Supporting Information

Kinetic Control in the Synthesis of a Möbius Tris((ethynyl)[5]helicene) Macrocycle Using Alkyne Metathesis

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Experimental Studies

General

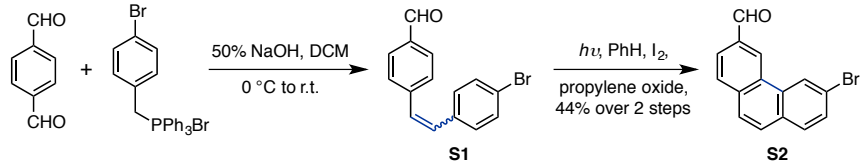
Unless stated otherwise, all compounds are used as received from commercial sources. Anhydrous chloroform and methanol were obtained from Sigma-Aldrich, and all other solvents were obtained from a solvent purification system. Reaction flasks are oven dried before cooled to room temperature under N_2. Silica gel (40–63 μm, 60 Å, bulk or pre-packed columns) was obtained from Silicycle. TLC plates with flourescent indicator F254 were used and visualized with UV lamps.

Instruments

All alkyne metathesis reactions were performed in an Ar-filled glovebox as the catalyst is sensitive to poisoning by N_2. Solution ^1H and ^{13}C NMR spectra were acquired on a Bruker 500 MHz instrument with a 5-mm cryo probe. Mass spectra were obtained on Waters Q-TOF Ultima ESI (ESI-TOF) and Bruker Daltonics UltrafleXtreme MALDI TOFTOF (MALDI-TOF). DCTB (*trans*-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malononitrile) was used as the matrix, and C_{70} (840.0000) and [70]PCBM ([6,6]-phenyl C71 butyric acid methyl ester, 1030.0994) were used as MALDI standards for HRMS of **2**. Infrared (IR) spectra were acquired on a PerkinElmer Frontier FT-IR instrument with a KRS5 thallium bromide/iodide universal attenuated total reflectance accessory, and the peaks are reported in wavenumbers (cm^{-1}) together with their relative intensity (s = strong, m = medium, w = weak). EFOS Novacure UV Spot Curing System with a 100-W mercury lamp and light guide was used in the synthesis of dibromo[5]helicene.

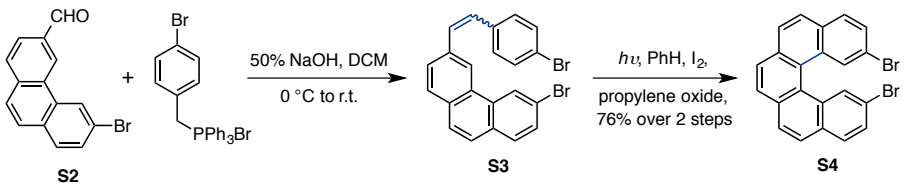
Synthesis

The synthesis of 2,13-dibromo-[5]helicene **S4** was achieved following literature procedures[1] with minor modifications:



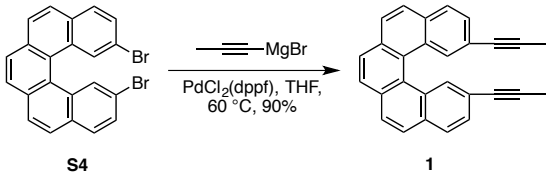
To a mixture of terephthalaldehyde (804 mg, 6.0 mmol) and (4-bromobenzyl)triphenylphosphonium bromide (3.07 g, 6.0 mmol) in DCM (100 mL) in an ice bath was added 50% (w/w) NaOH (4.0 mL) slowly. The ice bath was removed after the addition, and the reaction was stirred at r.t. for 3 h before water (100 mL) was added. The organic layer was separated from the aqueous layer, which was extracted with DCM (30 mL) twice. The organic layers were collected, dried over Na_2SO_4, and evaporated under vacuum to give a yellow solid. The crude mixture was passed through a short plug of silica, and **S1** (mixture of cis/trans isomers) was used in the next step without further purification.

S1 was dissolved in benzene (800 mL), and propylene oxide (20 mL) and iodine (500 mg) were added to the flask. The solution was degassed by bubbling N_2 for 1h. A Pyrex (50% transmission at 320 nm) tube was inserted into the flask to insulate the optical guide of the UV light. After 50 h of irradiation, the solvent was removed and the residue was passed through a short plug of silica. Pure **S2** was obtained by washing the solid with hot ether; the mother liquor was concentrated to give brown solids, which were subjected to another cycle of photoreaction. The overall yield of **S2** was 737 mg (44%, over two steps).



To a mixture of **S2** (550 mg, 1.99 mmol) and (4-bromobenzyl)triphenylphosphonium bromide (1.11 g, 2.17 mmol) in DCM (50 mL) in an ice bath was added 50% (w/w) NaOH (2.2 mL) slowly. The ice bath was removed after the addition, and the reaction was stirred overnight before water (50 mL) was added. The organic layer was separated, and the aqueous layer was extracted with DCM (20 mL) twice. The combined organic layers were dried over Na_2SO_4 and evaporated under vacuum to give a yellow solid. Triphenylphosphine oxide was removed by passing the crude mixture through a short plug of silica, and **S3** (mixture of cis/trans isomers) was used in the next step without further purification.

S3 was dissolved in benzene (500 mL) in a brown bottle, and propylene oxide (10 mL) and iodine (300 mg) were added to the solution. The solution was degassed by bubbling N_2 for 1h. A Pyrex (50% transmission at 320 nm) tube was inserted into the flask to insulate the optical guide of the UV light. *The cyclization of **S3** was much faster than that of **S1**, presumably because of the presence of two bromine atoms in the molecule.* After 5 h of irradiation, the solvent was removed to give a brown solid. Flash column chromatography (20% DCM in hexanes) gave 2,13-dibromo-[5]helicene (657 mg, 76% over two steps).



To a solution of 2,13-dibromo-[5]helicene **S4** (109 mg, 0.25 mmol) and $PdCl_2$(dppf) (11 mg, 0.015 mmol, 6 mol %) in 2 mL THF was added propynylmagnesium bromide (0.5 M in THF, 2 mL, 1.0 mmol) under nitrogen atmosphere. The reaction mixture was stirred overnight at 60 ˚C before it was quenched with saturated NH_4Cl. The reaction mixture was extracted with EtOAc, and the combined organic layers were washed with brine and dried over $MgSO_4$. After the removal of solvent *in vacuo*, flash column chromatography (10–20% DCM in hexanes) gave the desired product **1** (80 mg, 90%) as an off-white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 1.99 (s, 6H), 7.51 (dd, J = 8.3, 1.4 Hz, 2H), 7.90–7.81 (m, 8H), 8.57 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 4.5, 80.1, 85.7, 120.5, 126.5, 126.6, 127.2, 127.3, 127.7, 129.2, 130.5, 131.6, 131.7, 132.5. IR υ (cm^{-1}): 843 (s), 1438 (w), 1502 (w), 1606 (w), 2223 (w), 2847 (w), 2912 (w), 3048 (w). HRMS (ESI-TOF, m/z): calculated for $C_{28}H_{19}$ $[MH]^+$: 354.1408; found: 354.1400.

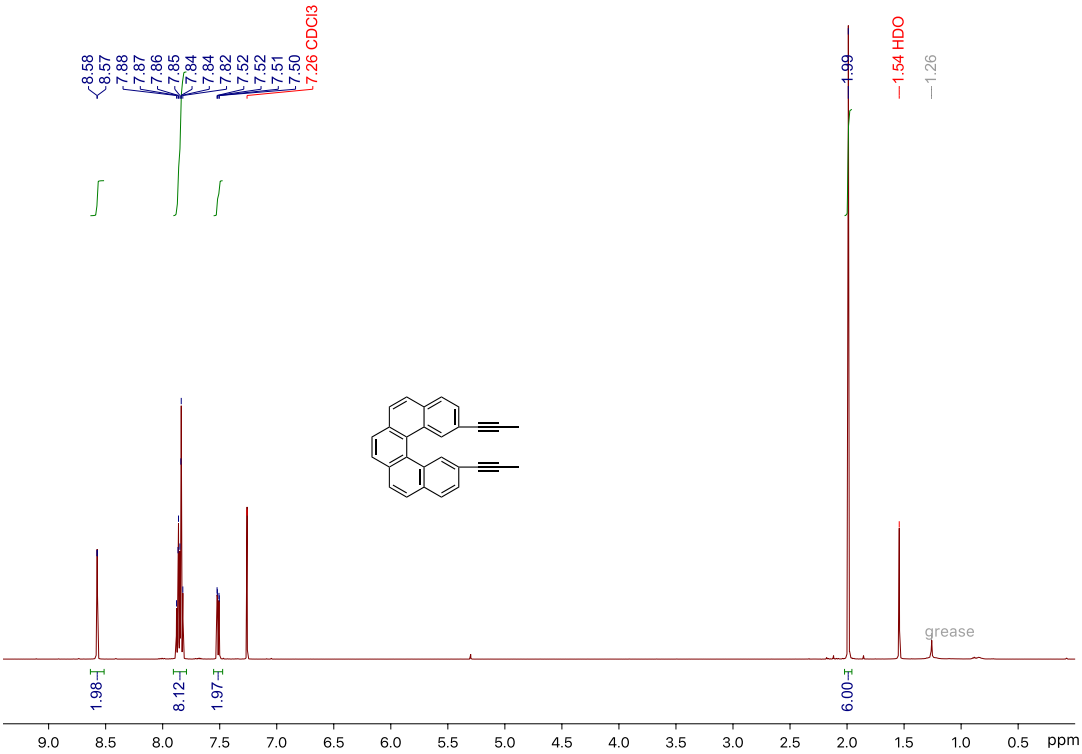


Figure S1. ^{1}H NMR spectrum of **1** at 500 MHz in $CDCl_3$.

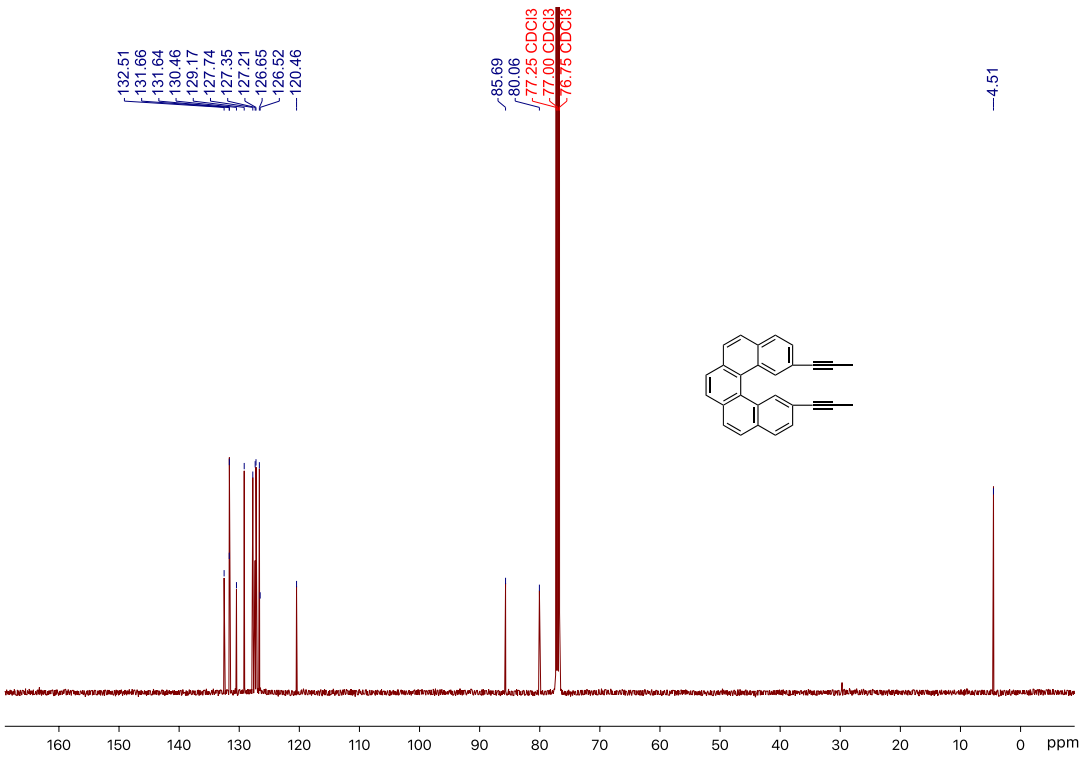
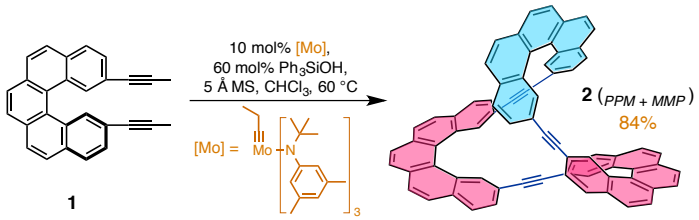


Figure S2. ^{13}C NMR spectrum of **1** at 126 MHz in $CDCl_3$.



In an argon-filled glovebox, [Mo] (5.61 mg, 0.0085 mmol, 0.1 equiv) and triphenyl silanol (14.0 mg, 0.0508 mmol, 0.6 equiv) were added to a 7.5-mL vial (**I**) with a stir bar followed by $CHCl_3$ (3 mL). The solution was stirred at room temperature for 15 min to allow for catalyst pre-activation. Monomer **1** (30 mg, 0.085 mmol), 5 Å molecular sieves (168 mg, 1 gram per mmol of alkyne), and $CHCl_3$ (82 mL) were added to a separate flask (**II**) equipped with a stir bar. After stirring, the catalyst solution in vial **I** was transferred to flask **II** *via* syringe. The flask was capped with a new septum which was secured with electrical tape. The flask was brought out of the glovebox and stirred at 60 °C overnight (no gas inlet). The reaction mixture was then cooled to r.t., filtered over celite, and concentrated to yield a brown solid. The crude solid was purified using flash column chromatography eluting with DCM in hexanes (10% to 30%). The product was obtained as a pale yellow solid (18.1 mg, 71% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73–7.79 (m, 4H), 7.80–7.89 (m, 12H), 7.91 (d, J = 4.1 Hz, 2H), 7.92 (dd, J = 8.5, 2.2 Hz, 4H), 7.89 (d, J = 7.9 Hz, 2H), 7.96 (d, J = 8.4 Hz, 2H), 8.02 (d, J = 8.6 Hz, 2H), 8.06 (dd, J = 8.1, 1.4 Hz, 2H), 8.10 (d, J = 8.1 Hz, 2H), 8.45 (s, 2H), 8.83 (s, 2H), 8.88 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 90.4, 90.7, 90.7, 119.2, 119.7, 120.3, 126.4, 126.5, 126.5, 126.7, 127.1, 127.1, 127.2, 127.3, 127.4, 127.4, 127.6, 127.8, 127.8, 128.0, 128.1, 129.4, 129.6, 129.6, 129.8, 129.9, 130.7, 131.0, 131.9, 132.0, 132.1, 132.1, 132.2, 132.3, 132.6, 132.8. IR υ (cm^{-1}): 3043 (w), 2922 (w), 2851 (w), 2203 (w), 2032 (w), 1892 (w), 1608 (m), 1505 (m), 1142 (m), 909 (m), 838 (s). HRMS (MALDI-TOF, m/z): calculated for $C_{72}H_{36}$ $[M]^+$: 900.2817; found: 900.2838. Optimization of the alkyne metathesis of **1**.

Table S1. Optimization of the alkyne metathesis of **1**.

Table entry	[Mo] loading	Temp	Conc.	Solvent	NMR (isolation) yield
1	10%	r.t.	[5 mM]	$CHCl_3$	23%
2	10%	r.t.	[1 mM]	$CHCl_3$	7%
3	10%	40 °C	[1 mM]	$CHCl_3$	38%
4	30%	40 °C	[1 mM]	$CHCl_3$	42%
5	10%	60 °C	[1 mM]	$CHCl_3$	84% (71%)
6	10%	r.t.	[1 mM]	Tol	15%
7	10%	40 °C	[1 mM]	Tol	27%
8	10%	60 °C	[1 mM]	Tol	26%

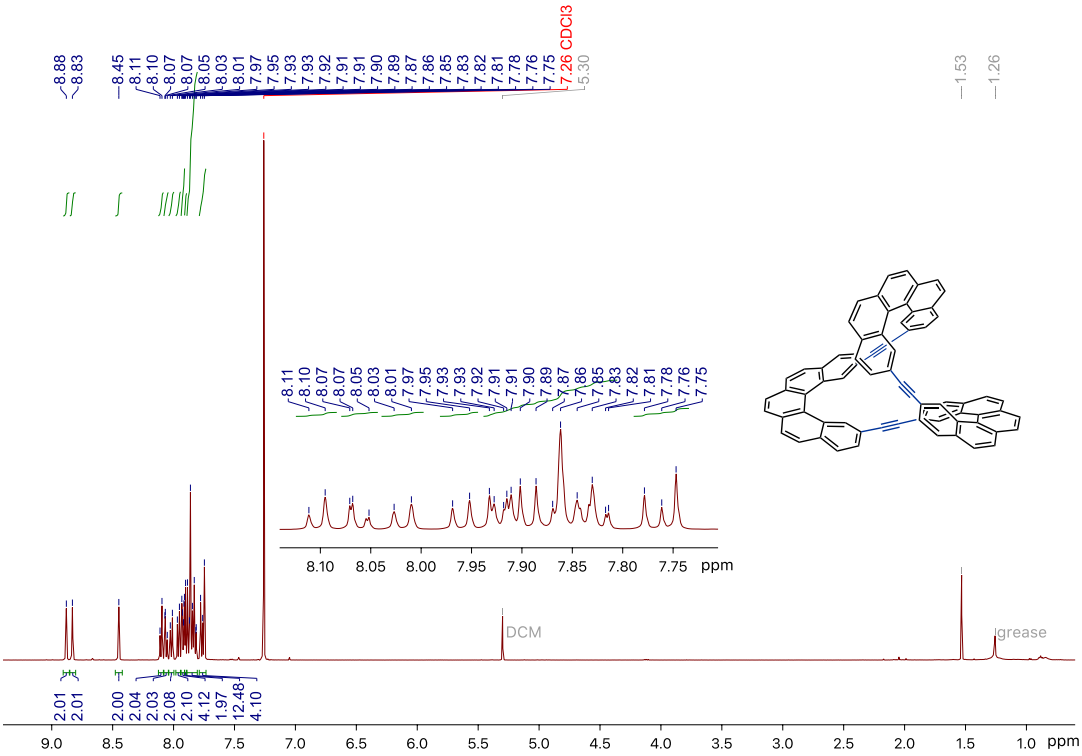


Figure S3. ^{1}H NMR spectrum of **2** at 500 MHz in $CDCl_3$.

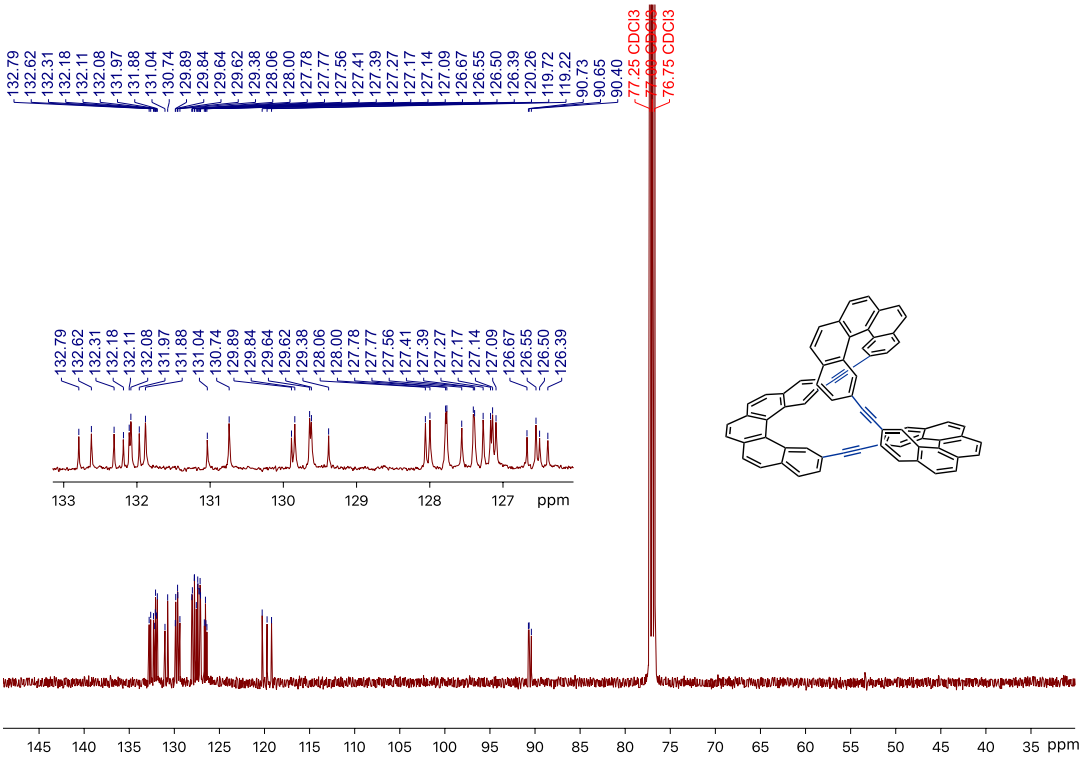
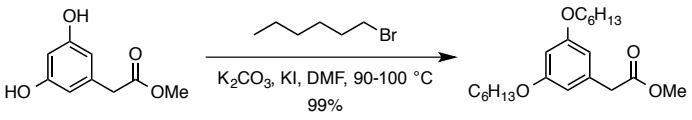


Figure S4. ^{13}C NMR spectrum of **2** at 126 MHz in $CDCl_3$.



S5 **S6**

To a solution of 3,5-dihydoxyphenylacetic acid **S5** (5.27 g, 29.0 mmol) and 1-bromohexane (15.4 mL, 18.1 g, 110 mmol) in anhydrous DMF (50 mL) was added potassium carbonate (19.0 g, 137 mmol) and potassium iodide (1.0 g, 6.0 mmol), and the mixture was stirred at 90°C overnight. TLC analysis showed that the reaction was incomplete, so an additional 5.0 mL of 1-bromohexane (36 mmol) was added to the reaction, which was heated to 100°C for 24 h before the heating bath was removed, and water (100 mL) was added to the reaction. The product was extracted with ethyl acetate (200 mL), and the organic layer was subsequently washed with water, 1M LiCl solution, and brine, and dried over Na_2SO_4. The solvent was removed *in vacuo*, and the crude oil was subject to flash column chromatography (5−10% ethyl acetate in hexanes) to give the desired **S6** as a yellowish oil (9.50 g, 99%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 0.90 (t, J = 6.4 Hz, 6H), 1.29−1.38 (m, 8H), 1.40−1.49 (m, 4H), 1.75 (app. quint, J = 7.1 Hz, 4H), 3.54 (s, 2H), 3.69 (s, 3H), 3.92 (t, J = 6.6 Hz, 4H), 6.36 (t, J = 2.2 Hz, 1H), 6.41 (d, J = 2.2 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 14.0, 22.6, 25.7, 29.2, 31.6, 41.5, 52.0, 68.0, 100.0, 107.7, 135.8, 160.3, 171.8. IR υ (cm^{-1}): 685 (w), 832 (w), 1061 (m), 1169 (s), 1460 (m), 1595 (s), 1741 (m), 2858 (w), 2930 (m). HRMS (ESI, TOF, m/z): calculated for $C_{21}H_{35}O_4$ $[MH]^+$: 351.2535, observed: 351.2532.

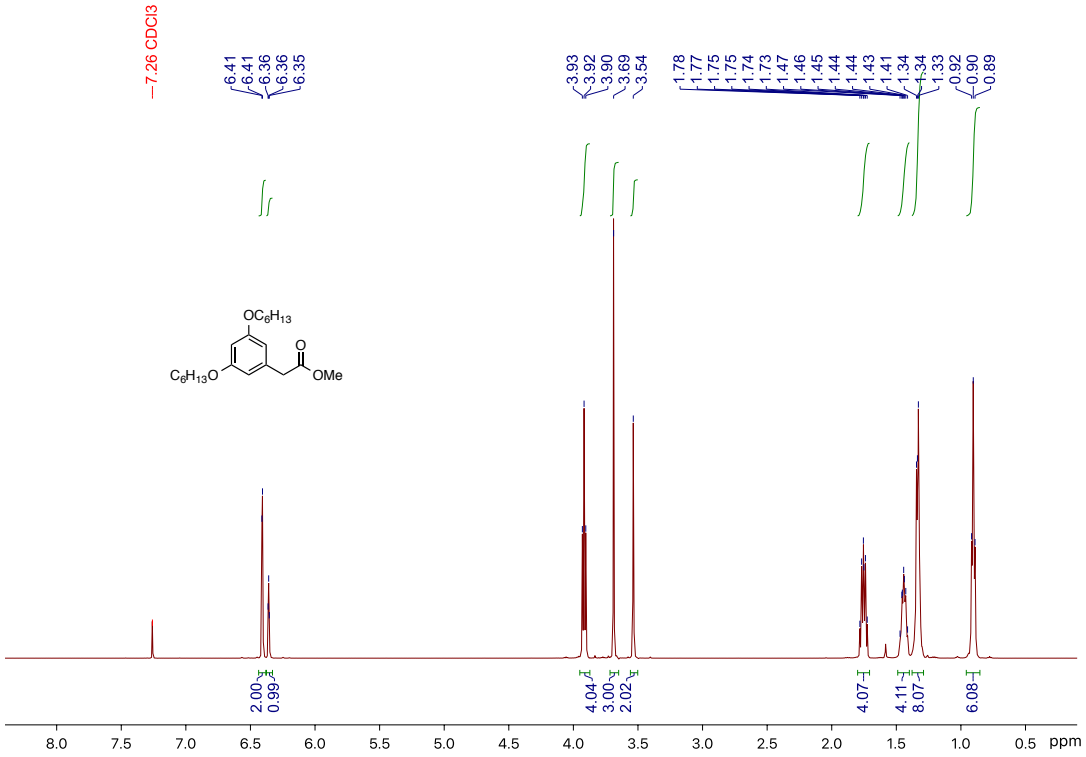


Figure S5. ^{1}H NMR spectrum of **S6** at 500 MHz in $CDCl_3$.

