.452564
H	-2.067313	-0.925966	-0.443534
C	-3.079567	-1.033460	1.430541
H	-2.902698	0.029545	1.657217
H	-3.055557	-1.578116	2.388262
H	-4.096403	-1.122759	1.016833
C	-0.619542	-1.461058	1.029065
H	-0.363887	-0.415107	1.258407
H	0.131577	-1.842372	0.319448
H	-0.517006	-2.031096	1.966494
C	-2.759557	-7.935567	1.421761
H	-1.882881	-8.231794	0.821550
H	-3.638928	-8.089192	0.773699
C	-2.869734	-8.883777	2.627365
H	-2.936231	-9.901017	2.202951
C	-4.143584	-8.652447	3.442840
H	-4.120593	-7.682671	3.965842
H	-4.266850	-9.431886	4.210517
H	-5.038504	-8.666595	2.801138
C	-1.626719	-8.847901	3.518758
H	-1.530864	-7.883266	4.042951
H	-0.707875	-9.003598	2.932050
H	-1.671695	-9.632838	4.289385
C	8.452507	-2.680978	-0.246035
C	8.756464	-1.348915	-0.010102
N	9.630375	-3.344451	-0.417231
N	10.608683	-2.522100	-0.300745
N	10.117911	-1.292512	-0.054597
Si	11.304953	0.085385	0.115215

C	12.848817	-0.488589	-0.753563
H	13.633234	0.281091	-0.677124
H	12.651584	-0.679634	-1.818955
H	13.221802	-1.422687	-0.310432
C	11.593271	0.353377	1.942780
H	10.691317	0.728665	2.448170
H	12.395654	1.092533	2.096532
H	11.899036	-0.586422	2.427485
C	10.559076	1.588891	-0.707777
H	9.696396	1.989488	-0.156100
H	10.233199	1.356862	-1.733417
H	11.322791	2.381293	-0.768011

Total Electronic Energy = -3737.7928740300003a.u.
N_{im}= 0

TS2

	X	Y	Z
H	0.057742	4.994914	3.621396
C	0.367904	4.730377	2.608240
C	1.171658	4.039994	-0.004692
C	-0.575399	4.473277	1.615097
C	1.718342	4.640741	2.292154
C	2.133818	4.289290	0.993443
C	-0.174288	4.136433	0.310792
H	2.476040	4.830613	3.054123
H	1.498651	3.772106	-1.011998
C	-2.040561	4.464143	1.666778
C	-4.768996	4.095215	1.254741
C	-2.921517	4.663296	2.729134
C	-2.521125	4.137289	0.388650
C	-3.875800	3.957299	0.174730
C	-4.284292	4.476355	2.519278
H	-2.551810	4.928791	3.721856
H	-4.259283	3.659128	-0.803392
H	-4.988039	4.585874	3.346153
C	-1.380855	3.961779	-0.602728
C	-1.409579	5.062888	-1.690885
H	-2.309229	4.896941	-2.307193
H	-0.546349	4.893299	-2.356049
C	-1.447629	2.580573	-1.286254
H	-2.386995	2.552565	-1.863737
H	-0.640991	2.518898	-2.035835
C	-6.132543	3.697780	1.076688
C	-7.218975	3.182518	0.903297
C	6.091608	3.636891	0.304520
C	8.717887	2.663561	0.011242
C	7.116004	4.069217	1.163322
C	6.416012	2.770210	-0.753629
C	7.707272	2.292319	-0.895927
C	8.416051	3.595633	1.013007
H	6.877016	4.758969	1.974851
H	5.630056	2.440059	-1.435129
H	7.941041	1.577907	-1.687510
H	9.200811	3.910834	1.702817
C	-8.347064	2.329984	0.680043
C	-10.184211	0.237606	0.307306

C	-9.156596	1.897301	1.743222
C	-8.548592	1.778024	-0.596384
C	-9.454846	0.743515	-0.776112
C	-10.061082	0.857263	1.556806
H	-9.017769	2.332608	2.734247
H	-7.935796	2.122936	-1.430673
H	-9.549995	0.265447	-1.753124
H	-10.617943	0.464044	2.410118
H	2.424839	-5.058444	-3.818863
C	2.837171	-4.777786	-2.847253
C	3.902826	-4.043177	-0.347172
C	2.000292	-4.409524	-1.794541
C	4.215518	-4.753447	-2.655492
C	4.760290	-4.363762	-1.418614
C	2.533433	-4.063973	-0.542586
H	4.889303	-5.003842	-3.476645
H	4.333099	-3.741103	0.610244
C	0.542214	-4.271861	-1.723890
C	-2.132911	-3.865957	-1.057404
C	-0.439427	-4.501852	-2.685866
C	0.196946	-3.838130	-0.432285
C	-1.131968	-3.631208	-0.094893
C	-1.772245	-4.301032	-2.347336
H	-0.172779	-4.839746	-3.689561
H	-1.416024	-3.300069	0.906716
H	-2.559526	-4.477442	-3.082132
C	1.433510	-3.718213	0.450544
C	1.383612	-4.749194	1.604963
H	0.545048	-4.467674	2.263687
H	2.300525	-4.621727	2.204794
C	1.633645	-2.310036	1.050169
H	0.864557	-2.149343	1.824273
H	2.597203	-2.319265	1.587646
C	6.164785	-4.131911	-1.259887
C	7.289859	-3.705474	-1.084983
C	8.422994	-2.863285	-0.842665
C	10.034756	-0.605734	-0.403628
C	9.136146	-2.281944	-1.904887
C	8.666678	-2.407411	0.464089
C	9.463567	-1.293220	0.680611
C	9.935794	-1.166266	-1.687138
H	8.981919	-2.652734	-2.919852
H	8.143840	-2.875854	1.299839
H	9.558224	-0.876841	1.685447
H	10.411137	-0.660022	-2.529561
C	-6.105432	-3.255370	-0.365414
C	-8.849993	-2.660498	-0.079996
C	-7.080856	-4.043579	-1.000224
C	-6.525849	-2.191238	0.447367
C	-7.876301	-1.903396	0.589237
C	-8.431533	-3.750564	-0.856213
H	-6.766962	-4.883665	-1.622451
H	-5.780367	-1.581158	0.960225
H	-8.171657	-1.072877	1.230633
H	-9.185414	-4.358080	-1.360210
C	-1.371293	1.384717	-0.335675

H	-0.314352	1.193429	-0.098903
H	-1.853481	1.642230	0.622505
C	-2.015665	0.090822	-0.861119
H	-1.762175	-0.699617	-0.131670
C	-3.542947	0.183172	-0.902815
H	-3.886057	0.925939	-1.642052
H	-3.953035	0.478369	0.076069
H	-3.986286	-0.785192	-1.179933
C	-1.448710	-0.343737	-2.213175
H	-1.736310	0.357612	-3.013500
H	-1.823540	-1.340158	-2.492634
H	-0.348855	-0.396647	-2.192777
C	-1.392874	6.495933	-1.165273
H	-0.505138	6.635402	-0.525714
H	-2.267623	6.649096	-0.510889
C	-1.391535	7.590588	-2.245195
H	-1.388868	8.550099	-1.698686
C	-2.654802	7.566883	-3.108072
H	-2.693186	8.442133	-3.774783
H	-3.564561	7.575645	-2.487374
H	-2.692711	6.669919	-3.747238
C	-0.129032	7.561547	-3.109189
H	-0.087397	8.437028	-3.775381
H	-0.095011	6.665061	-3.749169
H	0.781104	7.565865	-2.489216
C	1.599113	-1.162250	0.042358
H	0.551247	-0.985041	-0.244053
H	2.118998	-1.466818	-0.882097
C	2.218480	0.158549	0.534566
H	1.952556	0.923587	-0.217733
C	1.640883	0.620651	1.873774
H	1.980307	1.639493	2.114929
H	1.959621	-0.039622	2.696659
H	0.539791	0.631848	1.860587
C	3.746979	0.100285	0.585113
H	4.167735	1.079772	0.860535
H	4.170546	-0.189251	-0.389259
H	4.101565	-0.631261	1.329963
C	1.242104	-6.205446	1.169353
H	2.109722	-6.480018	0.546121
H	0.356156	-6.303730	0.519695
C	1.119199	-7.223037	2.315577
H	1.049410	-8.212944	1.831257
C	-0.159115	-7.032605	3.134787
H	-0.135197	-6.095535	3.714246
H	-0.292043	-7.855066	3.854478
H	-1.049383	-7.003663	2.487284
C	2.356409	-7.246882	3.215305
H	2.452802	-6.315170	3.796017
H	3.278380	-7.372121	2.625943
H	2.302850	-8.075873	3.937796
C	-3.519282	-3.666593	-0.755131
C	-4.707506	-3.502818	-0.562496
C	4.719452	3.980777	0.526121
C	3.531054	4.147504	0.716030
C	9.954919	1.918774	-0.047761

