

Supplementary Information for

Excited State Photochemically Driven Surface Formation of Benzene from Acetylene Ices on Pluto and in the Outer Solar System

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Determination of the Film Thickness

The film thickness of the acetylene ice exploited for the collection of the ultraviolet-visible (UV-Vis) absorption spectra was determined using the method by Swaenepoel.¹ This method was developed to determine the thickness and the refractive index of a thin film from its absorption along with the spacing and intensity of interference minima and maxima in the spectrum. Positions of the interference minima and maxima were determined by calculating the second derivative of the absorption spectrum and smoothing it using a pseudo-gaussian window. Table S5 shows the refractive indices at wavelengths between 302 and 220 nm. These values range from 1.41 to 1.43 and are in good agreement with refractive indices by Hudson *et al.* of 1.34 at 670 nm.² With these values for n , the thickness, d , of the film can be calculated using the equation

$$d = \frac{\lambda_1 \lambda_2}{2(\lambda_1 n_2 - \lambda_2 n_1)}$$

where λ_1 and λ_2 are the wavelengths of adjacent minima or maxima and n_1 and n_2 are the refractive indices at each wavelength. Thicknesses derived from the minima and maxima in this spectral region are compiled in Table S6. The mean value of these thicknesses is $1,330 \pm 80$ nm. The large deviation of individual values is mostly due to the low spectral resolution of the absorption spectra and the low prominence of the minima and maxima due to very similar refractive indices of the LiF substrate and the acetylene film.

Dose Calculation

From this film thickness and the absorptions at different wavelengths, the doses applied to the ices upon photon exposure can be calculated. The energy supplied to the sample by the photons was calculated from the average power of the laser beam and the irradiation time taking into account reflection losses from the two faces of the entrance window (CaF_2) and the vacuum–acetylene ice interface. Due to the low absorption of the acetylene ice (<1%), absorption losses in the film can be neglected. Light reflected by the silver surface underneath the acetylene film was also taken into account.³ The density of the acetylene ice was taken as 0.83 g cm^{-3} .⁴ Table S1 summarizes the doses and number of processed molecules inferred from this analysis.

Benzene Yield

A previously established calibration procedure for the detection efficiency of the PI-ReToF setup utilizing propyne, propene, and 1,2-butadiene along with their known ionization cross-sections was used to determine the amount of benzene formed in the present experiments.^{5, 6} In a separate experiment, an acetylene film on a rhodium-coated silver substrate was irradiated using the same conditions as those in the 222 nm irradiation REMPI experiment. During the TPD phase of the experiment, single photon ionization at 10.49 eV was used to determine the benzene yield in this experiment based on the ionization cross section of benzene at 10.49 eV of 30 ± 6 Mb.⁷ Correcting for the photon flux at 10.49 eV as measured by a NIST calibrated XUV photodiode (Opto. Diode Corp. SXUV100) and for quantitative differences in benzene formation between the experiments as determined by an electron impact quadrupole mass spectrometer, the total number of benzene molecules formed in the 222 nm REMPI experiment was determined to be $(6 \pm 1) \times 10^{15}$ molecules. From this number, the yield in the 249 nm and 288 nm irradiation experiments can be determined by comparing the integrated signal in each experiment as the REMPI TPD was carried out under identical conditions in each experiment. Knowing the total energy deposited in the ice and the photon energy (Table S1), this number can be correlated to the number of benzene molecules formed per absorbed photon at different irradiation wavelengths.

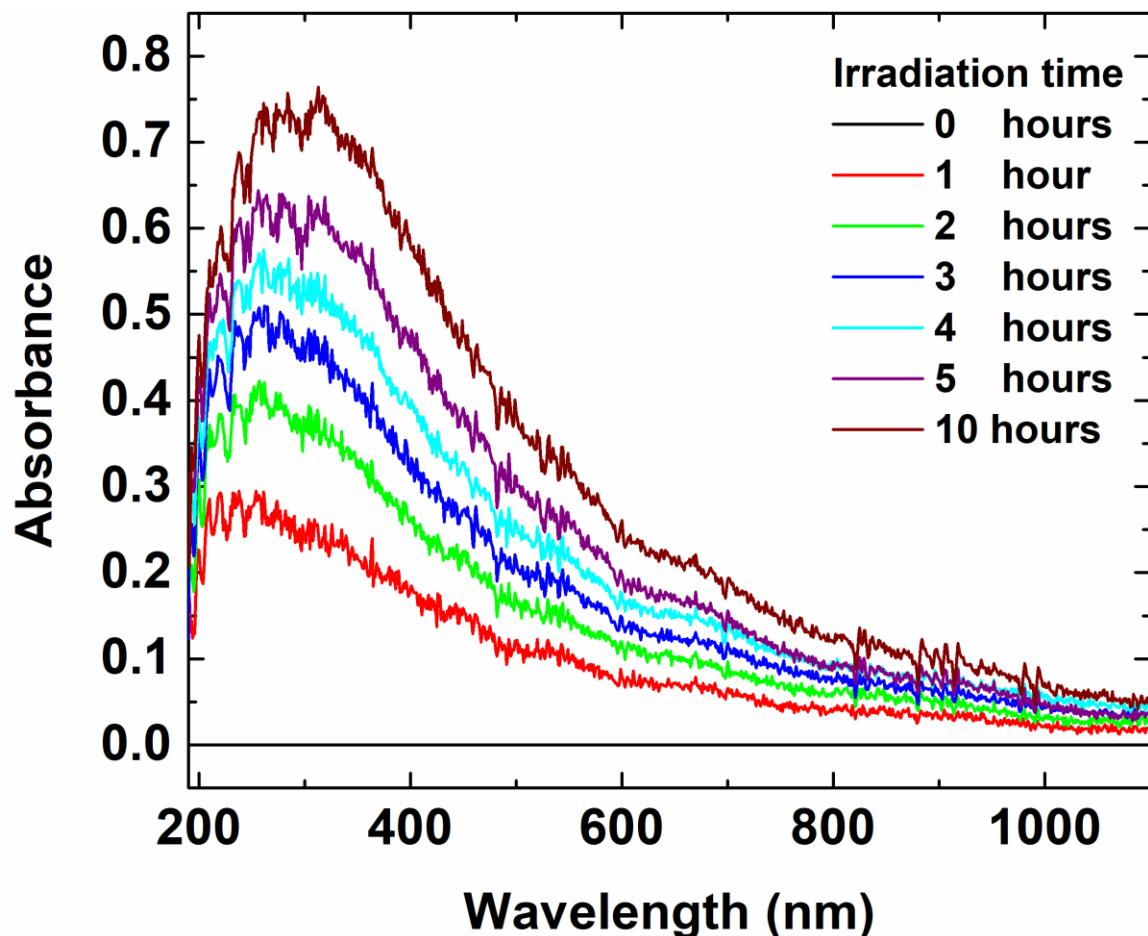


Fig. S1. UV-Vis spectra of the sample processed at 222 nm. Spectra were taken after each hour of irradiation. Spectra taken after 5–8 hours did not differ significantly from those taken after 4 hours and were therefore omitted for clarity. The absorbance was referenced to the unprocessed acetylene ice.

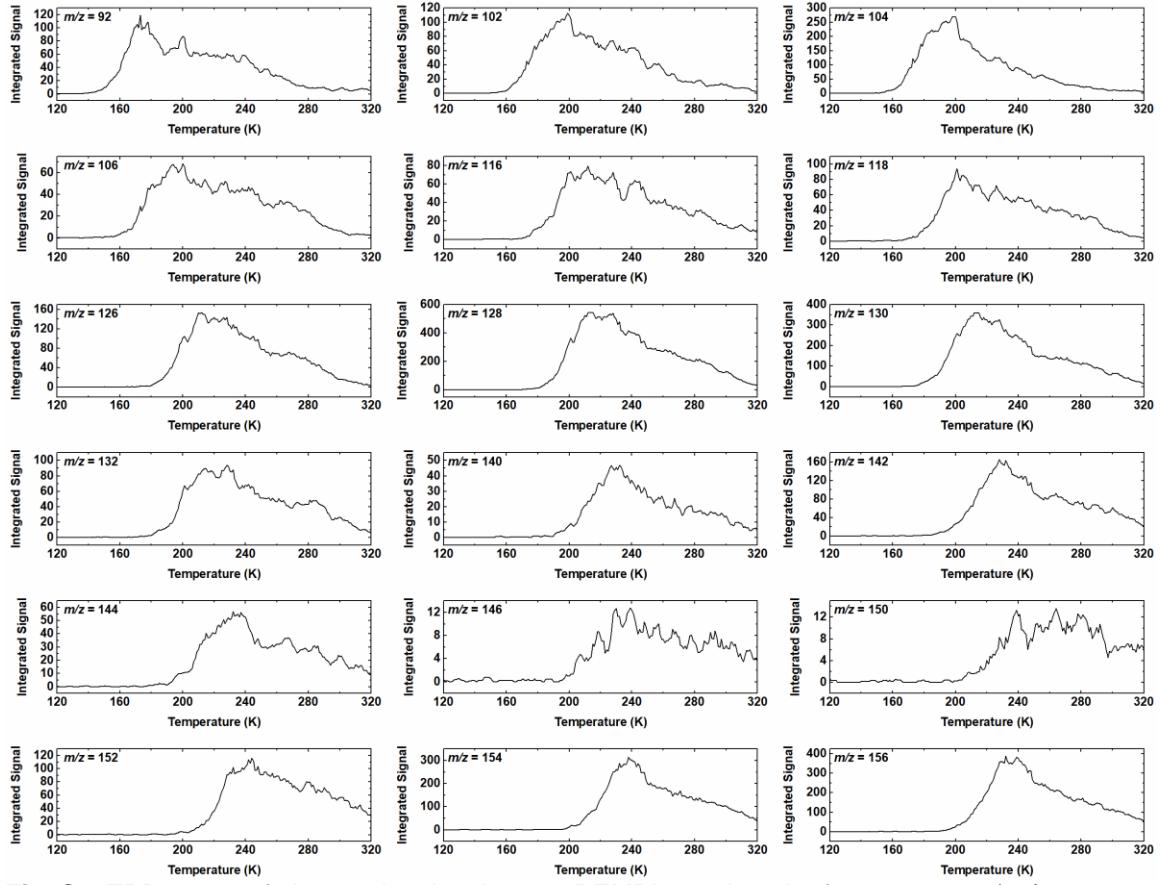


Fig. S2. TPD traces of observed molecules at a REMPI wavelength of 259.003 nm. ($m/z = 92$ – 156).

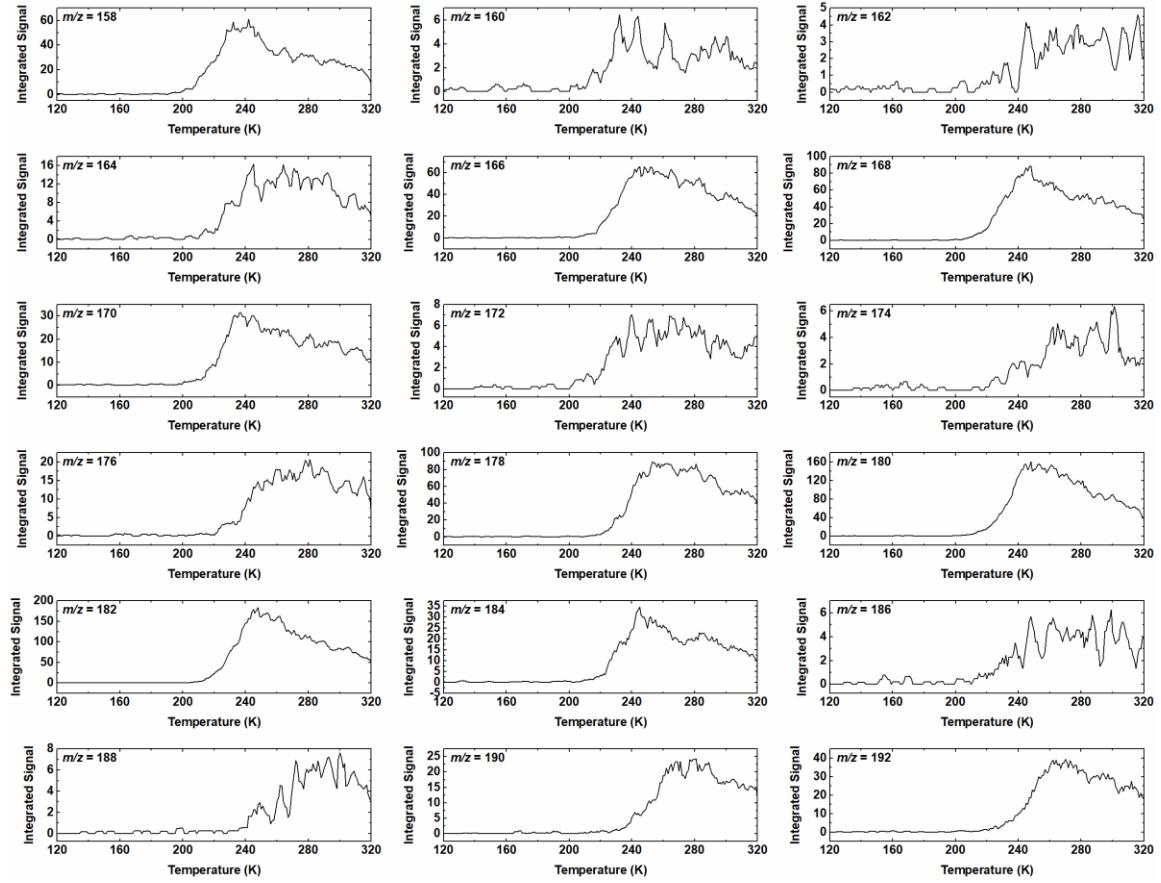


Fig. S3. TPD traces of observed molecules at a REMPI wavelength of 259.003 nm. ($m/z = 158\text{--}192$).

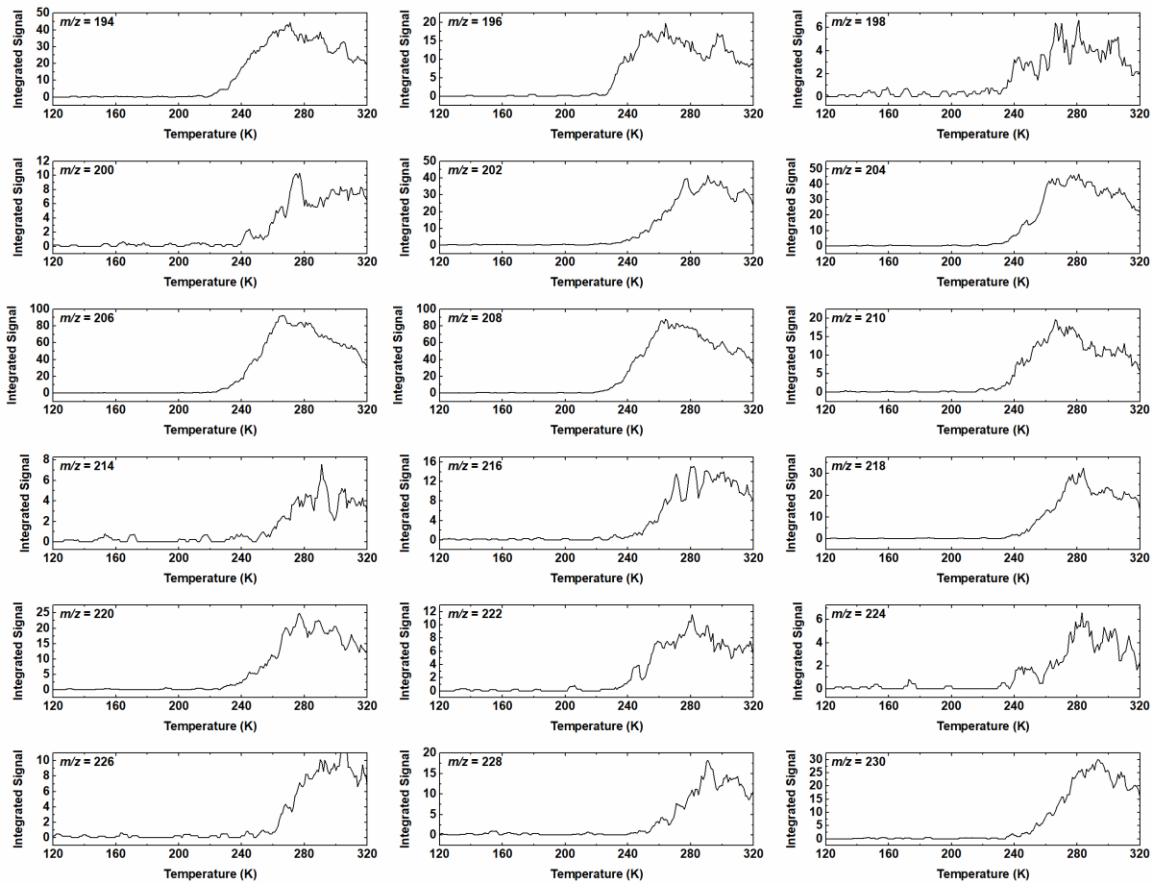


Fig. S4. TPD traces of observed molecules at a REMPI wavelength of 259.003 nm. ($m/z = 194\text{--}230$).

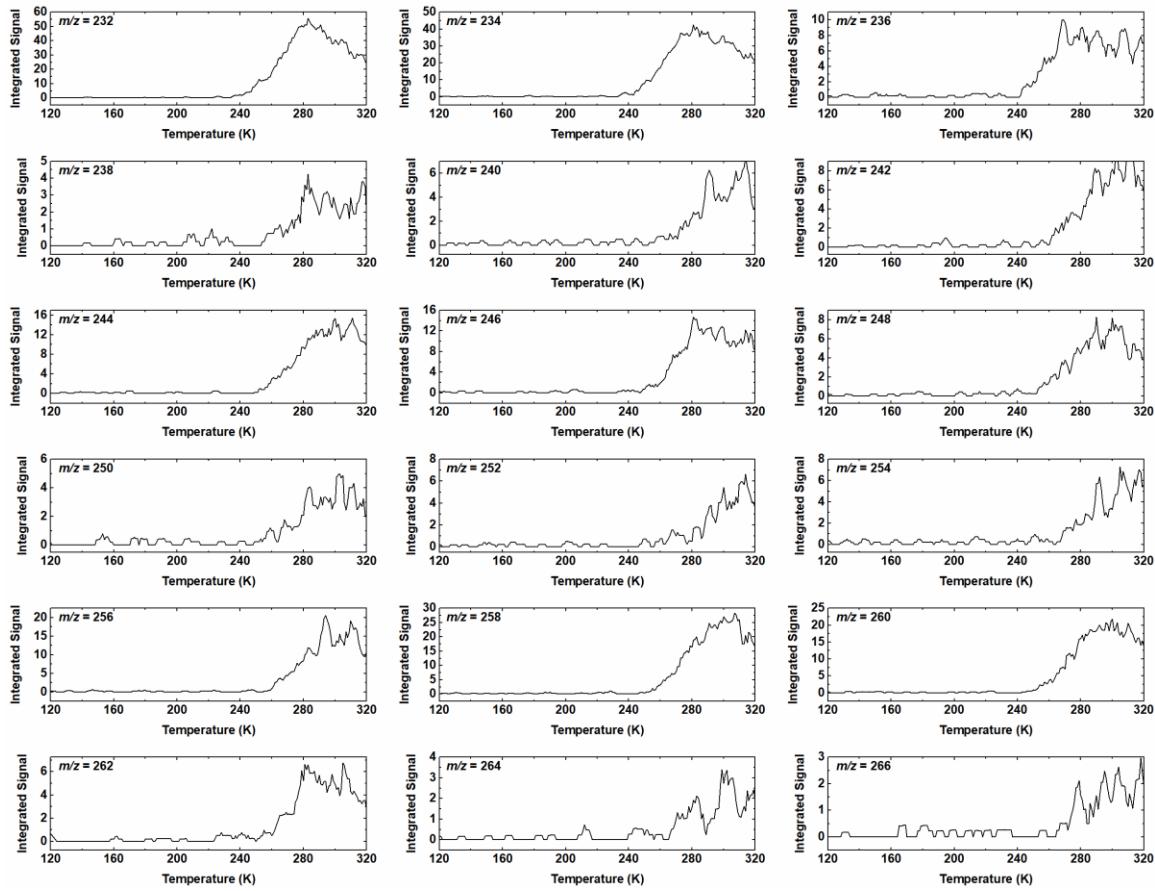


Fig. S5. TPD traces of observed molecules at a REMPI wavelength of 259.003 nm. ($m/z = 232 - 266$).

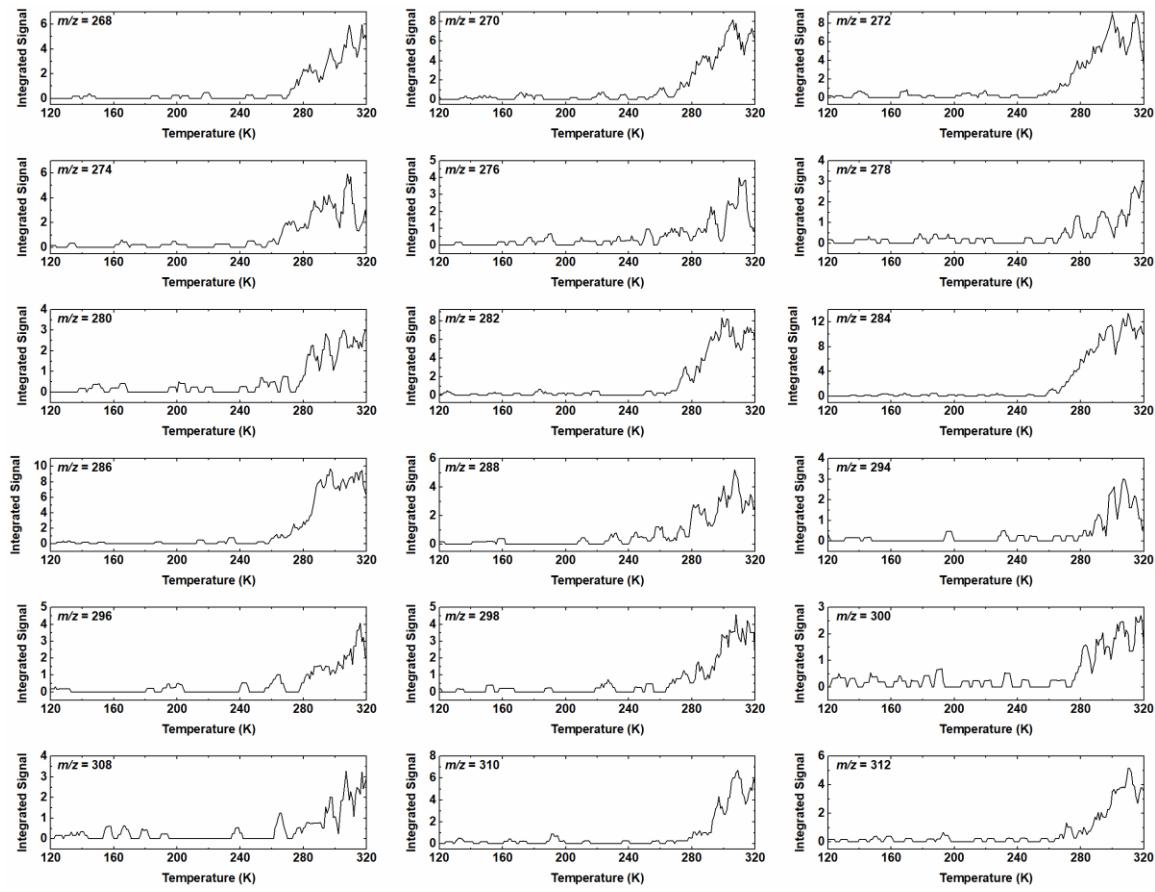


Fig. S6. TPD traces of observed molecules at a REMPI wavelength of 259.003 nm. ($m/z = 268$ – 312).

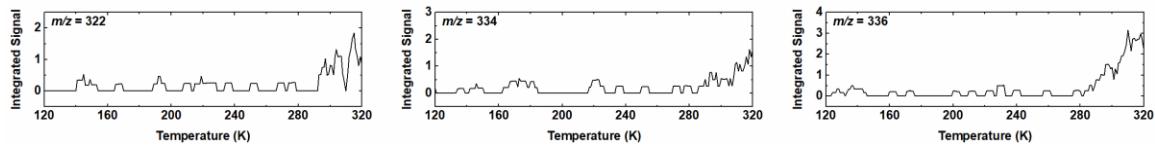


Fig. S7. TPD traces of observed molecules at a REMPI wavelength of 259.003 nm. ($m/z = 322$ – 336).

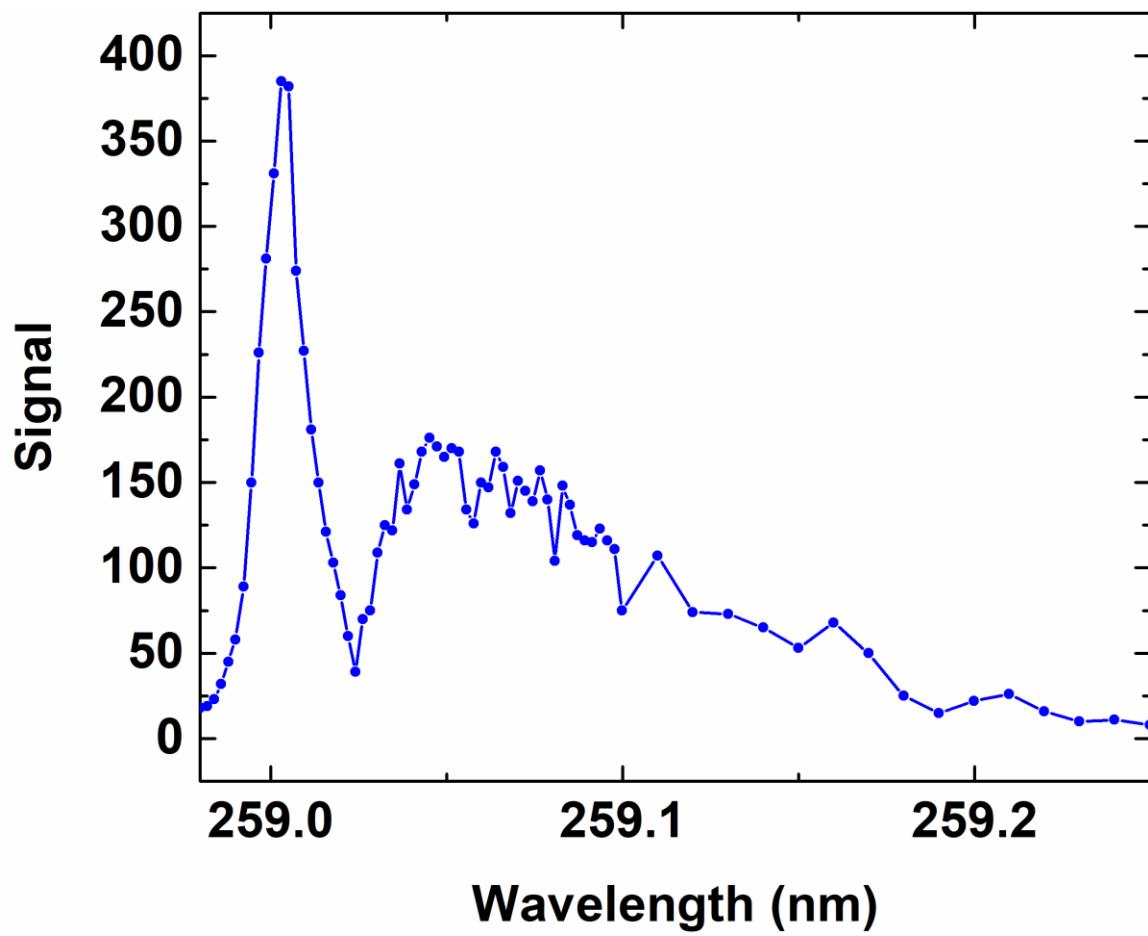


Fig. S8. Wavelength scan for the [1+1] REMPI transition of benzene. The maximum signal is achieved at 259.003 nm.

