

Supporting Information

Gas Phase Formation of Cyclopentanaphthalene (Benzindene) Isomers via Reactions of 5- and 6-Indenyl Radicals with Vinylacetylene

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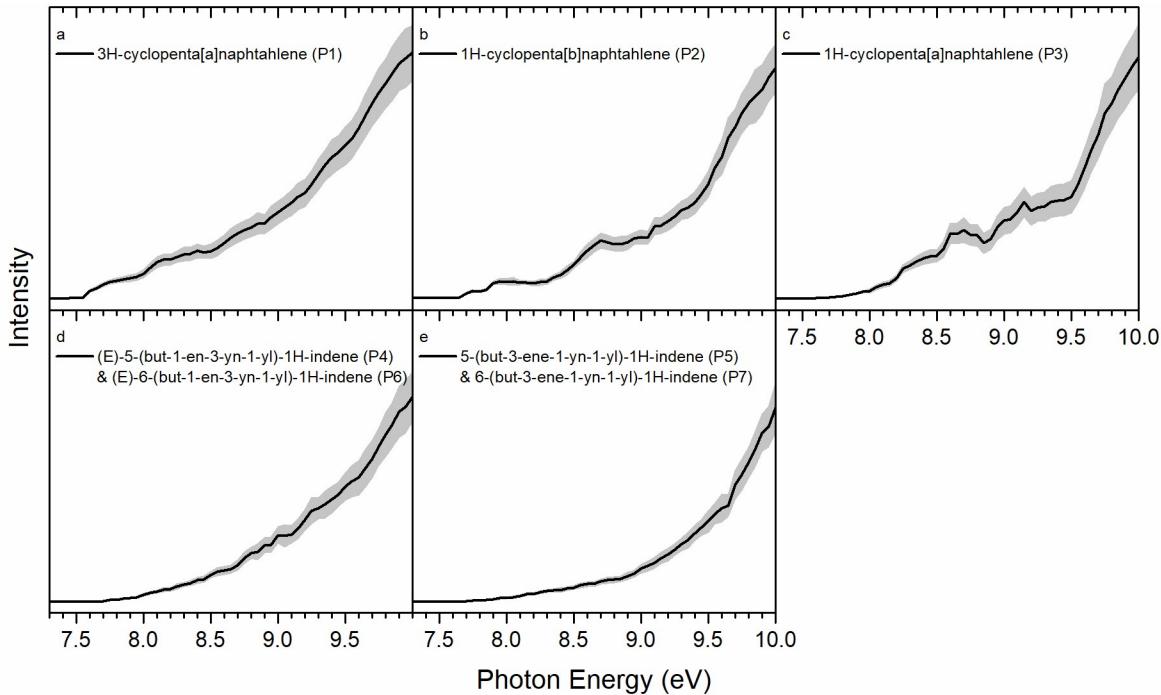


Figure S1. PIE calibration curves for distinct $C_{13}H_{10}$ isomers: a. 3*H*-cyclopenta[*a*]naphthalene (**P1**); b. 1*H*-cyclopenta[*b*]naphthalene (**P2**); c. 1*H*-cyclopenta[*a*]naphthalene (**P3**); d. (E)-5-(but-1-en-3-yn-1-yl)-1*H*-indene (**P4**) and (E)-6-(but-1-en-3-yn-1-yl)-1*H*-indene (**P6**) (as a 40:60 inseparable mixture); and e. 5-(but-3-ene-1-yn-1-yl)-1*H*-indene (**P5**) and 6-(but-3-ene-1-yn-1-yl)-1*H*-indene (**P7**) (as a 40:60 inseparable mixture). The values in the parenthesis indicates the ionization energies. The overall error bars (grey area) consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans.

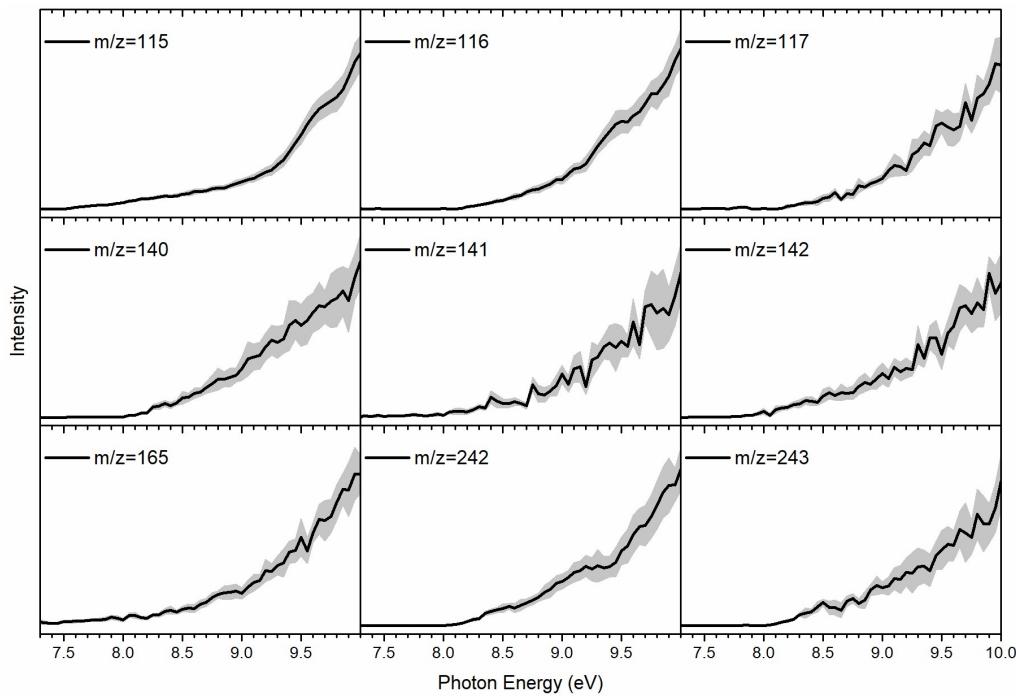


Figure S2. Photoionization efficiency (PIE) curves in the reaction of 5-indenyl ($C_9H_7\cdot$) and vinylacetylene (C_4H_4) along with the experimental errors (gray area). Signal at $m/z = 115$ is 5-indenyl radical produced from the C-I bond scission of the precursor. The H-addition to this radical leads to the formation of indene ($m/z = 116$), along with its ^{13}C -isotopologue at $m/z = 117$. In the high temperature condition, acetylene (C_2H_2) is produced in the pyrolysis process of vinylacetylene, reacting with 5-indenyl radical to produce 5-ethynylindene ($m/z = 140$) after H-elimination. And signal at $m/z = 141$ and 142 might be related to the ^{13}C - and doubly ^{13}C -counterpart. Signal at $m/z = 165$ should be the $C_{13}H_9\cdot$ radical from the H-loss of $C_{13}H_{10}$. Species at $m/z = 242$ and 243 are the precursor and the ^{13}C counterparts.