C	-10.864495	-1.062694	0.151723
C	-10.278853	-2.308175	-0.014077
N	-11.282553	-3.213752	-0.176550
N	-12.416403	-2.612527	-0.112524
N	-12.202633	-1.295753	0.088821
Si	-13.619192	-0.148580	0.100542
C	-13.286155	1.111064	-1.238881
H	-14.124162	1.822574	-1.311417
H	-13.170483	0.620160	-2.217439
H	-12.370649	1.685384	-1.030286
C	-13.697138	0.649879	1.789467
H	-14.626852	1.233674	1.883962
H	-12.853253	1.335865	1.953583
H	-13.692903	-0.109901	2.586147
C	-15.114047	-1.200525	-0.248806
H	-16.020475	-0.574604	-0.260651
H	-15.232877	-1.979366	0.518180
H	-15.020697	-1.704900	-1.221346
C	10.413028	0.774500	-0.216913
N	12.587837	1.038734	-0.092855
N	12.502010	2.223723	0.208280
N	11.848756	3.159835	0.348451
Si	13.717412	-0.204547	0.525649
C	13.609914	-1.596422	-0.709886
H	14.276309	-2.423506	-0.418085
H	13.903928	-1.255851	-1.714321
H	12.583485	-1.989851	-0.767880
C	15.426410	0.554204	0.607195
H	16.159461	-0.188021	0.961521
H	15.450667	1.408935	1.300954
H	15.751122	0.907612	-0.383333
C	13.115248	-0.736186	2.215732
H	13.779295	-1.502189	2.647213
H	12.104156	-1.165112	2.143018
H	13.078819	0.114982	2.913195

Total Electronic Energy = -4310.87371172 a.u.

N_{im}= 1

ν = 384.0*i* cm^{-1}

8

	X	Y	Z
H	2.325209	-4.722409	0.706148
C	2.736086	-3.712371	0.646062
C	3.795470	-1.103955	0.488703
C	2.444082	-2.762145	1.622179
C	3.557080	-3.353264	-0.415517
C	4.084170	-2.051042	-0.512865
C	2.982297	-1.466489	1.551756
H	3.794874	-4.076844	-1.197053
H	4.213770	-0.097697	0.414153
C	1.600144	-2.850468	2.816240
C	0.050272	-2.433813	5.089938
C	0.820325	-3.896602	3.306328
C	1.640010	-1.611595	3.475922
C	0.871840	-1.396438	4.607561
C	0.049206	-3.684299	4.443844

H	0.794567	-4.862832	2.798058
H	0.867865	-0.428530	5.113713
H	-0.590492	-4.479044	4.831226
C	2.576891	-0.642568	2.768024
C	3.812695	-0.328142	3.648360
H	3.461476	0.255638	4.515848
H	4.467274	0.345019	3.069870
C	1.870253	0.681682	2.414232
H	1.558541	1.147363	3.364275
H	2.616114	1.368309	1.979897
C	-0.865495	-2.182648	6.161373
C	-1.735908	-1.928001	6.969667
C	6.162858	-1.150596	-3.899825
C	7.195305	-0.587166	-6.461530
C	6.974146	-2.084270	-4.566574
C	5.933297	0.095908	-4.503508
C	6.446519	0.370491	-5.761972
C	7.485008	-1.803118	-5.829806
H	7.176958	-3.048359	-4.096616
H	5.324249	0.838700	-3.985593
H	6.241353	1.338873	-6.220302
H	8.089646	-2.544108	-6.356549
C	-2.890692	-1.526371	7.715038
C	-5.387464	-0.684821	8.692208
C	-3.816723	-2.463743	8.202500
C	-3.186338	-0.157805	7.829407
C	-4.420275	0.252986	8.309526
C	-5.053390	-2.044256	8.682577
H	-3.586440	-3.528501	8.137099
H	-2.463637	0.577012	7.471357
H	-4.674075	1.314798	8.319570
H	-5.799741	-2.786182	8.975835
H	-0.794567	4.862832	-2.798058
C	-0.820325	3.896602	-3.306328
C	-0.871840	1.396438	-4.607561
C	-1.600144	2.850468	-2.816240
C	-0.049206	3.684299	-4.443844
C	-0.050272	2.433813	-5.089938
C	-1.640010	1.611595	-3.475922
H	0.590492	4.479044	-4.831226
H	-0.867865	0.428530	-5.113713
C	-2.444082	2.762145	-1.622179
C	-4.084170	2.051042	0.512865
C	-2.736086	3.712371	-0.646062
C	-2.982297	1.466489	-1.551756
C	-3.795470	1.103955	-0.488703
C	-3.557080	3.353264	0.415517
H	-2.325209	4.722409	-0.706148
H	-4.213770	0.097697	-0.414153
H	-3.794874	4.076844	1.197053
C	-2.576891	0.642568	-2.768024
C	-3.812695	0.328142	-3.648360
H	-4.467274	-0.345019	-3.069870
H	-3.461476	-0.255638	-4.515848
C	-1.870253	-0.681682	-2.414232
H	-2.616114	-1.368309	-1.979897

H	-1.558541	-1.147363	-3.364275
C	0.865495	2.182648	-6.161373
C	1.735908	1.928001	-6.969667
C	2.890692	1.526371	-7.715038
C	5.387464	0.684821	-8.692208
C	3.816723	2.463743	-8.202500
C	3.186338	0.157805	-7.829407
C	4.420275	-0.252986	-8.309526
C	5.053390	2.044256	-8.682577
H	3.586440	3.528501	-8.137099
H	2.463637	-0.577012	-7.471357
H	4.674075	-1.314798	-8.319570
H	5.799741	2.786182	-8.975835
C	-6.162858	1.150596	3.899825
C	-7.195305	0.587166	6.461530
C	-6.974146	2.084270	4.566574
C	-5.933297	-0.095908	4.503508
C	-6.446519	-0.370491	5.761972
C	-7.485008	1.803118	5.829806
H	-7.176958	3.048359	4.096616
H	-5.324249	-0.838700	3.985593
H	-6.241353	-1.338873	6.220302
H	-8.089646	2.544108	6.356549
C	0.676428	0.545418	1.470772
H	1.055000	0.399227	0.447518
H	0.114751	-0.371618	1.719827
C	-0.304690	1.729298	1.474866
H	-1.044075	1.522807	0.682432
C	-1.082940	1.835264	2.787299
H	-0.426779	2.086216	3.637305
H	-1.595483	0.890015	3.024892
H	-1.851665	2.620280	2.723193
C	0.378258	3.048083	1.114204
H	1.116308	3.346900	1.876819
H	-0.360204	3.860158	1.034373
H	0.901003	2.974016	0.146994
C	4.602163	-1.545642	4.122410
H	4.910308	-2.139886	3.245744
H	3.937846	-2.197155	4.714785
C	5.852578	-1.230102	4.959936
H	6.288761	-2.208862	5.226599
C	5.517548	-0.514005	6.269855
H	6.408062	-0.429074	6.911565
H	4.743995	-1.055782	6.836521
H	5.148103	0.508592	6.090120
C	6.914087	-0.466295	4.165548
H	7.848973	-0.378667	4.740276
H	6.584005	0.557288	3.925233
H	7.147662	-0.974632	3.217003
C	-0.676428	-0.545418	-1.470772
H	-1.055000	-0.399227	-0.447518
H	-0.114751	0.371618	-1.719827
C	0.304690	-1.729298	-1.474866
H	1.044075	-1.522807	-0.682432
C	-0.378258	-3.048083	-1.114204
H	0.360204	-3.860158	-1.034373