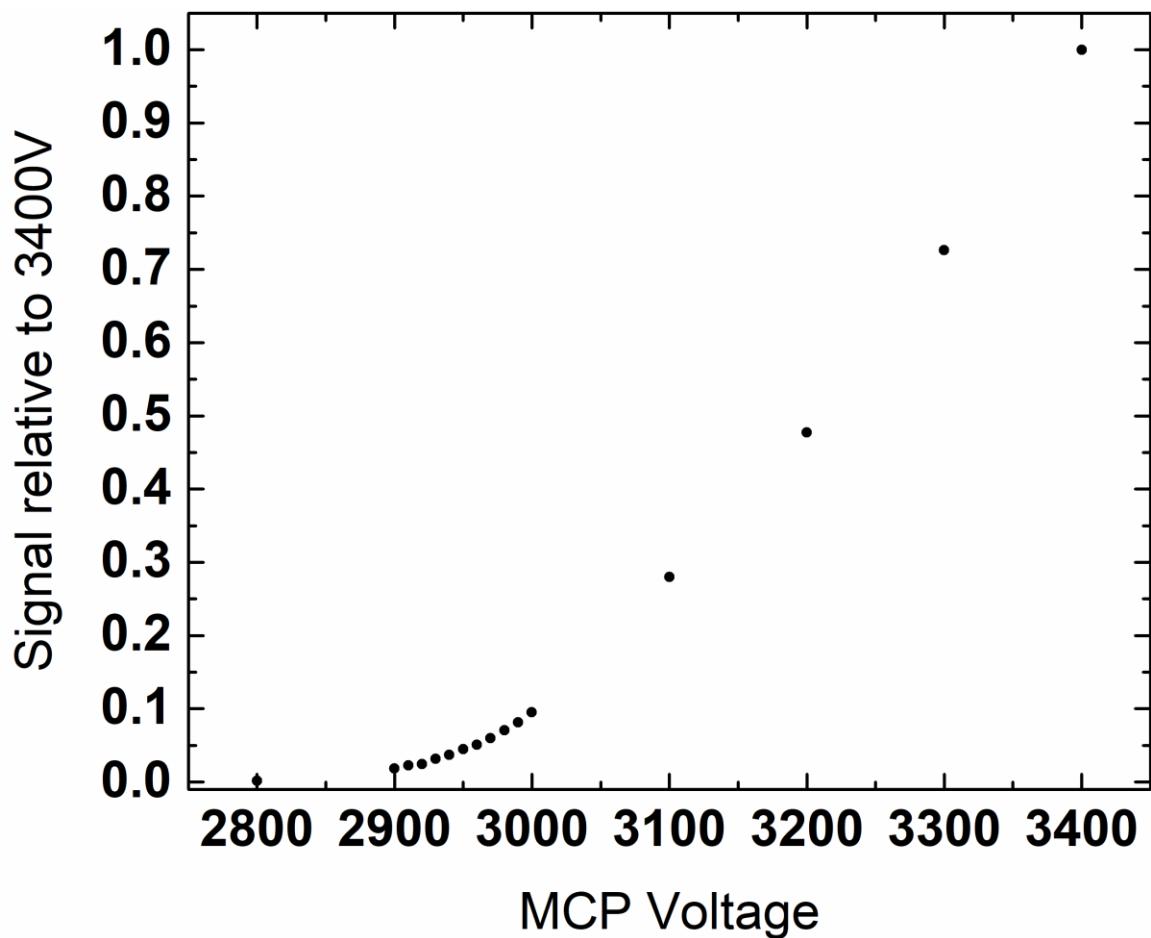


Fig. S9. Dependence of the signal at $m/z = 78$ for different MCP voltages. The relative signal is referenced to that at 3400 V, which is the standard operating voltage in the experiments.

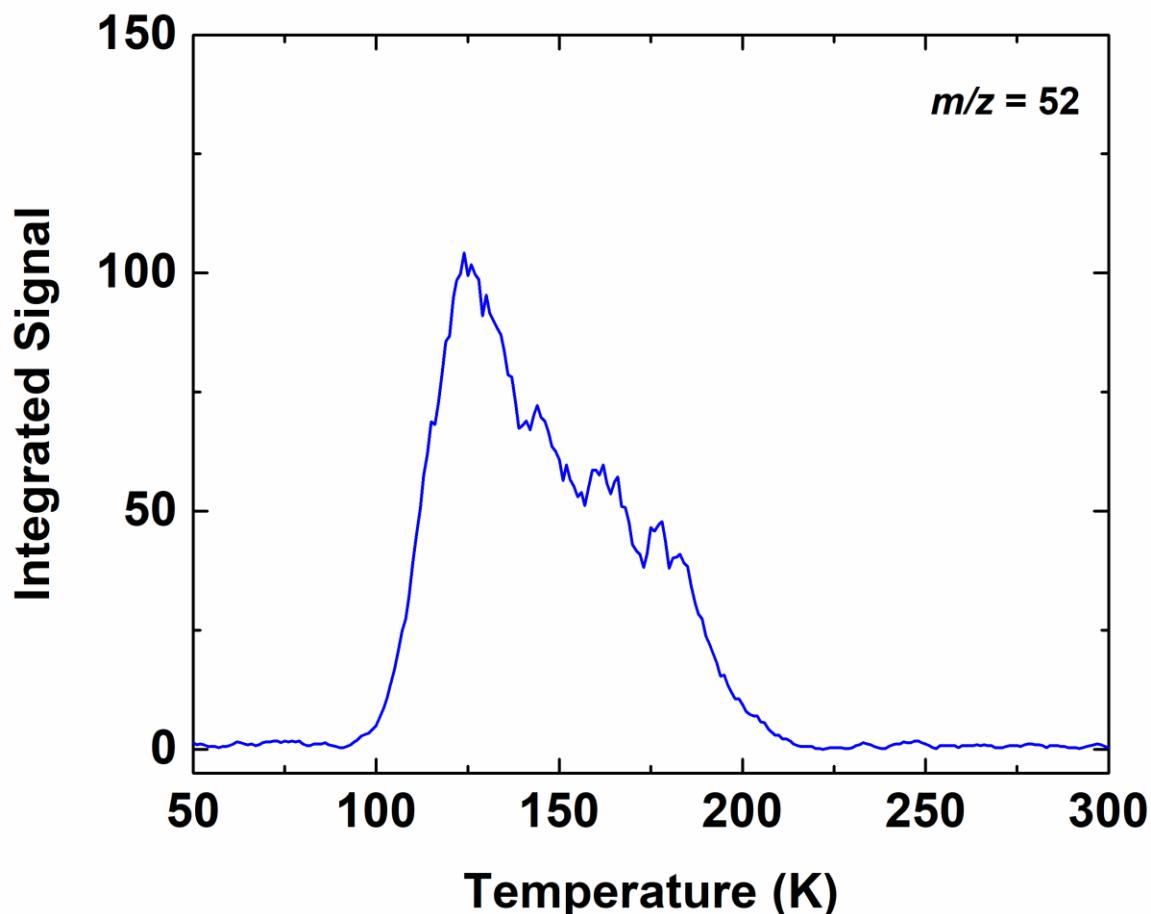


Fig. S10. TPD trace of $m/z = 52$ (C_4H_4) recorded at a photon energy of 10.49 eV after 222 nm irradiation of acetylene ice.

Table S1. Experimental parameters for the different wavelengths used in the experiments.

Wavelength (nm)	Total energy of irradiation (J)	Absorption (1330 nm film)	Dose (eV molecule ⁻¹)	Thickness (nm)	Processed molecules
288	560 ± 30	0.0010	1.7 ± 0.2	1200 ± 100	2.3 ± 0.2 × 10 ¹⁸
249	500 ± 70	0.0028	4.3 ± 0.7	1200 ± 100	2.3 ± 0.2 × 10 ¹⁸
222	480 ± 30	0.0055	8.4 ± 1.2	1000 ± 100	1.8 ± 0.2 × 10 ¹⁸

Table S2. Infrared absorptions of acetylene ice before irradiation

Wavenumber (cm ⁻¹)	Assignment	Carrier	Reference
4076	$\nu_1 + \nu_5$	Combination	2
3861	$\nu_2 + 2\nu_4 + \nu_5$	Combination	2
3434	$\nu_2 + 2 \nu_5$	Combination	2
3327	ν_1	CH stretch	2
3235	ν_3	CH stretch	2
3005	ν_3 (¹³ C ₂ H ₂)	CH stretch	
2737; 2715	$\nu_2 + \nu_5$	Combination	8
2545	ν_3 (C ₂ DH)	CD stretch	8
1962	ν_2	C≡C stretch	5
1391	$\nu_4 + \nu_5$	Combination	2
784	ν_5	CCH bend	2
743	ν_5	CCH bend	2

Table S3. New infrared absorptions in acetylene ice after irradiation at 222 nm.

Wavenumber (cm ⁻¹)	Assignment	Carrier	Reference
3287	ν_1 (C ₄ H ₄)	\equiv CH stretch	9
3089	$\nu_{16} + \nu_{13}$ (C ₆ H ₆)	Combination	10
3065	ν_{CH} (aromatic)	=CH stretch	11
3035	ν_{CH} (aromatic)	=CH stretch	12
2970	$\nu_6 + \nu_7$ (C ₄ H ₄)	Combination	9
2925	ν_{CH} (alkyl)	Asym. -CH stretch	11
2875	ν_{CH} (-CH ₃)	Sym. -CH stretch	11
2840	ν_{CH} (-CH ₂ -)	Sym. -CH stretch	11
2117	$\nu_{\text{C=C}}$ (R-C≡CH)	Alkyne C≡C stretch	11
1477	ν_{13} (C ₆ H ₆)	C=C aromatic stretch	10
1035	ν_{12} (C ₆ H ₆)	C-H in-plane bending	10
997	δ_{CH} (substituted benzenes/PAHs)	Aromatic =C-H in-plane deformation	11
959	δ_{CH} (substituted benzenes/PAHs)	Aromatic =C-H out-of-plane deformation	11

Table S4: Observed mass-to-charge ratios and possible molecular assignments (249 nm experiment)

m/z	Possible molecular formula	Possible assignment
78	C ₆ H ₆	Benzene
92	C ₇ H ₈	Toluene
102	C ₈ H ₆	Phenylacetylene
104	C ₈ H ₈	Styrene
106	C ₈ H ₁₀	Ethylbenzene, Dimethylbenzene, Xylene
116	C ₉ H ₈	Indene, 1-Propynylbenzene, Methylphenylacetylene
118	C ₉ H ₁₀	Indane, Methylstyrene
126	C ₁₀ H ₆	Aceanapentene, Diethynylbenzene
128	C ₁₀ H ₈	Naphthalene
130	C ₁₀ H ₁₀	Methylindene, Diethenylbenzene, Dihydronaphthalene
132	C ₁₀ H ₁₂	Tetrahydrobiphenyl, Dimethylstyrene
140	C ₁₁ H ₈	Pentadiynylbenzene, Norcapillene
142	C ₁₁ H ₁₀	Ethyldieneindene, Methylnaphthalene
144	C ₁₁ H ₁₂	Ethyldiene, Dimethylindene, Dihydromethylnaphthalene
146	C ₁₁ H ₁₄	Cyclopentylbenzene, Benzylcyclobutane
150	C ₁₂ H ₆	Triethynylbenzene, Dicyclopropnaphthalene
152	C ₁₂ H ₈	Acenaphthalene, Biphenylene
154	C ₁₂ H ₁₀	Heptalene, Acenaphthene, Benzocyclooctatetraene
156	C ₁₂ H ₁₂	Dimethylnaphthalene, Ethynaphthalene
158	C ₁₂ H ₁₄	Butylphenylacetylene, 1,3-hexadienylbenzene
160	C ₁₂ H ₁₆	Cyclohexylbenzene, Diethylstyrene
162	C ₁₂ H ₁₈	Hexamethylbenzene, Dipropylbenzene
164	C ₁₃ H ₈	Heptatriynylbenzene
166	C ₁₃ H ₁₀	Fluorene, Phenalene
168	C ₁₃ H ₁₂	Diphenylmethane, Dibenzofuran, Methylacenaphthene
170	C ₁₃ H ₁₄	Trimethylnaphthalene, Propylnaphthalene
172	C ₁₃ H ₁₆	Diallylphenylmethane
174	C ₁₄ H ₆	Tetraethynylbenzene
176	C ₁₄ H ₈	Diethylnaphthalene
178	C ₁₄ H ₁₀	Anthracene, Phenanthrene, Diphenylacetylene
180	C ₁₄ H ₁₂	Stilbene, 9,10-Dihydroanthracene
182	C ₁₄ H ₁₄	Dimethylbiphenyl, Diphenylethane
184	C ₁₄ H ₁₆	Butylnaphthalene, Tetramethylnaphthalene
186	C ₁₄ H ₁₈	Octahydroanthracene, Ethynylhexylbenzene
188	C ₁₄ H ₂₀	Cyclohexylethylbenzene, isobutyltetrahydronaphthalene
190	C ₁₅ H ₁₀	Methylenephenanthrene, Ethynylfluorene
192	C ₁₅ H ₁₂	Methylphenanthrene, Ethylidenefluorene
194	C ₁₅ H ₁₄	Ethylfluorene, Diphenylpropene, Methylstilbene
196	C ₁₅ H ₁₆	Diphenylpropane, Dibenzylmethane
198	C ₁₅ H ₁₈	Pentanylnaphthalene, Cadalene, Tripropenylbenzene
200	C ₁₅ H ₂₀	Nonnylnaphthalene
202	C ₁₆ H ₁₀	Pyrene, Fluoranthene
204	C ₁₆ H ₁₂	Phenylnaphthalene, Dihydropyrene
206	C ₁₆ H ₁₄	Dimethylphenanthrene, Tetrahydropyrene, Dimethylanthracene
208	C ₁₆ H ₁₆	Diphenylbutene, Phenyltetralin, Hexahydriopyrene
210	C ₁₆ H ₁₈	Diethylbiphenyl, Tetramethylacenaphthene
214	C ₁₇ H ₁₀	Diethynylfluorene
216	C ₁₇ H ₁₂	Benzofluorene, 1H-Benzo[de]anthracene, Methylpyrene
218	C ₁₇ H ₁₄	Cyclopentenophenanthrene, methylphenylnaphthalene
220	C ₁₇ H ₁₆	Methylphenyldihydronaphthalene, Propylanthracene

222	C ₁₇ H ₁₈	Diethylfluorene, 3,5-diphenyl-1-pentene
224	C ₁₈ H ₈	Tetraethynylnaphthalene,
226	C ₁₈ H ₁₀	Cyclopentapyrene, Ethynylpyrene, Diethynylanthracene
228	C ₁₈ H ₁₂	Chrysene, Vinylpyrene, Benzophenanthrene
230	C ₁₈ H ₁₄	Terphenyl, Dihydrochrysene, Dimethylpyrene
232	C ₁₈ H ₁₆	Tetrahydrochrysene, Dimethylphenylnaphthalene
234	C ₁₈ H ₁₈	Tetramethylphenanthrene, Retene
236	C ₁₈ H ₂₀	Dihydroanthracene
238	C ₁₈ H ₂₂	Diphenylhexane, Diisopropylbiphenyl
240	C ₁₉ H ₁₂	Olympicene, 2H-Benzopyrene
242	C ₁₉ H ₁₄	Dihydrobenzopyrene, Methylchrysene, Methylbenzanthracene
244	C ₁₉ H ₁₆	Triphenylmethane, Benzylbiphenyl, Diphenyltoluene
246	C ₁₉ H ₁₈	Methylcyclohexadienedibenzene
248	C ₁₉ H ₂₀	Isopropyldimethylphenanthrene, Diphenylheptadiene
250	C ₂₀ H ₁₀	Corannulene, Diethynylpyrene
252	C ₂₀ H ₁₂	Benzopyrene, Perylene
254	C ₂₀ H ₁₄	Binaphthyl, Dihydroperylene, Cholanthrene
256	C ₂₀ H ₁₆	Dimethylcrhrysene, Dimethylbenzophenanthrene
258	C ₂₀ H ₁₈	Tetramethylpyrene, Dibenzylbenzene, Triphenylethane
260	C ₂₀ H ₂₀	Dimethylphenyldimethylnaphthalene
262	C ₂₀ H ₂₂	Dipropylanthracene, Hexylanthracene, Decahydroperylene
264	C ₂₀ H ₂₄ /C ₂₁ H ₁₂	Diisopropylhydroanthracene / Sumanene
266	C ₂₁ H ₁₄	Methylbenzopyrene, Methylbenzotetraphene, Methylperylene
268	C ₂₁ H ₁₆	Methylcholanthrene, Dinaphthylmethane
270	C ₂₁ H ₁₈	Trimethylphenylene, Propylchrysene, Propanyltetracene
272	C ₂₁ H ₂₀	Dibenzyltoluene
274	C ₂₂ H ₁₀	Triethynylpyrene, Phenyldecapentaynylbenzene
276	C ₂₂ H ₁₂	Benzo[ghi]perylene, Anthanthrene
278	C ₂₂ H ₁₄	Pentacene, Picene, Pentaphene
280	C ₂₂ H ₁₆	Styrylanthracene, Dihydrobenzotetraphene
282	C ₂₂ H ₁₈	Distyrylbenzene, Dinaphthylethane
284	C ₂₂ H ₂₀	Tertbutylchrysene, Diethyltetraphene
286	C ₂₂ H ₂₂	Tribenzylmethane, Trismethylphenylmethane
288	C ₂₃ H ₁₂	Methylphenyldecapentaynylbenzene
294	C ₂₃ H ₁₈	Benzofulvene, Propylperylene
296	C ₂₃ H ₂₀	Isopropylphenylanthracene, Mesitylanthracene, Dinaphthylanthracene
298	C ₂₄ H ₁₀	Tetraethynylpyrene
300	C ₂₄ H ₁₂	Coronene, Hexadehydrotribenzoannulene
308	C ₂₄ H ₂₀	Tetramethylperylene, Octahydrocoronene
310	C ₂₄ H ₂₂	Bimethylstyrylbenzene
312	C ₂₄ H ₂₄	Hexamethyltriphenylene, Triphenylcyclohexane
322	C ₂₅ H ₂₂ /C ₂₆ H ₁₀	Isopropyldiphenylnaphthalene / Hexaethynylanthracene
334	C ₂₆ H ₂₂	Tetraphenylethane, Dimethylquarterphenyl
336	C ₂₆ H ₂₄	Dipropylperylene, Hexylperylene

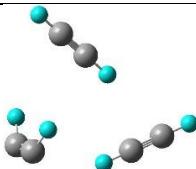
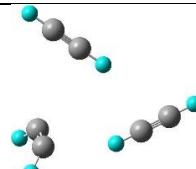
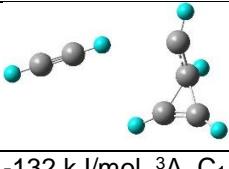
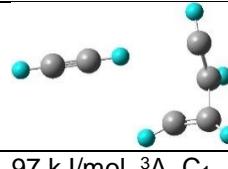
Table S5. Refractive indices derived from the absorption spectra of solid C₂H₂

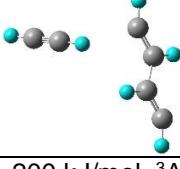
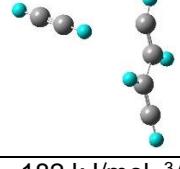
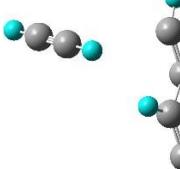
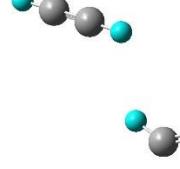
Wavelength (nm)	Refractive index <i>n</i>
304	1.41
280	1.42
261	1.42
245	1.42
231	1.43
220	1.43

Table S6. Film thicknesses derived from minima and maxima in the low absorption region of C₂H₂

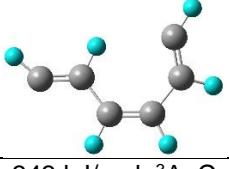
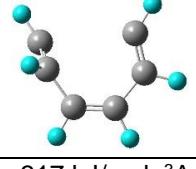
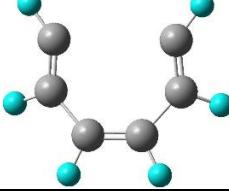
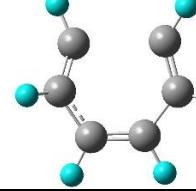
Film thickness (nm)
1448
1265
1327
1293
1389
1209
1281
1293
1366
1446

Table S7. Reactants, products, intermediates, and transition state structures relevant to the formation of triplet benzene from the T₁ state of acetylene. Geometries were optimized and frequencies were calculated at the B3LYP/6-311G** level. Relative energies were calculated at the CCSD(T)/CBS level.

Initial structure				TS1			
							
Relative energy, Electronic state & point group		0 kJ/mol, ³ A, C ₁		2.38 kJ/mol, ³ A, C ₁			
Imaginary frequency -31.45							
C	1.397390	-1.916634	0.665539	C	-0.787903	-1.747508	-0.032331
H	1.510777	-1.059001	1.335761	C	-1.338676	1.445089	0.568519
C	1.398304	-1.922153	-0.663714	C	-1.228957	2.150966	-0.550642
H	1.512691	-1.070154	-1.340936	H	-1.439787	3.211839	-0.720510
C	-2.264288	-0.537198	0.000816	C	-1.936064	-2.088734	-0.100799
H	-1.515287	-1.294549	0.002184	H	-2.955438	-2.382921	-0.161937
C	-3.099395	0.323514	-0.000713	H	-1.664242	1.787871	1.556199
H	-3.848129	1.078313	-0.002054	H	0.234955	-1.455547	0.022192
C	0.689420	1.746071	-0.000481	C	2.248765	0.431750	-0.022564
H	-0.337431	1.460501	-0.000505	H	1.466025	1.153475	-0.060637
C	1.846469	2.062281	-0.000450	C	3.119725	-0.391436	0.021930
H	2.869976	2.349611	-0.000436	H	3.897146	-1.115489	0.060011
[1]				TS2			
							
-132 kJ/mol, ³ A, C ₁				97 kJ/mol, ³ A, C ₁			
Imaginary frequency -618.72							
C	1.049540	-1.063915	-0.152105	C	0.999972	-1.227965	-0.346394
C	1.562413	0.348412	-0.426527	C	1.808445	0.447121	-0.288419
C	1.027572	1.501136	0.250724	C	1.131135	1.547479	0.167591
H	1.051032	2.566985	0.064413	H	0.847786	2.505927	-0.244222
C	2.215364	-0.811803	0.331526	C	1.927650	-0.845532	0.457882
H	3.062523	-1.088427	0.936551	H	2.518341	-1.175084	1.305533
H	1.926987	0.565414	-1.437026	H	2.449301	0.576562	-1.162920
H	0.189395	-1.704163	-0.255361	H	0.248090	-1.912785	-0.697290
C	-2.443555	0.294365	0.109654	C	-2.389495	0.237340	0.140582
H	-1.530479	0.835310	0.218309	H	-1.395771	0.595517	0.282166
C	-3.465606	-0.320438	-0.013967	C	-3.506164	-0.169044	-0.018487
H	-4.373826	-0.861654	-0.122717	H	-4.497007	-0.526530	-0.159799

[2]	TS3			
				
-200 kJ/mol, ^3A , C_1	-182 kJ/mol, ^3A , C_1			
	Imaginary frequency -693.55			
C 0.651658	1.718008	0.242384	C 0.642862	1.719499
C 1.896548	-0.413593	0.352793	C 1.980083	-0.350593
C 2.601044	-1.359135	-0.228036	C 2.634060	-1.350632
H 3.083311	-2.283651	0.049866	H 3.162126	-2.158474
C 1.360247	0.769688	-0.331372	C 1.303650	0.714639
H 1.583896	0.843694	-1.400596	H 1.374555	0.640246
H 1.679895	-0.486665	1.423258	H 1.901816	-0.251544
H 0.183069	2.648700	-0.039074	H 0.100397	2.590606
C -2.680831	-0.191233	-0.006730	C -2.699880	-0.225515
H -1.658668	0.107399	0.013096	H -1.671507	0.038731
C -3.831871	-0.525068	-0.028731	C -3.857915	-0.520309
H -4.852269	-0.821479	-0.048394	H -4.884541	-0.782099
[3]	TS4			
				
-196 kJ/mol, ^3A , C_1	-173 kJ/mol, ^3A , C_1			
	Imaginary frequency -176.68			
C -0.647128	1.696892	-0.141749	C -1.377783	1.617791
C -2.015263	-0.344439	-0.438280	C -1.844849	-0.828617
C -2.667275	-1.365463	0.072750	C -0.898286	-1.732793
H -2.893528	-1.781331	1.043718	H 0.123103	-1.816281
C -1.305410	0.670829	0.355757	C -1.678149	0.559560
H -1.341594	0.546665	1.443793	H -1.833843	0.680259
H -1.981676	-0.211914	-1.519607	H -2.815846	-1.071508
H -0.086509	2.540967	0.231462	H -1.213719	2.671194
C 2.714220	-0.222651	-0.085252	C 2.349784	0.342162
H 1.684570	0.024060	-0.198968	H 1.377220	0.709980
C 3.873701	-0.497838	0.043751	C 3.441370	-0.078838
H 4.901662	-0.742424	0.157736	H 4.410569	-0.449235
[4]	TS5			

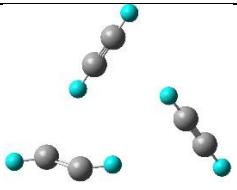
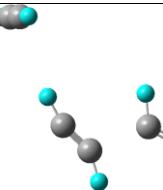
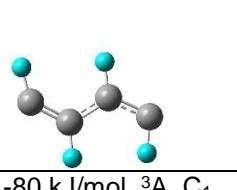
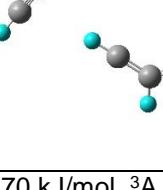
-187 kJ/mol, ${}^3\text{A}$, C_1	-174 kJ/mol, ${}^3\text{A}$, C_1				
	Imaginary frequency -665.31				
C 0.792664	-1.574404	-0.021458	C -0.750043	-1.521520	0.000419
C 2.072175	0.572748	-0.051910	C -2.104264	0.576978	-0.000276
C 1.131557	1.487391	0.001824	C -1.187568	1.515715	0.000406
H 1.064463	2.563220	-0.058005	H -1.141857	2.593820	0.000524
C 1.915390	-0.897616	0.057419	C -1.892277	-0.894819	-0.000215
H 2.846076	-1.446684	0.204093	H -2.824079	-1.473480	-0.000797
H 3.105371	0.915625	-0.186853	H -3.155812	0.887048	-0.000979
H -0.263888	-1.407550	-0.170761	H 0.180464	-2.039755	0.000904
C -2.509784	0.444874	0.092427	C 2.470880	0.331725	-0.000053
H -1.603660	0.990597	0.216448	H 1.458036	0.663759	0.000069
C -3.522886	-0.180278	-0.049909	C 3.607700	-0.049413	-0.000184
H -4.423052	-0.731502	-0.175274	H 4.616684	-0.383392	-0.000303
[5]	TS6				
-190 kJ/mol, ${}^3\text{A}$, C_1	-161 kJ/mol, ${}^3\text{A}$, C_1				
	Imaginary frequency -379.08				
C 1.006504	-1.535137	-0.026734	C -1.653416	-0.625861	0.119263
C 2.049685	0.739520	0.016623	C -0.238375	1.168486	-0.244147
C 1.006954	1.535172	-0.027035	C 1.049564	1.098143	0.042879
H 0.804369	2.594682	-0.035420	C 1.874376	-0.114137	0.192215
C 2.049490	-0.739786	0.016305	C 1.622472	-1.321153	-0.264463
H 3.043357	-1.198347	0.057348	C -2.827185	-0.317735	0.064074
H 3.043639	1.197800	0.058703	H -0.891232	2.021641	-0.359987
H 0.803619	-2.594588	-0.035355	H 2.107655	-2.285624	-0.267835
C -2.570189	0.000321	-0.001811	H -3.804441	0.092797	-0.020374
H -1.504688	0.000674	-0.015247	H 2.811795	0.031548	0.742226
C -3.768906	-0.000056	0.013212	H 1.588030	2.037151	0.207191
H -4.831520	-0.000421	0.026607	H -0.776425	-1.223967	0.239854
[6]	TS7				