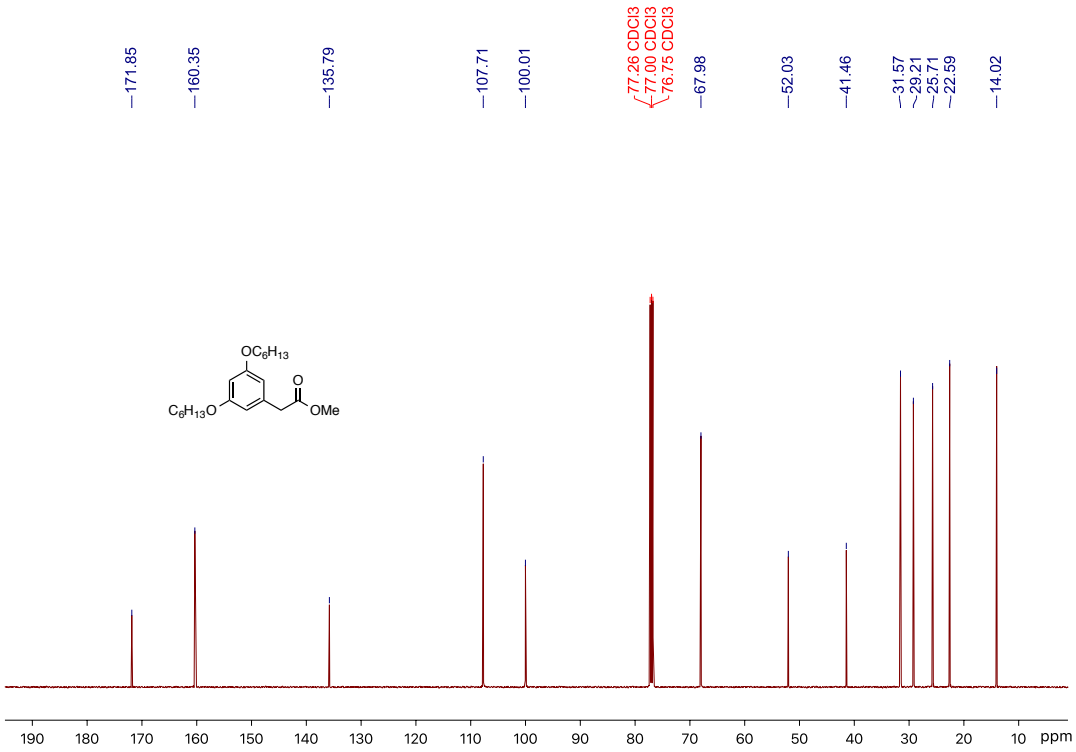
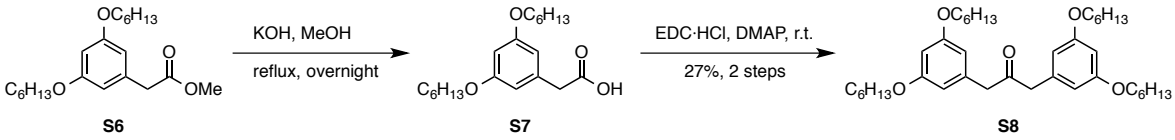


Figure S6. ^{13}C NMR spectrum of **S6** at 126 MHz in $CDCl_3$.



S6 **S7** **S8**

To a mixture of **S6** (4.17 g, 11.9 mmol), MeOH (1 mL), and water (30 mL) was added KOH (3.84 g, 68.5 mmol), and the reaction was heated to reflux overnight. The reaction mixture was allowed to cool down to rt before conc. HCl was slowly added to adjust its pH (< 3). The product was extracted with ethyl acetate, and the organic layer was washed with water and brine, and dried over Na_2SO_4. The solvent was removed *in vacuo*, and the crude **S7** was passed through a short plug of silica (EA) before it was concentrated and used in the next step.

To a solution of **S7** and DMAP (1.66 g, 13.6 mmol) in anhydrous DCM (25 mL) was added a slurry of EDC·HCl (2.61 g, 13.6 mmol) in anhydrous DCM (30 mL), and the reaction was stirred overnight. A large portion of the solvent was removed, and celite was added to the flask. The resulting slurry was filtered through a plug of silica, and the solution was concentrated to give a brown oil. Flash column chromatography (2−10% ethyl acetate in hexanes) gave **S8** (972 mg, 27% over two steps) as a yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 0.91 (t, J = 6.8 Hz, 12H), 1.29−1.38 (m, 16H), 1.40−1.49 (m, 8H), 1.75 (app. quint, J = 7.1 Hz, 8H), 3.61 (s, 4H), 3.89 (t, J = 6.7 Hz, 8H), 6.28 (t, J = 2.1 Hz, 4H), 6.35 (d, J = 2.1 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 14.0, 22.6, 25.7, 29.2, 31.6, 49.2, 68.0, 100.0, 107.9, 135.9, 160.5, 205.6. IR υ (cm^{-1}): 831 (w), 1059 (m), 1166 (s), 1456 (m), 1594 (s), 1713 (w), 2858 (w), 2930 (m). HRMS (ESI, TOF, m/z): calculated for $C_{39}H_{63}O_5$ $[MH]^+$: 611.4676, observed: 611.4677.

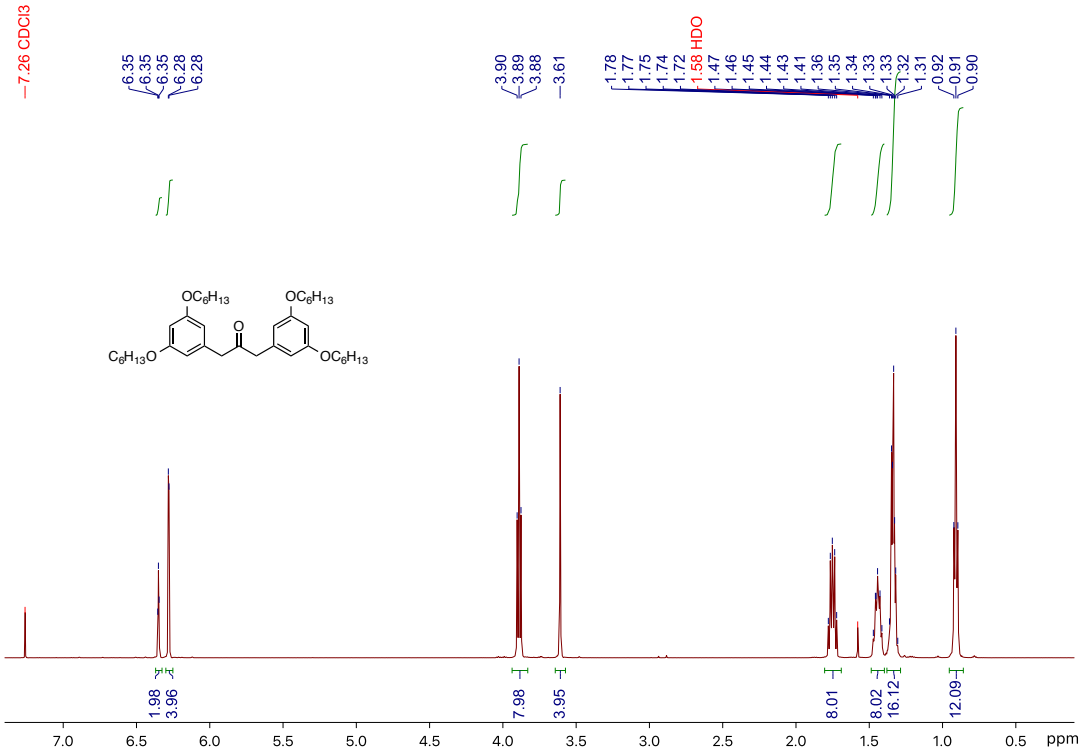


Figure S7. ^{1}H NMR spectrum of **S8** at 500 MHz in $CDCl_3$.

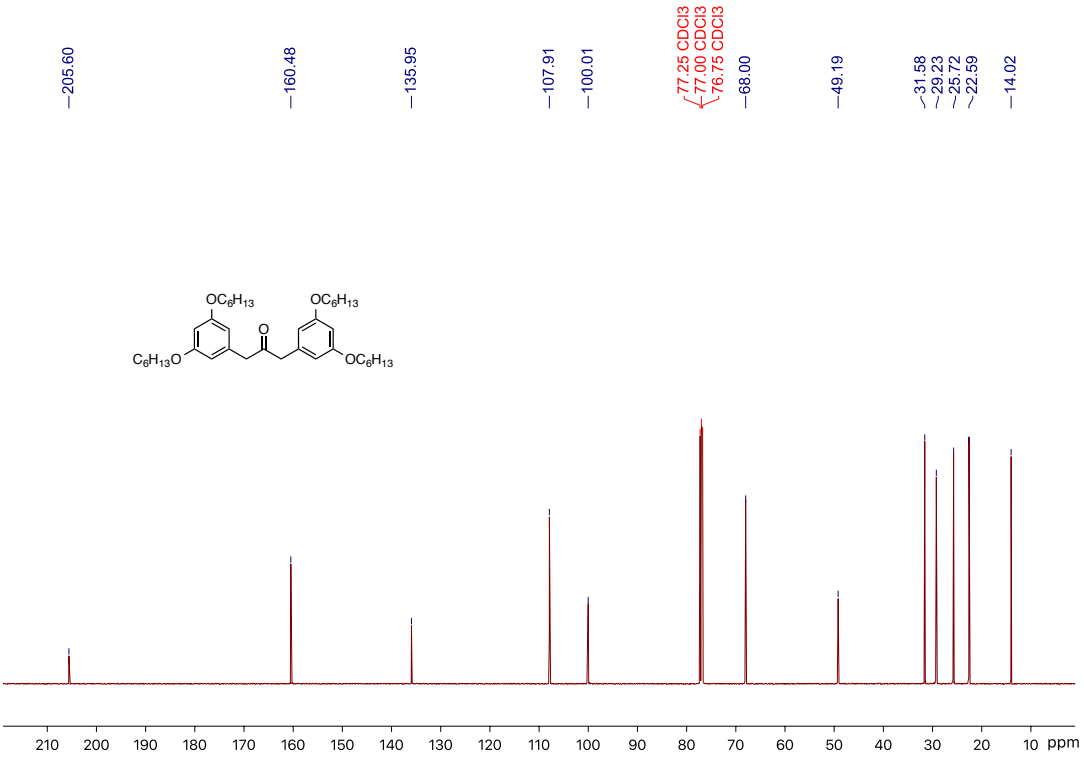
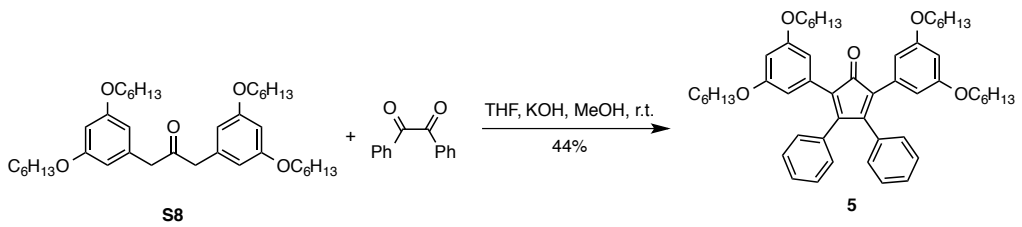


Figure S8. ^{13}C NMR spectrum of **S8** at 126 MHz in $CDCl_3$.



To a solution of **S8** (224 mg, 0.367 mmol) and benzil (77 mg, 0.367 mmol) in anhydrous THF (3 mL) was added a 5% (w/v) KOH solution in MeOH (0.25 mL), and the resulting mixture was stirred at r.t. for 48 h before it was concentrated under reduced pressure to give a dark violet crude. Flash column chromatography (5−10% ethyl acetate in hexanes) gave the desired product **5** as a violet oil (128 mg, 44%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 0.89 (t, J = 6.9 Hz, 12H), 1.23−1.38 (m, 24H), 1.60−1.68 (m, 8H), 3.71 (t, J = 6.6 Hz, 8H), 6.33 (t, J = 2.2 Hz, 2H), 6.35 (d, J = 2.2 Hz, 4H), 6.95 (app. dd, J = 7.8, 1.5 Hz, 4H), 7.15−7.25 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 14.0, 22.6, 25.6, 29.1, 31.5, 67.9, 102.0, 108.3, 125.3, 128.0, 128.4, 129.3, 132.1, 133.2, 154.6, 159.7, 199.9. IR υ (cm^{-1}): 697 (m), 846 (w), 1059 (m), 1159 (s), 1278 (m), 1432 (m), 1589 (s), 1712 (m), 2858 (w), 2929 (m). HRMS (ESI, TOF, m/z): $C_{53}H_{68}O_5$ $[MH]^+$: 785.5145, observed: 785.5154.

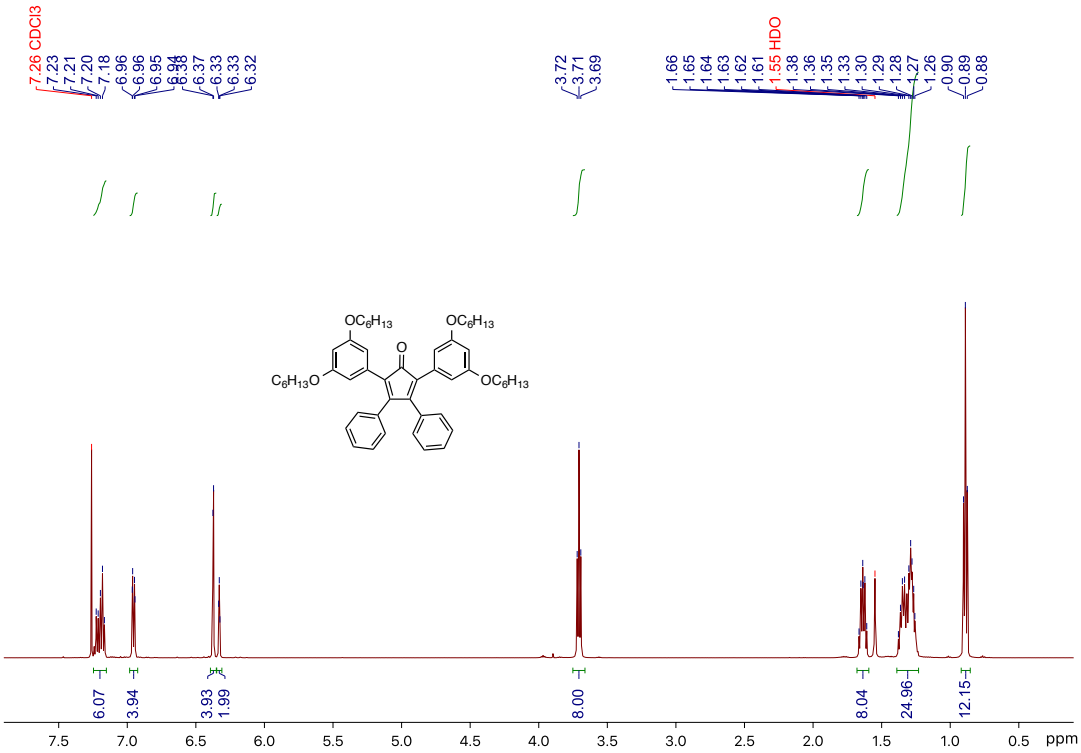


Figure S9. ^{1}H NMR spectrum of **5** at 500 MHz in $CDCl_3$.

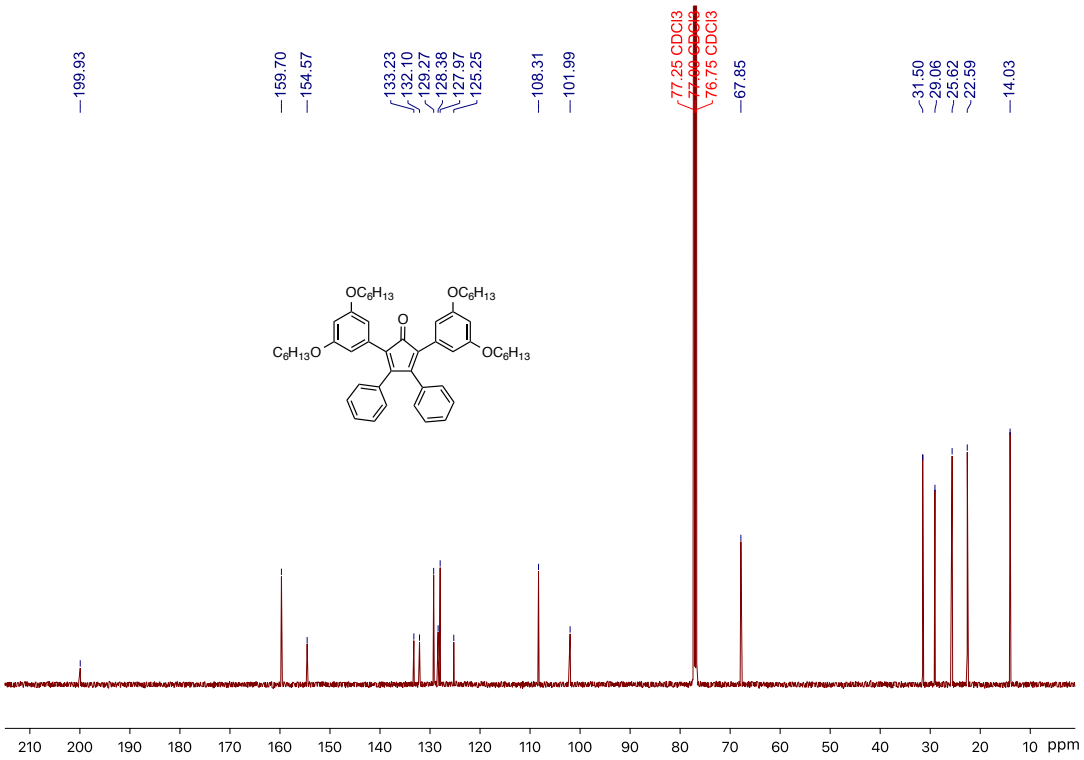
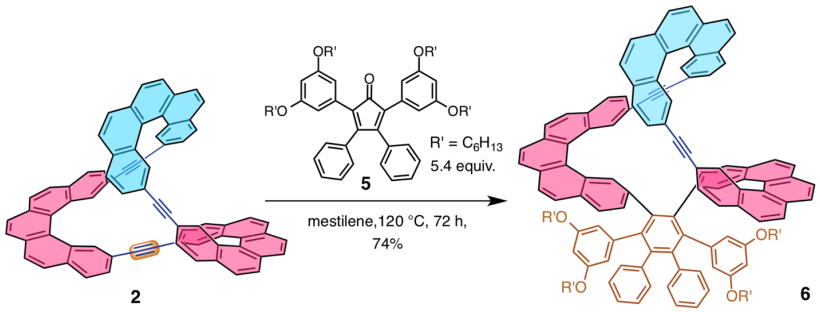


Figure S10. ^{13}C NMR spectrum of **5** at 126 MHz in $CDCl_3$.



To a 5-mL vial was charged **2** (10.1 mg, 11.2 μmol), cyclopentadieneone **5** (47.3 mg, 60.2 μmol), and mesitylene (0.4 mL) under N_2. The vial was sealed and the reaction was heated to 120°C for 72 h. The mixture was directly adsorbed onto silica (> 2 g) and purified *via* flash column chromatography (2−10% ethyl acetate in hexanes). The fractions containing the desired product were collected and concentrated to give a pale yellow solid, which was subject to another round of flash column chromatography (20−60% DCM in hexanes). The product was obtained as an off-white solid (13.8 mg, 74%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 0.94 (t, J = 7.2 Hz, 6H), 1.00 (t, J = 7.3 Hz, 6H), 1.08−1.15 (m, 4H), 1.20−1.42 (m, 24H), 1.45−1.52 (m, 4H), 1.88 (dt, J = 8.8, 6.7 Hz, 8H), 2.55 (dt, J = 8.8, 6.6 Hz, 8H), 3.34 (dt, J = 9.5, 6.8 Hz, 2H), 3.51 (dt, J = 9.4, 6.8 Hz, 2H), 4.83 (s, 2H), 5.51 (s, 2H), 5.60 (t, J = 2.2 Hz, 2H), 6.47−6.57 (m, 4H), 6.61 (dd, J = 8.4, 1.1 Hz, 2H), 6.62−6.67 (m, 6H), 6.69 (dd, J = 8.3, 1.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 7.49 (dd, J = 8.3, 1.5 Hz, 2H), 7.53 (d, J = 8.7 Hz, 2H), 7.59 (d, J = 8.7 Hz, 2H), 7.64 (s, 2H), 7.78 (dd, J = 11.9, 8.3 Hz, 4H), 7.81−7.97 (m, 10H), 8.09 (d, J = 8.5 Hz, 2H), 8.19 (s, 2H), 8.31 (s, 2H), 8.50 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 14.1, 14.2, 22.7, 22.8, 25.6, 28.9, 29.2, 31.5, 31.9, 66.8, 68.0, 90.2, 91.1, 99.9, 107.6, 110.5, 119.0, 121.8, 124.5, 124.9, 125.9, 126.0, 126.2, 126.2, 126.4, 126.5,

126.6, 126.8, 126.9, 127.0, 127.1, 127.2, 127.4, 127.7, 127.8, 128.0, 128.6, 129.5, 130.3, 130.6, 131.0, 131.3, 131.5, 131.5, 131.6, 131.7, 131.7, 132.0, 132.0, 132.2, 134.0, 134.3, 138.0, 138.4, 139.5, 140.3, 141.4, 141.5, 157.8, 158.0. IR υ (cm^{-1}): 3047 (w), 2927 (w), 2857 (w), 1592 (m), 1435 (w), 1378 (w), 1155 (m), 842 (s). LRMS (MALDI, TOF, m/z): $C_{124}H_{104}O_4$ $[M]^+$: 1656.8 (75%), 1657.8 (100%), 1658.8 (66%), 1659.8 (29%), observed: 1656.8 (88%), 1657.8 (100%), 1658.8 (66%), 1659.8 (30%).

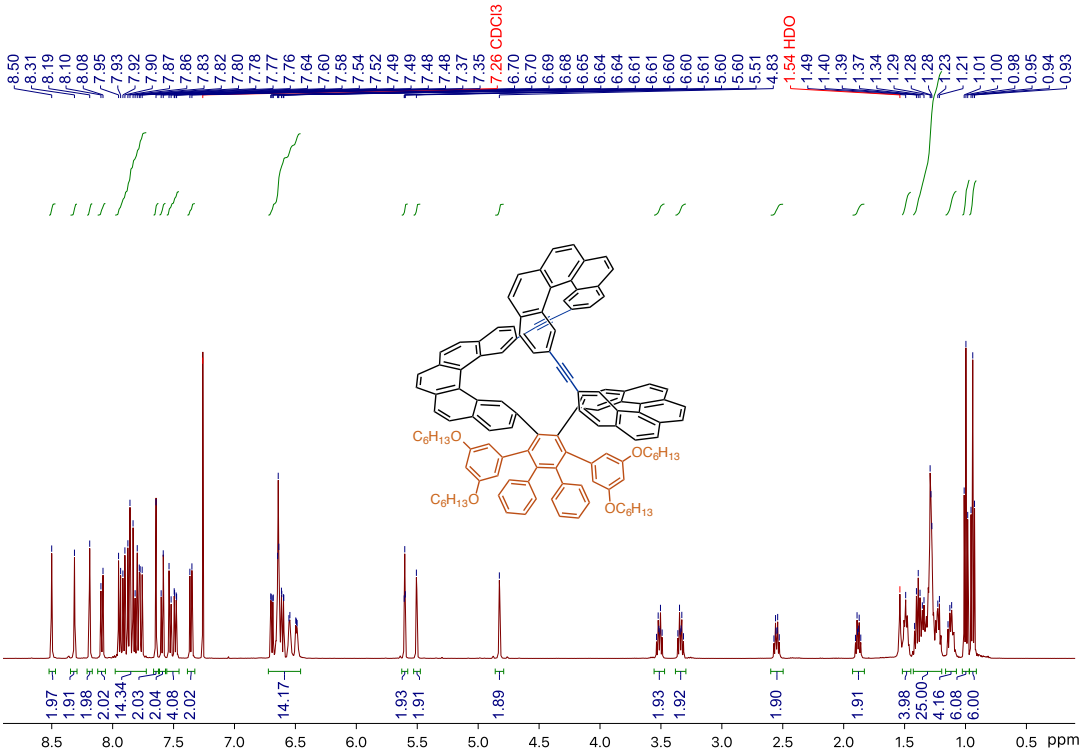


Figure S11. ^{1}H NMR spectrum of **5** at 500 MHz in $CDCl_3$.

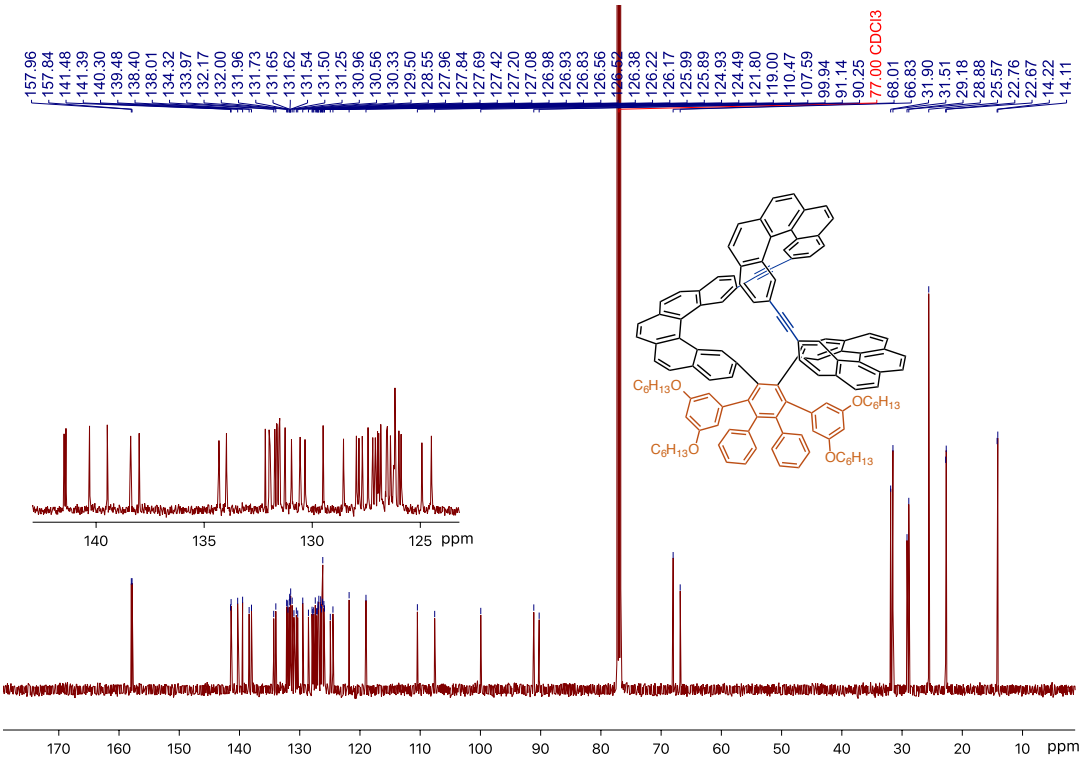
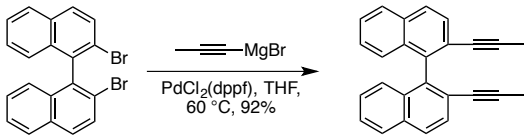


Figure S12. ^{13}C NMR spectrum of **6** at 126 MHz in $CDCl_3$.