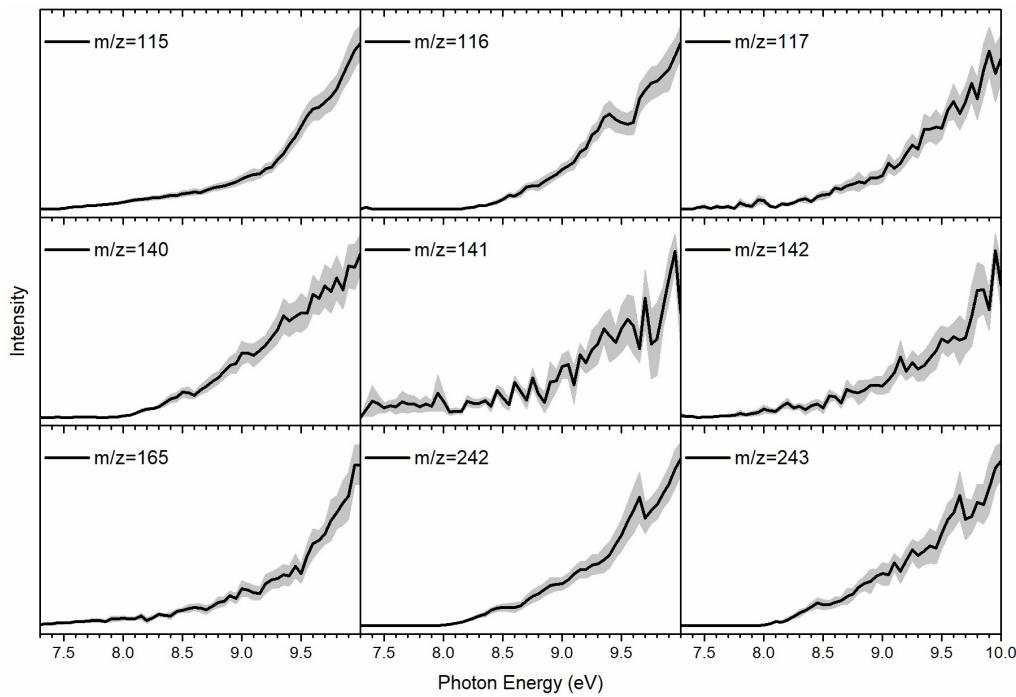


Figure S3. Photoionization efficiency (PIE) curves in the reaction of 6-indenyl ($C_9H_7\cdot$) and vinylacetylene (C_4H_4) along with the experimental errors (gray area). Signal at $m/z = 115$ is 6-indenyl radical produced from the C-I bond scission of the precursor. The H-addition to this radical leads to the formation of indene ($m/z = 116$), along with its ^{13}C -isotopologue at $m/z = 117$. In the high temperature condition, acetylene (C_2H_2) is produced in the pyrolysis process of vinylacetylene, reacting with 5-indenyl radical to produce 5-ethynylindene ($m/z = 140$) after H-elimination. And signal at $m/z = 141$ and 142 might be related to the ^{13}C - and doubly ^{13}C -counterpart. Signal at $m/z = 165$ should be the $C_{13}H_9\cdot$ radical from the H-loss of $C_{13}H_{10}$. Species at $m/z = 242$ and 243 are the precursor and the ^{13}C counterparts.

Synthesis of 5- and 6-iodoindene and calibration compounds **P4**, **P5**, **P6**, and **P7**.

The 5- and 6-iodoindene have been synthesized from 6- and 5-aminoindanone-1 by improving reported protocol.¹ The detailed synthesis and characterization have been published elsewhere.² The calibration compounds (*E*)-5-(but-1-en-3-yn-1-yl)-1*H*-indene (**P4**) and (*E*)-6-(but-1-en-3-yn-1-yl)-1*H*-indene (**P6**) (as a 40:60 inseparable mixture) have been synthesized from 5-iodoindene employing Stille and Sonogashira couplings. Similarly, 5-(but-3-ene-1-yn-1-yl)-1*H*-indene (**P5**), and 6-(but-3-ene-1-yn-1-yl)-1*H*-indene (**P7**) (as a 40:60 inseparable mixture) have been synthesized from 6-iodoindene utilizing Sonogashira couplings (Figure S4). The detailed synthesis and characterization of **P4**, **P5**, **P6**, and **P7** have been recently published.²

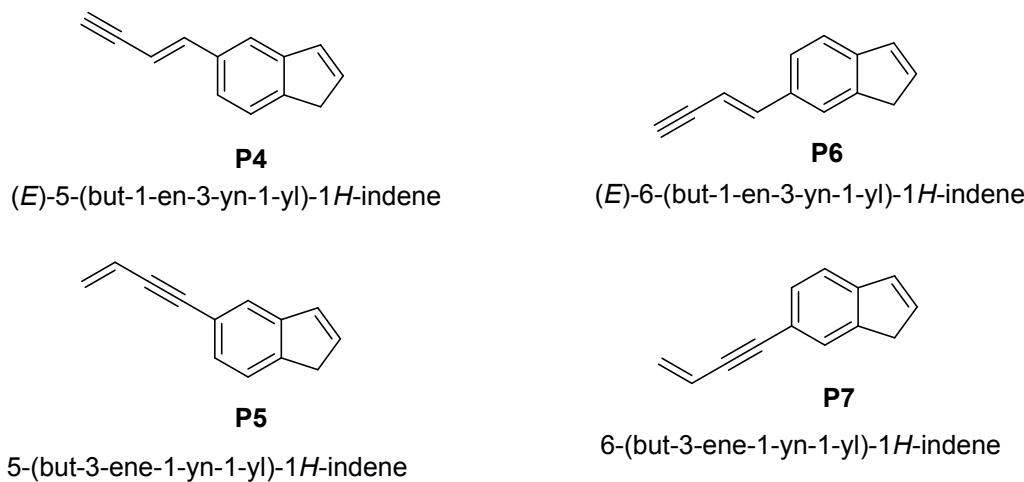
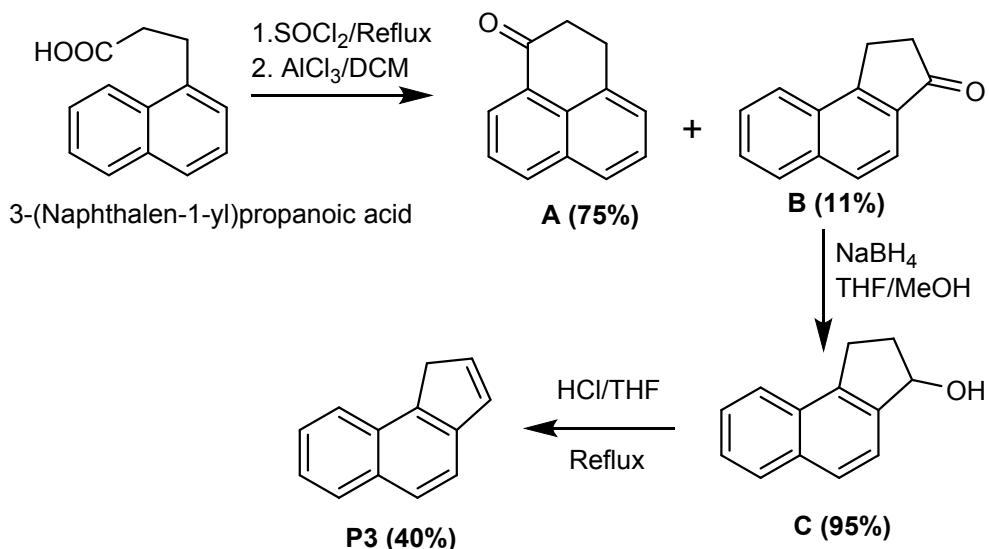


Figure S4. Structure of calibration compounds **P4**, **P5**, **P6**, and **P7**.

Synthesis of 1*H*-cyclopenta[a]naphthalene P3

Acylation of 3-(naphthalen-1-yl)propanoic acid³ with SOCl_2 and cyclization with AlCl_3 provided perinaphthanone-7 **A** (75%) and 1,2-dihydro-3*H*-cyclopenta[a]naphthalene-1-one **B** (11%). Reduction of ketone **B** with NaBH_4 and dehydration of the resulting **C** with HCl gave 1*H*-cyclopenta(a)naphthalene **P3** (**Scheme S1**).