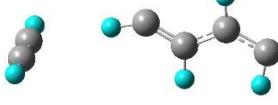
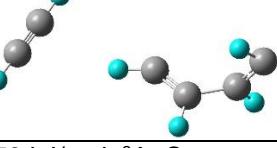
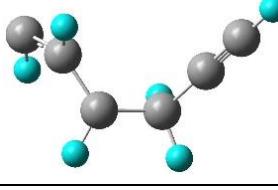
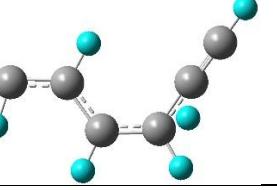
	
-343 kJ/mol, ^3A , C ₁	-317 kJ/mol, ^3A , C ₁
	Imaginary frequency -115.39
C -1.307989 -0.323881 0.090544	C -1.436566 -0.032277 0.365702
C -0.568953 0.922579 -0.046240	C -0.517977 -1.158748 0.073092
C 0.771138 1.073087 -0.029038	C 0.802648 -1.080115 -0.139880
C 1.808403 0.043831 0.090208	C 1.649540 0.120125 -0.113933
C 1.733053 -1.251054 -0.136998	C 1.310784 1.344402 0.230255
C -2.616791 -0.431695 -0.034015	C -1.890396 0.839270 -0.501773
H -1.175366 1.816903 -0.153204	H -1.803035 0.023439 1.400613
H 2.404195 -2.096058 -0.098371	H -0.977174 -2.145065 0.067253
H -3.358627 -1.213826 0.029283	H 1.807961 2.301347 0.289648
H 2.790717 0.430247 0.391120	H -2.559835 1.686909 -0.497761
H 1.152992 2.087515 -0.092959	H 2.694046 -0.054345 -0.398498
H -0.727075 -1.221976 0.317371	H 1.329839 -2.008219 -0.342027
[7]	TS8
	
-324 kJ/mol, ^3A , C ₁	-298 kJ/mol, ^3A , C ₁
	Imaginary frequency -482.17
C 1.632195 -0.048325 -0.136349	C 0.558515 -1.204142 -0.181003
C 0.675158 -1.129108 0.090618	C -0.794921 -1.138234 -0.025024
C -0.675161 -1.129106 0.090629	C -1.491641 0.093884 0.231663
C -1.632200 -0.048323 -0.136329	C -1.101861 1.247048 -0.326904
C -1.530873 1.242150 0.106786	C 1.268536 1.181413 0.087137
C 1.530885 1.242138 0.106821	C 1.506481 -0.124009 0.054346
H 2.586861 -0.392000 -0.557436	H 0.997180 -2.189500 -0.307807
H 1.142075 -2.104867 0.199957	H -1.350616 -2.069895 0.043596
H -2.165538 2.108596 -0.009118	H 1.899374 2.037626 0.287935
H 2.165547 2.108588 -0.009074	H 2.514933 -0.465119 0.312867
H -2.586886 -0.392006 -0.557365	H -1.455997 2.266205 -0.375042
H -1.142079 -2.104863 0.199980	H -2.275532 0.084920 0.997164
[8]	

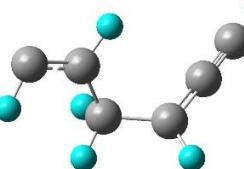
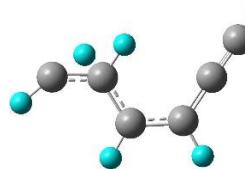
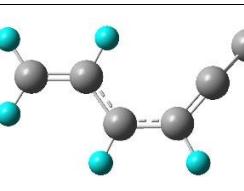
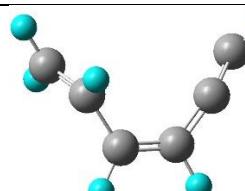
-569 kJ/mol, ${}^3\text{A}_1$, C_1

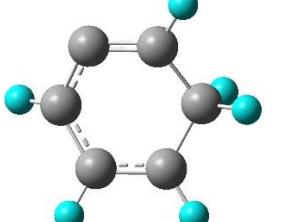
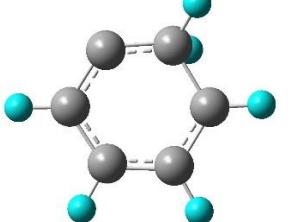
C	-1.244455	-0.668125	0.024402
C	-1.262166	0.683846	0.142259
C	0.000014	1.412251	-0.143256
C	1.262176	0.683829	0.142263
C	1.244443	-0.668147	0.024398
C	-0.000012	-1.365680	-0.147785
H	-2.157937	-1.244457	0.137926
H	-2.172140	1.224179	0.381147
H	2.157916	-1.244494	0.137915
H	-0.000021	-2.445185	-0.234841
H	2.172158	1.224144	0.381163
H	0.000022	2.017968	-1.057001

Table S8. Reactants, products, intermediates, and transition state structures relevant to the formation of triplet benzene from the T₂ state of acetylene. Geometries were optimized and frequencies were calculated at the TD-B3LYP/6-311G** level. Relative energies were calculated at the CASPT2/aug-cc-pVTZ level.

T ₂								
Initial structure				TS9				
								
Relative energy; Electronic state & point group		0 kJ/mol, ³ A, C ₁		6.09 kJ/mol, ³ A, C ₁				
				Imaginary frequency -490.05				
C	1.260816	1.781961	0.028412	C	-0.016374	1.206196		
H	0.195102	1.768825	0.051891	C	-1.247613	1.233411		
C	2.459981	1.786051	0.002136	C	-2.249481	-0.677301		
H	3.522758	1.800080	-0.020231	C	-3.595033	-0.976124		
C	0.915556	-1.948340	-0.053385	H	0.986969	0.842409		
H	1.399316	-0.998509	-0.047641	H	-4.307022	-0.138207		
C	0.364420	-3.013507	-0.058909	H	-1.463983	-1.435591		
H	-0.117163	-3.961178	-0.064465	H	-2.154951	1.800160		
C	-2.217865	0.237987	0.428095	C	3.540814	-0.415970		
H	-1.628479	-0.656925	0.281927	H	3.544754	-0.422612		
C	-2.781988	1.156473	-0.349132	C	3.542038	-0.410158		
H	-3.377062	2.043963	-0.184787	H	3.548124	-0.406488		
[9]					TS10			
								
-80 kJ/mol, ³ A, C ₁				-70 kJ/mol, ³ A, C ₁				
				Imaginary frequency -661.26				
C	-0.370719	1.622674	-0.001895	C	0.038402	-0.403059		
C	-1.515553	0.900142	-0.000797	C	1.361103	-0.587552		
C	-1.517739	-0.537586	0.000722	C	2.320365	0.481682		
C	-2.671574	-1.335448	0.001755	C	3.720239	0.330242		
H	0.669510	1.311759	-0.001888	H	-1.024004	-0.268287		
H	-3.567390	-0.682559	0.001167	H	3.931006	-0.762314		
H	-0.536875	-1.010549	0.001062	H	1.893174	1.484902		
H	-2.479945	1.401779	-0.001087	H	1.770938	-1.602025		
C	3.023854	-0.353087	-0.599335	C	-3.760057	-0.432208		
H	3.030086	-0.365475	-1.662643	H	-3.957471	-1.477230		

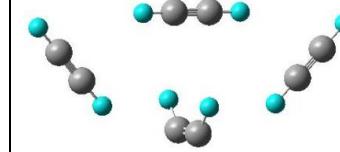
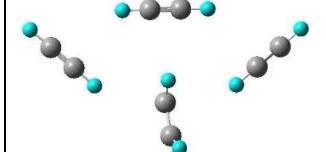
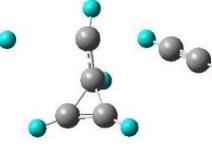
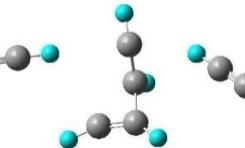
C	3.026338	-0.347515	0.599621	C	-3.552329	0.748686	0.000154
H	3.036977	-0.350031	1.662963	H	-3.379969	1.798213	-0.000769
[1]0				TS11			
							
-82 kJ/mol, ^3A , C_1				-53 kJ/mol, ^3A , C_1			
Imaginary frequency -524.46							
C	0.106754	-0.623336	-0.159903	C	0.167212	0.074769	0.165607
C	1.204242	0.130780	0.035145	C	1.327284	0.658743	0.031670
C	2.541177	-0.352249	-0.091077	C	2.646843	0.090876	0.400582
C	3.714588	0.403535	0.104185	C	3.500115	-0.666832	-0.439244
H	-0.968082	-0.502195	-0.127968	H	-0.876740	0.268368	-0.027879
H	3.391057	1.435158	0.371420	H	2.976243	-0.778497	-1.412223
H	2.629087	-1.404548	-0.364103	H	2.983407	0.322718	1.414144
H	1.080121	1.183130	0.308293	H	1.392014	1.669213	-0.408777
C	-3.674778	0.303450	-0.541783	C	-3.560963	-0.704089	0.178512
H	-3.679449	0.598777	-1.563411	H	-3.250919	-1.646826	0.560396
C	-3.683496	-0.027409	0.610549	C	-3.912183	0.357936	-0.252378
H	-3.703659	-0.318942	1.633079	H	-4.233854	1.296609	-0.634151
[11]				TS12			
							
-198 kJ/mol, ^3A , C_1				-136 kJ/mol, ^3A , C_1			
Imaginary frequency -1225.96							
C	1.015662	0.762651	-1.694470	C	1.638642	-0.009035	-0.021768
C	0.732058	0.769723	-0.258301	C	0.643377	0.989876	-0.009814
C	-0.743080	0.947158	0.056765	C	-0.726630	0.769975	-0.151273
C	-1.743504	-0.005202	-0.379549	C	-1.368676	-0.494710	0.015497
C	-2.060793	-1.176701	0.363244	C	-2.743316	-0.744635	0.072535
C	1.236923	0.754737	-2.874984	C	2.523546	-0.842808	-0.073735
H	1.107563	-0.166648	0.181865	H	1.018496	1.999008	-0.170241
H	1.291269	1.579317	0.219341	H	-3.262488	0.219389	-0.136627
H	-1.445762	-1.156818	1.292259	H	3.290845	-1.578720	-0.106647
H	1.437879	0.746337	-3.918227	H	-0.689767	-1.341403	0.152968
H	-2.288625	0.180413	-1.308927	H	-1.352178	1.647401	-0.273484
H	-1.007903	1.606882	0.880390	H	1.193443	1.042345	1.545382
[12]				TS13			

	
-256 kJ/mol, ${}^3\text{A}$, C ₁	-231 kJ/mol, ${}^3\text{A}$, C ₁
Imaginary frequency -1536.20	
C 1.749352 0.049799 -0.090258	C 1.680254 0.041038 0.009629
C 0.691721 0.902464 -0.288709	C 0.739250 1.055435 0.015090
C -0.646678 0.707324 0.364999	C -0.684097 0.886959 -0.046302
C -1.410656 -0.511425 -0.076895	C -1.243436 -0.438941 -0.014922
C -2.810975 -0.671749 -0.142637	C -2.607775 -0.678868 -0.113072
C 2.681149 -0.715156 0.100988	C 2.528032 -0.839923 -0.026411
H 0.800358 1.720008 -0.992770	H 1.118765 2.073331 0.006735
H -3.273496 0.302151 0.131759	H -3.516846 -0.115847 0.059757
H 3.498385 -1.374380 0.263492	H 3.270716 -1.596934 0.020113
H -0.774285 -1.360265 -0.335516	H -0.590590 -1.235143 -0.388436
H -1.276255 1.595594 0.275161	H -1.323864 1.734515 0.159258
H -0.498179 0.549347 1.452943	H -1.431547 -1.014122 1.198495
[13]	TS14
	
-395 kJ/mol, ${}^3\text{A}$, C ₁	-354 kJ/mol, ${}^3\text{A}$, C ₁
Imaginary frequency -165.66	
C -0.784834 0.948283 0.003180	C -2.317913 -1.073768 -0.171127
C 0.616337 0.828562 0.000874	C 2.038713 -0.958986 -0.304322
C 1.322320 -0.404941 0.007232	C 1.447412 -0.045754 0.462669
C 2.672149 -0.532040 -0.004532	C 0.634358 1.085278 -0.038816
H 3.147317 -1.504571 -0.000416	C -0.725227 1.038546 -0.155413
H 3.321773 0.336916 -0.021654	C -1.589971 0.022229 0.188431
H 0.723576 -1.314667 0.019797	H 2.626441 -1.762313 0.126899
H 1.184457 1.751293 -0.008206	H -1.252363 1.939943 -0.484847
C -2.730153 -0.854053 -0.177628	H 1.565103 -0.116672 1.546078
H -3.260962 -1.322096 0.659117	H 1.135926 2.016084 -0.281171
C -1.748364 0.029285 0.064673	H -2.951850 -1.548071 0.590092
H -1.200884 1.962550 -0.011434	H 1.952508 -0.934242 -1.385586
[14]	TS15

-399 kJ/mol, ${}^3\text{A}_1$, C ₁	-372 kJ/mol, ${}^3\text{A}_1$, C ₁
	Imaginary frequency -294.19
C 0.498713	C -2.268100
C -0.910278	C 1.315853
C -1.695861	C 1.702650
C -1.259626	C 0.852634
H -1.949630	C -0.554883
H -0.204464	C -1.412582
H -2.770645	H 2.066736
H -1.420251	H -0.916556
C 2.372396	H 2.767506
H 2.892411	H 1.372879
C 1.410215	H -3.377469
H 0.959218	H 0.273475
[15]	TS16
	
-486 kJ/mol, ${}^3\text{A}_1$, C ₁	-482 kJ/mol, ${}^3\text{A}_1$, C ₁
	Imaginary frequency -924.97
C 1.000846	C -1.191484
C 1.295372	C -1.221646
C 0.137972	C 0.028229
C -1.145270	C 1.218299
C -1.320779	C 1.301461
C -0.272694	C 0.063417
H 1.593487	H -2.182714
H -2.156702	H 2.249309
H 0.297827	H 0.047315
H -1.941910	H 2.151846
H 1.859040	H -2.085569
H 2.175577	H -1.369846
[16]	TS17

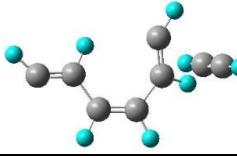
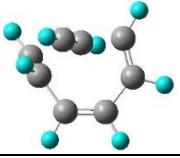
-498 kJ/mol, $^3\text{A}_1$, C ₁	-469 kJ/mol, $^3\text{A}_1$, C ₁
	Imaginary frequency -977.08
C 0.799405 1.028675 -0.245393	C 1.231979 0.675867 -0.030380
C -0.591506 1.219384 0.000402	C 0.002820 1.379188 -0.004311
C -1.407078 0.126440 0.247969	C -1.216343 0.652353 0.002354
C -0.826054 -1.111304 -0.183011	C -1.315562 -0.729648 -0.004771
C 0.556771 -1.349503 -0.174789	C -0.064219 -1.425876 -0.114557
C 1.430406 -0.191579 0.301729	C 1.223697 -0.754158 0.001646
H 1.310784 1.661134 -0.965215	H 2.186537 1.187456 -0.043751
H -1.018174 2.215843 -0.086507	H -0.014353 2.458541 0.029071
H -2.453484 0.223730 0.507750	H -2.144259 1.218028 0.045286
H -1.490098 -1.896364 -0.540933	H -2.262974 -1.244658 0.048870
H 1.408178 -0.220597 1.403754	H 0.934641 -1.106992 1.085257
H 2.471122 -0.316429 -0.000297	H 2.126179 -1.298730 -0.264615
[17]	
-509 kJ/mol, $^3\text{A}_1$, C ₁	
C 1.350965 0.467901 -0.000030	
C 1.077175 -0.939903 0.000039	
C -0.271692 -1.397337 0.000002	
C -1.350966 -0.467902 -0.000038	
C -1.077176 0.939905 0.000022	
C 0.271693 1.397337 -0.000001	
H 2.373577 0.823039 -0.000125	
H 1.892031 -1.652539 0.000089	
H -0.478448 -2.460390 0.000021	
H -2.373579 -0.823040 -0.000131	
H -1.892031 1.652542 0.000181	
H 0.478452 2.460390 0.000000	

Table S9. Reactants, products, intermediates, and transition state structures relevant to the formation of triplet benzene from the T₁ state of acetylene with increased size of the acetylene clusters. Geometries were optimized at the B3LYP/6-311G** level. Relative energies were calculated at the CCSD(T)/CBS level.

with 1 acetylene surrounding the reaction center							
Initial structure			TS1				
							
0 kJ/mol, ³ A, C ₁			1.14 kJ/mol, ³ A, C ₁				
C	-0.000008	1.959292	-0.665341	C	-1.629559	-2.671639	-0.000085
H	-0.000015	1.097120	-1.339187	C	-3.796942	0.840688	-0.664277
C	0.000007	1.959249	0.665327	C	-3.796777	0.840677	0.664721
H	0.000015	1.097032	1.339115	H	-3.369418	0.092055	1.338997
C	-3.710873	0.362959	0.000022	C	-1.008012	-1.645594	-0.000132
H	-2.979430	1.136671	0.000017	H	-0.460024	-0.730561	-0.000174
C	-4.531236	-0.511596	0.000029	H	-3.369752	0.092077	-1.338672
H	-5.266810	-1.279198	0.000035	H	-2.176582	-3.583150	-0.000045
C	-0.600009	-1.690285	-0.000035	C	1.143834	1.578702	-0.000277
H	-1.664957	-1.676631	-0.000033	H	2.155662	1.244397	-0.000301
C	0.600010	-1.690287	-0.000037	C	0.003819	1.952676	-0.000234
H	1.664958	-1.676635	-0.000038	H	-1.011840	2.271324	-0.000180
C	3.710874	0.362958	0.000002	C	4.111134	-0.811624	0.000018
H	2.979430	1.136668	-0.000030	C	4.849342	0.132954	0.000278
C	4.531237	-0.511595	0.000040	H	5.511322	0.965032	0.000520
H	5.266811	-1.279194	0.000074	H	3.459596	-1.652214	-0.000212
[1]	TS2						
							
-132 kJ/mol, ³ A, C ₁			-98 kJ/mol, ³ A, C ₁				
C	-0.643396	1.467979	-0.585667	C	-0.800195	1.620024	-0.718209
C	0.000007	1.175424	0.770906	C	0.227201	1.217508	0.785356
C	0.000006	-0.140891	1.356136	C	0.059950	0.038921	1.463171
H	0.000023	-0.515384	2.371955	H	-0.229539	-0.244065	2.465645
C	0.643314	1.467955	-0.585716	C	0.450099	1.324047	-0.692778
H	1.587943	1.508509	-1.101612	H	1.307802	1.154362	-1.333981
H	0.000050	1.977243	1.518202	H	0.386734	2.121275	1.376854
H	-1.588063	1.508565	-1.101490	H	-1.745053	1.818296	-1.191395
C	-3.356020	-1.007335	0.007657	C	-3.272588	-1.024975	-0.019708
H	-2.404752	-0.994465	0.488985	H	-2.272515	-0.877455	0.316423
C	-4.423777	-1.014560	-0.537752	C	-4.397312	-1.188391	-0.401245

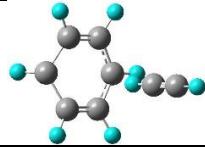
H	-5.371459	-1.025206	-1.018885	H	-5.394930	-1.335428	-0.737041
C	3.356049	-1.007316	0.007642	C	3.388739	-0.978654	0.092552
H	2.404777	-0.994455	0.488956	H	2.508846	-0.863294	0.683227
C	4.423812	-1.014530	-0.537747	C	4.375335	-1.101667	-0.577607
H	5.371500	-1.025166	-1.018863	H	5.251276	-1.214573	-1.168926
[2]				TS3			
-198 kJ/mol, 3A , C ₁				-180 kJ/mol, 3A , C ₁			
C	-0.000147	-0.760920	0.336196	C	0.000002	-0.719311	0.430178
C	0.000365	1.627120	-0.307051	C	0.000006	1.635285	-0.330176
C	0.000426	2.899091	0.024187	C	0.000001	2.919958	-0.051000
H	0.000710	3.856892	-0.472855	H	0.000005	3.857526	-0.585732
C	-0.000084	0.516581	0.653944	C	-0.000003	0.562815	0.684074
H	-0.000384	0.801916	1.711127	H	-0.000015	0.918216	1.721542
H	0.000665	1.346879	-1.365113	H	0.000018	1.310235	-1.375494
H	-0.000438	-1.713343	0.844295	H	0.000007	-1.759574	0.200417
C	-3.860141	-0.901281	-0.122460	C	-3.837365	-0.870270	-0.016140
H	-2.843064	-0.601957	-0.024918	H	-2.882367	-0.470250	0.231400
C	-5.004657	-1.239937	-0.232059	C	-4.911194	-1.323744	-0.295263
H	-6.019531	-1.540144	-0.329257	H	-5.863722	-1.725097	-0.542598
C	3.859856	-0.901712	-0.122120	C	3.837365	-0.870269	-0.016130
H	2.842769	-0.602543	-0.024174	H	2.882372	-0.470243	0.231425
C	5.004383	-1.240186	-0.232188	C	4.911187	-1.323749	-0.295268
H	6.019268	-1.540232	-0.329802	H	5.863709	-1.725108	-0.542618
[3]				TS4			
-194 kJ/mol, 3A , C ₁				-172 kJ/mol, 3A , C ₁			
C	0.000037	-0.689962	-0.224264	C	0.122254	-1.423382	0.491460
C	-0.000102	1.778228	-0.436855	C	0.322277	1.067630	0.449118
C	-0.000109	2.969567	0.119393	C	-0.668063	1.849616	0.098400
H	-0.000039	3.406124	1.107420	H	-1.748607	1.846783	0.122646
C	0.000030	0.512645	0.314128	C	0.114729	-0.264023	1.106149
H	0.000130	0.597910	1.406585	H	-0.044675	-0.249496	2.191943
H	-0.000200	1.688905	-1.523093	H	1.355591	1.375157	0.280648
H	0.000119	-1.715405	0.114677	H	-0.017082	-2.461153	0.761501

C	-3.894432	-0.916331	-0.072108	C	-3.617438	-0.523601	-0.555861
H	-2.904050	-0.553496	-0.216020	H	-2.602517	-0.841389	-0.512828
C	-5.008795	-1.326540	0.090683	C	-4.758376	-0.158267	-0.600897
H	-5.997077	-1.690026	0.234733	H	-5.770920	0.162432	-0.642437
C	3.894508	-0.916233	-0.072181	C	3.747269	-0.509113	-0.495965
H	2.904153	-0.553362	-0.216182	H	2.820969	-1.011081	-0.342497
C	5.008841	-1.326482	0.090711	C	4.786970	0.062876	-0.665872
H	5.997097	-1.690004	0.234851	H	5.709502	0.568328	-0.818166
[4]	TS5						
-188 kJ/mol, 3A , C ₁	-176 kJ/mol, 3A , C ₁						
C	0.421554	0.818004	-1.584932	C	-0.005686	0.669507	1.556065
C	-0.100989	1.751590	0.671667	C	0.004853	2.019971	-0.544057
C	-0.018722	0.694731	1.449046	C	0.000322	1.096998	-1.478511
H	-0.071260	0.470644	2.503544	H	0.001093	1.041031	-2.556047
C	-0.017724	1.783407	-0.809356	C	0.002480	1.812003	0.928501
H	-0.350590	2.714462	-1.268650	H	0.008470	2.744080	1.505891
H	-0.260925	2.727443	1.146263	H	0.011208	3.070288	-0.858164
H	0.841106	-0.173949	-1.506911	H	-0.012656	-0.266507	2.064337
C	3.182834	-0.889499	0.354725	C	-2.878939	-1.027820	-0.219823
H	2.552096	-0.154712	0.797224	H	-2.119331	-0.308929	-0.422292
C	3.886235	-1.720445	-0.147252	C	-3.731619	-1.838937	0.008476
H	4.511686	-2.456703	-0.590572	H	-4.487864	-2.557940	0.209954
C	-3.175313	-0.928624	-0.006787	C	2.877259	-1.030641	-0.215107
H	-2.301104	-0.325914	0.069998	H	2.117300	-0.310993	-0.413443
C	-4.159434	-1.607694	-0.091091	C	3.730443	-1.842543	0.008452
H	-5.031663	-2.210087	-0.167017	H	4.487103	-2.562254	0.205785
[5]	TS6						
-192 kJ/mol, 3A , C ₁	-162 kJ/mol, 3A , C ₁						
C	0.016862	0.629334	-1.533469	C	0.261170	1.818485	0.205670
C	0.018247	1.675001	0.739669	C	0.596976	-0.037908	-1.142560
C	-0.017268	0.629395	1.533471	C	1.688900	-0.771171	-1.015794
H	-0.002677	0.422683	2.592082	C	2.585147	-0.856597	0.151383

C	-0.017623	1.674996	-0.739697	C	2.317897	-0.520772	1.394381
H	-0.074910	2.667901	-1.198198	C	-0.789053	2.388581	-0.015325
H	0.076519	2.667866	1.198141	H	-0.091032	0.073352	-1.968453
H	0.002071	0.422605	-2.592074	H	2.824521	-0.534881	2.347574
C	3.215976	-0.927941	-0.013562	H	-1.736756	2.770240	-0.311349
H	2.274692	-0.430414	-0.032599	H	3.581359	-1.262047	-0.061136
C	4.275089	-1.488935	0.007509	H	1.992941	-1.385452	-1.869375
H	5.213902	-1.986585	0.026186	H	1.204810	1.593133	0.652309
C	-3.216144	-0.927716	0.013565	C	-2.845488	-0.762171	0.321434
H	-2.274859	-0.430187	0.032584	H	-1.843262	-0.413113	0.413751
C	-4.275253	-1.488718	-0.007484	C	-3.975069	-1.149409	0.213673
H	-5.214064	-1.986373	-0.026141	H	-4.975460	-1.495463	0.119510
[6]	TS7						
							
-343 kJ/mol, ³ A, C ₁	-319 kJ/mol, ³ A, C ₁						
C	0.072040	1.410904	1.281454	C	-0.681736	-1.311049	-1.313213
C	-2.791970	-1.837351	0.378793	C	-1.692410	1.838772	-0.870274
C	-2.089646	-0.722337	0.319336	C	-0.818357	1.435226	0.019749
C	-1.620266	-0.114130	-0.916896	C	-1.092625	0.515606	1.150892
C	-0.810923	0.958546	-1.033378	C	-1.210118	-0.817586	1.084294
C	-0.176081	1.742760	0.030598	C	-1.076619	-1.666086	-0.107944
H	0.518806	1.878939	2.146036	H	-0.559895	-1.800261	-2.268427
H	-3.242139	-2.453481	1.142768	H	-1.705281	2.499535	-1.724632
H	-0.603963	1.314889	-2.037699	H	-1.413555	-1.350150	2.008662
H	0.159171	2.739345	-0.284490	H	-1.317866	-2.723390	0.054118
H	-1.985089	-0.571530	-1.831501	H	-1.171033	0.986413	2.128389
H	-1.842684	-0.207398	1.251722	H	0.200713	1.844251	-0.021556
C	4.224944	-1.040178	-0.139416	C	3.772570	0.297587	0.117684
H	5.193383	-1.450047	-0.292755	H	4.712323	0.750313	0.321198
C	3.131950	-0.578937	0.032586	C	2.713276	-0.215532	-0.111135
H	2.162230	-0.166379	0.187452	H	1.770704	-0.668337	-0.318068
[7]	TS8						
							
-324 kJ/mol, ³ A, C ₁	-300 kJ/mol, ³ A, C ₁						
C	0.501459	-1.528321	1.174820	C	-0.740495	1.330969	1.086266
C	0.501382	1.528288	1.174836	C	-0.929671	-1.043133	1.420944
C	1.073894	1.628274	-0.007927	C	-0.733407	-1.498343	0.175553