S9 **7**

$PdCl_2$(dppf) (53 mg, 0.06 equiv, 0.07 mmol) was added to a dry flask followed by 2,2'-dibromo-1,1'-binaphthalene **S9** (500 mg, 1.2 mmol) which was then placed under inert atmosphere. THF (24 mL) was transferred to the flask via syringe with stirring. 1-Propynyl-1-magnesium bromide solution (0.5 M in THF, 14.4 mL, 6.0 equiv, 7.2 mmol) was transferred to the reaction mixture dropwise via syringe. The reaction flask was then heated to 60 °C overnight. After cooling to rt, a saturated NH_4Cl (aq) solution was added to the reaction to quench any remaining organometallic species. The reaction mixture was extracted three times with ethyl acetate. The combined organic layers were washed with brine then dried over $MgSO_4$. The solution was filtered followed by the removal of solvent *in vacuo*. The product **7** was purified *via* flash column chromatography eluting with DCM/Hexanes to give an off-white solid (365 mg, 92%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 1.63 (s, 6H), 7.13 (d, J = 8.4 Hz, 2H), 7.25 (ddd, J = 8.2, 6.7, 1.3 Hz, 2H), 7.43 (ddd, J = 8.1, 6.7, 1.2 Hz, 2H), 7.63 (d, J = 8.5 Hz, 2H), 7.86 (d, J = 8.8 Hz, 2H), 7.88 (d, J = 7.7 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 4.3, 79.1, 89.5, 122.3, 125.9, 126.3, 126.4, 127.5, 127.8, 129.0, 132.5, 132.6, 139.5. IR υ (cm^{-1}): 750 (s), 817(s), 1375 (w), 1500(m), 1592(w), 2226(w), 2846 (w), 2913 (w), 3056 (w). HRMS (EI, TOF, m/z): $C_{26}H_{18}$ $[M]^+$: 330.1409, observed: 330.1412.

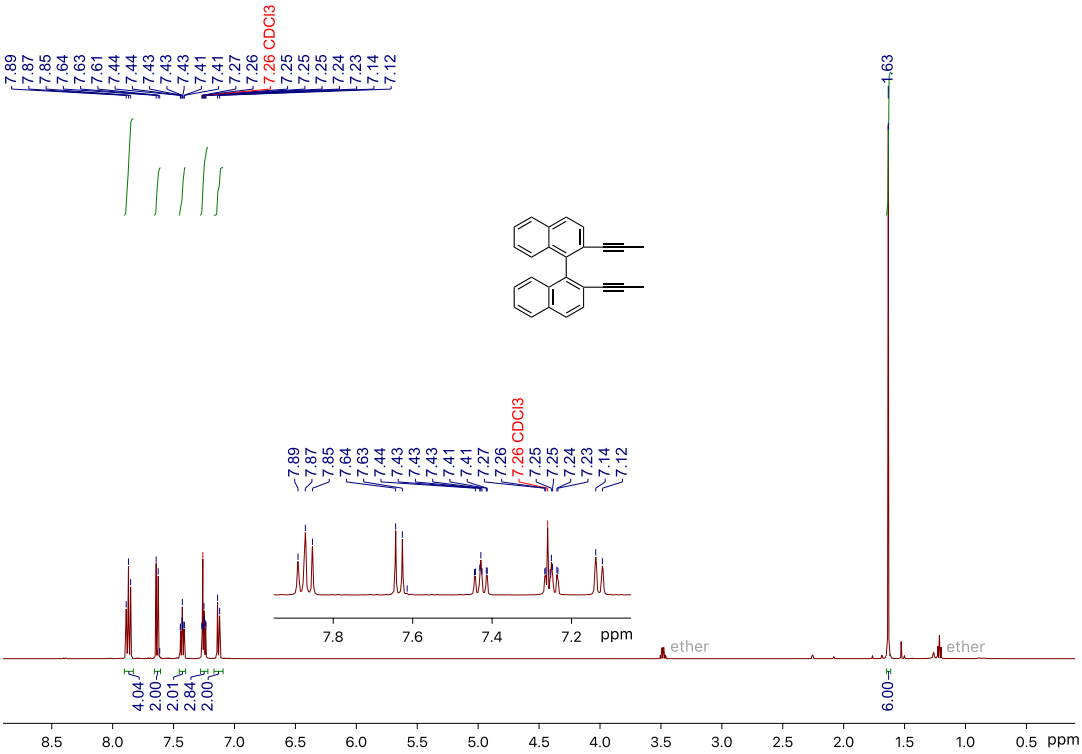


Figure S13. ^{1}H NMR spectrum of **7** at 500 MHz in $CDCl_3$.

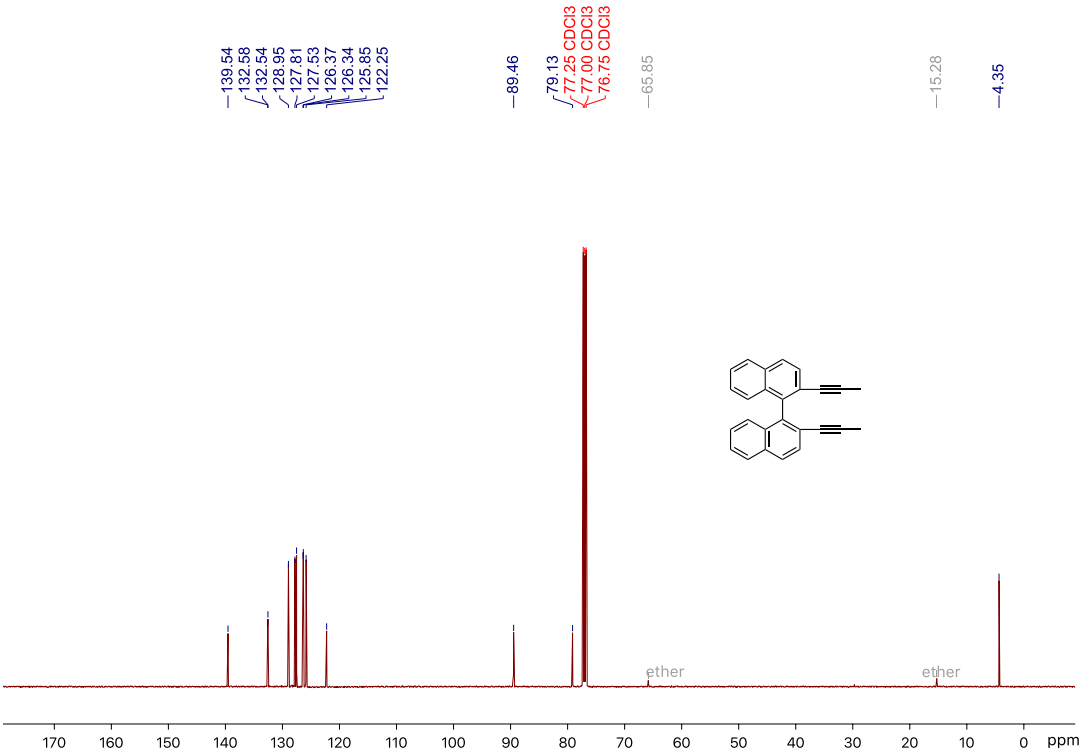
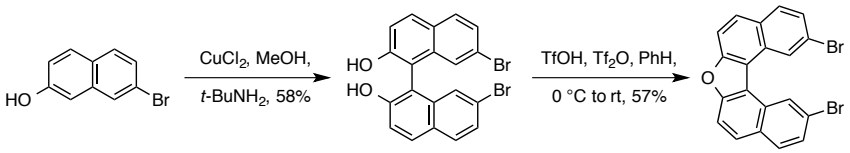


Figure S14. ^{13}C NMR spectrum of **7** at 126 MHz in $CDCl_3$.

The synthesis of **S10**[2] and **S11**[3] was achieved using literature procedures with minor modifications:



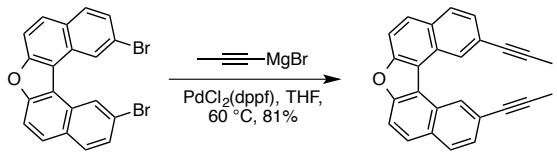
S10 **S11**

7-bromonaphthalen-2-ol (2.0 g, 9.0 mmol) along with $CuCl_2$ (2.4 g, 2.0 equiv, 18.0 mmol) was transferred to a dry 3-neck flask topped with an addition funnel and placed under inert atmosphere. Anhydrous MeOH (48 mL) was transferred to the flask *via* syringe and the solution was stirred at room temperature for 15 min. A solution of *tert*-butylamine (7.5 mL) in MeOH (27 mL) was added to the reaction mixture over 30 min *via* addition funnel. The reaction mixture stirred at rt overnight. The reaction was quenched at 0 °C by the addition of a 6 M solution of HCl until all solids dissolved. Most of the MeOH was removed *in vacuo* followed by extraction of the solution into ethyl acetate three times. The combined organic layers were washed with brine and dried over Na_2SO_4. The mixture was filtered and concentrated *in vacuo*. The crude brown oil was dissolved in boiling toluene. The hot solution was filtered over a coarse glass frit. The filtrate was cooled to –20 °C overnight. White crystals of product were filtered out of the solution while still cold. The crystals were rinsed with cold (–20 °C) toluene and dried over vacuum. The product **S10** was collected as a white solid (First crop: 750 mg; second crop: 413 mg; 58% combined).

S10: ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.01 (s, 2H), 7.23 (d, J = 1.8 Hz, 2H), 7.40 (d, J = 9.0 Hz, 2H), 7.48 (dd, J = 8.7, 1.9 Hz, 2H), 7.78 (d, J = 8.7 Hz, 2H), 7.97 (d, J = 8.9 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.76, 134.76, 131.91, 130.33, 128.12, 127.91, 126.09, 122.60, 118.43, 109.61.

7,7'-dibromo-[1,1'-binaphthalene]-2,2'-diol **S10** (200 mg, 0.45 mmol) was added to a dry flask which was then placed under inert atmosphere. Dry benzene (8 mL) was transferred to the flask *via* syringe, and the reaction mixture was cooled to 0 °C. Triflic acid (302 µL, 1.8 mmol, 4.0 equiv) was added to the reaction mixture *via* syringe. (*Note: No product was formed when the procedure in Ref. 3 was followed and TFA was used instead of TfOH*) A solution of triflic anhydride (160 µL, 1.8 mmol, 4.0 equiv) in benzene (2 mL) was transferred to the reaction mixture dropwise *via* syringe. The reaction mixture was warmed to room temperature and allowed to stir overnight. The reaction mixture was quenched with saturated $NaHCO_3$ solution and extracted with CH_2Cl_2. The combined organic layers were dried over $MgSO_4$. The solvent was removed *in vacuo* to yield an off-white solid **S11** (110 mg, 57%), which was used in the next reaction without further purification.

S11: ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.25 (d, J = 1.4 Hz, 2H), 7.93 (dd, J = 8.8, 3.2 Hz, 4H), 7.84 (d, J = 8.9 Hz, 2H), 7.69 (dd, J = 8.7, 1.7 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.01, 131.16, 129.73, 129.67, 128.53, 128.07, 128.01, 121.06, 118.52, 113.24.



S11 **8**

To a dry flask was added 2,12-dibromodinaphtho[2,1-b:1',2'-d]furan **S11** (88 mg, 0.21 mmol) then $PdCl_2$(dppf) (9.2 mg, 0.0126 mmol, 0.06 equiv). The flask was placed under inert atmosphere followed by the addition of anhydrous THF (3 mL). 1-Propynyl-1-magnesium bromide solution (0.5 M in THF, 2.52 mL, 1.26 mmol, 6.0 equiv) was then transferred to the flask *via* syringe. The reaction mixture was heated to 60 °C overnight. After cooling to room temperature, the reaction was quenched with a saturated NH_4Cl solution and extracted with EtOAc. The combined organic layers were dried over $MgSO_4$, and the solvent was removed *in vacuo*. The product was purified using flash column chromatography eluting with DCM/Hexanes. Pure product was obtained as a pale yellow solid (57 mg, 81%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 2.18 (s, 6H), 7.57 (dd, J = 8.4, 1.1 Hz, 2H), 7.80 (d, J = 8.8 Hz, 2H), 7.91 (d, J = 8.8 Hz, 2H), 7.97 (d, J = 8.4 Hz, 2H), 9.26 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 4.5, 80.3, 86.8, 112.9, 119.0, 122.0, 127.0, 128.1, 128.2, 129.2, 129.3, 130.2, 154.7. HRMS (ESI, TOF, m/z): $C_{26}H_{17}O$ $[MH]^+$: 345.1279, observed: 345.1287.

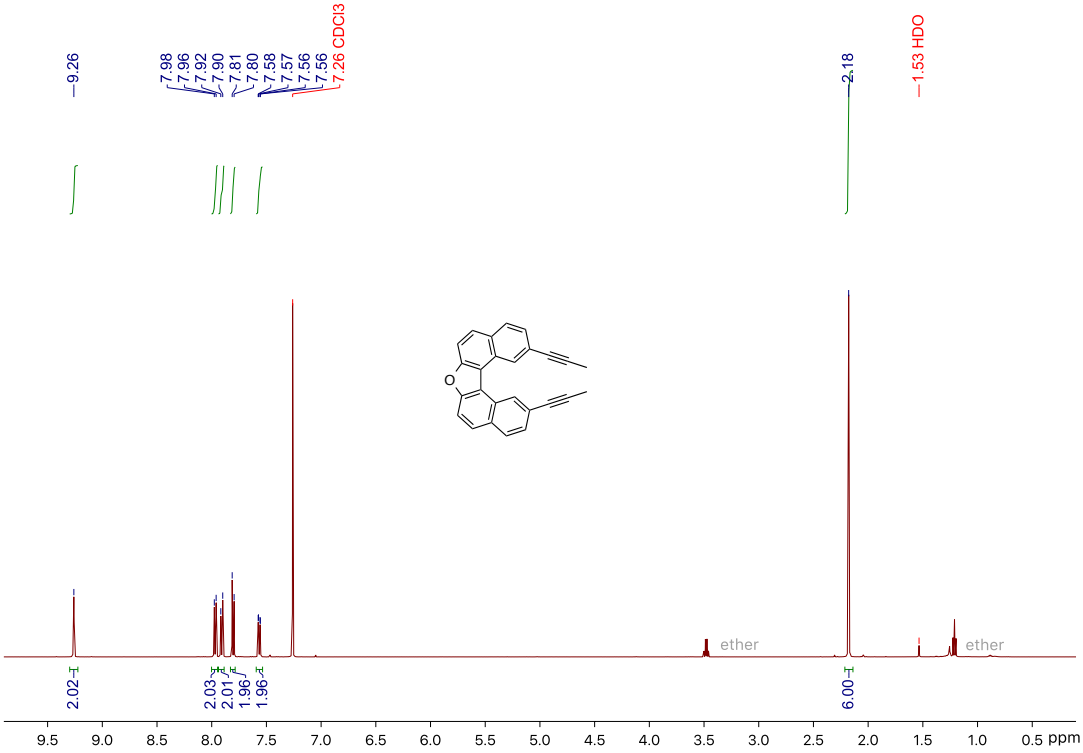


Figure S15. ^{1}H NMR spectrum of **8** at 500 MHz in $CDCl_3$.

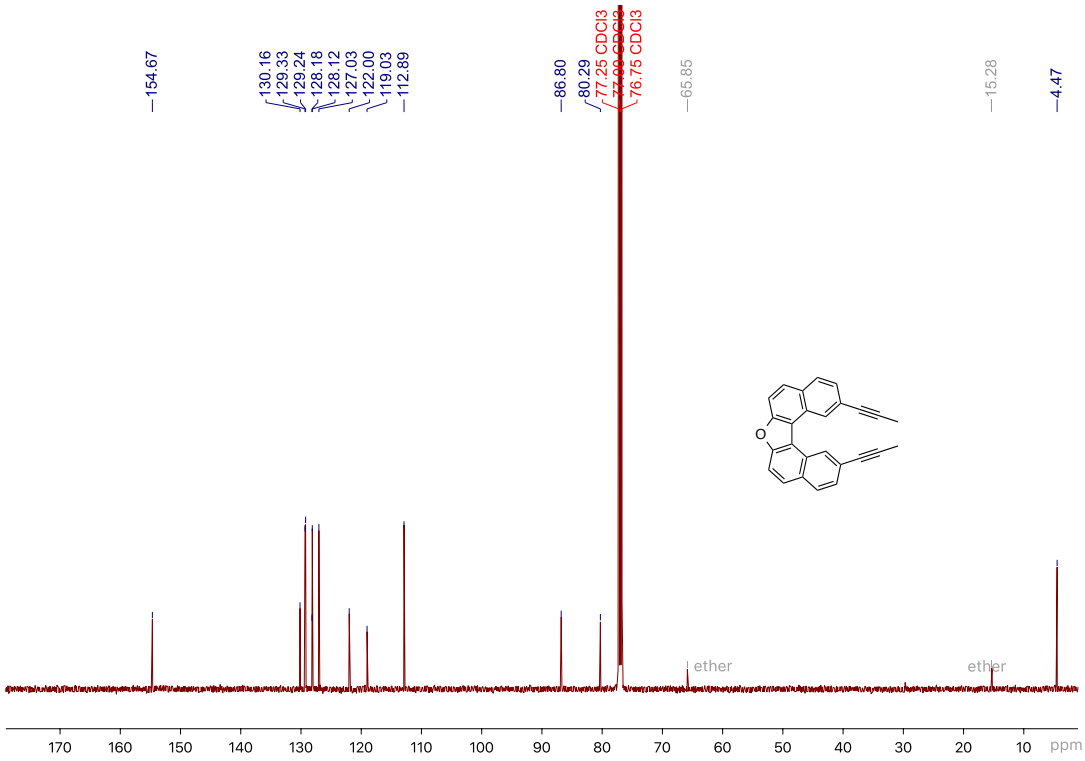
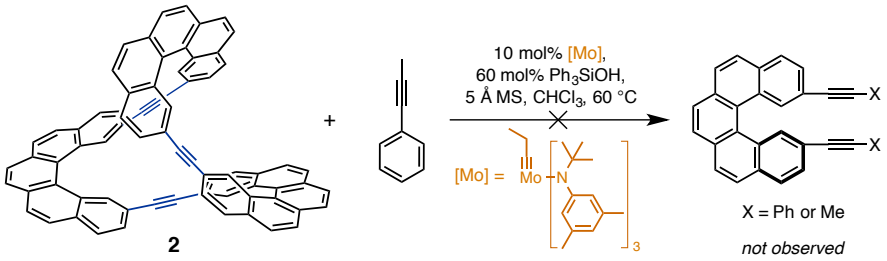


Figure S16. ^{13}C NMR spectrum of **8** at 126 MHz in $CDCl_3$.

Scrambling Experiments



Scrambling experiments under alkyne metathesis conditions demonstrated the kinetic stability of **2** (mixture of both enantiomers) over other linear- or cyclic-oligomers. Trimer **2** was subjected to the alkyne metathesis conditions described above in the presence of 12 equiv. 1-phenyl-1-propyne. After 24 hours, no evidence of trimer ring-opening was observed by ^{1}H or ^{13}C NMR studies (**Figure S17**). Meanwhile, the formation of diphenylacetylene was observed, indicating that metathesis of 1-phenyl-1-propyne did proceed.

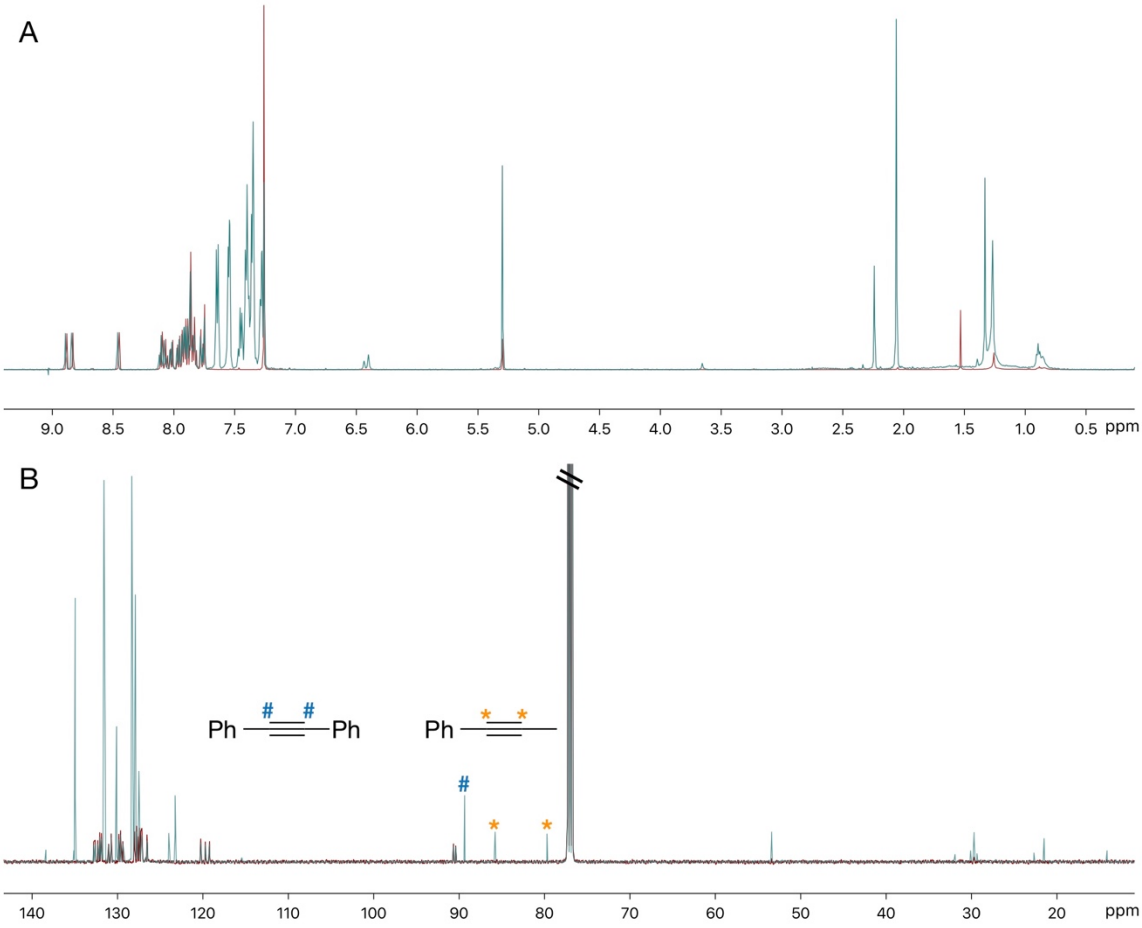


Figure S17. (A) The overlaid ^{1}H NMR and (B) ^{13}C NMR spectra of **2** (chestnut) and the crude product (cyan) of the scrambling experiment.

Crystallization and Single Crystal X-Ray Diffraction

A solution of trimer **2** in ethyl acetate in a vial was heated to reflux and was allowed to cool down on a stable shelf. Bright yellow crystals suitable for X-ray diffraction were formed overnight. A short prism of the crystal was covered in oil (Paratone-N, Exxon) before mounted onto a 0.3 mm cryo-loop (Hampton Research) for data collection with Mo K_{α} radiation at 100 K.

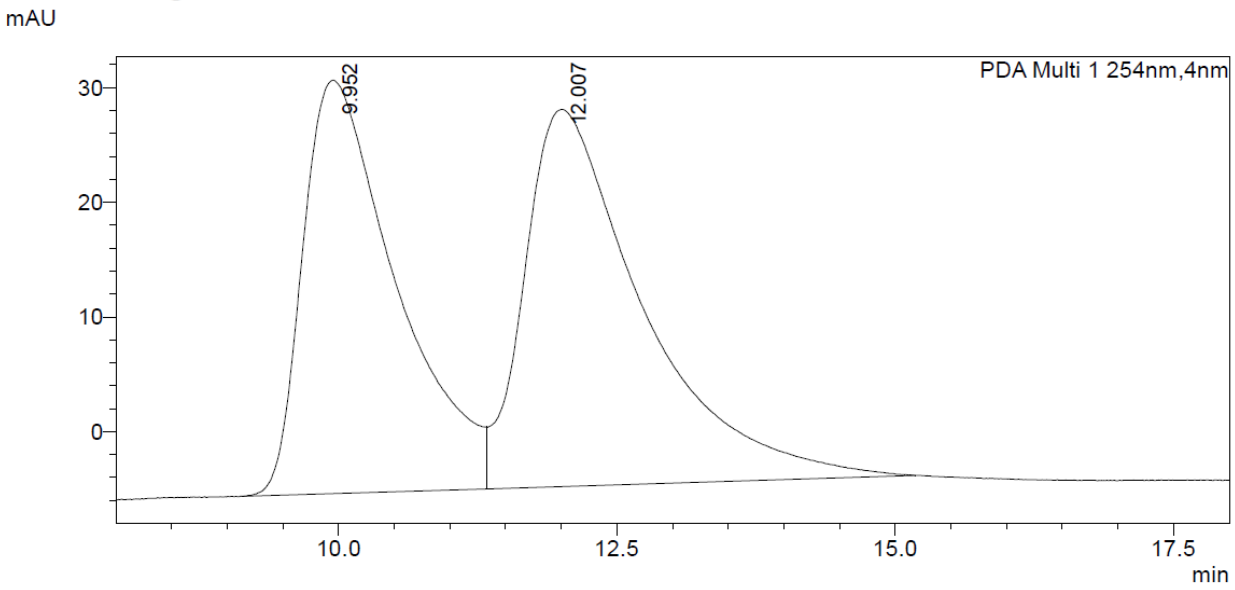
UV-Vis and Fluorescence Spectroscopy

UV-Vis spectra of **1** and **2** were obtained in spectrophotometric grade DCM at 9.0 and 3.0 μM, respectively. Fluorescence excitation and emission spectra of **1** and **2** were obtained in spectra grade DCM at ca. 3.0 and 1.0 μM, respectively. The solutions were purged with N_2 for 3 min to remove dissolved oxygen before each measurement. Diphenylanthracene in cyclohexane (90%) was used as the standard for quantum yield measurements.

Chiral HPLC Separation

Separation of enantiomers of **2** was achieved on an analytical HPLC by injection onto a ChiralPak IB-3column eluting with 2% to 10% IPA/Hexane over 20 minutes. Unfortunately, due to its limited solubility, the prep scale separation of **2** was not successful, and CD spectra of $\mathbf{2}_{PPM}$ and $\mathbf{2}_{MMP}$ were not obtained.

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%	Height%
1	9.952	2108963	36068	0.000	46.322	52.284
2	12.007	2443866	32917	0.000	53.678	47.716
Total		4552829	68986		100.000	100.000

Cyclic Voltammetry and Scan Rate Investigation of 1

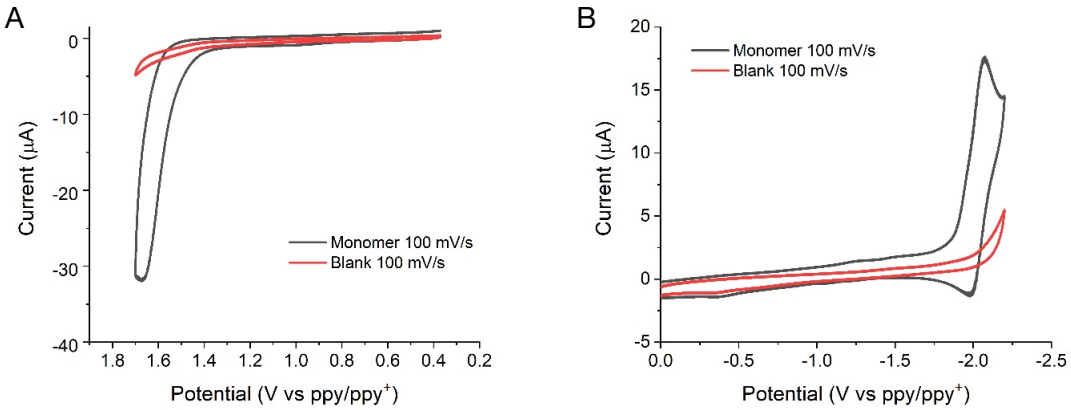


Figure S18. Cyclic voltammetry (CV) examining the first oxidation (A) and first reduction (B) of helicene **1**. CV was performed using solutions of 1.37 mM monomer and 0.125 M $TBAPF_6$ in MeCN (black trace) or 0.125 M $TBAPF_6$ in MeCN (red trace) in a glovebox under argon. The electrochemistry was performed at a scan rate of 100 mV/s utilizing a 2 mm Pt disc as a working electrode, a metal/ polypyrrole quasi-reference electrode (ppy/ppy^+), and a Pt wire as a counter electrode. Figure A displays an oxidative wave with an anodic peak at 1.675 V vs ppy/ppy^+, and the corresponding reverse cathodic wave is absent. Figure B displays a cathodic peak at -2.066 V vs ppy/ppy^+ and a smaller corresponding anodic peak at -1.972 V vs ppy/ppy^+. This equates to an approximate half wave potential for the 1st reduction of -2.019 V vs ppy/ppy^+. The current generated from the anodic peak (A) is roughly twice that generated from the cathodic peak (B).