Scheme S1. Synthesis of 1*H*-cyclopenta[a]naphthalene

1,2-Dihydro-3*H*-cyclopenta[a]naphthalene-3-one; B.

3-(Naphthalen-1-yl)propanoic acid³ (1.0 g, 4.99 mmol) was dissolved in SOCl_2 (15 mL) and the solution was refluxed at 85 °C for 1 h. The SOCl_2 was distilled off under reduced pressure. The resulted acid chloride was dissolved in 5 mL of dry dichloromethane and then added dropwise to a cold (-10°C) solution of 1.6 g (12.0 mmol) of aluminum chloride in 30 mL of dry dichloromethane. After stirring for 30 min at 0 °C, the mixture was poured into 100 mL of ice/water and the resulting solution was extracted with dichloromethane. The organic layer was separated, dried over anhydrous Na_2SO_4 , filtered, and evaporated. The residue was column chromatographed (5 → 10 % EtOAc/hexane) to give 2,3-dihydro-1*H*-phenalen-1-one³ **A** (682 mg, 75%) as off-white solid and **B** (100 mg, 11%) as pale yellow solid: ¹H NMR (400 MHz, CDCl_3) δ 8.06 (ddd, $J = 8.0, 2.0, 0.8$ Hz, 1H), 7.95 (dd, $J = 7.2, 1.6$ Hz, 1H), 7.81 (d, $J = 8.4$ Hz, 1H), 7.75 (d, $J = 8.4$ Hz, 1H), 7.71–7.62 (m, 2H), 3.47–3.43 (m, 2H), 2.87 – 2.83 (m, 2H); ¹³C NMR (101 MHz, CDCl_3) δ 206.96, 156.56, 136.69, 134.83, 130.70, 129.33, 129.06, 128.65, 127.21, 124.55, 119.65, 36.30, 24.48.

2,3-Dihydro-1*H*-cyclopenta[a]naphthalene-3-ol; C

NaBH₄ (74 mg, 1.96 mmol) was added to a stirred solution of **B** (90 mg, 0.49 mmol) in dry MeOH/THF (10 mL, 2:1) at 0 °C (ice-bath). After 5 min, the reaction mixture was allowed to warm to rt and stirring was continued for 1 h. Water (2 mL) was then added to quench the reaction. The mixture was concentrated under reduced pressure and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (EtOAc in hexane 20 → 30%) to give **C** (85 mg, 94%) as an off-white solid: ¹H NMR (400 MHz, CDCl₃) δ 7.88 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.85 (ddd, *J* = 7.6, 2.0, 0.8 Hz, 1H), 7.77 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.54 – 7.46 (m, 2H), 5.45 (t, *J* = 6.4 Hz, 1H), 3.43 (ddd, *J* = 16.0, 8.8, 4.8 Hz, 1H), 3.17–3.09 (m, 1H), 2.71 (dddd, *J* = 15.6, 11.6, 6.8, 4.4 Hz, 1H), 2.12 (dddd, *J* = 14.8, 10.4, 6.0, 4.8 Hz, 1H), 1.83 (s, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 141.68, 139.78, 133.85, 130.48, 128.65, 127.84, 126.35, 125.97, 124.66, 122.40, 77.57, 35.63, 28.36.

1*H*-Cyclopenta[a]naphthalene; P3

The secondary alcohol **C** (75 mg, 0.41 mmol) was dissolved in the mixture of THF/H₂O (6 mL, 1:1). Aqueous 4 N HCl (1.0 mL, 4 mmol) was then added and the reaction mixture was refluxed at 105 °C for 12 h. The reaction mixture was transferred to a separatory funnel and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (*n*-hexane) to give **P3** (27 mg, 40%) as a light yellow solid: ¹H NMR (400 MHz, CDCl₃) δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 7.2 Hz, 1H), 7.03 – 7.01 (m, 1H), 6.68 – 6.66 (m, 1H), 3.73 (s, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 142.39, 140.35, 133.80, 132.79, 131.63, 130.24, 128.97, 127.25, 126.29, 124.62, 123.66, 120.65, 38.19.

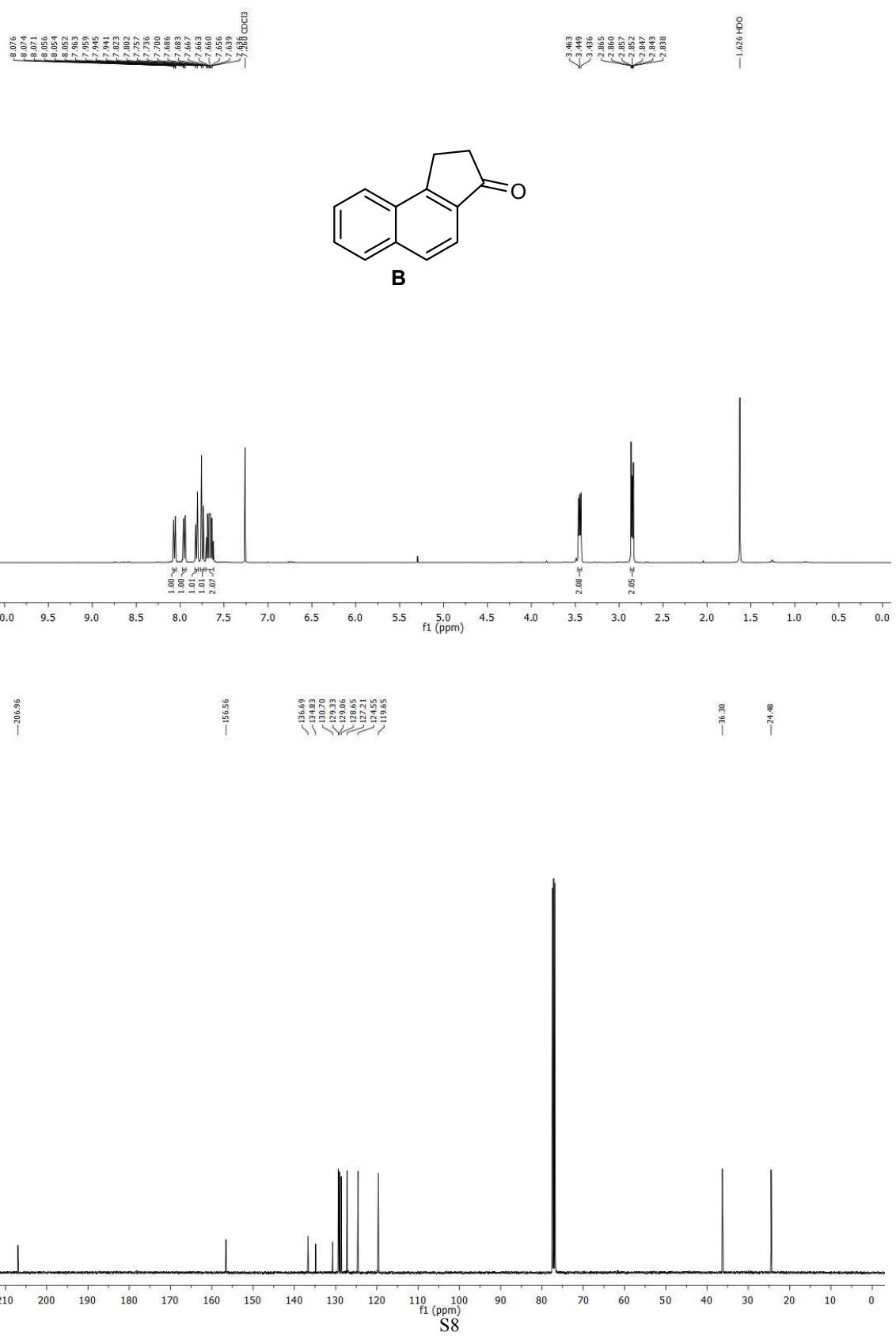


Figure S5. ^1H NMR and ^{13}C NMR spectra of compound **B** in CDCl_3 .

