Syntheses and Reactivity of Naphthalenyl-Substituted Arenediynes

Nadezhda V. Korovina, Michael L. Chang, Trang T. Nguyen, Ramiro Fernandez, Heather J. Walker, Marilyn M. Olmstead, Benjamin F. Gherman, and John D. Spence*

Department of Chemistry, California State University, Sacramento, 6000 J Street, Sacramento, CA, 95819 and Department of Chemistry, University of California, One Shields Ave., Davis, CA,95616

Fax: 916-278-4986; Tel: 916-278-4477; E-mail: jspence@csus.edu

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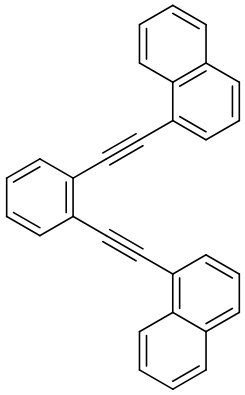
1. General Procedures

Reactions were carried out under an atmosphere of argon with magnetic stirring. Unless otherwise noted all reagents and solvents were obtained from commercial suppliers and used without further purification. Photochemical reactions were conducted in a quartz vessel with a Rayonet photochemical reactor equipped with sixteen 300 nm lamps that emit a Gaussian distribution of light from 275 to 350 nm or sixteen 350 nm lamps that emit a Gaussian distribution of light from 325 to 400 nm. TLC was performed on precoated silica plates and visualized with short (254 nm) or long (365 nm) wavelength UV light. Preparative thin layer chromatography was conducted on 20 cm x 20 cm glass plates with a silica gel layer thickness of 1,000 μm. Column chromatography was performed on 230-400 mesh silica gel packed in glass columns with the indicated solvent system. Melting points were determined in open capillary tubes on a Mel-Temp apparatus and are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were obtained on a Bruker 500 MHz or 300 MHz spectrometer. UV-visible absorbance spectra were recorded on a Shimadzu UV-2401 spectrometer. IR spectra were obtained on a Perkin Elmer 2000 FTIR spectrometer. Mass spectral determinations were performed at the OSU Mass Spectrometry and Proteomics Facility.

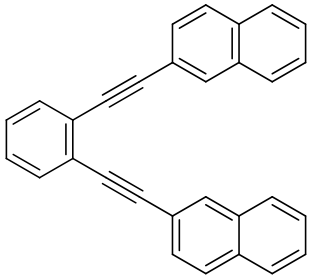
2. Experimental Details

1,2-bis(naphthalen-1-ylethynyl)benzene (1)



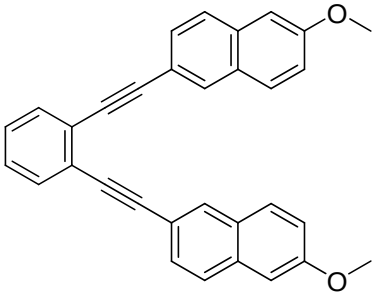
To a solution of 1,2-diiodobenzene (4.13 g, 12.5 mmol) in Et_3N (95 mL) was added CuI (0.048 g, 0.25 mmol) followed by $Pd(PPh_3)_4$ (0.289 g, 0.25 mmol) and the resulting solution was purged with argon for 5 minutes and wrapped in foil. A solution of 1-ethynylnaphthalene (4.0 g, 26.28 mmol) in Et_3N (25 mL) was then added dropwise over a 3 hour period. After stirring under argon overnight, the reaction mixture was diluted with ethyl acetate and washed with saturated aqueous NH_4Cl, saturated aqueous NaCl, and dried over Na_2SO_4. The solvent was removed under vacuum and the resulting solids were purified by silica gel column chromatography (4:1 hexanes/CH_2Cl_2) and recrystallized from EtOH/H_2O to afford naphthalen-1-yl arenediyne **1** as a white solid (3.07 g, 65%). mp = 96-98 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.53 (d, J = 8.4 Hz, 2H), 7.83 (d, J = 8.3 Hz, 2H), 7.81-7.78 (m, 4H), 7.73 (dd, J = 5.8, 3.4 Hz, 2H), 7.43-7.37 (m, 6H), 7.07 (dt, J = 6.9, 1.1 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 133.3, 133.1, 132.2, 130.8, 128.9, 128.1, 128.0, 126.8, 126.5, 126.4, 125.8, 125.1, 120.8, 93.3, 91.8; UV-vis (CH_3CN): λ_{max} nm (log ε) = 349 (4.37), 313 (4.53), 229 (4.89), 205 (4.84); IR (KBr): cm^{-1} = 2207; HRMS: calcd. for $C_{30}H_{18}$ $[M + Na]^+$ 401.1306 *m/z*, found 401.1311 *m/z*.

1,2-bis(naphthalen-2-ylethynyl)benzene (2)



To a solution of 1,2-diiodobenzene (1.25 g, 3.80 mmol) in Et_3N (30 mL) was added CuI (0.015 g, 0.078 mmol) followed by $Pd(PPh_3)_4$ (0.088 g, 0.076 mmol) and the resulting solution was purged with argon for 5 minutes and wrapped in foil. A solution of 2-ethynylnaphthalene (1.30 g, 8.54 mmol) in Et_3N (15 mL) was then added dropwise over a 3 hour period. After stirring under argon overnight, the reaction mixture was diluted with ethyl acetate and washed with saturated aqueous NH_4Cl, saturated aqueous NaCl, and dried over Na_2SO_4. The solvent was removed under vacuum and the resulting solids were purified by silica gel column chromatography (4:1 hexanes/CH_2Cl_2) and slowly recrystallized from CH_2Cl_2/hexanes to afford naphthalen-2-yl arenediyne **2** as a light yellow solid (0.84 g, 58%). mp = 139-140 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.13 (s, 2H), 7.83-7.79 (m, 4H), 7.72 (dd, *J* = 7.5, 1.8 Hz, 2H), 7.65 (dd, *J* = 8.5, 1.6 Hz, 2H), 7.62 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.50-7.45 (m, 4H), 7.34 (dd, *J* = 5.8, 3.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 133.0, 132.9, 131.71, 131.66, 128.4, 128.07, 128.06, 127.79, 127.78, 126.7, 126.6, 126.0, 120.6, 94.2, 88.8; UV-vis (CH_3CN): λ_{max} nm (log ε) = 330 (shoulder, 4.42), 300 (4.63), 262 (4.85), 246 (4.73), 219 (4.82); IR (KBr): cm^{-1} = 2197; HRMS: calcd. for $C_{30}H_{18}$ $[M + H]^+$ 379.1487 *m/z*, found 379.1489 *m/z*.

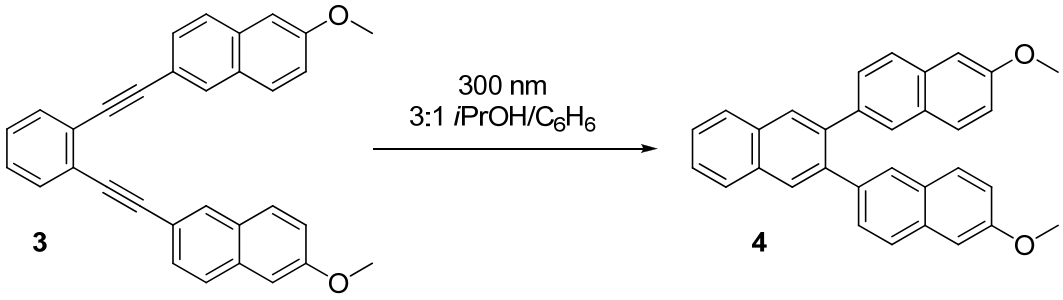
1,2-bis((6-methoxynaphthalen-2-yl)ethynyl)benzene (3)



To a solution of 1,2-diiodobenzene (0.425 g, 1.29 mmol) in Et_3N (15 mL) was added CuI (0.030 g, 0.16 mmol) followed by $Pd(PPh_3)_4$ (0.065 g, 0.056 mmol) and the resulting solution was purged with argon for 5 minutes and wrapped in foil. A solution of 2-ethynyl-6-methoxynaphthalene (0.50 g, 2.74 mmol) in Et_3N (5 mL) was then added dropwise over a 3 hour period. After stirring under argon overnight, the reaction mixture was diluted with chloroform and washed with saturated aqueous NH_4Cl, saturated aqueous NaCl, and dried over Na_2SO_4. The solvent was removed under vacuum and the resulting solids were purified by silica gel column chromatography (4:1 hexanes/CH_2Cl_2) and slowly recrystallized from CH_2Cl_2/hexanes to afford 6-methoxynaphthalen-2-yl arenediyne **3** as a light yellow solid (0.38 g, 67%). mp = 177-

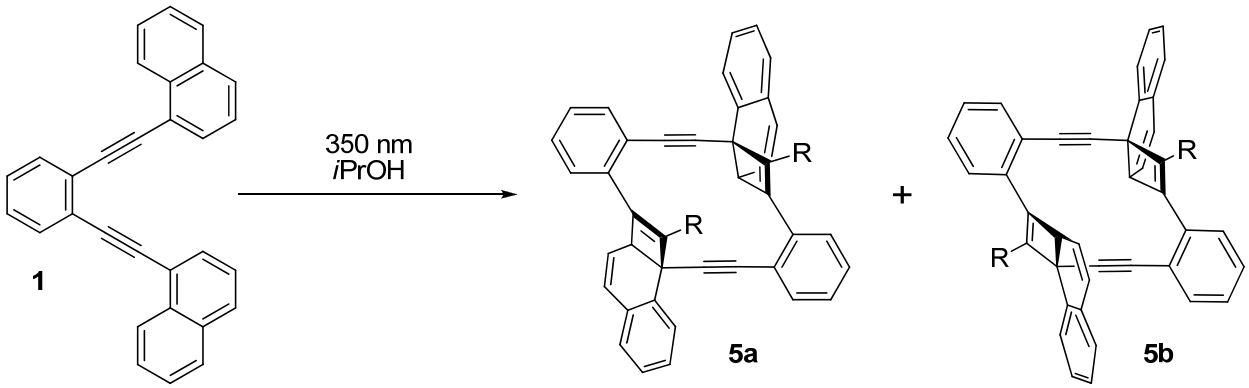
179 °C (dec); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.06 (s, 2H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.62-7.59 (m, 6H), 7.32 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.15-7.11 (m, 4H), 3.92 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 158.4, 134.2, 131.6, 131.5, 129.3, 129.0, 128.5, 127.9, 126.8, 126.1, 119.4, 118.2, 105.8, 94.4, 88.3, 55.3; UV-vis (CH_3CN): λ_{max} nm (log ε) = 307 (4.74), 265 (4.90), 250 (4.89), 227 (4.92); IR (KBr): cm^{-1} = 2202; HRMS: calcd. for $C_{32}H_{22}O_2$ $[M + Na]^+$ 461.1517 *m/z*, found 461.1501 *m/z*.

Photolysis of 1,2-bis((6-methoxynaphthalen-2-yl)ethynyl)benzene 3



1,2-bis((6-methoxynaphthalen-2-yl)ethynyl)benzene **3** (12.5 mg, 0.029 mmol) was placed in a quartz reaction tube, dissolved in 3:1 *i*PrOH/C_6H_6 (150 mL), and the resulting solution was purged with argon for 20 minutes and sealed. The solution was irradiated with a Rayonet photochemical reactor equipped with sixteen 300 nm lamps for 18 hours at 35-40 °C (reactor temperature with circulating fan). After removal of the solvents by rotary evaporation the crude product was purified by preparative thin layer chromatography (2:1 hexanes/THF) to afford 2,3-bis(6-methoxynaphthalen-2-yl)naphthalene **4** as a yellow solid (4.0 mg, 32%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.02 (s, 2H), 7.93 (dd, *J* = 6.1, 3.2 Hz, 2H), 7.85 (d, *J* = 1.2 Hz, 2H), 7.68 (d, *J* = 9.0 Hz, 2H), 7.53 (dd, *J* = 6.2, 3.3 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.17 (dd, *J* = 8.5, 1.8 Hz, 2H), 7.12 (dd, *J* = 9.0, 2.6 Hz, 2H), 7.05 (d, *J* = 2.4 Hz, 2H), 3.90 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 157.7, 139.1, 137.0, 133.2, 132.8, 129.8, 129.5, 129.0, 128.9, 128.2, 127.7, 126.3, 126.0, 118.7, 105.6, 55.3; HRMS: calcd. For $C_{32}H_{24}O_2$ $[M + Na]^+$ 463.1674 *m/z*, found 463.1662 *m/z*.

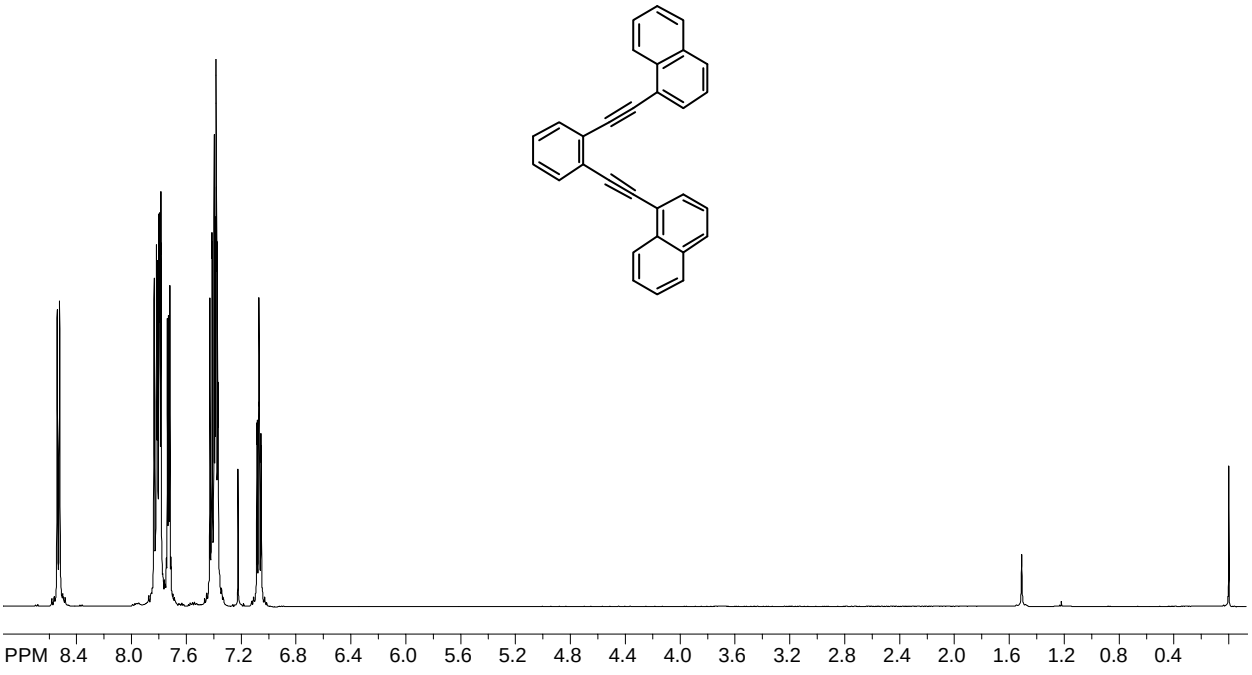
Photolysis of 1,2-bis(naphthalen-1-ylethynyl)benzene 1

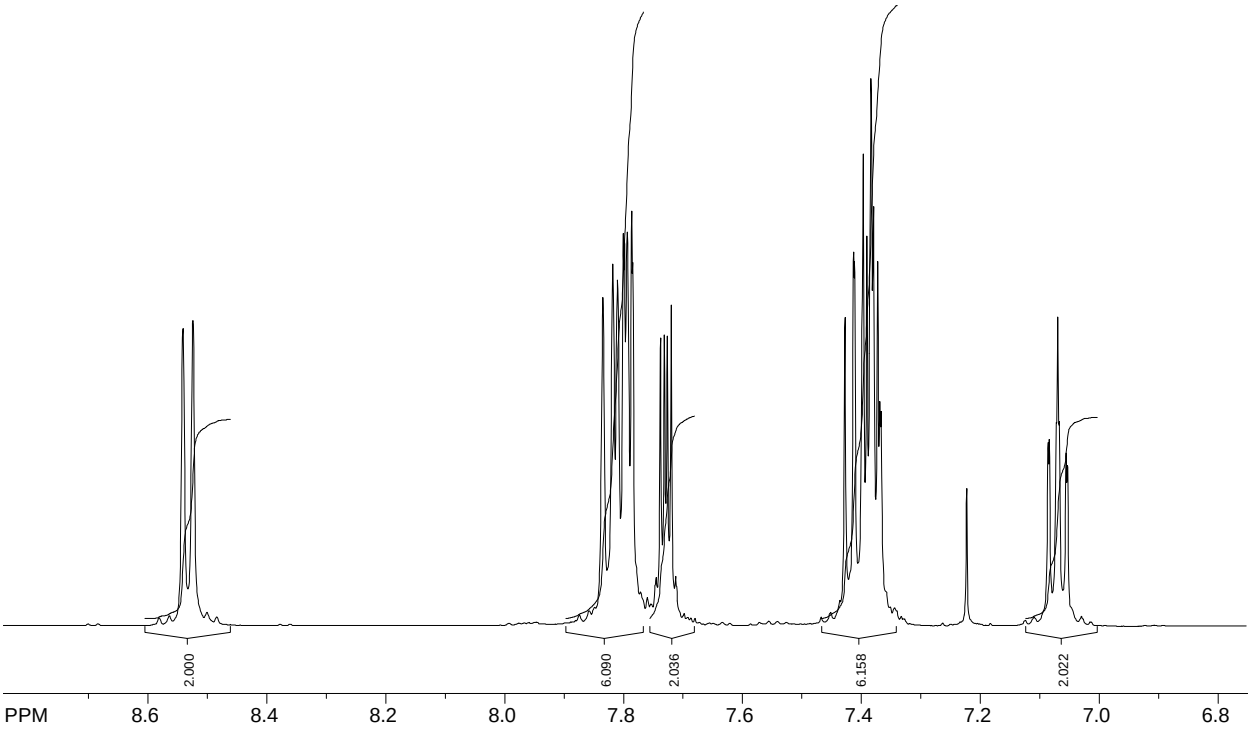


1,2-bis(naphthalen-1-ylethynyl)benzene **1** (0.201 g, 0.530 mmol) was placed in a quartz reaction tube, dissolved in isopropanol (450 mL), and the resulting solution was purged with argon for 20 minutes and sealed. The solution was irradiated with a Rayonet photochemical reactor equipped with sixteen 350 nm lamps for 24 hours at 35-40 °C (reactor temperature with circulating fan). After removal of the solvent by rotary evaporation the crude ^{1}H NMR spectrum indicated starting material was present along with two new products that were formed in a 4:1 ratio. Unreacted starting material (0.054 g) was subsequently removed by silica gel column chromatography (4:1 hexanes/CH_2Cl_2). The desired fractions containing the major, minor, and other byproducts were combined and further purified by slow recrystallization from 1:1 CH_2Cl_2/hexanes (60 mL) to afford the major product **5a** as a white solid (0.016 g, 11.0% based on recovered starting material). mp = 280-281 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.75-7.70 (m, 6H), 7.43 (dd, *J* = 7.0, 1.1 Hz, 2H), 7.37 (d, *J* = 7.5 Hz, 2H), 7.29-7.26 (m, 6H), 7.21-7.19 (m, 4H), 7.09-6.93 (m, 10H), 6.51 (d, *J* = 10.0 Hz, 2H), 6.05 (dd, *J* = 9.9, 4.4 Hz, 2H), 5.25 (dd, *J* = 4.4, 0.9 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 149.9, 144.2, 135.7, 133.6, 133.1, 132.3, 132.2, 131.0, 130.6, 128.5, 128.3, 128.2, 128.1, 127.9, 127.7, 127.65, 127.63, 127.62, 127.60, 127.5, 126.3, 126.1, 125.7, 125.5, 125.1, 122.2, 98.0, 80.9, 51.1, 47.0; HRMS: calcd. For $C_{60}H_{36}$ $[M + H]^+$ 757.2895 *m/z*, found 757.2922 *m/z*.

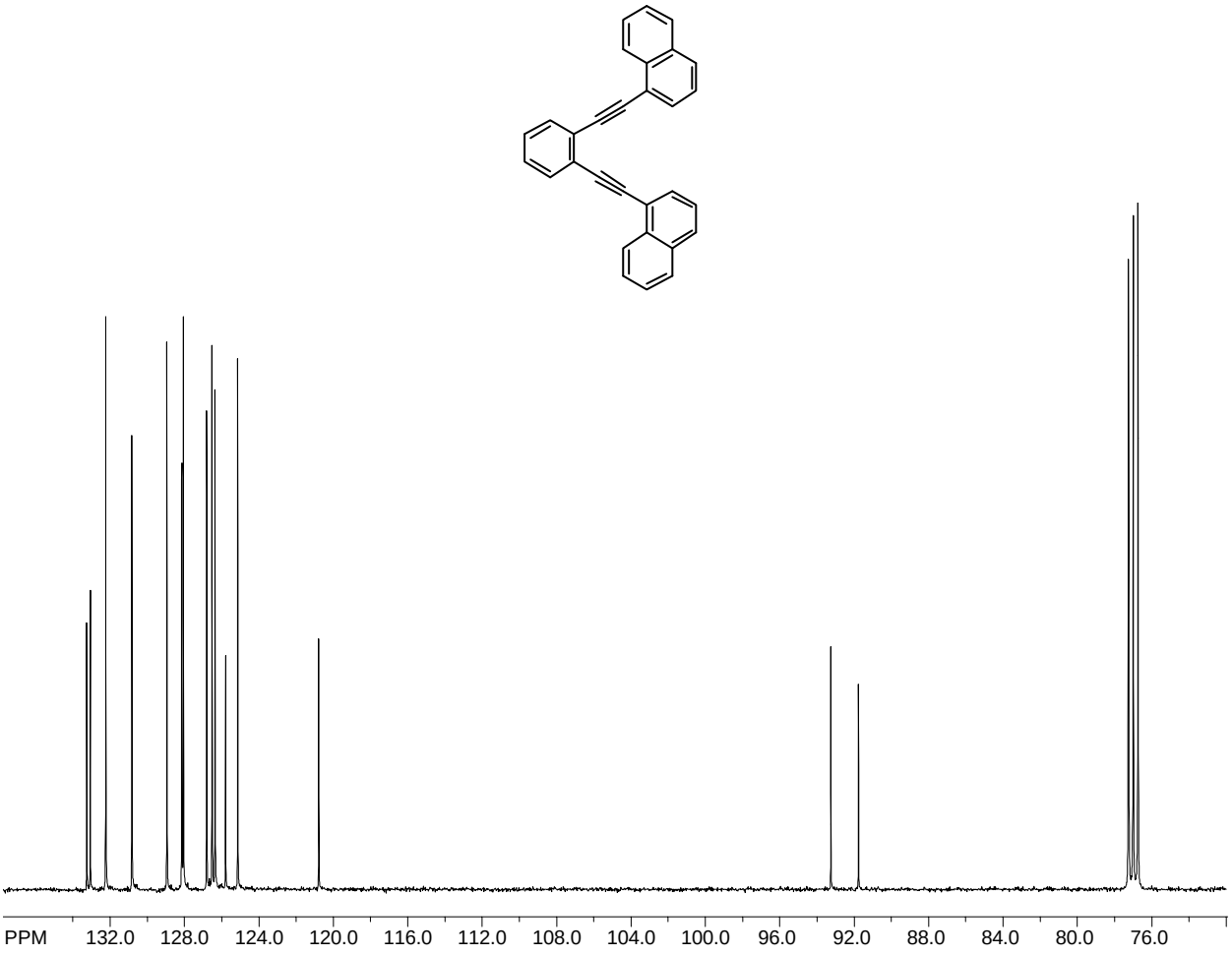
For characterization of the minor product, **5b**, the remaining filtrate from multiple recrystallizations were combined and purified by preparative thin layer chromatography (95% CCl_4 / 5% hexanes) to afford an analytically pure sample of **5b** as a white solid. mp = 278-280 ^{o}C (dec); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.09 (d, *J* = 6.8 Hz, 2H), 7.93 (dd, *J* = 7.0, 0.7 Hz, 2H), 7.74-7.70 (m, 4H), 7.46-7.39 (m, 4H), 7.33-7.27 (m, 2H), 7.23-7.20 (m, 6H), 7.16-7.05 (m, 8H), 6.94 (dt, *J* = 7.4, 2.0 Hz, 2H), 6.29 (d, *J* = 10.0 Hz, 2H), 5.23 (dd, *J* = 7.6, 4.1 Hz, 2H), 4.35 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 147.4, 142.9, 133.1, 133.0, 132.6, 130.9, 130.8, 130.0, 129.8, 128.7, 127.8, 127.5, 127.0, 126.9, 126.8, 126.5, 126.3, 126.1, 126.0, 125.6, 125.4, 124.9, 124.7, 124.4, 97.0, 80.9, 53.2, 44.9; HRMS: calcd. For $C_{60}H_{36}$ $[M + H]^+$ 757.2895 *m/z*, found 757.2949 *m/z*.