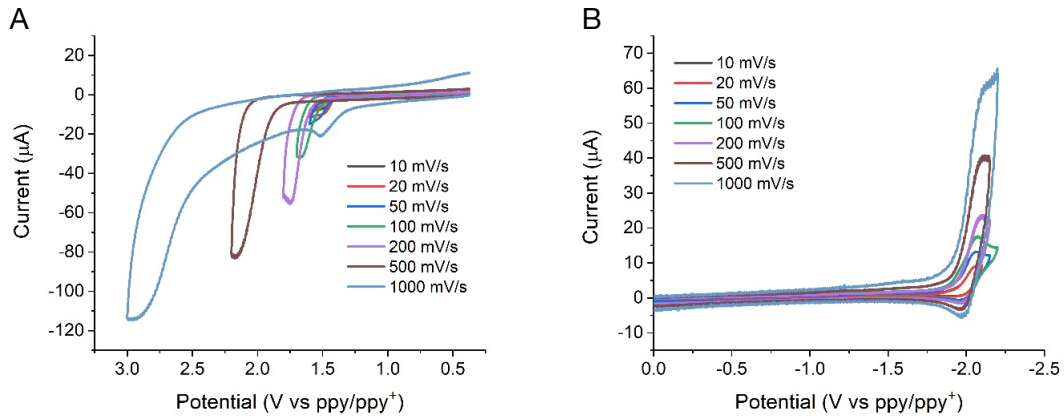


Figure S19. CV comparing the effect of scan rate on the 1st oxidation (A) and reduction (B) of helicene **1**. CV was performed with varying scan rates using a solution of 1.37 mM monomer and 0.125 M $TBAPF_6$ in MeCN in a glovebox under argon. The electrochemistry was performed utilizing a 2 mm Pt disc as a working electrode, ppy/ppy^+ reference electrode, and a Pt wire as a counter electrode. The 1st oxidation (A) demonstrated a large shift in potential upon increasing the scan rate and an absence of a corresponding cathodic peak even with probing at higher scan rates. In contrast, the 1st reduction (B) demonstrated very little shift upon increasing the scan rate and at faster scan rates the reverse anodic peak becomes more prominent. This indicates that the electrochemical products of the reduction are relatively more stable than the electrochemical oxidized species in Figure A.

Cyclic Voltammetry and Scan Rate Investigation of 2

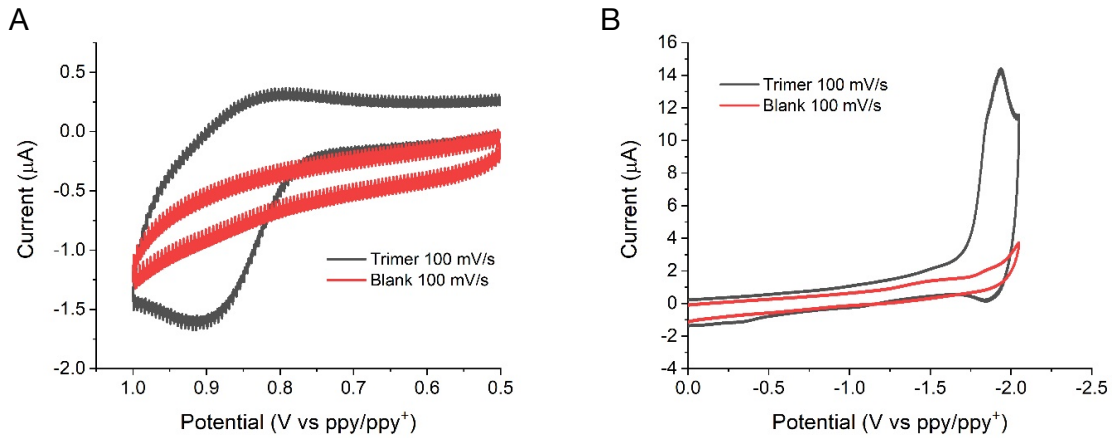


Figure S20. CV examining a prominent oxidative surface process (A) and the first reduction (B) of macrocycle **2**. CVs were performed using solutions of 376 µM of **2** and 0.125 M $TBAPF_6$ in MeCN (black trace) or 0.125 M $TBAPF_6$ in MeCN (red trace) in a glovebox under argon. The electrochemistry was performed at a scan rate of 100 mV/s utilizing a 2 mm Pt disc as a working electrode, ppy/ppy^+ reference electrode, and a Pt wire as a counter electrode. The oxidative process displayed an anodic peak at 0.914 V vs ppy/ppy^+, which is roughly 600 mV less anodic than the monomers 1st oxidation (Figure S1A). The y-offset in the blank is most likely due to a difference in sensitivity setting during the two measurements. Regardless, no peaks are observed in the blank, which indicates the observed process is faradaic. The 1st reduction (B) displays a cathodic peak at -1.938 V vs ppy/ppy^+ and corresponding anodic peak at -1.853 V vs ppy/ppy^+. This equates to an approximate half wave potential of 1.896 V vs ppy/ppy^+ for the 1st reduction. This is less 100 mV less cathodic than the corresponding 1st reduction for the monomer **1** (Figure S18B).

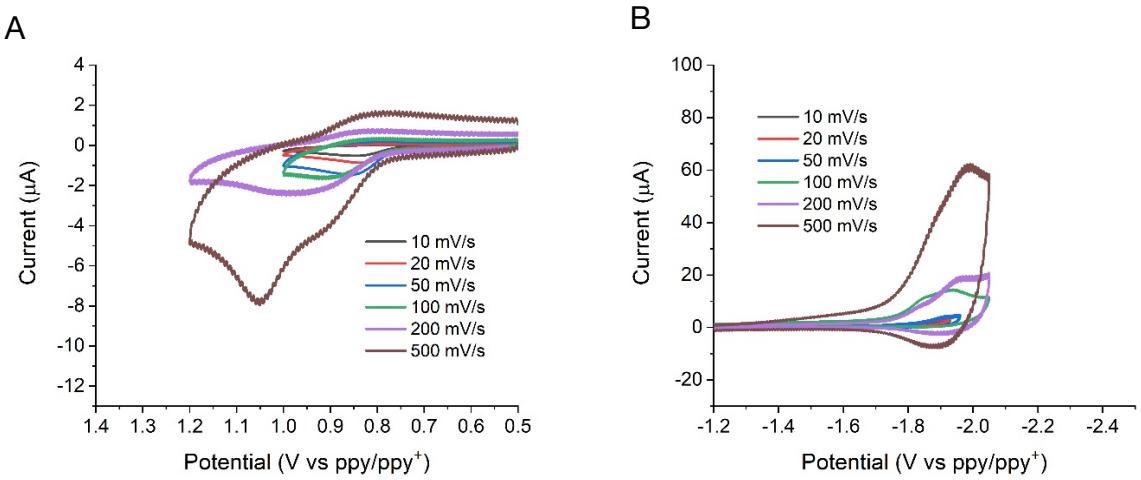


Figure S21. CV comparing the effect of scan rate on the oxidative surface process and 1st reduction of macrocycle **2** using a solution of 376 µM macrocycle **2** and 0.1 M $TBAPF_6$ in MeCN in a glovebox under argon. The electrochemistry was performed at varied scan rates utilizing a 2 mm Pt disc as a working electrode, a ppy/ppy^+ reference electrode, and a Pt wire as a counter electrode. Unlike Figure S19A displaying a faradaic oxidation, the oxidative surface process observed for **2** (A) demonstrates a complex mixture of absorption and precipitation. Similar to Figure S19B, increasing the scan rate for the trimer reduction wave (B) causes the corresponding anodic peak to become more prominent.

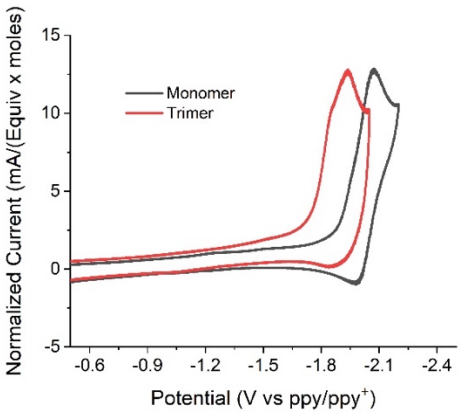


Figure S22. Comparison of monomer **1** (black trace) and macrocycle **2** (red trace) CV normalizing the cathodic currents. Normalization was performed through dividing the current by the product of the number of moles in solution and the hypothesized number of redox active centers (monomer equal to one and trimer equal to three). The close correlation in normalized currents for the monomer and macrocycle CVs, as well as the presence of a single three-electron wave indicates that the global macrocycle structure is capable of accepting three electrons in redox centers that act independently of each other.

Computational Studies

General

All the DFT calculations in this study were carried out using the Gaussian 09 software package.[4] EDDB calculations were based on density matrix of natural atomic orbitals (NAOs) obtained using the NBO 6.0 program,[5] analyzed by the RunEDDB script.[6] Visualization of transition dipole moments was implemented by Multiwfn (v3.7)[7] and VMD (v1.9.3)[8] programs.

Unless stated otherwise, all DFT calculation were performed at B3LYP/6-31G(d) level of theory for C, H, O, and Si atoms, and B3LYP/SDD for Mo. Frequency calculations were performed to confirm that all optimized structures were minima and every transition state has only one imaginary frequency. Intrinsic reaction coordinate (IRC) calculations[9] confirmed the transition states are saddle points in the proposed potential energy surfaces (PES). SMD solvation models[10] were used for C, H, O, and Si atoms in PES calculations ($CHCl_3$), and the SDD basis set were applied to only molybdenum atoms in the solvation models.[11] The SMD model (DCM) was also used in the TD-DFT calculation. The long-range corrected CAM-B3LYP functional[12] was used in the time-dependent DFT (TD-DFT)[13,14] and electron density of delocalized bonds (EDDB)[15] calculations, in conjunction with basis sets 6-31G(d) for TD-DFT and 6-311G(d,p) for EDDB.

[5]Helicene Helicity Inversion Barrier

DFT calculation (in vacuum) suggests that the barriers of inversion at 298.15 K are essentially the same for [5]helicene and 2,13-diproprynyl-[5]helicene **1**. Coordinates of both compounds at the ground and transition states are in SI Appendix.

Table S2. Inversion barrier of parent and substituted [5]helicenes.

	Inversion barrier (kcal mol^{-1})		
	ΔE	ΔH	ΔG
[5]helicene	24.3(8)	23.6(0)	24.3(5)
2,13-diproprynyl-[5]helicene **1**	24.4(4)	23.6(1)	25.6(1)

$\mathbf{2}_{PPM}$ and $\mathbf{4}_{PPP}$ Thermodynamic Stability

Both macrocycles **2** and **4** are optimized at B3LYP/6-31G(d) level of theory. High-level single-point energy calculations were performed on the optimized structures, suggesting that $\mathbf{4}_{PPP}$ is thermodynamically more stable than $\mathbf{2}_{PPM}$ by 1−2 kcal/mol. Minimal entropy/temperature contribution to the relative stability was observed (less than 0.1 kcal/mol over 100 K). ($\Delta E = E_{PPP} - E_{PPM}$)

Table S3. Thermodynamic stabilities of cyclic trimers **2** and **4**.

Methods	Relative energy differences (kcal/mol)			
	ΔE	ΔZPE	ΔH	ΔG
M06-2X/def2-TZVP	-1.1	-1.2	-1.2	-0.9
B3LYP/def2-TZVP	-2.9	-3.0	-3.0	-2.8
PBE0/def2-TZVP	-2.1	-2.2	-2.2	-2.0

Mechanism for *PPM*/*PPP* Selectivity

The energy barriers of the last step of macrocyclic 3mer formation were studied. Basis set superposition error (BSSE) values calculated in gas phase for $\mathbf{2}_{PPM}\cdots$Mo and $\mathbf{4}_{PPP}\cdots$Mo are 0.00425 a.u. and 0.00332 a.u., respectively. The BSSE correction has been applied to the sum of product energies. Uncorrected energies are provided in parentheses.

Table S4. Relative energies of intermediates and transition states of $\mathbf{2}_{PPM}$ and $\mathbf{4}_{PPP}$ formation.

	O3	**TS1**	**IM1(IM)**	**IM2**	**TS2**	3mer + Mo
$\mathbf{2}_{PPM}$ *G* (kcal/mol)	0.0	21.6	13.6	-	-	-16.5 (-13.8)
$\mathbf{2}_{PPM}$ *H* (kcal/mol)	0.0	15.1	5.5	-	-	-4.2 (-1.6)
$\mathbf{4}_{PPP}$ *G* (kcal/mol)	0.0	37.0	26.0	24.5	28.2	-14.4 (-12.3)
$\mathbf{4}_{PPP}$ *H* (kcal/mol)	0.0	29.9	18.8	18.6	21.2	-3.1 (-1.0)

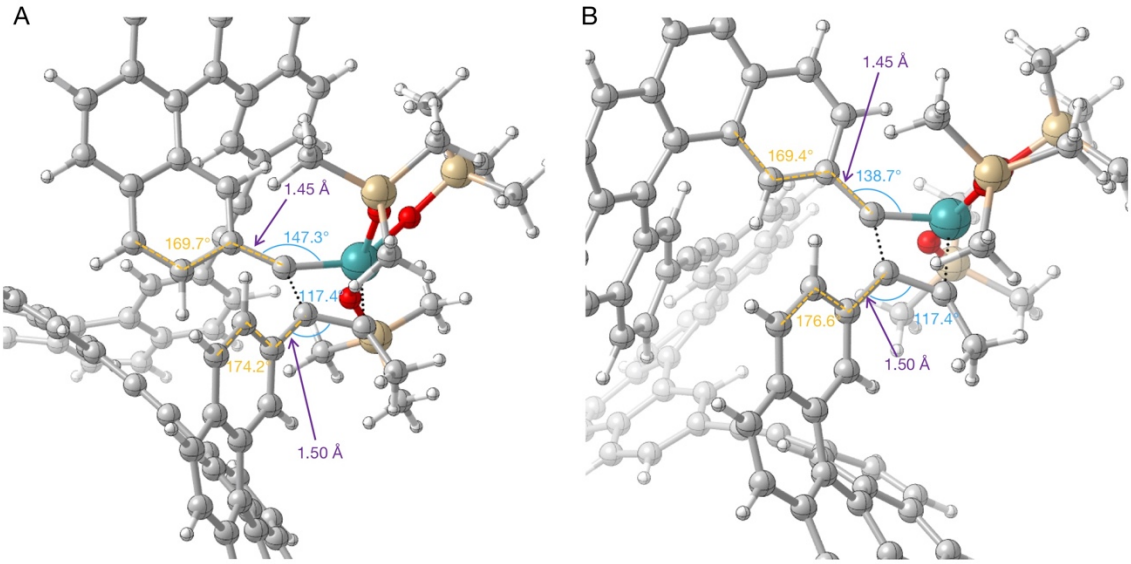


Figure S23. Key structure parameters, including bond angles (blue), bond length (purple), and dihedral angles (yellow) in **TS1**$_{PPM}$ (A) and **TS1**$_{PPP}$ (B).

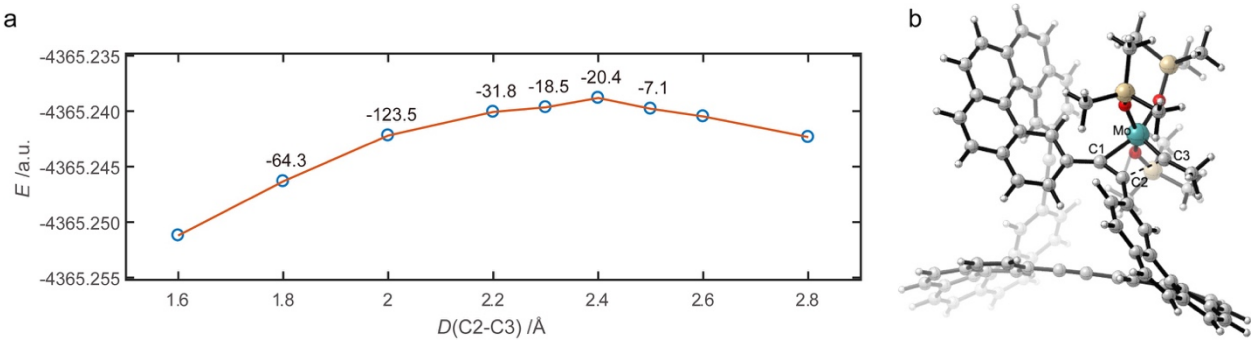


Figure S24. Relaxed potential energy surface (PES) scan (**a**) with fixed C2-C3 distances (**b**). Imaginary frequencies correspond to the C2-C3 stretching vibration, and the values are given in cm^{-1}. Transition state searches based on the points including the one with the most negative imaginary frequency (C2-C3: 2.0 Å) and the one with highest energy (C2-C3: 2.4 Å), all failed to locate the **TS2** of PPM but directly lead to the product.

Calculated UV and ECD Spectra

The TD-DFT calculation was performed at CAM-B3LYP/6-31G(d) level of theory. A total of 10 and 50 states were calculated for the monomer and 3mer. The SMD was also applied to TD-DFT calculations in the singlet electronic state (solvent: DCM). The ECD of **2**$_{PPM}$ is predicted to have a (+) peak at around 300 nm, and a (-) peak at approximately 380 nm.

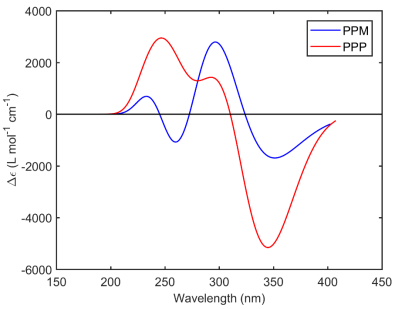


Figure S25. Calculated ECD of $\mathbf{2}_{PPM}$ and $\mathbf{4}_{PPP}$.

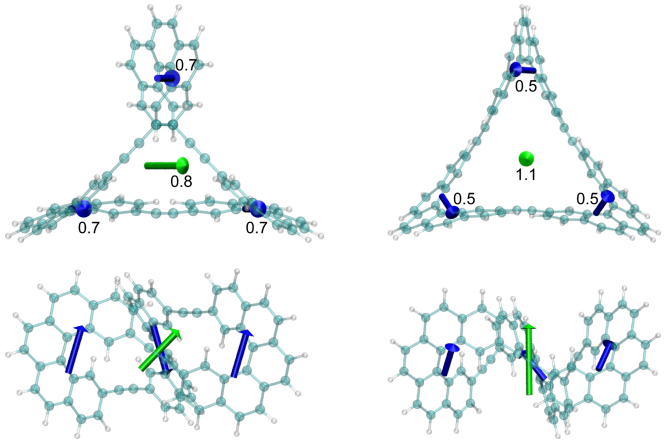


Figure S26. Electric transition dipole moments ($S_0 \rightarrow S_1$) of $\mathbf{2}_{PPM}$ (left) and $\mathbf{4}_{PPP}$ (right). Unit: Debye. Blue arrows indicate the contribution of transition dipole moments from helicene fragments, not including bridging moieties.

Table S5. Calculated oscillator strength of **1** (right, 10 states) and **2** (left, 50 states)

Index	Excit. energy(eV)	nm	Oscil.str.
1	3.4224	362.5237	0.0073
2	3.6167	343.04783	0.3322
3	3.6219	342.55532	0.2537
4	3.6354	341.28324	0.0002
5	3.6694	338.12097	0.5353
6	3.6887	336.35186	0.8579
7	3.9902	310.93707	0.7701
8	4.0003	310.15201	1.0035
9	4.0444	306.77013	0.0353
10	4.1825	296.64103	0.2784
11	4.2127	294.51447	0.5901
12	4.2611	291.16921	0.0311
13	4.2654	290.87567	0.0011
14	4.299	288.60226	0.7402
15	4.3461	285.47459	0.0179
16	4.3493	285.26455	0.3253
17	4.3828	283.08412	0.1002
18	4.4678	277.69844	0.149
19	4.4836	276.71985	0.2453
20	4.4926	276.16549	0.0602
21	4.5168	274.68586	0.0375
22	4.5825	270.74765	0.0099

Index	Excit. energy(eV)	nm	Oscil.str.
1	3.6675	338.29614	0
2	3.8187	324.90143	0.1997
3	4.1565	298.4966	0.3642
4	4.3328	286.35088	0.0609
5	4.4539	278.5651	0.506
6	4.5023	275.57051	0.6415
7	4.7618	260.55296	0.021
8	4.9199	252.18015	0.2637
9	5.0559	245.39669	0.1907
10	5.0928	243.61866	0.5567

23	4.7096	263.44087	0.0266
24	4.7138	263.20614	0.1152
25	4.741	261.69608	0.2973
26	4.7567	260.83232	0.0155
27	4.7774	259.70216	0.8144
28	4.8161	257.61531	0.1038
29	4.8831	254.08063	0.1246
30	4.8992	253.24565	0.3653
31	4.919	252.22629	0.0063
32	4.9381	251.2507	0.199
33	4.9573	250.27759	0.0111
34	5.0022	248.03109	0.0043
35	5.03	246.66026	0.0115
36	5.0328	246.52303	0.0064
37	5.0658	244.91711	0.0146
38	5.0898	243.76225	0.0047
39	5.1036	243.10312	0.0452
40	5.1774	239.63787	0.005
41	5.1845	239.30969	0.1345
42	5.2045	238.39007	0.0623
43	5.219	237.72774	0.306
44	5.2192	237.71864	0.0356
45	5.2645	235.67311	0.2188
46	5.2813	234.92343	0.3211
47	5.2828	234.85672	0.012
48	5.3131	233.51736	0.0028
49	5.3593	231.50432	0.009
50	5.3681	231.12481	0.047

ACID and EDDB Plots

Anisotropy of the induced ring current density (ACID)[16,17] calculations were performed at the B3LYP/6-311G(d,p) level, using the continuous set of gauge transformation (CSGT)[18] method. EDDB calculation utilized the CAM-B3LYP functional with 6-311G(d,p) basis set.

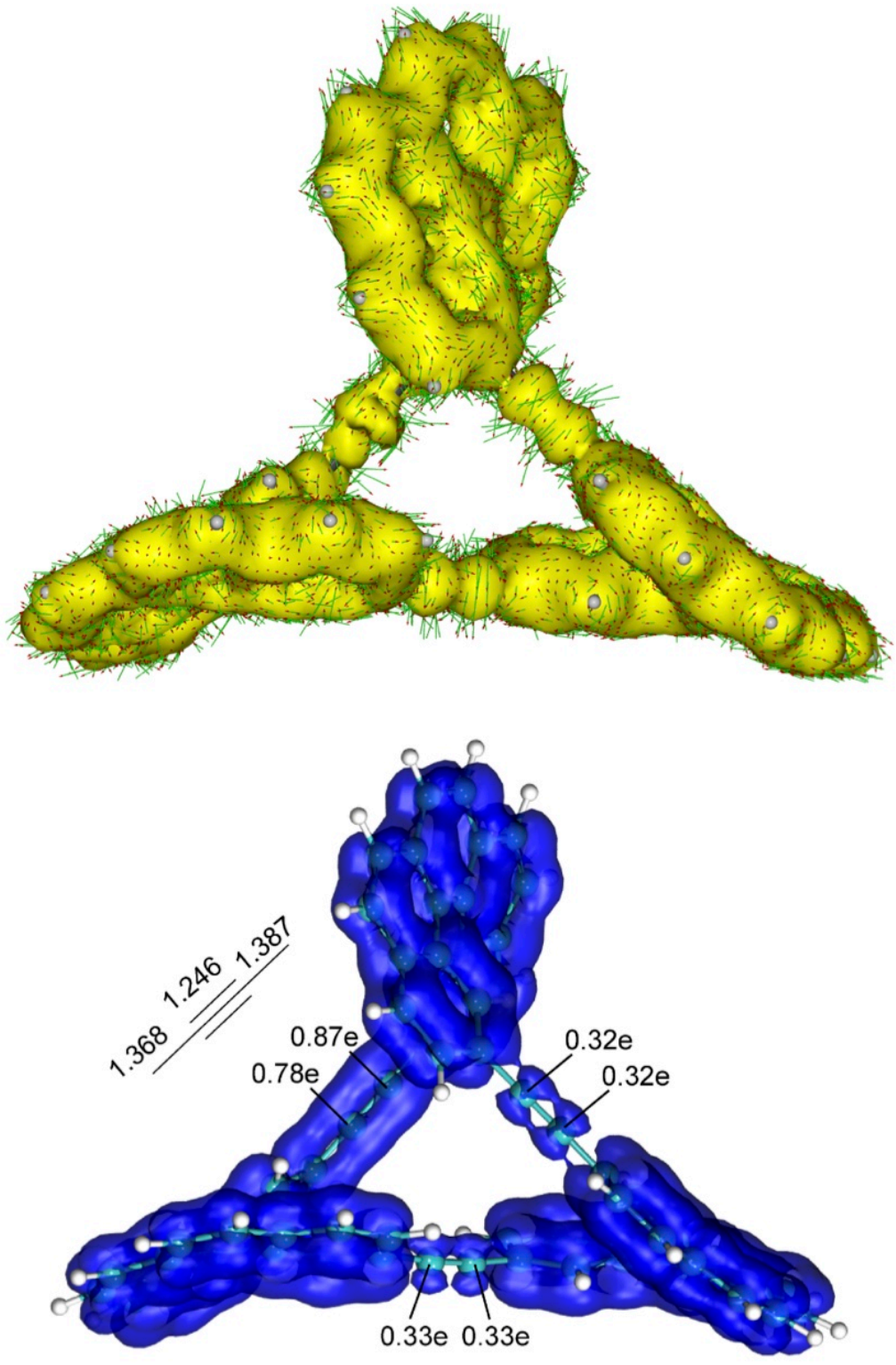


Figure S27. The ACID and EDDB plots of $\mathbf{2}_{PPM}$ showing a higher level of conjugation through one of the three triple bonds at the T_1 excited state (isovalue 0.015).