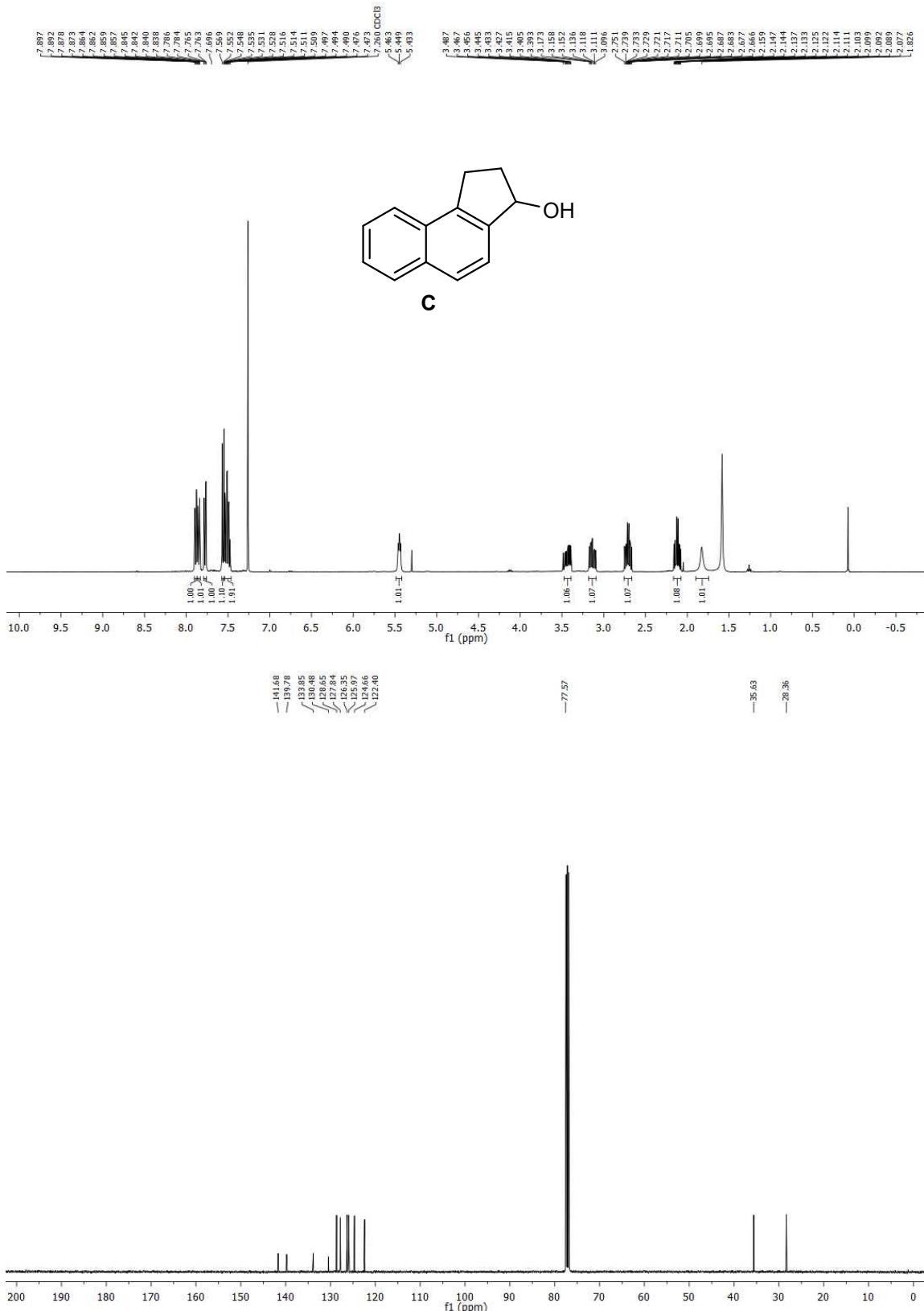


Figure S6. ^1H NMR and ^{13}C NMR spectra of compound **C** in CDCl_3

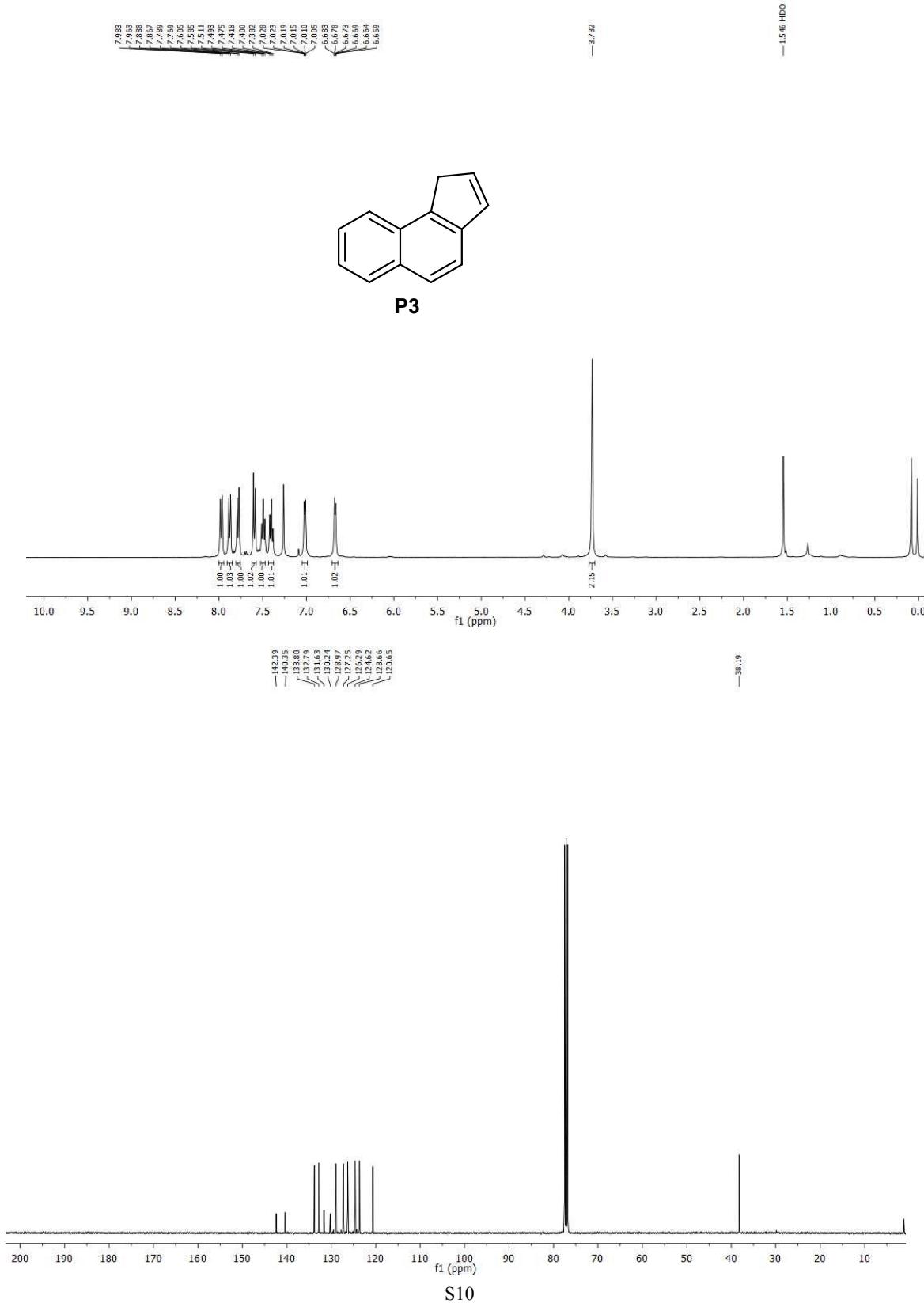


Figure S7. ^1H NMR and ^{13}C NMR spectra of compound **P3** in CDCl_3 .