C	1.914100	0.675134	-0.729989	C	-1.415969	-0.918286	-0.949595
C	1.914126	-0.675077	-0.730001	C	-1.692978	0.414426	-1.042152
C	1.073957	-1.628261	-0.007953	C	-1.210239	1.459744	-0.150038
H	-0.110589	-2.162343	1.799817	H	-0.349703	2.048593	1.796450
H	-0.110693	2.162278	1.799839	H	-0.630662	-1.317041	2.422019
H	2.589436	-1.143817	-1.441307	H	-2.155981	0.763932	-1.959948
H	0.927238	-2.576026	-0.543399	H	-1.170207	2.453466	-0.609314
H	2.589394	1.143912	-1.441285	H	-1.595516	-1.541777	-1.821488
H	0.927151	2.576047	-0.543351	H	0.046474	-2.239812	-0.028389
C	-4.067650	-0.000023	-0.454628	C	3.874521	-0.025754	-0.335305
H	-5.113395	-0.000028	-0.643828	H	4.893747	-0.242198	-0.544470
C	-2.887754	-0.000017	-0.241881	C	2.724760	0.220077	-0.100171
H	-1.839619	-0.000011	-0.050143	H	1.702718	0.436639	0.112118

[8]



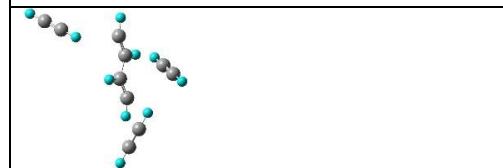
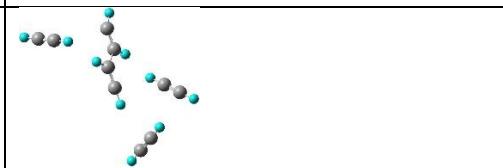
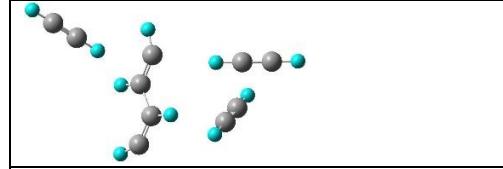
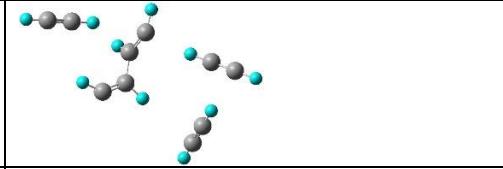
-571 kJ/mol, ^3A , C_1

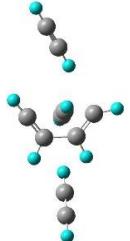
C	-0.888793	1.190910	0.789138
C	-1.007452	1.319422	-0.558141
C	-1.521991	0.148288	-1.312084
C	-1.208528	-1.188572	-0.746925
C	-1.085989	-1.283123	0.602475
C	-1.036347	-0.096390	1.411104
H	-0.604327	2.040819	1.402332
H	-0.797698	2.256451	-1.062980
H	-0.943401	-2.248756	1.078171
H	-0.933701	-0.185353	2.485413
H	-1.139534	-2.060190	-1.389047
H	-2.529115	0.261028	-1.729828
C	2.791435	0.004407	-0.132054
H	1.730110	0.091880	-0.127086
C	3.986344	-0.091434	-0.138862
H	5.045593	-0.176925	-0.144883

with 2 acetylenes surrounding the reaction center

Initial structure			TS1		
0 kJ/mol, ^3A , C_1			0.66 kJ/mol, ^3A , C_1		
C	-3.416583	-0.843573	-2.213793	C	-3.510809
C	-1.233845	-2.465145	1.048616	C	-0.619567
					-2.020211
					2.003126

C	-0.743337	-1.740376	2.050195	C	0.220363	-1.122523	2.509944
H	-0.828853	-0.660171	2.208018	H	0.244752	-0.041222	2.338654
C	-2.935779	0.008305	-1.520043	C	-3.048812	-0.780561	-0.895810
H	-2.510163	0.765430	-0.902680	H	-2.641471	0.203494	-0.850859
H	-1.818807	-2.125410	0.187552	H	-1.454925	-1.863141	1.313139
H	-3.843328	-1.595460	-2.832352	H	-3.921847	-2.865089	-1.000142
C	2.560969	-2.113940	-0.003268	C	2.344883	-2.151098	-0.622366
H	1.595765	-2.220421	0.437162	H	1.666551	-2.245084	0.194444
C	3.647605	-1.999266	-0.498154	C	3.107558	-2.041164	-1.541542
H	4.611989	-1.906849	-0.936135	H	3.783203	-1.954099	-2.357817
C	-0.881043	2.184004	1.005373	C	-1.179745	2.630860	-0.322331
H	0.085736	2.193786	0.553805	H	-0.142030	2.396594	-0.395729
C	-1.966346	2.180542	1.517337	C	-2.343021	2.909558	-0.231913
H	-2.926394	2.183606	1.974710	H	-3.372519	3.162661	-0.149991
C	2.592259	1.699196	-0.586790	C	2.606005	1.574439	-0.107566
C	2.468565	2.887183	-0.698818	C	2.535957	2.707992	0.279182
H	2.367912	3.940563	-0.802565	H	2.482731	3.712655	0.623355
H	2.711344	0.643337	-0.491447	H	2.678677	0.565831	-0.447183
[1]				TS2			
	-133 kJ/mol, 3A_1 , C ₁			-98 kJ/mol, 3A_1 , C ₁			
C	1.201986	-1.603966	-0.123680	C	1.569969	-1.557082	0.951857
C	0.890144	-0.968265	1.228642	C	0.671199	-0.070947	1.638038
C	1.011372	0.447864	1.460536	C	0.903413	1.183145	1.140252
H	1.126276	1.062364	2.344659	H	1.302524	2.109258	1.530743
C	-0.050343	-1.551850	0.167946	C	0.325840	-1.270226	0.805606
H	-1.089399	-1.684327	-0.087499	H	-0.585474	-1.612279	0.326948
H	1.078714	-1.566131	2.127978	H	0.560474	-0.171845	2.719692
H	2.003979	-1.813406	-0.811657	H	2.472385	-2.110979	0.766371
C	4.220838	0.586278	-0.418416	C	3.970830	0.518298	-0.991620
H	3.370425	0.766335	0.199036	H	3.011557	0.712907	-0.571055
C	5.173356	0.377203	-1.116007	C	5.049749	0.295440	-1.464396
H	6.019595	0.196058	-1.733058	H	6.006691	0.100802	-1.883860
C	-1.801606	2.419041	0.097252	C	-2.409960	2.256310	-0.073344
H	-0.937094	1.882548	0.419792	H	-1.440968	1.981730	0.281076
C	-2.772213	3.024038	-0.264274	C	-3.498610	2.565336	-0.471206
H	-3.627709	3.568509	-0.583720	H	-4.461500	2.847850	-0.822448
C	-3.777205	-0.768489	-0.523074	C	-3.313605	-1.357822	-0.781755
H	-3.482676	0.251808	-0.427486	H	-3.317871	-0.294486	-0.703615
C	-4.105913	-1.917026	-0.629419	C	-3.308468	-2.553962	-0.869142

H	-4.404606	-2.932723	-0.725079	H	-3.309962	-3.613887	-0.949596
[2]				TS3			
							
-200 kJ/mol, 3A , C ₁				-182 kJ/mol, 3A , C ₁			
C	1.606961	1.559982	0.101725	C	2.259840	2.025508	0.416110
C	0.215927	-0.432823	0.562243	C	0.565864	0.478484	-0.513702
C	-0.351631	-1.259212	1.413145	C	-0.338408	-0.451650	-0.359181
H	-1.014188	-2.110230	1.373062	H	-1.071618	-1.213841	-0.211221
C	1.071215	0.699058	0.941458	C	1.349598	1.089229	0.578030
H	1.254016	0.819176	2.014530	H	1.136607	0.717982	1.585995
H	0.044954	-0.571218	-0.509958	H	0.797663	0.865288	-1.513311
H	2.235589	2.436403	0.145370	H	2.926648	2.610718	1.031279
C	4.882087	-0.389072	-0.512819	C	5.116043	-0.528569	-0.129629
H	3.863313	-0.169143	-0.295472	H	4.172100	-0.037083	-0.090322
C	6.029517	-0.633988	-0.757915	C	6.179585	-1.079738	-0.172835
H	7.046841	-0.851694	-0.975124	H	7.122364	-1.568774	-0.211424
C	-2.449519	2.264840	-0.230825	C	-3.469343	1.719394	-0.231962
H	-1.424938	2.146603	0.034149	H	-2.420311	1.554813	-0.317784
C	-3.602363	2.401409	-0.531400	C	-4.651094	1.899005	-0.134901
H	-4.623390	2.529616	-0.798700	H	-5.697149	2.069254	-0.050454
C	-3.599717	-1.519311	-0.425470	C	-3.706822	-2.002444	0.181266
H	-3.423878	-0.474458	-0.309833	H	-4.063143	-1.000215	0.113122
C	-3.798780	-2.694332	-0.559405	C	-3.298228	-3.127554	0.256721
H	-3.980500	-3.734365	-0.682450	H	-2.945383	-4.128142	0.324614
[3]				TS4			
							
-196 kJ/mol, 3A , C ₁				-173 kJ/mol, 3A , C ₁			
C	-0.708497	-1.320581	-0.071643	C	-0.691092	-0.660348	1.566264
C	-0.208517	0.415910	1.627702	C	-0.366290	1.306553	0.057390
C	-0.340578	0.872553	2.853954	C	-1.224917	1.645718	-0.871934
H	-0.822770	0.589926	3.778610	H	-2.288568	1.581334	-1.053478
C	-0.816085	-0.836156	1.149000	C	-0.774111	0.627040	1.330444
H	-1.404040	-1.399623	1.882597	H	-1.160736	1.276746	2.126094
H	0.378436	0.977675	0.900733	H	0.696062	1.525264	-0.063160
H	-1.067877	-2.177596	-0.622171	H	-0.924305	-1.336249	2.377286
C	-4.254704	-0.032981	-1.009316	C	-4.284077	-0.601066	-0.267252
H	-3.249301	0.029891	-0.665313	H	-3.331860	-0.796263	0.166469

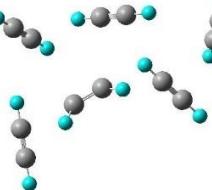
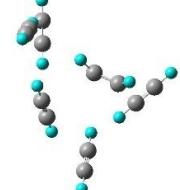
C	-5.386504	-0.107521	-1.396794	C	-5.353803	-0.373103	-0.758158
H	-6.390030	-0.172721	-1.740672	H	-6.303196	-0.174328	-1.192895
C	3.015243	-1.821015	-0.437638	C	2.130650	-2.393955	-0.184067
H	2.002394	-1.801113	-0.107134	H	1.210783	-1.956797	0.131042
C	4.154304	-1.839282	-0.812236	C	3.166534	-2.884599	-0.536834
H	5.164604	-1.862996	-1.142405	H	4.081401	-3.326341	-0.850198
C	2.589921	1.875012	-0.980998	C	3.667550	1.063692	-0.285825
H	3.043672	0.910922	-0.982907	H	3.531004	0.007633	-0.330643
C	2.075828	2.958373	-0.976496	C	3.818475	2.252323	-0.236114
H	1.622439	3.919760	-0.974555	H	3.955896	3.305467	-0.194003
[4]	TS5						
							
-188 kJ/mol, $^3\text{A}_1$, C_1	-175 kJ/mol, $^3\text{A}_1$, C_1						
C	-1.408429	-1.241715	-1.323885	C	-1.275692	-1.002857	-1.380892
C	-0.054718	-0.841267	0.737234	C	0.015747	-1.013355	0.756325
C	-0.841819	-0.095462	1.480552	C	-0.815481	-0.448446	1.601834
H	-0.839871	0.297495	2.486606	H	-0.844970	-0.205426	2.653178
C	-0.273798	-1.278644	-0.663119	C	-0.191488	-1.244219	-0.698912
H	0.612598	-1.677644	-1.156480	H	0.687849	-1.659452	-1.204549
H	0.889997	-1.182484	1.177548	H	0.985775	-1.354484	1.135661
H	-2.439873	-0.955552	-1.178529	H	-2.163631	-0.814467	-1.938329
C	-4.443567	0.449141	0.354371	C	-4.385259	0.192141	0.250499
H	-3.539166	0.507378	0.913242	H	-3.424173	-0.025840	0.655871
C	-5.455582	0.377020	-0.284370	C	-5.463392	0.436571	-0.213641
H	-6.354801	0.315110	-0.847851	H	-6.420529	0.654367	-0.621205
C	1.823695	2.421280	-0.167207	C	1.556477	2.420634	-0.018338
H	0.941697	1.854731	0.022324	H	0.729851	1.776656	0.173065
C	2.820265	3.054368	-0.377754	C	2.491170	3.141233	-0.231401
H	3.697969	3.624145	-0.565704	H	3.313357	3.788099	-0.420761
C	3.738554	-0.834680	-0.023288	C	3.778739	-0.649773	-0.091885
H	3.521173	0.202020	-0.142517	H	3.441891	0.359940	-0.149810
C	3.980233	-2.001755	0.111256	C	4.155592	-1.786511	-0.025923
H	4.201280	-3.034917	0.228609	H	4.496104	-2.791898	0.030885
[5]	TS6						

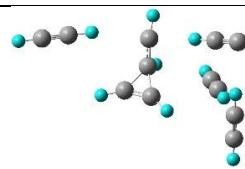
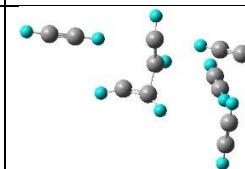
-192 kJ/mol, ${}^3\text{A}_1$, C ₁	-165 kJ/mol, ${}^3\text{A}_1$, C ₁
C -1.096706 -0.951414 -1.471394	C -0.109988 -1.622622 0.034141
C -0.066390 -0.859970 0.805643	C 2.518401 1.439051 1.939012
C -0.945842 -0.170174 1.495722	C 2.050205 0.373604 1.590453
H -1.098452 0.135473 2.519351	C 2.531075 -0.150609 -0.618201
C -0.097692 -1.154366 -0.644511	C 2.050399 -1.252871 -1.167410
H 0.825614 -1.589966 -1.040008	C 0.871802 -2.029222 -0.739983
H 0.805092 -1.262744 1.332417	H -1.045622 -1.994064 0.423181
H -1.311900 -1.094016 -2.519072	H 2.975116 2.385737 2.100801
C -4.526210 0.119939 -0.043263	H 2.575163 -1.661438 -2.036967
H -3.487848 -0.111298 -0.103928	H 0.820336 -3.049469 -1.137613
C -5.694239 0.381133 0.024490	H 3.386844 0.456190 -0.877285
H -6.729768 0.612294 0.084523	H 1.519413 -0.551919 1.636811
C 1.733024 2.426000 -0.067091	C -3.497906 -0.236828 0.450468
H 0.851637 1.862842 0.134952	H -2.842837 0.484176 0.016795
C 2.728514 3.055961 -0.291890	C -4.233293 -1.048733 0.938701
H 3.604945 3.623548 -0.491961	H -4.890641 -1.762977 1.371610
C 3.733347 -0.796644 0.039531	C -1.577529 2.699589 -1.289332
H 3.469607 0.232727 -0.046551	H -2.394597 3.329617 -1.545239
C 4.027917 -1.955256 0.137193	C -0.649761 1.994454 -1.004575
H 4.296738 -2.980111 0.223693	H 0.176395 1.369269 -0.751734
[6]	TS7
-343 kJ/mol, ${}^3\text{A}_1$, C ₁	-318 kJ/mol, ${}^3\text{A}_1$, C ₁
C -0.053410 -0.979623 0.223289	C -0.222043 -0.945223 0.349243
C -3.895363 0.027646 -1.728371	C -2.855556 -1.005551 -1.694720
C -2.977399 -0.277406 -0.831407	C -2.691627 0.149733 -1.097421
C -2.967910 0.222151 0.535726	C -2.993454 0.444121 0.324651
C -2.002585 0.032372 1.458624	C -2.246196 0.108011 1.385032
C -0.725219 -0.673297 1.315104	C -0.960912 -0.604780 1.385389
H 0.873452 -1.478708 -0.021427	H 0.709310 -1.469781 0.189334
H -4.111233 -0.215279 -2.758136	H -2.725817 -1.411451 -2.687143
H -2.184687 0.432087 2.451548	H -2.611263 0.398357 2.365999

H	-0.261802	-0.961412	2.267700	H	-0.579382	-0.857125	2.382123
H	-3.845632	0.787747	0.833512	H	-3.901339	1.016955	0.501182
H	-2.168161	-0.954327	-1.118370	H	-2.357261	1.006263	-1.699837
C	3.746434	-1.066519	-0.370559	C	3.654698	-1.049986	-0.180381
H	3.568594	-0.015985	-0.339911	H	3.461401	-0.002974	-0.226751
C	3.941405	-2.249364	-0.404706	C	3.866868	-2.229093	-0.127640
H	4.121755	-3.296459	-0.436276	H	4.060824	-3.273192	-0.082076
C	2.896296	2.862829	-0.229622	C	2.653618	2.885138	-0.325210
H	3.768175	3.453670	-0.374388	H	3.472753	3.526032	-0.545316
C	1.905926	2.206564	-0.065493	C	1.722835	2.170846	-0.075964
H	1.030491	1.616543	0.080230	H	0.901390	1.527621	0.144609
[7]				TS8			
-326 kJ/mol, ³ A, C ₁				-301 kJ/mol, ³ A, C ₁			
C	0.134881	-1.481846	0.346233	C	0.291491	-1.274930	0.128987
C	1.825785	0.693598	1.673085	C	1.648402	-0.095824	1.724956
C	2.728409	0.743022	0.713495	C	2.396866	0.678153	0.925662
C	3.039612	-0.218597	-0.342446	C	3.034865	0.145812	-0.246828
C	2.262443	-1.136389	-0.956592	C	2.471413	-0.826058	-1.022995
C	0.856017	-1.480322	-0.756892	C	1.112997	-1.337372	-0.913802
H	-0.884028	-1.724828	0.613212	H	-0.729616	-1.600089	0.284209
H	1.533288	1.327166	2.497944	H	1.133111	-0.001429	2.669343
H	2.723562	-1.657193	-1.792297	H	3.005607	-1.114354	-1.923303
H	0.349338	-1.812903	-1.673163	H	0.716379	-1.751007	-1.847561
H	4.042943	-0.108854	-0.745707	H	3.937276	0.631892	-0.608372
H	3.370206	1.634248	0.694427	H	2.440597	1.761524	1.082683
C	-3.606644	-0.619713	0.199512	C	-3.644550	-0.681891	0.093035
H	-3.138290	0.305253	-0.048797	H	-3.257208	0.296172	-0.077656
C	-4.131373	-1.660953	0.480246	C	-4.076416	-1.783859	0.285934
H	-4.601439	-2.581415	0.728453	H	-4.463635	-2.758901	0.456555
C	-2.037003	2.895715	-0.747218	C	-1.996649	2.974789	-0.481560
H	-2.848981	3.530325	-1.008256	H	-2.718721	3.747259	-0.591318
C	-1.113874	2.187583	-0.454993	C	-1.174129	2.110133	-0.359539
H	-0.296117	1.555611	-0.192401	H	-0.449526	1.335216	-0.247676
[8]							
-576 kJ/mol, ³ A, C ₁							

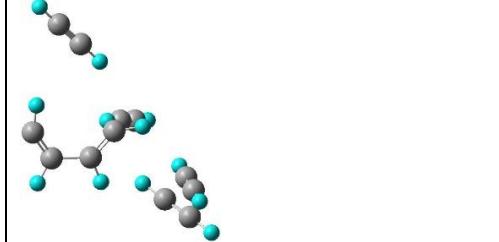
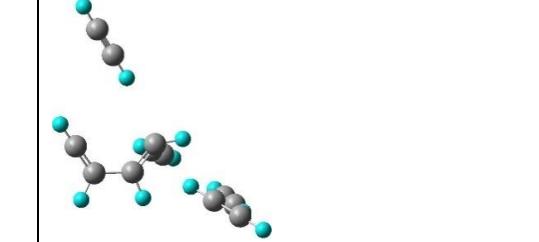
C	0.844996	-0.413635	1.092425
C	1.941751	0.336688	1.371347
C	2.842712	0.680839	0.241974
C	2.902825	-0.293293	-0.877101
C	1.791028	-1.029609	-1.127289
C	0.688901	-1.020471	-0.203418
H	0.112239	-0.633593	1.863233
H	2.137708	0.711606	2.370480
H	1.749743	-1.694337	-1.984944
H	-0.193486	-1.613179	-0.409243
H	3.787989	-0.365920	-1.500111
H	2.870756	1.738402	-0.043648
C	-3.305536	-1.088829	-0.000934
H	-3.103507	-0.053499	-0.152846
C	-3.530488	-2.253969	0.172144
H	-3.734723	-3.285649	0.326029
C	-2.557379	2.842994	-0.442393
H	-3.454062	3.371514	-0.658866
C	-1.540687	2.255489	-0.198351
H	-0.641396	1.727423	0.019504

with 3 acetylenes surrounding the reaction center

Initial structure				TS1			
							
0 kJ/mol, 3A , C ₁				-0.30 kJ/mol, 3A , C ₁			
C	-2.677631	1.891158	-1.197265	C	-0.385397	-1.954991	-1.173150
H	-2.604815	0.918031	-1.627330	C	2.217680	2.761977	-0.718154
C	-2.766460	2.982681	-0.706812	C	2.986393	2.271333	0.250245
H	-2.850685	3.953904	-0.281646	H	2.681757	1.773827	1.176873
C	1.882354	-2.823311	-0.194123	C	-1.499463	-1.944706	-0.726963
H	2.070139	-3.869394	-0.226575	H	-2.488570	-1.923701	-0.330902
C	1.664618	-1.643873	-0.157019	H	1.124327	2.772970	-0.779494
H	1.481188	-0.593222	-0.123277	H	0.608248	-1.967394	-1.557840
C	-3.034827	-1.888911	-1.399416	C	3.337925	-1.150239	-1.357210
H	-3.240985	-1.887573	-0.324003	H	3.258043	-0.092197	-1.251622
C	-1.868163	-2.035170	-2.021466	C	3.433842	-2.340909	-1.469203
H	-0.876752	-2.191081	-1.583344	H	3.530988	-3.395044	-1.569794
C	5.153022	-0.322015	0.476895	C	-4.604932	-0.143990	0.398307
H	4.417770	-1.074448	0.308762	H	-4.061575	0.726817	0.112765
C	5.977514	0.528070	0.665981	C	-5.213000	-1.126831	0.718458

H	6.715800	1.274188	0.834682	H	-5.760269	-1.991879	1.005579
C	-3.765340	0.021928	1.941552	C	-1.661480	1.750405	-1.032681
H	-3.565062	0.844234	1.294798	C	-2.055849	2.878227	-0.922203
C	-3.989690	-0.905401	2.667878	H	-2.401217	3.879532	-0.828802
H	-4.189481	-1.723213	3.316908	H	-1.319111	0.744453	-1.127338
C	1.076116	2.206466	-0.262491	C	1.818848	-0.781472	2.443403
H	0.046121	2.382699	-0.471348	C	1.823371	-0.150061	3.462609
C	2.236948	2.011577	-0.029296	H	1.824725	0.403988	4.369791
H	3.266003	1.826685	0.175861	H	1.815028	-1.343830	1.540024
[1]				TS2			
							
-134 kJ/mol, 3A , C ₁				-101 kJ/mol, 3A , C ₁			
C	-1.620597	-1.002495	1.098815	C	-1.710010	-1.354839	1.020494
C	-0.921995	-0.718801	-0.235327	C	-0.753007	-0.642188	-0.414142
C	-1.345186	0.338638	-1.117013	C	-1.287229	0.360831	-1.179306
H	-1.448832	0.424545	-2.191762	H	-1.575885	0.468826	-2.216066
C	-0.460479	-0.455687	1.197976	C	-0.660648	-0.616237	1.082235
H	0.335881	-0.021893	1.779764	H	0.020400	-0.144928	1.781884
H	-0.465086	-1.562744	-0.763709	H	-0.196967	-1.430164	-0.925913
H	-2.539481	-1.355758	1.535521	H	-2.549597	-1.893618	1.420805
C	-4.929023	0.280903	-0.098647	C	-4.875473	0.344812	0.011740
H	-3.961755	0.501828	-0.488939	H	-3.845385	0.483355	-0.222921
C	-6.013700	0.027441	0.344983	C	-6.033554	0.187345	0.278870
H	-6.976946	-0.194759	0.735413	H	-7.060917	0.048985	0.513262
C	1.190339	2.973637	-0.999495	C	1.300828	2.966263	-0.978500
H	0.393934	2.262542	-1.029239	H	0.509436	2.253707	-1.059227
C	2.084060	3.773283	-0.967719	C	2.190275	3.766111	-0.887236
H	2.870237	4.488777	-0.946162	H	2.973392	4.481494	-0.813969
C	3.240832	0.808529	1.291259	C	3.099695	0.779785	1.477278
H	2.913950	1.575644	0.625822	H	2.832923	1.569667	0.811689
C	3.604979	-0.052186	2.043746	C	3.396811	-0.107032	2.228885
H	3.933342	-0.810731	2.712715	H	3.664463	-0.888345	2.898630
C	2.440481	-3.409811	-1.585743	C	2.537830	-3.233420	-1.673035
H	2.215672	-4.244831	-2.203689	H	2.327999	-4.020640	-2.355693
C	2.697105	-2.468314	-0.889004	C	2.778756	-2.346216	-0.903138
H	2.928188	-1.633433	-0.268714	H	2.994502	-1.559630	-0.217346
[2]				TS3			

-200 kJ/mol, ^3A , C_1	-183 kJ/mol, ^3A , C_1
C -0.864978 -0.887014 0.665890	C -0.924716 0.650809 -0.785179
C -2.718041 0.491170 1.562049	C -2.629009 -0.995284 -1.522701
C -3.258343 1.170926 2.549189	C -3.060395 -1.874317 -2.385459
H -4.154209 1.746087 2.726434	H -3.392302 -2.586864 -3.103602
C -1.431176 -0.211647 1.643067	C -1.375545 -0.227850 -1.655048
H -0.919523 -0.157028 2.610082	H -0.790892 -0.419612 -2.561499
H -3.244740 0.426909 0.604623	H -3.210873 -0.778169 -0.619456
H 0.028629 -1.472707 0.501797	H -0.081646 1.318425 -0.673451
C -3.403560 -1.024764 -2.111695	C -3.533198 1.392855 1.844032
H -2.508375 -1.268093 -1.588814	H -2.669961 1.402381 1.220063
C -4.413806 -0.743815 -2.692840	C -4.507324 1.375407 2.542483
H -5.308089 -0.497043 -3.211586	H -5.370129 1.360877 3.162938
C 0.649860 2.518604 -0.479367	C 0.765476 -2.398696 0.985743
H 0.087351 1.715382 -0.061521	H 0.155529 -1.717475 0.438025
C 1.277093 3.425463 -0.951348	C 1.446471 -3.168083 1.604496
H 1.825089 4.234408 -1.370566	H 2.042271 -3.854972 2.155540
C 4.191917 0.973599 -0.410850	C 4.215475 -0.737486 0.493174
H 3.286612 1.531779 -0.491731	H 3.343810 -1.311028 0.714408
C 5.214042 0.352233 -0.320842	C 5.199999 -0.098319 0.245940
H 6.124205 -0.191675 -0.242093	H 6.077222 0.461845 0.028851
C 2.694074 -2.531114 0.174271	C 2.511022 2.577859 -0.489000
H 3.258541 -1.643027 0.000888	H 3.132034 1.753743 -0.219750
C 2.064861 -3.533533 0.369307	C 1.817805 3.508645 -0.792120
H 1.512842 -4.425641 0.541500	H 1.208566 4.337615 -1.060235
[3]	TS4
-197 kJ/mol, ^3A , C_1	-176 kJ/mol, ^3A , C_1
C -0.882586 0.872737 -0.657519	C 0.850398 0.738911 -0.452148
C -2.697870 -0.544895 -1.582184	C 2.226008 2.797791 -0.765493
C -3.189104 -1.256732 -2.572783	C 3.323083 3.035512 -0.091036
H -2.917582 -1.545976 -3.577674	H 4.124220 2.474129 0.368383
C -1.407929 0.161739 -1.633705	C 1.762463 1.413950 -1.110100