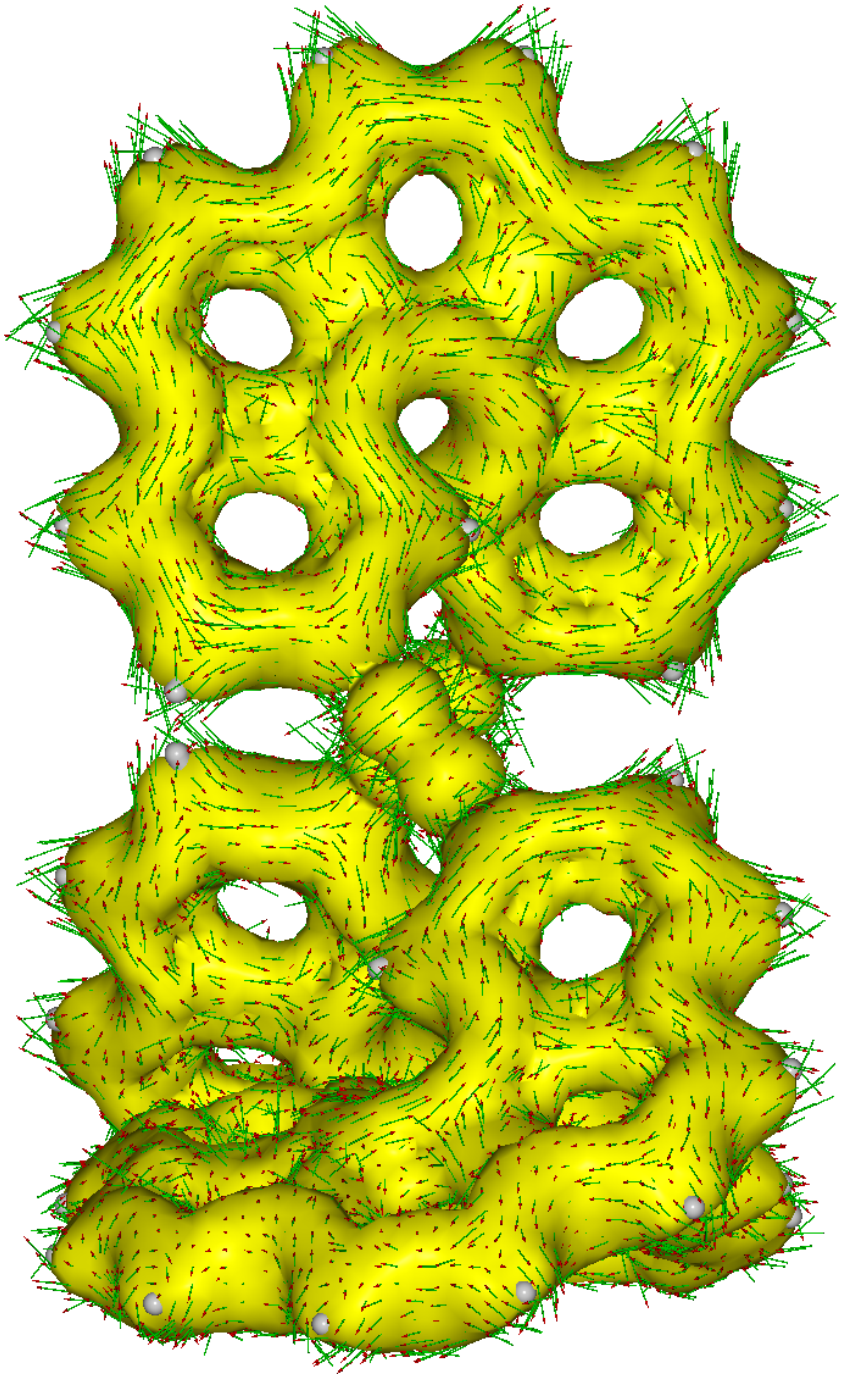


Figure S28. The ACID plot of $\mathbf{4}_{PPP}$.

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SI Appendix

Coordinates of the following calculated structures (ground state, activated state, and transition state) are included:

[5]helicene, [5]helicene-TS-inversion

2,13-diproprynyl-[5]helicene, 2,13-diproprynyl-[5]helicene **1**-TS-inversion

$\mathbf{2}_{PPM}$ (S_0 and T_1), $\mathbf{4}_{PPP}$ (S_0)

All intermediates ($\mathbf{O3}_{PPM}$, $\mathbf{IM}_{PPM}$, $\mathbf{O3}_{PPP}$, $\mathbf{IM1}_{PPP}$, $\mathbf{IM2}_{PPP}$) and transition states ($\mathbf{TS1}_{PPM}$, $\mathbf{TS1}_{PPP}$, $\mathbf{TS2}_{PPP}$) leading to the macrocycle formation (see Figure 2)

[5]helicene					[5]helicene-TS-inversion			
H	4.555336	0.949222	-0.98515		C	-0.679435	3.215508	-0.495794
C	3.510183	0.921359	-0.687014		C	0.679435	3.215508	-0.495794
H	3.185969	3.009016	-0.969962		C	-1.383648	2.008037	-0.260679
C	2.752604	2.052022	-0.689539		C	1.383648	2.008037	-0.260679
C	1.589218	-0.369998	0.187167		C	-0.739224	0.727467	-0.33137
C	1.367764	2.020969	-0.328894		C	0.739224	0.727467	-0.33137
C	2.969198	-0.303422	-0.186363		C	-2.732141	2.165262	0.199849
C	0.723656	0.781456	-0.05489		C	-3.434533	1.112203	0.681245
C	0.650128	3.2446	-0.207992		C	-2.938463	-0.209041	0.467312
C	-0.649986	3.244616	0.208005		C	-1.678516	-0.413464	-0.199193
H	1.17697	4.177572	-0.391941		H	-1.241104	4.143685	-0.560205
H	-1.176785	4.1776	0.392021		H	1.241104	4.143685	-0.560205
C	-1.367668	2.021008	0.328865		H	-3.131242	3.174692	0.254455
C	-2.752492	2.052107	0.689566		H	-4.409313	1.241776	1.144099
C	-0.723618	0.781481	0.054783		C	-3.777857	-1.302842	0.78324
C	-3.510115	0.921474	0.687048		C	-1.525204	-1.705504	-0.755389
H	-3.185805	3.009109	0.970041		C	-2.384121	-2.759667	-0.488885
H	-4.555252	0.94937	0.985233		C	-3.492977	-2.580785	0.349525
C	-2.969195	-0.303325	0.186372		H	-4.692685	-1.099481	1.33493
C	-1.589228	-0.369954	-0.187223		H	-0.774315	-1.870818	-1.501767
C	3.812744	-1.421601	0.027452		H	-2.202317	-3.7221	-0.959561
C	3.350515	-2.551767	0.667242		H	-4.151741	-3.410799	0.588884
C	2.022574	-2.582521	1.138039		C	3.434533	1.112203	0.681245
C	1.17017	-1.521444	0.903756		C	2.732141	2.165262	0.199849
H	4.84983	-1.354917	-0.293268		C	2.938463	-0.209041	0.467312
H	4.011769	-3.396794	0.83851		C	1.678516	-0.413464	-0.199193
H	0.161714	-1.562811	1.29474		C	3.777857	-1.302842	0.78324
C	-1.170271	-1.521427	-0.903815		C	3.492977	-2.580785	0.349525
C	-2.02273	-2.582475	-1.138046		C	2.384121	-2.759667	-0.488885
C	-3.350641	-2.551669	-0.667184		C	1.525204	-1.705504	-0.755389
C	-3.812792	-1.421472	-0.027386		H	4.409314	1.241776	1.144099
H	-0.16185	-1.562842	-1.294877		H	3.131242	3.174692	0.254455
H	-4.011945	-3.396664	-0.83841		H	4.692685	-1.099481	1.33493
H	-4.849861	-1.354745	0.293381		H	4.151742	-3.410799	0.588883
H	-1.666211	-3.441588	-1.700011		H	0.774315	-1.870818	-1.501766
H	1.666001	-3.441625	1.699984		H	2.202316	-3.7221	-0.95956

2,13-diproprynyl-[5]helicene **1**				2,13-diproprynyl-[5]helicene **1** TS-inversion			
C	3.603109	1.597886	2.298642	C	4.249422	0.671204	-1.105547
C	2.64073	1.861661	1.609781	C	4.2461	-0.687612	-1.105948
H	-2.022389	4.318259	-1.756481	C	3.134826	1.377149	-0.58705
C	-1.996179	3.340322	-1.2823	C	3.128305	-1.388506	-0.587406
H	-4.085064	2.974894	-1.503965	C	1.871687	0.734936	-0.356193
C	-3.128635	2.595141	-1.153033	C	1.8682	-0.74055	-0.355875
C	-0.707133	1.598806	-0.087565	C	3.401919	2.720415	-0.166151
C	-3.09884	1.293899	-0.558037	C	2.493329	3.419754	0.556344
C	-0.774024	2.892523	-0.695668	C	1.157901	2.929964	0.649061
C	-1.859973	0.704476	-0.178009	C	0.794427	1.677436	0.038593
C	-4.323285	0.609078	-0.316022	H	5.13696	1.230961	-1.38845
C	-4.32458	-0.600582	0.316487	H	5.130898	-1.251513	-1.389214
H	-5.255499	1.097668	-0.588096	H	4.397091	3.117519	-0.34764
H	-5.257836	-1.087128	0.588649	H	2.73103	4.390026	0.984254
C	-3.101616	-1.288065	0.558405	C	0.167832	3.772437	1.207503
C	-3.134192	-2.589228	1.153416	C	-0.584996	1.534668	-0.222638
C	-1.861503	-0.701343	0.178244	C	-1.562797	2.411225	0.258512
C	-2.003345	-3.33687	1.282602	C	-1.173052	3.511958	1.056197
H	-4.091417	-2.966912	1.504408	H	0.494693	4.67713	1.714449
H	-2.031667	-4.314747	1.756785	H	-0.923223	0.787086	-0.91179
C	-0.780256	-2.891723	0.695911	H	-1.92748	4.174233	1.46836
C	-0.71062	-1.59817	0.087772	C	2.478449	-3.428182	0.556333
C	0.347051	3.756944	-0.625835	C	3.389619	-2.73301	-0.166885
C	1.471326	3.417207	0.087816	C	1.145401	-2.932231	0.65035
C	1.512504	2.184978	0.795074	C	0.786865	-1.678016	0.040343
C	0.435476	1.30693	0.694206	C	0.152263	-3.770473	1.20974
H	0.287462	4.722512	-1.122513	C	-1.187634	-3.504638	1.059246
H	2.318527	4.092893	0.149719	C	-1.573335	-2.402163	0.262001
H	0.478798	0.38331	1.255351	C	-0.59235	-1.529105	-0.219012
C	0.432578	-1.308781	-0.694058	H	2.712023	-4.399589	0.983942
C	1.507722	-2.189138	-0.79497	H	4.382828	-3.134613	-0.349193
C	1.463974	-3.421228	-0.087633	H	0.475786	-4.676538	1.716378
C	0.338991	-3.758527	0.626065	H	-1.944504	-4.164149	1.471364
H	0.47796	-0.385301	-1.255272	H	-0.928496	-0.779321	-0.906648
H	2.309717	-4.098751	-0.149416	C	-2.946576	-2.222064	-0.086257
H	0.277354	-4.72395	1.122779	C	-4.120037	-2.118608	-0.373908
C	2.636279	-1.867725	-1.609907	C	-2.93679	2.234537	-0.088287
C	3.598425	-1.604333	-2.299224	C	-4.11094	2.131391	-0.373153
C	4.752633	-1.275212	-3.129219	C	-5.531265	-1.997437	-0.723994
H	5.516499	-2.06066	-3.079488	H	-5.680924	-1.264047	-1.525448
H	4.46589	-1.157421	-4.181784	H	-5.940204	-2.955013	-1.070095
H	5.219286	-0.335901	-2.807127	H	-6.130719	-1.676093	0.137428

2$_{PPM}$ (S_0)				**2**$_{PPM}$ (T_1)			
C	-2.301474	0.430184	-2.362412	C	-2.198107	0.071439	-2.475935
H	-6.624014	-3.658922	-4.237931	H	-5.870211	-4.619623	-4.097814
C	-6.423273	-3.348161	-3.215804	C	-5.770468	-4.166605	-3.114506
H	-8.205603	-4.196765	-2.410121	H	-7.611689	-5.015982	-2.362213
C	-7.285673	-3.653801	-2.207983	C	-6.741024	-4.40865	-2.130893
C	-4.993812	-2.106039	-1.619879	C	-4.617726	-2.629175	-1.579857
C	-7.004708	-3.289623	-0.853371	C	-6.597025	-3.900708	-0.82381

C	-5.289446	-2.5218	-2.957952
C	-5.771383	-2.663012	-0.511314
C	-7.986309	-3.544003	0.145168
C	-7.766284	-3.174355	1.439478
H	-8.931186	-3.989081	-0.156028
H	-8.541532	-3.289041	2.19278
C	-6.484024	-2.710312	1.846502
C	-6.261261	-2.423709	3.230337
C	-5.429453	-2.574276	0.897909
C	-5.023544	-2.10265	3.697384
H	-7.113162	-2.469805	3.904236
H	-4.866478	-1.865823	4.746707
C	-3.893357	-2.16406	2.829386
C	-4.075069	-2.453328	1.438287
C	-4.500987	-2.040645	-4.033192
C	-3.506323	-1.116409	-3.833405
C	-3.281273	-0.591008	-2.529617
C	-4.028078	-1.082704	-1.459172
H	-4.720335	-2.399023	-5.036061
H	-2.912516	-0.745591	-4.662759
H	-3.855346	-0.658377	-0.479158
C	-2.911816	-2.713273	0.679192
C	-1.629265	-2.556326	1.201783
C	-1.471105	-2.182293	2.564288
C	-2.583664	-2.012859	3.351662
H	-2.999723	-3.03694	-0.347815
H	-0.471672	-2.044173	2.963815
H	-2.474384	-1.770864	4.406223
C	-0.49009	-2.69506	0.360481
C	2.301589	0.430397	2.362407
C	1.454187	1.303524	2.318229
H	-2.612365	5.774767	3.848808
C	-1.943634	5.757213	2.991928
H	-2.120501	7.843295	2.584026
C	-1.681061	6.894037	2.287529
C	-0.387754	4.491547	1.545316
C	-0.823276	6.876243	1.142273
C	-1.246352	4.548721	2.687958
C	-0.319288	5.641358	0.648779
C	-0.441235	8.099976	0.521474
C	0.440735	8.099995	-0.521769
H	-0.812916	9.033185	0.937101
H	0.812336	9.033221	-0.937429
C	0.822886	6.876272	-1.14252
C	1.680678	6.894099	-2.287769
C	0.319004	5.641362	-0.64898
C	1.943362	5.757269	-2.992119
H	2.120036	7.843384	-2.5843
H	2.612099	5.77485	-3.848993
C	1.246189	4.548725	-2.688105
C	0.387585	4.49152	-1.54547
C	-1.309053	3.439603	3.568635
C	-0.47586	2.358481	3.416195
C	0.480169	2.34265	2.361353
C	0.48753	3.384718	1.435503
H	-2.000057	3.481735	4.407145
C	-4.734313	-3.275364	-2.876684
C	-5.422246	-3.157266	-0.460442
C	-7.614966	-4.139531	0.1496
C	-7.473917	-3.679017	1.423666
H	-8.51626	-4.662628	-0.159897
H	-8.273493	-3.797765	2.15064
C	-6.243704	-3.100893	1.855628
C	-6.106421	-2.700032	3.216379
C	-5.157103	-2.94392	0.937034
C	-4.92094	-2.234516	3.708889
H	-6.979764	-2.772421	3.86005
H	-4.835386	-1.912953	4.743728
C	-3.75156	-2.249871	2.893361
C	-3.842521	-2.653019	1.522093
C	-3.815461	-2.888224	-3.929523
C	-2.968842	-1.836551	-3.79075
C	-2.984296	-1.043278	-2.584316
C	-3.846246	-1.485645	-1.494056
H	-3.841741	-3.454326	-4.857527
H	-2.296366	-1.548056	-4.592839
H	-3.821862	-0.908615	-0.577916
C	-2.629834	-2.852289	0.8299
C	-1.38932	-2.541643	1.387149
C	-1.326171	-2.061241	2.722771
C	-2.484917	-1.940741	3.452012
H	-2.641325	-3.248513	-0.174545
H	-0.362203	-1.804995	3.150418
H	-2.445372	-1.616966	4.489453
C	-0.215681	-2.637783	0.588473
C	2.354892	0.764122	2.295877
C	1.402767	1.519385	2.22273
H	-3.27371	5.336266	3.760675
C	-2.614326	5.419643	2.900503
H	-3.095577	7.458728	2.499656
C	-2.523843	6.584395	2.198462
C	-0.894574	4.399771	1.443139
C	-1.681382	6.693943	1.048368
C	-1.747672	4.328836	2.589427
C	-1.003027	5.547231	0.545408
C	-1.497542	7.962273	0.426984
C	-0.647731	8.095115	-0.632795
H	-1.998499	8.828034	0.852686
H	-0.429827	9.072972	-1.054608
C	-0.099755	6.941936	-1.265924
C	0.708574	7.094992	-2.430543
C	-0.395593	5.641535	-0.762355
C	1.116645	6.007611	-3.158868
H	0.986483	8.100443	-2.73608
H	1.740938	6.134337	-4.039851
C	0.629705	4.715571	-2.84537
C	-0.174366	4.513265	-1.670663
C	-1.641753	3.223864	3.470619
C	-0.656104	2.280587	3.316313
C	0.288259	2.406785	2.258314
C	0.135952	3.435868	1.330167
H	-2.328524	3.162841	4.3114

H	-0.506062	1.528659	4.114849	H	-0.559487	1.455671	4.014653
H	1.22649	3.363141	0.645192	H	0.864942	3.522774	0.534695
C	-0.487599	3.384614	-1.435623	C	-0.851723	3.288414	-1.544197
C	-0.480127	2.342505	-2.361426	C	-0.725793	2.25098	-2.504527
C	0.475911	2.358383	-3.41626	C	0.182029	2.440801	-3.602739
C	1.309004	3.439576	-3.568735	C	0.833197	3.63037	-3.751676
H	-1.226569	3.363001	-0.645322	H	-1.542848	3.134806	-0.725971
H	0.5062	1.528534	-4.114877	H	0.314574	1.634835	-4.317215
H	2.000015	3.481737	-4.407238	H	1.48818	3.790944	-4.60474
C	-1.454041	1.303283	-2.318269	C	-1.490638	1.095936	-2.438472
C	0.490174	-2.695081	-0.360023	C	0.763162	-2.620414	-0.134237
H	4.86618	-1.86618	-4.746698	H	4.942499	-1.790675	-4.706166
C	5.023339	-2.102889	-3.697362	C	5.147824	-1.936931	-3.648671
H	7.112955	-2.469983	-3.904341	H	7.253186	-2.157544	-3.90006
C	6.261105	-2.423849	-3.230379	C	6.419791	-2.127154	-3.202561
C	4.075056	-2.453359	-1.438152	C	4.294249	-2.193446	-1.339222
C	6.483989	-2.710293	-1.846531	C	6.703725	-2.291436	-1.810191
C	3.893223	-2.164248	-2.829268	C	4.051463	-2.019801	-2.740218
C	5.429488	-2.574198	-0.89787	C	5.668977	-2.167552	-0.838122
C	7.7663	-3.174243	-1.439559	C	8.030636	-2.621111	-1.415227
C	7.98644	-3.54375	-0.145227	C	8.317755	-2.870953	-0.105612
H	8.541494	-3.288977	-2.192909	H	8.790141	-2.732603	-2.184862
H	8.931357	-3.988762	0.15594	H	9.304071	-3.215542	0.194491
C	7.004904	-3.289313	0.853361	C	7.348714	-2.616883	0.905111
C	7.285983	-3.653354	2.207986	C	7.699877	-2.848097	2.272394
C	5.771528	-2.662784	0.511335	C	6.058245	-2.119492	0.561018
C	6.423639	-3.347664	3.215841	C	6.846315	-2.533029	3.284748
H	8.205951	-4.19626	2.410108	H	8.667498	-3.297294	2.481824
H	6.624466	-3.658327	4.23798	H	7.103273	-2.743815	4.319717
C	5.289753	-2.521383	2.957995	C	5.638916	-1.826662	3.005846
C	4.994008	-2.10575	1.619907	C	5.269143	-1.543771	1.651611
C	2.583482	-2.01315	-3.351454	C	2.71977	-2.003289	-3.227165
C	1.470992	-2.182535	-2.56397	C	1.646612	-2.19586	-2.39245
C	1.629275	-2.55641	-1.201436	C	1.870977	-2.458937	-1.012868
C	2.911875	-2.713262	-0.678934	C	3.176193	-2.485203	-0.524776
H	2.474108	-1.771272	-4.406032	H	2.562425	-1.846386	-4.291676
H	0.471522	-2.04449	-2.96343	H	0.628406	-2.161457	-2.766352
H	2.999877	-3.036807	0.348104	H	3.31862	-2.728053	0.518326
C	4.028211	-1.082478	1.459178	C	4.209904	-0.625766	1.449169
C	3.28145	-0.590732	2.529632	C	3.447301	-0.127275	2.50464
C	3.506615	-1.116011	3.833448	C	3.759336	-0.523468	3.835876
C	4.501341	-2.040178	4.033246	C	4.842523	-1.332998	4.069453
H	3.85539	-0.658242	0.479141	H	3.970966	-0.295756	0.447257
H	2.912845	-0.745155	4.662811	H	3.155724	-0.146188	4.655132
H	4.720775	-2.398461	5.03613	H	5.123433	-1.589558	5.088055

4$_{PPP}$ (S_0)				—≡Mo(OSiMe$_3$)$_3$			
H	-4.712596	-4.813078	-4.457678	C	7.38070489	-2.82150249	1.05243951
C	-4.499456	-4.929537	-3.39802	H	8.44534226	-3.05876659	0.91162818
H	-5.298727	-6.902939	-3.272194	H	7.23061309	-2.57918246	2.11393159
C	-4.811634	-6.085505	-2.746164	Mo	6.58706933	-0.36058922	-0.86244818
C	-3.684147	-3.949408	-1.28138	C	6.98171778	-1.69879582	0.18010674
C	-4.507105	-6.262917	-1.358858	H	6.80316999	-3.72934739	0.82991477

C	-3.993767	-3.809506	-2.670601
C	-3.774733	-5.265985	-0.657689
C	-4.96889	-7.421654	-0.67113
C	-4.746648	-7.565737	0.669324
H	-5.55468	-8.154489	-1.220328
H	-5.176766	-8.39948	1.218596
C	-3.877616	-6.670941	1.357087
C	-3.591647	-6.876107	2.744541
C	-3.266515	-5.595402	0.65583
C	-2.664013	-6.119089	3.396482
H	-4.139034	-7.654441	3.270587
H	-2.470866	-6.265946	4.456197
C	-1.8482	-5.200004	2.669173
C	-2.102135	-4.974634	1.279907
C	-3.89263	-2.533235	-3.281046
C	-3.609144	-1.407115	-2.546045
C	-3.4336	-1.508787	-1.137271
C	-3.455515	-2.768058	-0.539377
H	-4.091585	-2.451508	-4.346971
H	-3.56328	-0.430384	-3.016928
H	-3.33173	-2.825322	0.533883
C	-1.117145	-4.283311	0.538045
C	0.023144	-3.748711	1.136112
C	0.187535	-3.867515	2.544897
C	-0.724639	-4.586325	3.279749
H	-1.219695	-4.194016	-0.535218
H	1.060173	-3.426465	3.015869
H	-0.569119	-4.73435	4.345748
C	-3.301482	-0.335591	-0.341969
C	-3.250924	0.67442	0.335599
C	1.039703	-3.148647	0.340706
C	1.939617	-2.689184	-0.337967
H	6.520942	-1.676178	-4.456776
C	6.516184	-1.4334	-3.397097
H	8.624961	-1.139036	-3.273136
C	7.673971	-1.125867	-2.746268
C	5.261544	-1.216796	-1.279426
C	7.67672	-0.773309	-1.358985
C	5.293887	-1.554864	-2.668733
C	6.447802	-0.637511	-0.656593
C	8.91182	-0.593585	-0.672606
C	8.926827	-0.328699	0.667758
H	9.838845	-0.734242	-1.222755
H	9.864505	-0.2838	1.215994
C	7.71809	-0.023454	1.356642
C	7.75433	0.327199	2.743949
C	6.480335	-0.032274	0.656713
C	6.635463	0.751643	3.3971
H	8.70271	0.242815	3.268917
H	6.667161	0.992351	4.456781
C	5.43076	0.998211	2.671105
C	5.361278	0.666005	1.281799
C	4.137151	-2.104621	-3.278239
C	3.020453	-2.42134	-2.54242
C	3.021887	-2.218381	-1.133693
C	4.124407	-1.60875	-0.536575
O	8.3049524	0.01212873	-1.67078573
O	5.90939973	1.01442558	0.29263933
O	5.26708189	-0.99887326	-2.09935587
Si	8.88697241	1.08852785	-2.82900963
Si	5.60807136	1.34774107	1.92148982
Si	4.35467054	-2.32527417	-2.60703672
C	7.48322469	2.17151221	-3.483185
H	6.69847291	1.56990707	-3.96116323
H	7.01483851	2.75345442	-2.67777597
H	7.85063173	2.8860023	-4.23207906
C	9.63271657	0.06738566	-4.2271028
H	10.0510446	0.71218198	-5.01154408
H	10.44092702	-0.57747603	-3.85937833
H	8.87809672	-0.57788458	-4.69523327
C	10.20524244	2.15363519	-2.00445582
H	9.78256313	2.74559653	-1.18228406
H	11.01213879	1.53600948	-1.59008249
H	10.6555152	2.85395932	-2.72054846
C	4.7117494	3.0053446	1.9611444
H	4.4726185	3.30524485	2.99012116
H	5.32463753	3.80031148	1.5173668
H	3.76913454	2.96013091	1.40077648
C	7.25086321	1.45659004	2.83917585
H	7.09973625	1.68327628	3.90298193
H	7.80658197	0.51237924	2.77427038
H	7.88716488	2.24594127	2.41850496
C	4.51587802	-0.00610812	2.64939667
H	3.57736672	-0.09837993	2.08737166
H	5.01516372	-0.98259678	2.62692822
H	4.25700483	0.21250418	3.69411364
C	4.57500098	-2.45732348	-4.47470128
H	3.97704855	-3.28086223	-4.8872299
H	4.26303333	-1.53423705	-4.97961735
H	5.62383309	-2.64427061	-4.73938748
C	2.55460846	-1.97357653	-2.17097298
H	2.2060796	-1.04312663	-2.63695806
H	1.89677427	-2.78388252	-2.51253142
H	2.4213204	-1.87313347	-1.08594094
C	4.934876	-3.9111433	-1.7688139
H	4.77792283	-3.87597057	-0.68415216
H	4.37532697	-4.77343169	-2.15639553
H	6.00024996	-4.09778631	-1.95210341