Optimized Cartesian Coordinates (\AA) and Calculated Vibrational Frequencies (cm^{-1}) for the 5-Indenyl + Vinylacetylene System

Reactants

Vinylacetylene C_4H_4 , C_s , $^1\text{A}'$

6	0	0.121125	-1.700404	0.000000
6	0	-0.579921	-0.557132	0.000000
6	0	0.000000	0.743992	0.000000
6	0	0.453986	1.866353	0.000000
1	0	1.206897	-1.705189	0.000000
1	0	-0.382460	-2.662132	0.000000
1	0	-1.669070	-0.596050	0.000000
1	0	0.873491	2.846518	0.000000

Frequencies

229.5891	339.4361	558.9958
588.1117	631.2114	714.7025
899.2819	944.5974	1013.3805
1122.3708	1335.8813	1463.2716
1690.9964	2223.9797	3158.4122
3178.0551	3263.9634	3495.5663

5-1H-indenyl C_9H_7 , C_s , $^2\text{A}'$

6	0	-0.340876	-0.684507	0.000000
6	0	0.000000	0.685392	0.000000
6	0	1.325254	1.095426	0.000000
6	0	2.342318	0.123184	0.000000
6	0	1.950136	-1.195996	0.000000
6	0	0.658505	-1.668764	0.000000
6	0	-1.802274	-0.794823	0.000000
6	0	-2.347930	0.433727	0.000000
6	0	-1.275313	1.496181	0.000000
1	0	1.586154	2.149465	0.000000
1	0	3.386931	0.413175	0.000000
1	0	0.419882	-2.726900	0.000000
1	0	-2.343252	-1.732589	0.000000
1	0	-3.406242	0.659317	0.000000
1	0	-1.351195	2.149305	0.878439
1	0	-1.351195	2.149305	-0.878439

Frequencies			
193.0636		221.9687	390.3952
391.4342		419.3922	532.9600
546.9856		603.7417	695.8004
734.6857		738.9651	781.4171
827.7034		858.4912	865.7767
928.0563		956.3110	956.3483
964.2426		1041.1762	1086.0045
1124.6772		1148.9166	1170.5416
1205.3139		1238.7476	1287.2114
1320.6399		1376.0584	1417.5719
1438.0175		1458.8385	1564.1300
1620.1414		1633.3490	3015.3295
3038.1201		3152.6851	3164.7501
3174.5852		3190.8419	3213.4939

Intermediates

[i0a] C₁₃H₁₁, C₁, ²A

6	0	-2.413803	0.473979	0.152369
6	0	-1.394140	-0.405553	-0.271135
6	0	-0.117763	0.057977	-0.556227
6	0	0.157350	1.431766	-0.418521
6	0	-0.875500	2.240951	-0.001904
6	0	-2.158958	1.846114	0.295972
6	0	-3.633788	-0.307793	0.372200
6	0	-3.394977	-1.602963	0.102358
6	0	-1.962959	-1.804384	-0.331149
6	0	4.260536	-0.518160	0.830946
6	0	3.396277	-0.252923	1.816116
6	0	3.826817	-0.120138	-1.730197
6	0	4.003282	-0.294555	-0.550864
1	0	0.669654	-0.614756	-0.881557
1	0	1.145962	1.818890	-0.637541
1	0	-2.927261	2.539988	0.619931
1	0	-4.575972	0.111415	0.701899
1	0	-4.111652	-2.410340	0.176577
1	0	-1.900667	-2.233919	-1.338914
1	0	-1.430826	-2.497090	0.332860
1	0	5.237101	-0.933306	1.067952
1	0	2.414668	0.160879	1.618233

1	0	3.659157	-0.447416	2.848826
1	0	3.665595	0.039752	-2.768061

Frequencies

7.9503	14.0869	15.0599
27.9534	40.5263	43.3326
195.1020	222.4223	228.3440
319.3288	390.4235	392.3506
421.5745	532.6202	548.3044
559.3361	604.0084	646.1855
681.8311	696.0756	704.4418
735.0659	738.5748	793.2958
827.8719	858.1796	865.4396
891.9652	934.0723	956.2115
960.6860	964.4556	969.7989
1010.5092	1040.6757	1085.6784
1112.4783	1124.6234	1148.7042
1170.3438	1204.7077	1238.2372
1287.1256	1319.8954	1322.5491
1375.8913	1415.8596	1437.8725
1445.8026	1458.4111	1562.7481
1619.1952	1632.5605	1668.1787
2201.4000	3015.6658	3038.2534
3135.6727	3146.9947	3158.6992
3164.0422	3176.7023	3190.2502
3212.9811	3236.6107	3475.6129

[i0b] C₁₃H₁₁, C₁, ²A

6	0	1.956554	-0.594057	-0.101893
6	0	2.926697	0.412771	0.092960
6	0	2.569518	1.751326	0.162833
6	0	1.213590	2.105650	0.036311
6	0	0.315959	1.080064	-0.151125
6	0	0.599369	-0.263177	-0.230547
6	0	2.637908	-1.891067	-0.130980
6	0	3.959412	-1.709792	0.035809
6	0	4.283792	-0.244003	0.194417
6	0	-3.367705	0.630730	-0.164410
6	0	-4.484900	0.183954	-0.230916
6	0	-5.802952	-0.336074	-0.355905
6	0	-6.534200	-0.804186	0.661030

1	0	3.316744	2.524683	0.312436
1	0	0.903514	3.143106	0.085761
1	0	-0.164296	-1.018456	-0.381070
1	0	2.136211	-2.840576	-0.267124
1	0	4.709988	-2.488898	0.057549
1	0	4.972551	0.105968	-0.584701
1	0	4.772757	-0.038080	1.154834
1	0	-2.379542	1.021590	-0.094003
1	0	-6.218269	-0.339751	-1.360933
1	0	-6.153799	-0.815656	1.675499
1	0	-7.534106	-1.186771	0.496238

Frequencies

4.1975	6.2751	10.2151
20.3332	37.0028	50.2474
193.2095	222.3959	226.3791
321.0334	391.1724	391.3840
419.3702	532.4940	543.9750
557.2327	604.7971	693.0024
694.5777	702.9853	709.0506
734.5147	738.9394	777.7118
828.0454	859.4834	866.0302
892.5266	927.2492	951.9828
956.0291	956.5659	965.0345
1010.4641	1042.4906	1086.0790
1111.7345	1124.9486	1149.4485
1170.7252	1205.9217	1239.4749
1287.7240	1320.1117	1321.0168
1376.3105	1417.8115	1437.7179
1443.2442	1458.8706	1563.8833
1619.4625	1633.3771	1668.0570
2200.4372	3016.0109	3038.9804
3133.4321	3146.0366	3154.5878
3167.8927	3177.0800	3192.2166
3214.5148	3234.8585	3436.0646