H	-1.116308	-3.346900	-1.876819
H	-0.901003	-2.974016	-0.146994
C	1.082940	-1.835264	-2.787299
H	1.851665	-2.620280	-2.723193
H	1.595483	-0.890015	-3.024892
H	0.426779	-2.086216	-3.637305
C	-4.602163	1.545642	-4.122410
H	-3.937846	2.197155	-4.714785
H	-4.910308	2.139886	-3.245744
C	-5.852578	1.230102	-4.959936
H	-6.288761	2.208862	-5.226599
C	-6.914087	0.466295	-4.165548
H	-6.584005	-0.557288	-3.925233
H	-7.848973	0.378667	-4.740276
H	-7.147662	0.974632	-3.217003
C	-5.517548	0.514005	-6.269855
H	-5.148103	-0.508592	-6.090120
H	-4.743995	1.055782	-6.836521
H	-6.408062	0.429074	-6.911565
C	-4.883358	1.708996	1.651938
C	-5.516601	1.463829	2.659045
C	5.516601	-1.463829	-2.659045
C	4.883358	-1.708996	-1.651938
C	7.572567	-0.345357	-7.865698
C	6.777496	0.217559	-8.851940
C	-6.777496	-0.217559	8.851940
C	-7.572567	0.345357	7.865698
N	8.757714	-0.691444	-8.434457
N	8.739626	-0.366345	-9.679316
N	7.545297	0.189659	-9.972885
Si	7.242494	0.749883	-11.680259
C	5.443703	0.415362	-12.059636
H	5.190249	-0.639110	-11.870248
H	5.250029	0.623788	-13.124311
H	4.766111	1.041796	-11.461651
C	8.390456	-0.254332	-12.747753
H	8.152954	-1.326374	-12.677611
H	9.433235	-0.121062	-12.426510
H	8.299055	0.054099	-13.801231
C	7.644787	2.574717	-11.732438
H	8.676707	2.751102	-11.392399
H	6.965701	3.157687	-11.092195
H	7.552347	2.961965	-12.759602
N	-8.757714	0.691444	8.434457
N	-8.739626	0.366345	9.679316
N	-7.545297	-0.189659	9.972885
Si	-7.242494	-0.749883	11.680259
C	-5.443703	-0.415362	12.059636
H	-5.250029	-0.623788	13.124311
H	-5.190249	0.639110	11.870248
H	-4.766111	-1.041796	11.461651
C	-7.644787	-2.574717	11.732438
H	-7.552347	-2.961965	12.759602
H	-6.965701	-3.157687	11.092195
H	-8.676707	-2.751102	11.392399
C	-8.390456	0.254332	12.747753

H	-8.299055	-0.054099	13.801231
H	-9.433235	0.121062	12.426510
H	-8.152954	1.326374	12.677611

Total Electronic Energy = -4311.03689646 a.u.
N_{im}= 0

TS3

	X	Y	Z
H	-9.635158	-3.005260	3.282875
C	-9.484152	-2.432176	2.365383
C	-9.080698	-0.927910	0.028041
C	-8.518413	-2.816086	1.432971
C	-10.193682	-1.247739	2.164457
C	-9.958628	-0.460457	1.024254
C	-8.347962	-2.076248	0.251155
H	-10.883614	-0.887835	2.929700
H	-8.896583	-0.306816	-0.850533
C	-7.440110	-3.815718	1.498193
C	-5.037007	-5.223032	1.271725
C	-7.088214	-4.734228	2.487788
C	-6.619813	-3.644838	0.368857
C	-5.434941	-4.345677	0.244824
C	-5.887124	-5.431499	2.372833
H	-7.721117	-4.881226	3.365679
H	-4.772759	-4.183809	-0.608626
H	-5.576292	-6.119643	3.160815
C	-7.167685	-2.577287	-0.561896
C	-7.600255	-3.167079	-1.922532
H	-6.691204	-3.521575	-2.436986
H	-7.995739	-2.338421	-2.533894
C	-6.156707	-1.431587	-0.795895
H	-5.319727	-1.818656	-1.400603
H	-6.656633	-0.685144	-1.435219
C	-3.710851	-5.764264	1.213289
C	-2.527248	-6.023609	1.118620
C	-9.588261	3.406590	0.530597
C	-7.707202	5.450119	0.095912
C	-9.069679	4.137340	1.613014
C	-9.261061	3.807247	-0.776272
C	-8.332643	4.815546	-0.991027
C	-8.139126	5.144102	1.398165
H	-9.337586	3.849083	2.630869
H	-9.681070	3.261995	-1.623288
H	-8.024701	5.067487	-2.007229
H	-7.680138	5.653346	2.247316
C	-1.104002	-6.106287	0.978026
C	1.683936	-5.824696	0.692763
C	-0.263318	-6.148004	2.103280
C	-0.522253	-6.004171	-0.297938
C	0.850471	-5.866683	-0.438762
C	1.110860	-6.007234	1.962678
H	-0.704393	-6.243230	3.096926
H	-1.166762	-5.989489	-1.178510
H	1.289568	-5.743029	-1.430200
H	1.751976	-5.993626	2.845739
C	3.064166	-5.471073	0.546513

H	5.518480	5.745106	-2.965674
C	4.804662	5.457212	-2.190803
C	2.952860	4.716521	-0.206709
C	5.070272	4.386292	-1.337523
C	3.598705	6.144635	-2.066043
C	2.657402	5.773802	-1.089480
C	4.145127	4.029761	-0.340283
H	3.364708	6.967789	-2.743382
H	2.219758	4.429970	0.550747
C	6.182732	3.424484	-1.294517
C	7.820627	1.188113	-0.948011
C	7.308495	3.266342	-2.103366
C	5.916978	2.503023	-0.268311
C	6.727085	1.399081	-0.087079
C	8.126158	2.150499	-1.923916
H	7.534195	3.984573	-2.894851
H	6.492830	0.649983	0.672888
H	8.990338	1.989614	-2.570038
C	4.635417	2.842821	0.471359
C	4.918504	3.244266	1.938659
H	5.297979	2.348648	2.458909
H	3.951815	3.487546	2.411143
C	3.645834	1.658013	0.458413
H	4.095396	0.852079	1.062337
H	2.734553	1.962595	1.000206
C	1.359685	6.378344	-1.006768
C	0.203083	6.734766	-0.897775
C	-1.204453	6.953957	-0.741440
C	-4.003229	6.935641	-0.428172
C	-2.048656	7.087151	-1.856943
C	-1.780254	6.903730	0.540213
C	-3.158281	6.896387	0.694967
C	-3.428703	7.076647	-1.702775
H	-1.610563	7.146280	-2.854707
H	-1.131050	6.822563	1.413688
H	-3.596840	6.806271	1.690239
H	-4.076792	7.126524	-2.579450
C	7.456435	-2.428611	-0.335450
C	5.382385	-4.263703	0.180753
C	7.004198	-3.296569	-1.343105
C	6.922150	-2.559406	0.957175
C	5.902606	-3.466239	1.213073
C	5.977151	-4.195326	-1.091011
H	7.436168	-3.219685	-2.342266
H	7.281304	-1.902146	1.751954
H	5.457528	-3.523179	2.207960
H	5.590759	-4.823277	-1.895705
C	4.176045	-5.006507	0.389200
C	-5.626487	-0.768069	0.481245
H	-6.390464	-0.830369	1.273454
H	-4.761958	-1.341907	0.853326
C	-5.227520	0.710372	0.329988
H	-4.782105	1.005327	1.296343
C	-4.161459	0.919787	-0.746328
H	-4.551191	0.681060	-1.749544
H	-3.280668	0.282453	-0.568694

H	-3.821804	1.966764	-0.768598
C	-6.439572	1.618810	0.103065
H	-6.916378	1.431353	-0.873285
H	-6.150758	2.681678	0.117566
H	-7.208251	1.469101	0.877438
C	-8.628391	-4.291924	-1.836300
H	-9.529437	-3.914996	-1.323450
H	-8.228286	-5.096788	-1.196773
C	-9.049974	-4.902809	-3.182925
H	-9.792615	-5.682747	-2.938945
C	-7.890390	-5.595001	-3.902276
H	-8.246772	-6.141214	-4.789224
H	-7.383408	-6.316840	-3.242930
H	-7.136569	-4.869745	-4.249031
C	-9.743430	-3.890210	-4.096581
H	-10.157243	-4.383695	-4.989463
H	-9.043270	-3.115456	-4.448791
H	-10.571789	-3.383136	-3.577376
C	3.281090	1.129016	-0.928176
H	4.194168	1.060844	-1.542410
H	2.628425	1.861332	-1.432588
C	2.595815	-0.248572	-0.937142
H	2.346468	-0.455109	-1.992959
C	3.527497	-1.369719	-0.468888
H	3.060143	-2.357394	-0.605201
H	3.769993	-1.280592	0.602485
H	4.480025	-1.368550	-1.023010
C	1.284063	-0.256697	-0.149941
H	0.758301	-1.216886	-0.267968
H	0.606984	0.544227	-0.487141
H	1.461950	-0.114347	0.928473
C	5.894997	4.404160	2.114307
H	5.496501	5.291891	1.594947
H	6.843025	4.155186	1.608444
C	6.204284	4.787465	3.570907
H	6.910011	5.634894	3.514580
C	6.909081	3.665691	4.336587
H	6.240439	2.805603	4.503159
H	7.243283	4.013350	5.326354
H	7.793411	3.302399	3.789935
C	4.967345	5.280672	4.324432
H	4.242402	4.467383	4.490486
H	4.452802	6.080619	3.769252
H	5.240810	5.678994	5.313743
C	-5.401968	6.669755	-0.271110
C	-6.524421	6.231584	-0.109153
C	-10.190763	2.123607	0.747726
C	-10.321070	0.925310	0.918334
C	8.468744	-0.102417	-0.871999
C	8.321617	-1.318617	-0.645907
N	10.577188	0.070124	-1.495215
N	10.779662	-1.058498	-1.362751
N	10.293017	-2.160365	-1.119129
Si	11.039182	-3.485045	-0.167442
C	12.839185	-3.607717	-0.666480
H	12.939158	-3.813954	-1.743070