H	-0.850451	0.081511	-2.574152	H	2.223986	0.952447	-1.992533
H	-3.260483	-0.451923	-0.653231	H	1.606298	3.625258	-1.114083
H	0.003962	1.467169	-0.483967	H	0.381635	-0.235919	-0.492446
C	-3.480715	1.036200	2.077753	C	3.546956	-1.885575	0.670060
H	-2.579880	1.294374	1.572458	H	3.058278	-0.944600	0.571630
C	-4.497423	0.737538	2.638290	C	4.095192	-2.946480	0.778529
H	-5.398024	0.474122	3.137559	H	4.588420	-3.883155	0.876806
C	0.648037	-2.503038	0.588528	C	-2.201390	2.304566	1.009601
H	0.066222	-1.706614	0.184530	H	-1.226419	1.973863	0.731664
C	1.296700	-3.402943	1.044554	C	-3.295260	2.682252	1.324772
H	1.863332	-4.205910	1.450314	H	-4.261603	3.023788	1.607608
C	4.178795	-0.936454	0.426278	C	-4.356144	-0.662290	-0.320140
H	3.277923	-1.496760	0.536716	H	-3.899329	0.210852	0.087593
C	5.196084	-0.312844	0.303075	C	-4.874777	-1.641772	-0.778835
H	6.102089	0.233032	0.195232	H	-5.342102	-2.505673	-1.185786
C	2.654888	2.555000	-0.158652	C	-1.123861	-2.682377	-0.163256
H	3.227989	1.672416	0.014558	H	-2.141895	-2.403202	-0.311912
C	2.016023	3.551391	-0.353254	C	0.021980	-2.992763	0.011488
H	1.455512	4.438364	-0.524626	H	1.040614	-3.258130	0.172422
[4]				TS5			
							
-189 kJ/mol, ^3A , C_1				-175 kJ/mol, ^3A , C_1			
C	-0.379236	-0.000664	-0.119165	C	-0.357284	-0.006150	-0.169214
C	-2.612189	-0.004777	2.006114	C	-2.570786	-0.045957	1.959612
C	-1.315831	-0.003175	2.218436	C	-1.284814	-0.031650	2.169723
C	-0.247310	-0.001203	1.190341	C	-0.214005	-0.012498	1.137934
H	0.287519	0.000633	-0.969216	H	0.291269	0.006628	-1.032614
H	-0.956737	-0.003273	3.247905	H	-0.905252	-0.033291	3.198535
H	0.776653	-0.000084	1.583599	H	0.809614	-0.002731	1.530247
C	3.323832	0.603402	-0.647048	C	3.354151	0.637657	-0.655095
H	3.307815	1.668124	-0.641893	H	3.326688	1.702106	-0.647600
C	3.325146	-0.596409	-0.647410	C	3.368039	-0.562045	-0.658328
H	3.311462	-1.661166	-0.642897	H	3.365232	-1.626869	-0.656585
C	2.094654	4.506124	-0.339280	C	2.082233	4.528601	-0.318196
H	2.810944	5.254896	-0.577034	H	2.795084	5.288893	-0.528014
C	1.278774	3.669943	-0.069136	C	1.270154	3.679139	-0.079913
H	0.555223	2.926269	0.170029	H	0.550158	2.923544	0.131058
C	1.286436	-3.667474	-0.071246	C	1.354599	-3.654059	-0.100742

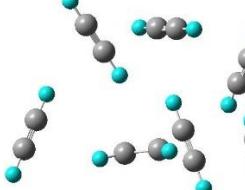
H	0.561529	-2.925146	0.167997	H	0.616891	-2.915582	0.109684
C	2.103844	-4.502133	-0.341471	C	2.186643	-4.484185	-0.338306
H	2.821501	-5.249569	-0.579303	H	2.917356	-5.227490	-0.547535
H	-3.318512	-0.005233	1.188745	H	-3.623391	-0.057552	1.795988
C	-3.922782	-0.001510	-1.591556	C	-5.248816	-0.028428	-1.629226
H	-2.858568	-0.000743	-1.612039	H	-6.286585	-0.034321	-1.858820
C	-5.121164	-0.002385	-1.556159	C	-4.076777	-0.021680	-1.376588
H	-6.183877	-0.003149	-1.530410	H	-3.037092	-0.015805	-1.144313
[5]				TS6			
-189 kJ/mol, ³ A, C ₁				-164 kJ/mol, ³ A, C ₁			
C	-0.357284	-0.006150	-0.169214	C	-0.100766	-0.433731	-0.654478
C	-2.570786	-0.045957	1.959612	C	-4.552027	-1.470943	-0.947456
C	-1.284814	-0.031650	2.169723	C	-3.354686	-1.268569	-0.988510
C	-0.214005	-0.012498	1.137934	C	-2.317160	-1.887938	0.987856
H	0.291269	0.006628	-1.032614	C	-1.198037	-1.333642	1.420466
H	-0.905252	-0.033291	3.198535	C	-0.222583	-0.539576	0.652677
H	0.809614	-0.002731	1.530247	H	0.552196	0.088990	-1.338087
C	3.354151	0.637657	-0.655095	H	-5.574093	-1.705619	-0.770637
H	3.326688	1.702106	-0.647600	H	-0.947227	-1.457411	2.478730
C	3.368039	-0.562045	-0.658328	H	0.498442	0.024016	1.256704
H	3.365232	-1.626869	-0.656585	H	-3.063798	-2.466648	1.512405
C	2.082233	4.528601	-0.318196	H	-2.400933	-0.961447	-1.357566
H	2.795084	5.288893	-0.528014	C	2.468285	2.301380	-0.075557
C	1.270154	3.679139	-0.079913	H	1.792784	3.123571	-0.033831
H	0.550158	2.923544	0.131058	C	3.214578	1.363139	-0.122322
C	1.354599	-3.654059	-0.100742	H	3.863508	0.520043	-0.163742
H	0.616891	-2.915582	0.109684	C	-0.873675	4.645714	0.073317
C	2.186643	-4.484185	-0.338306	H	-0.693671	5.693410	0.085204
H	2.917356	-5.227490	-0.547535	C	-1.088496	3.466077	0.060113
H	-3.456903	-0.045626	2.550950	H	-1.278184	2.418420	0.048075
C	-4.715427	0.560191	-2.553413	C	3.364516	-2.363251	-0.277773
H	-5.433384	0.778961	-3.306002	H	2.311945	-2.204109	-0.244145
C	-3.900892	0.313110	-1.709002	C	4.549988	-2.539820	-0.315548
H	-3.177150	0.093570	-0.958715	H	5.599410	-2.706254	-0.349824
[6]				TS7			

-346 kJ/mol, ${}^3\text{A}$, C_1	-325 kJ/mol, ${}^3\text{A}$, C_1				
C 0.284278	-0.005382	-0.719514	C -0.006265	-0.469308	0.077985
C 4.739912	-0.022879	-0.893701	C -3.192069	-0.536449	1.131520
C 3.475348	-0.016238	-0.515921	C -2.657856	-1.725804	0.996496
C 3.040303	-0.018811	0.872386	C -2.388972	-2.421347	-0.285590
C 1.770688	-0.013975	1.330173	C -1.388624	-2.166412	-1.139601
C 0.510888	-0.005511	0.580989	C -0.325163	-1.162066	-0.996655
H -0.594441	0.000324	-1.348202	H 0.711401	0.299704	0.327916
H 5.292221	-0.022717	-1.821664	H -3.489303	0.116299	1.939023
H 1.642586	-0.016229	2.407859	H -1.339608	-2.763834	-2.045455
H -0.386680	0.001485	1.212721	H 0.276440	-0.999460	-1.899213
H 3.837862	-0.025027	1.609253	H -3.069605	-3.235508	-0.525079
H 2.700036	-0.008272	-1.285524	H -2.434946	-2.302363	1.905269
C -3.431176	-0.578461	-0.016551	C 2.940607	2.081386	0.151473
H -3.422116	-1.643194	-0.017763	H 3.795318	1.454324	0.245002
C -3.423015	0.621255	-0.016543	C 1.964741	2.770571	0.043601
H -3.399478	1.685766	-0.017730	H 1.086318	3.364666	-0.053679
C -2.145295	-4.490255	-0.153869	C 4.965708	-1.590141	0.306314
H -2.885395	-5.253344	-0.142981	H 6.027709	-1.550586	0.331846
C -1.302374	-3.637461	-0.166833	C 3.768226	-1.644580	0.277310
H -0.555705	-2.878087	-0.178472	H 2.704762	-1.694993	0.251061
C -1.252561	3.650800	-0.165589	C -1.857630	2.865222	-0.289981
H -0.516507	2.881154	-0.178102	H -1.819514	1.800381	-0.315025
C -2.083559	4.515198	-0.151622	C -1.904699	4.063351	-0.260570
H -2.813005	5.288464	-0.139826	H -1.957000	5.124823	-0.235475
[7]	TS8				
-329 kJ/mol, ${}^3\text{A}$, C_1	-311 kJ/mol, ${}^3\text{A}$, C_1				
C 0.121927	0.386757	1.061491	C 0.209601	0.282436	0.542971
C 1.452219	-0.942804	-1.365457	C 1.039002	-0.966027	-1.343423
C 1.760969	-2.053365	-0.726778	C 0.828009	-2.226468	-0.939194
C 1.881558	-2.317110	0.706187	C 1.204021	-2.662831	0.378131
C 1.252550	-1.754368	1.759832	C 1.114829	-1.860759	1.479036
C 0.252829	-0.689034	1.810574	C 0.478640	-0.551863	1.541860
H -0.551655	1.230938	1.011084	H -0.287013	1.243393	0.493195

H	1.358588	-0.632471	-2.395934	H	0.948493	-0.392520	-2.253934
H	1.449625	-2.213680	2.725319	H	1.364256	-2.303110	2.438571
H	-0.476267	-0.805884	2.624009	H	0.117335	-0.279249	2.539499
H	2.523324	-3.162777	0.938896	H	1.439661	-3.713379	0.525942
H	1.985196	-2.927567	-1.352789	H	0.255598	-2.921105	-1.563543
C	-3.352771	1.810124	0.395704	C	-2.939700	2.602556	0.163679
H	-3.407896	0.900163	-0.156804	H	-3.377623	1.660911	-0.075023
C	-3.285585	2.834042	1.016537	C	-2.440721	3.659621	0.431479
H	-3.231012	3.743433	1.564232	H	-2.002240	4.598714	0.667637
C	-3.610091	-1.565778	-1.690101	C	-4.275050	-1.126364	-0.780901
H	-4.610304	-1.643515	-2.041929	H	-5.308063	-1.169469	-1.028339
C	-2.479141	-1.487269	-1.298180	C	-3.108814	-1.088055	-0.502957
H	-1.474292	-1.413911	-0.949838	H	-2.072374	-1.045288	-0.255539
C	2.755285	2.482380	-0.649499	C	3.581401	1.626917	-0.345182
H	2.259083	1.612781	-0.284500	H	2.801933	0.970973	-0.032694
C	3.311991	3.460506	-1.062590	C	4.456656	2.365761	-0.699355
H	3.805164	4.328003	-1.428071	H	5.232785	3.020595	-1.012651
[8]							
							
-577 kJ/mol, ³ A, C ₁							
C	-0.295350	-0.674323	0.783620				
C	-0.973780	-1.651412	1.441099				
C	-1.291941	-2.890355	0.686824				
C	-1.491997	-2.740436	-0.776233				
C	-0.811716	-1.747851	-1.403864				
C	-0.106240	-0.753629	-0.639766				
H	0.045584	0.215777	1.303436				
H	-1.221101	-1.564591	2.493884				
H	-0.856968	-1.644261	-2.483809				
H	0.407420	0.052543	-1.148363				
H	-2.115816	-3.438998	-1.323821				
H	-0.747153	-3.788031	1.001056				
C	1.799076	2.693624	-0.014126				
H	2.814719	2.376616	0.014379				
C	0.648105	3.030204	-0.046788				
H	-0.378708	3.311165	-0.074064				
C	5.008066	0.045728	0.019026				
H	5.988445	0.455068	0.056592				
C	3.906193	-0.425190	-0.023045				

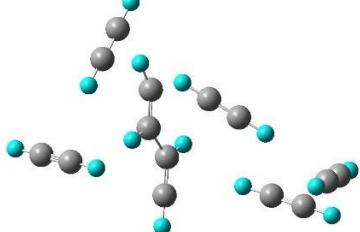
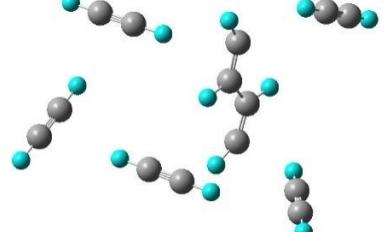
H	2.928146	-0.844084	-0.061797
C	-3.004176	1.989228	0.082963
H	-2.606292	1.011528	0.225463
C	-3.452717	3.090226	-0.074445
H	-3.859406	4.062390	-0.214544

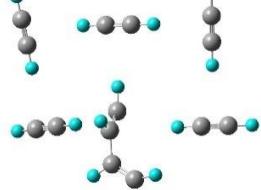
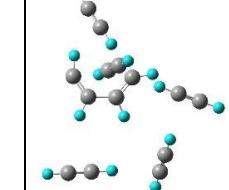
with 4 acetylenes surrounding the reaction center

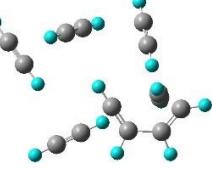
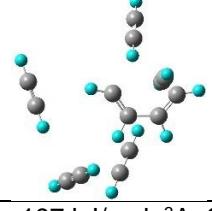
Initial structure				vdW			
							
0 kJ/mol, ${}^3\text{A}_1$, C ₁				-2.12 kJ/mol, ${}^3\text{A}_1$, C ₁			
C	-4.419138	1.624659	-0.332902	C	2.425872	-2.444260	0.694626
H	-4.206726	0.890243	-1.076387	H	2.650882	-2.161126	-0.309725
C	-4.663081	2.443745	0.509396	C	2.176550	-2.769390	1.822701
H	-4.887551	3.174496	1.248847	H	1.960434	-3.064376	2.821500
C	1.127269	-1.859187	-1.161355	C	-2.434263	2.778298	-0.313965
H	1.545137	-2.773546	-1.508045	H	-2.678170	3.790559	-0.529584
C	0.650314	-0.831111	-0.766981	C	-2.152209	1.638323	-0.067501
H	0.237519	0.087919	-0.415725	H	-1.913117	0.622009	0.152174
C	-3.987695	-1.854410	-1.801620	C	2.587706	2.627432	-1.106497
H	-4.043506	-2.247035	-0.780972	H	2.754271	2.458006	-0.037509
C	-2.910321	-1.504464	-2.498907	C	1.435894	2.651797	-1.771675
H	-1.859088	-1.544987	-2.194924	H	0.421728	2.510662	-1.383356
C	3.839907	1.097033	-0.469443	C	-5.642677	0.203542	-0.184785
H	3.191563	0.282631	-0.700015	H	-4.902754	0.967539	-0.248746
C	4.562791	2.018827	-0.210098	C	-6.471128	-0.660512	-0.111853
H	5.207598	2.833951	0.015251	H	-7.212840	-1.419602	-0.049670
C	-4.535579	-1.347190	2.046779	C	2.979017	0.977623	2.526736
H	-4.634894	-0.340652	1.712766	H	2.858115	-0.016371	2.161986
C	-4.422360	-2.480945	2.420411	C	3.114330	2.094175	2.942897
H	-4.322727	-3.483940	2.758160	H	3.234465	3.082026	3.316811
C	-0.733972	2.667020	0.231483	C	-1.488202	-2.194135	0.620120
H	-1.798057	2.609635	0.218002	H	-0.445955	-2.381085	0.739958
C	0.463823	2.735992	0.244394	C	-2.663569	-1.992747	0.486316
H	1.527358	2.790029	0.251087	H	-3.705418	-1.805230	0.364367
C	7.002094	-0.945738	0.656137	C	3.269419	-1.996722	-3.015903
H	6.217685	-0.272225	0.399940	H	3.523875	-2.994033	-3.282622
C	7.885463	-1.702941	0.944616	C	2.983893	-0.867785	-2.727765
H	8.668611	-2.374256	1.200555	H	2.730683	0.137199	-2.476299
TS1				[1]			

-1.81 kJ/mol, ${}^3\text{A}$, C_1	-135 kJ/mol, ${}^3\text{A}$, C_1
C 2.506498 2.815262 0.230118	C -1.979459 0.526943 -0.030590
C -1.491321 -1.964768 1.087287	C -1.632889 -0.021719 1.349348
C -1.491935 -2.319664 -0.196114	C -1.540084 -1.434803 1.607979
H -1.309916 -1.683860 -1.068685	H -1.484061 -2.042394 2.502246
C 1.857417 3.760979 0.581179	C -0.746276 0.679516 0.310271
H 1.284606 4.601560 0.891042	H 0.269430 0.968714 0.089959
H -1.303799 -0.978204 1.524026	H -1.954127 0.556849 2.222821
H 3.079296 1.979581 -0.099826	H -2.772508 0.583243 -0.757981
C 3.458115 -0.411957 -1.715083	C -4.756865 -1.894844 -0.229941
H 3.221275 -1.231617 -1.074510	H -3.914397 -2.031074 0.408769
C 3.732265 0.501224 -2.443512	C -5.700467 -1.733583 -0.951906
H 3.979063 1.304719 -3.094844	H -6.539168 -1.596223 -1.590259
C -0.093275 1.389797 2.911884	C 0.826855 -3.504581 -0.348868
C -0.773566 0.918297 3.779744	H 0.158759 -2.833877 0.143449
H -1.374501 0.504142 4.552647	C 1.567428 -4.266774 -0.905075
H 0.514516 1.815234 2.146733	H 2.217486 -4.946854 -1.400469
C -0.712489 1.277574 -1.791241	C 4.382260 -1.873231 0.050195
C -1.898701 1.105879 -1.738757	H 3.457498 -2.385062 -0.092042
H -2.951140 0.949290 -1.684585	C 5.426728 -1.305512 0.210194
H 0.338655 1.436139 -1.833192	H 6.355644 -0.808664 0.353824
C 3.429297 -3.470440 0.580488	C 2.410256 2.747186 -0.345437
C 2.252533 -3.241515 0.619498	H 1.830836 3.638899 -0.404565
H 1.205929 -3.042997 0.657461	C 3.054154 1.736995 -0.276090
H 4.471058 -3.681092 0.551493	H 3.627232 0.840163 -0.213426
C -5.026320 -0.658620 -0.644470	C -0.871068 4.603693 -0.174398
H -4.332311 -1.301383 -0.155278	H -1.259729 3.630072 0.010855
C -5.802590 0.068166 -1.198696	C -0.431181 5.699382 -0.383199
H -6.498293 0.707206 -1.686416	H -0.049249 6.674203 -0.568079
TS2	[2]
-102 kJ/mol, ${}^3\text{A}$, C_1	-202 kJ/mol, ${}^3\text{A}$, C_1

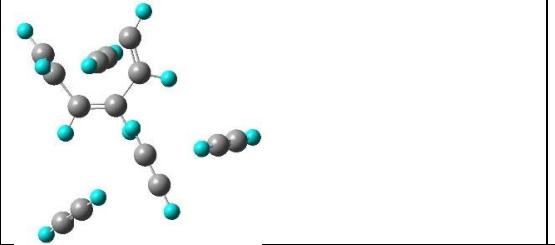
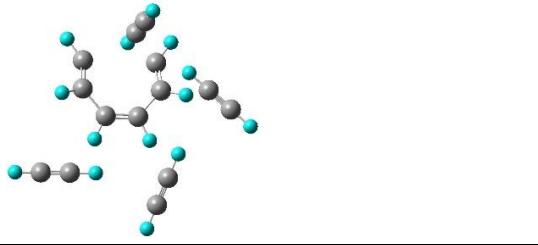
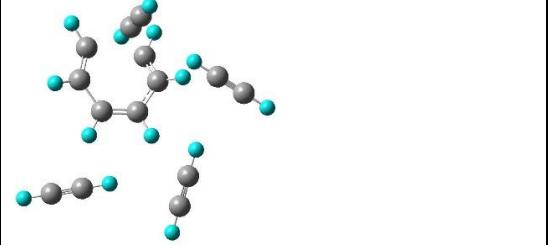
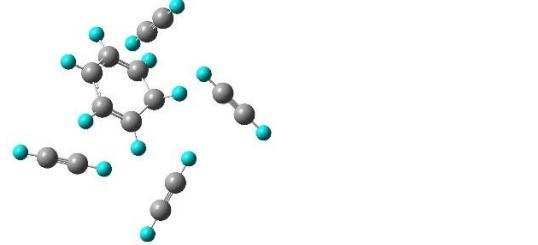
C	-1.361989	-1.439243	1.620772	C	-0.758193	-0.024265	-0.274699
C	-0.782994	-0.615136	0.050890	C	-2.382163	-1.503090	-1.423071
C	-1.465257	-0.794481	-1.123921	C	-2.934678	-1.942161	-2.532328
H	-1.234200	-1.222556	-2.090028	H	-3.690599	-2.656871	-2.819762
C	-1.409238	-0.185635	1.343733	C	-1.331767	-0.478041	-1.369984
H	-1.720261	0.773159	1.742934	H	-1.014015	-0.071363	-2.336403
H	0.307957	-0.605805	0.007970	H	-2.708802	-1.911200	-0.461371
H	-1.559604	-2.316263	2.210122	H	-0.003511	0.701340	-0.003444
C	-3.602352	-3.763066	-0.191578	C	-2.556145	-1.849356	2.545059
H	-3.131885	-2.838908	-0.436711	H	-1.815877	-1.144793	2.248260
C	-4.131306	-4.801989	0.088084	C	-3.391938	-2.644679	2.870800
H	-4.600679	-5.723510	0.333104	H	-4.131429	-3.348903	3.165869
C	-2.174862	2.683530	-2.088728	C	2.036514	-2.738866	-0.529079
H	-2.013403	1.654142	-1.854429	H	1.151383	-2.149455	-0.597091
C	-2.355766	3.840093	-2.351105	C	3.027171	-3.410621	-0.453257
H	-2.520699	4.862173	-2.593016	H	3.900735	-4.013150	-0.387405
C	-0.573741	3.742047	1.139335	C	4.831291	-0.094964	0.255259
H	-1.025146	3.734154	0.172851	H	4.159276	-0.894826	0.041131
C	-0.070265	3.749565	2.228362	C	5.592636	0.800060	0.496150
H	0.373605	3.761706	3.194488	H	6.273606	1.588156	0.709593
C	3.359194	0.550814	0.243176	C	2.129010	2.621461	0.345057
H	4.083894	-0.189725	-0.004542	H	3.047978	2.082510	0.385092
C	2.545375	1.387102	0.521847	C	1.094601	3.228008	0.298032
H	1.822911	2.129680	0.770341	H	0.171327	3.757567	0.253494
C	6.256481	-1.739039	-1.049153	C	-2.710608	4.613112	-0.029943
H	6.797164	-1.009400	-1.602245	H	-2.781045	5.664168	0.113582
C	5.650624	-2.565591	-0.427297	C	-2.642267	3.427189	-0.193560
H	5.116922	-3.302671	0.122657	H	-2.579818	2.374098	-0.338163

TS3	[3]				
					
-188 kJ/mol, ³ A, C ₁	-201 kJ/mol, ³ A, C ₁				
C -0.283989	-2.306651	0.956385	C -1.215259	-1.144359	1.562269
C 0.832875	-2.143836	-1.243790	C -1.410155	-0.226217	-0.733537
C 1.277606	-1.412148	-2.241644	C -0.959285	0.578675	-1.673015
H 1.794641	-1.558796	-3.177542	H -0.160839	1.296017	-1.801501
C 0.144720	-1.598636	-0.056476	C -0.818525	-0.323780	0.611560
H 0.008915	-0.510251	-0.065127	H 0.016092	0.355083	0.819752
H 0.972788	-3.229575	-1.265645	H -2.266633	-0.870173	-0.933569

H	-0.623336	-2.900249	1.773127	H	-0.940833	-1.366102	2.583364
C	-3.889696	-1.918737	-0.408559	C	-4.406953	-2.730790	0.269041
H	-2.827290	-1.921134	-0.325126	H	-3.684045	-2.484586	1.010528
C	-5.085407	-1.923780	-0.501790	C	-5.214640	-3.002107	-0.574209
H	-6.145117	-1.934495	-0.587609	H	-5.932540	-3.244744	-1.319586
C	3.554756	-1.296219	1.797018	C	1.869024	-3.232665	0.185413
H	2.545513	-1.487793	1.514193	H	0.984702	-2.646984	0.287197
C	4.689882	-1.082183	2.119509	C	2.858929	-3.900702	0.074678
H	5.695519	-0.896664	2.410407	H	3.731876	-4.499699	-0.023842
C	4.157046	1.678230	-0.594395	C	4.736106	-0.563747	-0.213615
H	4.166405	0.840511	0.065134	H	4.022199	-1.352450	-0.139259
C	4.149894	2.622149	-1.334442	C	5.546560	0.316543	-0.297667
H	4.148179	3.457766	-1.991654	H	6.271087	1.091012	-0.373161
C	0.372226	2.422599	-0.204323	C	2.264978	2.373137	0.118794
H	1.414163	2.407343	-0.427678	H	3.123763	1.750552	0.010810
C	-0.800715	2.441759	0.048235	C	1.297484	3.072834	0.241305
H	-1.842929	2.459265	0.270167	H	0.432615	3.686247	0.346207
C	-4.581808	2.884789	1.023014	C	-2.310818	4.916400	0.360881
H	-4.603759	3.897873	1.344637	H	-2.255137	5.910903	0.732564
C	-4.563047	1.741304	0.661502	C	-2.386250	3.795792	-0.059417
H	-4.549757	0.724362	0.341257	H	-2.449487	2.800838	-0.434392
TS4	[4]						
							
-179 kJ/mol, ³ A, C ₁				-194 kJ/mol, ³ A, C ₁			
C	0.035483	0.962233	-0.376381	C	1.150006	-0.516289	-1.055331
C	0.340303	3.336532	-1.091111	C	5.966074	0.260145	-1.123908
C	1.513049	3.918153	-1.139233	C	4.800029	0.213215	-1.398768
H	2.543330	3.641980	-1.313156	C	2.198569	1.389215	1.110243
C	0.150238	1.866880	-1.319799	C	1.032116	1.439673	0.505289
H	0.100593	1.540525	-2.366511	C	0.609186	0.612079	-0.651608
H	-0.555997	3.925468	-0.890211	H	0.967434	-1.255116	-1.821190
H	-0.081518	-0.111808	-0.304242	H	7.000579	0.301675	-0.883432
C	3.527008	1.230810	1.111275	H	0.283651	2.151493	0.855309
H	2.505292	1.372443	0.843470	H	-0.262343	0.990347	-1.198873
C	4.678219	1.079628	1.412215	H	3.762334	0.170125	-1.634453
H	5.698509	0.952198	1.683026	C	-1.734212	-3.174581	-0.250427
C	-3.319295	1.841091	1.066507	H	-1.182056	-2.814812	0.588570
H	-2.317025	1.684742	0.738545	C	-2.354403	-3.590995	-1.189350
C	-4.445794	2.021617	1.436515	H	-2.901981	-3.968575	-2.018883

H	-5.442256	2.188659	1.767684	C	-0.127787	-2.684967	3.195877
C	-4.698353	-1.581239	-0.046280	H	-0.505621	-3.575239	3.637409
H	-4.502085	-0.598826	0.319035	C	0.303467	-1.679022	2.705099
C	-4.924388	-2.685109	-0.457505	H	0.688650	-0.782431	2.275887
H	-5.132125	-3.662013	-0.822007	C	-3.157475	0.069541	-1.874255
C	-1.026281	-2.789909	-0.140592	H	-2.893264	-0.857510	-1.417441
H	-2.086373	-2.677891	-0.155894	C	-3.454739	1.105614	-2.401385
C	0.166830	-2.918464	-0.121264	H	-3.720626	2.020593	-2.873511
H	1.226440	-3.034208	-0.102186	C	-2.739465	2.875627	0.898225
C	4.003326	-3.635815	-0.285996	H	-3.067410	2.139209	0.201517
H	4.010637	-4.646865	-0.614777	C	-2.369691	3.706935	1.679399
C	4.003442	-2.495263	0.085312	H	-2.046185	4.443838	2.373914
H	4.009860	-1.481264	0.415240	H	3.146787	0.879259	1.020578
TS5				[5]			
							