[i1] C₁₃H₁₁, C₁, ^2A

6	0	1.709350	-0.631600	-0.031487
6	0	1.907258	0.761988	-0.013615
6	0	0.833326	1.620914	-0.193702
6	0	-0.439666	1.082355	-0.390551

6	0	-0.649950	-0.303698	-0.414497
6	0	0.436073	-1.164395	-0.231046
6	0	3.006643	-1.279969	0.180494
6	0	3.962579	-0.345520	0.323494
6	0	3.373695	1.041143	0.216450
6	0	-2.967770	-0.573553	0.536329
6	0	-2.052173	-0.854287	-0.626320
6	0	-5.286082	0.562651	0.289041
6	0	-4.194865	0.026438	0.411503
1	0	0.970561	2.697495	-0.183876
1	0	0.284693	-2.239439	-0.249538
1	0	3.155440	-2.352036	0.214354
1	0	5.014897	-0.532038	0.492700
1	0	3.821449	1.611227	-0.607426
1	0	3.546003	1.628355	1.127360
1	0	-2.629070	-0.864208	1.526341
1	0	-2.488451	-0.438342	-1.538475
1	0	-1.983717	-1.939563	-0.779087
1	0	-6.235767	1.027191	0.188302
1	0	-1.286545	1.746563	-0.527216

Frequencies

19.1898	24.6641	99.5756
167.2659	195.6223	208.6313
273.1625	333.5220	388.2351
398.2869	412.9301	437.4730
440.4372	487.7944	553.5826
594.2484	607.5389	644.1581
650.9059	715.1717	751.2293
752.6254	775.4405	832.9936
856.0138	875.1782	896.5276
939.6754	945.5221	960.5454
961.9726	968.1893	1024.0670
1091.6673	1138.3501	1143.7370
1147.2101	1156.1514	1187.5556
1204.0527	1239.4310	1258.6515
1294.5096	1313.8051	1344.5907
1379.6060	1401.4142	1436.8149
1463.2378	1474.8897	1501.7280
1601.9483	1629.7418	1653.8693
2013.3749	2995.7770	3014.0799

3036.5019		3065.8727		3150.2805
3154.3204		3155.5169		3172.9620
3188.7274		3212.7094		3469.3721

[i2] C₁₃H₁₁, C₁, ²A

6	0	1.293982	-0.620372	-0.063401
6	0	2.182098	0.468893	0.071297
6	0	1.690722	1.761556	0.139692
6	0	0.310112	1.965227	0.073051
6	0	-0.583625	0.891814	-0.061390
6	0	-0.078190	-0.416865	-0.129518
6	0	2.089505	-1.851272	-0.108185
6	0	3.395852	-1.551864	-0.007991
6	0	3.596094	-0.059628	0.115903
6	0	-2.033744	1.173306	-0.128051
6	0	-2.999540	0.302277	-0.260839
6	0	-4.013282	-0.575132	-0.408303
6	0	-4.706204	-1.202113	0.625856
1	0	2.358783	2.610470	0.243531
1	0	-0.084661	2.974514	0.125522
1	0	-0.762115	-1.252711	-0.231317
1	0	1.670380	-2.844688	-0.207459
1	0	4.213083	-2.261106	-0.012503
1	0	4.213410	0.337924	-0.699723
1	0	4.109056	0.206594	1.048839
1	0	-2.302941	2.230169	-0.056224
1	0	-4.310233	-0.810025	-1.431229
1	0	-4.459367	-1.010604	1.662222
1	0	-5.508072	-1.895493	0.409626

Frequencies

37.3302	51.9800	115.4053
156.1684	198.8267	227.4695
239.2652	333.8724	361.0310
397.6764	434.2973	445.3417
515.2342	544.0238	583.0848
600.9403	611.4748	711.4759
746.3576	748.3893	749.6278
785.5882	796.2849	850.2891
852.7829	908.9120	919.6846
936.0838	940.6584	953.4673

961.9971	965.9968	968.5694
1082.3080	1094.4621	1140.2472
1148.0051	1156.9634	1191.1496
1202.9389	1236.0820	1252.4510
1278.8366	1327.0621	1346.8922
1376.1227	1417.9304	1438.2388
1465.3835	1490.4663	1497.5140
1603.1148	1628.0953	1654.1083
1888.4606	3012.8439	3034.8010
3057.3787	3093.6820	3149.1097
3154.7445	3168.0359	3171.6106
3189.5679	3212.7673	3249.7519

[i3] C₁₃H₁₁, C₁, ²A

6	0	1.571703	-0.668259	-0.170905
6	0	2.148314	0.599564	0.101288
6	0	1.359030	1.738704	0.120656
6	0	-0.013317	1.633497	-0.129517
6	0	-0.621653	0.393707	-0.404915
6	0	0.219896	-0.701367	-0.406476
6	0	2.633158	-1.677657	-0.130378
6	0	3.805834	-1.084261	0.150399
6	0	3.630275	0.405410	0.325708
6	0	-2.109133	0.275618	-0.653059
6	0	-2.862071	-0.307481	0.569100
6	0	-4.299738	-0.425118	0.345242
6	0	-5.480210	-0.510267	0.136319
1	0	1.794645	2.711297	0.324378
1	0	-0.630986	2.526716	-0.120181
1	0	2.472883	-2.733395	-0.303405
1	0	4.761627	-1.582470	0.243980
1	0	4.233292	0.973818	-0.393553
1	0	3.942737	0.737781	1.323703
1	0	-2.523915	1.257968	-0.891614
1	0	-2.293606	-0.368788	-1.516381
1	0	-2.445950	-1.291656	0.809123
1	0	-2.678758	0.326704	1.443300
1	0	-6.524505	-0.590508	-0.040127

Frequencies

26.3390	58.1487	60.8122
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152.2198	191.6722	197.5596
270.7359	329.4724	352.8966
397.2419	421.7177	439.5967
478.8960	546.6679	594.4029
620.8555	663.9575	674.7589
697.0232	747.3365	750.8051
767.7881	784.2304	816.9490
852.7346	928.7575	944.6726
954.4810	958.5765	963.0623
974.1759	1011.2260	1027.1384
1079.1923	1136.2829	1146.4051
1160.0811	1180.4798	1219.9485
1252.5205	1262.8411	1292.1092
1310.5651	1331.9455	1360.1402
1371.6427	1434.5292	1446.8275
1454.0743	1476.7182	1497.7769
1565.2409	1615.3197	1646.6747
2220.2512	3014.5055	3023.6031
3037.9630	3048.1293	3052.3756
3091.6110	3148.8040	3169.9316
3197.7203	3219.5324	3478.1161

[i4] C₁₃H₁₁, C₁, ²A

6	0	-0.940202	-0.465611	0.050457
6	0	-1.683552	0.730445	-0.034588
6	0	-1.044084	1.956753	-0.057570
6	0	0.354395	1.987868	0.013452
6	0	1.106435	0.818648	0.103415
6	0	0.458258	-0.438655	0.118220
6	0	-1.885571	-1.586874	0.037801
6	0	-3.144187	-1.121516	-0.043986
6	0	-3.153271	0.386491	-0.098985
6	0	2.613736	0.866150	0.273815
6	0	3.338402	-0.327765	-0.398614
6	0	2.579314	-1.558119	-0.079203
6	0	1.286190	-1.664589	0.169653
1	0	-1.606101	2.882051	-0.129621
1	0	0.866851	2.944681	0.003861
1	0	-1.605820	-2.631104	0.085320
1	0	-4.043196	-1.723099	-0.069460
1	0	-3.717318	0.822119	0.735535