^{1}H NMR Spectrum of **1**
(500 MHz, $CDCl_3$)

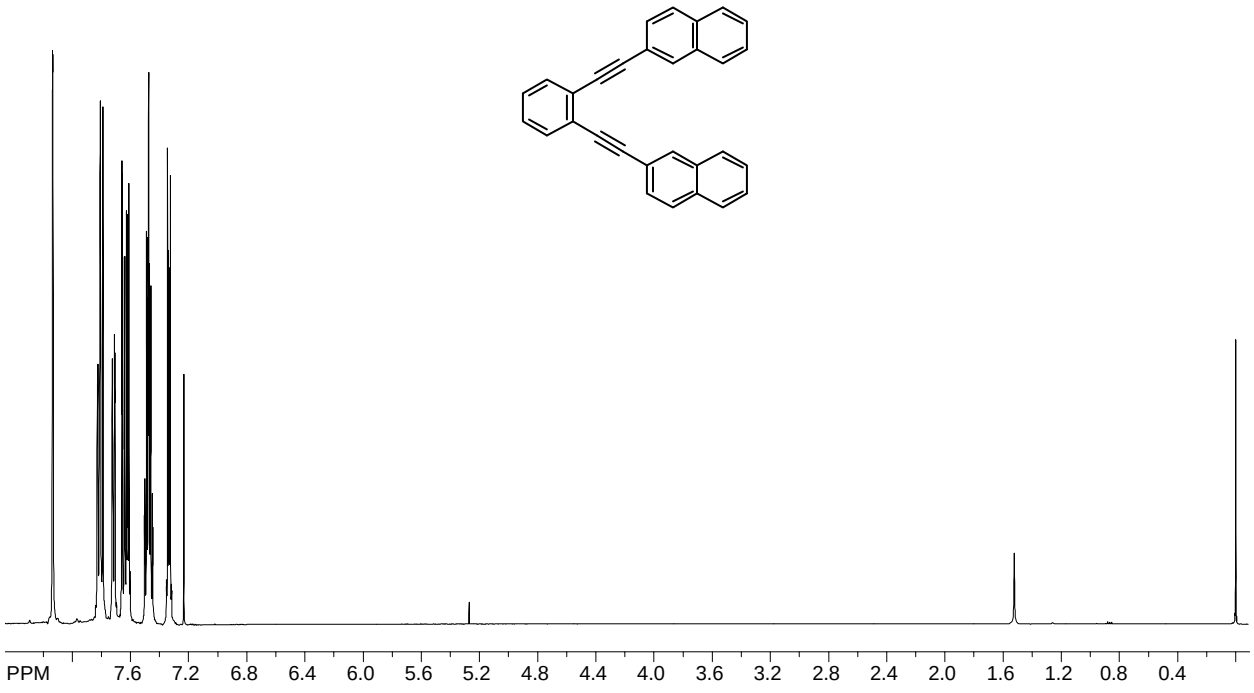


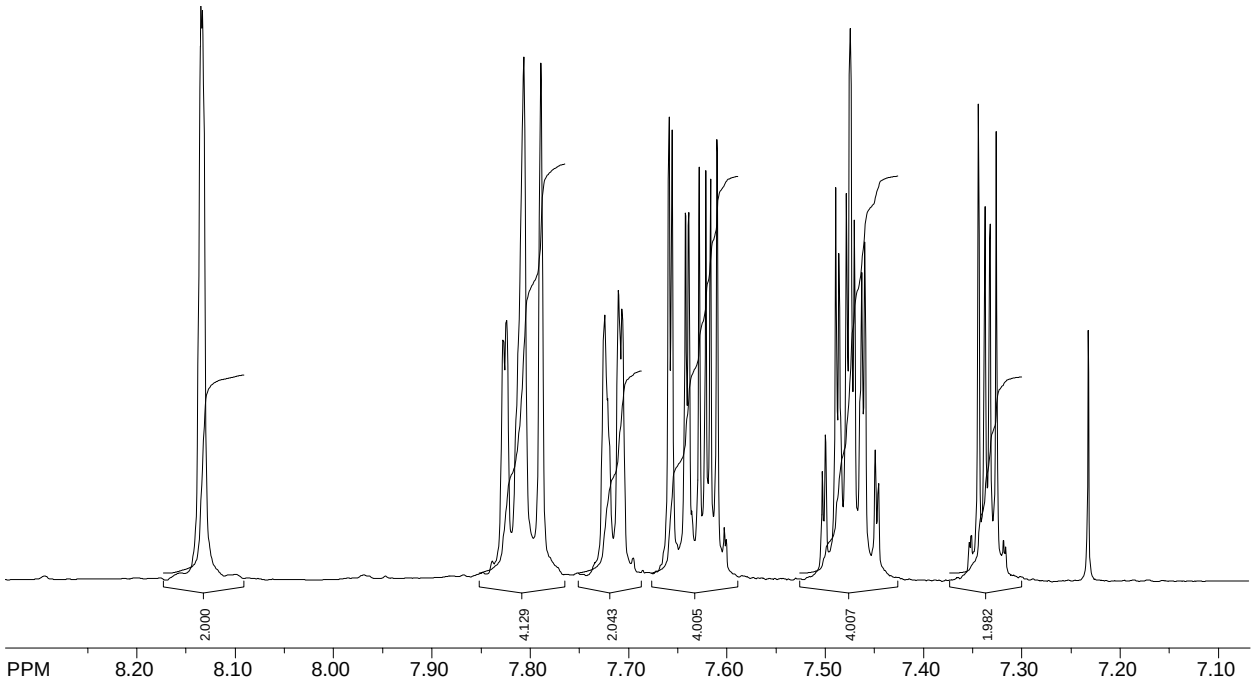


^{13}C NMR Spectrum of **1**
(125 MHz, $CDCl_3$)

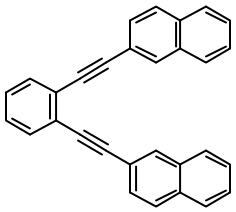


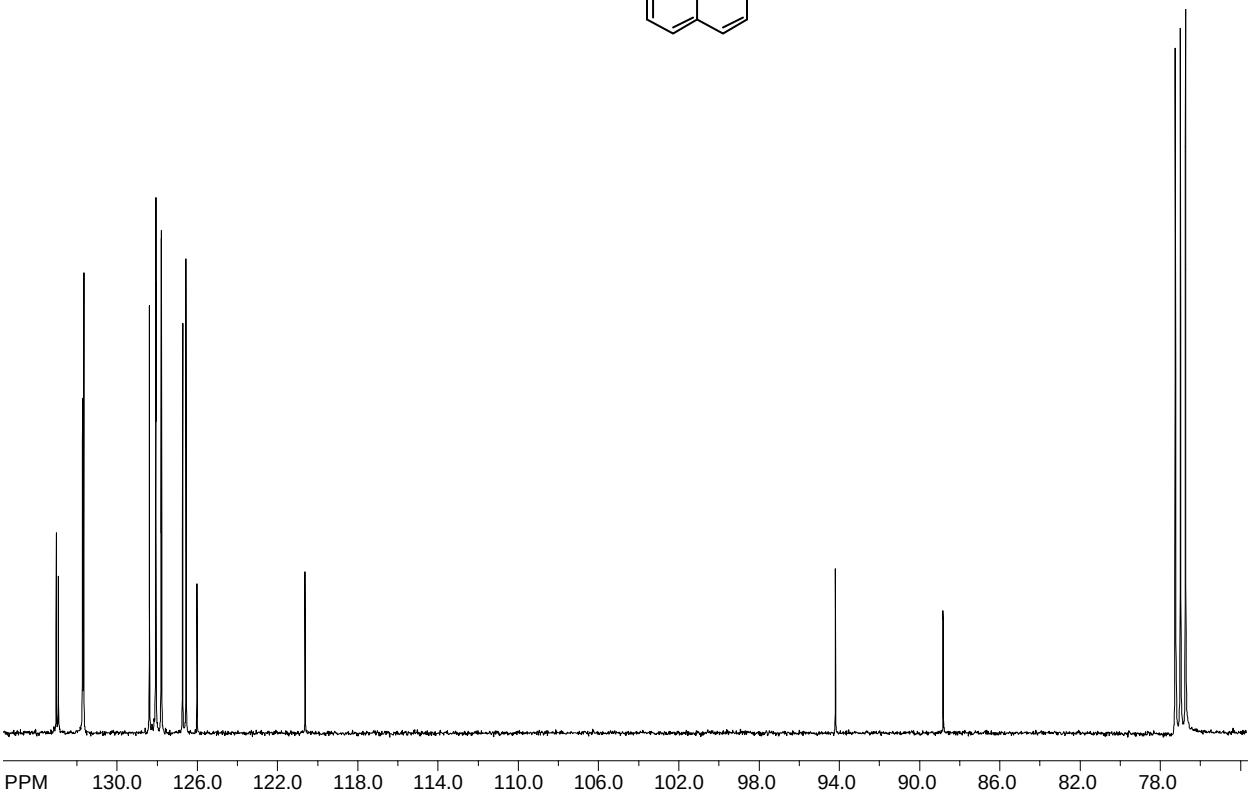
^{1}H NMR Spectrum of **2**
(500 MHz, $CDCl_3$)



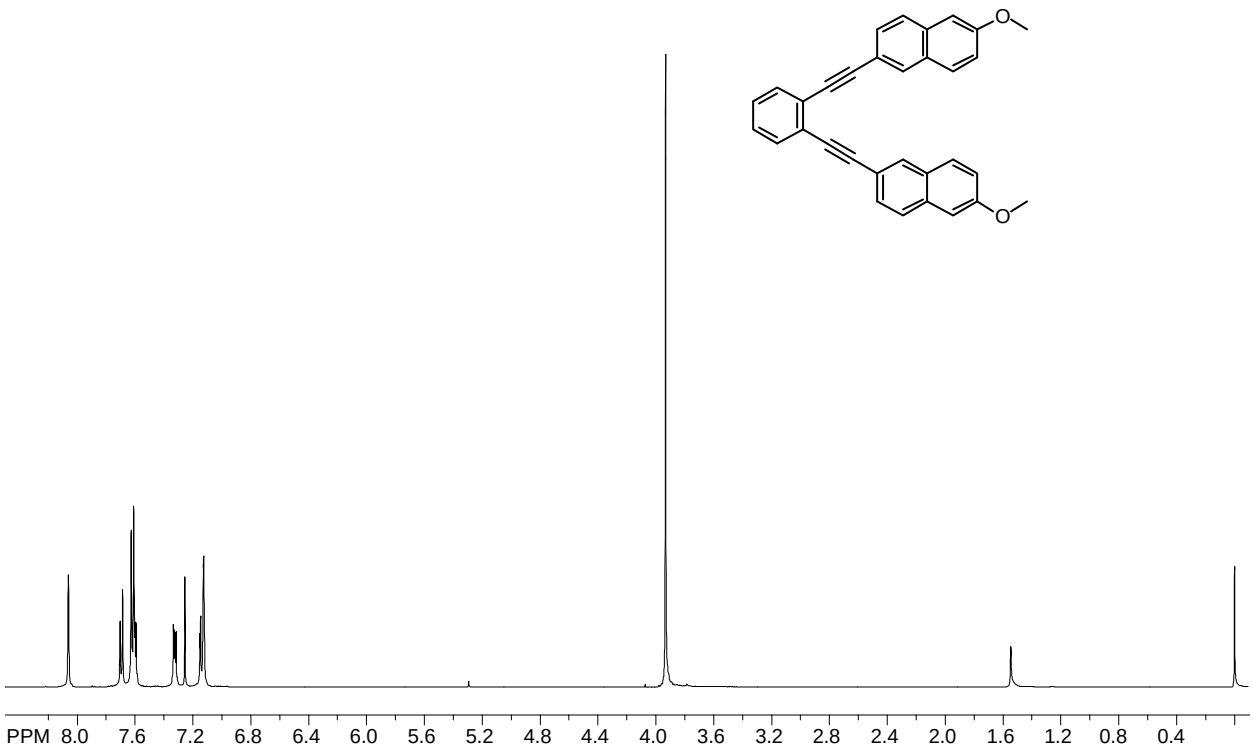


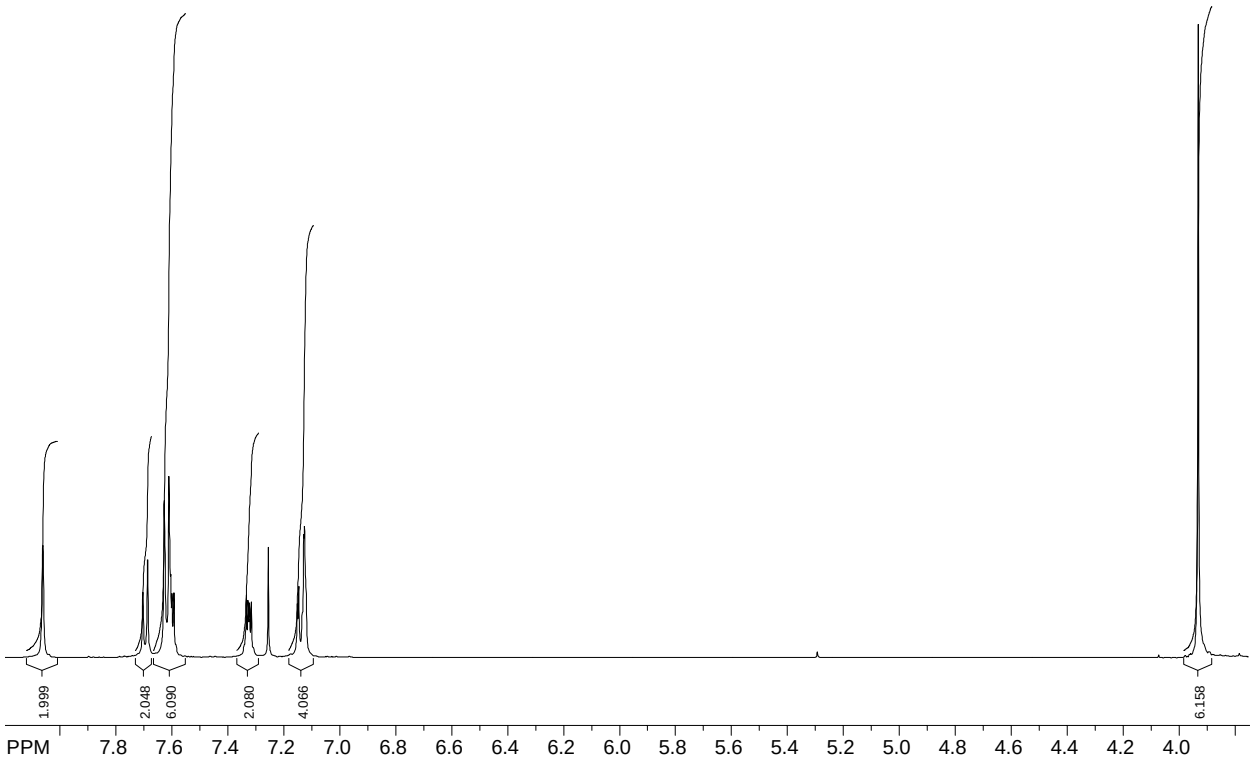
^{13}C NMR Spectrum of **2**
(125 MHz, $CDCl_3$)



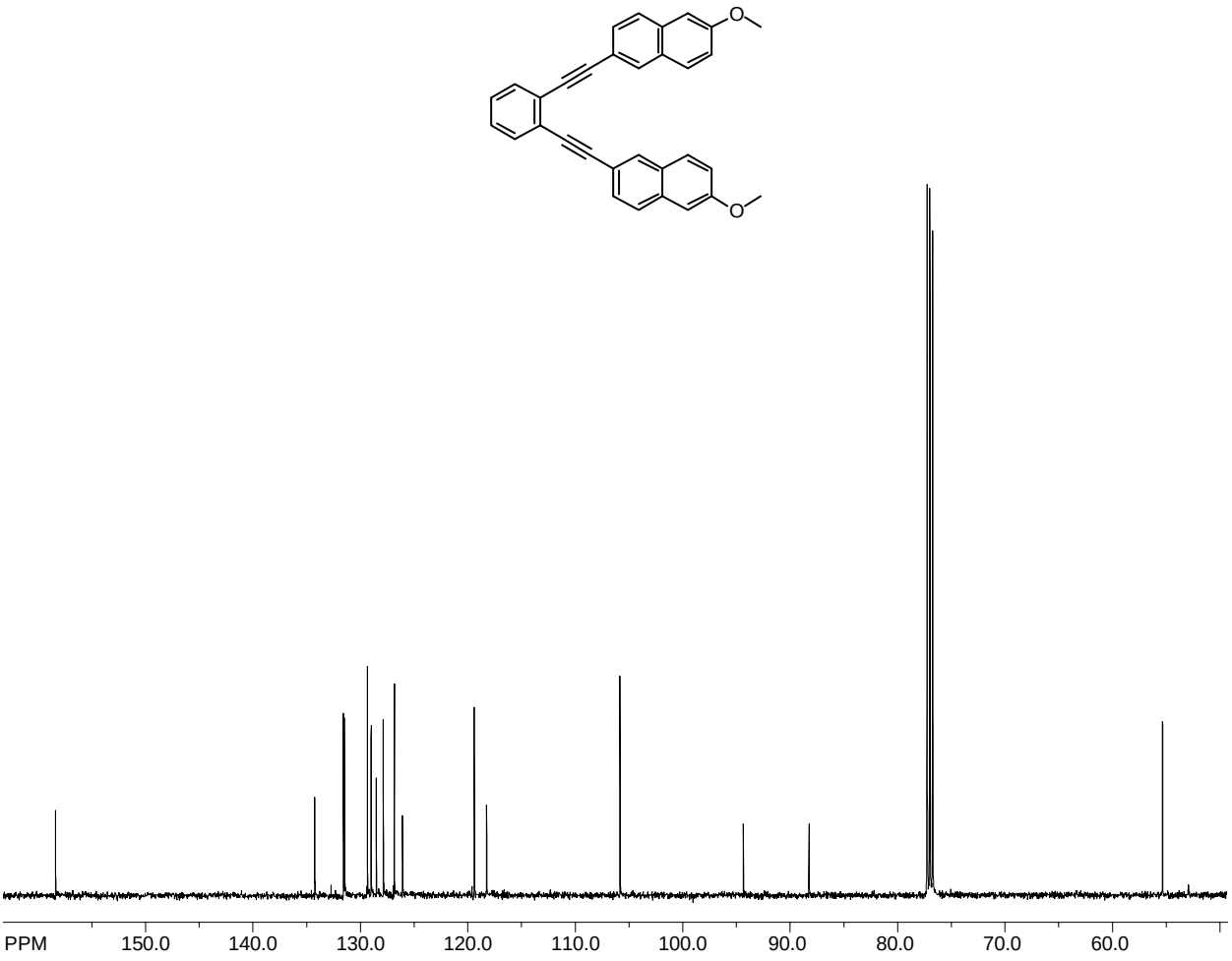


^{1}H NMR Spectrum of **3**
(500 MHz, $CDCl_3$)