H	4.164787	-2.317459	-4.344257
H	2.150798	-2.869009	-3.012669
H	4.113218	-1.473072	0.536699
C	4.269318	1.17346	0.541137
C	3.236494	1.893026	1.140452
C	3.258198	2.09375	2.549358
C	4.337679	1.663388	3.283021
H	4.242492	1.040397	-0.532199
H	2.44005	2.628208	3.021405
H	4.388928	1.871634	4.34908
C	2.207849	2.473756	0.346122
C	1.359806	3.023876	-0.331899
H	-1.796084	6.492365	-4.45338
C	-2.006832	6.365321	-3.394458
H	-3.314728	8.045505	-3.271179
C	-2.852928	7.213962	-2.744457
C	-1.57347	5.166876	-1.277501
C	-3.16338	7.038041	-1.358261
C	-1.293195	5.365827	-2.66577
C	-2.669468	5.904239	-0.656418
C	-3.937403	8.017377	-0.672286
C	-4.178336	7.89561	0.667132
H	-4.27666	8.89185	-1.221844
H	-4.686941	8.684649	1.215366
C	-3.841643	6.694517	1.354776
C	-4.168229	6.548234	2.740672
C	-3.213824	5.627718	0.654866
C	-3.980296	5.365444	3.392059
H	-4.569954	7.411261	3.265989
H	-4.208402	5.270716	4.450758
C	-3.590442	4.199834	2.665039
C	-3.262431	4.308166	1.277174
C	-0.237784	4.639063	-3.273725
C	0.59233	3.828692	-2.536918
C	0.412379	3.726606	-1.128683
C	-0.667981	4.376279	-0.533376
H	-0.06443	4.770931	-4.339095
H	1.415733	3.299562	-3.005813
H	-0.782795	4.297372	0.539536
C	-3.153893	3.110002	0.534727
C	-3.264441	1.854745	1.131188
C	-3.455361	1.7707	2.539116
C	-3.624074	2.919479	3.274287
H	-3.020149	3.155313	-0.537862
H	-3.512442	0.794086	3.009033
H	-3.834428	2.857935	4.339379

O3$_{PPM}$					**TS1**$_{PPM}$ Imaginary frequency: 109.2009 cm^{-1}		
C	-2.329632	-3.179118	-1.995547		C	-3.435773	2.183112	-1.390591
H	1.162462	-7.656813	-4.54533		H	-7.604081	-1.120998	-4.654457
C	1.009372	-7.449701	-3.48922		C	-7.521424	-1.04291	-3.573399
H	1.62343	-9.386779	-2.837046		H	-9.480001	-1.795844	-3.185559

C	1.274366	-8.399278	-2.545296	C	-8.549387	-1.425002	-2.763166
C	0.225646	-5.906272	-1.724077	C	-6.21418	-0.336901	-1.593122
C	1.09857	-8.130038	-1.149078	C	-8.442027	-1.342667	-1.33734
C	0.398378	-6.213842	-3.110461	C	-6.365901	-0.414658	-3.014673
C	0.762914	-6.817357	-0.719172	C	-7.206132	-0.978008	-0.732967
C	1.216125	-9.180123	-0.19147	C	-9.590993	-1.579781	-0.528108
C	0.96724	-8.94098	1.132564	C	-9.527287	-1.412492	0.82698
H	1.440127	-10.183836	-0.5437	H	-10.53017	-1.82596	-1.016817
H	0.956577	-9.754836	1.853183	H	-10.420198	-1.489983	1.441988
C	0.805861	-7.605876	1.607026	C	-8.270726	-1.215789	1.469871
C	0.637055	-7.349664	3.006579	C	-8.211269	-1.120646	2.897521
C	0.858193	-6.520184	0.691061	C	-7.076276	-1.152886	0.698432
C	0.645673	-6.077344	3.500319	C	-7.017315	-1.083584	3.554913
H	0.504599	-8.199938	3.671046	H	-9.148454	-1.079417	3.447048
H	0.499561	-5.890865	4.561215	H	-6.978164	-0.990531	4.637183
C	0.979966	-4.979604	2.647444	C	-5.799982	-1.294787	2.837274
C	1.134453	-5.197971	1.242322	C	-5.819846	-1.383069	1.408316
C	-0.156537	-5.348326	-4.088678	C	-5.426588	0.235884	-3.855441
C	-0.978582	-4.303199	-3.735707	C	-4.43852	1.039935	-3.337704
C	-1.282273	-4.075329	-2.362931	C	-4.348317	1.228014	-1.929721
C	-0.640056	-4.83919	-1.386941	C	-5.206346	0.51858	-1.087886
H	0.024615	-5.567118	-5.138218	H	-5.53566	0.131709	-4.932152
H	-1.446165	-3.683742	-4.494822	H	-3.749228	1.565935	-3.990807
H	-0.885175	-4.657028	-0.348105	H	-5.127604	0.683172	-0.021015
C	1.749394	-4.177498	0.4798	C	-4.656445	-1.870422	0.765016
C	2.163389	-2.975041	1.055012	C	-3.502343	-2.20248	1.47794
C	1.868118	-2.721168	2.42457	C	-3.463669	-1.978613	2.883593
C	1.288512	-3.705699	3.191214	C	-4.589757	-1.537184	3.536034
H	1.987254	-4.357774	-0.560975	H	-4.670462	-2.051179	-0.302385
H	2.153991	-1.770648	2.863983	H	-2.55724	-2.208535	3.433927
H	1.119416	-3.539548	4.252241	H	-4.583647	-1.422762	4.617167
C	2.990344	-2.079857	0.312974	C	-2.405707	-2.848388	0.834498
C	3.585733	4.108032	0.287452	C	3.356264	-0.700681	-0.496361
C	-2.326966	2.222321	0.325531	C	1.799246	0.792069	-0.163141
H	-2.758404	-0.762176	5.823795	H	-0.480464	0.071849	5.625181
C	-3.506903	-0.698831	5.037871	C	-0.288245	0.997642	5.08881
H	-5.115729	-1.371698	6.268408	H	-0.330555	2.227699	6.832755
C	-4.804295	-1.046471	5.27878	C	-0.219023	2.189122	5.751909
C	-4.099742	-0.069056	2.7216	C	0.255661	2.145796	2.971334
C	-5.793138	-0.996433	4.243464	C	-0.026733	3.423173	5.049186
C	-3.135329	-0.138655	3.777147	C	0.003585	0.936476	3.691053
C	-5.412832	-0.679142	2.909733	C	0.024408	3.426831	3.628236
C	-7.164748	-1.224676	4.557632	C	0.127355	4.645345	5.766112
C	-8.12647	-1.096014	3.594018	C	0.337924	5.819782	5.096539
H	-7.434309	-1.437516	5.58905	H	0.125039	4.616416	6.852849
H	-9.181514	-1.171915	3.844884	H	0.540009	6.740605	5.637777
C	-7.760597	-0.936392	2.225602	C	0.206607	5.876995	3.67811
C	-8.775459	-0.863429	1.217468	C	0.327269	7.130881	2.996016
C	-6.387159	-0.87908	1.859238	C	-0.087268	4.694297	2.944512
C	-8.456675	-0.831293	-0.108625	C	0.066932	7.239883	1.661069
H	-9.813474	-0.826483	1.538605	H	0.632692	8.00046	3.572716
H	-9.231149	-0.745846	-0.866591	H	0.18147	8.191308	1.148006
C	-7.104042	-1.029123	-0.525177	C	-0.465435	6.127564	0.937854
C	-6.066601	-1.122523	0.455467	C	-0.597214	4.85949	1.586533
C	-1.853899	0.442351	3.58884	C	0.137491	-0.305371	3.018952
C	-1.549369	1.160663	2.455113	C	0.630208	-0.379871	1.736623

C	-2.544597	1.355884	1.452941	C	1.094362	0.801913	1.088931
C	-3.784437	0.727529	1.597767	C	0.875032	2.039926	1.704664
H	-1.118764	0.342727	4.384	H	-0.125182	-1.215799	3.551673
H	-0.57103	1.61524	2.331495	H	0.721814	-1.336816	1.238841
H	-4.530345	0.898811	0.832516	H	1.221103	2.93363	1.19986
C	-4.806476	-1.608344	0.03342	C	-1.35901	3.864503	0.931924
C	-4.536897	-1.901399	-1.303927	C	-1.884977	4.052676	-0.345595
C	-5.540283	-1.658085	-2.285867	C	-1.640772	5.279703	-1.024536
C	-6.791773	-1.244163	-1.893103	C	-0.958965	6.289027	-0.383373
H	-4.036714	-1.810284	0.767091	H	-1.581642	2.935694	1.438925
H	-5.32336	-1.858217	-3.33054	H	-2.03643	5.42506	-2.024861
H	-7.582394	-1.12691	-2.630192	H	-0.825782	7.250844	-0.872403
C	-3.315244	-2.536858	-1.675637	C	-2.703509	3.041274	-0.930758
C	3.809187	-1.408446	-0.290787	C	-1.490238	-3.479391	0.334473
H	8.604343	0.17725	-3.936353	H	1.6657	-7.855171	-2.779906
C	8.466445	0.411162	-2.88379	C	1.961489	-7.366704	-1.855042
H	10.51992	0.872255	-2.529765	H	3.423572	-8.830244	-1.332373
C	9.518972	0.805416	-2.110694	C	2.937101	-7.896022	-1.063582
C	6.974439	0.510903	-0.912936	C	1.614443	-5.542351	-0.21592
C	9.342525	1.141915	-0.729523	C	3.349964	-7.244144	0.142504
C	7.188548	0.177627	-2.287946	C	1.224369	-6.226022	-1.412299
C	8.036314	1.181851	-0.167736	C	2.829099	-5.962695	0.47967
C	10.479034	1.398098	0.092108	C	4.253865	-7.904719	1.024306
C	10.325662	1.645511	1.428221	C	4.596961	-7.331819	2.216421
H	11.468762	1.328217	-0.351932	H	4.608951	-8.89695	0.758076
H	11.190066	1.745784	2.079662	H	5.206236	-7.867853	2.939563
C	9.028147	1.864459	1.976554	C	4.237111	-5.981441	2.495302
C	8.884439	2.214061	3.358473	C	4.690772	-5.367095	3.706597
C	7.880323	1.779374	1.140797	C	3.473402	-5.234566	1.553774
C	7.676161	2.580014	3.874848	C	4.513118	-4.035303	3.933857
H	9.76963	2.182889	3.989016	H	5.190158	-5.993711	4.441371
H	7.571719	2.82612	4.928561	H	4.847386	-3.576533	4.860775
C	6.552701	2.763281	3.009862	C	3.995338	-3.197461	2.897902
C	6.658413	2.412447	1.627012	C	3.509161	-3.779363	1.683831
C	6.167175	-0.49158	-3.010816	C	0.038002	-5.837069	-2.085657
C	5.027819	-0.944075	-2.387736	C	-0.812511	-4.898907	-1.552032
C	4.861967	-0.744244	-0.987258	C	-0.510654	-4.305756	-0.292259
C	5.808964	0.006042	-0.288589	C	0.701095	-4.608867	0.332699
H	6.328187	-0.696827	-4.066283	H	-0.218834	-6.33916	-3.014989
H	4.275742	-1.499783	-2.939177	H	-1.739629	-4.638993	-2.052599
H	5.672362	0.139794	0.77688	H	0.912745	-4.158898	1.294822
C	5.636114	2.85837	0.756433	C	3.257718	-2.904727	0.595277
C	4.522447	3.557774	1.218432	C	3.417174	-1.525655	0.706711
C	4.373137	3.780655	2.615718	C	3.779926	-0.960635	1.957083
C	5.371717	3.393315	3.479848	C	4.067541	-1.786908	3.018636
H	5.738015	2.706504	-0.310268	H	2.987162	-3.316778	-0.368561
H	3.491354	4.297618	2.981856	H	3.874987	0.11532	2.053365
H	5.290054	3.615991	4.541006	H	4.408212	-1.363425	3.960103
C	1.978813	5.27289	-1.506116	C	4.976546	-1.0206	-2.549425
H	1.7613	6.309352	-1.219269	H	5.677813	-0.218914	-2.808152
H	2.458777	5.292534	-2.492284	H	5.537507	-1.85241	-2.105434
Mo	-2.233754	3.315352	-1.041418	Mo	2.631367	1.169623	-1.708905
C	2.842211	4.627279	-0.521215	C	3.929886	-0.52489	-1.6266
H	1.023034	4.746639	-1.610954	H	4.518241	-1.368434	-3.483536
O	-4.021048	3.200888	-1.750244	O	1.919367	2.798043	-2.48826
O	-1.865352	5.053682	-0.323424	O	4.226033	2.205559	-1.162276

O	-0.889742	2.651583	-2.235028	O	1.70354	0.135481	-3.09954
Si	-4.859614	3.92428	-3.023558	Si	2.19251	3.918174	-3.69932
Si	-1.821351	5.899579	1.143241	Si	5.410008	2.818727	-0.178699
Si	-0.009673	1.277998	-2.695711	Si	0.493768	-0.825115	-3.710088
C	-3.500239	5.747851	1.985735	C	6.359129	4.145176	-1.137014
H	-3.519991	6.297563	2.93636	H	7.141948	4.60052	-0.514956
H	-4.300563	6.151631	1.352062	H	6.848517	3.724814	-2.025439
H	-3.742535	4.699668	2.201141	H	5.695217	4.951374	-1.474022
C	-1.467358	7.697502	0.699948	C	6.62844	1.457675	0.320153
H	-0.499424	7.804895	0.194358	H	6.140521	0.648335	0.87656
H	-2.238766	8.102438	0.032409	H	7.109989	1.011649	-0.559838
H	-1.443257	8.327046	1.599454	H	7.425491	1.863433	0.95861
C	-0.455219	5.20444	2.238294	C	4.655472	3.593974	1.37222
H	-0.668203	4.169231	2.530846	H	3.936569	4.380787	1.10987
H	0.514632	5.214665	1.724988	H	4.12547	2.852769	1.983503
H	-0.353174	5.796215	3.158074	H	5.43022	4.050483	2.003654
C	-0.944621	0.479763	-4.126259	C	-0.158192	-0.048723	-5.307531
H	-1.067901	1.177863	-4.964446	H	0.648405	0.125033	-6.031733
H	-0.410135	-0.40271	-4.502775	H	-0.898623	-0.703649	-5.787484
H	-1.942979	0.151418	-3.810461	H	-0.646486	0.913928	-5.111542
C	0.161444	0.07557	-1.261512	C	-0.915789	-0.969089	-2.469615
H	-0.811267	-0.302034	-0.926988	H	-1.311259	0.024275	-2.224008
H	0.765941	-0.789057	-1.563667	H	-1.746911	-1.570042	-2.861951
H	0.660396	0.541287	-0.403085	H	-0.585164	-1.427839	-1.531688
C	1.684038	1.872831	-3.27118	C	1.220069	-2.523447	-4.122422
H	2.260226	1.040281	-3.696666	H	0.453694	-3.200554	-4.522558
H	1.599195	2.646476	-4.044923	H	2.009523	-2.436837	-4.881123
H	2.270505	2.284078	-2.440769	H	1.657596	-3.004697	-3.239404
C	-5.334658	2.564073	-4.237381	C	0.669524	3.998227	-4.812894
H	-5.93489	2.96222	-5.066461	H	0.772077	4.793592	-5.563864
H	-4.445117	2.087432	-4.668871	H	0.515123	3.053272	-5.347645
H	-5.922946	1.781792	-3.741987	H	-0.23777	4.203486	-4.231112
C	-3.771627	5.213386	-3.875351	C	3.701031	3.424895	-4.72805
H	-4.30554	5.692095	-4.707315	H	3.882919	4.141465	-5.540661
H	-3.465446	6.006933	-3.180851	H	4.60648	3.386856	-4.109401
H	-2.860318	4.760401	-4.288736	H	3.563323	2.435904	-5.185673
C	-6.394255	4.73595	-2.291621	C	2.479949	5.607155	-2.905668
H	-6.126774	5.51005	-1.560907	H	3.362729	5.59855	-2.254354
H	-7.003192	5.211281	-3.072229	H	2.634695	6.383089	-3.667818
H	-7.024297	3.997994	-1.779105	H	1.619628	5.905153	-2.293409

IM$_{PPM}$				**2**$_{PPM}$ + [Mo] pair			
C	-3.363393	2.002178	-1.900292	C	-4.548635	-1.565391	2.467277
H	-8.189354	-0.996971	-4.486466	H	-10.773427	-2.00129	2.504971
C	-8.023321	-0.800248	-3.430365	C	-10.11363	-2.190998	1.662276
H	-10.030608	-1.227767	-2.847071	H	-11.60541	-3.134625	0.46459
C	-9.033355	-0.938159	-2.525216	C	-10.572795	-2.802188	0.534818
C	-6.50357	-0.043826	-1.628006	C	-7.834077	-2.110097	0.693212
C	-8.817788	-0.704484	-1.128834	C	-9.721298	-3.011367	-0.596878
C	-6.759324	-0.27828	-3.017264	C	-8.725617	-1.883308	1.79161
C	-7.507906	-0.434586	-0.640291	C	-8.386104	-2.511477	-0.602674
C	-9.929642	-0.702637	-0.237423	C	-10.22286	-3.745513	-1.709551
C	-9.754857	-0.401829	1.083964	C	-9.424453	-3.995887	-2.788013
H	-10.92238	-0.880021	-0.643064	H	-11.232891	-4.143625	-1.656873
H	-10.606646	-0.302814	1.751972	H	-9.76856	-4.624989	-3.604912

C	-8.443224	-0.295546	1.630661	C	-8.153182	-3.364099	-2.90319
C	-8.280465	-0.061425	3.0341	C	-7.384631	-3.571698	-4.093136
C	-7.303289	-0.460607	0.793937	C	-7.674742	-2.506599	-1.869732
C	-7.050251	-0.098476	3.620517	C	-6.225559	-2.891697	-4.317087
H	-9.169559	0.148352	3.623619	H	-7.754418	-4.291765	-4.818819
H	-6.931145	0.101136	4.68237	H	-5.636527	-3.069832	-5.213141
C	-5.911505	-0.517235	2.866483	C	-5.816082	-1.862232	-3.416869
C	-6.034833	-0.751824	1.459278	C	-6.562076	-1.621693	-2.217181
C	-5.795747	0.112073	-3.982484	C	-8.210532	-1.433507	3.034396
C	-4.664942	0.80768	-3.625935	C	-6.860309	-1.288545	3.239047
C	-4.451088	1.154219	-2.261757	C	-5.947969	-1.634381	2.201015
C	-5.352892	0.709223	-1.293918	C	-6.444632	-2.042028	0.962039
H	-5.992436	-0.108245	-5.02887	H	-8.910092	-1.231893	3.841809
H	-3.951394	1.131714	-4.376637	H	-6.474267	-0.952537	4.196346
H	-5.180252	0.997783	-0.2654	H	-5.735017	-2.319948	0.193998
C	-4.964547	-1.412343	0.811438	C	-6.240644	-0.457453	-1.482599
C	-3.791742	-1.759748	1.484128	C	-5.157283	0.356714	-1.81234
C	-3.643952	-1.40791	2.855145	C	-4.373037	0.049001	-2.958641
C	-4.686092	-0.806921	3.519905	C	-4.716882	-1.026068	-3.742982
H	-5.062822	-1.703986	-0.226001	H	-6.841758	-0.17457	-0.63032
H	-2.722628	-1.655962	3.37169	H	-3.520507	0.673828	-3.205188
H	-4.601	-0.586067	4.581011	H	-4.153064	-1.24538	-4.646403
C	-2.783032	-2.519024	0.823759	C	-4.800072	1.445477	-0.966316
C	2.757883	-0.862213	0.213358	C	-0.207542	1.443253	-1.535806
C	1.973176	0.327519	0.416444	C	-0.140962	0.249298	-1.300913
H	-1.035277	1.606519	5.768646	H	0.903849	-5.86701	-1.866955
C	-0.693398	2.303673	5.007782	C	1.069344	-5.250127	-0.98739
H	-0.787088	4.018632	6.276322	H	2.354664	-6.651726	-0.018671
C	-0.569342	3.635116	5.282516	C	1.857615	-5.686429	0.036435
C	0.175319	2.690505	2.725463	C	0.727376	-3.098293	0.186337
C	-0.165787	4.567746	4.273235	C	2.053596	-4.893252	1.212542
C	-0.260187	1.790275	3.747467	C	0.550389	-3.91889	-0.972452
C	0.024737	4.126871	2.934082	C	1.334871	-3.676841	1.38134
C	0.070684	5.932037	4.612076	C	2.996418	-5.307259	2.19799
C	0.503785	6.816339	3.662889	C	3.239318	-4.525825	3.293249
H	-0.044448	6.238974	5.648563	H	3.558395	-6.222282	2.029196
H	0.772899	7.83486	3.930954	H	4.021573	-4.785506	4.001882
C	0.52364	6.444984	2.286634	C	2.408127	-3.402503	3.575222
C	0.880717	7.409376	1.289889	C	2.613736	-2.652215	4.777527
C	0.142694	5.129797	1.90024	C	1.349841	-3.056796	2.688532
C	0.75934	7.131518	-0.040341	C	1.746189	-1.670102	5.155908
H	1.249597	8.376699	1.621906	H	3.48219	-2.890072	5.386788
H	1.048935	7.8627	-0.790758	H	1.916611	-1.092829	6.061027
C	0.137971	5.916816	-0.466428	C	0.533128	-1.467096	4.428583
C	-0.222649	4.926577	0.501552	C	0.298077	-2.191104	3.21614
C	-0.160181	0.393365	3.520827	C	-0.037712	-3.363282	-2.137832
C	0.480857	-0.11305	2.414894	C	-0.322838	-2.021161	-2.222882
C	1.10116	0.771438	1.48213	C	-0.0187	-1.161443	-1.12788
C	0.887164	2.14663	1.630627	C	0.463218	-1.712689	0.059291
H	-0.564587	-0.28334	4.2697	H	-0.212659	-4.013308	-2.991596
H	0.544941	-1.184345	2.271365	H	-0.740955	-1.597844	-3.130752
H	1.337951	2.814254	0.906255	H	0.694332	-1.045806	0.880131
C	-1.075761	3.878632	0.082269	C	-1.012119	-2.163508	2.679278
C	-1.497086	3.753466	-1.241817	C	-2.032168	-1.408969	3.259344
C	-1.013224	4.671548	-2.217235	C	-1.740403	-0.595682	4.391867
C	-0.223682	5.727778	-1.826067	C	-0.487832	-0.635129	4.955603

H	-1.464696	3.178169	0.809555	H	-1.256328	-2.784161	1.827005
H	-1.31702	4.557926	-3.253141	H	-2.525429	0.017998	4.822402
H	0.092618	6.469998	-2.554812	H	-0.275316	-0.05927	5.852974
C	-2.471313	2.775678	-1.599661	C	-3.375706	-1.489867	2.788324
C	-1.951199	-3.222757	0.278393	C	-4.418823	2.313111	-0.201845
H	0.854862	-7.525011	-3.255791	H	-2.552459	5.845691	4.607404
C	1.146204	-7.203901	-2.259117	C	-2.283029	5.966032	3.561218
H	2.429948	-8.868915	-1.895203	H	-1.323203	7.851238	3.831488
C	2.022243	-7.935825	-1.514531	C	-1.596356	7.062468	3.135111
C	0.892301	-5.598111	-0.390063	C	-2.382465	5.12042	1.234506
C	2.434274	-7.502358	-0.213625	C	-1.212131	7.215311	1.764504
C	0.506108	-6.061517	-1.68934	C	-2.740599	4.998483	2.616905
C	2.018651	-6.236151	0.289041	C	-1.45619	6.175652	0.819714
C	3.233652	-8.367129	0.588231	C	-0.618229	8.442669	1.353503
C	3.583254	-8.003691	1.857341	C	-0.323105	8.658564	0.038646
H	3.504772	-9.341882	0.191068	H	-0.467905	9.222181	2.095983
H	4.11293	-8.691841	2.510898	H	0.039909	9.624783	-0.30209
C	3.338493	-6.678131	2.318326	C	-0.421483	7.596883	-0.905413
C	3.810141	-6.29391	3.614255	C	-0.0659	7.851127	-2.268613
C	2.676958	-5.734293	1.480574	C	-0.847829	6.299423	-0.494847
C	3.750166	-4.999848	4.034838	C	-0.054044	6.852262	-3.194461
H	4.228187	-7.066384	4.254851	H	0.181993	8.871738	-2.549139
H	4.09937	-4.715139	5.0239	H	0.179	7.05601	-4.236413
C	3.330518	-3.976225	3.13072	C	-0.251004	5.498935	-2.785371
C	2.826408	-4.324216	1.837034	C	-0.570196	5.199114	-1.421061
C	-0.585162	-5.448301	-2.35707	C	-3.61019	3.956677	3.031289
C	-1.351534	-4.487361	-1.742591	C	-4.161256	3.078468	2.129376
C	-1.060537	-4.102613	-0.402245	C	-3.887922	3.238065	0.742408
C	0.055375	-4.644359	0.237977	C	-3.039486	4.262347	0.322783
H	-0.838031	-5.789095	-3.357976	H	-3.846473	3.872787	4.089215
H	-2.204882	-4.047508	-2.248548	H	-4.809254	2.271348	2.455947
H	0.250035	-4.353136	1.262357	H	-2.885281	4.384954	-0.739531
C	2.657724	-3.26989	0.901415	C	-0.491943	3.841873	-1.021349
C	2.878694	-1.942294	1.24062	C	-0.263031	2.811991	-1.934619
C	3.278752	-1.607831	2.559028	C	-0.077385	3.128239	-3.311281
C	3.507353	-2.611957	3.471527	C	-0.050814	4.441974	-3.709936
H	2.368946	-3.50441	-0.11402	H	-0.610329	3.58132	0.021982
H	3.441339	-0.570479	2.829254	H	0.080582	2.325455	-4.024593
H	3.870052	-2.368678	4.466981	H	0.152947	4.69383	-4.747718
C	4.542668	-2.056371	-1.359689	C	7.920538	1.678674	-1.668007
H	5.321054	-1.662014	-2.021462	H	8.837097	1.273105	-2.118358
H	5.025505	-2.509293	-0.485754	H	7.412643	2.283686	-2.432116
Mo	2.891017	0.773832	-1.24477	Mo	6.006875	-0.676602	-0.580683
C	3.606067	-0.967902	-0.982963	C	7.043604	0.596508	-1.168697
H	4.024882	-2.857088	-1.904602	H	8.221289	2.355169	-0.855539
O	3.069243	2.199411	-2.521007	O	7.187756	-2.053498	0.056548
O	4.405355	1.744321	-0.306624	O	4.943309	-1.214396	-2.088053
O	1.365557	0.205055	-2.388062	O	4.95747	0.122514	0.813489
Si	4.021089	3.455914	-3.089834	Si	8.776291	-2.533184	0.340188
Si	5.594038	1.84663	0.830442	Si	4.735738	-0.847938	-3.723549
Si	0.890377	-0.478164	-3.820241	Si	4.819641	1.609923	1.606296
C	6.904941	3.119548	0.326382	C	3.929758	0.849248	-3.871585
H	7.680871	3.187263	1.101838	H	3.781489	1.134082	-4.921856
H	7.404487	2.845124	-0.61134	H	2.949281	0.862999	-3.379049
H	6.484179	4.123982	0.196461	H	4.547514	1.623189	-3.398722
C	6.493319	0.191469	1.061819	C	6.407043	-0.876448	-4.600216