1	0	-3.624890	0.757678	-1.017644
1	0	3.014785	1.808764	-0.108644
1	0	2.839934	0.835444	1.347864
1	0	3.379445	-0.198968	-1.488969
1	0	4.373272	-0.378062	-0.047512
1	0	0.807862	-2.618863	0.366070

Frequencies

100.8064	122.8722	191.6841
221.0765	239.8362	320.7981
362.9138	398.3263	420.6233
466.0411	487.5212	525.2545
552.7059	616.9461	626.6907
708.0155	718.5461	756.8742
766.9664	819.3274	831.3602
842.7495	874.6128	904.9534
934.4935	950.4602	954.1875
959.8006	961.7809	977.4639
1020.0962	1043.2416	1125.3655
1147.6095	1159.7515	1175.7962
1197.9630	1214.9531	1229.3850
1244.5555	1267.4100	1291.2724
1323.8411	1340.6771	1358.0440
1395.5525	1435.6760	1450.7272
1465.2809	1475.1137	1479.3824
1604.0711	1624.1568	1640.5093
1683.2755	2992.5872	3002.0328
3013.4345	3035.6397	3055.3536
3064.8116	3152.2334	3153.6689
3170.3515	3193.1758	3215.2857

[i5] C₁₃H₁₁, C_s, ²A"

6	0	0.962260	-0.405998	0.000000
6	0	0.578094	-1.755926	0.000000
6	0	-0.763742	-2.110416	0.000000
6	0	-1.724899	-1.094570	0.000000
6	0	-1.372350	0.253468	0.000000
6	0	0.000000	0.632552	0.000000
6	0	2.426113	-0.351308	0.000000
6	0	2.929986	-1.599008	0.000000
6	0	1.817978	-2.617982	0.000000

6	0	-2.459318	1.312404	0.000000
6	0	0.357674	2.018229	0.000000
6	0	-0.627422	3.022483	0.000000
6	0	-1.961741	2.724719	0.000000
1	0	-1.069703	-3.151280	0.000000
1	0	-2.777713	-1.361093	0.000000
1	0	3.011483	0.558680	0.000000
1	0	3.979605	-1.861394	0.000000
1	0	1.865237	-3.274119	0.878406
1	0	1.865237	-3.274119	-0.878406
1	0	-3.119421	1.157344	-0.868423
1	0	-3.119421	1.157344	0.868423
1	0	1.403869	2.296540	0.000000
1	0	-0.314070	4.061737	0.000000
1	0	-2.700903	3.518479	0.000000

Frequencies

79.2257	111.2371	165.6439
237.3644	240.0496	304.3759
399.3095	418.5838	457.8222
461.7358	495.9142	529.2433
599.3024	600.9960	659.8510
662.9974	698.9020	730.9872
744.9458	798.9261	809.5701
833.4705	874.7439	925.1218
936.0879	942.7873	953.8186
954.5730	956.3344	964.7983
966.3135	1033.2506	1099.3012
1132.2813	1145.2536	1167.5734
1177.2311	1203.1482	1219.5623
1233.4672	1255.8415	1271.1454
1306.0796	1342.4045	1384.1335
1402.8621	1430.0805	1436.8785
1439.1890	1448.2143	1488.9798
1562.1478	1595.2184	1613.4987
1624.2574	2950.8735	2951.1885
3013.6398	3036.0542	3147.6114
3151.3053	3169.6435	3171.2872
3189.9296	3196.0160	3216.3533

[i6] C₁₃H₁₁, C₁, ²A

6	0	1.640915	-0.642017	-0.100144
6	0	2.107443	0.680929	0.042607
6	0	1.221489	1.753411	-0.058059
6	0	-0.092378	1.417606	-0.296795
6	0	-0.623971	0.151450	-0.451231
6	0	0.293564	-0.909937	-0.343437
6	0	2.787718	-1.543814	0.048278
6	0	3.904074	-0.829599	0.271416
6	0	3.597375	0.649434	0.291937
6	0	-2.098080	-0.087695	-0.689845
6	0	-2.934974	0.077789	0.603698
6	0	-4.359928	-0.156224	0.390086
6	0	-5.527803	-0.355283	0.188030
1	0	1.548659	2.783228	0.043148
1	0	-0.056299	-1.932199	-0.458704
1	0	2.726110	-2.622961	-0.015168
1	0	4.898063	-1.230534	0.419220
1	0	4.156584	1.193533	-0.479457
1	0	3.865244	1.109336	1.251418
1	0	-2.473649	0.612243	-1.440416
1	0	-2.250030	-1.094904	-1.085669
1	0	-2.561432	-0.613131	1.367330
1	0	-2.783925	1.087299	1.000455
1	0	-6.561983	-0.528204	0.018605

Frequencies

25.4125	58.5970	62.0210
152.5493	197.6583	206.4384
266.5540	326.6006	352.5619
400.4553	409.9303	430.0956
458.5614	541.9977	601.9792
636.6865	664.1884	675.0781
702.6663	743.0876	745.4636
770.0182	778.4355	847.1947
854.4484	886.0556	921.2584
946.6530	955.3004	961.6237
966.8069	1013.0825	1019.5340
1092.4480	1141.7706	1146.2568
1163.1230	1179.9113	1233.5662
1254.7443	1263.5073	1290.7891
1306.3146	1331.3049	1361.2946

1369.2691		1424.7420		1436.1169
1460.9959		1476.8013		1497.7355
1567.1408		1611.5006		1640.6182
2220.3563		3016.1417		3023.6769
3039.2244		3048.3474		3052.4401
3091.8024		3146.7371		3158.6879
3190.0836		3213.6753		3478.1275

[i7] C₁₃H₁₁, C₁, ²A

6	0	-1.458342	-0.726582	0.005456
6	0	-1.512287	0.679683	0.008386
6	0	-0.346567	1.425305	0.062222
6	0	0.892588	0.769751	0.115608
6	0	0.949878	-0.644243	0.124359
6	0	-0.228392	-1.384604	0.065503
6	0	-2.828699	-1.237062	-0.064409
6	0	-3.695349	-0.209130	-0.102417
6	0	-2.959271	1.109425	-0.060749
6	0	2.298058	-1.321738	0.288521
6	0	3.453244	-0.559556	-0.410096
6	0	3.288078	0.883275	-0.120756
6	0	2.162632	1.529107	0.126801
1	0	-0.375620	2.510953	0.054840
1	0	-0.184497	-2.469681	0.073081
1	0	-3.089028	-2.288119	-0.081434
1	0	-4.773277	-0.286106	-0.155135
1	0	-3.253567	1.713053	0.807158
1	0	-3.168323	1.720931	-0.947573
1	0	2.528069	-1.371668	1.361025
1	0	2.257412	-2.351967	-0.075882
1	0	4.415040	-0.944593	-0.058843
1	0	3.426531	-0.717380	-1.497119
1	0	2.123835	2.602797	0.289300

Frequencies

92.2730	125.5395	187.1191
253.3751	256.8313	317.0229
367.2295	392.2872	414.0118
432.0562	441.8394	519.1787
560.8412	638.9912	700.5585
718.6662	737.2266	755.0903

761.1461	779.8554	828.2434
865.1479	891.4462	894.0891
897.0562	927.1677	950.4545
954.9695	960.4073	973.8320
1021.0725	1066.5038	1112.5173
1146.7393	1171.0745	1180.5467
1196.2513	1212.9779	1232.5584
1246.0069	1278.7382	1292.8437
1323.7607	1327.8382	1356.3870
1381.2511	1436.6238	1455.7690
1467.5598	1476.9355	1499.8780
1574.0832	1624.8854	1649.5160
1685.2828	2992.0443	3001.7825
3014.1254	3036.6400	3055.4043
3064.1101	3140.1302	3151.5972
3153.5449	3188.1796	3212.7715