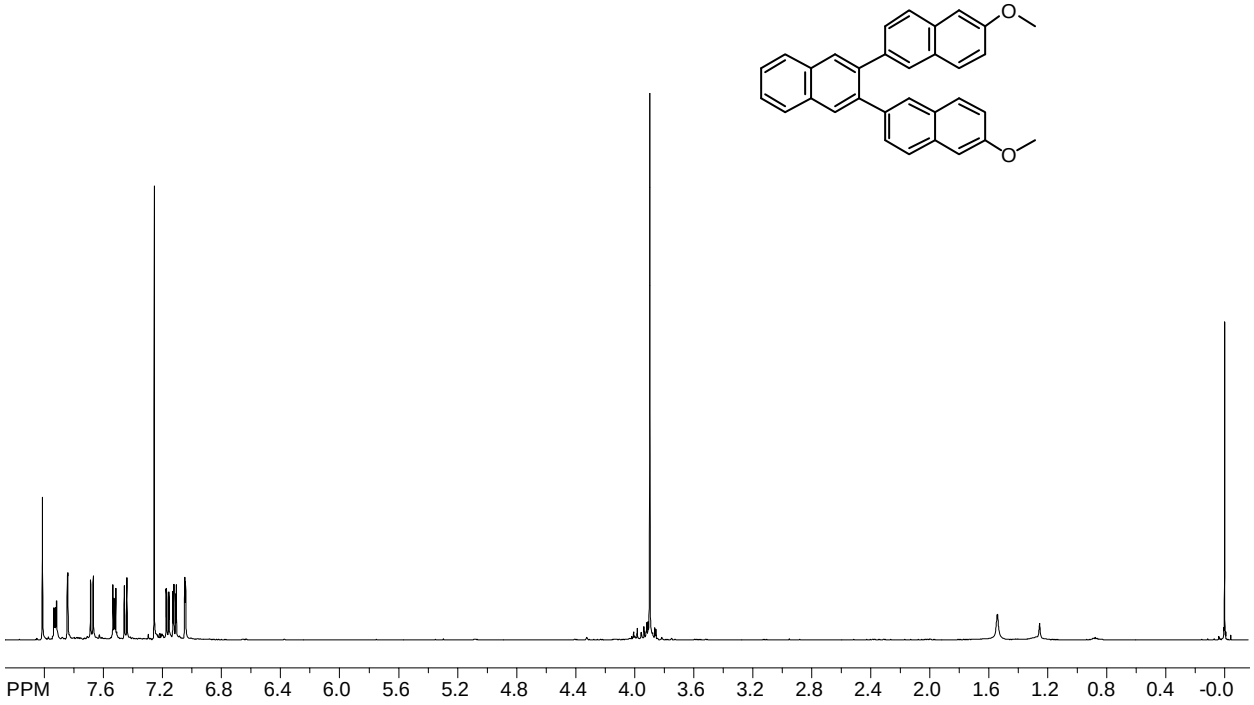


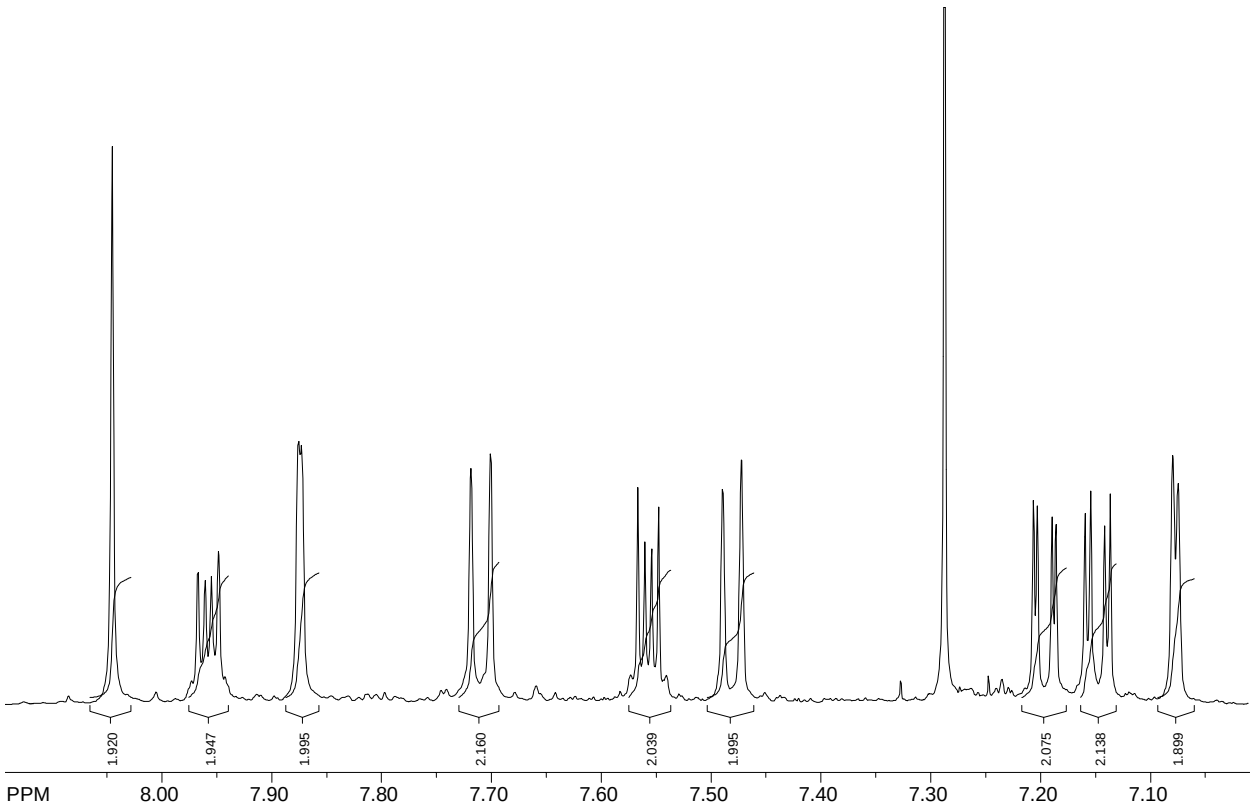


^{13}C NMR Spectrum of **3**
(125 MHz, $CDCl_3$)

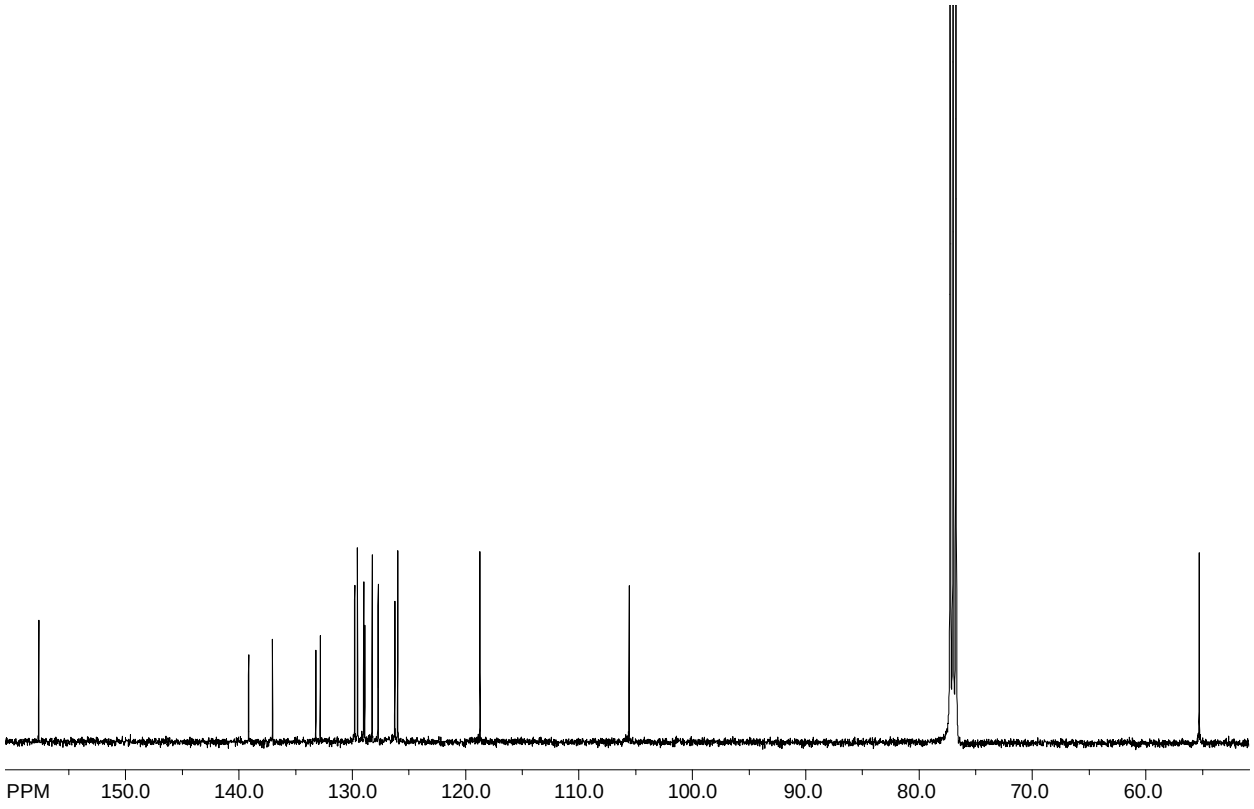


^{1}H NMR Spectrum of **4**
(500 MHz, $CDCl_3$)

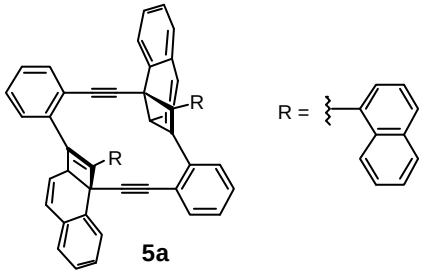




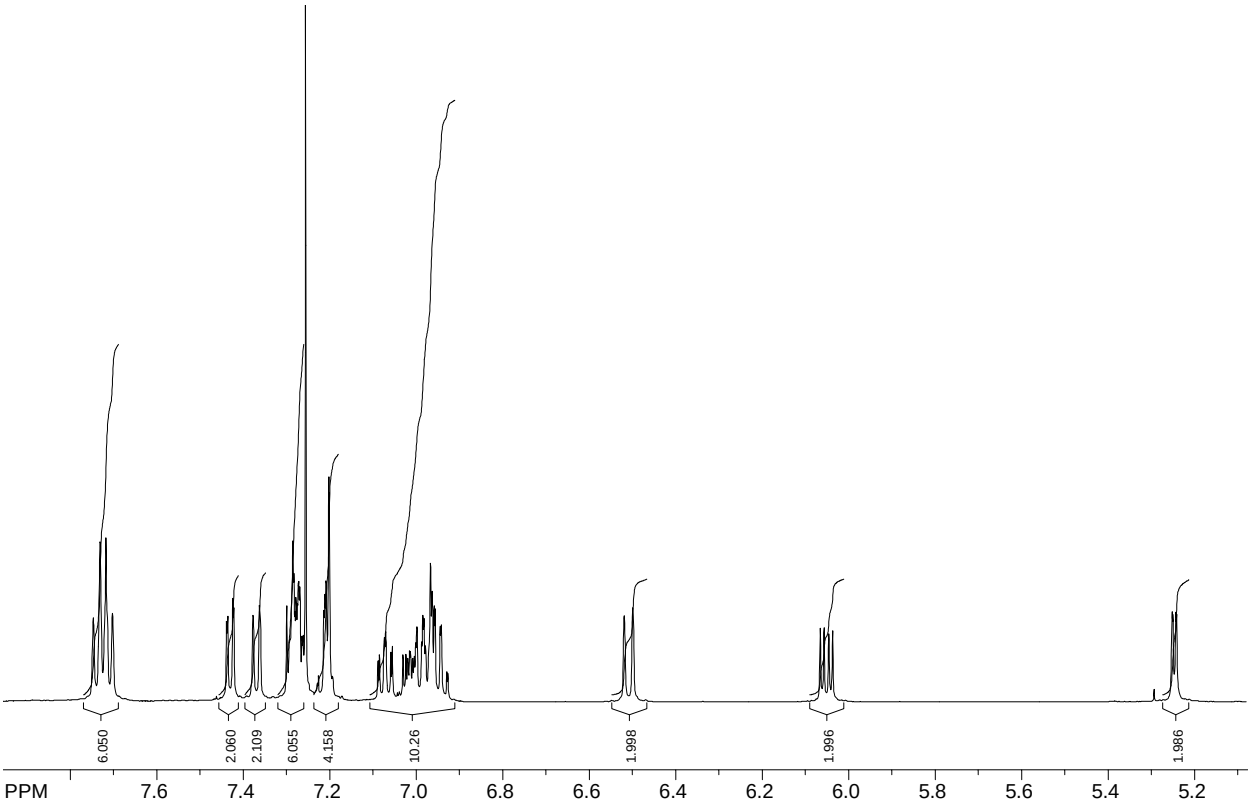
^{13}C NMR Spectrum of **4**
(125 MHz, $CDCl_3$)



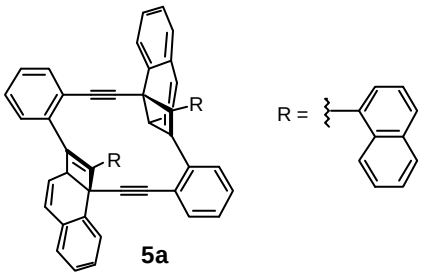
^{1}H NMR Spectrum of **5a**
(500 MHz, $CDCl_3$)



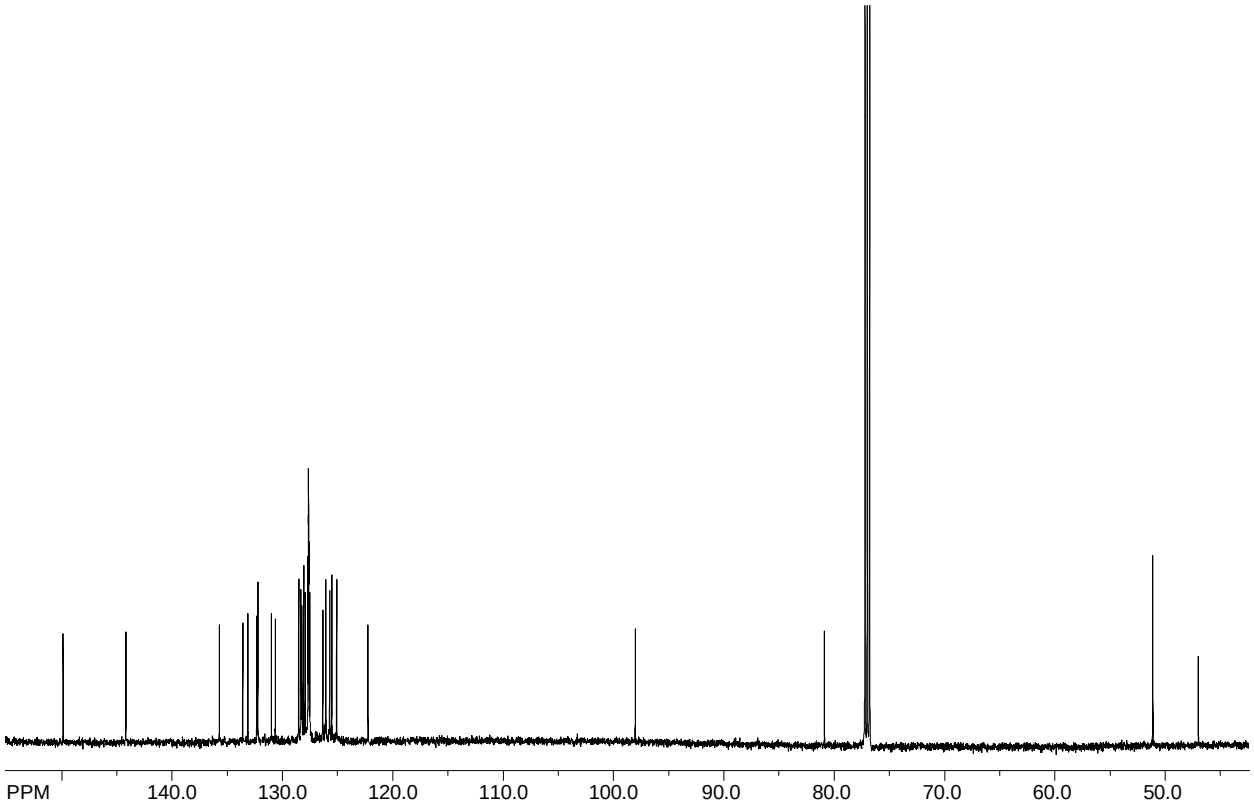
5a



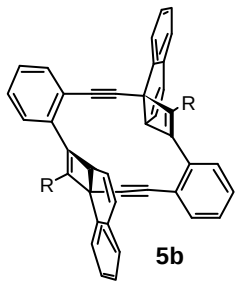
^{13}C NMR Spectrum of **5a**
(125 MHz, $CDCl_3$)



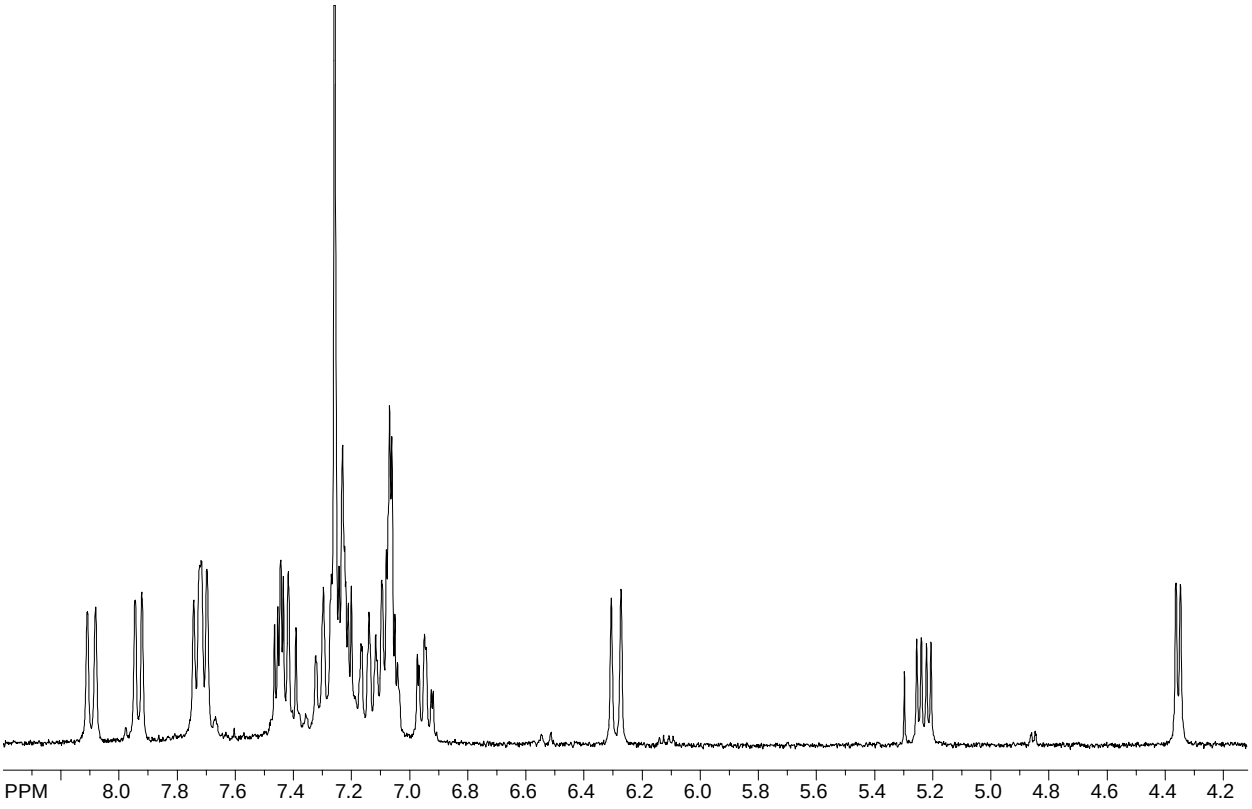
5a



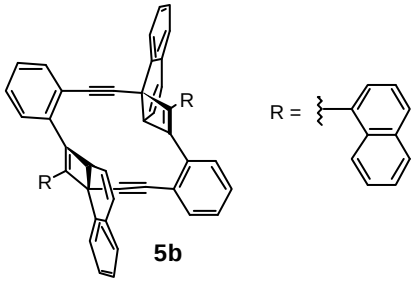
^{1}H NMR Spectrum of **5b**
(300 MHz, $CDCl_3$)



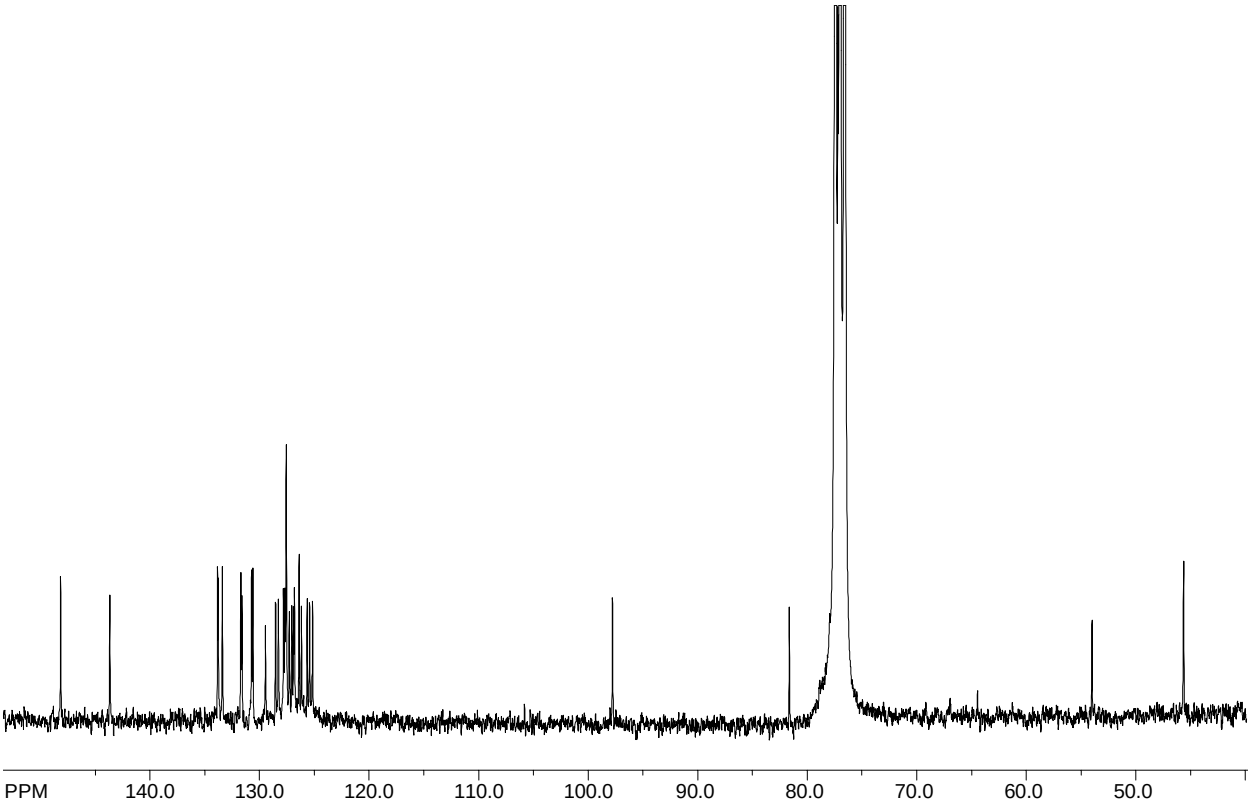
5b



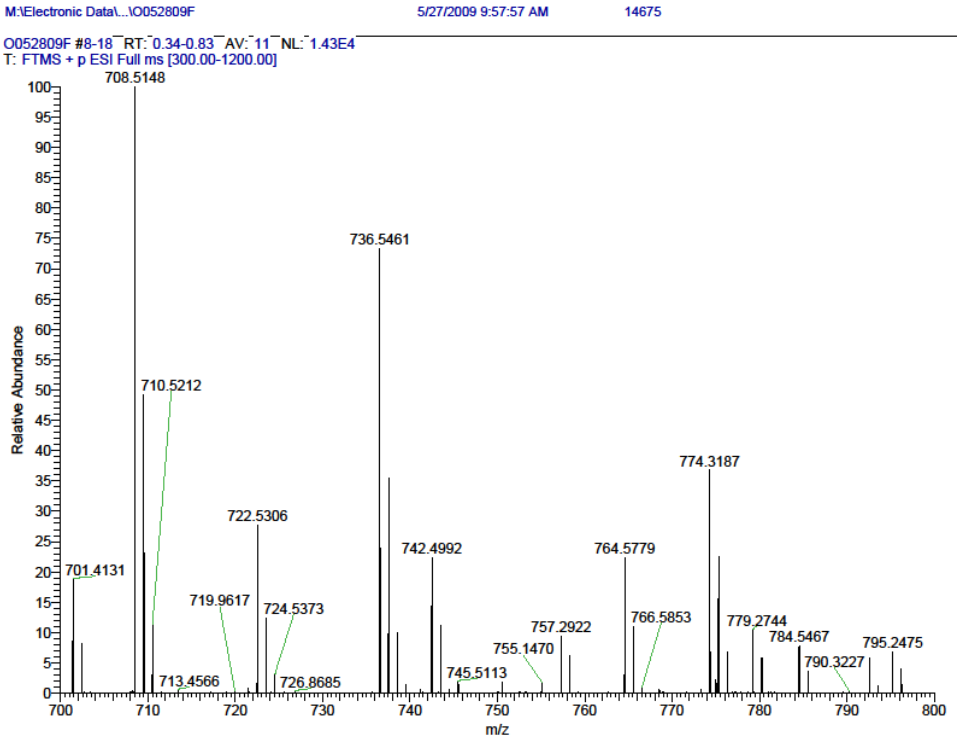
^{13}C NMR Spectrum of **5b**
(75 MHz, $CDCl_3$)