H	13.335726	-4.422599	-0.115868
H	13.378278	-2.673498	-0.445245
C	10.849114	-3.049339	1.642565
H	9.782884	-2.959687	1.901408
H	11.339929	-2.091612	1.875120
H	11.292356	-3.826229	2.285828
C	10.078169	-5.021936	-0.604973
H	9.025100	-4.933341	-0.298271
H	10.510064	-5.897422	-0.094374
H	10.104246	-5.210085	-1.689088

Total Electronic Energy = -a.u.

N_{im}= 1

ν = 440.2*i* cm^{-1}

7'

	X	Y	Z
H	-9.535817	-3.419751	3.282525
C	-9.476096	-2.767842	2.408188
C	-9.313298	-1.063368	0.182421
C	-8.458700	-2.927437	1.465852
C	-10.372627	-1.706434	2.273527
C	-10.266412	-0.818267	1.190671
C	-8.405376	-2.090523	0.338544
H	-11.118354	-1.519643	3.048171
H	-9.230649	-0.363499	-0.651757
C	-7.245489	-3.760787	1.465317
C	-4.680033	-4.813603	1.125438
C	-6.758970	-4.690290	2.385219
C	-6.470428	-3.399236	0.349087
C	-5.204298	-3.922406	0.169755
C	-5.477791	-5.211120	2.213768
H	-7.354681	-4.984384	3.252083
H	-4.583515	-3.615481	-0.674897
H	-5.067799	-5.908481	2.946296
C	-7.174455	-2.362337	-0.507366
C	-7.542264	-2.927249	-1.898748
H	-6.600608	-3.117316	-2.440764
H	-8.061120	-2.128452	-2.455017
C	-6.332222	-1.078768	-0.686450
H	-5.456794	-1.322575	-1.311505
H	-6.933833	-0.374145	-1.284298
C	-3.302978	-5.188143	1.003083
C	-2.104507	-5.324564	0.855927
C	-10.355590	3.013973	0.753723
C	-8.457365	5.013769	0.233858
C	-9.793737	3.748956	1.811506
C	-10.093055	3.417710	-0.566956
C	-9.154257	4.406378	-0.824049
C	-8.852041	4.735372	1.553515
H	-10.018778	3.464625	2.840811
H	-10.555091	2.875437	-1.393864
H	-8.878772	4.643445	-1.853082
H	-8.341029	5.230765	2.380917
C	-0.688779	-5.293465	0.648132
C	2.084611	-4.949329	0.303698
C	0.217194	-5.822299	1.582494

C	-0.184279	-4.632820	-0.487020
C	1.180178	-4.463558	-0.657075
C	1.585455	-5.651070	1.413239
H	-0.164074	-6.343886	2.461901
H	-0.881991	-4.227234	-1.221479
H	1.561423	-3.922277	-1.524638
H	2.281358	-6.037147	2.159937
C	3.470850	-4.617844	0.179182
H	4.608495	4.516747	-3.619272
C	4.058877	4.292591	-2.702508
C	2.634075	3.715583	-0.343243
C	4.631871	3.514411	-1.697568
C	2.764937	4.776378	-2.529569
C	2.038857	4.489609	-1.358773
C	3.919707	3.234690	-0.519147
H	2.295565	5.379039	-3.309037
H	2.069322	3.499330	0.566496
C	5.938347	2.848014	-1.612479
C	8.177642	1.309910	-0.986305
C	7.016141	2.821200	-2.496368
C	5.996828	2.149949	-0.395767
C	7.102897	1.374045	-0.086434
C	8.135724	2.058070	-2.172309
H	6.986183	3.380749	-3.434018
H	7.146101	0.811697	0.850038
H	8.989927	2.015614	-2.850894
C	4.758977	2.412942	0.447371
C	5.124817	3.253953	1.698173
H	5.775424	2.630116	2.333586
H	4.196508	3.414917	2.272265
C	4.039693	1.132834	0.910908
H	4.623511	0.687127	1.733372
H	3.081158	1.440027	1.363387
C	0.690988	4.946744	-1.197343
C	-0.466491	5.279190	-1.036376
C	-1.850495	5.570644	-0.815581
C	-4.616035	5.931233	-0.408367
C	-2.658373	6.116656	-1.827833
C	-2.438881	5.254384	0.422066
C	-3.798406	5.433839	0.622933
C	-4.021798	6.293655	-1.627996
H	-2.208934	6.376003	-2.787858
H	-1.817570	4.840137	1.217798
H	-4.252826	5.155286	1.575329
H	-4.645619	6.687415	-2.432210
C	8.114092	-1.815795	-0.233379
C	5.821087	-3.437566	-0.038631
C	7.259646	-1.977626	-1.331939
C	7.809426	-2.476085	0.962819
C	6.681415	-3.283715	1.060776
C	6.130247	-2.777971	-1.239905
H	7.484248	-1.454895	-2.263681
H	8.451950	-2.335407	1.834349
H	6.441041	-3.780335	2.002355
H	5.461429	-2.884861	-2.095370
C	4.589604	-4.157363	0.075867

C	-5.880098	-0.412488	0.614529
H	-6.701359	-0.453038	1.349247
H	-5.054208	-0.999042	1.050445
C	-5.440171	1.055491	0.477083
H	-5.079020	1.356957	1.476367
C	-4.276218	1.235673	-0.499028
H	-4.581024	1.009293	-1.533931
H	-3.431609	0.575362	-0.245502
H	-3.908785	2.273944	-0.487563
C	-6.604052	1.985151	0.125244
H	-6.994533	1.789398	-0.886932
H	-6.283636	3.037804	0.143392
H	-7.443515	1.875865	0.830858
C	-8.398988	-4.190238	-1.874462
H	-9.336190	-3.977159	-1.333044
H	-7.878707	-4.967020	-1.288978
C	-8.750903	-4.772681	-3.253324
H	-9.372394	-5.663113	-3.052745
C	-7.516596	-5.249411	-4.021758
H	-7.806107	-5.786397	-4.938184
H	-6.902929	-5.930467	-3.411519
H	-6.877760	-4.405363	-4.328293
C	-9.594126	-3.815362	-4.097974
H	-9.947836	-4.307697	-5.016930
H	-9.015576	-2.929421	-4.406033
H	-10.477614	-3.463036	-3.542814
C	3.804593	0.081152	-0.171419
H	4.759992	-0.426766	-0.381345
H	3.509926	0.576782	-1.112664
C	2.741547	-0.972853	0.188825
H	2.865449	-1.801301	-0.530698
C	2.945454	-1.556122	1.588100
H	2.277084	-2.414568	1.755326
H	2.726544	-0.809911	2.368841
H	3.980200	-1.903538	1.732518
C	1.318464	-0.436225	0.023474
H	0.575450	-1.219942	0.240539
H	1.142540	-0.074218	-1.001302
H	1.120228	0.403919	0.709584
C	5.803065	4.591194	1.412402
H	5.129329	5.214139	0.800482
H	6.700769	4.415660	0.796134
C	6.216816	5.394310	2.656707
H	6.670469	6.325550	2.274297
C	7.286589	4.681776	3.486975
H	6.888396	3.775348	3.971153
H	7.665475	5.336689	4.286785
H	8.142648	4.380518	2.863254
C	5.020420	5.797406	3.521002
H	4.556988	4.922524	4.005191
H	4.244535	6.299788	2.922141
H	5.327205	6.487321	4.322287
C	-6.036773	5.918276	-0.223563
C	-7.210168	5.672880	-0.018776
C	-10.880721	1.699547	0.991282
C	-10.856350	0.491883	1.147615