-183 kJ/mol, ³ A, C ₁				-197 kJ/mol, ³ A, C ₁			
C	3.215491	-1.976005	0.170400	C	2.195666	-1.967916	-1.477832
C	4.599941	2.763359	0.324241	C	6.055122	0.475904	0.330944
C	4.151324	1.671943	0.109855	C	4.885914	0.326195	0.112700
C	0.977175	-0.383665	-1.199604	C	1.088569	0.474983	0.020042
C	1.523534	-1.489754	-1.622696	C	0.786481	0.081329	-1.196446
C	2.638029	-2.236790	-0.980350	C	1.392448	-1.040701	-1.946923
H	4.002226	-2.383700	0.786318	H	2.730591	-2.829416	-1.845888
H	5.006114	3.727504	0.513068	H	7.091577	0.608808	0.524328
H	1.154557	-1.954947	-2.544418	H	0.007265	0.632896	-1.733302
H	2.995472	-3.103784	-1.548511	H	1.117938	-1.086836	-3.006369
H	0.548888	0.529298	-0.845458	H	0.776688	1.236914	0.719332
H	3.754364	0.700525	-0.078102	H	3.846439	0.192800	-0.079313
C	-3.127901	-1.944342	-0.541852	C	-3.722399	-1.730948	0.280332
H	-2.358719	-2.069001	0.186453	H	-2.776069	-2.072420	0.635385
C	-3.994689	-1.814860	-1.361047	C	-4.793297	-1.359423	-0.112580
H	-4.760502	-1.706751	-2.090574	H	-5.746508	-1.038424	-0.457270
C	-1.093219	-2.633418	2.650253	C	-0.885858	-3.564847	2.072470
H	-1.915242	-2.841376	3.291607	H	-1.504164	-4.119607	2.735954
C	-0.160428	-2.398594	1.933750	C	-0.181194	-2.942159	1.327835
H	0.671416	-2.190919	1.300716	H	0.449740	-2.391730	0.668252
C	-4.261731	1.767988	-0.054867	C	-2.904418	1.674905	-1.404293
H	-4.042065	0.740079	-0.235421	H	-3.229249	0.762615	-0.956260
C	-4.514449	2.923193	0.146213	C	-2.544591	2.700176	-1.913403

H	-4.745111	3.945496	0.325052	H	-2.230092	3.608170	-2.368816
C	-0.599830	2.897440	0.214581	C	-1.007064	3.287599	1.596615
H	-1.662041	2.826217	0.158196	H	-1.680375	3.069784	0.800005
C	0.595575	2.977535	0.283906	C	-0.245531	3.531122	2.490482
H	1.657714	3.037176	0.344373	H	0.427139	3.749139	3.284308
TS6				[6]			
	-171 kJ/mol, ${}^3\text{A}$, C_1			-351 kJ/mol, ${}^3\text{A}$, C_1			
C	-2.432298	-1.023080	2.279401	C	2.332067	-1.827269	-1.926187
C	-3.627165	1.490963	-1.071416	C	3.948444	0.593633	1.396838
C	-3.345816	1.257340	0.087580	C	3.295549	0.221376	0.312578
C	-1.057929	1.090023	0.474571	C	1.973495	0.705589	-0.058078
C	-0.598929	0.533812	1.582216	C	1.216316	0.270649	-1.086854
C	-1.324773	-0.353006	2.510696	C	1.505773	-0.806747	-2.038707
H	-3.072486	-1.711387	2.809932	H	2.634847	-2.665836	-2.535609
H	-3.709902	1.684822	-2.113835	H	4.902769	0.387498	1.858330
H	0.435085	0.749563	1.869137	H	0.275323	0.782840	-1.261385
H	-0.860245	-0.465827	3.497305	H	0.916205	-0.758152	-2.963517
H	-0.586998	1.748720	-0.241903	H	1.577827	1.513857	0.549349
H	-3.475768	1.061241	1.128382	H	3.772202	-0.492004	-0.365770
C	1.990225	-2.975943	-0.742727	C	-3.428619	-1.817315	0.726614
H	0.970870	-2.746280	-0.958540	H	-2.444248	-2.213332	0.837560
C	3.134971	-3.247816	-0.508373	C	-4.540813	-1.383070	0.609972
H	4.148326	-3.496229	-0.304093	H	-5.529581	-1.004732	0.511832
C	-1.512497	-2.988247	-2.228170	C	-0.395780	-3.917373	1.647359
H	-1.347438	-3.828062	-2.858686	H	-0.922860	-4.535524	2.333190
C	-1.706242	-2.040345	-1.518699	C	0.206282	-3.222263	0.877170
H	-1.881744	-1.195397	-0.891649	H	0.748701	-2.612705	0.190875
C	3.376775	0.236450	0.971243	C	-2.802169	1.359040	-1.387888
H	3.062549	-0.671629	0.507507	H	-3.095575	0.512089	-0.809169
C	3.736829	1.253215	1.496860	C	-2.477388	2.310158	-2.043327
H	4.059380	2.151666	1.965198	H	-2.192917	3.152106	-2.627155
C	1.915372	2.989856	-1.411275	C	-0.789487	3.538398	1.194036
H	2.469350	2.299997	-0.817311	H	-1.473239	3.095868	0.507267
C	1.292571	3.769629	-2.076124	C	-0.016625	4.035677	1.964185
H	0.742461	4.461702	-2.666130	H	0.668273	4.475132	2.647938
TS7				[7]			

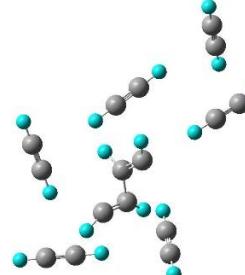
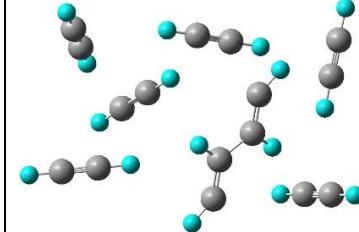
	
-332 kJ/mol, ${}^3\text{A}$, C_1	-334 kJ/mol, ${}^3\text{A}$, C_1
C -2.360329 2.022462 -0.488751	C -2.559714 -1.165033 -1.935378
C -4.041632 -0.847963 -0.882985	C -1.199417 -3.326193 -0.249826
C -2.925044 -0.955373 -0.204252	C -0.060741 -2.671164 -0.135212
C -1.556289 -0.950218 -0.777663	C 0.495591 -1.591020 -0.947508
C -0.854895 0.131306 -1.145809	C -0.114303 -0.622168 -1.664476
C -1.270640 1.537277 -1.049337	C -1.533496 -0.340306 -1.872189
H -2.800337 3.002256 -0.370966	H -3.623069 -1.071429 -2.102707
H -5.101109 -0.855373 -0.672826	H -1.681825 -4.139351 0.273511
H 0.138527 -0.028657 -1.553484	H 0.545740 0.127762 -2.092852
H -0.557480 2.250911 -1.477770	H -1.751924 0.726529 -2.014934
H -1.078579 -1.922675 -0.872788	H 1.577449 -1.517814 -0.881620
H -2.985951 -1.125178 0.880036	H 0.601304 -2.979138 0.685151
C 2.518460 -0.100073 1.876896	C -1.683832 2.997032 0.490529
H 1.547129 0.122350 2.259313	H -1.948188 2.129994 1.053339
C 3.613853 -0.350162 1.455065	C -1.396283 3.976416 -0.140172
H 4.586917 -0.571509 1.087188	H -1.147151 4.847096 -0.697286
C -0.691731 0.556824 3.892499	C -2.885769 0.278772 2.962167
H -0.395534 0.229461 4.859756	H -3.213206 0.861847 3.788648
C -1.034846 0.929051 2.804629	C -2.518045 -0.387725 2.034881
H -1.345811 1.262495 1.839204	H -2.193139 -0.983077 1.211574
C 1.767925 -3.127295 -0.543716	C 2.145830 2.650569 -0.401010
H 2.065810 -2.386050 0.161205	H 1.135211 2.758992 -0.078811
C 1.434836 -3.959990 -1.339722	C 3.281061 2.542418 -0.773555
H 1.141916 -4.698072 -2.046317	H 4.286903 2.449523 -1.105515
C 2.699965 2.220309 -1.321837	C 3.730478 -0.702598 1.124804
H 2.782376 1.668793 -0.413918	H 3.310368 0.241671 0.865274
C 2.611217 2.838235 -2.345734	C 4.209382 -1.763982 1.411669
H 2.537024 3.384901 -3.254334	H 4.637079 -2.702716 1.667890
TS8	[8]
	
-313 kJ/mol, ${}^3\text{A}$, C_1	-578 kJ/mol, ${}^3\text{A}$, C_1

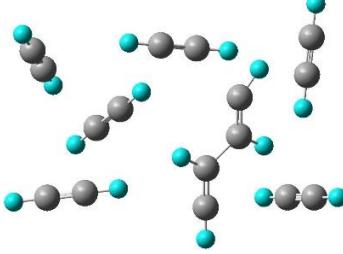
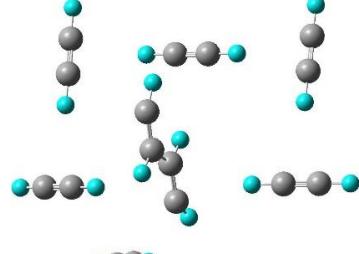
C	-2.347509	-1.167423	-2.067489	C	-2.897760	-0.796735	-1.657944
C	-2.087766	-2.752001	-0.275675	C	-2.940142	-1.719940	-0.664458
C	-0.777640	-2.687209	-0.056261	C	-1.734844	-2.101379	0.023618
C	0.209950	-1.864398	-0.739472	C	-0.453370	-1.681900	-0.480530
C	-0.040841	-0.733757	-1.463734	C	-0.379022	-0.758316	-1.472811
C	-1.367628	-0.292581	-1.796399	C	-1.628846	-0.049949	-1.848829
H	-3.370140	-1.125761	-2.413195	H	-3.769281	-0.571072	-2.263422
H	-2.875092	-3.324958	0.198312	H	-3.865018	-2.239107	-0.431222
H	0.791582	-0.067713	-1.675092	H	0.565607	-0.500720	-1.939612
H	-1.583927	0.777819	-1.709275	H	-1.660024	1.018571	-1.609899
H	1.244142	-2.070568	-0.482025	H	0.443292	-2.168449	-0.109151
H	-0.372496	-3.255206	0.788392	H	-1.780063	-2.858205	0.797523
C	-1.277462	3.225729	0.303122	C	-0.197332	3.373727	0.312001
H	-1.627457	2.475044	0.975842	H	-0.596164	2.766644	1.093262
C	-0.893988	4.073394	-0.454648	C	0.244373	4.062851	-0.565240
H	-0.560088	4.827762	-1.125533	H	0.630728	4.677807	-1.341842
C	-2.774849	0.904310	2.968814	C	-1.729740	1.585968	3.397235
H	-3.014204	1.587141	3.747804	H	-1.725899	2.335889	4.150878
C	-2.508212	0.125610	2.095883	C	-1.737969	0.733486	2.553442
H	-2.275551	-0.574591	1.324404	H	-1.746764	-0.026843	1.805589
C	2.501794	2.393718	-0.445810	C	2.989585	1.460400	-0.982551
H	1.522544	2.677641	-0.134048	H	2.161608	2.013008	-0.600250
C	3.602984	2.086820	-0.809774	C	3.922482	0.848470	-1.423642
H	4.579151	1.817567	-1.134193	H	4.750094	0.309217	-1.817109
C	3.676463	-1.137138	1.145491	C	3.274377	-1.925189	1.103572
H	3.347950	-0.158877	0.880588	H	3.277826	-0.968841	0.633518
C	4.052391	-2.237387	1.438782	C	3.274418	-3.003191	1.628725
H	4.387461	-3.211413	1.701037	H	3.276802	-3.957722	2.096214

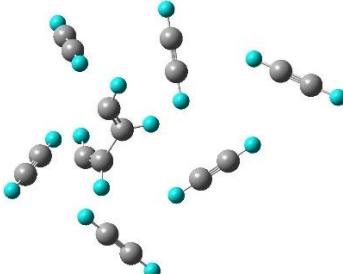
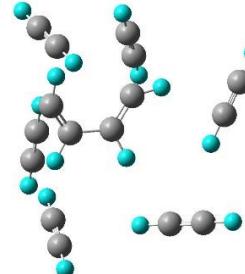
5_ace (with 5 acetylenes surrounding the reaction center)

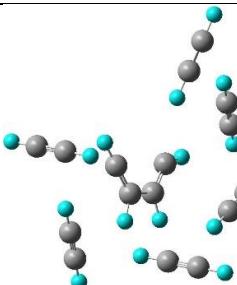
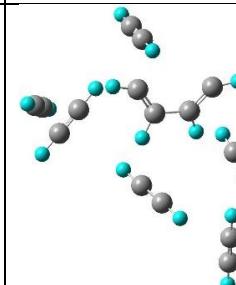
Initial structure	vdW						
0 kJ/mol, ³ A, C ₁	-3.83 kJ/mol, ³ A, C ₁						
C	1.630422	1.932301	-1.112469	C	3.731453	3.089956	0.000279
H	0.865859	2.654376	-0.936664	C	2.536170	-2.287948	0.665433
C	2.488552	1.118697	-1.320090	C	2.536235	-2.287447	-0.665510
H	3.259101	0.403596	-1.499531	H	1.963581	-1.643806	-1.340013
C	-4.667109	2.039008	-0.072574	C	2.861946	3.916463	-0.000038
H	-5.509520	2.672141	0.070967	H	2.093852	4.652134	-0.000326

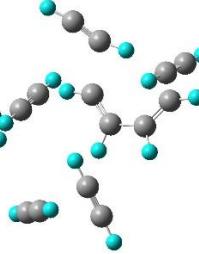
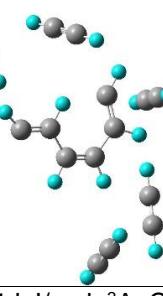
C	-3.714792	1.326831	-0.235311	H	1.963451	-1.644811	1.340364
H	-2.875505	0.683016	-0.378135	H	4.506471	2.357341	0.000553
C	-1.310628	4.216517	0.246131	C	0.601102	0.880110	0.000963
H	-1.891586	3.654259	0.983457	C	-0.334608	0.126844	0.000903
C	-1.511712	4.302462	-1.065191	H	-1.168365	-0.539986	0.000853
H	-2.296801	3.827249	-1.661101	H	1.426828	1.555956	0.001012
C	-5.469892	-1.960744	0.131499	C	6.765626	0.652218	0.001395
H	-5.339406	-0.903392	0.094433	C	5.849430	-0.121731	0.001025
C	-5.610041	-3.151584	0.172133	H	5.039240	-0.813773	0.000697
H	-5.737373	-4.206760	0.208841	H	7.584128	1.330902	0.001726
C	4.644771	1.971618	1.648345	C	-2.990214	-2.601802	0.000014
H	3.802657	2.091764	1.006478	H	-2.371388	-3.470057	-0.000503
C	5.594833	1.831135	2.366712	C	-3.691240	-1.627528	0.000592
H	6.433163	1.715477	3.010226	H	-4.318888	-0.765442	0.001103
C	-0.717330	-1.072280	-0.680069	C	-5.444365	1.867872	0.001797
H	0.147871	-0.467503	-0.829861	C	-6.402219	1.145867	0.003580
C	-1.689606	-1.754921	-0.510952	H	-7.255915	0.512138	0.005170
H	-2.555401	-2.356052	-0.359758	H	-4.597609	2.515966	0.000222
C	-9.298556	-1.740014	0.739930	C	-0.132842	-5.214924	-0.001609
H	-8.284563	-2.025898	0.583254	C	-1.048179	-5.989803	-0.002067
C	-10.439706	-1.418121	0.916222	H	-1.854197	-6.683214	-0.002478
H	-11.451688	-1.133564	1.072544	H	0.683453	-4.530273	-0.001205
C	5.484162	-1.538330	-1.619617	C	-2.659615	4.640375	-0.003894
H	5.387896	-2.189399	-2.454599	H	-3.225075	5.540801	-0.004767
C	5.603768	-0.810422	-0.673842	C	-2.016663	3.627607	-0.002922
H	5.703205	-0.160088	0.164949	H	-1.441683	2.729353	-0.002061
TS1				[1]			
-2.77 kJ/mol, 3A , C ₁				-134 kJ/mol, 3A , C ₁			
C	-0.781147	3.165755	-0.904598	C	1.099758	1.004355	-1.008420
C	1.529722	-2.105647	1.563729	C	1.055750	0.977097	0.516689
C	2.443601	-2.380906	0.635552	C	0.319641	1.954699	1.274358
H	2.393065	-2.176065	-0.438459	H	0.291871	2.243270	2.317436
C	-1.951808	2.921765	-0.802220	C	0.373768	0.062604	-0.511574
H	-2.990102	2.701565	-0.704024	H	-0.320410	-0.756247	-0.617035
H	0.556252	-1.620350	1.441378	H	1.932439	0.587838	1.045366
H	0.257398	3.377799	-1.011431	H	1.459218	1.575797	-1.848427
C	2.980273	2.558450	-1.547988	C	1.742773	4.650830	-0.868106

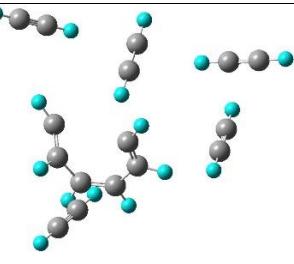
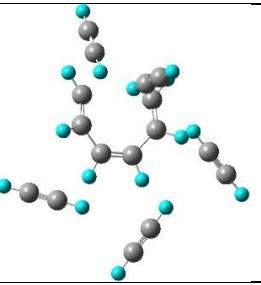
H	3.343306	2.247678	-0.594182	H	1.302826	4.088480	-0.076367
C	2.581371	2.909197	-2.623839	C	2.237248	5.275897	-1.763902
H	2.236068	3.219736	-3.580443	H	2.674889	5.834744	-2.555023
C	-4.984117	1.282892	0.687391	C	-3.302158	2.405803	0.670108
H	-4.272724	0.784811	1.304915	H	-2.259471	2.196318	0.758264
C	-5.779674	1.847324	-0.010343	C	-4.471030	2.656973	0.572756
H	-6.492742	2.342469	-0.624004	H	-5.505358	2.887594	0.486393
C	-1.553344	0.522653	2.036747	C	-5.180131	-1.066274	0.351615
C	-1.884511	-0.246496	2.895958	H	-4.717260	-0.109651	0.441249
H	-2.171071	-0.926834	3.661207	C	-5.710883	-2.137440	0.252874
H	-1.267763	1.210878	1.273889	H	-6.187876	-3.083828	0.168004
C	0.081556	-0.712513	-2.029655	C	-0.942302	-3.532763	-0.799388
C	-0.174486	-1.881671	-1.945188	H	0.038515	-3.894331	-1.000544
H	-0.401775	-2.919375	-1.864089	C	-2.044060	-3.116902	-0.569699
H	0.299847	0.326183	-2.105462	H	-3.022946	-2.748716	-0.362256
C	4.489531	2.115620	1.957434	C	2.757707	-2.827647	-1.419510
C	3.927555	1.060151	1.863202	H	2.375884	-1.836911	-1.505020
H	3.430145	0.120729	1.784152	C	3.185996	-3.943491	-1.317477
H	4.990908	3.048645	2.050083	H	3.570664	-4.931486	-1.234612
C	-0.023909	-5.304361	-0.414873	C	4.558859	-0.773915	2.695961
H	0.625489	-4.813630	0.271668	H	4.840208	-0.092511	3.461679
C	-0.755987	-5.849441	-1.192624	C	4.245447	-1.545103	1.833061
H	-1.404050	-6.340877	-1.877312	H	3.968508	-2.228695	1.064815
TS2			[2]				
							
-103 kJ/mol, 3A , C ₁				-205 kJ/mol, 3A , C ₁			
C	-1.903488	2.264246	1.544447	C	1.273004	-3.470515	0.724926
C	-0.165533	1.586695	1.649937	C	2.079799	-2.121035	-1.183521
C	0.404015	0.957669	0.575169	C	1.969459	-1.070492	-1.966375
H	0.744760	-0.044480	0.347541	H	2.501505	-0.620655	-2.790049
C	-0.811091	2.938325	1.603665	C	1.149200	-2.446590	-0.094171
H	-0.430812	3.954137	1.591130	H	0.299381	-1.766392	0.027990
H	0.003465	1.152526	2.637470	H	2.917045	-2.812160	-1.324737
H	-2.959976	2.110736	1.415740	H	0.738178	-3.884252	1.566860
C	-1.538440	1.462425	-2.554804	C	-2.378471	-4.595931	-0.367739
H	-0.882650	1.419643	-1.714348	H	-1.364392	-4.394158	-0.621455
C	-2.274109	1.511132	-3.501017	C	-3.519491	-4.823268	-0.077391

H	-2.916749	1.555471	-4.346865	H	-4.529770	-5.034499	0.177739
C	3.844104	2.254811	0.279398	C	3.641864	-0.421270	2.092438
H	2.820863	1.966536	0.379242	H	3.013189	-1.189055	1.704753
C	4.992311	2.583904	0.167993	C	4.349062	0.440218	2.535221
H	6.007996	2.882541	0.070073	H	4.975875	1.201029	2.933563
C	5.403706	-1.231427	-0.392162	C	3.608138	2.324951	-0.728389
H	5.123604	-0.216071	-0.225018	H	3.646590	1.578743	0.032525
C	5.724099	-2.371793	-0.580987	C	3.573590	3.167245	-1.581997
H	6.014732	-3.380482	-0.749297	H	3.548138	3.912723	-2.339656
C	0.657603	-2.865793	0.010779	C	-0.053797	3.606683	-0.253436
H	-0.389148	-3.026960	0.130195	H	0.977710	3.417195	-0.444689
C	1.836590	-2.685871	-0.122411	C	-1.214428	3.823474	-0.038996
H	2.883567	-2.524471	-0.240877	H	-2.247152	4.003000	0.151223
C	-2.898397	-4.117079	0.858379	C	-5.260249	3.668543	0.645580
H	-2.560786	-5.094423	1.105746	H	-5.718509	4.617803	0.783366
C	-3.284848	-3.016311	0.580021	C	-4.753409	2.592561	0.491612
H	-3.638924	-2.040862	0.336564	H	-4.298876	1.638467	0.354335
C	-4.589131	0.546980	-0.534071	C	-2.526356	-0.859387	-0.075721
H	-3.892442	0.803777	-1.300484	H	-3.024661	-1.800208	-0.043174
C	-5.373005	0.261226	0.328384	C	-1.939826	0.187001	-0.122491
H	-6.073829	0.007547	1.086870	H	-1.422779	1.119289	-0.165896
TS3				[3]			
							
-188 kJ/mol, ³ A, C ₁				-200 kJ/mol, ³ A, C ₁			
C	1.166350	-3.641802	0.508444	C	0.047596	-1.669944	1.250006
C	2.001603	-2.091175	-1.227185	C	0.059163	-1.131117	-1.175845
C	1.887017	-0.962552	-1.892314	C	0.030602	-0.223224	-2.127838
H	2.424921	-0.412924	-2.649164	H	-0.017938	0.853289	-2.210773
C	1.048852	-2.545816	-0.194899	C	0.023029	-0.801203	0.258543
H	0.195024	-1.876091	-0.036664	H	-0.028882	0.266284	0.502967
H	2.853087	-2.750747	-1.423934	H	0.112385	-2.189520	-1.430594
H	1.276703	-4.533312	1.080697	H	0.030448	-1.638592	2.329981
C	-2.603294	-4.469690	-0.242765	C	0.272396	-5.081174	-0.442741
H	-1.565354	-4.268570	-0.371648	H	0.201380	-4.492196	0.440495
C	-3.771762	-4.695752	-0.096167	C	0.352441	-5.735197	-1.444134
H	-4.806194	-4.904460	0.032809	H	0.423695	-6.317978	-2.330234
C	3.511863	-0.588323	2.109672	C	3.935341	-0.998002	1.108792

H	2.815481	-1.274590	1.687002	H	2.918186	-1.202666	0.866645
C	4.295635	0.181461	2.590741	C	5.080273	-0.774962	1.387630
H	4.989562	0.860856	3.023498	H	6.096234	-0.584639	1.636842
C	3.748067	2.184966	-0.659405	C	4.288479	2.697852	-0.085937
H	3.728777	1.437658	0.101213	H	4.318955	1.682631	0.239086
C	3.777476	3.028055	-1.512472	C	4.263312	3.840089	-0.451279
H	3.808659	3.775192	-2.268310	H	4.248746	4.852345	-0.776121
C	0.124411	3.587987	-0.260391	C	0.451690	3.221276	-0.146295
H	1.149731	3.358785	-0.440544	H	1.517045	3.266077	-0.145791
C	-1.028817	3.850105	-0.057034	C	-0.747837	3.174370	-0.146842
H	-2.055282	4.070358	0.124327	H	-1.813435	3.135883	-0.147205
C	-5.071705	3.908108	0.638759	C	-4.600147	3.498132	-0.423118
H	-5.480176	4.881267	0.765905	H	-4.667871	4.513937	-0.729646
C	-4.621209	2.805656	0.497177	C	-4.532596	2.351257	-0.078265
H	-4.216004	1.827992	0.370741	H	-4.480528	1.331283	0.228622
C	-2.608160	-0.750717	-0.050712	C	-5.037897	-1.201990	1.325028
H	-3.167661	-1.655323	0.003650	H	-6.067525	-1.102581	1.571022
C	-1.952552	0.252409	-0.120793	C	-3.876851	-1.322401	1.049651
H	-1.373914	1.146379	-0.183516	H	-2.844853	-1.436135	0.810575
TS4				[4]			
							
-178 kJ/mol, ³ A, C ₁				-193 kJ/mol, ³ A, C ₁			
C	1.248755	-0.699275	0.450402	C	1.752004	-1.850003	-1.943669
C	2.541545	0.277470	-1.454382	C	-0.625900	-3.905246	2.192100
C	3.678686	-0.207136	-1.887700	C	-0.104465	-3.002527	1.598838
H	4.179061	-1.163295	-1.950018	C	1.585803	0.110838	0.420299
C	1.473367	-0.573916	-0.836099	C	0.971238	0.189280	-0.739709
H	0.822250	-1.118950	-1.531375	C	0.905439	-0.856825	-1.789818
H	2.323277	1.342734	-1.545622	H	2.661681	-2.226446	-1.499465
H	0.556511	-1.233294	1.087474	H	-1.080621	-4.708655	2.719417
C	3.984553	-3.607673	-0.062263	H	0.427170	1.113617	-0.969579
H	3.280506	-2.859918	0.218027	H	0.074181	-0.754742	-2.487907
C	4.778811	-4.445520	-0.385545	H	1.722462	0.733742	1.292740
H	5.482574	-5.189849	-0.669273	H	0.364960	-2.201167	1.075123
C	2.082219	2.302497	2.494714	C	-3.183125	0.130529	-2.128417
H	2.086970	1.355287	2.005062	H	-3.431029	-0.505401	-1.308292
C	2.073870	3.369068	3.043224	C	-2.914038	0.840543	-3.057601

H	2.070698	4.310253	3.537787	H	-2.680105	1.465818	-3.885298
C	0.761082	3.896179	-0.634427	C	-4.901314	-1.735722	0.701478
H	1.094394	3.715841	0.362548	H	-5.885063	-1.400765	0.476783
C	0.393699	4.100648	-1.758155	C	-3.795075	-2.119321	0.962776
H	0.071971	4.287677	-2.754237	H	-2.815460	-2.466866	1.203272
C	-2.562721	1.765110	-0.929058	C	5.092159	-0.399848	-0.761332
H	-1.693925	2.381205	-0.883939	H	4.144856	0.063172	-0.610586
C	-3.545048	1.078543	-0.992028	C	6.155161	-0.928281	-0.929203
H	-4.413508	0.463291	-1.043628	H	7.098313	-1.395077	-1.078245
C	-6.553284	-1.667923	-0.804919	C	-1.601090	3.448636	-0.691545
H	-7.367933	-1.456985	-1.454619	H	-2.234136	2.637976	-0.971282
C	-5.639897	-1.915404	-0.068249	C	-0.884959	4.365697	-0.399081
H	-4.826175	-2.130529	0.584982	H	-0.252092	5.181269	-0.143808
C	-2.248692	-2.266232	2.259086	C	0.406903	2.861501	2.811233
H	-2.186312	-3.146785	2.851919	H	-0.286576	3.034524	2.021201
C	-2.316458	-1.268481	1.595861	C	1.189868	2.671458	3.699486
H	-2.383282	-0.384405	1.002150	H	1.879798	2.504746	4.490927
TS5				[5]			
							