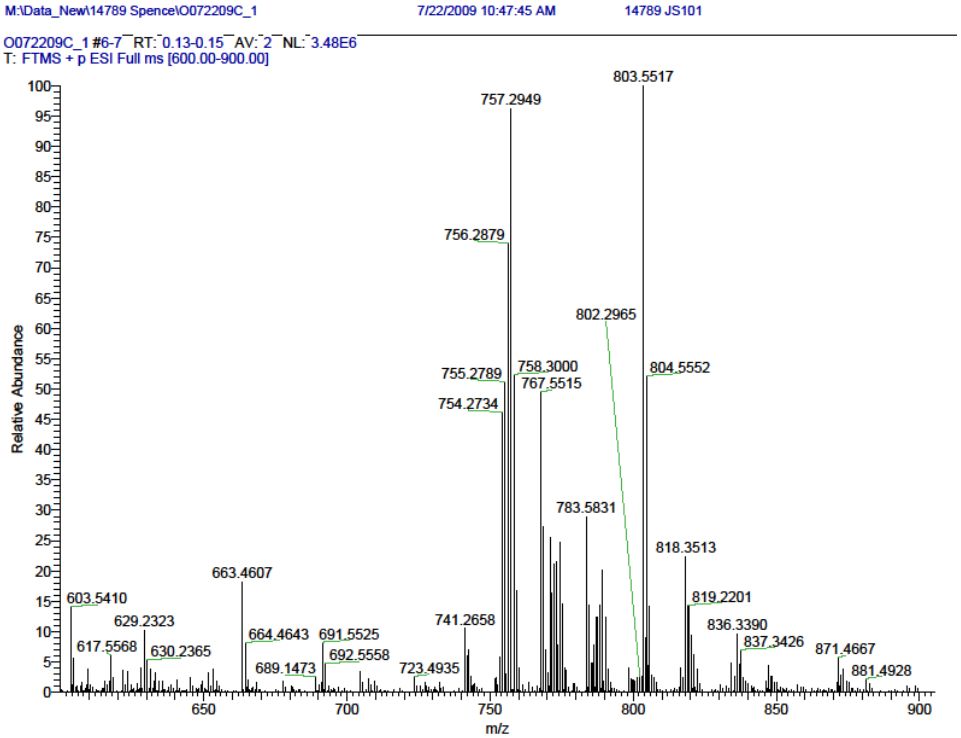
5b



4. HRMS Data



Compound **5a** Theoretical M + H = 757.2895, Observed 757.2922

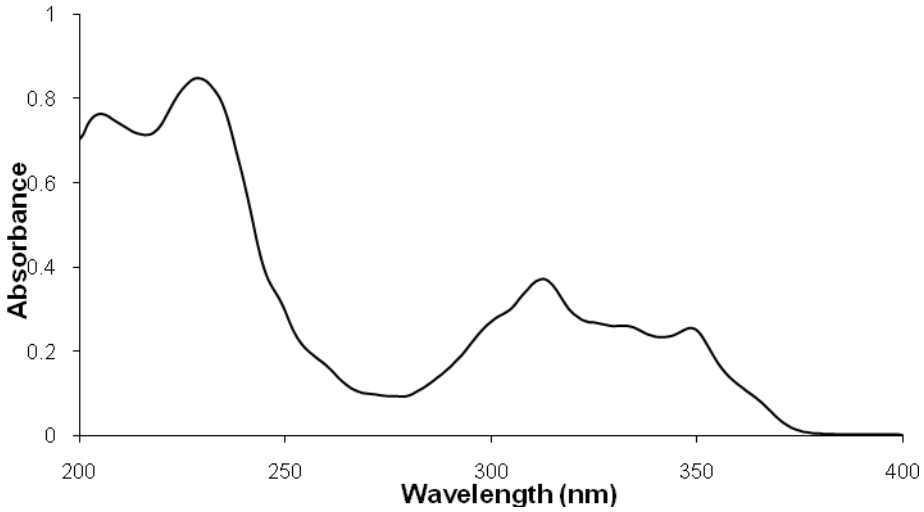


Compound **5b** Theoretical M + H = 757.2895, Observed 757.2949

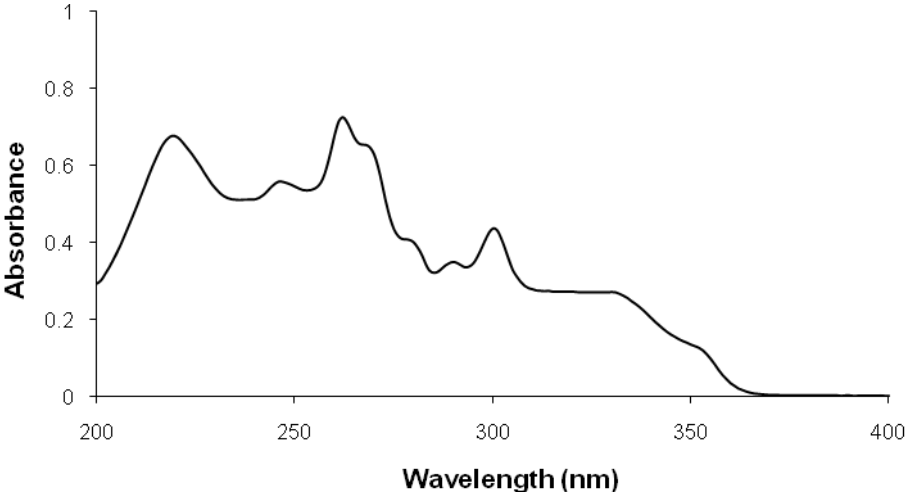
5. Absorbance Spectra

Measured in CH_3CN. Concentration for compound **1** is 1.1×10^{-5}. Concentration for compounds **2** and **3** is 1.0×10^{-5}.

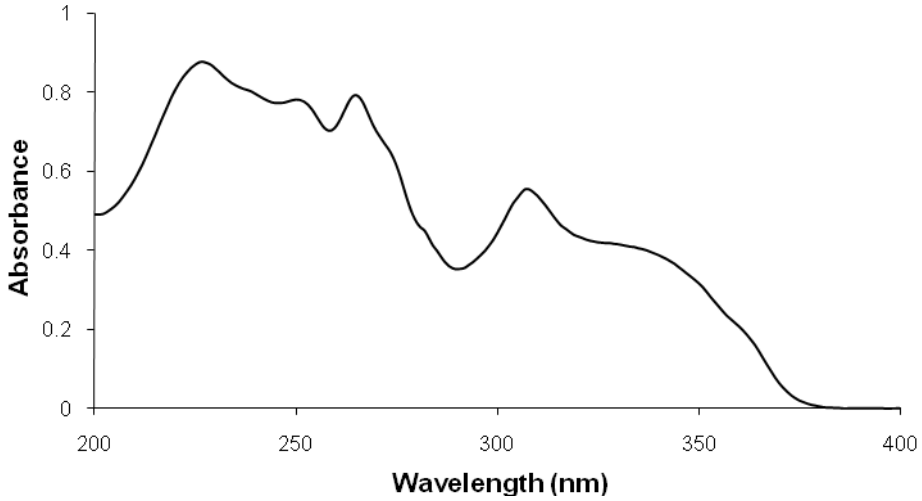
UV/Visible Absorbance Spectrum of **1**



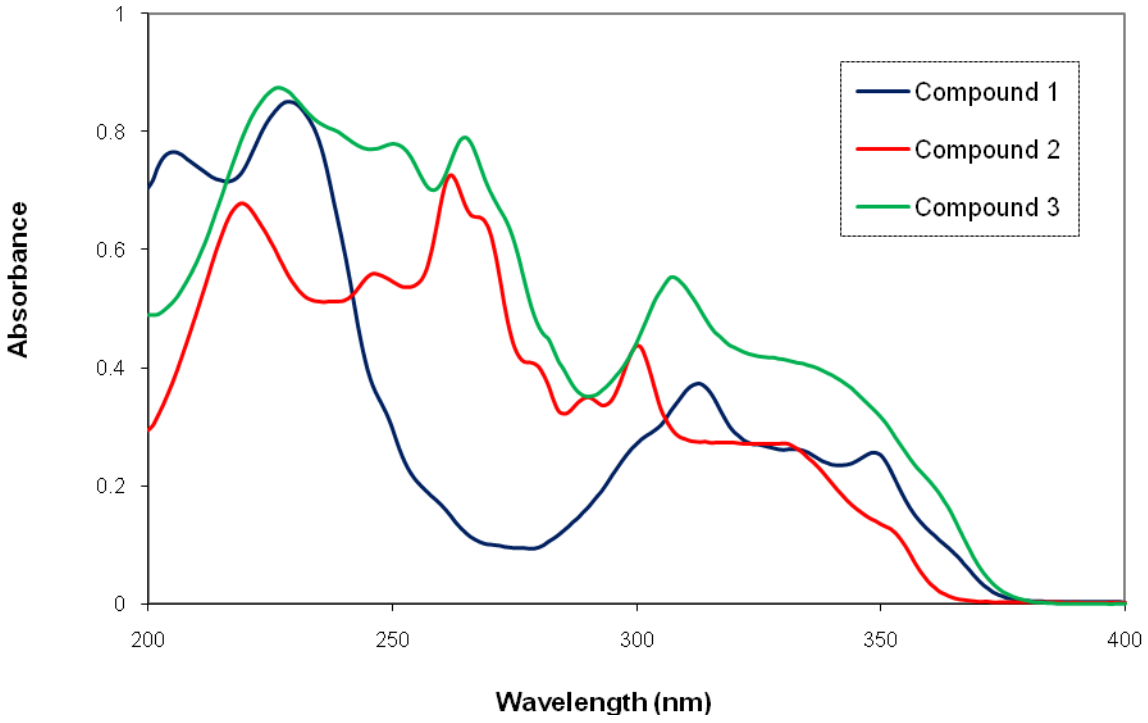
UV/Visible Absorbance Spectrum of **2**



UV/Visible Absorbance Spectrum of **3**



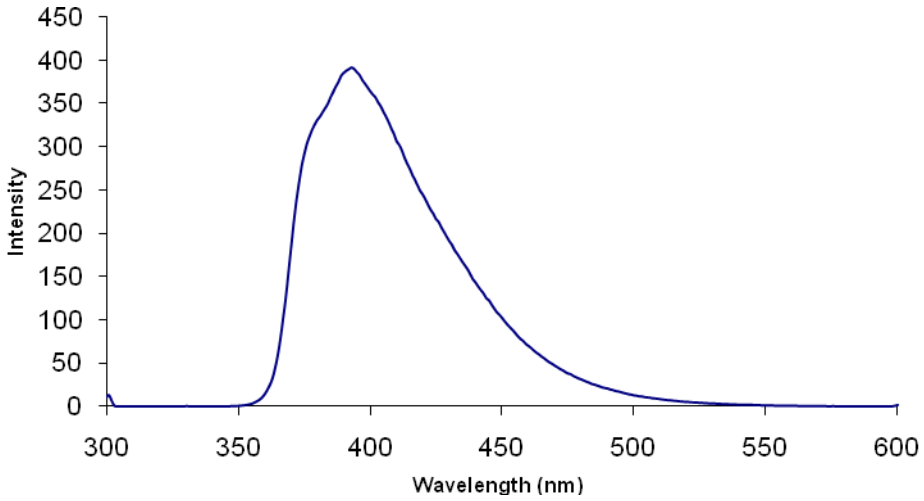
UV/Visible Absorbance Spectra of Compounds **1-3**



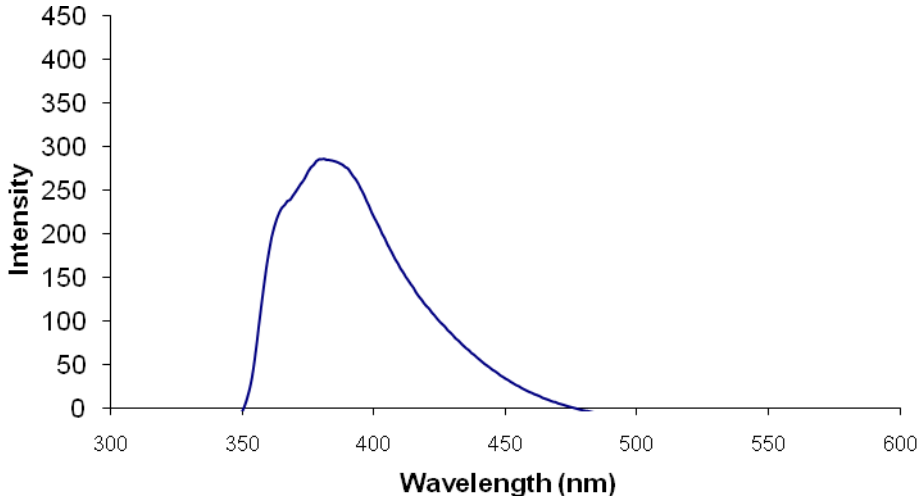
6. Emission Spectra

Measured in CH_3CN at room temperature. Concentration for compound **1** is 1.1×10^{-5}. Concentration for compounds **2** and **3** is 1.0×10^{-5}. Excitation wavelength used is 300 nm.

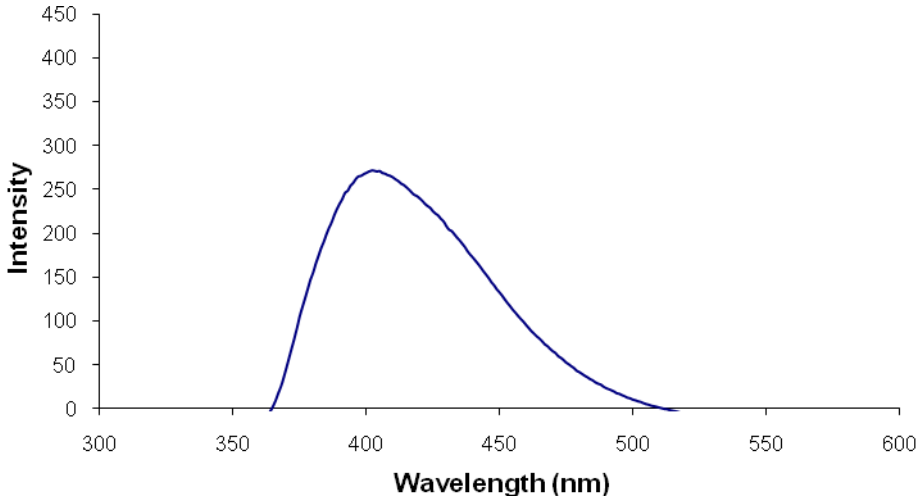
Fluorescence Spectrum of **1**



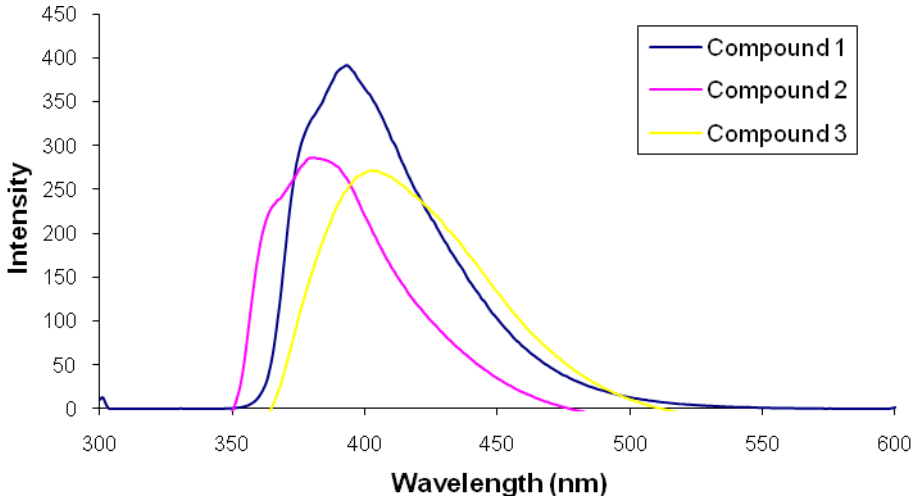
Fluorescence Spectrum of **2**



Fluorescence Spectrum of **3**

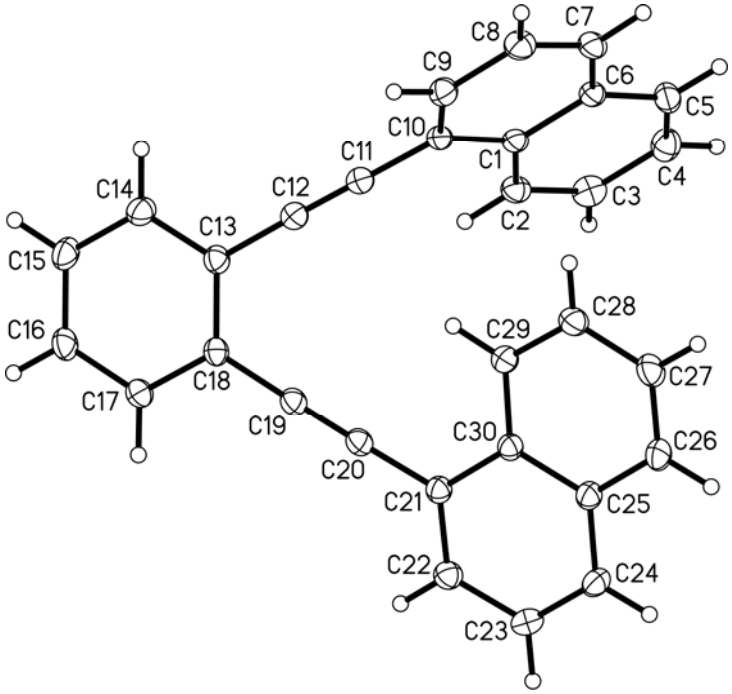


Fluorescence Spectra of Compounds **1-3**

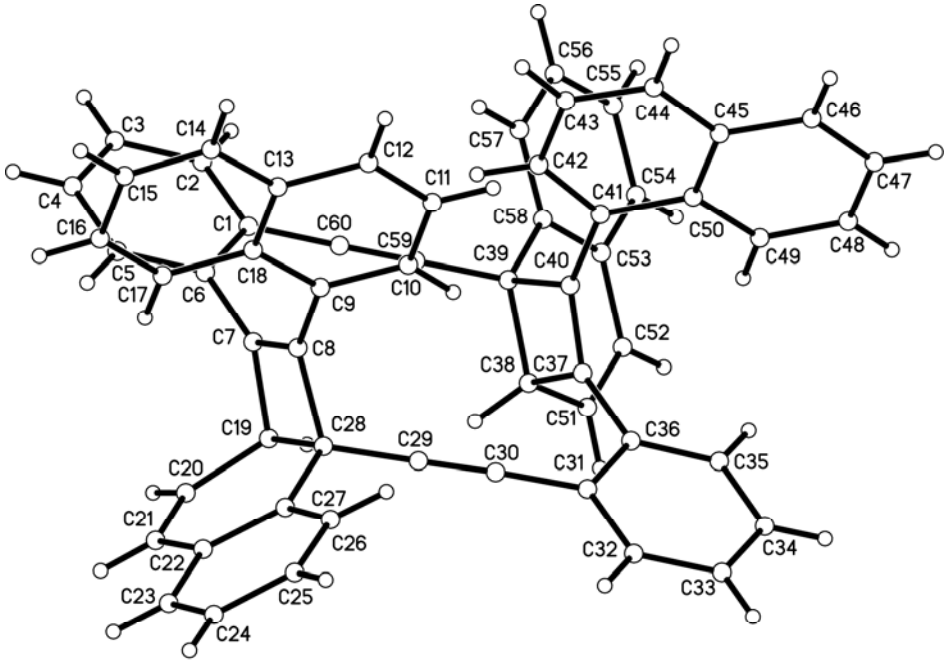


7. X-Ray Crystal Structures

X-Ray Crystal Structure of **1** with numbering scheme.



X-Ray Crystal Structure of **5a** with numbering scheme.



5a

8. Computational Methods

All calculations were carried out using Gaussian 03.[1] For the cyclization reaction coordinates, geometry optimizations were performed with mPW1PW91/6-31G(d,p), with single-point energies then calculated for the optimized geometries with mPW1PW91/cc-pVTZ. Calculations involving the closed-shell reactant arenediynes used restricted wave functions. Calculations on the open-shell transition states and diradical products used broken-symmetry unrestricted wave functions.[2,3] Both singlet and triplet states were calculated for the transition states and diradical products. In all cases, the singlet states were lower in energy (Tables S1 and S2) and were used in the calculation of the activation energies and free energies of reaction for the cyclization reactions. Vibrational frequencies were computed for each optimized structure to confirm that each geometry was a stationary point and to obtain free energies for all species. Solvation energies were determined for each of the optimized geometries in benzene, isopropanol, and acetonitrile using the IEF-PCM implicit solvent model. The density functional mPW1PW91 was chosen based on its ability to most accurately reproduce the geometry of the crystal structure of 1,2-bis(naphthalene-1-ylethynyl)benzene versus other commonly used density functionals (Table S3).

Optimized geometries for the dimer isomers were obtained at the mPW1PW91/6-31G(d,p) level, with single-point energies computed using mPW1PW91/cc-pVDZ. Again, vibrational frequencies were computed for each optimized structure to confirm that each geometry was a stationary point and to obtain free energies for the species. Solvation energies were determined for each of the optimized geometries in isopropanol using the IEF-PCM implicit solvent model.

TD-DFT calculations on the arenediynes were carried out on geometries optimized at the mPW1PW91/6-31G(d,p) level using mPW1PW91/6-311++G(d,p) with the IEF-PCM implicit solvent model with dichloromethane as the solvent.

Table S1. Singlet versus triplet gas phase electronic energies for the cyclization transition states at the mPW1PW91/cc-pVTZ//mPW1PW91/6-31G(d,p) level of theory (kcal/mol). Computed as singlet minus triplet.

Arylethynyl Substituent	C^1-C^5	C^1-C^6
phenylethynyl	-40.46	-38.92
(naphthalen-1-yl)ethynyl (1)	-36.58	-34.40
(naphthalen-2-yl)ethynyl (2)	-38.02	-36.98
(6-methoxynaphthalen-2-yl)ethynyl (3)	-38.51	-36.48

Table S2. Singlet versus triplet gas phase electronic energies for the cyclization diradical products at the mPW1PW91/cc-pVTZ//mPW1PW91/6-31G(d,p) level of theory (kcal/mol). Computed as singlet minus triplet.