C	9.317585	0.416932	-0.712169
C	9.278351	-0.922415	-0.365941
N	10.622920	0.788753	-0.797217
N	11.368639	-0.222493	-0.522246
N	10.587070	-1.288134	-0.255730
Si	11.413938	-2.883453	0.065218
C	13.113447	-2.718019	-0.677629
H	13.052055	-2.540649	-1.761648
H	13.691068	-3.640506	-0.507293
H	13.653636	-1.871252	-0.231374
C	11.494788	-3.118905	1.918666
H	10.499060	-3.257171	2.364761
H	11.971116	-2.248713	2.395744
H	12.095591	-4.010126	2.160811
C	10.413070	-4.216755	-0.780203
H	9.434541	-4.379904	-0.306531
H	10.971913	-5.165963	-0.744235
H	10.243152	-3.965838	-1.838660

Total Electronic Energy = -3737.79586266 a.u.
N_{im}= 0

TS4

	X	Y	Z
H	-8.124023	4.536461	-2.820061
C	-8.081563	3.743658	-2.069760
C	-7.977039	1.689374	-0.160177
C	-6.973828	3.612394	-1.231153
C	-9.127571	2.824540	-1.971030
C	-9.070276	1.771772	-1.044216
C	-6.941447	2.595977	-0.262163
H	-9.986459	2.891203	-2.640488
H	-7.934766	0.871185	0.562247
C	-5.685383	4.321793	-1.181213
C	-3.039056	5.132894	-0.796810
C	-5.163417	5.351776	-1.964443
C	-4.897531	3.727604	-0.179115
C	-3.591009	4.129629	0.022714
C	-3.842161	5.750895	-1.772370
H	-5.767965	5.824582	-2.741483
H	-2.965532	3.649167	0.778488
H	-3.409130	6.531780	-2.399917
C	-5.649152	2.617850	0.534037
C	-5.906936	2.964055	2.018871
H	-4.929781	2.993574	2.529752
H	-6.460229	2.119620	2.463757
C	-4.916260	1.261723	0.450821
H	-4.045944	1.291427	1.127764
H	-5.592028	0.498354	0.872385
C	-1.641026	5.414343	-0.662353
C	-0.435691	5.485537	-0.525947
C	-9.460414	-1.764548	-0.316838
C	-7.562388	-3.713612	0.399118
C	-9.078614	-2.756303	-1.234776
C	-8.992580	-1.854444	1.005971
C	-8.057098	-2.816378	1.360261
C	-8.137190	-3.714442	-0.883141

H	-9.468154	-2.714960	-2.253436
H	-9.313980	-1.109344	1.737065
H	-7.638299	-2.827337	2.368129
H	-7.777011	-4.424436	-1.629721
C	0.981626	5.390235	-0.351425
C	3.746834	4.925033	-0.091194
C	1.884475	5.906102	-1.296400
C	1.488123	4.683062	0.754174
C	2.848752	4.455130	0.883250
C	3.248264	5.674802	-1.169126
H	1.501889	6.464117	-2.152565
H	0.793891	4.288241	1.497739
H	3.229595	3.877905	1.727482
H	3.939456	6.049252	-1.926077
C	5.118525	4.523843	-0.020886
H	5.695111	-4.583441	3.592765
C	5.132060	-4.316145	2.695914
C	3.671603	-3.625449	0.389082
C	5.735750	-3.610049	1.656533
C	3.788727	-4.664991	2.586150
C	3.045040	-4.318153	1.443159
C	5.005442	-3.274142	0.504348
H	3.293888	-5.204691	3.395459
H	3.091451	-3.359741	-0.497545
C	7.092689	-3.065172	1.514368
C	9.426505	-1.719409	0.798665
C	8.201490	-3.127885	2.357007
C	7.163680	-2.377751	0.292334
C	8.317779	-1.696215	-0.060944
C	9.367700	-2.461032	1.987929
H	8.159730	-3.680591	3.298265
H	8.372047	-1.138030	-0.999337
H	10.246779	-2.487780	2.634866
C	5.875388	-2.534275	-0.500477
C	6.116160	-3.404997	-1.760735
H	6.792236	-2.840696	-2.424598
H	5.155043	-3.485670	-2.296477
C	5.252357	-1.196383	-0.938861
H	5.847546	-0.794245	-1.775600
H	4.259619	-1.420616	-1.365388
C	1.646547	-4.621536	1.359569
C	0.450089	-4.815211	1.278283
C	-0.973421	-4.944708	1.183837
C	-3.782926	-4.962505	0.967640
C	-1.780232	-4.778697	2.322839
C	-1.593819	-5.174700	-0.056242
C	-2.977498	-5.186432	-0.162428
C	-3.163567	-4.786319	2.216524
H	-1.306733	-4.610721	3.291579
H	-0.975646	-5.317621	-0.944128
H	-3.450526	-5.331520	-1.135234
H	-3.781340	-4.619702	3.100562
C	9.575248	1.413456	0.114666
C	7.397891	3.198054	0.068158
C	8.784888	1.604475	1.255730
C	9.266851	2.129210	-1.048247

C	8.196456	3.016849	-1.072998
C	7.712987	2.484948	1.236836
H	9.011899	1.039964	2.162166
H	9.858439	1.969182	-1.951967
H	7.950455	3.555755	-1.989536
H	7.091781	2.613277	2.124635
C	6.212265	3.998384	0.026033
C	-4.467928	0.856281	-0.954482
H	-5.228482	1.174034	-1.687809
H	-3.551177	1.412289	-1.210529
C	-4.219128	-0.650135	-1.141711
H	-3.739752	-0.762474	-2.130181
C	-3.257379	-1.224561	-0.099190
H	-3.706168	-1.220738	0.907479
H	-2.320106	-0.647380	-0.052626
H	-2.998642	-2.269676	-0.329296
C	-5.527619	-1.439489	-1.183889
H	-6.080101	-1.368329	-0.232982
H	-5.338879	-2.509568	-1.360613
H	-6.194883	-1.072394	-1.979126
C	-6.661332	4.269577	2.255477
H	-7.622462	4.232406	1.715782
H	-6.091225	5.099960	1.805599
C	-6.941431	4.608684	3.728802
H	-7.479122	5.573114	3.717954
C	-5.660090	4.816149	4.538775
H	-5.887804	5.192864	5.547933
H	-4.990972	5.542127	4.050814
H	-5.101069	3.874385	4.661754
C	-7.862548	3.587908	4.400407
H	-8.158417	3.924969	5.405915
H	-7.367370	2.610355	4.517944
H	-8.780879	3.430557	3.813179
C	5.134138	-0.138350	0.156429
H	6.130306	0.299077	0.333251
H	4.839658	-0.618699	1.105578
C	4.136003	0.990505	-0.157036
H	4.336194	1.794922	0.571878
C	4.342210	1.583277	-1.551795
H	3.728367	2.486867	-1.687706
H	4.054010	0.867032	-2.338174
H	5.393982	1.863563	-1.717954
C	2.684485	0.549875	0.040727
H	1.992455	1.388189	-0.137326
H	2.513813	0.178210	1.063007
H	2.407107	-0.258779	-0.655641
C	6.686861	-4.795612	-1.495725
H	5.984941	-5.358113	-0.857459
H	7.618308	-4.698081	-0.913235
C	6.984383	-5.631435	-2.751677
H	7.370423	-6.598113	-2.383168
C	8.079978	-5.013144	-3.622780
H	7.743080	-4.076236	-4.095296
H	8.372126	-5.698269	-4.433594
H	8.980805	-4.785733	-3.031675
C	5.727033	-5.930572	-3.570540

H	5.322296	-5.019090	-4.039616
H	4.933733	-6.365276	-2.942246
H	5.944225	-6.643736	-4.380739
C	-5.194551	-4.773698	0.823777
C	-6.347709	-4.425291	0.660106
C	-10.112641	-0.554647	-0.751018
C	-9.990577	0.655483	-1.019314
C	10.621407	-0.915654	0.483478
C	10.672119	0.431080	0.168715
N	11.895164	-1.391622	0.492789
N	12.704781	-0.435519	0.201253
N	11.998726	0.695026	-0.001171
Si	12.934399	2.226344	-0.333493
C	14.644976	1.916374	0.334504
H	14.614292	1.726281	1.417698
H	15.286110	2.793570	0.152524
H	15.097886	1.037555	-0.145602
C	12.956744	2.485766	-2.185340
H	11.956139	2.702073	-2.587417
H	13.348399	1.590993	-2.692982
H	13.610164	3.335121	-2.441208
C	12.077603	3.618885	0.572536
H	11.096954	3.867707	0.142564
H	12.708770	4.521254	0.528156
H	11.930474	3.362542	1.633116
N	-12.143785	-1.038596	-1.447679
N	-12.381181	0.123641	-1.763267
N	-11.976223	1.194062	-1.899629
Si	-13.204642	-2.159202	-0.534373
C	-14.955422	-1.933304	-1.156646
H	-15.310132	-0.905314	-0.983936
H	-15.640424	-2.618963	-0.632826
H	-15.023485	-2.142491	-2.235156
C	-13.048549	-1.722104	1.278232
H	-13.346844	-0.678394	1.462373
H	-12.005901	-1.843661	1.610110
H	-13.683101	-2.374416	1.899240
C	-12.540602	-3.865587	-0.886962
H	-13.150952	-4.626942	-0.375739
H	-11.503491	-3.965643	-0.532537
H	-12.556666	-4.081003	-1.966215

Total Electronic Energy = -a.u.