-180 kJ/mol, ³ A, C ₁				-198 kJ/mol, ³ A, C ₁			
C	-3.149804	-2.460307	1.512740	C	-0.753139	-2.580756	-1.368608
C	-0.489565	-3.498894	-2.750642	C	-0.567452	-1.363071	-0.908518
C	-0.799058	-2.815378	-1.814772	C	0.129008	-0.970050	0.336649
C	-1.365782	-0.067210	0.796208	C	0.905174	-1.722536	1.083861
C	-1.116306	-1.013464	1.671778	H	-1.213380	-3.040863	-2.230100
C	-2.003111	-2.147418	2.047890	H	1.488010	-1.604458	1.985534
H	-4.082791	-2.711387	1.065041	H	-0.021804	0.073773	0.629928
H	-0.223489	-4.104785	-3.582755	H	-0.962097	-0.522233	-1.489238
H	-0.153765	-0.984336	2.195220	C	-5.020084	1.486643	-0.225692
H	-1.607217	-2.763683	2.864031	H	-4.813533	0.499318	0.120666
H	-0.895955	0.818228	0.393008	C	-5.262696	2.595507	-0.613509
H	-1.075438	-2.206215	-0.984673	H	-5.486354	3.576788	-0.956223
C	2.892962	-0.360166	1.708393	C	3.708922	2.729959	-0.259963
H	3.047146	-1.059603	0.917428	H	3.736147	3.689833	0.197206
C	2.721473	0.422598	2.601649	C	3.685486	1.647838	-0.778403
H	2.570276	1.113415	3.395888	H	3.671591	0.685600	-1.239912
C	4.166386	-2.799295	-0.938872	C	-0.169480	2.600660	-0.979958

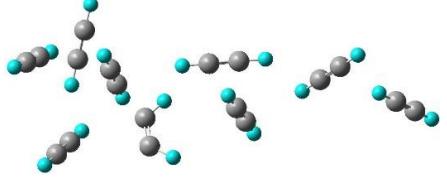
H	5.196542	-2.753444	-0.679723	H	0.891387	2.624272	-1.073329
C	3.006617	-2.857688	-1.240041	C	-1.363839	2.568323	-0.867655
H	1.977771	-2.916105	-1.516094	H	-2.424223	2.535669	-0.762991
C	-4.553275	1.441715	-0.326562	C	-3.976461	-2.147464	0.848289
H	-3.869258	0.746053	0.103308	H	-2.983023	-2.234996	0.472177
C	-5.316954	2.227875	-0.813385	C	-5.095269	-2.056244	1.270942
H	-6.000251	2.919738	-1.242957	H	-6.086291	-1.983088	1.649020
C	3.599372	3.063667	-0.072119	C	3.315954	0.551158	2.997195
H	3.461763	2.172736	0.496805	H	3.487499	0.943027	2.021231
C	3.755569	4.067091	-0.710279	C	3.123200	0.114231	4.097234
H	3.900619	4.955531	-1.275934	H	2.954798	-0.268520	5.074532
C	-0.142484	3.457618	-0.837122	C	4.200633	-1.731767	-2.613758
H	0.916211	3.565770	-0.778819	H	5.086902	-1.559301	-3.175116
C	-1.334438	3.337187	-0.903464	C	3.200396	-1.938069	-1.984563
H	-2.391770	3.220514	-0.958176	H	2.312253	-2.120998	-1.424649
TS6			[6]				
							
-171 kJ/mol, 3A , C ₁				-351 kJ/mol, 3A , C ₁			
C	1.832439	2.690793	-0.435159	C	1.138205	-0.091819	2.281446
C	1.543572	-1.080425	-3.044028	C	1.217852	-1.020715	-2.038279
C	1.649035	-0.044502	-2.416028	C	0.819714	-0.811201	-0.796516
C	1.151477	-0.329130	-0.185773	C	-0.297340	-1.497294	-0.163132
C	0.692207	0.685502	0.528498	C	-0.679952	-1.401900	1.127643
C	0.875085	2.124705	0.266188	C	-0.059498	-0.639245	2.215695
H	2.139945	3.690372	-0.702972	H	1.715081	0.466082	3.003504
H	1.422215	-2.057894	-3.445848	H	1.970595	-0.620917	-2.701929
H	0.093010	0.451558	1.414250	H	-1.574578	-1.946402	1.411453
H	0.124858	2.777041	0.727427	H	-0.690847	-0.540511	3.108422
H	1.039667	-1.396343	-0.053310	H	-0.892146	-2.131967	-0.812709
H	1.822054	0.990657	-2.212406	C	-5.209360	1.315032	-1.198975
C	-3.229231	2.341334	0.153168	H	-6.164951	0.986924	-1.529969
H	-3.024361	1.761508	-0.718647	C	-4.132688	1.691022	-0.827505
C	-3.466258	2.991006	1.133712	H	-3.179084	2.036800	-0.500159
H	-3.679259	3.571975	1.998421	C	-4.254562	-3.409373	0.091653
C	-3.415752	-0.120969	-2.736032	H	-4.266272	-4.451281	0.301711
H	-4.471568	-0.088588	-2.856916	C	-4.245240	-2.234343	-0.148483
C	-2.223862	-0.165869	-2.606726	H	-4.240107	-1.190264	-0.363517

H	-1.163655	-0.213353	-2.500800	C	6.010365	-1.605499	-0.496294
C	4.725956	0.392507	1.048534	H	7.062706	-1.459814	-0.456924
H	3.707653	0.355376	0.736506	C	4.824989	-1.781485	-0.541089
C	5.871455	0.432139	1.400036	H	3.772060	-1.935635	-0.584339
H	6.886883	0.467453	1.711250	C	-1.137900	3.965932	0.234907
C	-2.642237	-0.507080	2.633454	H	-1.513975	4.869183	-0.181575
H	-3.012276	0.305151	2.050568	C	-0.716199	2.947121	0.707915
C	-2.222452	-1.413442	3.297905	H	-0.338655	2.044031	1.131282
H	-1.849833	-2.215560	3.888164	C	2.947684	2.657322	-0.311734
C	-0.874289	-3.591838	0.563342	H	2.169970	3.383321	-0.315168
H	-1.550433	-2.820163	0.848983	C	3.814583	1.828304	-0.304361
C	-0.109111	-4.461969	0.254429	H	4.572384	1.080033	-0.300192
H	0.566906	-5.235780	-0.017794	H	1.353917	-0.060740	-0.207231
TS7				[7]			
							
-330 kJ/mol, ³ A, C ₁				-334 kJ/mol, ³ A, C ₁			
C	0.501167	-0.915303	-0.323207	C	-2.220391	1.378901	-0.867149
C	1.898317	1.963770	0.589694	C	-2.211072	-1.168742	0.857710
C	2.610702	0.921342	0.940882	C	-1.015208	-1.552994	0.458114
C	2.291927	-0.013210	2.048206	C	-0.259613	-1.200249	-0.742665
C	1.385330	-1.000565	2.024618	C	-0.246321	-0.064434	-1.472750
C	0.523328	-1.399625	0.903272	C	-0.994542	1.180676	-1.306932
H	-0.071381	-1.119100	-1.216640	H	-2.872795	2.227988	-0.723009
H	1.939678	2.770882	-0.127157	H	-2.858730	-1.381434	1.696225
H	1.276745	-1.601121	2.922852	H	0.499423	-0.023013	-2.262365
H	-0.166198	-2.223643	1.120770	H	-0.438250	2.072870	-1.624076
H	2.887763	0.110337	2.949838	H	0.471701	-1.951887	-1.025894
C	-1.592412	-4.056641	-1.429573	H	-0.487324	-2.266857	1.104276
H	-0.800080	-4.697509	-1.732194	C	2.204723	3.193356	0.024734
C	-2.487996	-3.335043	-1.089241	H	1.627631	2.889333	0.869053
H	-3.284309	-2.693902	-0.786889	C	2.853157	3.542863	-0.922404
C	-5.647516	-1.351643	-0.011648	H	3.428009	3.858976	-1.759178
H	-6.412817	-2.067763	-0.190317	C	0.454275	2.418093	3.392794
C	-4.789977	-0.538286	0.192738	H	0.973300	3.041825	4.079751
H	-4.033153	0.189979	0.375958	C	-0.137138	1.709740	2.626236
C	-2.804763	2.678681	0.821247	H	-0.665179	1.079703	1.946847
H	-3.669296	3.298047	0.815309	C	-5.479558	-0.399546	-0.702614

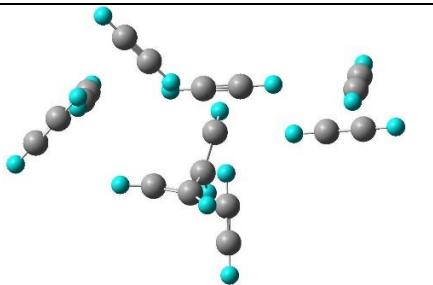
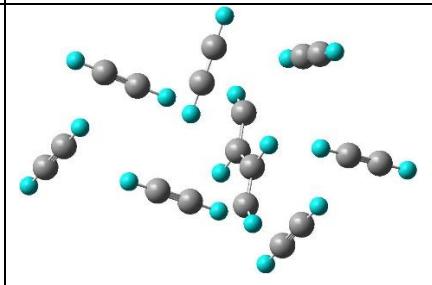
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H	-0.954825	1.368648	0.848809	C	-6.677895	-0.418005	-0.669411
C	5.160143	-2.438664	-1.221820	H	-7.740138	-0.435055	-0.641353
H	6.168414	-2.648136	-1.484598	C	4.076355	-0.066220	-1.154444
C	4.022289	-2.203780	-0.925458	H	3.588093	0.811275	-0.796103
H	3.011061	-1.991498	-0.664042	C	4.633859	-1.043982	-1.569535
C	0.770806	5.221268	-1.988169	H	5.130177	-1.908041	-1.940480
H	1.486998	5.766133	-2.553882	C	2.676155	-3.265414	0.793954
C	-0.042256	4.610587	-1.352677	H	3.136634	-2.384621	0.409278
H	-0.761624	4.064916	-0.787058	C	2.161667	-4.261314	1.220469
H	3.560403	0.733558	0.420687	H	1.710981	-5.146557	1.598857
TS8				[8]			
	-314 kJ/mol, ³ A, C ₁				-579 kJ/mol, ³ A, C ₁		
C	-2.204613	1.364438	-0.867495	C	-2.014414	-2.994925	0.998753
C	-2.715872	0.639437	1.375880	C	-1.200682	-2.024514	1.487378
C	-1.522504	0.181058	1.779369	C	-1.240889	-0.694238	0.826818
C	-0.732770	-0.689457	0.951019	C	-1.595630	-0.679392	-0.615144
C	-0.684948	-0.577969	-0.408974	C	-2.399370	-1.670804	-1.076958
C	-1.251710	0.501322	-1.207333	C	-2.720093	-2.798327	-0.239143
H	-2.655995	2.195753	-1.394301	H	-2.088095	-3.956640	1.497667
H	-3.534340	1.204200	1.797629	H	-0.587143	-2.185034	2.367541
H	-0.006202	-1.239289	-0.938107	H	-2.744174	-1.667766	-2.106936
H	-0.759590	0.642296	-2.175922	H	-3.360688	-3.583468	-0.620636
H	-0.040789	-1.374916	1.432903	H	-1.260086	0.131795	-1.251591
H	-1.068011	0.555385	2.702915	H	-1.624636	0.137744	1.423737
C	3.861161	2.039240	-0.728910	C	2.838446	1.757582	0.660615
H	2.986385	2.373767	-0.218328	H	2.530320	0.757332	0.453259
C	4.852596	1.677277	-1.299135	C	3.196741	2.879046	0.893137
H	5.734933	1.364156	-1.803067	H	3.511929	3.872652	1.103668
C	1.383461	3.994357	1.406262	C	-5.857121	2.163486	-0.577865
H	2.118166	4.633941	1.832367	H	-6.575073	2.947345	-0.593351
C	0.549594	3.276050	0.928662	C	-5.054238	1.272856	-0.561531
H	-0.198857	2.642727	0.507666	H	-4.339727	0.482591	-0.547739
C	-5.362603	-0.620612	-0.932235	C	-1.918989	3.222328	0.000872
H	-4.333652	-0.401876	-0.762347	H	-2.970953	3.237132	-0.162801

C	-6.521466	-0.863206	-1.120980	C	-0.734130	3.186125	0.185000
H	-7.548299	-1.079234	-1.289208	H	0.317445	3.144654	0.348614
C	2.995608	-1.572734	-1.907999	C	2.147883	-2.069096	-0.276396
H	3.306328	-0.591178	-1.628416	H	1.124779	-2.330727	-0.138112
C	2.650948	-2.676110	-2.229654	C	3.302442	-1.782406	-0.433509
H	2.347223	-3.652833	-2.520393	H	4.326199	-1.521284	-0.572067
C	2.438301	-3.202299	1.595401	C	6.254829	0.535265	-0.438361
H	2.723930	-2.891355	0.616997	H	5.530503	1.237845	-0.096346
C	2.114560	-3.555769	2.694580	C	7.065097	-0.260490	-0.823664
H	1.830304	-3.871686	3.668858	H	7.790108	-0.959141	-1.164928

with 6 acetylenes surrounding the reaction center

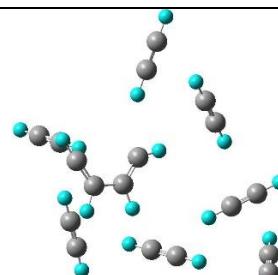
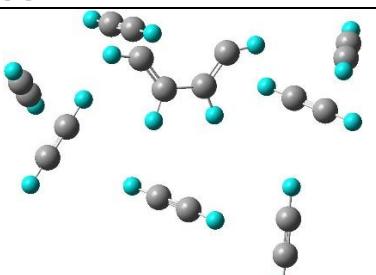
Initial structure				vdW			
							
0 kJ/mol, ³ A, C ₁				-5.01 kJ/mol, ³ A, C ₁			
C	1.616798	1.888854	-1.121387	C	2.799834	-2.671572	-1.306527
H	0.852702	2.609900	-0.938853	C	-2.891593	2.664728	0.335798
C	2.473919	1.076191	-1.336002	C	-2.873571	2.191404	1.579473
H	3.242227	0.361915	-1.524154	H	-2.926490	1.147642	1.906159
C	-4.669292	2.039983	0.026435	C	3.899577	-2.260284	-1.058008
H	-5.504066	2.678895	0.187927	H	4.877322	-1.896782	-0.836325
C	-3.725683	1.321124	-0.156395	H	-2.973788	2.100369	-0.598628
H	-2.894290	0.671466	-0.317512	H	1.822263	-3.035342	-1.524224
C	-1.282308	4.181569	0.280529	C	-1.051894	-3.238176	-1.212288
H	-1.859557	3.630420	1.029061	H	-1.144647	-2.944534	-0.191037
C	-1.505603	4.269620	-1.027079	C	-0.954142	-3.564496	-2.362869
H	-2.309583	3.807724	-1.608074	H	-0.871952	-3.858813	-3.381526
C	-5.513476	-1.959147	0.113928	C	6.960479	-0.227468	0.077837
H	-5.375641	-0.902108	0.108725	H	6.425365	0.611749	0.461037
C	-5.662011	-3.149653	0.118729	C	7.569721	-1.167692	-0.350720
H	-5.796949	-4.204521	0.123664	H	8.117352	-1.997129	-0.728284
C	4.673615	2.044214	1.583318	C	1.596375	0.613680	-0.025780
H	3.807597	2.165032	0.974437	C	0.897551	1.507404	0.367079
C	5.651164	1.901566	2.263472	H	0.258502	2.289650	0.703198
H	6.514721	1.783250	2.872528	H	2.204982	-0.186554	-0.384727
C	-0.759103	-1.097796	-0.708649	C	-3.896117	-0.726041	-1.847240
H	0.110945	-0.499218	-0.854487	C	-4.837081	-0.012800	-1.634166
C	-1.736839	-1.773786	-0.544498	H	-5.671596	0.619365	-1.436658
H	-2.607649	-2.368831	-0.397857	H	-3.065576	-1.366564	-2.031982

C	-9.343965	-1.725728	0.707583	C	-1.864678	-2.065931	2.457374
H	-8.331455	-2.016179	0.549821	C	-0.992704	-1.340868	2.065454
C	-10.48346	-1.398706	0.885115	H	-0.221453	-0.694140	1.713202
H	-11.49400	-1.109632	1.042501	H	-2.636778	-2.705825	2.811265
C	5.625791	-1.564802	-1.532975	C	-6.760155	2.701381	0.117695
H	5.590883	-2.267613	-2.330400	H	-5.829365	2.876886	0.604647
C	5.669503	-0.774462	-0.631076	C	-7.804722	2.499218	-0.435512
H	5.700109	-0.068164	0.167984	H	-8.734861	2.327061	-0.920744
C	9.066166	-2.402711	0.317305	C	4.586073	2.609742	1.322766
H	8.135447	-2.109611	-0.109606	C	5.654528	3.036448	1.661949
C	10.113659	-2.732424	0.797877	H	6.597798	3.421747	1.965690
H	11.042440	-3.025090	1.223573	H	3.633077	2.236508	1.024275
TS1			[1]				
			-2.98 kJ/mol, ³ A, C ₁				-137 kJ/mol, ³ A, C ₁
C	0.291953	-2.765104	2.943917	C	-0.719292	-0.978838	0.033217
C	-0.338508	1.751446	-0.938150	C	-0.777701	-0.707742	-1.466670
C	-0.372448	0.969978	-2.014485	C	-1.755798	0.176829	-2.042835
H	-0.409872	-0.123489	-2.050840	H	-1.973679	0.523822	-3.045498
C	0.551698	-2.667137	4.110826	C	0.232046	-0.231101	-0.408936
H	0.781795	-2.586701	5.145687	H	1.094522	0.398834	-0.256422
H	-0.328845	1.471691	0.120076	H	-0.470781	-1.516783	-2.139077
H	0.060188	-2.852944	1.906796	H	-1.254880	-1.453372	0.840498
C	-4.717082	-1.369712	0.316740	C	-4.950427	-1.500648	-1.259847
H	-4.800357	-0.546886	-0.356694	H	-4.058057	-0.975315	-1.519879
C	-4.628474	-2.291301	1.079522	C	-5.954703	-2.089580	-0.970907
H	-4.556704	-3.104336	1.761028	H	-6.849129	-2.607991	-0.722622
C	0.997824	1.006255	2.795786	C	-2.610441	3.492402	-0.651730
C	1.131510	2.165163	2.514144	H	-2.278634	2.509225	-0.899787
H	1.245592	3.193003	2.258271	C	-2.995453	4.595420	-0.380070
H	0.880715	-0.022347	3.050417	H	-3.343788	5.571532	-0.142694
C	-1.194529	-2.641692	-0.593062	C	0.409377	5.095755	1.263522
C	-0.061375	-2.870396	-0.918364	H	-0.457497	4.730110	0.761338
H	0.943628	-3.077021	-1.211038	C	1.378918	5.515372	1.831604
H	-2.202193	-2.442230	-0.304797	H	2.234888	5.891548	2.337746
C	-5.437177	1.557740	-2.139709	C	3.743143	1.484799	-0.051031
C	-4.244603	1.621470	-2.029527	H	4.365379	0.675734	-0.358689
H	-3.184923	1.680718	-1.934303	C	3.047296	2.398576	0.297141

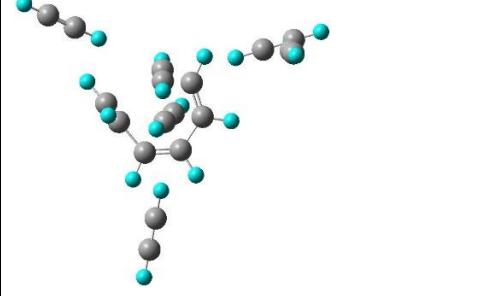
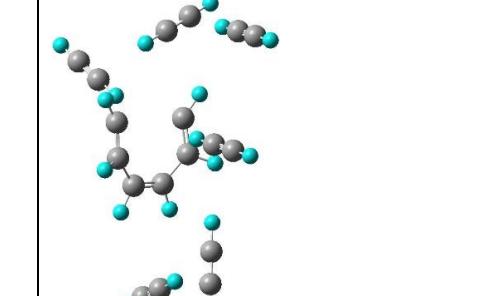
H	-6.494268	1.508522	-2.242863	H	2.435094	3.213942	0.608867
C	3.646186	-2.919875	-1.828281	C	2.287903	-3.516143	0.670635
H	3.844922	-1.882286	-1.681098	H	1.590626	-2.744919	0.438380
C	3.430333	-4.087868	-1.996272	C	3.067707	-4.388058	0.935034
H	3.248223	-5.124502	-2.147041	H	3.753167	-5.165297	1.172998
C	3.825783	0.908986	-1.213023	C	6.221634	-1.198481	-1.458188
C	4.939126	0.683410	-1.597181	H	6.954151	-0.593172	-1.935069
H	5.928553	0.492933	-1.936595	C	5.398971	-1.887715	-0.922614
H	2.839224	1.118333	-0.872522	H	4.668720	-2.502773	-0.447942
C	0.841826	5.203230	0.278976	C	-2.655654	-3.260639	2.778235
C	1.341480	5.937482	1.084507	H	-1.981331	-3.536161	3.552591
H	1.784110	6.595855	1.792310	C	-3.422174	-2.955937	1.907461
H	0.399065	4.549238	-0.434965	H	-4.100885	-2.684585	1.131133
TS2	[2]						
							
-106 kJ/mol, ^3A , C_1				-206 kJ/mol, ^3A , C_1			
C	1.909357	-1.671329	1.978644	C	0.000071	1.219649	0.457385
C	0.166585	-1.206173	1.496345	C	0.000032	1.989495	-1.898498
C	-0.210301	-1.192730	0.179168	C	-0.000029	1.716894	-3.184672
H	-0.534637	-0.434439	-0.521789	H	-0.000032	2.261231	-4.116613
C	0.841453	-2.357647	2.177634	C	0.000013	0.974154	-0.836916
H	0.494264	-3.301823	2.583533	H	-0.000056	-0.070156	-1.168860
H	-0.192734	-0.393207	2.130671	H	0.000103	3.034188	-1.571363
H	2.966526	-1.476103	1.961881	H	0.000071	0.655060	1.379692
C	2.369289	-2.649139	-2.034753	C	0.000325	4.984339	0.796289
H	1.568978	-2.406153	-1.372153	H	0.000277	3.988388	1.172139
C	3.267629	-2.922287	-2.781311	C	0.000379	6.102294	0.363454
H	4.056413	-3.170128	-3.449758	H	0.000428	7.095283	-0.015748
C	-3.561707	-2.726777	0.099292	C	-3.921236	1.202496	0.176374
H	-2.563042	-2.360005	0.191182	H	-2.863940	1.268750	0.061231
C	-4.682041	-3.143326	-0.003185	C	-5.111345	1.134918	0.308564
H	-5.672575	-3.519464	-0.091111	H	-6.166624	1.083230	0.427401
C	-5.256294	0.438971	-1.346878	C	-4.414865	-2.581778	-0.461761
H	-4.933187	-0.491819	-0.938257	H	-4.432342	-1.534371	-0.261312
C	-5.626641	1.483131	-1.806791	C	-4.403343	-3.759891	-0.687211
H	-5.963271	2.405506	-2.214507	H	-4.401081	-4.804176	-0.886853
C	-0.655303	2.430955	-1.299380	C	-0.600497	-3.130191	-0.601436

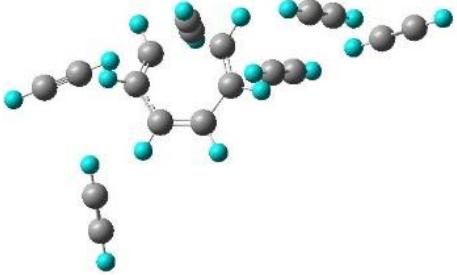
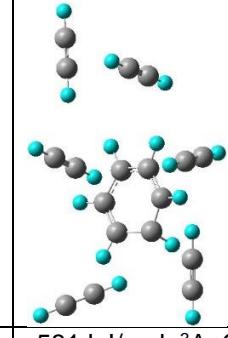
H	0.375837	2.692743	-1.224472	H	-1.667134	-3.135482	-0.607301
C	-1.815728	2.136032	-1.388792	C	0.600200	-3.130258	-0.601394
H	-2.845294	1.870325	-1.472765	H	1.666837	-3.135666	-0.607181
C	2.795863	4.095595	-1.126398	C	4.402978	-3.760440	-0.686530
H	2.431006	5.059688	-1.386871	H	4.400614	-4.804778	-0.885893
C	3.215679	3.011190	-0.832299	C	4.414616	-2.582269	-0.461393
H	3.601185	2.053029	-0.568393	H	4.432195	-1.534811	-0.261219
C	4.857073	-0.531409	-0.150895	C	5.111486	1.134563	0.307918
H	4.357482	-1.163898	-0.850080	H	6.166780	1.082821	0.426606
C	5.419200	0.176243	0.638480	C	3.921363	1.202204	0.175894
H	5.923795	0.802518	1.334164	H	2.864054	1.268515	0.060896
C	-1.535542	2.185378	3.673499	C	-0.000053	-1.018576	3.912983
H	-1.566592	2.060949	4.728571	H	-0.000017	-0.424421	4.794493
C	-1.503423	2.329314	2.483405	C	-0.000096	-1.696845	2.923718
H	-1.475040	2.456332	1.425449	H	-0.000133	-2.298158	2.043287
TS3			[3]				
-189 kJ/mol, 3A_1 , C ₁				-203 kJ/mol, 3A_1 , C ₁			
C	0.047957	-3.559562	1.351658	C	0.001148	1.264256	0.536039
C	1.569042	-2.593211	-0.343247	C	-0.000207	1.888259	-1.869292
C	1.822024	-1.678573	-1.253879	C	-0.001159	1.521265	-3.132298
H	2.626284	-1.398535	-1.918298	H	-0.001805	0.608505	-3.710457
C	0.309719	-2.676782	0.422868	C	0.000313	0.941271	-0.742410
H	-0.434497	-1.913963	0.163419	H	-0.000061	-0.124265	-1.001218
H	2.326017	-3.350277	-0.113223	H	0.000239	2.947565	-1.612400
H	-0.149741	-4.279305	2.111475	H	0.001630	0.744178	1.484671
C	-3.349660	-4.328706	-0.424426	C	0.002026	5.079782	0.575377
H	-2.306952	-4.231280	-0.229588	H	0.000645	4.151074	1.094725
C	-4.523898	-4.436736	-0.642407	C	0.003608	6.120102	-0.020201
H	-5.564119	-4.541116	-0.835567	H	0.005009	7.044349	-0.545180
C	2.173897	-0.632408	3.164704	C	-3.913835	1.232085	0.308743
H	1.577716	-1.269389	2.552810	H	-2.859680	1.316605	0.177755
C	2.841681	0.078416	3.862860	C	-5.100478	1.144432	0.459141
H	3.431193	0.704277	4.488373	H	-6.152813	1.075455	0.594316
C	3.294961	2.242786	0.773864	C	-4.406491	-2.517692	-0.504365
H	3.046030	1.442533	1.434464	H	-4.418595	-1.482066	-0.249242
C	3.578229	3.149637	0.040595	C	-4.402135	-3.682435	-0.791343
H	3.831050	3.955659	-0.605673	H	-4.407238	-4.714853	-1.045358