Arylethynyl Substituent	C^1-C^5	C^1-C^6
phenylethynyl	-3.12	-1.22
(naphthalen-1-yl)ethynyl (1)	-1.65	-2.44
(naphthalen-2-yl)ethynyl (2)	-1.96	-1.19
(6-methoxynaphthalen-2-yl)ethynyl (3)	-2.99	-1.12

Table S3. RMSD (10^{-3} Å) for the geometries optimized with various density functionals with the 6-31G(d,p) basis set versus the crystal structure for 1,2-bis(naphthalen-1-ylethynyl)benzene.

	pure density functionals					
	BLYP[4,5]	mPWPW91[6,7]	TPSS[8]	HCTH[9]		
RMSD (10^{-3} Å)	11	8	8	3		
	hybrid density functionals					
	B3LYP[4,5,10]	mPW1PW91[6,7,11]	TPSSh[8]	O3LYP[5,12,13]	X3LYP[14]	B97-1[9,15]
RMSD (10^{-3} Å)	3	2	4	3	3	6

Table S4. Activation energies ($\Delta G^{‡}$, 25 °C) for cyclization of 1,2-bis(arylethynyl)benzenes (kcal/mol) in solvent.

a) benzene

Arylethynyl Substituent	$\Delta G^{‡}$ C^1-C^5	$\Delta G^{‡}$ C^1-C^6	$\Delta\Delta G^{‡}$
phenylethynyl	42.45	45.87	-3.42
(naphthalen-1-yl)ethynyl (1)	40.93	46.14	-5.21
(naphthalen-2-yl)ethynyl (2)	41.94	46.01	-4.07
(6-methoxynaphthalen-2-yl)ethynyl (3)	40.67	45.37	-4.70

b) isopropanol

Arylethynyl Substituent	$\Delta G^{‡}$ C^1-C^5	$\Delta G^{‡}$ C^1-C^6	$\Delta\Delta G^{‡}$
phenylethynyl	42.49	46.28	-3.79
(naphthalen-1-yl)ethynyl (1)	41.00	45.85	-4.85
(naphthalen-2-yl)ethynyl (2)	41.49	46.19	-4.70
(6-methoxynaphthalen-2-yl)ethynyl (3)	40.53	45.98	-5.45

c) acetonitrile

Arylethynyl Substituent	$\Delta G^{‡}$ C^1-C^5	$\Delta G^{‡}$ C^1-C^6	$\Delta\Delta G^{‡}$
phenylethynyl	42.44	46.31	-3.87
(naphthalen-1-yl)ethynyl (1)	41.07	46.64	-5.57
(naphthalen-2-yl)ethynyl (2)	41.51	46.28	-4.77
(6-methoxynaphthalen-2-yl)ethynyl (3)	40.63	45.96	-5.33

Table S5. Free energies of reaction (ΔG, 25 °C) for cyclization of 1,2-bis(arylethynyl)benzenes (kcal/mol) in solvent.

a) benzene

Arylethynyl Substituent	ΔG C^1-C^5	ΔG C^1-C^6	ΔΔG
phenylethynyl	35.92	29.48	6.44
(naphthalen-1-yl)ethynyl (1)	34.58	30.84	3.74
(naphthalen-2-yl)ethynyl (2)	35.48	28.90	6.58
(6-methoxynaphthalen-2-yl)ethynyl (3)	34.08	28.93	5.15

b) isopropanol

Arylethynyl Substituent	ΔG C^1-C^5	ΔG C^1-C^6	ΔΔG
phenylethynyl	36.55	30.50	6.05
(naphthalen-1-yl)ethynyl (1)	35.09	31.52	3.57
(naphthalen-2-yl)ethynyl (2)	35.62	29.32	6.30
(6-methoxynaphthalen-2-yl)ethynyl (3)	34.59	29.63	4.96

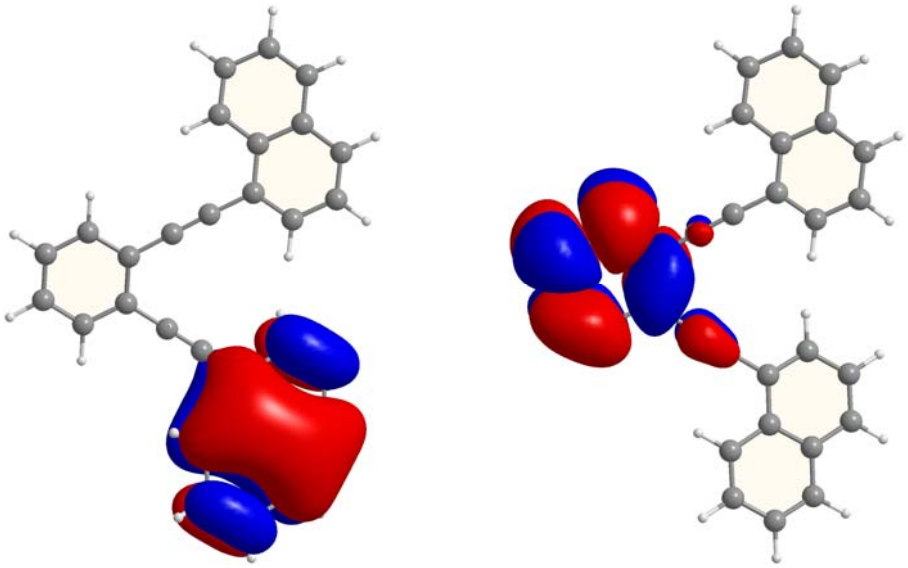
c) acetonitrile

Arylethynyl Substituent	ΔG C^1-C^5	ΔG C^1-C^6	ΔΔG
phenylethynyl	36.63	30.55	6.08
(naphthalen-1-yl)ethynyl (1)	35.17	32.31	2.86
(naphthalen-2-yl)ethynyl (2)	35.75	29.43	6.32
(6-methoxynaphthalen-2-yl)ethynyl (3)	34.69	29.75	4.94

Table S6. Wavelength of maximum absorption λ_{max} (nm) predicted by TD-DFT calculations.

Arylethynyl Substituent	λ (nm)
phenylethynyl	287
(naphthalen-1-yl)ethynyl (1)	334
(naphthalen-2-yl)ethynyl (2)	320
(6-methoxynaphthalen-2-yl)ethynyl (3)	333

Figure S1. Initial (left) and final (right) molecular orbitals for λ_{max} electronic excitation of arenediyne **1**.



9. Cartesian Coordinates of Optimized Geometries from DFT Calculations

1,2-bis(phenylethynyl)benzene – enediyne

H	4.061594	-1.912823	1.473429
C	-2.716295	-0.674645	0.180580
C	-3.932718	-1.350571	0.354964
C	-5.143048	-0.697326	0.177570
C	-5.162533	0.650740	-0.177989
C	-3.971602	1.337537	-0.359753
C	-2.736119	0.695882	-0.189829
C	-1.527907	1.409707	-0.399551
C	-1.487783	-1.354389	0.385767
C	-0.499176	2.024730	-0.595549
C	-0.441354	-1.940157	0.577639
C	3.093325	2.685378	-1.303843
C	1.904476	2.007558	-1.072853
C	0.718153	2.720432	-0.831247
C	0.755321	4.124237	-0.829853
C	1.949384	4.793033	-1.061403
C	3.121021	4.078118	-1.298438
C	3.238144	-3.890274	1.266814
C	2.088151	-4.637897	1.024831
C	0.874788	-4.003145	0.797779
C	0.796083	-2.601110	0.808738
C	1.960839	-1.855104	1.055261
C	3.169258	-2.499036	1.281704
H	-3.908137	-2.396731	0.636782
H	-6.072354	-1.237985	0.318739
H	-6.107113	1.165188	-0.315734
H	-3.977272	2.383961	-0.641611
H	4.002641	2.124543	-1.491675
H	1.874837	0.924042	-1.083291
H	-0.158682	4.676395	-0.644056
H	1.966194	5.877605	-1.057109
H	4.051930	4.604393	-1.479488
H	4.184263	-4.389965	1.444342
H	2.137027	-5.721442	1.013091
H	-0.022482	-4.580839	0.608111
H	1.899145	-0.773040	1.073131

1,2-bis(phenylethynyl)benzene – C^1C^5 singlet transition state

C	-3.154084	0.106956	-0.075984
C	0.209294	-1.262473	-0.045426
C	0.177517	1.962104	-0.079792
C	1.301292	1.639440	-0.850349
C	2.436460	2.439872	-0.810023
C	2.467369	3.576554	-0.007694
C	1.351246	3.911527	0.755895
C	0.217068	3.112350	0.724954
C	1.543447	-1.684055	0.048996
C	2.247975	-2.110188	-1.099114
C	3.558404	-2.546640	-0.992947
C	-4.539256	-0.014803	-0.058790
C	4.194515	-2.573924	0.248141
C	3.508769	-2.158841	1.389653
C	2.198629	-1.718093	1.299885
C	-5.109293	-1.286324	-0.073140
C	-4.309424	-2.427453	-0.103643
C	-2.918918	-2.321908	-0.119483
C	-2.340890	-1.058320	-0.105413
C	-2.312727	1.267943	-0.070732
C	-1.031061	1.169444	-0.109260
C	-0.927055	-0.726534	-0.105590

H	-5.161139	0.872419	-0.035077
H	-6.189096	-1.388631	-0.060634
H	-4.771012	-3.408792	-0.114760
H	-2.297795	-3.209787	-0.141838
H	1.273111	0.767248	-1.491307
H	3.298341	2.176558	-1.413775
H	3.354785	4.199689	0.021129
H	1.366061	4.797132	1.382412
H	-0.653157	3.362571	1.320691
H	1.747041	-2.094215	-2.060382
H	4.088988	-2.870640	-1.881747
H	5.220058	-2.917716	0.325403
H	4.002134	-2.177461	2.355340
H	1.662403	-1.390012	2.182398

1,2-bis(phenylethynyl)benzene – C^1C^5 triplet transition state

C	0.607538	3.061952	-0.250068
C	-1.623909	0.144305	-0.021381
C	1.871550	-0.550125	-0.174083
C	1.410494	-1.584324	-1.042894
C	1.882733	-2.873434	-0.909345
C	2.803479	-3.196369	0.095874
C	3.254516	-2.201226	0.971512
C	2.804059	-0.902759	0.849488
C	-2.228563	-1.126009	0.079854
C	-2.825161	-1.730401	-1.045840
C	-3.422051	-2.976658	-0.937243
C	0.863340	4.436186	-0.239534
C	-3.447787	-3.642070	0.287886
C	-2.867001	-3.051212	1.409304
C	-2.260687	-1.808494	1.313105
C	-0.187527	5.338304	-0.147076
C	-1.502400	4.878885	-0.051115
C	-1.771692	3.515348	-0.040606
C	-0.725684	2.594603	-0.144799
C	1.604409	2.035678	-0.359699
C	1.375309	0.738708	-0.261274
C	-0.957790	1.179193	-0.102055
H	1.888395	4.781710	-0.312855
H	0.014046	6.403975	-0.148281
H	-2.320646	5.587386	0.017875
H	-2.789699	3.151846	0.045421
H	0.688492	-1.332792	-1.810482
H	1.530262	-3.645681	-1.584892
H	3.161622	-4.214613	0.198495
H	3.969476	-2.450176	1.748826
H	3.150987	-0.125978	1.520924
H	-2.809447	-1.206369	-1.994614
H	-3.874628	-3.432078	-1.811628
H	-3.919206	-4.615407	0.368384
H	-2.883723	-3.566260	2.363802
H	-1.801109	-1.348641	2.180013

1,2-bis(phenylethynyl)benzene – C^1C^6 singlet transition state

C	-2.586453	1.096263	0.036366
C	-1.823905	-1.218497	0.011791
C	1.306988	1.065402	-0.152326
C	0.624962	-1.968864	0.145116
C	0.811068	-2.999188	-0.787685
C	1.906091	-3.847942	-0.686837
C	2.830687	-3.680550	0.340958
C	2.067200	0.523742	-1.196041
C	3.418173	0.824571	-1.309388
C	4.030873	1.665465	-0.384297

C	2.651097	-2.661023	1.271877
C	-3.642730	2.018107	0.054559
C	1.558523	-1.809175	1.176437
C	3.282012	2.210250	0.655741
C	1.930232	1.913247	0.774522
C	-4.962923	1.600767	0.052202
C	-5.270175	0.238887	0.029948
C	-4.256994	-0.704602	0.010452
C	-2.907187	-0.325303	0.010977
C	-1.224817	1.438153	0.017583
C	-0.118623	0.802624	-0.036544
C	-0.551395	-1.119358	0.048420
H	-3.402219	3.074351	0.066060
H	-5.758683	2.337293	0.067114
H	-6.305129	-0.084833	0.028481
H	-4.493212	-1.761814	-0.001080
H	0.084867	-3.125778	-1.582550
H	2.036780	-4.643219	-1.413050
H	3.686022	-4.343232	0.417084
H	1.590578	-0.130878	-1.915875
H	3.994566	0.400999	-2.124702
H	5.086677	1.897186	-0.474429
H	3.364782	-2.528387	2.077756
H	1.419025	-1.015650	1.900810
H	3.751458	2.870221	1.377536
H	1.339786	2.336763	1.579016

1,2-bis(phenylethynyl)benzene – C^1C^6 triplet transition state

C	-2.284962	1.287676	0.417826
C	-1.889409	-0.949276	-0.383466
C	1.562667	0.945285	-0.131624
C	0.239742	-2.331626	0.131314
C	0.170382	-3.524596	-0.625291
C	1.052639	-4.563324	-0.380536
C	2.027005	-4.442606	0.611251
C	2.178328	0.176066	-1.141753
C	3.528735	0.326524	-1.411596
C	4.302671	1.223972	-0.675531
C	2.112372	-3.267228	1.357808
C	-3.239349	2.217779	0.906180
C	1.240666	-2.217309	1.119253
C	3.710585	1.979649	0.337411
C	2.360577	1.844394	0.613733
C	-4.550773	2.119077	0.522456
C	-4.982554	1.084426	-0.358709
C	-4.119206	0.105081	-0.774059
C	-2.774710	0.104693	-0.319770
C	-0.914686	1.427876	0.449539
C	0.181124	0.833810	0.163879
C	-0.682667	-1.288076	-0.131381
H	-2.899379	3.040436	1.525640
H	-5.270132	2.853388	0.867897
H	-6.018573	1.060584	-0.678257
H	-4.463021	-0.716351	-1.393027
H	-0.591622	-3.610987	-1.391183
H	0.981906	-5.475156	-0.964075
H	2.718774	-5.256921	0.796740
H	1.576982	-0.525978	-1.706191
H	3.985183	-0.264241	-2.198427
H	5.361315	1.329744	-0.885628
H	2.869514	-3.168227	2.128123
H	1.310367	-1.300389	1.691515
H	4.307794	2.679219	0.912653
H	1.891714	2.429612	1.396286

1,2-bis(phenylethynyl)benzene – C^1C^5 singlet cyclized diradical

C	3.454636	-4.418823	-0.042325
C	2.086618	-4.259791	-0.228334
C	1.621783	-3.058462	-0.762825
C	2.505168	-2.035990	-1.106471
C	3.881532	-2.187991	-0.922899
C	4.352525	-3.375775	-0.390633
C	4.270218	-5.487125	0.468277
C	5.589613	-5.231975	0.497071
C	5.727173	-3.834598	-0.087086
C	6.835035	-3.183870	-0.328189
C	6.672224	-6.098437	0.957612
C	7.894345	-5.594256	1.419345
C	8.893017	-6.453170	1.864474
C	8.691020	-7.829438	1.863559
C	7.476539	-8.343371	1.413263
C	6.480737	-7.489147	0.963044
C	8.026036	-2.540679	-0.578559
C	8.603427	-1.663918	0.386207
C	9.796248	-1.019720	0.119254
C	10.454675	-1.212943	-1.098700
C	9.901706	-2.067675	-2.057329
C	8.711681	-2.725647	-1.814625
H	1.397725	-5.053685	0.036836
H	0.556823	-2.918208	-0.913659
H	2.119913	-1.110628	-1.520574
H	4.567462	-1.391193	-1.190266
H	8.058894	-4.524181	1.447060
H	9.831779	-6.041603	2.219952
H	9.472256	-8.497109	2.210639
H	7.308492	-9.415215	1.405503
H	5.540729	-7.888397	0.596943
H	8.089318	-1.510312	1.328005
H	10.222101	-0.356562	0.864685
H	11.389814	-0.702550	-1.299144
H	10.411375	-2.220598	-3.002639
H	8.284362	-3.391957	-2.554471

1,2-bis(phenylethynyl)benzene – C^1C^5 triplet cyclized diradical

C	3.660629	-4.417570	-0.077198
C	2.321715	-4.138827	-0.324701
C	1.996467	-2.903991	-0.884721
C	2.987043	-1.970470	-1.190617
C	4.333426	-2.248191	-0.943379
C	4.664317	-3.471126	-0.386550
C	4.359645	-5.548697	0.474183
C	5.701977	-5.409215	0.550100
C	5.983846	-4.054515	-0.013873
C	7.143203	-3.456184	-0.195559
C	6.665548	-6.380024	1.062913
C	7.997232	-6.044933	1.337785
C	8.881498	-6.996241	1.834280
C	8.455101	-8.298658	2.071382
C	7.131244	-8.645022	1.805039
C	6.249564	-7.699593	1.304521
C	8.051599	-2.483813	-0.572199
C	8.479345	-1.485302	0.350624
C	9.418419	-0.543402	-0.024060
C	9.970007	-0.557982	-1.308705
C	9.567999	-1.534981	-2.224574
C	8.630703	-2.487879	-1.874085
H	1.550978	-4.863822	-0.088339
H	0.957545	-2.665645	-1.085804

H	2.708725	-1.016609	-1.625301
H	5.103617	-1.521531	-1.181321
H	8.340352	-5.030661	1.167273
H	9.908829	-6.714381	2.039901
H	9.146526	-9.039029	2.459103
H	6.787440	-9.658576	1.983092
H	5.222606	-7.974637	1.086097
H	8.050647	-1.475817	1.346025
H	9.727718	0.214084	0.688294
H	10.707594	0.184022	-1.592841
H	9.993947	-1.548127	-3.222192
H	8.319951	-3.247652	-2.581595

1,2-bis(phenylethynyl)benzene – C^1C^6 singlet cyclized diradical

C	3.728257	-5.586421	0.052784
C	2.489489	-6.266521	0.122123
C	1.307781	-5.568307	0.066121
C	1.307190	-4.162339	-0.061677
C	2.488327	-3.464092	-0.128283
C	3.727686	-4.144162	-0.070076
C	4.987186	-6.184940	0.106627
C	6.209775	-5.589493	0.070634
C	6.208944	-4.141017	-0.110233
C	4.986062	-3.545606	-0.135238
C	7.437019	-6.400945	0.257116
C	7.434438	-3.329539	-0.307776
C	7.560489	-2.099138	0.348139
C	8.673396	-1.293190	0.137977
C	9.677295	-1.702587	-0.734555
C	8.458275	-6.000245	1.126560
C	9.570657	-6.808741	1.327027
C	9.683685	-8.027816	0.663679
C	9.558238	-2.921567	-1.397015
C	8.447734	-3.730106	-1.186538
C	8.671886	-8.437345	-0.199611
C	7.557101	-7.631433	-0.399745
H	2.493977	-7.345970	0.222307
H	0.364284	-6.100358	0.119878
H	0.363233	-3.630317	-0.106963
H	2.491887	-2.384643	-0.228499
H	6.777470	-1.784623	1.029962
H	8.756608	-0.344741	0.658092
H	10.546695	-1.075198	-0.899469
H	8.373667	-5.056223	1.652324
H	10.350864	-6.486029	2.008157
H	10.554561	-8.655169	0.820763
H	10.332207	-3.244186	-2.085269
H	8.358367	-4.674062	-1.711634
H	8.750356	-9.385869	-0.720326
H	6.767913	-7.946060	-1.074365

1,2-bis(phenylethynyl)benzene – C^1C^6 triplet cyclized diradical

C	3.733787	-5.581740	0.046047
C	2.498649	-6.270090	0.107468
C	1.318311	-5.569887	0.058293
C	1.317790	-4.160750	-0.053935
C	2.497620	-3.460516	-0.113706
C	3.733278	-4.148836	-0.063386
C	4.999798	-6.173509	0.098247
C	6.229556	-5.585488	0.067286
C	6.228756	-4.145018	-0.107066
C	4.998752	-3.557033	-0.126969
C	7.444488	-6.413566	0.255623
C	7.441922	-3.316916	-0.306348

C	7.542315	-2.075771	0.333463
C	8.642167	-1.253152	0.119082
C	9.659117	-1.657292	-0.740669
C	8.478976	-6.017969	1.111946
C	9.578653	-6.842663	1.316217
C	9.665555	-8.073120	0.669955
C	9.566365	-2.887690	-1.386230
C	8.468599	-3.712420	-1.172062
C	8.640847	-8.477354	-0.180491
C	7.539084	-7.654768	-0.384959
H	2.504853	-7.350824	0.196075
H	0.373693	-6.100646	0.105652
H	0.372771	-3.630016	-0.092812
H	2.503001	-2.379782	-0.202361
H	6.749875	-1.766362	1.006861
H	8.705746	-0.296485	0.626785
H	10.518724	-1.017256	-0.908365
H	8.413906	-5.065726	1.625589
H	10.369255	-6.524084	1.987255
H	10.526657	-8.713130	0.829902
H	10.350846	-3.206201	-2.064447
H	8.398891	-4.664619	-1.685177
H	8.699826	-9.434069	-0.688657
H	6.740568	-7.964252	-1.051107

1 – enediyne

C	-1.397977	6.243901	-9.637946
H	-3.939234	16.492293	-7.605366
H	-2.443634	16.861320	-9.532954
H	-1.415795	14.921431	-10.700936
H	-1.886968	12.621491	-9.940301
H	-4.548059	10.724443	-6.447083
H	-5.559186	12.668681	-5.284112
H	-4.262063	7.074177	-1.390963
H	-3.149733	4.682341	-6.270349
H	-3.781373	2.559304	-5.182203
H	-4.495006	2.537554	-2.800177
H	-4.575581	4.642485	-1.515120
H	-3.628156	9.206487	-2.466318
H	-5.075048	14.966130	-6.053735
H	-2.904770	9.240242	-4.839191
H	-1.510121	9.624322	-11.508919
H	-0.620279	7.613093	-12.642379
H	-0.555980	5.439953	-11.436856
H	-1.367084	5.301570	-9.103500
C	-3.488188	15.649886	-8.120603
C	-2.656428	15.853695	-9.192493
C	-2.073934	14.752351	-9.855444
C	-2.334019	13.470850	-9.435895
C	-4.327530	11.730846	-6.783766
C	-4.900405	12.835011	-6.129359
C	-3.905876	5.878313	-3.153556
C	-3.947793	7.094705	-2.429726
C	-3.459763	4.666861	-5.231440
C	-3.812760	3.487788	-4.622270
C	-4.218535	3.474968	-3.270624
C	-4.263763	4.644639	-2.554988
C	-3.596413	8.279657	-3.028527
C	-4.632750	14.112278	-6.557248
C	-3.777306	14.340371	-7.662458
C	-3.188724	13.229358	-8.335626
C	-3.132300	7.137617	-5.122299
C	-2.923668	10.768611	-8.512104
C	-3.494392	5.887807	-4.519033