H	5.830349	-0.602353	1.425606	H	6.291583	-0.686866	-5.676055
H	6.942896	-0.152381	0.120925	H	7.08792	-0.116021	-4.199087
H	7.307767	0.29681	1.792297	H	6.893619	-1.854181	-4.487089
C	4.869032	2.397183	2.493496	C	3.614687	-2.185028	-4.434731
H	4.371757	3.371455	2.398481	H	4.075903	-3.17702	-4.345621
H	4.124935	1.689464	2.879146	H	2.652588	-2.217348	-3.908958
H	5.654433	2.499416	3.255245	H	3.409981	-2.007348	-5.499111
C	1.251582	0.673671	-5.278214	C	10.001778	-1.382164	-0.515118
H	2.329595	0.800298	-5.435756	H	9.834845	-1.351475	-1.599093
H	0.826345	0.269344	-6.207569	H	9.932981	-0.356947	-0.132021
H	0.818844	1.668476	-5.117733	H	11.030886	-1.728976	-0.348807
C	-0.969743	-0.790745	-3.73788	C	9.051464	-2.513924	2.205753
H	-1.509756	0.150947	-3.582385	H	10.059271	-2.864155	2.465861
H	-1.345923	-1.247285	-4.663629	H	8.935764	-1.501515	2.614217
H	-1.229442	-1.455883	-2.905211	H	8.330223	-3.163192	2.718284
C	1.797958	-2.115739	-4.12011	C	8.948767	-4.284167	-0.338613
H	1.46788	-2.582127	-5.058871	H	8.225882	-4.964125	0.129799
H	2.882742	-1.9641	-4.193479	H	8.773352	-4.308566	-1.421985
H	1.610626	-2.835325	-3.313311	H	9.953617	-4.687679	-0.155486
C	3.194336	4.08848	-4.667562	C	4.432853	2.964505	0.353492
H	3.734729	4.96	-5.062834	H	3.496884	2.752818	-0.179051
H	3.174051	3.326017	-5.455361	H	4.320325	3.939134	0.847297
H	2.159404	4.39877	-4.476284	H	5.22957	3.058479	-0.394556
C	5.74797	2.82026	-3.516887	C	6.439178	1.971307	2.505882
H	6.388205	3.628933	-3.894748	H	7.280514	2.031034	1.80386
H	6.240346	2.383505	-2.641302	H	6.390974	2.923092	3.051741
H	5.698149	2.047638	-4.296077	H	6.668711	1.182252	3.233939
C	4.09138	4.866194	-1.840952	C	3.409782	1.434759	2.842125
H	4.447475	4.515478	-0.867922	H	3.604087	0.625573	3.556874
H	4.760897	5.666765	-2.184205	H	3.26821	2.361379	3.414503
H	3.095971	5.303465	-1.694097	H	2.462895	1.209174	2.335984

O3$_{PPP}$					**TS1**$_{PPP}$ Imaginary frequency: 115.5362 cm^{-1}		
H	4.798776	5.156577	-3.81664	H	-0.221405	3.913769	-6.996126
C	5.314452	4.927352	-2.887635	C	-0.482205	4.166602	-5.971749
H	6.643793	6.592421	-2.999184	H	-1.629992	5.890755	-6.487366
C	6.322188	5.723497	-2.430485	C	-1.266509	5.245344	-5.691687
C	5.642446	3.402873	-0.965011	C	-0.221415	3.731129	-3.546171
C	6.986365	5.447097	-1.192129	C	-1.647263	5.555909	-4.34651
C	4.997689	3.713061	-2.205357	C	0.129195	3.44046	-4.904061
C	6.535125	4.387483	-0.354871	C	-1.306163	4.673594	-3.281818
C	8.125764	6.218556	-0.821929	C	-2.349429	6.765443	-4.077833
C	8.817522	5.925411	0.319233	C	-2.708247	7.081811	-2.79873
H	8.46603	7.000037	-1.496441	H	-2.545496	7.447661	-4.900855
H	9.740257	6.445916	0.562606	H	-3.171928	8.0372	-2.567462
C	8.296706	4.98702	1.256495	C	-2.597987	6.109111	-1.762978
C	8.997222	4.755937	2.484363	C	-3.178022	6.398786	-0.486151
C	7.069986	4.314514	0.991101	C	-2.007837	4.83798	-2.021564
C	8.467733	3.971848	3.465623	C	-3.357756	5.42138	0.44377
H	9.969699	5.2246	2.6133	H	-3.514933	7.414971	-0.296954
H	9.015235	3.781806	4.385295	H	-3.827066	5.636159	1.400158
C	7.132747	3.477078	3.343828	C	-3.041308	4.065942	0.121096

C	6.401767	3.69122	2.131754	C	-2.335988	3.756001	-1.087777
C	4.124983	2.764375	-2.79866	C	1.18357	2.532595	-5.174765
C	3.957051	1.509702	-2.262372	C	1.985946	2.055362	-4.1664
C	4.683626	1.140602	-1.095569	C	1.762081	2.475145	-2.823106
C	5.49529	2.086705	-0.467382	C	0.6379	3.2484	-2.526031
H	3.616728	3.034848	-3.720826	H	1.399534	2.27972	-6.20987
H	3.307753	0.782152	-2.738993	H	2.835062	1.41651	-4.386895
H	6.053493	1.778599	0.406636	H	0.467845	3.549367	-1.498294
C	5.014273	3.415193	2.151177	C	-2.175755	2.38444	-1.403703
C	4.381108	2.861271	3.262774	C	-2.709385	1.363659	-0.611512
C	5.151336	2.546867	4.416319	C	-3.414752	1.698625	0.56834
C	6.490117	2.861916	4.448708	C	-3.541809	3.019602	0.93328
H	4.40618	3.664947	1.292111	H	-1.674254	2.10237	-2.318394
H	4.665586	2.09451	5.275481	H	-3.884766	0.921866	1.157358
H	7.072127	2.676396	5.348201	H	-4.090288	3.282307	1.834136
C	4.624275	-0.194538	-0.600822	C	2.788112	2.210393	-1.862705
C	4.614148	-1.345707	-0.202715	C	3.803364	2.048039	-1.207341
C	2.968664	2.639665	3.245754	C	-2.640141	0.012129	-1.161715
C	-4.54002	0.896865	-0.855918	C	-2.316036	-1.501983	0.397886
H	-8.376853	-3.989366	-0.298686	H	-4.072963	-2.89539	6.195011
C	-7.735905	-3.57376	0.474671	C	-3.733513	-1.917676	5.862992
H	-8.763665	-4.513525	2.092246	H	-4.493991	-0.864981	7.55693
C	-7.940549	-3.871159	1.789453	C	-3.954179	-0.803643	6.615368
C	-5.870254	-2.067686	1.098238	C	-2.664074	-0.534208	4.100322
C	-7.081634	-3.350548	2.809681	C	-3.488919	0.479372	6.187542
C	-6.750083	-2.608759	0.105884	C	-3.158882	-1.795239	4.563377
C	-5.924084	-2.598773	2.459383	C	-2.678726	0.607044	5.02069
C	-7.413082	-3.559354	4.179885	C	-3.882714	1.633819	6.924661
C	-6.641525	-3.016087	5.167873	C	-3.517185	2.880376	6.505307
H	-8.322376	-4.105567	4.417425	H	-4.529147	1.501165	7.788389
H	-6.935836	-3.090181	6.211594	H	-3.887749	3.771144	7.005965
C	-5.385071	-2.421608	4.853438	C	-2.566255	3.031658	5.455697
C	-4.541994	-1.957124	5.913494	C	-2.119808	4.345381	5.102424
C	-4.950197	-2.338111	3.500136	C	-2.029172	1.886047	4.800521
C	-3.26654	-1.540845	5.673289	C	-1.09852	4.532793	4.219257
H	-4.945207	-1.95463	6.923134	H	-2.614872	5.194563	5.567133
H	-2.635097	-1.179824	6.481044	H	-0.773359	5.532705	3.94352
C	-2.700849	-1.688489	4.369858	C	-0.367812	3.410348	3.725063
C	-3.521666	-2.121732	3.279372	C	-0.795772	2.081566	4.045117
C	-6.711435	-2.096171	-1.216548	C	-3.17943	-2.904133	3.679712
C	-5.937397	-1.007584	-1.538427	C	-2.871259	-2.765141	2.351976
C	-5.16001	-0.36099	-0.529542	C	-2.484843	-1.486229	1.831318
C	-5.111572	-0.922638	0.750112	C	-2.333065	-0.420384	2.721767
H	-7.353224	-2.550559	-1.967662	H	-3.514137	-3.866127	4.060265
H	-5.94838	-0.594707	-2.542761	H	-2.949128	-3.609192	1.675156
H	-4.517318	-0.42641	1.506654	H	-2.004947	0.533172	2.338028
C	-2.869117	-2.491466	2.078816	C	0.080193	1.018964	3.725547
C	-1.486367	-2.387942	1.924511	C	1.272048	1.22634	3.034616
C	-0.701442	-1.855041	2.985873	C	1.635429	2.546308	2.643709
C	-1.305654	-1.518832	4.174747	C	0.831756	3.604165	2.994017
H	-3.441592	-2.922547	1.268081	H	-0.15829	0.011245	4.037634
H	0.37218	-1.758508	2.858315	H	2.55646	2.703469	2.092624
H	-0.705757	-1.165295	5.009763	H	1.123474	4.619763	2.738238
C	-0.850359	-2.870982	0.742045	C	2.123457	0.135361	2.701341
C	-0.284785	-3.323215	-0.236988	C	2.871287	-0.756593	2.345045
H	1.454105	-5.917107	-5.649334	H	6.243372	-5.463898	-0.038391

C	1.933036	-6.026837	-4.679785	C	6.567211	-4.443557	0.150288
H	3.11601	-7.708318	-5.248983	H	8.624251	-4.823761	-0.264196
C	2.856493	-7.005286	-4.461424	C	7.875284	-4.087014	0.015293
C	2.136899	-5.300816	-2.321111	C	6.010563	-2.138118	0.861308
C	3.507159	-7.145117	-3.193404	C	8.310421	-2.741917	0.243775
C	1.494797	-5.203528	-3.597559	C	5.613949	-3.495963	0.631219
C	3.291309	-6.18435	-2.164988	C	7.366659	-1.709639	0.518293
C	4.336952	-8.278484	-2.953976	C	9.707013	-2.463181	0.243438
C	4.894149	-8.477847	-1.722544	C	10.160312	-1.218333	0.572639
H	4.459806	-9.010352	-3.748108	H	10.400093	-3.277055	0.046932
H	5.446236	-9.387259	-1.4995	H	11.223834	-1.019143	0.676565
C	4.830194	-7.458062	-0.729419	C	9.247539	-0.136115	0.728062
C	5.483037	-7.658399	0.529339	C	9.759261	1.160031	1.057063
C	4.15313	-6.235231	-1.000773	C	7.84808	-0.338706	0.546514
C	5.563805	-6.65813	1.451979	C	8.938711	2.244135	1.138434
H	5.914073	-8.63579	0.731451	H	10.8233	1.251719	1.260179
H	6.040421	-6.822829	2.414925	H	9.322913	3.217965	1.430625
C	5.126894	-5.34015	1.116636	C	7.573789	2.13625	0.73288
C	4.468465	-5.102454	-0.13249	C	7.035883	0.864918	0.35072
C	0.357447	-4.369351	-3.749292	C	4.294459	-3.908602	0.952505
C	-0.206633	-3.722822	-2.674811	C	3.384182	-3.043599	1.515002
C	0.355668	-3.89061	-1.378552	C	3.783489	-1.712802	1.815456
C	1.513006	-4.65507	-1.227346	C	5.08298	-1.302042	1.519378
H	-0.095968	-4.28689	-4.734053	H	4.014071	-4.940176	0.754413
H	-1.09753	-3.114742	-2.795111	H	2.372686	-3.365718	1.742196
H	1.907748	-4.78837	-0.228956	H	5.36804	-0.301218	1.807546
C	4.302279	-3.756195	-0.536705	C	5.782519	0.864304	-0.313155
C	4.686919	-2.686876	0.273624	C	5.029235	2.028149	-0.472831
C	5.221946	-2.948119	1.567249	C	5.52337	3.257319	0.051538
C	5.437853	-4.245895	1.964581	C	6.773329	3.301517	0.619167
H	3.911622	-3.536296	-1.521941	H	5.394816	-0.057826	-0.727201
H	5.493202	-2.115681	2.208924	H	4.925829	4.157642	-0.051765
H	5.900725	-4.451495	2.926622	H	7.186127	4.248503	0.957741
C	0.321357	2.278755	3.16647	C	-2.950976	-0.231216	-3.754374
H	-0.192312	2.920918	3.893239	H	-3.615641	-0.975615	-4.20668
H	-0.068433	2.519786	2.169769	H	-3.400045	0.763055	-3.870812
Mo	-4.087076	2.488817	-1.439815	Mo	-2.372804	-2.303249	-1.212197
C	1.766891	2.470273	3.218333	C	-2.69973	-0.538779	-2.3249
H	0.045786	1.239955	3.385992	H	-2.009234	-0.249412	-4.315155
O	-5.638481	2.896881	-2.510267	O	-2.214505	-4.224039	-0.978019
O	-3.930165	3.66417	0.061084	O	-4.316691	-2.613346	-1.462006
O	-2.463978	2.310579	-2.440335	O	-0.501459	-2.232678	-1.826752
Si	-6.111139	4.189658	-3.491205	Si	-2.770653	-5.775704	-1.249407
Si	-4.235912	3.95738	1.696593	Si	-5.929507	-2.267245	-1.286512
Si	-1.284864	1.206381	-2.947569	Si	0.725245	-2.622816	-2.876247
C	-4.806877	5.554705	-3.435974	C	-3.359878	-5.964631	-3.034805
H	-5.102203	6.409265	-4.059527	H	-3.714106	-6.986053	-3.22938
H	-4.659639	5.928945	-2.414139	H	-4.185595	-5.277614	-3.257067
H	-3.835429	5.199462	-3.805326	H	-2.550272	-5.756681	-3.746943
C	-7.759598	4.81691	-2.830394	C	-4.181848	-6.158709	-0.052188
H	-8.511705	4.017887	-2.822939	H	-3.830729	-6.162217	0.988004
H	-7.661502	5.191454	-1.803443	H	-4.989523	-5.42217	-0.12989
H	-8.149275	5.636799	-3.448343	H	-4.610876	-7.149231	-0.256696
C	-6.298978	3.527652	-5.245509	C	-1.357278	-6.982604	-0.911682
H	-5.34741	3.136438	-5.628173	H	-0.535159	-6.865703	-1.627225
H	-7.034972	2.714711	-5.286498	H	-0.945569	-6.835741	0.095334

H	-6.634276	4.316013	-5.932556	H	-1.709662	-8.021289	-0.976593
C	-4.027398	2.383247	2.709488	C	-6.428561	-2.288829	0.537855
H	-4.827206	1.66371	2.499705	H	-6.202283	-3.254355	1.007203
H	-3.068702	1.890959	2.503922	H	-5.905929	-1.512731	1.110426
H	-4.060759	2.609615	3.783845	H	-7.507098	-2.110993	0.649977
C	-2.99747	5.271131	2.23717	C	-6.357118	-0.573082	-2.017569
H	-3.102874	6.185916	1.640054	H	-6.112651	-0.518534	-3.085985
H	-3.144218	5.543131	3.290945	H	-7.434707	-0.380382	-1.919946
H	-1.964061	4.919473	2.125447	H	-5.831608	0.2456	-1.511558
C	-5.999238	4.606404	1.847657	C	-6.926375	-3.5768	-2.220536
H	-6.249081	4.836834	2.891959	H	-8.003907	-3.374588	-2.148116
H	-6.1383	5.524511	1.262465	H	-6.666897	-3.591377	-3.287336
H	-6.725948	3.86655	1.487883	H	-6.754027	-4.584828	-1.823004
C	-0.135581	2.163754	-4.095008	C	0.338525	-2.005111	-4.625006
H	0.652583	1.511841	-4.495183	H	1.125508	-2.319432	-5.324692
H	-0.681453	2.586032	-4.948527	H	-0.610898	-2.411136	-4.998364
H	0.353136	2.992346	-3.566959	H	0.281192	-0.910496	-4.669094
C	-0.35621	0.585508	-1.434261	C	2.325761	-1.831385	-2.270861
H	-1.034037	0.088835	-0.729543	H	2.638973	-2.262987	-1.312567
H	0.424819	-0.136239	-1.705825	H	3.141779	-1.989851	-2.9895
H	0.130176	1.415042	-0.904696	H	2.214304	-0.75092	-2.122248
C	-2.117182	-0.20209	-3.883222	C	0.964273	-4.497727	-2.950712
H	-2.7883	-0.774189	-3.231101	H	1.107019	-4.919299	-1.948468
H	-2.713034	0.180472	-4.722334	H	0.106234	-5.002754	-3.410728
H	-1.372398	-0.895784	-4.294905	H	1.85278	-4.747971	-3.547016

IM1$_{PPP}$				**IM2**$_{PPP}$			
H	-0.290697	1.701293	-7.51246	H	-0.212649	1.968755	-7.423577
C	-0.460476	2.27839	-6.607251	C	-0.367718	2.514894	-6.496746
H	-1.560549	3.832338	-7.572494	H	-1.469803	4.107493	-7.393713
C	-1.168507	3.442266	-6.636633	C	-1.06856	3.683193	-6.476852
C	-0.03497	2.604203	-4.187092	C	0.085791	2.749728	-4.070495
C	-1.427013	4.182931	-5.438415	C	-1.299419	4.387948	-5.251895
C	0.199571	1.8838	-5.403222	C	0.306003	2.07594	-5.315964
C	-1.051181	3.65272	-4.170888	C	-0.915021	3.811335	-4.007341
C	-2.036951	5.466762	-5.526561	C	-1.882713	5.686454	-5.291681
C	-2.27255	6.192445	-4.394474	C	-2.072695	6.386486	-4.135235
H	-2.259247	5.872117	-6.510219	H	-2.115949	6.12438	-6.258699
H	-2.660479	7.206116	-4.449171	H	-2.433437	7.411443	-4.153273
C	-2.141371	5.581463	-3.113502	C	-1.927668	5.73779	-2.874366
C	-2.618775	6.295863	-1.968596	C	-2.347456	6.43708	-1.698185
C	-1.647199	4.249947	-2.988461	C	-1.475048	4.387837	-2.797347
C	-2.818437	5.665034	-0.779905	C	-2.534494	5.780343	-0.521747
H	-2.873337	7.345656	-2.090424	H	-2.567508	7.498202	-1.784488
H	-3.224574	6.195871	0.076917	H	-2.895571	6.300637	0.36136
C	-2.619085	4.253849	-0.685517	C	-2.390447	4.359917	-0.473884
C	-1.986524	3.53508	-1.751811	C	-1.815693	3.647045	-1.576204
C	1.194437	0.874981	-5.437287	C	1.302363	1.071678	-5.401848
C	2.056533	0.694635	-4.382872	C	2.174566	0.849042	-4.364509
C	1.952524	1.526632	-3.23042	C	2.077583	1.627895	-3.175202
C	0.878903	2.412735	-3.119698	C	1.005616	2.508944	-3.017875
H	1.320006	0.297728	-6.349927	H	1.418963	0.532249	-6.338475
H	2.864747	-0.027028	-4.442178	H	2.982083	0.130642	-4.46096
H	0.797052	3.027776	-2.230177	H	0.931043	3.084479	-2.101794

C	-1.936898	2.121036	-1.63193	C	-1.832902	2.22721	-1.505371
C	-2.536164	1.436931	-0.574305	C	-2.453084	1.538524	-0.462913
C	-3.177035	2.173908	0.45209	C	-3.031248	2.273696	0.602271
C	-3.175475	3.548075	0.408234	C	-2.955739	3.645882	0.60927
H	-1.458051	1.546993	-2.410447	H	-1.397633	1.660508	-2.314623
H	-3.694516	1.659016	1.251147	H	-3.566006	1.757391	1.389156
H	-3.670016	4.114832	1.192634	H	-3.405589	4.208719	1.422901
C	3.043008	1.517743	-2.307315	C	3.169602	1.568697	-2.256222
C	4.105078	1.510138	-1.709478	C	4.230554	1.520276	-1.658271
C	-2.599504	-0.057156	-0.572152	C	-2.627291	0.051179	-0.482136
C	-2.494837	-0.893095	0.624285	C	-2.589843	-0.810015	0.633894
H	-3.449541	-1.584018	6.744722	H	-3.350258	-1.847179	6.739638
C	-3.11515	-0.674373	6.252544	C	-2.980903	-0.928959	6.290371
H	-3.632065	0.616344	7.872446	H	-3.348398	0.282159	8.00874
C	-3.204374	0.534687	6.876325	C	-2.969073	0.240161	6.990818
C	-2.216192	0.426052	4.22075	C	-2.099303	0.245539	4.29168
C	-2.738308	1.730187	6.242333	C	-2.458847	1.445608	6.411115
C	-2.695258	-0.743973	4.890366	C	-2.62346	-0.934781	4.908236
C	-2.066686	1.664975	4.98771	C	-1.845342	1.422667	5.12596
C	-2.98215	2.990951	6.861401	C	-2.601171	2.675426	7.117293
C	-2.600727	4.15057	6.24775	C	-2.179923	3.848787	6.55806
H	-3.529713	3.010553	7.800196	H	-3.105267	2.665333	8.080296
H	-2.862487	5.117779	6.66897	H	-2.366867	4.800564	7.048671
C	-1.771493	4.109718	5.08993	C	-1.407513	3.835791	5.361154
C	-1.291741	5.332572	4.519221	C	-0.889347	5.06462	4.83904
C	-1.382368	2.858303	4.534066	C	-1.113756	2.602249	4.713967
C	-0.374559	5.332591	3.509751	C	-0.022526	5.078042	3.786275
H	-1.675453	6.267956	4.918889	H	-1.202879	5.992591	5.310896
H	-0.02687	6.264465	3.071205	H	0.353789	6.015302	3.384439
C	0.227502	4.106988	3.090354	C	0.492777	3.850545	3.268124
C	-0.23679	2.86612	3.631766	C	-0.010888	2.60462	3.759832
C	-2.852862	-1.945675	4.154088	C	-2.886242	-2.073453	4.107227
C	-2.705441	-1.967383	2.790697	C	-2.790813	-2.016154	2.739314
C	-2.386225	-0.77389	2.067041	C	-2.42414	-0.803473	2.076401
C	-2.08164	0.373587	2.808089	C	-2.023906	0.27503	2.874932
H	-3.156089	-2.845426	4.683791	H	-3.226172	-2.985231	4.59208
H	-2.882433	-2.885139	2.237156	H	-3.043906	-2.888885	2.147084
H	-1.784592	1.270306	2.286546	H	-1.697366	1.185559	2.396621
C	0.538209	1.711278	3.381942	C	0.69171	1.428816	3.410429
C	1.665769	1.740399	2.564811	C	1.783569	1.450847	2.546221
C	2.051362	2.964488	1.948229	C	2.201572	2.688354	1.978825
C	1.346139	4.113456	2.217977	C	1.568776	3.852839	2.343818
H	0.280495	0.77595	3.8598	H	0.407814	0.481711	3.849084
H	2.91626	2.981759	1.293548	H	3.036321	2.700945	1.28613
H	1.663802	5.060943	1.789751	H	1.915219	4.806775	1.953907
C	2.435152	0.560363	2.35829	C	2.499756	0.255829	2.249655
C	3.105558	-0.435434	2.156733	C	3.143741	-0.738753	1.970066
H	6.129544	-5.731071	0.725674	H	6.147346	-5.921703	0.133643
C	6.524149	-4.718264	0.725319	C	6.550852	-4.917215	0.232306
H	8.550355	-5.311462	0.424436	H	8.577188	-5.503353	-0.078836
C	7.854919	-4.484891	0.547212	C	7.887119	-4.683321	0.103466
C	6.13365	-2.289109	0.989077	C	6.176475	-2.517204	0.704609
C	8.38343	-3.154053	0.516491	C	8.4284	-3.361075	0.204434
C	5.638612	-3.633412	1.003311	C	5.669454	-3.852044	0.588858
C	7.513702	-2.027029	0.581113	C	7.567891	-2.234638	0.351359
C	9.795377	-2.973949	0.464504	C	9.842791	-3.193236	0.200236

C	10.333561	-1.721034	0.534393	C	10.391119	-1.957876	0.39357
H	10.4317	-3.85473	0.436001	H	10.471595	-4.074914	0.10728
H	11.409235	-1.576843	0.594126	H	11.466469	-1.832359	0.489714
C	9.496058	-0.570892	0.467822	C	9.566481	-0.796792	0.410667
C	10.095135	0.728767	0.51994	C	10.177123	0.48632	0.58826
C	8.083856	-0.712781	0.337933	C	8.156195	-0.910477	0.239134
C	9.347177	1.859519	0.384528	C	9.44397	1.633572	0.535862
H	11.166976	0.789525	0.691086	H	11.245448	0.518898	0.786989
H	9.799641	2.844194	0.468753	H	9.90485	2.601716	0.713754
C	7.967712	1.763877	0.028095	C	8.071153	1.585612	0.14559
C	7.345264	0.479145	-0.084576	C	7.43871	0.322645	-0.090509
C	4.288805	-3.882673	1.364931	C	4.310661	-4.118656	0.900968
C	3.44285	-2.865033	1.742233	C	3.46539	-3.129933	1.349933
C	3.941891	-1.535569	1.812247	C	3.973117	-1.817082	1.545924
C	5.271408	-1.283376	1.476346	C	5.312087	-1.550222	1.26157
H	3.931836	-4.909361	1.34928	H	3.946033	-5.136538	0.788185
H	2.407892	-3.064339	2.002145	H	2.424117	-3.341415	1.57221
H	5.633149	-0.272767	1.593125	H	5.679852	-0.558025	1.476342
C	6.073419	0.429328	-0.706248	C	6.178414	0.342197	-0.735861
C	5.372673	1.583795	-1.056837	C	5.493102	1.530163	-0.992322
C	5.956152	2.858034	-0.803378	C	6.085043	2.770985	-0.621095
C	7.231365	2.93226	-0.29675	C	7.352482	2.786154	-0.089929
H	5.621121	-0.52863	-0.926352	H	5.721462	-0.587218	-1.048681
H	5.404544	3.757235	-1.059616	H	5.546735	3.69539	-0.80601
H	7.710897	3.898989	-0.164649	H	7.83939	3.732255	0.133101
C	-3.236186	-0.171676	-3.17724	C	-3.325039	0.122348	-3.114538
H	-3.956475	-0.837186	-3.666873	H	-3.985367	-0.511348	-3.715816
H	-3.667212	0.834837	-3.132334	H	-3.802427	1.102105	-2.992191
Mo	-2.887955	-2.245737	-0.6911	Mo	-3.262099	-2.067122	-0.756349
C	-2.903886	-0.718705	-1.838584	C	-3.073459	-0.549422	-1.813165
H	-2.348954	-0.128572	-3.822968	H	-2.402292	0.26853	-3.689738
O	-3.158201	-4.15716	-0.689101	O	-3.947647	-3.784248	-1.291549
O	-4.887709	-2.201561	-0.420083	O	-5.135256	-1.748923	-0.076383
O	-0.979078	-2.728829	-0.999653	O	-1.455497	-2.873893	-0.999513
Si	-4.289323	-5.385017	-0.828143	Si	-4.476954	-5.299609	-0.807593
Si	-6.338512	-1.461485	-0.15894	Si	-6.656711	-1.151799	-0.311178
Si	0.070108	-3.607831	-1.933613	Si	-0.336947	-3.387977	-2.111781
C	-5.346682	-5.152463	-2.375067	C	-4.15005	-5.564068	1.033511
H	-6.118448	-5.930414	-2.450042	H	-3.081399	-5.474633	1.267722
H	-5.847399	-4.178965	-2.375477	H	-4.698224	-4.83912	1.648202
H	-4.728882	-5.214554	-3.281141	H	-4.471413	-6.567633	1.34397
C	-5.340881	-5.497644	0.735867	C	-3.548682	-6.596604	-1.817751
H	-4.712679	-5.735275	1.605011	H	-3.883094	-7.608018	-1.54884
H	-5.858355	-4.556643	0.945866	H	-3.72584	-6.46682	-2.892986
H	-6.09602	-6.290827	0.649367	H	-2.466632	-6.549229	-1.647501
C	-3.318958	-6.99905	-0.997413	C	-6.32159	-5.459415	-1.173035
H	-2.695935	-7.009903	-1.900287	H	-6.919448	-4.751806	-0.587477
H	-2.663092	-7.166521	-0.13377	H	-6.53148	-5.280677	-2.235332
H	-4.004987	-7.855357	-1.060306	H	-6.675781	-6.471504	-0.933228
C	-6.580712	-1.106845	1.686895	C	-7.839013	-1.986534	0.909585
H	-6.525154	-2.028283	2.280885	H	-8.860344	-1.594161	0.810324
H	-5.819322	-0.420083	2.077015	H	-7.886157	-3.072253	0.75642
H	-7.562808	-0.651105	1.874811	H	-7.518636	-1.814594	1.945862
C	-6.479942	0.173097	-1.111257	C	-7.251393	-1.466174	-2.082758
H	-6.375546	0.021268	-2.193379	H	-8.275284	-1.098145	-2.235492
H	-7.466664	0.625927	-0.939954	H	-6.606881	-0.958757	-2.812958