N_{im}= 1

ν = 421.9*i* cm^{-1}

8'

	X	Y	Z
H	-8.289500	-3.491564	3.420374
C	-8.367620	-2.951589	2.474055
C	-8.575743	-1.546803	0.046826
C	-7.322032	-2.968656	1.552012
C	-9.514366	-2.215938	2.180788
C	-9.614734	-1.485215	0.987672
C	-7.443695	-2.295484	0.325549
H	-10.341152	-2.176585	2.892811
H	-8.664111	-0.997373	-0.894042

C	-5.984252	-3.574654	1.610922
C	-3.321881	-4.331957	1.253082
C	-5.330706	-4.272591	2.625867
C	-5.322993	-3.289745	0.404313
C	-4.005118	-3.664769	0.217802
C	-4.001555	-4.647046	2.443846
H	-5.839841	-4.504102	3.563945
H	-3.474900	-3.425490	-0.706604
H	-3.465246	-5.169388	3.237968
C	-6.230469	-2.539482	-0.556941
C	-6.609505	-3.432914	-1.766374
H	-5.694767	-3.585421	-2.364005
H	-7.298818	-2.850849	-2.400673
C	-5.573666	-1.251616	-1.082737
H	-4.647145	-1.548189	-1.603395
H	-6.222194	-0.820858	-1.863763
C	-1.925307	-4.606542	1.095517
C	-0.728557	-4.734948	0.930088
C	-9.568256	1.640155	0.288122
C	-7.254983	3.232326	0.081450
C	-8.709841	1.797218	1.384312
C	-9.261128	2.296262	-0.909679
C	-8.122712	3.088872	-1.013628
C	-7.571255	2.583663	1.286894
H	-8.936850	1.278476	2.317690
H	-9.907973	2.161283	-1.779020
H	-7.878626	3.578591	-1.957890
H	-6.897658	2.683048	2.139476
C	0.684730	-4.756711	0.707181
C	3.468199	-4.583567	0.313189
C	1.575527	-5.275228	1.662612
C	1.207446	-4.189959	-0.469185
C	2.577053	-4.105934	-0.663772
C	2.948028	-5.188985	1.468948
H	1.178929	-5.725031	2.574296
H	0.522210	-3.791867	-1.219288
H	2.974010	-3.638313	-1.566390
H	3.632891	-5.566407	2.230176
C	4.868099	-4.328423	0.162844
H	5.839844	4.504100	-3.563946
C	5.330709	4.272589	-2.625869
C	4.005118	3.664767	-0.217805
C	5.984254	3.574653	-1.610923
C	4.001558	4.647044	-2.443850
C	3.321882	4.331955	-1.253086
C	5.322994	3.289743	-0.404314
H	3.465249	5.169385	-3.237972
H	3.474899	3.425488	0.706601
C	7.322034	2.968655	-1.552012
C	9.614736	1.485215	-0.987669
C	8.367623	2.951589	-2.474054
C	7.443696	2.295484	-0.325548
C	8.575744	1.546803	-0.046824
C	9.514368	2.215938	-2.180786
H	8.289504	3.491564	-3.420373
H	8.664111	0.997373	0.894044

H	10.341155	2.176585	-2.892808
C	6.230469	2.539481	0.556941
C	6.609503	3.432913	1.766373
H	7.298815	2.850848	2.400674
H	5.694764	3.585420	2.364003
C	5.573665	1.251614	1.082735
H	6.222193	0.820857	1.863762
H	4.647144	1.548187	1.603392
C	1.925308	4.606540	-1.095522
C	0.728558	4.734945	-0.930095
C	-0.684729	4.756710	-0.707187
C	-3.468198	4.583567	-0.313196
C	-1.575526	5.275224	-1.662620
C	-1.207446	4.189960	0.469180
C	-2.577053	4.105936	0.663766
C	-2.948027	5.188981	-1.468957
H	-1.178928	5.725025	-2.574305
H	-0.522210	3.791870	1.219284
H	-2.974010	3.638317	1.566385
H	-3.632890	5.566403	-2.230186
C	9.568258	-1.640155	-0.288121
C	7.254984	-3.232325	-0.081453
C	8.709844	-1.797217	-1.384312
C	9.261127	-2.296263	0.909679
C	8.122712	-3.088873	1.013626
C	7.571258	-2.583662	-1.286897
H	8.936855	-1.278475	-2.317690
H	9.907971	-2.161285	1.779022
H	7.878624	-3.578593	1.957887
H	6.897662	-2.683046	-2.139480
C	6.004805	-3.917560	0.044780
C	-5.271440	-0.192721	-0.023292
H	-6.199198	0.357193	0.203907
H	-4.971790	-0.684734	0.917974
C	-4.173342	0.807361	-0.424199
H	-4.222413	1.632919	0.305999
C	-2.773001	0.199298	-0.325300
H	-2.638994	-0.631990	-1.037439
H	-2.576972	-0.195779	0.683559
H	-2.001808	0.952528	-0.551512
C	-4.411917	1.411720	-1.808648
H	-4.275386	0.660369	-2.603273
H	-3.704210	2.231698	-2.005242
H	-5.431057	1.818515	-1.898457
C	-7.236100	-4.779748	-1.415601
H	-8.123935	-4.611012	-0.783420
H	-6.527365	-5.357883	-0.799100
C	-7.652927	-5.640621	-2.619670
H	-8.068887	-6.570321	-2.193139
C	-6.464674	-6.039296	-3.497160
H	-6.768523	-6.766364	-4.266057
H	-5.660604	-6.496696	-2.899456
H	-6.038877	-5.169212	-4.022746
C	-8.762554	-4.991401	-3.449495
H	-9.138628	-5.686005	-4.216456
H	-8.403459	-4.091474	-3.974623

H	-9.613478	-4.693708	-2.817111
C	5.271441	0.192720	0.023289
H	6.199200	-0.357195	-0.203906
H	4.971794	0.684733	-0.917977
C	4.173341	-0.807361	0.424193
H	4.222413	-1.632919	-0.306005
C	4.411912	-1.411721	1.808642
H	3.704203	-2.231699	2.005235
H	4.275382	-0.660371	2.603268
H	5.431051	-1.818519	1.898453
C	2.773001	-0.199296	0.325292
H	2.001806	-0.952526	0.551500
H	2.576975	0.195784	-0.683566
H	2.638993	0.631990	1.037432
C	7.236098	4.779747	1.415602
H	6.527366	5.357881	0.799096
H	8.123937	4.611011	0.783426
C	7.652919	5.640623	2.619671
H	8.068882	6.570322	2.193140
C	8.762539	4.991404	3.449505
H	8.403440	4.091479	3.974633
H	9.138608	5.686010	4.216467
H	9.613468	4.693709	2.817127
C	6.464659	6.039301	3.497153
H	6.038859	5.169218	4.022738
H	5.660594	6.496700	2.899443
H	6.768504	6.766370	4.266050
C	-4.868098	4.328424	-0.162851
C	-6.004805	3.917561	-0.044785
C	-10.733641	0.747762	0.423852
C	-10.766909	-0.596850	0.749653
C	10.766910	0.596850	-0.749649
C	10.733642	-0.747761	-0.423848
N	12.070132	0.971082	-0.850764
N	12.820665	-0.044185	-0.603503
N	12.043690	-1.114289	-0.340854
Si	12.871098	-2.713673	-0.045529
C	14.563213	-2.543435	-0.803900
H	14.490999	-2.355996	-1.885564
H	15.141762	-3.467866	-0.647980
H	15.108683	-1.701259	-0.355335
C	12.967285	-2.967491	1.804664
H	11.973755	-3.102471	2.256771
H	13.453528	-2.105227	2.286095
H	13.563173	-3.865408	2.033795
C	11.857304	-4.035764	-0.893033
H	10.882565	-4.198065	-0.411172
H	12.411850	-4.987880	-0.869956
H	11.678346	-3.775521	-1.947732
N	-12.043688	1.114290	0.340860
N	-12.820663	0.044186	0.603511
N	-12.070130	-0.971082	0.850772
Si	-12.871095	2.713675	0.045539
C	-14.563210	2.543436	0.803910
H	-15.108683	1.701265	0.355340
H	-15.141758	3.467869	0.647997