C	-2.712192	7.194954	-6.477659
C	-3.188538	8.303574	-4.373398
C	-1.472679	8.674785	-10.987812
C	-3.483302	11.905086	-7.870223
C	-2.464240	9.775961	-9.041929
C	-1.942954	8.614607	-9.667716
C	-0.977145	7.544939	-11.620723
C	-1.899853	7.374480	-8.976627
C	-2.344708	7.276937	-7.633244
C	-0.941794	6.325847	-10.944799

1– C^1C^5 singlet transition state

C	-0.055988	-0.070570	0.392682
C	-0.124091	-0.150595	1.783209
C	1.530728	-0.692579	-5.998591
C	-0.896060	-0.874588	-0.368658
C	-1.018624	-1.021794	2.402986
C	-0.284580	2.476272	-6.755944
C	1.114110	0.438744	-6.663234
C	-1.864676	-1.832260	1.648697
C	-1.211951	3.311850	-6.183369
C	-1.808639	-1.763141	0.260860
C	-0.981869	-0.954064	-1.815416
C	-1.735737	3.016327	-4.908886
C	-2.551748	-2.465822	-0.744367
H	-2.463939	3.681987	-4.458468
C	-1.325788	1.891195	-4.231444
C	-2.367137	-2.246697	-1.999027
H	-1.056932	-1.069829	3.485944
C	-0.430305	-0.517677	-2.860055
H	-1.721199	1.667604	-3.246100
C	-3.444661	-6.744818	-4.303529
C	-3.620028	-3.392193	-5.910916
C	-2.799979	-5.077520	-2.674640
C	-0.379965	1.010846	-4.799479
C	-2.996214	-4.044753	-3.622059
C	1.011458	-1.008729	-4.737273
C	-2.782863	-2.654803	-3.321308
H	-2.560011	-2.509880	2.130193
C	-2.994620	-1.707896	-4.306995
H	0.526704	0.472558	2.386803
C	0.062420	-0.185510	-4.123162
C	-3.410261	-2.073284	-5.599927
C	0.156189	1.309531	-6.085125
C	-3.018424	-6.392536	-3.006093
C	-3.640070	-5.767904	-5.246149
H	1.514907	0.679937	-7.642553
H	-3.616174	-7.786617	-4.552455
H	-3.967333	-6.026388	-6.248632
H	-2.850873	-0.660921	-4.070644
C	-3.422360	-4.401972	-4.937982
H	2.262457	-1.351993	-6.451908
H	1.335112	-1.905248	-4.222213
H	-1.541463	4.201592	-6.708738
H	0.125880	2.698618	-7.735989
H	-2.861375	-7.167541	-2.263376
H	-2.479453	-4.809010	-1.675131
H	-3.943019	-3.681667	-6.906124
H	-3.566900	-1.301036	-6.344946
H	0.640523	0.606412	-0.088222

1– C^1C^5 triplet transition state

C	-0.097478	-0.324564	0.595365
C	-0.264347	-0.210307	1.971581

C	1.389926	-1.612856	-5.844777
C	-1.091986	-0.928988	-0.175692
C	-1.423424	-0.687048	2.583642
C	0.044614	1.721903	-6.832235
C	1.129726	-0.486593	-6.593948
C	-2.423882	-1.286229	1.826174
C	-0.739992	2.725335	-6.319122
C	-2.261695	-1.415175	0.447890
C	-1.001246	-1.058959	-1.606381
C	-1.280341	2.604845	-5.023090
C	-3.187149	-2.019843	-0.474011
H	-1.901711	3.398859	-4.623156
C	-1.025369	1.486920	-4.263248
C	-3.056306	-2.105700	-1.771226
H	-1.546008	-0.590475	3.656977
C	-0.428842	-0.887236	-2.692760
H	-1.442843	1.390568	-3.267039
C	-1.817700	-5.632965	-5.282013
C	-4.446175	-3.005494	-5.643503
C	-1.904036	-4.332624	-3.249109
C	-0.221524	0.440920	-4.764179
C	-2.932166	-3.536693	-3.778138
C	0.868634	-1.744543	-4.552932
C	-3.530708	-2.452381	-3.015500
H	-3.327976	-1.659001	2.294245
C	-4.561718	-1.682984	-3.626516
H	0.512709	0.253576	2.569247
C	0.067912	-0.744417	-3.994362
C	-5.003522	-1.966323	-4.910305
C	0.324555	0.557806	-6.075600
C	-1.352365	-5.365072	-3.986070
C	-2.826967	-4.864991	-5.824065
H	1.537188	-0.384980	-7.594746
H	-1.383866	-6.443972	-5.857186
H	-3.191088	-5.066952	-6.826731
H	-4.999038	-0.870512	-3.058645
C	-3.406380	-3.803912	-5.093924
H	2.002831	-2.408590	-6.253686
H	1.070197	-2.636480	-3.972198
H	-0.946226	3.611590	-6.909511
H	0.463701	1.806125	-7.830157
H	-0.559522	-5.970023	-3.559336
H	-1.545926	-4.120359	-2.247649
H	-4.796715	-3.219983	-6.647533
H	-5.798544	-1.368600	-5.343429
H	0.797962	0.049010	0.110834

1– C^1C^6 singlet transition state

C	-0.165120	0.169362	0.172251
C	-0.175712	0.114949	1.555295
C	3.398461	-0.037350	-6.148301
C	0.868182	-0.418199	-0.572297
C	0.853959	-0.532307	2.242298
C	0.428493	-1.831597	-7.495698
C	2.514136	-0.587122	-7.041682
C	1.892024	-1.126188	1.545427
C	-0.691030	-2.484708	-7.045860
C	1.940658	-1.095318	0.144014
C	0.962855	-0.388438	-1.973069
C	-0.936645	-2.589409	-5.660522
C	2.945302	-1.690745	-0.635889
H	-1.822881	-3.107449	-5.309817
C	-0.064279	-2.038474	-4.753692
C	3.178902	-1.811600	-1.887873

H	0.842668	-0.572506	3.325886
C	1.798201	-0.817497	-2.841765
H	-0.258119	-2.111552	-3.689949
C	8.248117	-1.471260	-2.801415
C	5.898013	-3.809321	-4.499774
C	6.024929	-1.096605	-1.927874
C	1.099146	-1.357269	-5.185784
C	5.504397	-2.108679	-2.769843
C	3.159551	-0.130676	-4.765204
C	4.116900	-2.466251	-2.785519
H	2.688618	-1.634031	2.075737
C	3.673344	-3.453466	-3.644495
H	-0.987648	0.578644	2.104522
C	2.035599	-0.767769	-4.275295
C	4.563437	-4.127572	-4.500159
C	1.351575	-1.255957	-6.587706
C	7.362591	-0.784744	-1.944076
C	7.773642	-2.456427	-3.630014
H	2.693951	-0.518775	-8.110042
H	9.302884	-1.218163	-2.802865
H	8.447546	-2.990381	-4.293002
H	2.620251	-3.709677	-3.654270
C	6.398990	-2.800012	-3.642261
H	4.287598	0.473539	-6.500698
H	3.865627	0.303932	-4.067117
H	-1.388940	-2.921177	-7.752268
H	0.625745	-1.745760	-8.559899
H	7.742492	-0.006060	-1.291318
H	5.346726	-0.575059	-1.262642
H	6.589241	-4.325749	-5.158492
H	4.184326	-4.900903	-5.158944
H	-0.959403	0.675993	-0.362666

1– C^1C^6 triplet transition state

C	0.341561	0.821440	0.394070
C	0.068756	0.525760	1.721450
C	3.728958	0.129330	-5.975447
C	1.097531	-0.065892	-0.382147
C	0.539565	-0.658889	2.294921
C	1.185175	-2.291699	-7.259808
C	3.031978	-0.701785	-6.843921
C	1.303677	-1.542897	1.547346
C	0.092036	-3.005313	-6.814413
C	1.600922	-1.249244	0.212493
C	1.337586	0.136815	-1.780041
C	-0.313161	-2.900680	-5.475903
C	2.435708	-2.042976	-0.625016
H	-1.174905	-3.458001	-5.124757
C	0.383714	-2.086532	-4.600878
C	2.955843	-2.193823	-1.752433
H	0.313624	-0.884889	3.331186
C	1.943562	-0.422807	-2.782663
H	0.074042	-2.005508	-3.564394
C	7.754879	-1.221178	-3.301234
C	5.504703	-3.832841	-4.714940
C	5.653258	-1.156941	-2.107898
C	1.501664	-1.353235	-5.028477
C	5.151590	-2.210823	-2.906212
C	3.358456	0.242355	-4.645128
C	3.831712	-2.748312	-2.731172
H	1.689321	-2.456407	1.986560
C	3.399494	-3.789007	-3.540903
H	-0.519294	1.216316	2.316070
C	2.244324	-0.481722	-4.126096

C	4.238310	-4.331841	-4.527859
C	1.912253	-1.450893	-6.388516
C	6.925029	-0.673239	-2.300554
C	7.295465	-2.246862	-4.088881
H	3.331274	-0.786713	-7.883203
H	8.757016	-0.831230	-3.443716
H	7.928737	-2.676145	-4.859206
H	2.397898	-4.178806	-3.406556
C	5.990335	-2.770049	-3.915006
H	4.577020	0.698908	-6.340303
H	3.910923	0.886192	-3.971897
H	-0.455194	-3.644891	-7.498734
H	1.502649	-2.366094	-8.295461
H	7.295408	0.134348	-1.678153
H	5.014081	-0.738654	-1.338555
H	6.152595	-4.248381	-5.480389
H	3.873818	-5.144525	-5.146142
H	-0.034577	1.731066	-0.061647

1– C^1C^5 singlet cyclized diradical

C	0.490639	0.549783	0.325627
C	-0.517373	-0.397879	0.516161
C	3.598761	5.773686	0.817218
C	1.810075	0.144544	0.435044
C	-0.204300	-1.724464	0.811023
C	3.650752	6.024742	-2.907900
C	3.671069	6.315522	-0.452639
C	1.121521	-2.141466	0.925101
C	3.557044	5.215678	-4.017117
C	2.129877	-1.203843	0.737220
C	3.077803	0.894367	0.296294
C	3.384392	3.829587	-3.862148
C	3.566688	-1.270626	0.775719
H	3.303817	3.192985	-4.736396
C	3.312445	3.275545	-2.600571
C	4.198747	-0.113311	0.516339
H	-1.003970	-2.443157	0.954390
C	3.209370	2.180779	0.099760
H	3.166664	2.206648	-2.481945
C	8.541739	-1.703126	2.905608
C	8.373246	0.803055	0.161328
C	6.224642	-1.393709	2.289828
C	3.414043	4.080207	-1.451652
C	6.585173	-0.461634	1.286101
C	3.443472	4.402715	1.003028
C	5.627290	0.192310	0.436581
H	1.362565	-3.172984	1.155470
C	6.076357	1.116225	-0.490103
H	-1.556120	-0.097624	0.432453
C	3.350861	3.520368	-0.105410
C	7.441895	1.424722	-0.628560
C	3.581081	5.484425	-1.602992
C	7.174173	-1.999505	3.076260
C	8.926285	-0.791834	1.955633
H	3.796596	7.384473	-0.588845
H	9.283698	-2.189427	3.529850
H	9.975160	-0.545986	1.820396
H	5.362832	1.597298	-1.148131
C	7.971317	-0.147065	1.131071
H	3.668418	6.419890	1.685542
H	3.397875	3.985119	2.001486
H	3.612676	5.646006	-5.011111
H	3.779508	7.096839	-3.019627
H	6.868204	-2.707461	3.839152

H	5.175983	-1.624175	2.437458
H	9.429997	1.027491	0.054986
H	7.749040	2.149979	-1.374109
H	0.245972	1.581288	0.095130

1– C^1C^5 triplet cyclized diradical

C	0.594367	0.649606	0.303718
C	-0.440965	-0.267795	0.493538
C	3.370492	5.834307	0.770028
C	1.899712	0.210849	0.443533
C	-0.167692	-1.597194	0.817885
C	3.452038	6.052761	-2.958570
C	3.414960	6.368932	-0.506353
C	1.144216	-2.046249	0.962551
C	3.442008	5.228024	-4.061208
C	2.176829	-1.135064	0.774323
C	3.193638	0.930509	0.312198
C	3.386526	3.834822	-3.894092
C	3.613559	-1.229826	0.834174
H	3.373314	3.184706	-4.761962
C	3.345444	3.289162	-2.626248
C	4.272188	-0.082487	0.562602
H	-0.988663	-2.291755	0.959840
C	3.321683	2.218833	0.086463
H	3.292436	2.212727	-2.498106
C	8.563734	-1.904078	2.883820
C	8.476015	0.697301	0.225425
C	6.257077	-1.483421	2.297175
C	3.361467	4.109928	-1.486280
C	6.647204	-0.535928	1.319397
C	3.327977	4.459854	0.970915
C	5.710202	0.176715	0.494462
H	1.355167	-3.079244	1.215319
C	6.189459	1.114836	-0.403343
H	-1.470135	0.056981	0.386107
C	3.325960	3.556598	-0.132137
C	7.564441	1.379684	-0.537132
C	3.411096	5.521252	-1.649500
C	7.186962	-2.151970	3.056126
C	8.977380	-0.976915	1.961593
H	3.451970	7.443202	-0.652281
H	9.290117	-2.438563	3.486592
H	10.034177	-0.766722	1.827934
H	5.491574	1.641691	-1.042886
C	8.043418	-0.269104	1.165474
H	3.371722	6.493763	1.631268
H	3.302468	4.049623	1.973078
H	3.474252	5.652795	-5.058649
H	3.491069	7.130794	-3.080229
H	6.858218	-2.870242	3.799607
H	5.200991	-1.674162	2.450687
H	9.539910	0.885410	0.120097
H	7.894806	2.118440	-1.259126
H	0.383213	1.683615	0.050177

1– C^1C^6 singlet cyclized diradical

C	-1.219668	-0.993371	-0.748972
C	-0.143482	-0.142322	-0.811531
C	4.705563	2.106286	0.374864
C	4.946021	-1.936203	1.233501
C	6.916415	2.439691	-0.649755
C	1.127872	-0.557648	-0.348479
C	5.785585	0.324246	-0.871711
C	-1.078664	-2.295664	-0.222172

H	7.112603	-1.006504	3.686822
H	5.777810	-0.687506	-1.261982
C	6.893574	1.154388	-1.126506
C	1.273607	-1.894987	0.187089
C	0.138186	-2.738634	0.235460
C	5.834370	2.943710	0.110947
H	-1.941456	-2.951370	-0.179992
H	0.250399	-3.737242	0.642088
C	3.536502	-0.129520	0.046049
C	5.849620	4.265275	0.622283
C	3.675337	-1.466909	0.621755
H	7.724483	0.769398	-1.707420
C	2.552921	-2.232815	0.628443
H	8.204131	-3.125253	3.023037
C	7.299999	-2.788896	2.525148
C	2.289264	0.214569	-0.369216
H	-0.247113	0.857829	-1.216641
H	-2.188910	-0.663701	-1.106782
C	7.380018	-4.792052	1.086489
C	5.519354	-1.191077	2.243440
C	4.701456	0.773375	-0.145884
H	7.350397	-6.472820	-0.229205
H	8.281725	-5.105618	1.603626
C	3.651864	2.631714	1.165750
C	4.807856	4.745028	1.374155
C	3.701382	3.915041	1.651803
H	2.797830	2.002230	1.385597
H	2.884234	4.293453	2.256682
C	6.758213	-3.582998	1.486209
C	5.564827	-3.159130	0.821896
C	6.694846	-1.614562	2.891943
H	7.764782	3.088117	-0.845461
C	6.862905	-5.550375	0.067528
H	4.833736	5.758180	1.760752
H	6.709695	4.892628	0.408907
C	5.696236	-5.125240	-0.602093
C	5.065133	-3.962205	-0.235096
H	5.047119	-0.264152	2.549725
H	5.296223	-5.721168	-1.415520
H	4.170199	-3.644220	-0.756569

1– C^1C^6 triplet cyclized diradical

C	-1.191528	-0.983408	-0.735153
C	-0.118988	-0.127902	-0.789601
C	4.695123	2.140545	0.374967
C	4.979804	-1.953783	1.225765
C	6.905242	2.507711	-0.639678
C	1.151232	-0.555437	-0.333198
C	5.823686	0.364414	-0.836941
C	-1.046085	-2.294444	-0.226007
H	7.179148	-1.061277	3.664402
H	5.840609	-0.652528	-1.213231
C	6.915275	1.214585	-1.095520
C	1.299721	-1.888221	0.180768
C	0.171464	-2.742492	0.223456
C	5.806749	2.999136	0.105310
H	-1.908628	-2.951030	-0.192029
H	0.288763	-3.746264	0.616578
C	3.575813	-0.123819	0.064517
C	5.789385	4.328628	0.595823
C	3.717634	-1.458144	0.618710
H	7.759193	0.839407	-1.663987
C	2.587371	-2.219774	0.614983
H	8.211239	-3.214091	3.015861

C	7.315337	-2.857620	2.517094
C	2.319875	0.213154	-0.343681
H	-0.224009	0.878063	-1.180580
H	-2.163347	-0.653197	-1.085533
C	7.339539	-4.873125	1.094263
C	5.576700	-1.215731	2.227709
C	4.723158	0.800383	-0.127259
H	7.264157	-6.561965	-0.209142
H	8.233415	-5.206349	1.612709
C	3.626682	2.654056	1.154266
C	4.732865	4.796461	1.334349
C	3.644681	3.945435	1.620516
H	2.787005	2.008694	1.382802
H	2.816903	4.313786	2.217086
C	6.750273	-3.645126	1.485718
C	5.567039	-3.194698	0.820383
C	6.743010	-1.664301	2.875571
H	7.740138	3.172009	-0.840030
C	6.801613	-5.624775	0.081256
H	4.733674	5.815889	1.704982
H	6.636657	4.971543	0.377578
C	5.647012	-5.172653	-0.591620
C	5.047122	-3.990949	-0.232337
H	5.128798	-0.275311	2.529445
H	5.231970	-5.762224	-1.402139
H	4.162509	-3.652262	-0.758201

2 – enediyne

C	-2.622556	-4.348808	-3.164529
C	-2.937889	-5.224371	-4.213746
C	-3.990116	-6.120733	-4.101787
C	-4.752584	-6.159547	-2.935042
C	-4.455863	-5.305688	-1.883264
C	-3.393464	-4.394614	-1.972674
C	-3.090630	-3.540875	-0.880829
C	-1.556882	-3.422817	-3.300867
C	-0.894562	-0.563598	2.285575
C	2.605428	2.388916	-2.017358
C	3.523749	1.172000	-3.892428
C	2.391825	-0.894874	-4.671828
C	3.583439	2.235025	-3.025034
C	-0.656661	-2.615639	-3.417703
C	-1.853170	-0.217345	3.271859
C	-3.167620	-0.765604	3.172172
C	0.390130	-1.663009	-3.537838
C	-1.212769	-1.403316	1.253549
C	-3.473689	-1.631275	2.099008
C	-1.551358	0.648720	4.349348
C	1.379048	-1.806999	-4.553750
C	-2.524036	-1.952900	1.144436
C	-4.128788	-0.422942	4.156672
C	-2.504157	0.961486	5.287605
C	0.461886	-0.584698	-2.671259
C	-2.834565	-2.819020	0.061950
C	-3.805137	0.420372	5.189618
C	1.498172	0.368675	-2.774907
C	2.486530	0.214556	-3.793586
C	1.586905	1.477566	-1.895456
H	-2.343959	-5.183260	-5.119307
H	-4.218468	-6.788440	-4.925121
H	-5.577164	-6.857994	-2.845157
H	-5.039411	-5.333396	-0.970470
H	-4.549380	0.674830	5.936490
H	-2.260277	1.626462	6.109050

H	-0.294677	-0.466972	-1.902806
H	-0.473085	-1.671656	0.508102
H	-4.472374	-2.047413	2.021276
H	-0.550387	1.062624	4.422791
H	0.107497	-0.153036	2.363136
H	0.832638	1.592962	-1.123222
H	-5.127878	-0.840258	4.078851
H	3.141771	-1.012549	-5.447816
H	1.314378	-2.652884	-5.228069
H	2.662716	3.233575	-1.339280
H	4.383491	2.962313	-3.111342
H	4.273952	1.052448	-4.668011

2– C^1C^5 singlet transition state

C	-0.708189	3.625828	-0.066435
C	0.072481	4.764255	0.093859
H	1.142848	4.679913	0.241611
C	-0.544382	6.014500	0.061179
H	0.055334	6.909695	0.184353
C	-1.921167	6.123983	-0.127390
H	-2.382880	7.105283	-0.149488
C	-2.712501	4.988336	-0.288906
H	-3.782808	5.073427	-0.436129
C	-2.111779	3.734498	-0.260580
C	-2.671974	2.421952	-0.404365
C	-1.934721	1.369188	-0.364844
C	-1.982828	-0.074445	-0.398968
C	-3.006516	-0.738672	0.253625
H	-3.745553	-0.164670	0.802230
C	-3.106128	-2.147302	0.221132
C	-4.149063	-2.841590	0.885625
H	-4.894659	-2.268640	1.428130
C	-4.217122	-4.211409	0.844828
H	-5.020150	-4.731028	1.356504
C	-3.244863	-4.953159	0.137106
H	-3.310013	-6.035654	0.112011
C	-2.222987	-4.309766	-0.516268
H	-1.474772	-4.877119	-1.061299
C	-2.124275	-2.897760	-0.493089
C	-1.086882	-2.197451	-1.157073
H	-0.344174	-2.763268	-1.710823
C	-1.015990	-0.830600	-1.115507
H	-0.228613	-0.307520	-1.643308
C	-0.272683	2.240859	-0.057400
C	0.746421	1.527925	0.132313
C	1.753570	0.580659	0.352923
C	2.659976	0.248570	-0.653855
H	2.575600	0.725302	-1.624741
C	3.686570	-0.691470	-0.432120
C	4.615236	-1.040442	-1.446145
H	4.529160	-0.566876	-2.419090
C	5.605294	-1.959666	-1.203821
H	6.309550	-2.218437	-1.986991
C	5.713624	-2.573118	0.063100
H	6.499953	-3.298188	0.242540
C	4.828861	-2.254629	1.066361
H	4.911289	-2.724982	2.041221
C	3.799062	-1.312345	0.849814
C	2.868916	-0.958272	1.864439
H	2.954039	-1.432119	2.837309
C	1.880568	-0.045542	1.634813
H	1.172202	0.215580	2.411764