H	-5.726866	0.907901	-0.801555	H	-7.242592	-2.536611	-2.323485
C	-7.759443	-2.57301	-0.739086	C	-6.71047	0.714886	0.016646
H	-8.727363	-2.107824	-0.505464	H	-6.36514	0.951305	1.03149
H	-7.731124	-2.736872	-1.823952	H	-6.086444	1.279018	-0.687971
H	-7.742666	-3.556907	-0.254587	H	-7.736483	1.097443	-0.077951
C	-0.66415	-3.965759	-3.645072	C	0.472125	-4.976442	-1.477826
H	0.040041	-4.532649	-4.269616	H	1.237158	-5.341351	-2.176747
H	-1.589734	-4.551385	-3.577452	H	0.962567	-4.808518	-0.510349
H	-0.898548	-3.034128	-4.177766	H	-0.261958	-5.7807	-1.340813
C	1.657834	-2.608964	-2.158935	C	0.990729	-2.061534	-2.323349
H	2.119394	-2.365445	-1.19411	H	1.48984	-1.833244	-1.373175
H	2.398317	-3.165905	-2.749766	H	1.762925	-2.378747	-3.037293
H	1.462478	-1.662486	-2.677777	H	0.55545	-1.128072	-2.699266
C	0.493565	-5.240771	-1.077618	C	-1.147309	-3.721396	-3.790755
H	0.946563	-5.061548	-0.093651	H	-1.634159	-2.818462	-4.183096
H	-0.398132	-5.859861	-0.923289	H	-0.406488	-4.047181	-4.533943
H	1.209876	-5.826624	-1.670134	H	-1.912523	-4.503351	-3.716788

TS2$_{PPP}$ Imaginary frequency: 143.7685 cm^{-1}				**4**$_{PPP}$ + [Mo] pair			
H	-0.3675	7.672677	-0.660765	H	0.639279	-6.545526	-2.792103
C	-0.454996	6.991984	0.182062	C	0.510057	-6.331861	-1.734083
H	-1.568383	8.34661	1.399585	H	1.805546	-7.894542	-1.074017
C	-1.126841	7.357057	1.31158	C	1.161761	-7.066797	-0.786924
C	0.133687	4.828494	1.230896	C	-0.616385	-5.031892	0.043783
C	-1.266236	6.455954	2.416399	C	1.020343	-6.775967	0.608683
C	0.268863	5.759825	0.152065	C	-0.446737	-5.345102	-1.342322
C	-0.819543	5.110317	2.297707	C	0.273571	-5.640032	1.029107
C	-1.809117	6.919112	3.649792	C	1.597404	-7.648522	1.576653
C	-1.877338	6.081401	4.727676	C	1.404482	-7.424982	2.911593
H	-2.103173	7.96231	3.731626	H	2.137456	-8.526023	1.230476
H	-2.196932	6.446796	5.700124	H	1.759028	-8.136557	3.652876
C	-1.637165	4.684769	4.570143	C	0.805425	-6.212304	3.360954
C	-1.863081	3.804494	5.676587	C	0.674165	-5.95942	4.764642
C	-1.24875	4.162069	3.304109	C	0.36975	-5.240817	2.416863
C	-1.885735	2.453138	5.507136	C	0.225006	-4.758126	5.229176
H	-2.046297	4.245487	6.65329	H	0.939078	-6.756285	5.455097
H	-2.071379	1.786592	6.345346	H	0.102865	-4.58231	6.294933
C	-1.81199	1.90034	4.190897	C	0.019339	-3.671361	4.324468
C	-1.489079	2.735635	3.073722	C	0.150758	-3.885654	2.915702
C	1.227184	5.514012	-0.864083	C	-1.302669	-4.745745	-2.303014
C	2.135713	4.48831	-0.751626	C	-2.360441	-3.952295	-1.925648
C	2.119095	3.649914	0.399953	C	-2.624754	-3.741205	-0.542373
C	1.090229	3.789194	1.332806	C	-1.746988	-4.264162	0.407622
H	1.282016	6.200593	-1.705163	H	-1.134098	-4.963717	-3.354821
H	2.910076	4.347845	-1.499058	H	-3.02595	-3.522066	-2.667461
H	1.083038	3.139295	2.200128	H	-1.973254	-4.105411	1.453718
C	-1.661448	2.187771	1.774693	C	0.218154	-2.744335	2.08236
C	-2.175468	0.907729	1.570014	C	0.070223	-1.45125	2.585133
C	-2.411749	0.075469	2.698524	C	-0.1988	-1.269956	3.972069
C	-2.203863	0.557851	3.969263	C	-0.210121	-2.358467	4.811879
H	-1.45829	2.807154	0.912601	H	0.433527	-2.861958	1.028287
H	-2.81204	-0.920625	2.555036	H	-0.344938	-0.266456	4.35928
H	-2.422203	-0.070124	4.829243	H	-0.350762	-2.21954	5.881011

C	3.226324	2.780878	0.636152
C	4.266229	2.176364	0.82932
C	-2.549907	0.372834	0.253326
C	-2.539032	-0.742921	-0.420586
H	-3.0032	-6.877386	-1.446424
C	-2.711964	-6.388583	-0.520317
H	-3.141569	-8.072809	0.717702
C	-2.775882	-7.050043	0.671084
C	-1.970031	-4.340045	0.651361
C	-2.35438	-6.427728	1.890652
C	-2.380053	-4.998537	-0.549696
C	-1.766325	-5.133141	1.860738
C	-2.545783	-7.092743	3.137057
C	-2.188486	-6.485711	4.309488
H	-3.031811	-8.065035	3.138821
H	-2.412262	-6.948552	5.267234
C	-1.430949	-5.278309	4.293556
C	-0.965065	-4.706103	5.521504
C	-1.094373	-4.669066	3.053268
C	-0.105231	-3.646409	5.529384
H	-1.310743	-5.144848	6.454229
H	0.232165	-3.210338	6.46625
C	0.457341	-3.16849	4.305306
C	0.00161	-3.707023	3.060827
C	-2.560389	-4.233256	-1.72983
C	-2.508677	-2.859588	-1.700312
C	-2.276605	-2.170934	-0.474501
C	-1.957295	-2.922576	0.657602
H	-2.807309	-4.750113	-2.653893
H	-2.69549	-2.288859	-2.604842
H	-1.752623	-2.406748	1.584967
C	0.751321	-3.406712	1.901173
C	1.853172	-2.554136	1.932532
C	2.221017	-1.934189	3.160497
C	1.535788	-2.245785	4.311904
H	0.505251	-3.885017	0.962766
H	3.062534	-1.248761	3.180155
H	1.845621	-1.817464	5.261973
C	2.625873	-2.347797	0.753835
C	3.299539	-2.197225	-0.249222
H	6.394193	-1.617656	-5.665581
C	6.771289	-1.442758	-4.661186
H	8.813354	-1.29041	-5.258061
C	8.102195	-1.250097	-4.436653
C	6.334487	-1.266213	-2.23299
C	8.607654	-0.986867	-3.122428
C	5.862042	-1.512825	-3.561853
C	7.713731	-0.828628	-2.02514
C	10.015877	-0.922957	-2.916141
C	10.523382	-0.75921	-1.658291
H	10.674256	-1.071067	-3.76821
H	11.594295	-0.805089	-1.477844
C	9.660789	-0.458362	-0.565084
C	10.220857	-0.255217	0.73736
C	8.256101	-0.343817	-0.770082
C	9.443132	0.115514	1.793909
C	-3.808296	-3.062185	-0.132118
C	-4.853526	-2.537007	0.207667
C	0.2506	-0.317554	1.740449
C	0.459462	0.669658	1.057368
H	2.828218	5.134876	-2.610569
C	2.283336	5.262671	-1.678671
H	2.876149	7.293262	-1.399028
C	2.298618	6.455264	-1.016641
C	0.898184	4.278295	0.118474
C	1.555958	6.644837	0.193325
C	1.641869	4.127138	-1.094715
C	0.701893	5.613947	0.67565
C	1.700926	7.855044	0.932061
C	1.052956	8.020065	2.124568
H	2.383849	8.613759	0.558428
H	1.231119	8.898563	2.739496
C	0.067286	7.080526	2.54558
C	-0.659755	7.305842	3.758942
C	-0.218948	5.940667	1.743437
C	-1.698638	6.500433	4.123587
H	-0.358309	8.139698	4.388086
H	-2.228718	6.663063	5.058563
C	-2.17951	5.499891	3.223861
C	-1.481241	5.252192	1.999492
C	1.816528	2.832237	-1.649147
C	1.383209	1.705094	-0.990622
C	0.766069	1.828907	0.286936
C	0.519609	3.100783	0.80524
H	2.343616	2.739897	-2.595646
H	1.544689	0.718372	-1.412643
H	0.060377	3.174192	1.782258
C	-2.132868	4.464885	1.021787
C	-3.368619	3.862217	1.258644
C	-3.98209	4.010477	2.53535
C	-3.398878	4.820617	3.48105
H	-1.689328	4.353109	0.041183
H	-4.929227	3.51791	2.732067
H	-3.894546	4.988408	4.434038
C	-4.040323	3.161225	0.215849
C	-4.650673	2.612011	-0.683975
H	-7.633699	1.115241	-5.961345
C	-7.951928	0.916739	-4.941086
H	-9.974379	0.481666	-5.464205
C	-9.238574	0.555685	-4.66728
C	-7.420814	0.872074	-2.525911
C	-9.660475	0.259569	-3.330911
C	-7.030956	1.151878	-3.874131
C	-8.71106	0.236921	-2.271377
C	-11.039234	0.022448	-3.058298
C	-11.464979	-0.18941	-1.776436
H	-11.748921	0.076387	-3.879923
H	-12.524133	-0.275951	-1.547613
C	-10.521428	-0.382251	-0.725614
C	-10.979252	-0.677692	0.599113
C	-9.126846	-0.315644	-1.000038
C	-10.10531	-0.995495	1.597175

H	11.287289	-0.422391	0.866128	H	-12.048595	-0.638377	0.79123
H	9.867379	0.228173	2.788284	H	-10.458802	-1.192233	2.606132
C	8.072984	0.46256	1.586407	C	-8.720226	-1.187071	1.302886
C	7.491067	0.316683	0.286878	C	-8.229597	-0.908795	-0.012257
C	4.512753	-1.90466	-3.764525	C	-5.771995	1.757014	-4.125292
C	3.655601	-2.111556	-2.70853	C	-4.961928	2.180684	-3.098013
C	4.13767	-1.967658	-1.378037	C	-5.397643	2.033063	-1.750229
C	5.45923	-1.575333	-1.168682	C	-6.598007	1.371429	-1.489637
H	4.167976	-2.061414	-4.78359	H	-5.474209	1.923749	-5.157569
H	2.625358	-2.408799	-2.876805	H	-4.014062	2.669075	-3.301471
H	5.810842	-1.518074	-0.148762	H	-6.918276	1.281996	-0.459958
C	6.235635	0.931205	0.064664	C	-6.932943	-1.370183	-0.338577
C	5.509217	1.528675	1.094418	C	-6.109438	-1.99097	0.600973
C	6.045971	1.53403	2.413577	C	-6.566882	-2.133284	1.942145
C	7.306585	1.032707	2.636125	C	-7.845711	-1.748209	2.269609
H	5.819552	0.956462	-0.933756	H	-6.572619	-1.283394	-1.355154
H	5.473033	1.979916	3.220597	H	-5.915877	-2.588609	2.68189
H	7.751381	1.096626	3.62606	H	-8.223105	-1.913244	3.275812
C	-4.018946	3.060642	0.072018	C	7.773643	-2.734859	0.918562
H	-4.876616	3.473552	-0.477212	H	8.811618	-2.933149	0.613993
H	-4.343667	2.857254	1.099358	H	7.782049	-2.480362	1.987617
Mo	-3.618161	0.470719	-1.788517	Mo	6.553765	-0.355413	-0.87132
C	-3.622341	1.836337	-0.645208	C	7.1941	-1.645499	0.107207
H	-3.23928	3.830467	0.093565	H	7.204685	-3.667583	0.801544
O	-4.631696	0.901925	-3.38318	O	8.100469	0.135809	-1.928181
O	-5.185053	-0.598965	-1.197714	O	5.973415	1.010685	0.351088
O	-1.963904	0.645663	-2.841168	O	5.148226	-1.12309	-1.930002
Si	-5.221254	0.486306	-4.887467	Si	8.399676	1.294311	-3.114568
Si	-6.541109	-0.715236	-0.251047	Si	5.935216	1.33486	2.010576
Si	-0.48346	1.256588	-3.272129	Si	4.350177	-2.540805	-2.377795
C	-4.63111	-1.241493	-5.375564	C	6.82374	2.265493	-3.495745
H	-3.53529	-1.292384	-5.414602	H	6.021287	1.605412	-3.851519
H	-4.980176	-1.99672	-4.659169	H	6.452338	2.795451	-2.608358
H	-5.010816	-1.526507	-6.36614	H	7.001408	3.017063	-4.276791
C	-4.600941	1.761513	-6.135445	C	8.999892	0.3855	-4.653086
H	-4.970143	1.543847	-7.146828	H	9.245188	1.088328	-5.460552
H	-4.939203	2.771249	-5.868547	H	9.901333	-0.202283	-4.437891
H	-3.504662	1.780272	-6.177263	H	8.235402	-0.304375	-5.033168
C	-7.109525	0.528815	-4.843178	C	9.738843	2.449383	-2.461998
H	-7.516532	-0.232497	-4.166372	H	9.406291	2.974926	-1.557497
H	-7.476763	1.506932	-4.506619	H	10.651165	1.89464	-2.20843
H	-7.529903	0.343316	-5.841145	H	10.007097	3.209042	-3.208364
C	-7.551681	-2.196162	-0.852835	C	5.177754	3.049212	2.201611
H	-8.462287	-2.332251	-0.253738	H	5.132882	3.345897	3.258025
H	-7.859112	-2.073029	-1.899452	H	5.765395	3.807569	1.668479
H	-6.969788	-3.12488	-0.787139	H	4.15557	3.079458	1.804128
C	-7.587116	0.856825	-0.384256	C	7.699122	1.312556	2.679922
H	-8.511746	0.770746	0.202842	H	7.72105	1.531237	3.75599
H	-7.041335	1.734298	-0.013876	H	8.170023	0.333253	2.527683
H	-7.87058	1.059236	-1.425054	H	8.322803	2.062185	2.175698
C	-6.077084	-0.993067	1.563375	C	4.871914	0.04187	2.876108
H	-5.466752	-1.897392	1.683447	H	3.84573	0.050825	2.487425
H	-5.510436	-0.14848	1.97484	H	5.27374	-0.969358	2.734215
H	-6.976763	-1.117485	2.181962	H	4.818652	0.230864	3.956778
C	0.040142	0.440826	-4.897326	C	5.039846	-3.078585	-4.04923
H	1.022333	0.804794	-5.228352	H	4.546888	-3.992204	-4.407535

H	0.111944	-0.649371	-4.78696	H	4.893893	-2.301845	-4.810852
H	-0.677464	0.645104	-5.702567	H	6.116211	-3.285009	-3.985386
C	0.790745	0.844761	-1.941297	C	2.521073	-2.111502	-2.523153
H	0.80296	-0.232502	-1.732775	H	2.358946	-1.299831	-3.243754
H	1.804448	1.131125	-2.251313	H	1.935537	-2.976448	-2.860928
H	0.577294	1.357147	-0.996574	H	2.109178	-1.793462	-1.557008
C	-0.608274	3.126732	-3.523386	C	4.60769	-3.901751	-1.099346
H	-0.946987	3.629872	-2.609042	H	4.335489	-3.564917	-0.091345
H	0.359788	3.562556	-3.803984	H	3.978927	-4.770742	-1.335971
H	-1.325024	3.367546	-4.319676	H	5.649816	-4.242088	-1.074847

2$_{PPM}$ product				**4**$_{PPP}$ product			
C	-2.318857	0.446618	-2.346153	H	-4.78147	4.787044	4.449216
H	-6.638053	-3.638309	-4.237331	C	-4.559687	4.905844	3.391701
C	-6.43544	-3.335748	-3.213271	H	-5.367913	6.876275	3.257254
H	-8.216482	-4.189802	-2.407859	C	-4.871359	6.061139	2.736697
C	-7.295471	-3.649182	-2.204612	C	-3.718846	3.930581	1.280123
C	-5.001123	-2.104306	-1.609921	C	-4.55399	6.240705	1.351507
C	-7.009911	-3.295492	-0.847125	C	-4.040635	3.7888	2.667225
C	-5.300395	-2.510832	-2.950937	C	-3.810421	5.247324	0.655186
C	-5.775201	-2.670769	-0.502911	C	-5.015378	7.399838	0.662271
C	-7.990142	-3.559666	0.151637	C	-4.781942	7.547562	-0.676715
C	-7.767027	-3.20137	1.449566	H	-5.607878	8.129094	1.208833
H	-8.934844	-4.003185	-0.152066	H	-5.210507	8.379846	-1.229183
H	-8.539988	-3.322195	2.204189	C	-3.902784	6.656516	-1.358456
C	-6.482537	-2.740886	1.857168	C	-3.607035	6.868046	-2.743931
C	-6.257567	-2.469043	3.244703	C	-3.292661	5.580993	-0.654481
C	-5.429582	-2.594718	0.906965	C	-2.671488	6.116202	-3.392167
C	-5.018266	-2.153983	3.714026	H	-4.153464	7.646811	-3.270162
H	-7.108885	-2.522328	3.918637	H	-2.470805	6.266056	-4.44995
H	-4.858274	-1.928544	4.76529	C	-1.857778	5.197456	-2.660188
C	-3.889534	-2.207179	2.841975	C	-2.120631	4.966779	-1.272544
C	-4.073628	-2.479413	1.44685	C	-3.938244	2.512655	3.280065
C	-4.514891	-2.022295	-4.026239	C	-3.641206	1.386971	2.548238
C	-3.520508	-1.097249	-3.823417	C	-3.453378	1.490761	1.140347
C	-3.294585	-0.579716	-2.515632	C	-3.477065	2.749899	0.540067
C	-4.036076	-1.080154	-1.444442	H	-4.1456	2.43088	4.344217
H	-4.735778	-2.375513	-5.030435	H	-3.59382	0.411427	3.021908
H	-2.92948	-0.722477	-4.65322	H	-3.346858	2.806723	-0.532614
H	-3.862579	-0.659684	-0.462693	C	-1.137081	4.277399	-0.525659
C	-2.91102	-2.730488	0.68258	C	0.009958	3.750255	-1.119517
C	-1.627336	-2.583372	1.207964	C	0.184536	3.873381	-2.527588
C	-1.46627	-2.227459	2.575749	C	-0.726951	4.590507	-3.266324
C	-2.578617	-2.065117	3.36623	H	-1.244725	4.185725	0.547093
H	-2.999962	-3.04265	-0.348016	H	1.061636	3.438127	-2.996163
H	-0.467039	-2.099095	2.979633	H	-0.565503	4.742261	-4.330767
H	-2.46814	-1.836426	4.423383	C	-3.309741	0.317817	0.344362
C	-0.488727	-2.715807	0.362673	C	-3.249595	-0.690794	-0.335991
C	2.318319	0.446521	2.345714	C	1.026532	3.153928	-0.318806
C	1.476371	1.326173	2.304194	C	1.928228	2.697947	0.361544
H	-2.560755	5.806656	3.887393	H	6.535155	1.706644	4.459823
C	-1.903703	5.788587	3.021672	C	6.527443	1.465982	3.399799
H	-2.081945	7.875681	2.614159	H	8.638192	1.184885	3.263003
C	-1.648573	6.925307	2.312702	C	7.68427	1.166224	2.741842

C	-0.368262	4.519641	1.552434
C	-0.806656	6.905407	1.154579
C	-1.211817	4.578563	2.707263
C	-0.310476	5.669267	0.653726
C	-0.433848	8.130473	0.528564
C	0.433198	8.130533	-0.528232
H	-0.800366	9.062942	0.950036
H	0.799739	9.06305	-0.949578
C	0.805982	6.905542	-1.154408
C	1.647908	6.925577	-2.312521
C	0.309773	5.669347	-0.65372
C	1.903024	5.788943	-3.021634
H	2.081302	7.875981	-2.61385
H	2.560085	5.807111	-3.887347
C	1.211115	4.578891	-2.707388
C	0.367544	4.519836	-1.552576
C	-1.265937	3.46946	3.590147
C	-0.437301	2.385348	3.4271
C	0.504502	2.368396	2.358252
C	0.503807	3.410612	1.431282
H	-1.946083	3.513276	4.437139
H	-0.461563	1.556107	4.127104
H	1.234254	3.387049	0.632919
C	-0.504546	3.410806	-1.431578
C	-0.505246	2.368708	-2.358681
C	0.436573	2.385779	-3.427513
C	1.265227	3.4699	-3.590413
H	-1.235006	3.387155	-0.633231
H	0.460828	1.556629	-4.127625
H	1.945382	3.513814	-4.437393
C	-1.477148	1.326506	-2.304783
C	0.489244	-2.715857	-0.36262
H	4.85878	-1.92877	-4.76529
C	5.018777	-2.154023	-3.713987
H	7.109467	-2.522037	-3.918477
C	6.258119	-2.468797	-3.244577
C	4.074128	-2.479236	-1.446785
C	6.483095	-2.74039	-1.856993
C	3.890029	-2.207254	-2.841958
C	5.43008	-2.594277	-0.906848
C	7.767658	-3.20057	-1.449276
C	7.990796	-3.558634	-0.151286
H	8.540671	-3.321353	-2.203852
H	8.935573	-4.001925	0.152516
C	7.010467	-3.294529	0.8474
C	7.296034	-3.647991	2.204945
C	5.775643	-2.67011	0.503049
C	6.435876	-3.334639	3.213521
H	8.217156	-4.18838	2.408306
H	6.638498	-3.637041	4.237626
C	5.300641	-2.510034	2.951026
C	5.001352	-2.103729	1.609948
C	2.579103	-2.065461	-3.366264
C	1.466763	-2.227809	-2.575775
C	1.627848	-2.583446	-1.20792
C	2.91154	-2.730305	-0.682486
C	5.263218	1.243408	1.285991
C	7.681779	0.814708	1.35328
C	5.300478	1.580422	2.676319
C	6.449881	0.671422	0.655798
C	8.916469	0.643152	0.662112
C	8.927902	0.378597	-0.679249
H	9.844138	0.789351	1.209521
H	9.86297	0.340706	-1.232267
C	7.717132	0.06612	-1.363371
C	7.752171	-0.282995	-2.752086
C	6.480785	0.06756	-0.659013
C	6.633273	-0.711639	-3.404137
H	8.699323	-0.193327	-3.278134
H	6.662379	-0.949578	-4.464387
C	5.431183	-0.964812	-2.674241
C	5.363448	-0.635881	-1.28316
C	4.143014	2.122156	3.293808
C	3.019231	2.432608	2.564476
C	3.015857	2.230931	1.154734
C	4.119259	1.6291	0.54928
H	4.175089	2.333294	4.359867
H	2.150022	2.873798	3.042135
H	4.103413	1.497124	-0.524517
C	4.275176	-1.1511	-0.541039
C	3.24458	-1.874225	-1.142216
C	3.262975	-2.071879	-2.552429
C	4.33987	-1.634058	-3.286954
H	4.249591	-1.023527	0.533152
H	2.446811	-2.608131	-3.026357
H	4.390327	-1.838323	-4.353623
C	2.220513	-2.463479	-0.345943
C	1.376456	-3.020431	0.333152
H	-1.755171	-6.519587	4.449139
C	-1.968819	-6.390673	3.39109
H	-3.271248	-8.076142	3.263182
C	-2.813716	-7.240569	2.739313
C	-1.545368	-5.182181	1.275237
C	-3.128402	-7.060242	1.353575
C	-1.261192	-5.385097	2.663022
C	-2.640283	-5.921703	0.653454
C	-3.901426	-8.041763	0.667508
C	-4.145565	-7.918344	-0.672089
H	-4.236478	-8.917793	1.216939
H	-4.651359	-8.708117	-1.221631
C	-3.813558	-6.713758	-1.357913
C	-4.142195	-6.568207	-2.744414
C	-3.188375	-5.644921	-0.657075
C	-3.958044	-5.384207	-3.396483
H	-4.541757	-7.432823	-3.268612
H	-4.185728	-5.289518	-4.455177
C	-3.571646	-4.217227	-2.667924
C	-3.243138	-4.324967	-1.279233
C	-0.207775	-4.655612	3.273327
C	0.617647	-3.837153	2.538704
C	0.433393	-3.731044	1.130486
C	-0.644548	-4.384154	0.532312

H	2.468617	-1.836965	-4.423458	H	-0.032837	-4.790861	4.337826
H	0.467522	-2.099646	-2.979701	H	1.438283	-3.305997	3.010673
H	3.000506	-3.042254	0.348174	H	-0.759422	-4.302759	-0.540529
C	4.036023	-1.079873	1.444286	C	-3.139819	-3.126194	-0.535737
C	3.294328	-0.579517	2.515373	C	-3.254788	-1.871163	-1.13396
C	3.520308	-1.096843	3.823231	C	-3.444905	-1.786209	-2.542849
C	4.514932	-2.021592	4.026222	C	-3.609637	-2.936438	-3.27825
H	3.862463	-0.659574	0.462474	H	-3.009977	-3.170163	0.537652
H	2.92912	-0.722143	4.652953	H	-3.505211	-0.81053	-3.01481
H	4.735844	-2.374644	5.030471	H	-3.819568	-2.876028	-4.343335