H	-14.490996	2.355989	1.885573
C	-12.967282	2.967498	-1.804653
H	-13.453525	2.105235	-2.286087
H	-11.973753	3.102481	-2.256760
H	-13.563172	3.865414	-2.033781
C	-11.857301	4.035763	0.893046
H	-10.882561	4.198064	0.411185
H	-11.678343	3.775517	1.947745
H	-12.411846	4.987879	0.869972

Total Electronic Energy = -4311.04031128 a.u.
N_{im}= 0

6

	X	Y	Z
H	0.838396	-3.720227	-3.685374
C	1.153553	-3.651629	-2.642067
C	1.967881	-3.471728	0.051696
C	0.218641	-3.676184	-1.609470
C	2.500708	-3.530844	-2.324755
C	2.920609	-3.428837	-0.984669
C	0.624592	-3.600620	-0.266550
H	3.252133	-3.501664	-3.115613
H	2.298608	-3.401462	1.090339
C	-1.243210	-3.761299	-1.648884
C	-3.983218	-3.759997	-1.158231
C	-2.125129	-3.810215	-2.727032
C	-1.720240	-3.752475	-0.328543
C	-3.081731	-3.751695	-0.076219
C	-3.493036	-3.811828	-2.476775
H	-1.755023	-3.825051	-3.754404
H	-3.468712	-3.712505	0.944426
H	-4.203943	-3.821561	-3.304661
C	-0.571401	-3.722020	0.670128
C	-0.501731	-5.046860	1.470966
H	-1.393135	-5.088912	2.119228
H	0.367015	-4.978645	2.146976
C	-0.705958	-2.549342	1.662270
H	-1.637148	-2.710581	2.230920
H	0.108423	-2.624286	2.402328
C	-5.386438	-3.600270	-0.921866
C	-6.552659	-3.320785	-0.728239
C	6.886449	-2.745710	-0.343864
C	9.553677	-1.877104	-0.100567
C	7.878026	-3.226182	-1.215494
C	7.260901	-1.874210	0.691741
C	8.575259	-1.448981	0.807888
C	9.196035	-2.796585	-1.092755
H	7.599683	-3.917725	-2.012683
H	6.502321	-1.507553	1.385031
H	8.842609	-0.744262	1.597424
H	9.953996	-3.146941	-1.796336
C	-7.843663	-2.751247	-0.480754
C	-10.158994	-1.196591	-0.141887
C	-8.870346	-2.785028	-1.438499
C	-8.040067	-2.015287	0.699739
C	-9.181859	-1.247034	0.860631

C	-10.017257	-2.014704	-1.267654
H	-8.736997	-3.375574	-2.346623
H	-7.257042	-2.003353	1.459532
H	-9.292037	-0.621995	1.749224
H	-10.783262	-1.994569	-2.045733
H	1.754885	3.824970	3.754466
C	2.125027	3.810143	2.727107
C	3.081719	3.751645	0.076327
C	1.243143	3.761255	1.648927
C	3.492942	3.811742	2.476898
C	3.983169	3.759926	1.158370
C	1.720219	3.752438	0.328603
H	4.203820	3.821456	3.304808
H	3.468735	3.712464	-0.944305
C	-0.218707	3.676166	1.609460
C	-2.920656	3.428859	0.984563
C	-1.153656	3.651629	2.642024
C	-0.624612	3.600612	0.266526
C	-1.967891	3.471739	-0.051768
C	-2.500802	3.530865	2.324664
H	-0.838536	3.720230	3.685342
H	-2.298583	3.401479	-1.090423
H	-3.252256	3.501702	3.115494
C	0.571416	3.722010	-0.670109
C	0.501787	5.046864	-1.470928
H	-0.366943	4.978674	-2.146960
H	1.393208	5.088911	-2.119168
C	0.706003	2.549348	-1.662265
H	-0.108326	2.624327	-2.402375
H	1.637234	2.710576	-2.230852
C	5.386395	3.600201	0.922040
C	6.552619	3.320729	0.728414
C	7.843627	2.751213	0.480896
C	10.158966	1.196594	0.141917
C	8.870306	2.784926	1.438647
C	8.040037	2.015344	-0.699653
C	9.181834	1.247109	-0.860600
C	10.017222	2.014621	1.267746
H	8.736952	3.375402	2.346816
H	7.257015	2.003465	-1.459448
H	9.292017	0.622139	-1.749241
H	10.783224	1.994429	2.045827
C	-6.886487	2.745747	0.343688
C	-9.553713	1.877127	0.100414
C	-7.878072	3.226263	1.215285
C	-7.260930	1.874196	-0.691877
C	-8.575287	1.448959	-0.808012
C	-9.196079	2.796660	1.092557
H	-7.599736	3.917846	2.012443
H	-6.502344	1.507504	-1.385141
H	-8.842630	0.744200	-1.597515
H	-9.954046	3.147051	1.796114
C	-0.705057	-1.161420	1.024020
H	0.330485	-0.899542	0.757858
H	-1.262888	-1.195919	0.072231
C	-1.296804	-0.037009	1.889527

H	-1.141187	0.900410	1.328997
C	-2.806100	-0.187811	2.086441
H	-3.057558	-1.081243	2.681846
H	-3.328462	-0.268891	1.120367
H	-3.219939	0.685110	2.613816
C	-0.564626	0.113917	3.222477
H	-0.695018	-0.774582	3.862132
H	-0.947455	0.981227	3.781542
H	0.515864	0.265206	3.068024
C	-0.409548	-6.315187	0.626531
H	0.460818	-6.238512	-0.046697
H	-1.296185	-6.377954	-0.026550
C	-0.293972	-7.625388	1.423119
H	-0.251529	-8.431153	0.669273
C	-1.520062	-7.891347	2.298805
H	-1.474918	-8.896657	2.745275
H	-2.451810	-7.822921	1.715647
H	-1.589721	-7.170083	3.129135
C	0.998185	-7.704374	2.238848
H	1.122576	-8.703512	2.684110
H	1.000973	-6.977468	3.067146
H	1.880833	-7.501960	1.612139
C	0.705027	1.161412	-1.024042
H	-0.330553	0.899501	-0.758057
H	1.262697	1.195904	-0.072158
C	1.296950	0.037036	-1.889475
H	1.141194	-0.900409	-1.329029
C	0.565070	-0.113810	-3.222597
H	0.948014	-0.981097	-3.781620
H	0.695622	0.774720	-3.862177
H	-0.515457	-0.265089	-3.068398
C	2.806293	0.187824	-2.086044
H	3.220236	-0.685070	-2.613384
H	3.328442	0.268829	-1.119848
H	3.057900	1.081292	-2.681330
C	0.409607	6.315181	-0.626476
H	1.296242	6.377937	0.026607
H	-0.460761	6.238500	0.046749
C	0.294034	7.625392	-1.423047
H	0.251605	8.431149	-0.669192
C	-0.998130	7.704399	-2.238764
H	-1.000933	6.977503	-3.067070
H	-1.122517	8.703543	-2.684013
H	-1.880773	7.501986	-1.612048
C	1.520118	7.891351	-2.298743
H	1.589762	7.170097	-3.129082
H	2.451871	7.822908	-1.715595
H	1.474980	8.896667	-2.745199
C	-4.315472	3.255477	0.706191
C	-5.503279	3.071269	0.531987
C	5.503241	-3.071230	-0.532156
C	4.315431	-3.255444	-0.706339
C	10.892636	-1.258552	-0.054250
C	11.177074	0.130463	0.067831
C	-11.177102	-0.130455	-0.067877
C	-10.892669	1.258568	0.054121

N	12.049977	-1.907854	-0.119995
N	12.947015	-0.950181	-0.023388
N	12.495639	0.280859	0.094463
N	-12.050012	1.907872	0.119813
N	-12.947047	0.950191	0.023256
N	-12.495667	-0.280856	-0.094513
H	-13.939630	1.150786	0.038023
H	13.939597	-1.150778	-0.038179