2– C^1C^5 triplet transition state

C	-0.377371	0.097296	0.214179
C	-0.581434	-0.110997	1.580227
H	0.274747	-0.273176	2.225630
C	-1.871815	-0.105508	2.097832
H	-2.023363	-0.256709	3.161066
C	-2.969378	0.090804	1.258019
H	-3.972454	0.088103	1.670494
C	-2.782860	0.289139	-0.103680
H	-3.628509	0.440908	-0.764933
C	-1.491116	0.303660	-0.634690
C	-1.151201	0.510119	-2.013551
C	0.059998	0.438635	-2.519265
C	0.881946	0.406556	-3.626759
C	0.675051	-0.553741	-4.651019
H	-0.179139	-1.217610	-4.576335
C	1.548673	-0.659523	-5.745977
C	1.349877	-1.613642	-6.778068
H	0.498782	-2.284081	-6.711644
C	2.215369	-1.688772	-7.845092
H	2.049156	-2.421732	-8.627252
C	3.318152	-0.818377	-7.927459
H	3.996143	-0.884741	-8.771269
C	3.537268	0.120691	-6.935755
H	4.387818	0.792607	-6.998827
C	2.670646	0.224731	-5.836516
C	2.870608	1.185995	-4.794816
H	3.726147	1.850760	-4.865023
C	2.027865	1.272380	-3.732542
H	2.198928	1.994541	-2.943258
C	0.931448	0.070323	-0.378346
C	2.162334	-0.045884	-0.351819
C	3.553274	-0.177200	-0.510513
C	4.408855	0.893786	-0.262040
H	3.993524	1.843223	0.058630
C	5.803748	0.767901	-0.421047
C	6.687994	1.850633	-0.177926
H	6.273094	2.802892	0.137539
C	8.043005	1.699867	-0.336789
H	8.708052	2.535522	-0.147203
C	8.579300	0.459870	-0.746730
H	9.651624	0.352748	-0.869100
C	7.747915	-0.608240	-0.989568
H	8.158010	-1.562849	-1.304544
C	6.349127	-0.486475	-0.834729
C	5.461347	-1.569428	-1.075283
H	5.874963	-2.521954	-1.391643
C	4.111924	-1.428147	-0.922039
H	3.441216	-2.256919	-1.115023

2– C^1C^6 singlet transition state

C	-0.014241	-0.001614	0.204462
C	-0.045822	0.004693	1.606225
H	0.896275	0.011145	2.141051
C	-1.244382	-0.003742	2.299402
H	-1.237302	0.001599	3.383748
C	-2.457171	-0.019602	1.607672
H	-3.394090	-0.025462	2.153595
C	-2.470705	-0.027332	0.223160
H	-3.410643	-0.033732	-0.315451
C	-1.280269	-0.020386	-0.517638
C	-1.208037	-0.007099	-1.919143
C	-0.278912	0.040764	-2.794513
C	-0.136091	0.143007	-4.236394
C	0.634128	1.121509	-4.831726

H	1.183794	1.823758	-4.214867
C	0.723446	1.229080	-6.238093
C	1.509977	2.228745	-6.863752
H	2.060799	2.925828	-6.240211
C	1.578704	2.312962	-8.231728
H	2.185140	3.081379	-8.698907
C	0.863617	1.401058	-9.039306
H	0.925911	1.478219	-10.119471
C	0.093544	0.421206	-8.462723
H	-0.457161	-0.281151	-9.080901
C	0.001968	0.308076	-7.055065
C	-0.783828	-0.687993	-6.422696
H	-1.338968	-1.388011	-7.039611
C	-0.852329	-0.773069	-5.058172
H	-1.459182	-1.532564	-4.579004
C	1.155274	-0.013901	-0.571197
C	1.435915	-0.060522	-1.816548
C	2.604372	-0.161569	-2.673492
C	2.724566	-1.138350	-3.641282
H	1.913590	-1.839994	-3.801895
C	3.889823	-1.245021	-4.433879
C	4.027803	-2.242900	-5.431185
H	3.210383	-2.939246	-5.589487
C	5.170503	-2.326298	-6.186467
H	5.263781	-3.093339	-6.947673
C	6.230032	-1.415328	-5.979991
H	7.128231	-1.491831	-6.583296
C	6.125919	-0.437205	-5.021866
H	6.938648	0.264439	-4.860949
C	4.960692	-0.324955	-4.226670
C	4.816549	0.669331	-3.226606
H	5.630428	1.368649	-3.061248
C	3.676703	0.753588	-2.473272
H	3.573278	1.511768	-1.705698

2– C^1C^6 triplet transition state

C	-0.053727	0.314954	0.133775
C	-0.202370	0.746105	1.475627
H	0.598967	1.315497	1.933550
C	-1.307149	0.375313	2.199627
H	-1.399595	0.680811	3.236058
C	-2.320221	-0.436890	1.621020
H	-3.162017	-0.748839	2.229405
C	-2.263029	-0.799578	0.299124
H	-3.064945	-1.368774	-0.158028
C	-1.188109	-0.360036	-0.513191
C	-1.147811	-0.394218	-1.894343
C	-0.389841	-0.147712	-2.895867
C	-0.282632	0.062468	-4.287675
C	0.589448	1.001936	-4.843401
H	1.198180	1.612951	-4.187650
C	0.678730	1.184485	-6.238351
C	1.550460	2.145130	-6.811846
H	2.162732	2.752226	-6.152751
C	1.623130	2.302586	-8.174339
H	2.294237	3.040386	-8.600500
C	0.829383	1.506404	-9.026175
H	0.894401	1.639401	-10.100634
C	-0.024885	0.563970	-8.498828
H	-0.636435	-0.049516	-9.153344
C	-0.123657	0.379529	-7.104100
C	-0.994970	-0.584449	-6.522975
H	-1.608103	-1.194578	-7.179246
C	-1.072173	-0.746518	-5.171290

H	-1.738271	-1.480902	-4.733802
C	1.111942	0.356875	-0.607728
C	1.584695	0.117263	-1.772900
C	2.726787	-0.085136	-2.577631
C	2.761076	-1.017397	-3.617643
H	1.888053	-1.629683	-3.809567
C	3.914715	-1.191376	-4.408871
C	3.964426	-2.144735	-5.457810
H	3.086587	-2.752908	-5.651133
C	5.098587	-2.293892	-6.218011
H	5.123662	-3.026164	-7.017695
C	6.234330	-1.496315	-5.965995
H	7.124813	-1.622741	-6.572158
C	6.215386	-0.560807	-4.955780
H	7.088894	0.053748	-4.760708
C	5.066798	-0.384968	-4.156506
C	5.010250	0.571724	-3.104026
H	5.886070	1.182943	-2.908493
C	3.887657	0.725558	-2.345503
H	3.850203	1.454463	-1.544446

2– C^1C^5 singlet cyclized diradical

C	8.325684	3.902304	-3.908574
C	9.081690	2.703824	-3.822404
C	10.470044	3.008095	-4.237143
C	10.501693	4.493304	-4.558393
C	11.657834	5.261044	-5.014371
C	8.487108	1.522864	-3.412162
C	6.975597	3.907244	-3.578926
C	9.240735	4.915105	-4.360281
C	7.129794	1.536175	-3.082880
C	6.386303	2.712919	-3.165491
C	11.453866	2.155101	-4.356044
C	12.507640	1.290535	-4.508256
C	11.467348	6.374017	-5.813703
C	12.550281	7.162326	-6.259489
C	13.877216	6.796943	-5.881211
C	12.983419	4.911490	-4.639802
C	12.363071	8.303520	-7.080680
C	14.053876	5.655390	-5.061924
C	14.962599	7.585175	-6.334116
C	13.435527	9.047445	-7.503492
C	14.748555	8.685437	-7.126752
C	12.739154	0.642320	-5.777409
C	13.383192	1.001406	-3.439409
C	14.458308	0.105682	-3.596051
C	14.668619	-0.525470	-4.861410
C	15.344458	-0.193890	-2.529606
C	13.775647	-0.223955	-5.933193
C	15.745011	-1.420883	-5.011104
C	16.590343	-1.692644	-3.956305
C	16.386078	-1.072941	-2.706925
H	6.649332	0.619689	-2.758235
H	5.333624	2.699485	-2.904251
H	6.395351	4.820661	-3.643190
H	9.064192	0.606560	-3.346860
H	10.459997	6.642267	-6.116924
H	12.070200	0.865532	-6.599876
H	13.939470	-0.702747	-6.893679
H	13.219141	1.475796	-2.477879
H	15.900412	-1.896856	-5.974401
H	17.415296	-2.384583	-4.085517
H	15.059459	5.377036	-4.761857
H	13.145069	4.054825	-3.997263

H	11.353341	8.579448	-7.368654
H	13.278898	9.918871	-8.130248
H	15.587945	9.281933	-7.467735
H	15.970141	7.303878	-6.043235
H	17.055914	-1.292688	-1.882630
H	15.185527	0.284009	-1.568060

2– C^1C^5 triplet cyclized diradical

C	8.526599	3.852639	-3.976983
C	9.365144	2.715345	-3.924191
C	10.725716	3.119709	-4.373498
C	10.649599	4.581529	-4.681711
C	11.730942	5.441068	-5.155851
C	8.869818	1.491519	-3.509525
C	7.188692	3.764512	-3.610229
C	9.364328	4.925663	-4.446251
C	7.525445	1.406203	-3.141085
C	6.698177	2.528592	-3.191132
C	11.749646	2.304541	-4.498682
C	12.633610	1.260875	-4.540722
C	11.433577	6.615691	-5.824365
C	12.444906	7.489520	-6.277552
C	13.811867	7.147165	-6.048872
C	13.096011	5.113769	-4.932323
C	12.147758	8.696115	-6.961783
C	14.098941	5.939648	-5.366927
C	14.825656	8.021713	-6.508533
C	13.153030	9.523536	-7.394208
C	14.505611	9.183890	-7.165560
C	12.799198	0.493495	-5.755099
C	13.439567	0.929196	-3.425848
C	14.374527	-0.121384	-3.485318
C	14.517502	-0.868910	-4.695824
C	15.185038	-0.465939	-2.373098
C	13.699825	-0.522123	-5.814832
C	15.454053	-1.917675	-4.748351
C	16.229309	-2.229822	-3.650589
C	16.091098	-1.496719	-2.455302
H	7.120332	0.455794	-2.811219
H	5.657304	2.438129	-2.899643
H	6.544278	4.635497	-3.649527
H	9.514250	0.619029	-3.470304
H	10.395190	6.868763	-6.016984
H	12.187942	0.748660	-6.612504
H	13.810343	-1.092249	-6.732162
H	13.328447	1.494877	-2.507237
H	15.558505	-2.481263	-5.670397
H	16.946979	-3.040956	-3.705178
H	15.136138	5.675709	-5.184435
H	13.342159	4.203726	-4.398301
H	11.107939	8.954795	-7.136382
H	12.912480	10.444252	-7.914930
H	15.291018	9.846527	-7.512919
H	15.863759	7.757174	-6.331891
H	16.704137	-1.748665	-1.596727
H	15.077611	0.099840	-1.453017

2– C^1C^6 singlet cyclized diradical

C	4.204766	11.812376	-0.619470
C	5.257893	12.804426	-0.658100
C	2.858115	12.245766	-0.605966
C	4.630514	10.483915	-0.614419
C	5.901443	10.000648	-0.653706
C	6.965156	11.002677	-0.623402

C	6.136239	8.542480	-0.777073
C	8.406697	10.681314	-0.499795
C	6.558584	12.300172	-0.662913
C	4.905629	14.174536	-0.671835
C	2.558095	13.586389	-0.623514
C	3.585295	14.554017	-0.654512
C	9.349363	11.417800	-1.266700
C	8.867050	9.731197	0.388249
C	10.248643	9.471448	0.538695
C	11.186735	10.211342	-0.241448
C	10.731910	8.495545	1.446378
C	10.694521	11.187780	-1.141883
C	12.569111	9.945627	-0.087435
C	12.077823	8.261544	1.574081
C	13.005809	8.993451	0.799832
C	7.057296	8.026138	-1.664944
C	7.234174	6.631487	-1.815172
C	6.439545	5.739322	-1.034986
C	5.344741	7.645544	-0.010126
C	8.179605	6.090727	-2.722673
C	5.494113	6.289042	-0.134733
C	6.622328	4.343534	-1.188778
C	7.546850	3.850677	-2.075874
C	8.332902	4.733232	-2.850165
H	2.071903	11.499683	-0.584691
H	1.522129	13.906996	-0.612792
H	3.327075	15.607266	-0.665413
H	5.697297	14.914828	-0.693109
H	8.981669	12.164983	-1.961727
H	11.402020	11.755480	-1.738523
H	7.660019	8.693818	-2.271088
H	8.164519	9.169446	0.994360
H	10.016264	7.932630	2.037335
H	12.435216	7.511031	2.270893
H	4.885153	5.616755	0.461936
H	4.620754	8.057261	0.684766
H	6.016547	3.668010	-0.592464
H	7.677383	2.779428	-2.185799
H	9.060832	4.331600	-3.546839
H	8.784277	6.771429	-3.313663
H	14.067347	8.799248	0.909923
H	13.279654	10.509957	-0.683719

2– C^1C^6 triplet cyclized diradical

C	4.212754	11.811472	-0.615237
C	5.258098	12.796249	-0.662463
C	2.863340	12.236984	-0.594828
C	4.648761	10.482627	-0.611171
C	5.918990	9.988616	-0.653167
C	6.975962	10.984355	-0.623222
C	6.133231	8.528290	-0.780102
C	8.420929	10.683380	-0.496311
C	6.558578	12.281762	-0.666003
C	4.913759	14.168609	-0.683415
C	2.565095	13.577558	-0.617786
C	3.593331	14.546219	-0.661004
C	9.356424	11.449782	-1.242358
C	8.891164	9.723249	0.376011
C	10.275802	9.483488	0.530997
C	11.206633	10.254119	-0.227938
C	10.769300	8.498223	1.423046
C	10.704350	11.239853	-1.112575
C	12.592196	10.008032	-0.069716
C	12.118020	8.284122	1.555600

C	13.038799	9.046094	0.801922
C	7.063972	8.001710	-1.652015
C	7.220782	6.605236	-1.807045
C	6.395595	5.721964	-1.048637
C	5.312015	7.640118	-0.034479
C	8.175315	6.053944	-2.698648
C	5.441172	6.282087	-0.164363
C	6.558616	4.324214	-1.206965
C	7.492627	3.821107	-2.078205
C	8.308597	4.694862	-2.831324
H	2.078171	11.489661	-0.564862
H	1.529778	13.900211	-0.602464
H	3.332966	15.598922	-0.676773
H	5.706540	14.907850	-0.713418
H	8.980902	12.203157	-1.926622
H	11.406367	11.829855	-1.693859
H	7.689497	8.662704	-2.242176
H	8.194130	9.138729	0.966711
H	10.059246	7.912216	1.998104
H	12.483215	7.526285	2.240347
H	4.810060	5.616457	0.416547
H	4.582043	8.059894	0.649432
H	5.929867	3.655440	-0.627048
H	7.607578	2.748469	-2.191946
H	9.043618	4.285185	-3.515774
H	8.802932	6.727827	-3.273323
H	14.102681	8.867372	0.915584
H	13.297203	10.595443	-0.650059

3 – enediyne

C	6.307254	-4.400297	0.559306
C	-1.537491	4.506510	0.001578
C	3.812455	-1.000852	0.336602
C	4.344415	0.184071	-0.252083
C	1.716506	0.161508	0.729802
C	3.542450	1.339927	-0.335349
C	-2.326593	5.666074	-0.020502
C	4.616651	-2.163459	0.425594
C	2.241596	1.347934	0.142637
C	5.678987	0.155656	-0.737899
C	5.907477	-2.150639	-0.055623
C	1.431846	2.511849	0.059022
C	6.440104	-0.974685	-0.644710
C	-1.745450	6.923071	-0.092390
C	-0.357694	7.048120	-0.145868
C	0.442130	5.915518	-0.120299
C	-0.123580	4.634461	-0.042306
C	0.709813	3.487387	0.004718
C	2.480255	-0.971418	0.821205
H	7.136247	-5.103596	0.493145
H	5.445099	-4.806521	0.018016
H	-3.404544	5.559564	0.014723
H	6.035490	-4.259608	1.611677
H	-2.374111	7.806498	-0.109720
H	0.100177	8.029358	-0.204478
H	1.521784	6.003525	-0.154716
H	-1.462336	-0.173926	-0.477532
H	3.952322	2.238269	-0.784583
H	2.068210	-1.866806	1.276475
H	0.702384	0.176253	1.112471
H	-1.290894	-2.629949	-0.766450
H	-2.313489	-4.850291	-0.727989
H	-6.080783	-3.143013	0.419576
H	-6.261519	-0.663142	0.715492

H	-5.214324	1.564578	0.671801
H	6.091980	1.052481	-1.188585
H	4.192897	-3.051097	0.879288
H	7.459371	-1.007137	-1.011459
H	-4.901261	-7.311612	-0.313393
H	-3.363792	-6.644662	0.282455
H	-3.812781	-6.465623	-1.437313
O	6.763424	-3.199306	-0.021063
C	-4.197364	-6.486004	-0.411244
C	-2.913200	-3.982798	-0.483332
C	-5.035412	-3.010386	0.163887
C	-5.212775	-0.557345	0.456999
C	-4.280671	-4.124644	-0.144523
C	-2.666277	2.128882	0.075341
C	-3.256616	0.837819	0.096207
C	-4.634173	0.680734	0.433023
C	-2.508196	-0.285564	-0.211644
C	-3.084092	-1.574145	-0.193720
C	-4.463806	-1.724552	0.146883
C	-2.339211	-2.735119	-0.504813
C	-2.147263	3.227225	0.051746
O	-4.923244	-5.318515	-0.099982

3– C^1C^5 singlet transition state

C	-7.198985	-2.233913	1.060355
C	4.803178	-1.576978	-0.122136
C	6.304213	-3.441639	0.075060
C	1.199240	-1.955282	0.126230
C	-0.190461	-1.979931	0.288968
C	3.703792	-2.465865	0.025556
C	-0.773569	-1.657105	1.554999
C	-1.033735	-2.342081	-0.763361
C	-2.429348	-2.387113	-0.598231
C	-3.000413	-2.060831	0.668635
C	-3.302947	-2.751249	-1.658621
C	-2.127613	-1.697916	1.729541
C	-4.402898	-2.105686	0.838816
C	-5.218412	-2.463507	-0.214950
C	2.434577	-1.761640	-0.014014
C	-4.656134	-2.789021	-1.476347
C	3.052685	0.015301	-0.288920
C	3.915467	-3.828941	0.193795
C	6.102211	-2.073371	-0.095664
C	4.314029	-0.238368	-0.283741
C	5.223968	-4.310911	0.217457
H	3.075856	-4.505070	0.306280
H	6.942276	-1.397669	-0.206672
H	5.400342	-5.372961	0.348763
H	7.315097	-3.834593	0.096580
H	-6.879580	-2.914951	1.857113
H	-2.788225	7.568236	-0.406089
H	-2.982488	5.814886	-0.155437
H	-0.118285	-1.373710	2.369971
H	3.307469	2.378231	0.869057
H	-2.555826	-1.446328	2.694741
H	-0.603403	-2.597450	-1.726085
H	-4.814367	-1.854562	1.808787
H	-0.913342	1.945528	-1.700284
H	0.673766	0.075053	-1.603788
H	1.095174	6.594823	1.364764
H	2.699300	4.707778	1.475583
H	-1.542754	4.249728	-1.078088
H	-5.331417	-3.065607	-2.277507
H	-2.878072	-3.001995	-2.625307

H	-2.157084	6.422919	-1.616353
H	-8.267346	-2.357184	0.889105
H	-6.998790	-1.201485	1.368117
O	-6.567671	-2.539498	-0.163666
C	-2.319026	6.595171	-0.546030
C	2.383553	2.289426	0.307561
C	1.496719	3.383595	0.256879
C	0.276432	3.266373	-0.471146
C	0.888444	0.995298	-1.075330
C	1.772416	4.609653	0.919392
C	0.007131	2.043629	-1.133202
C	-0.622374	4.361256	-0.517846
C	0.894584	5.654744	0.864132
C	-0.318727	5.533490	0.137839
C	2.100369	1.099975	-0.344018
O	-1.100889	6.640374	0.160767

3– C^1C^5 triplet transition state

C	6.097383	-3.766674	-0.613132
C	-5.290350	0.235862	0.023861
C	-7.386509	-0.952632	0.121902
C	-2.033268	-1.452414	-0.216890
C	-0.680365	-1.821855	-0.295611
C	-4.598702	-0.996908	-0.069760
C	-0.066296	-2.041702	-1.568126
C	0.087044	-2.007567	0.855059
C	1.435800	-2.398175	0.778332
C	2.041342	-2.604850	-0.497494
C	2.231593	-2.593219	1.939839
C	1.245702	-2.412067	-1.659193
C	3.397672	-2.993648	-0.577868
C	4.137287	-3.172956	0.573147
C	-3.164273	-0.959341	-0.131116
C	3.541816	-2.968675	1.843836
C	-3.127222	1.368791	0.017063
C	-5.319436	-2.193279	-0.063623
C	-6.683396	0.244937	0.126975
C	-4.439308	1.391649	-0.000411
C	-6.706941	-2.167986	0.024142
H	-4.785127	-3.134523	-0.131210
H	-7.201916	1.193998	0.204393
H	-7.261665	-3.100010	0.017129
H	-8.468646	-0.943207	0.195234
H	5.625197	-4.576548	-1.180854
H	5.465146	5.385380	0.499156
H	4.390834	4.521422	1.627232
H	-0.665185	-1.909420	-2.462080
H	-1.083281	1.145515	-1.694967
H	1.697179	-2.571648	-2.633634
H	-0.365743	-1.844337	1.826887
H	3.835300	-3.144530	-1.557256
H	-0.184133	4.076879	2.223046
H	-2.374402	2.986884	1.990768
H	3.414012	2.681711	-2.275145
H	1.213718	1.567968	-2.535727
H	2.081453	4.501200	1.380144
H	4.156742	-3.119698	2.723380
H	1.781448	-2.437766	2.915044
H	3.781384	5.927267	0.710374
H	7.118056	-4.052092	-0.362020
H	6.117270	-2.860857	-1.229823
O	5.439041	-3.543090	0.613246
C	4.441975	5.053813	0.670777
C	-0.880570	1.788183	-0.846212

C	0.371949	2.403471	-0.724994
C	0.644180	3.248338	0.396479
C	-1.601214	2.836873	1.246130
C	1.404921	2.213615	-1.684923
C	-0.387433	3.435250	1.370850
C	1.899873	3.865785	0.521524
C	2.622781	2.822269	-1.548072
C	2.880405	3.659708	-0.437391
C	-1.906316	1.999675	0.112288
O	4.117410	4.208191	-0.410047