C	-0.317901	3.682907	0.141866	C	-0.602857	-3.093328	-0.622382			
H	0.715330	3.443364	0.243952	H	-1.669639	-3.098167	-0.626922			
C	-1.480433	3.957691	0.028821	C	0.597920	-3.093929	-0.622780			
H	-2.515653	4.188999	-0.071301	H	1.664694	-3.099826	-0.627992			
C	-5.552315	4.087780	-0.372958	C	4.396329	-3.686967	-0.792619			
H	-5.961439	5.068707	-0.351035	H	4.400050	-4.719435	-1.046463			
C	-5.101714	2.976604	-0.398889	C	4.402229	-2.522185	-0.505824			
H	-4.696087	1.991176	-0.421468	H	4.415729	-1.486536	-0.250861			
C	-3.085622	-0.610551	-0.452544	C	5.102362	1.139314	0.455956			
H	-3.663401	-1.500949	-0.542907	H	6.154675	1.068486	0.590337			
C	-2.411081	0.377005	-0.349361	C	3.915763	1.229057	0.306446			
H	-1.816418	1.257659	-0.257413	H	2.861660	1.315414	0.176244			
C	5.232852	-0.326849	-3.238244	C	0.003840	-1.052995	3.957586			
H	5.566236	-0.928373	-4.048829	H	0.005819	-0.480794	4.853509			
C	4.861865	0.356500	-2.325235	C	0.001622	-1.706649	2.951956			
H	4.530828	0.965126	-1.515454	H	-0.000313	-2.287552	2.058160			
TS4	[4]									
-182 kJ/mol, ³ A, C ₁				-193 kJ/mol, ³ A, C ₁						
C	1.408479	-0.361399	0.766637	C	2.946498	-1.269010	1.620495			
C	2.870875	0.339047	-1.135531	C	2.092244	0.705240	-0.557727			
C	4.051358	-0.172189	-1.382130	C	1.372574	-0.272900	-0.052399			
H	4.568777	-1.111609	-1.247294	C	1.748519	-1.132493	1.097910			
C	1.760238	-0.438818	-0.495350	H	3.402293	-1.806586	2.438171			
H	1.192154	-1.108271	-1.153975	H	0.396877	-0.489783	-0.489016			
H	2.646939	1.370513	-1.412311	H	0.924260	-1.708739	1.535048			
H	0.668121	-0.812096	1.414334	H	3.049732	1.185593	-0.409967			
C	4.216527	-3.218399	1.000634	C	-3.573884	2.584540	0.254285			
H	3.467628	-2.463223	1.053032	H	-2.653828	3.048449	0.529185			
C	5.062605	-4.065247	0.933895	C	-4.611925	2.067557	-0.054841			
H	5.812093	-4.816829	0.878006	H	-5.528063	1.600744	-0.333728			
C	1.790377	2.987735	2.291557	C	-0.425424	4.568638	1.352521			
H	1.907083	1.970533	1.992553	H	-0.874972	5.457546	1.724196			
C	1.656088	4.132039	2.625093	C	0.090494	3.569218	0.935742			
H	1.541014	5.143801	2.930897	H	0.555236	2.683358	0.566126			
C	0.699615	3.862331	-1.181491	C	5.109260	-2.101836	-1.225739			

H	0.947774	3.911209	-0.145221	H	4.255113	-1.966940	-0.601939
C	0.428877	3.807022	-2.349099	C	6.074181	-2.251854	-1.922163
H	0.195564	3.763695	-3.385658	H	6.925877	-2.392381	-2.542720
C	-2.489678	1.635479	-1.019993	C	-2.737222	-0.915772	-1.118040
H	-1.630970	2.245325	-1.189479	H	-2.978087	0.051980	-0.736150
C	-3.462427	0.956478	-0.834364	C	-2.476156	-2.001923	-1.557620
H	-4.323301	0.352511	-0.658515	H	-2.237622	-2.960122	-1.952960
C	-6.374444	-1.616538	0.205827	C	-6.531583	-0.834607	-1.525844
H	-7.206503	-1.594397	-0.455656	H	-5.561809	-1.259844	-1.639552
C	-5.441435	-1.652170	0.958555	C	-7.622246	-0.353327	-1.396301
H	-4.610241	-1.680192	1.624628	H	-8.593351	0.064983	-1.285618
C	-2.006720	-1.304670	3.211755	C	5.740790	2.706959	-0.407704
H	-1.904500	-2.013511	3.997773	H	5.621278	3.726122	-0.130125
C	-2.117406	-0.498726	2.329869	C	5.880544	1.557959	-0.721702
H	-2.220253	0.213395	1.542977	H	5.998760	0.536007	-1.000335
C	-1.259218	-1.667225	-2.710181	C	-1.753414	-2.992347	2.088682
H	-1.800228	-0.856510	-2.279027	H	-2.185336	-2.533636	1.229606
C	-0.650018	-2.579050	-3.195597	C	-1.268576	-3.511450	3.054802
H	-0.113310	-3.388541	-3.627584	H	-0.844396	-3.972316	3.913636
TS5				[5]			
							
-182 kJ/mol, ³ A, C ₁				-200 kJ/mol, ³ A, C ₁			
C	3.665411	0.164575	2.666549	C	0.939814	2.010475	0.528332
C	3.954929	2.676467	-1.735691	C	0.389190	0.847981	0.252163
C	3.417336	1.910625	-0.985122	C	-0.687373	0.160517	0.999312
C	1.375414	-0.737546	0.830812	C	-1.455881	0.670249	1.935524
C	1.309942	0.114219	1.828050	H	1.711509	2.642489	0.112628
C	2.412356	0.515612	2.742808	H	-2.275022	0.335453	2.554769
H	4.688103	-0.122643	2.592618	H	-0.850648	-0.880602	0.702691
H	4.438381	3.349625	-2.401593	H	0.745663	0.302355	-0.628588
H	0.345138	0.595302	2.025915	C	3.975041	-3.158733	-0.503194
H	2.091882	1.184513	3.550534	H	3.992641	-2.356795	0.198737
H	0.726695	-1.166741	0.080809	C	3.965253	-4.063145	-1.290871
H	2.939773	1.227542	-0.320085	H	3.963975	-4.866478	-1.987363
C	-1.966773	2.191659	0.688574	C	-4.611339	-1.361095	-1.874403
H	-1.332583	2.893297	0.195150	H	-4.986576	-2.345278	-2.021525
C	-2.683556	1.409619	1.250797	C	-4.194247	-0.247478	-1.712305

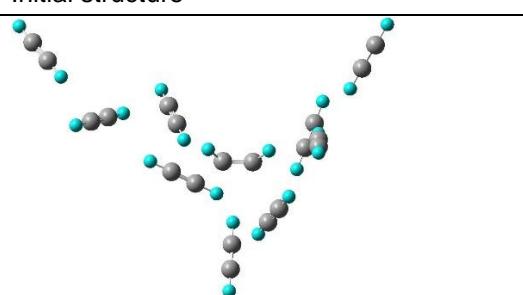
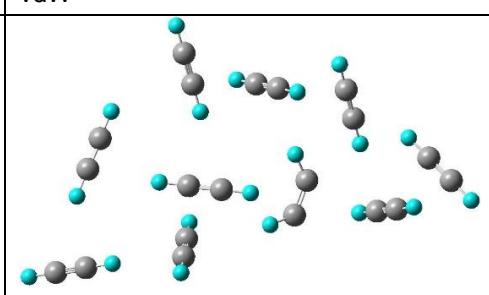
H	-3.326258	0.714672	1.740928	H	-3.830052	0.745637	-1.569771
C	-0.389698	5.184421	-1.094300	C	-0.745519	-2.196258	-2.016228
H	-1.243634	5.815699	-1.042235	H	-1.731381	-1.832090	-2.190112
C	0.578678	4.479162	-1.157281	C	0.364951	-2.603465	-1.813532
H	1.444480	3.858819	-1.217600	H	1.351129	-2.963534	-1.629343
C	3.587190	-3.587158	-0.054223	C	3.810657	-0.063396	1.978665
H	3.229771	-2.710077	0.435187	H	2.806478	0.277836	1.867483
C	3.984821	-4.573068	-0.609291	C	4.944074	-0.438039	2.100966
H	4.344379	-5.446924	-1.096323	H	5.947051	-0.771158	2.220188
C	-3.782507	-0.230477	-1.909664	C	-4.778611	-1.224792	2.058941
H	-3.290024	0.493565	-1.300431	H	-4.717625	-1.044192	1.010505
C	-4.342446	-1.047126	-2.587534	C	-4.848809	-1.431078	3.238196
H	-4.839560	-1.763003	-3.196986	H	-4.915228	-1.616762	4.282723
C	-0.740339	-2.639004	-2.056704	C	4.405721	3.764128	-1.083859
H	-1.661948	-2.132682	-2.227166	H	4.225886	4.584076	-1.736115
C	0.297271	-3.209733	-1.864409	C	4.615428	2.839398	-0.349826
H	1.221241	-3.708052	-1.683923	H	4.798249	2.017459	0.302515
C	-5.207934	-1.354833	1.414699	C	-3.506401	3.549445	-1.489418
H	-5.086282	-1.371015	0.356364	H	-4.303322	3.934435	-2.078470
C	-5.340728	-1.332461	2.606384	C	-2.603877	3.126323	-0.822011
H	-5.465745	-1.321606	3.662111	H	-1.801161	2.750925	-0.229663
TS6	[6]						
	-175 kJ/mol, ³ A, C ₁			-355 kJ/mol, ³ A, C ₁			
C	0.819906	-1.371101	0.695794	C	1.124775	-0.388472	1.542753
C	1.140257	-0.140904	-3.156715	C	0.005102	-0.658517	-2.704601
C	0.870408	0.370901	-2.086408	C	-0.067309	-0.604807	-1.387071
C	-1.219411	-0.387207	-1.404468	C	-0.999843	-1.375911	-0.576721
C	-1.375505	-1.344666	-0.507957	C	-1.015265	-1.466239	0.769615
C	-0.357689	-1.884313	0.414423	C	-0.084490	-0.876085	1.737286
H	1.684366	-1.612014	1.296769	H	1.924699	0.033648	2.132754
H	1.200523	-0.682398	-4.070510	H	0.574256	-0.168519	-3.480986
H	-2.363833	-1.807443	-0.424484	H	-1.823047	-2.041375	1.210566
H	-0.642726	-2.815158	0.918740	H	-0.451547	-0.878304	2.772022
H	-1.905736	0.036116	-2.124094	H	-1.771738	-1.910578	-1.121399
C	-5.325713	2.007287	-0.898347	C	-5.899050	1.388564	-0.163655

H	-6.168910	2.090348	-1.540597	H	-6.921148	1.135589	-0.310917
C	-4.372413	1.921340	-0.175205	C	-4.747370	1.680170	0.001301
H	-3.525956	1.849500	0.469131	H	-3.727037	1.951651	0.147151
C	4.434829	-2.420233	2.556865	C	5.099815	-0.018406	3.075812
H	4.291003	-2.984423	3.446154	H	5.304380	0.381711	4.039073
C	4.603929	-1.783156	1.555059	C	4.875532	-0.470391	1.988006
H	4.756058	-1.216112	0.665590	H	4.677471	-0.870625	1.020609
C	-5.446157	-2.998555	-0.027080	C	-4.721829	-3.455792	0.328309
H	-5.523170	-4.057712	0.017362	H	-4.659970	-4.514495	0.400014
C	-5.363772	-1.803219	-0.077241	C	-4.795719	-2.261591	0.245270
H	-5.291306	-0.740734	-0.123904	H	-4.863427	-1.200341	0.170147
C	5.805956	0.466388	-1.430278	C	5.063711	-1.532241	-1.757128
H	6.804546	0.648703	-1.113441	H	6.124933	-1.486642	-1.807962
C	4.682519	0.257414	-1.796627	C	3.866736	-1.594142	-1.704343
H	3.682599	0.077618	-2.123427	H	2.803382	-1.649676	-1.664176
C	-1.885215	2.345929	2.755443	C	-1.606835	3.866889	0.599124
H	-2.347472	3.196335	3.195839	H	-2.101253	4.778317	0.363251
C	-1.366490	1.380158	2.267079	C	-1.051197	2.839027	0.871738
H	-0.902522	0.521279	1.835935	H	-0.554727	1.927439	1.116105
C	1.732149	2.860900	0.928170	C	2.003802	2.782389	-1.390817
H	0.823920	2.999606	1.466212	H	1.171600	3.397555	-1.143263
C	2.755359	2.687925	0.326402	C	2.937205	2.077826	-1.656799
H	3.662102	2.520707	-0.205214	H	3.758294	1.440785	-1.884936
H	0.968844	0.986460	-1.219518	H	0.608249	0.080230	-0.866531
TS7				[7]			
							
-333 kJ/mol, ³ A, C ₁				-335 kJ/mol, ³ A, C ₁			
C	0.059964	-0.624483	0.838537	C	1.062653	0.421422	0.206063
C	-0.466114	2.577290	-0.031630	C	-0.009806	-0.510545	-2.512249
C	-1.543521	1.831076	-0.029539	C	-1.144037	-0.960527	-2.014854
C	-1.908830	0.830589	-1.062882	C	-1.470320	-1.410083	-0.662844
C	-1.422192	-0.413915	-1.173833	C	-0.988050	-1.017057	0.536665
C	-0.447590	-1.072893	-0.293252	C	0.013195	-0.008520	0.878274
H	0.767177	-1.000141	1.563984	H	1.854136	1.142410	0.359791
H	-0.021617	3.361777	0.563439	H	0.344809	-0.176016	-3.476229
H	-1.797290	-1.026194	-1.988246	H	-1.482769	-1.454336	1.399487

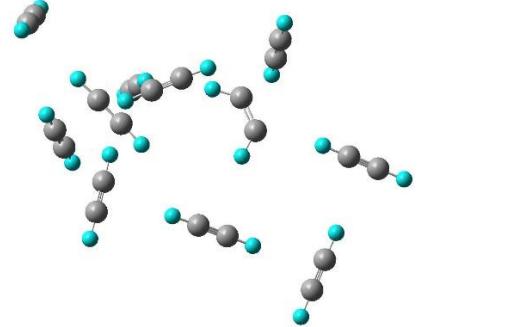
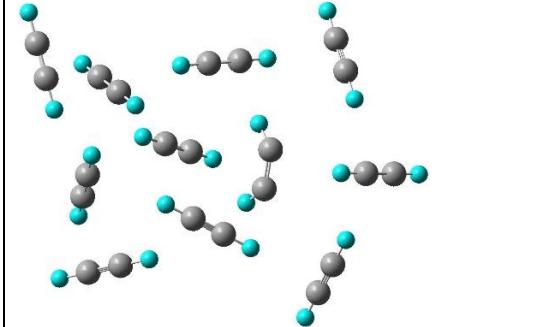
H	-0.136179	-2.074183	-0.612939	H	-0.141284	0.441572	1.868583
H	-2.675471	1.142135	-1.768251	H	-2.295784	-2.115434	-0.621850
C	1.276315	-4.278863	1.667004	H	-1.984857	-1.039255	-2.717332
H	0.422342	-4.626520	2.196049	C	3.467658	3.564048	0.818150
C	2.241346	-3.889525	1.070580	H	2.801665	4.382281	0.687157
H	3.099581	-3.544654	0.540364	C	4.222187	2.643382	0.965444
C	5.517073	-3.055550	-0.839028	H	4.891749	1.823571	1.094328
H	6.050745	-3.970998	-0.751834	C	-6.414487	0.906071	0.604485
C	4.921188	-2.019682	-0.941924	H	-7.358348	0.531458	0.919436
H	4.397784	-1.095683	-1.036701	C	-5.353142	1.335209	0.246212
C	-6.073434	-0.266027	-2.415956	H	-4.415964	1.729222	-0.076060
H	-6.527974	-0.097923	-3.361882	C	6.729897	-0.237288	1.744939
C	-5.563450	-0.456883	-1.347554	H	7.412129	0.215717	2.422917
H	-5.111034	-0.625945	-0.397588	C	5.964366	-0.756803	0.981378
C	3.930653	1.623120	-1.517345	H	5.287218	-1.223245	0.301850
H	4.916748	1.901446	-1.802396	C	-4.205562	-3.387212	1.900396
C	2.815461	1.309292	-1.203720	H	-3.904824	-4.363106	2.195614
H	1.820641	1.042479	-0.925852	C	-4.548942	-2.286849	1.568902
C	-4.699782	-0.879340	2.449671	H	-4.855516	-1.309399	1.273419
H	-5.696258	-0.845584	2.818810	C	4.216538	-2.746638	-1.774448
C	-3.573130	-0.918015	2.039478	H	5.074958	-3.304731	-2.060692
H	-2.570373	-0.951656	1.678118	C	3.242559	-2.121682	-1.458386
C	2.315165	5.342146	1.742459	H	2.373268	-1.567648	-1.184382
H	1.998196	6.121673	2.391862	C	-2.688672	3.729337	-1.059205
C	2.679377	4.465184	1.010231	H	-3.359228	4.553503	-1.096943
H	2.998536	3.684259	0.359455	C	-1.928346	2.802251	-1.019434
H	-2.286543	1.984591	0.765837	H	-1.247501	1.982334	-0.986041
TS8			[8]				
							
-317 kJ/mol, ³ A, C ₁			-581 kJ/mol, ³ A, C ₁				
C	0.951213	-0.010302	-0.918998	C	0.740385	0.155126	-1.277139
C	-0.647352	-1.327189	-2.147317	C	0.017022	-0.539608	-2.194775
C	-1.684562	-1.321499	-1.298611	C	-1.222547	-1.208419	-1.724360
C	-1.514325	-1.608781	0.101163	C	-1.233022	-1.664844	-0.311789
C	-0.416007	-1.213425	0.807644	C	-0.491621	-0.958540	0.580411
C	0.632799	-0.318301	0.335569	C	0.432737	0.045220	0.124362

H	1.679017	0.678195	-1.330136	H	1.601315	0.745046	-1.576490
H	-0.491738	-1.231129	-3.211898	H	0.290806	-0.553584	-3.244505
H	-0.409655	-1.417469	1.873855	H	-0.534143	-1.193749	1.639285
H	1.158419	0.222030	1.130197	H	1.032790	0.593409	0.839956
H	-2.353789	-2.029478	0.647857	H	-1.867043	-2.486582	0.002290
H	-2.670709	-0.977381	-1.629270	H	-2.161703	-0.773916	-2.084943
C	2.357188	3.273067	0.601120	C	2.326624	3.479156	0.652369
H	1.437112	3.802493	0.528648	H	1.478367	4.118964	0.599705
C	3.389855	2.667569	0.679741	C	3.279201	2.752371	0.711363
H	4.304293	2.124072	0.748040	H	4.122651	2.102520	0.763303
C	-5.787667	0.637480	-1.248084	C	-5.675289	0.455033	-0.844282
H	-6.622903	0.030273	-1.501731	H	-6.439619	-0.239384	-1.097441
C	-4.847116	1.327080	-0.966542	C	-4.815371	1.242337	-0.561959
H	-4.012079	1.944244	-0.723693	H	-4.055580	1.948847	-0.317242
C	6.805284	0.794579	1.071572	C	6.466716	0.538462	1.050318
H	7.424106	1.559244	1.474885	H	7.159886	1.260885	1.408100
C	6.114258	-0.074246	0.617161	C	5.691599	-0.283402	0.647070
H	5.506411	-0.852099	0.213322	H	5.010286	-1.021802	0.289272
C	-5.042665	-2.348328	2.663853	C	-4.373862	-3.055805	2.415804
H	-5.002218	-3.165003	3.343006	H	-4.294198	-3.956008	2.975288
C	-5.091061	-1.425551	1.899609	C	-4.465910	-2.038833	1.787081
H	-5.137185	-0.608339	1.217434	H	-4.551632	-1.136766	1.226537
C	4.635013	-3.292000	-0.913012	C	4.037174	-3.521596	-0.550383
H	5.549483	-3.827993	-0.995250	H	4.907379	-4.107772	-0.378599
C	3.598421	-2.694903	-0.823892	C	3.050744	-2.867851	-0.746203
H	2.676251	-2.164897	-0.746190	H	2.172186	-2.292024	-0.926029
C	-1.977058	3.920257	-0.199125	C	-2.199900	4.211419	0.157709
H	-2.470107	4.853613	-0.070723	H	-2.746288	5.116959	0.267774
C	-1.418106	2.868346	-0.344554	C	-1.580598	3.191531	0.032593
H	-0.913381	1.936524	-0.472141	H	-1.029937	2.284422	-0.075404

with 7 acetylenes surrounding the reaction center

Initial structure			vdW				
							
0 kJ/mol, 3A_1 , C ₁				-4.48 kJ/mol, 3A_1 , C ₁			
C	-2.456257	-2.650633	-1.766010	C	-5.254074	-1.078858	1.081848
H	-1.962136	-3.571305	-1.548929	H	-5.084330	-0.324892	0.345629
C	-3.014283	-1.616047	-2.010607	C	-5.455737	-1.922526	1.911118

H	-3.513993	-0.697934	-2.217409	H	-5.631687	-2.671266	2.645494
C	2.975730	0.073305	1.956379	C	2.416116	2.360845	0.222501
H	3.525415	0.193987	2.858783	H	2.769543	1.575807	-0.406755
C	2.350218	-0.062386	0.941295	C	2.013814	3.244029	0.927923
H	1.804981	-0.175234	0.031133	H	1.652988	4.024638	1.553389
C	-0.568684	-3.326820	3.178156	C	-1.060297	0.004917	-2.167502
H	-1.313327	-2.525524	3.128673	H	-1.048364	-0.772678	-1.396329
C	0.719411	-3.280290	2.849993	C	-0.650452	1.268546	-2.081359
H	1.295901	-2.431952	2.466881	H	-0.211646	1.785560	-1.221341
C	4.960263	1.478435	-1.249609	C	5.989580	3.324991	1.337731
H	4.480658	1.117938	-0.368141	H	4.938514	3.247088	1.177422
C	5.493161	1.881658	-2.246085	C	7.171954	3.416255	1.517459
H	5.968118	2.239917	-3.127554	H	8.218944	3.507953	1.677982
C	-3.318904	-0.872859	1.638050	C	-1.695530	-2.631515	0.810078
H	-3.156534	-1.459373	0.762459	H	-2.698548	-2.337131	1.016719
C	-3.504947	-0.202680	2.615747	C	-0.566697	-2.969663	0.588316
H	-3.669474	0.386751	3.485522	H	0.434800	-3.276679	0.388498
C	0.654703	-0.439578	-2.581273	C	-5.740342	1.801761	-1.189620
H	-0.285669	-0.929627	-2.473177	H	-6.740417	1.914915	-0.840164
C	1.712366	0.111962	-2.711310	C	-4.612334	1.663458	-1.574653
H	2.652410	0.600101	-2.821552	H	-3.610726	1.541350	-1.916287
C	8.161760	2.661333	0.605984	C	2.974728	-0.188168	-2.614129
H	7.387112	2.410472	-0.080701	H	2.042233	-0.078452	-3.116002
C	9.033577	2.943604	1.378765	C	4.021997	-0.300489	-2.038389
H	9.806895	3.194067	2.063417	H	4.942234	-0.404730	-1.510261
C	-4.789651	2.107712	-1.927107	C	3.067281	-3.631498	-0.636385
H	-5.022110	2.519453	-2.879760	H	3.101026	-2.757177	-1.245853
C	-4.528033	1.649177	-0.849642	C	3.032273	-4.613776	0.051628
H	-4.292306	1.236170	0.104656	H	2.999301	-5.487619	0.656707
C	-6.171894	4.921672	0.517807	C	5.947375	-1.566864	0.887356
H	-5.764993	4.105455	-0.032198	H	5.605734	-2.566324	0.756325
C	-6.629870	5.840462	1.136630	C	6.316507	-0.435539	1.040348
H	-7.035933	6.655364	1.684870	H	6.629638	0.572876	1.186246
C	-0.623026	-6.013890	-1.225212	C	-8.596794	0.727528	1.027675
H	-0.784602	-6.533334	-2.138782	H	-7.903613	-0.013835	1.351078
C	-0.432550	-5.438347	-0.190148	C	-9.374973	1.563275	0.661553
H	-0.258963	-4.930124	0.731001	H	-10.07199	2.300343	0.343515
with 8 acetylenes surrounding the reaction center							
Initial structure				vdW			

						
0 kJ/mol, 3A_1 , C ₁	-5.14 kJ/mol, 3A_1 , C ₁					
C 2.004584	0.788633	-2.812674	C -3.742030	-2.587763	-0.869229	
C -2.386037	-0.444902	1.202860	H -3.246042	-2.939066	-1.745990	
C -1.432315	-0.753432	2.076754	C -4.304381	-2.195128	0.116322	
H -0.349854	-0.773081	1.914762	H -4.804277	-1.834277	0.986278	
C 1.816168	1.209108	-3.920693	C 1.378007	2.545945	-0.722353	
H 1.648958	1.574693	-4.905479	H 2.403435	2.837254	-0.752670	
H -2.297728	-0.151595	0.152074	C 0.226923	2.206783	-0.686331	
H 2.167975	0.413317	-1.827415	H -0.797666	1.914052	-0.649281	
C 1.340325	3.849754	1.811309	C 1.606747	-2.283901	-1.621524	
H 0.602492	3.676930	2.561177	H 1.141550	-2.434217	-0.641116	
C 2.162679	4.051502	0.960466	C 1.734142	-1.152241	-2.312731	
H 2.884873	4.235931	0.198241	H 1.402267	-0.146179	-2.034082	
C -1.875544	0.260731	-2.796243	C -1.313910	5.552089	0.054868	
C -3.033807	-0.040120	-2.707045	H -0.522308	4.859427	-0.117173	
H -4.064025	-0.305418	-2.636466	C -2.208350	6.327471	0.247984	
H -0.848370	0.528408	-2.887137	H -2.993174	7.023691	0.420100	
C 2.266069	0.252583	0.909101	C -0.688154	-2.596649	1.582169	
C 2.308411	-0.912856	0.621240	H -1.644284	-2.631364	1.112832	
H 2.344552	-1.949316	0.370076	C 0.386358	-2.554069	2.114797	
H 2.224134	1.288657	1.163113	H 1.338588	-2.514065	2.592176	
C -1.372669	3.557640	4.610440	C -3.658842	1.391166	-0.686704	
C -1.609805	2.605716	3.920627	H -3.809323	0.354784	-0.886729	
H -1.822403	1.758523	3.310211	C -3.493238	2.557127	-0.453570	
H -1.170094	4.399931	5.226688	H -3.328717	3.591760	-0.256330	
C 1.749282	-4.498399	-0.643642	C -2.416377	-3.784604	-4.296347	
H 0.758437	-4.424606	-1.023684	H -3.299460	-4.210769	-4.707554	
C 2.865867	-4.590058	-0.214275	C -1.414490	-3.306373	-3.842370	
H 3.858263	-4.675238	0.166766	H -0.521279	-2.882912	-3.444065	
C -6.740218	-1.013050	-1.991506	C -5.431037	0.445470	2.504408	
C -6.774875	-0.893211	-3.184567	H -4.938415	1.119341	1.841970	
H -6.811311	-0.789104	-4.242093	C -5.984317	-0.317423	3.246250	
H -6.714884	-1.120160	-0.930684	H -6.476894	-0.984226	3.911877	
C -5.975491	-1.297700	1.781809	C 5.198228	-1.187490	-0.423654	
C -7.156156	-1.503491	1.830052	H 4.291706	-1.404113	-0.942222	

H	-8.202996	-1.684151	1.881398	C	6.220715	-0.948096	0.157083
H	-4.925422	-1.114970	1.743613	H	7.131389	-0.742272	0.666689
C	4.843362	4.823847	-1.835662	C	4.116131	-2.239267	3.202053
C	4.173899	3.927682	-2.268827	H	4.535728	-1.921699	2.275313
H	3.580107	3.130634	-2.654550	C	3.650962	-2.596092	4.248318
H	5.439615	5.619838	-1.459220	H	3.244096	-2.911887	5.178471
C	6.438163	-4.147177	1.230959	C	5.199900	2.712236	-0.777434
C	6.224996	-5.270000	1.593399	H	5.345570	1.668839	-0.615216
H	6.040000	-6.265036	1.920705	C	5.042790	3.887160	-0.960333
H	6.636348	-3.150996	0.914595	H	4.912846	4.929797	-1.123317

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