Total Electronic Energy = -3494.06595598 a.u.
N_{im}= 0

6′

	X	Y	Z
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C	8.549961	1.801782	2.527558
C	8.659203	0.499662	0.037192
C	7.539019	1.984677	1.585795
C	9.612685	0.952154	2.221659
C	9.662387	0.279599	0.993285
C	7.610988	1.356565	0.331329
H	10.405555	0.780324	2.952448
H	8.704068	-0.020105	-0.923586
C	6.281120	2.742836	1.647190
C	3.743363	3.841024	1.273022
C	5.698053	3.479549	2.677417
C	5.615590	2.584284	0.420424
C	4.358346	3.127512	0.226153
C	4.431225	4.025306	2.486702
H	6.211971	3.612508	3.631912
H	3.822410	2.988716	-0.715370
H	3.947970	4.584249	3.289844
C	6.442207	1.761031	-0.553846
C	6.930995	2.632747	-1.738635
H	6.045933	2.899340	-2.340579
H	7.558413	1.992341	-2.380955
C	5.654146	0.561729	-1.112797
H	4.780047	0.961949	-1.654671
H	6.275795	0.067567	-1.877905
C	2.399334	4.304807	1.101340
C	1.235178	4.602723	0.922757
C	9.299724	-2.886712	0.361978
C	6.848568	-4.262756	0.215350
C	8.291364	-2.648518	1.305735
C	9.087506	-3.858740	-0.623798
C	7.876179	-4.537902	-0.701151
C	7.085411	-3.329590	1.238588
H	8.447984	-1.909426	2.093403
H	9.876529	-4.060588	-1.350736
H	7.706181	-5.267738	-1.494532
H	6.296485	-3.119858	1.962747
C	-0.156253	4.832726	0.678855
C	-2.927742	5.082802	0.238456
C	-0.971138	5.497346	1.611052
C	-0.742352	4.331425	-0.497226
C	-2.105378	4.455073	-0.714079
C	-2.337569	5.620911	1.394034

H	-0.524074	5.896943	2.522821
H	-0.115503	3.819526	-1.229172
H	-2.556318	4.038154	-1.616166
H	-2.967334	6.113650	2.136732
C	-4.347107	5.044573	0.061973
H	-6.211965	-3.612506	-3.631915
C	-5.698049	-3.479547	-2.677419
C	-4.358346	-3.127513	-0.226153
C	-6.281118	-2.742835	-1.647193
C	-4.431221	-4.025305	-2.486702
C	-3.743362	-3.841024	-1.273021
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H	-3.822412	-2.988718	0.715371
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C	-9.662385	-0.279598	-0.993291
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C	-7.610987	-1.356565	-0.331333
C	-8.659203	-0.499662	-0.037197
C	-9.612681	-0.952152	-2.221665
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H	-8.704069	0.020104	0.923581
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C	-6.442209	-1.761032	0.553844
C	-6.930998	-2.632748	1.738632
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H	-6.045937	-2.899342	2.340576
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C	-1.235178	-4.602723	-0.922753
C	0.156254	-4.832726	-0.678850
C	2.927742	-5.082802	-0.238448
C	0.971139	-5.497348	-1.611044
C	0.742352	-4.331423	0.497231
C	2.105378	-4.455071	0.714085
C	2.337570	-5.620914	-1.394025
H	0.524075	-5.896948	-2.522813
H	0.115503	-3.819522	1.229176
H	2.556318	-4.038149	1.616171
H	2.967336	-6.113655	-2.136722
C	-9.299723	2.886712	-0.361978
C	-6.848567	4.262756	-0.215345
C	-8.291362	2.648520	-1.305734
C	-9.087506	3.858738	0.623800
C	-7.876180	4.537901	0.701156
C	-7.085409	3.329593	-1.238584
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H	-9.876530	4.060585	1.350738
H	-7.706183	5.267735	1.494539
H	-6.296482	3.119862	-1.962743
C	-5.529488	4.800868	-0.073077
C	5.212664	-0.462424	-0.071330
H	6.101921	-1.012360	0.274110
H	4.811185	0.060407	0.813855

C	4.164224	-1.473291	-0.565341
H	4.112983	-2.264090	0.202567
C	2.766260	-0.862031	-0.674111
H	2.725224	-0.072480	-1.442905
H	2.448939	-0.413597	0.280294
H	2.025017	-1.628714	-0.950115
C	4.574663	-2.145497	-1.875914
H	4.548122	-1.434087	-2.717492
H	3.890956	-2.972591	-2.120838
H	5.593223	-2.559813	-1.812688
C	7.697460	3.893841	-1.348660
H	8.547486	3.614890	-0.703463
H	7.045013	4.535936	-0.733363
C	8.233632	4.725051	-2.526040
H	8.737175	5.596713	-2.072161
C	7.117006	5.265072	-3.421779
H	7.515936	5.969474	-4.167934
H	6.351750	5.795041	-2.833172
H	6.614074	4.455657	-3.975348
C	9.286313	3.973629	-3.343792
H	9.753239	4.636353	-4.088708
H	8.845230	3.126909	-3.894224
H	10.084915	3.574935	-2.698760
C	-5.212663	0.462423	0.071332
H	-6.101920	1.012358	-0.274111
H	-4.811181	-0.060407	-0.813852
C	-4.164225	1.473291	0.565346
H	-4.112983	2.264090	-0.202562
C	-4.574669	2.145496	1.875918
H	-3.890964	2.972591	2.120844
H	-4.548129	1.434086	2.717496
H	-5.593229	2.559812	1.812690
C	-2.766261	0.862031	0.674120
H	-2.025019	1.628715	0.950127
H	-2.448937	0.413598	-0.280284
H	-2.725227	0.072480	1.442915
C	-7.697464	-3.893841	1.348655
H	-7.045015	-4.535937	0.733358
H	-8.547488	-3.614890	0.703457
C	-8.233637	-4.725052	2.526033
H	-8.737180	-5.596714	2.072152
C	-9.286319	-3.973631	3.343783
H	-8.845236	-3.126912	3.894217
H	-9.753247	-4.636355	4.088699
H	-10.084920	-3.574936	2.698751
C	-7.117013	-5.265075	3.421774
H	-6.614081	-4.455660	3.975344
H	-6.351757	-5.795044	2.833167
H	-7.515944	-5.969477	4.167927
C	4.347107	-5.044573	-0.061965
C	5.529488	-4.800868	0.073084
C	10.544952	-2.101194	0.408551
C	10.712608	-0.722072	0.714622
C	-10.712606	0.722073	-0.714628
C	-10.544951	2.101194	-0.408554
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N	-12.562324	1.600753	-0.353454
N	-11.749235	2.617122	-0.176655
N	11.749236	-2.617122	0.176650
N	12.562325	-1.600753	0.353446
N	12.013195	-0.450351	0.676575
H	13.564865	-1.698677	0.248146
H	-13.564864	1.698677	-0.248156

Total Electronic Energy = -3494.0722229499997 a.u.

N_{im}= 0

S9. References

1. H. E. Gottlieb, V. Kotlyar and A. Nudelman, *J. Org. Chem.*, 1997, **62**, 7512-7515.
2. D. Göbel, N. Clamor, E. Lork and B. J. Nachtsheim, *Org. Lett.*, 2019, **21**, 5373-5377.
3. M. Linseis, S. Záliš, M. Zabel and R. F. Winter, *J. Am. Chem. Soc.*, 2012, **134**, 16671-16692.
4. X. Zhou, H. Kwon, R. R. Thompson, R. J. Herman, F. R. Fronczek, C. J. Bruns and S. Lee, *Chem. Commun.*, 2021, **57**, 10887-10890.
5. P. J. Wilson, T. J. Bradley and D. J. Tozer, *J. Chem. Phys.*, 2001, **115**, 9233-9242.
6. R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650-654.
7. T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294-301.
8. D. Flaig, M. Maurer, M. Hanni, K. Braunger, L. Kick, M. Thubauville and C. Ochsenfeld, *J. Chem. Theory Comput.*, 2014, **10**, 572-578.
9. G. Herzberg, *Electronic Spectra and Electronic Structure of Polyatomic Molecules*, Van Nostrand, 1966.
10. R. J. Abraham, M. Canton, M. Reid and L. Griffiths, *J. Chem. Soc., Perkin Trans. 2*, 2000, 803-812.
11. J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615-6620.
12. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.

15. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford CT, 2016.