3– C^1C^6 singlet transition state

C	-5.162123	-4.678174	-0.400146
C	4.961957	-0.709660	-0.165415
C	6.195426	1.359558	0.315807
C	7.391529	-0.679888	-0.158358
C	7.391480	0.680225	0.157907
C	4.961910	0.709684	0.165545
C	0.253345	-1.425168	0.817856
C	-1.010213	-2.049501	0.769296
C	-1.360641	-2.844137	-0.360874
C	0.808250	-2.360222	-1.337870
C	-1.957184	-1.915027	1.819055
C	-0.413076	-2.977779	-1.406033
C	-2.628209	-3.474631	-0.412181
C	-3.519233	-3.320909	0.626948
C	6.195522	-1.359378	-0.315948
C	-3.175198	-2.530131	1.753765
C	3.709133	-1.330245	-0.287911
C	2.487856	-0.973669	-0.166419
C	2.487782	0.973522	0.166606
C	1.163598	-1.567637	-0.212097
C	3.709035	1.330105	0.288336
H	-5.191163	-4.106215	-1.334693
H	-4.502519	-5.543714	-0.530913
H	-6.166220	5.025433	0.159901
H	-4.502254	5.543799	0.530672
H	-5.191332	4.106536	1.334502
H	-6.166407	-5.024996	-0.160297
H	6.193284	-2.415944	-0.555504
H	8.329963	-1.209304	-0.281058
H	8.329877	1.209762	0.280375
H	6.193111	2.416117	0.555391
H	0.508855	-0.822798	1.682595
H	-0.665817	-3.584523	-2.270215
H	1.529461	-2.473226	-2.139199
H	-2.872210	-4.073849	-1.280956
H	-3.905767	-2.433235	2.548364
H	-1.700307	-1.308655	2.681662
O	-4.753398	-3.876317	0.684582
C	-5.162047	4.678402	0.399906
C	0.808095	2.359988	1.338055
C	0.253320	1.425098	-0.817775
C	-1.010222	2.049470	-0.769266
C	-1.360703	2.844051	0.360926
C	-1.957128	1.915080	-1.819096
C	-0.413208	2.977596	1.406160
C	-2.628259	3.474575	0.412186
C	-3.175133	2.530202	-1.753845
C	-3.519223	3.320921	-0.627004
C	1.163497	1.567450	0.212261
H	1.529243	2.472904	2.139452
H	-0.665990	3.584297	2.270361
H	0.508867	0.822780	-1.682537

H	-1.700203	1.308757	-2.681722
H	-3.905650	2.433377	-2.548501
H	-2.872305	4.073758	1.280970
O	-4.753368	3.876354	-0.684700

3– C^1C^6 triplet transition state

C	5.097999	4.956374	-0.137169
C	-4.886813	0.543684	-0.495811
C	-6.126665	-0.944241	1.054999
C	-7.303276	0.457808	-0.543733
C	-7.303115	-0.457208	0.545145
C	-4.886748	-0.544446	0.495314
C	-0.247984	1.473138	0.669949
C	0.994471	2.130863	0.703645
C	1.343527	3.041322	-0.338685
C	-0.797637	2.611524	-1.405105
C	1.931288	1.915532	1.750528
C	0.406238	3.254074	-1.387808
C	2.592278	3.699077	-0.308755
C	3.475014	3.465591	0.727575
C	-6.126950	0.944207	-1.054491
C	3.135193	2.562043	1.765787
C	-3.668507	1.162349	-0.700724
C	-2.423148	1.064039	-0.420739
C	-2.423156	-1.065018	0.419467
C	-1.166598	1.705418	-0.357887
C	-3.668458	-1.163229	0.699939
H	5.154067	4.479993	-1.122507
H	4.420620	5.816082	-0.192318
H	6.091033	-5.298546	-0.152124
H	4.421222	-5.815758	0.192029
H	5.154272	-4.480230	1.123338
H	6.090280	5.299068	0.152869
H	-6.127601	1.687456	-1.844346
H	-8.249195	0.793735	-0.954374
H	-8.248902	-0.792558	0.956562
H	-6.127107	-1.687361	1.844974
H	-0.506616	0.783969	1.465050
H	0.661943	3.946823	-2.183851
H	-1.507108	2.781734	-2.206576
H	2.835450	4.385514	-1.110584
H	3.856275	2.404580	2.559279
H	1.676655	1.221685	2.545035
O	4.692498	4.042029	0.856788
C	5.098630	-4.956021	0.137691
C	-0.798028	-2.612763	1.403872
C	-0.247402	-1.473051	-0.670225
C	0.995171	-2.130556	-0.703628
C	1.343783	-3.041601	0.338340
C	1.932533	-1.914452	-1.749864
C	0.405947	-3.255122	1.386830
C	2.592645	-3.699150	0.308702
C	3.136537	-2.560786	-1.764860
C	3.475918	-3.464914	-0.727010
C	-1.166563	-1.706089	0.356985
H	-1.507896	-2.783515	2.204876
H	0.661333	-3.948295	2.182606
H	-0.505718	-0.783454	-1.465055
H	1.678240	-1.220153	-2.544085
H	3.858028	-2.402744	-2.557864
H	2.835485	-4.386015	1.110264
O	4.693563	-4.041078	-0.855894

3– C^1C^5 singlet cyclized diradical

C	7.241916	-3.570824	1.047865
C	-1.594960	4.488685	-0.113967
C	-0.835742	6.758132	-0.051527
C	0.785093	1.781807	0.104605
C	1.827939	0.904107	0.262700
C	-0.248382	4.046572	-0.027916
C	2.205793	0.453020	1.579539
C	2.570265	0.427226	-0.839752
C	3.644821	-0.461669	-0.667609
C	4.003328	-0.896940	0.644096
C	4.402441	-0.950295	-1.766501
C	3.246390	-0.407417	1.749676
C	5.081217	-1.788605	0.819914
C	5.794249	-2.243039	-0.273816
C	-0.252388	2.566161	-0.030453
C	5.445515	-1.814532	-1.578408
C	-1.709475	2.145704	-0.151353
C	0.789911	4.959010	0.047854
C	-1.888924	5.847015	-0.126306
C	-2.399807	3.298838	-0.175507
C	0.485862	6.322409	0.034962
H	1.818669	4.621052	0.114211
H	-2.915692	6.188553	-0.192387
H	1.288183	7.049955	0.091857
H	-1.048503	7.821782	-0.060587
H	7.562001	-2.750991	1.700832
H	-5.640345	-6.578712	-0.309433
H	-4.052560	-5.910258	0.145196
H	1.638410	0.812602	2.429706
H	-4.076788	1.306322	0.716591
H	3.513620	-0.737835	2.748735
H	2.307055	0.759374	-1.838246
H	5.332824	-2.104185	1.825196
H	-1.369244	-2.364012	-1.223274
H	-0.472155	-0.090638	-1.137991
H	-6.830311	-2.590774	1.049112
H	-5.928534	-0.284028	1.150737
H	-3.197611	-3.965030	-0.778137
H	6.028154	-2.191831	-2.410660
H	4.141262	-0.626128	-2.768761
H	-4.742666	-5.559750	-1.463055
H	8.084619	-4.237397	0.870048
H	6.437738	-4.129143	1.540310
O	6.842073	-3.097579	-0.219044
C	-4.980919	-5.716913	-0.404719
C	-3.488834	0.502713	0.283716
C	-4.033702	-0.795799	0.237868
C	-3.261604	-1.861780	-0.309752
C	-1.459836	-0.290256	-0.740868
C	-5.333901	-1.088697	0.729899
C	-1.965492	-1.564184	-0.794900
C	-3.802225	-3.171457	-0.356031
C	-5.839206	-2.356740	0.678156
C	-5.067926	-3.413932	0.128572
C	-2.218556	0.777571	-0.194475
O	-5.683983	-4.621704	0.134874

3– C^1C^5 triplet cyclized diradical

C	7.904136	-3.467519	0.937599
C	-0.838796	4.250604	-0.119918
C	0.472705	6.249490	-0.109711
C	0.810933	1.046332	0.157325
C	1.985611	0.344012	0.293559
C	0.343120	3.482163	-0.008189

C	2.477036	-0.010476	1.602830
C	2.713386	-0.105833	-0.830804
C	3.887248	-0.864233	-0.686478
C	4.362084	-1.197141	0.618354
C	4.633964	-1.318140	-1.807676
C	3.615346	-0.742458	1.746111
C	5.540576	-1.956427	0.766047
C	6.240062	-2.380193	-0.348858
C	-0.039259	2.043197	0.025448
C	5.775628	-2.053589	-1.646773
C	-1.529742	2.000474	-0.085455
C	1.581546	4.096233	0.053808
C	-0.779145	5.638588	-0.171585
C	-1.914293	3.294872	-0.156453
C	1.638303	5.490866	0.001603
H	2.487744	3.505079	0.139425
H	-1.683917	6.229852	-0.257457
H	2.600307	5.989597	0.047753
H	0.541470	7.331379	-0.148733
H	8.160002	-2.582983	1.531745
H	-7.639386	-5.368292	-0.128249
H	-6.038084	-5.049864	0.585411
H	1.919835	0.323916	2.470014
H	-4.157320	1.931026	0.339243
H	3.973407	-0.991943	2.740297
H	2.358505	0.145649	-1.824343
H	5.879963	-2.196137	1.766472
H	-2.274047	-2.562421	-0.566958
H	-0.809885	-0.602165	-0.539001
H	-7.896186	-1.042290	0.490102
H	-6.422091	0.949611	0.532962
H	-4.523901	-3.560657	-0.353033
H	6.350985	-2.403148	-2.496032
H	4.284164	-1.071398	-2.804949
H	-6.299664	-4.814111	-1.164220
H	8.809183	-4.039193	0.737172
H	7.202112	-4.089861	1.503993
O	7.379065	-3.110226	-0.321665
C	-6.760198	-4.726749	-0.173348
C	-3.745644	0.947833	0.130101
C	-4.612653	-0.161350	0.109263
C	-4.083560	-1.461246	-0.142480
C	-1.870358	-0.481357	-0.350144
C	-6.009390	-0.035458	0.339201
C	-2.691439	-1.579780	-0.369305
C	-4.949376	-2.583348	-0.159674
C	-6.829584	-1.127400	0.317556
C	-6.297761	-2.419138	0.065409
C	-2.384837	0.817143	-0.097273
O	-7.216202	-3.416211	0.071395

3– C^1C^6 singlet cyclized diradical

C	-4.663189	-5.723105	-0.362461
C	4.731059	-0.702077	-0.176480
C	5.970319	1.365027	0.337865
C	7.151841	-0.685844	-0.168783
C	7.151980	0.684912	0.168202
C	4.731203	0.701515	0.176385
C	0.012206	-1.437023	0.722862
C	-1.120869	-2.276839	0.683603
C	-1.227704	-3.269830	-0.333116
C	0.915698	-2.547562	-1.212642
C	-2.171110	-2.168382	1.633491
C	-0.175162	-3.377043	-1.274144

C	-2.366276	-4.113446	-0.376617
C	-3.363965	-3.976096	0.562350
C	5.970043	-1.365771	-0.338237
C	-3.260747	-2.990291	1.578101
C	3.472107	-1.287470	-0.311909
C	2.248574	-0.716799	-0.143935
C	2.248710	0.716565	0.144527
C	1.025979	-1.551275	-0.208277
C	3.472364	1.287109	0.312038
H	-4.696386	-5.294776	-1.370875
H	-3.863744	-6.471638	-0.318367
H	-5.615844	6.203574	0.144321
H	-3.863022	6.472416	0.317440
H	-4.695477	5.295810	1.370388
H	-5.616573	-6.202905	-0.144965
H	5.965919	-2.419086	-0.594764
H	8.095454	-1.205210	-0.295477
H	8.095697	1.204135	0.294698
H	5.966407	2.418354	0.594344
H	0.079847	-0.693639	1.509865
H	-0.241888	-4.129166	-2.054320
H	1.713313	-2.638359	-1.942317
H	-2.425840	-4.860116	-1.159237
H	-4.068604	-2.914749	2.296546
H	-2.099050	-1.413826	2.410225
O	-4.492010	-4.725223	0.617689
C	-4.662425	5.723857	0.361851
C	0.916243	2.547981	1.212667
C	0.012362	1.436758	-0.722269
C	-1.120604	2.276729	-0.683217
C	-1.227163	3.270182	0.333081
C	-2.170996	2.167983	-1.632904
C	-0.174498	3.377641	1.273942
C	-2.365596	4.114000	0.376338
C	-3.260502	2.990081	-1.577744
C	-3.363421	3.976391	-0.562452
C	1.026270	1.551279	0.208688
H	1.713954	2.638969	1.942213
H	-0.241027	4.130104	2.053807
H	0.079794	0.692988	-1.508929
H	-2.099165	1.413047	-2.409289
H	-4.068474	2.914319	-2.296037
H	-2.424968	4.861004	1.158655
O	-4.491330	4.725700	-0.618034

3– C^1C^6 triplet cyclized diradical

C	-4.620625	-5.809182	-0.353953
C	4.721594	-0.696089	-0.177871
C	5.956957	1.365661	0.346308
C	7.137335	-0.685268	-0.173068
C	7.137362	0.685111	0.172956
C	4.721622	0.696030	0.177745
C	-0.012583	-1.445291	0.710118
C	-1.134004	-2.300532	0.672685
C	-1.215563	-3.313128	-0.327093
C	0.928661	-2.578454	-1.194115
C	-2.196933	-2.188862	1.608043
C	-0.150365	-3.423419	-1.253466
C	-2.342808	-4.171964	-0.368980
C	-3.353492	-4.030639	0.555391
C	5.956904	-1.365764	-0.346447
C	-3.275146	-3.025722	1.554556
C	3.455449	-1.275135	-0.309974
C	2.224654	-0.712393	-0.142418

C	2.224677	0.712359	0.142548
C	1.014089	-1.563138	-0.206601
C	3.455496	1.275112	0.309892
H	-4.645767	-5.398498	-1.369903
H	-3.813808	-6.548071	-0.287170
H	-5.571104	6.296191	0.139364
H	-3.813477	6.548225	0.286749
H	-4.645888	5.399123	1.369638
H	-5.571423	-6.295657	-0.140042
H	5.951105	-2.417845	-0.609143
H	8.082059	-1.201944	-0.302731
H	8.082107	1.201747	0.302629
H	5.951199	2.417751	0.608965
H	0.036055	-0.687381	1.484556
H	-0.198639	-4.189530	-2.021288
H	1.735555	-2.670792	-1.913480
H	-2.383389	-4.933314	-1.138534
H	-4.092547	-2.947943	2.261870
H	-2.143838	-1.419703	2.371867
O	-4.472659	-4.792893	0.610931
C	-4.620469	5.809534	0.353585
C	0.928812	2.578615	1.194076
C	-0.012624	1.445155	-0.709888
C	-1.134030	2.300415	-0.672495
C	-1.215472	3.313193	0.327108
C	-2.197058	2.188584	-1.607719
C	-0.150199	3.423608	1.253376
C	-2.342677	4.172089	0.368920
C	-3.275229	3.025504	-1.554309
C	-3.353428	4.030663	-0.555372
C	1.014136	1.563143	0.206717
H	1.735760	2.671048	1.913368
H	-0.198394	4.189846	2.021077
H	0.035928	0.687096	-1.484187
H	-2.144085	1.419239	-2.371365
H	-4.092708	2.947595	-2.261518
H	-2.383218	4.933500	1.138413
O	-4.472561	4.792960	-0.611014

dimer major product **5a**

C	-0.550743	3.244759	-0.317530
C	-0.304526	4.581539	0.025524
H	0.707895	4.961174	-0.050751
C	-1.333245	5.400407	0.469990
H	-1.125451	6.432424	0.730824
C	-2.623660	4.892321	0.590281
H	-3.428950	5.524956	0.947308
C	-2.884290	3.570853	0.245744
H	-3.889682	3.173652	0.330485
C	-1.867893	2.734691	-0.220856
C	-2.158540	1.351822	-0.615210
C	-2.687910	0.283854	0.007722
C	-3.169819	-0.006772	1.366540
C	-2.291755	-0.533294	2.292756
H	-1.265172	-0.720689	1.998360
C	-2.707798	-0.826995	3.607044
H	-1.993008	-1.235959	4.312932
C	-4.003176	-0.591039	3.990665
H	-4.327976	-0.809324	5.003386
C	-4.942551	-0.061238	3.073130
C	-6.287344	0.184664	3.446737
H	-6.591945	-0.035812	4.465373
C	-7.190089	0.687643	2.544535
H	-8.216686	0.869513	2.844119

C	-6.786295	0.964558	1.220735
H	-7.507501	1.350590	0.508349
C	-5.489871	0.741111	0.827243
H	-5.186282	0.942110	-0.194253
C	-4.530296	0.229801	1.737060
C	-1.943369	0.630374	-1.939769
H	-0.893253	0.550601	-2.233518
C	-2.775828	1.140811	-3.066696
H	-2.414431	2.026083	-3.582158
C	-3.929133	0.571720	-3.432758
H	-4.506181	0.996065	-4.249699
C	-4.461172	-0.634192	-2.804940
C	-5.661849	-1.192925	-3.256796
H	-6.192883	-0.706838	-4.069885
C	-6.174344	-2.351676	-2.687910
H	-7.107582	-2.768100	-3.051602
C	-5.482276	-2.975756	-1.655048
H	-5.871791	-3.881887	-1.203908
C	-4.283495	-2.434624	-1.199343
H	-3.736148	-2.921884	-0.399015
C	-3.768087	-1.267898	-1.756547
C	-2.494798	-0.658109	-1.204330
C	-1.448344	-1.642193	-0.953004
C	-0.532248	-2.392415	-0.686196
C	0.550749	-3.244745	-0.317534
C	0.304525	-4.581507	0.025585
H	-0.707908	-4.961123	-0.050626
C	1.333248	-5.400381	0.470027
H	1.125445	-6.432382	0.730915
C	2.623683	-4.892321	0.590218
H	3.428982	-5.524963	0.947214
C	2.884318	-3.570869	0.245625
H	3.889720	-3.173682	0.330305
C	1.867911	-2.734698	-0.220936
C	2.158565	-1.351829	-0.615293
C	1.943394	-0.630336	-1.939823
H	0.893269	-0.550566	-2.233542
C	2.494805	0.658129	-1.204338
C	2.687893	-0.283874	0.007694
C	3.169770	0.006724	1.366528
C	2.291690	0.533231	2.292738
H	1.265111	0.720624	1.998329
C	2.707711	0.826905	3.607037
H	1.992909	1.235849	4.312923
C	4.003083	0.590946	3.990676
H	4.327860	0.809208	5.003410
C	4.942480	0.061175	3.073147
C	6.287271	-0.184712	3.446770
H	6.591850	0.035739	4.465418
C	7.190043	-0.687638	2.544567
H	8.216639	-0.869496	2.844162
C	6.786280	-0.964510	1.220748
H	7.507511	-1.350490	0.508359
C	5.489858	-0.741082	0.827242
H	5.186296	-0.942040	-0.194270
C	4.530249	-0.229838	1.737063
C	2.775834	-1.140706	-3.066794
H	2.414419	-2.025932	-3.582321
C	3.929146	-0.571608	-3.432820
H	4.506180	-0.995902	-4.249797
C	4.461210	0.634250	-2.804917
C	5.661915	1.192973	-3.256713
H	6.192948	0.706923	-4.069825
C	6.174437	2.351670	-2.687742

H	7.107696	2.768086	-3.051391
C	5.482370	2.975704	-1.654852
H	5.871910	3.881790	-1.203642
C	4.283562	2.434582	-1.199206
H	3.736219	2.921807	-0.398854
C	3.768124	1.267911	-1.756499
C	1.448360	1.642218	-0.953000
C	0.532254	2.392414	-0.686156

dimer minor product **5b**

C	-1.034280	-2.302430	1.969226
C	-0.857806	-3.490974	2.694828
C	-1.792772	-3.897677	3.634559
C	1.716762	-0.152012	-3.021075
C	-2.918657	-3.115290	3.877122
C	2.833457	-2.036655	-1.098692
C	-3.109597	-1.939505	3.161271
C	0.878581	-1.512626	0.334711
C	-2.195000	-1.524945	2.187889
C	-2.407869	-0.262500	1.462296
C	-0.018304	-1.873189	1.066982
C	2.606345	-1.080397	-3.389786
C	-2.704899	0.111976	0.198601
C	-2.264705	1.158494	1.986790
C	-3.017464	-0.540684	-1.075650
C	-2.559637	1.621802	0.501724
C	-3.263768	1.566986	3.015698
C	-3.825913	2.433565	0.289336
C	-1.383880	2.245862	-0.097646
C	3.191331	-2.042079	-2.459647
C	-2.469691	-0.014178	-2.233205
C	-3.871439	-1.689264	-1.175845
C	-2.666544	-0.616904	-3.489101
C	4.102228	-3.001745	-2.915324
C	-3.427473	-1.751816	-3.595814
C	3.381691	-2.985130	-0.240267
C	-4.053808	-2.304887	-2.453546
C	-4.880834	-3.450450	-2.560036
C	-4.583096	-2.221944	-0.074007
C	4.652956	-3.937827	-2.049490
C	-5.529058	-3.958715	-1.463743
C	4.290846	-3.930366	-0.706291
C	-5.387751	-3.326023	-0.211626
C	2.917838	0.553056	2.447990
C	4.898872	0.393416	1.051981
C	3.725491	0.684949	3.595586
C	-4.389428	2.221526	2.709611
C	5.092234	0.680723	3.482870
C	-4.713093	2.664750	1.357388
C	-5.898027	3.368814	1.115936
C	-4.137078	2.928356	-0.973925
C	5.711470	0.536168	2.217667
C	-6.208790	3.840411	-0.152583
C	7.121763	0.526819	2.078513
C	-5.322256	3.622028	-1.201650
C	5.536598	0.233665	-0.203953
C	7.708442	0.377631	0.847431
C	6.905948	0.226306	-0.303849
C	-0.357197	2.740376	-0.515961
C	0.865028	3.341556	-0.941205
C	0.913883	4.721698	-1.183704
C	2.049619	2.575003	-1.047946
C	2.110890	5.340651	-1.515748
C	3.281209	4.591455	-1.597512

C	3.246047	3.220912	-1.365455
C	2.015383	1.121559	-0.845158
C	2.593468	0.275833	0.025094
C	1.274917	0.030006	-1.608614
C	1.895970	-0.975428	-0.558656
C	3.476342	0.415885	1.193231
H	0.031585	-4.082652	2.511597
H	-1.638563	-4.819887	4.184055
H	-3.648013	-3.420526	4.619525
H	-3.986960	-1.327801	3.345439
H	-1.245199	1.400641	2.308442
H	-1.848927	0.872135	-2.163398
H	-2.200660	-0.183277	-4.367297
H	-3.572872	-2.233971	-4.557456
H	-4.999359	-3.913852	-3.534703
H	-6.161137	-4.835043	-1.559468
H	-5.923189	-3.711168	0.649529
H	-4.499748	-1.734750	0.887044
H	-3.052345	1.293882	4.045753
H	-5.097483	2.476962	3.493117
H	-6.577974	3.548806	1.943331
H	-7.134015	4.381186	-0.319821
H	-5.548502	3.990998	-2.196155
H	-3.441167	2.769800	-1.790211
H	4.713157	-4.657483	-0.021238
H	3.090573	-2.978892	0.805098
H	1.298671	0.525814	-3.760187
H	0.001025	5.299111	-1.092549
H	2.131555	6.409231	-1.699976
H	1.837921	0.562202	2.544225
H	4.221415	5.072051	-1.845007
H	3.256825	0.795717	4.567478
H	2.908351	-1.157485	-4.430639
H	0.186201	0.091132	-1.535190
H	4.373670	-3.009536	-3.966889
H	5.719393	0.787496	4.362654
H	4.154373	2.632751	-1.434516
H	7.732082	0.639079	2.969503
H	5.358572	-4.672584	-2.422168
H	4.922898	0.102353	-1.088229
H	7.375538	0.096571	-1.273038
H	8.789318	0.371427	0.755633

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