[i8] C₁₃H₁₁, C_s, ²A"

6	0	1.469071	-0.759783	0.000000
6	0	0.350461	-1.625977	0.000000
6	0	-0.926193	-1.114347	0.000000
6	0	-1.130087	0.289727	0.000000
6	0	0.000000	1.157229	0.000000
6	0	1.286041	0.622449	0.000000
6	0	2.678448	-1.577148	0.000000
6	0	2.348170	-2.882850	0.000000
6	0	0.846992	-3.054326	0.000000
6	0	-0.190609	2.662649	0.000000
6	0	-2.448736	0.840891	0.000000
6	0	-1.617947	3.117347	0.000000
6	0	-2.659370	2.232408	0.000000
1	0	-1.793058	-1.768642	0.000000
1	0	2.144565	1.288396	0.000000
1	0	3.685302	-1.178285	0.000000
1	0	3.040769	-3.714094	0.000000
1	0	0.500437	-3.613050	0.878429
1	0	0.500437	-3.613050	-0.878429
1	0	0.331467	3.095317	0.868482
1	0	0.331467	3.095317	-0.868482
1	0	-3.296117	0.164824	0.000000
1	0	-1.804949	4.185688	0.000000

1	0	-3.677772	2.607959	0.000000
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Frequencies

70.4352		120.7611		159.2442
255.1103		266.9734		307.6414
398.2054		408.3799		414.8067
429.6699		495.9819		558.6225
585.5938		631.3007		664.7430
706.6247		724.0272		746.1902
747.9620		782.7334		783.8659
863.2247		883.1577		885.2209
899.5266		946.6566		950.1786
952.1518		954.1532		959.5561
964.6461		1048.3517		1100.4563
1124.4145		1148.8423		1166.1281
1180.9999		1203.7761		1227.6961
1241.9142		1253.3917		1272.7095
1311.9502		1331.2744		1367.7929
1392.6479		1434.8241		1440.4195
1447.3931		1464.9132		1493.8426
1561.3115		1576.4664		1614.8079
1641.0103		2950.2364		2950.6348
3014.2562		3036.5516		3146.4447
3150.5680		3152.1584		3168.7983
3179.8973		3188.0434		3212.4721

Products

3H-cyclopenta[a]naphthalene [P1] C₁₃H₁₀, C_s, ¹A'

6	0	0.924373	-0.413419	0.000000
6	0	0.483046	-1.732947	0.000000
6	0	-0.887360	-2.042206	0.000000
6	0	-1.807157	-1.016884	0.000000
6	0	-1.397836	0.344203	0.000000
6	0	0.000000	0.667509	0.000000
6	0	2.390825	-0.418136	0.000000
6	0	2.839112	-1.686514	0.000000
6	0	1.680062	-2.650712	0.000000
6	0	0.386186	2.032362	0.000000
6	0	-0.556046	3.032961	0.000000
6	0	-1.933972	2.716786	0.000000
6	0	-2.341373	1.405165	0.000000

1	0	-1.219072	-3.075382	0.000000
1	0	-2.869477	-1.237091	0.000000
1	0	3.013043	0.467065	0.000000
1	0	3.875258	-1.997286	0.000000
1	0	1.695725	-3.308892	0.878281
1	0	1.695725	-3.308892	-0.878281
1	0	1.440453	2.284459	0.000000
1	0	-0.244318	4.071476	0.000000
1	0	-2.667798	3.514960	0.000000
1	0	-3.398687	1.160579	0.000000

Frequencies

114.2372	132.0570	229.1156
242.3782	268.5622	387.5335
433.0191	439.3947	463.9684
506.3711	519.7729	565.1862
613.0959	666.4571	682.1473
723.5469	748.9623	753.2205
798.5637	818.1915	841.1685
879.3718	882.5764	933.2719
950.4223	955.5959	959.0772
967.2270	969.3689	992.6970
1044.1496	1074.2564	1126.8287
1141.8636	1167.2558	1178.6990
1191.9635	1216.4784	1236.8079
1283.6730	1293.2675	1352.2697
1378.6488	1389.4194	1430.2038
1431.5527	1469.4414	1486.5783
1555.3473	1585.0322	1619.0469
1634.2600	1664.4750	3013.2641
3035.9395	3155.0041	3156.8946
3164.8202	3173.8559	3176.9878
3187.3411	3195.5485	3217.5782

1H-cyclopenta[b]naphthalene [P2] C₁₃H₁₀, C_s, ¹A'

6	0	-0.274495	-1.600869	0.000000
6	0	-1.428382	-0.755109	0.000000
6	0	-1.297784	0.604896	0.000000
6	0	0.000000	1.192878	0.000000
6	0	1.157970	0.345205	0.000000
6	0	0.991533	-1.065552	0.000000

6	0	-0.739094	-2.988790	0.000000
6	0	-2.082493	-3.023472	0.000000
6	0	-2.664072	-1.628432	0.000000
6	0	2.442505	0.949854	0.000000
6	0	0.184026	2.598751	0.000000
6	0	2.584192	2.316613	0.000000
6	0	1.443138	3.150646	0.000000
1	0	-2.167492	1.255386	0.000000
1	0	1.870386	-1.702573	0.000000
1	0	-0.082590	-3.849851	0.000000
1	0	-2.692519	-3.917436	0.000000
1	0	-3.297001	-1.450501	0.878396
1	0	-3.297001	-1.450501	-0.878396
1	0	3.318424	0.309101	0.000000
1	0	-0.692984	3.238165	0.000000
1	0	3.573446	2.760523	0.000000
1	0	1.565067	4.227980	0.000000

Frequencies

101.6939	135.6973	251.2229
263.6581	278.7787	393.8545
406.0427	417.1045	426.3078
485.8694	560.0141	577.9544
628.7414	686.3422	732.7069
737.9740	751.3041	764.3906
782.9561	806.1093	856.7377
857.4651	888.3833	900.8895
913.7686	955.7244	957.3809
962.2859	970.1595	991.2861
1043.3698	1077.5211	1121.5879
1154.8071	1169.1007	1174.4976
1180.5263	1244.3719	1251.1493
1268.1191	1282.2110	1348.0689
1373.3486	1387.6188	1434.8920
1446.7381	1470.2751	1486.6068
1537.3062	1611.9868	1627.0489
1654.9286	1677.6559	3012.8723
3034.3514	3151.7288	3154.3238
3157.7318	3161.0250	3172.2271
3185.5638	3188.8036	3211.4998

5-((E)-but-1-en-3-ynyl)-1H-indene [P4] C₁₃H₁₀, C_s, ¹A'

6	0	-1.383771	-0.816307	0.000000
6	0	-2.201038	0.335263	0.000000
6	0	-1.626000	1.595005	0.000000
6	0	-0.234456	1.701523	0.000000
6	0	0.597423	0.566598	0.000000
6	0	0.000000	-0.708454	0.000000
6	0	-2.258334	-1.993120	0.000000
6	0	-3.544230	-1.602736	0.000000
6	0	-3.647800	-0.095741	0.000000
6	0	2.046048	0.772235	0.000000
6	0	3.005191	-0.175064	0.000000
6	0	4.392769	0.111153	0.000000
6	0	5.580868	0.318742	0.000000
1	0	-2.238065	2.490951	0.000000
1	0	0.224720	2.684297	0.000000
1	0	0.611902	-1.603194	0.000000
1	0	-1.904273	-3.016311	0.000000
1	0	-4.406924	-2.255799	0.000000
1	0	-4.190590	0.276330	0.878190
1	0	-4.190590	0.276330	-0.878190
1	0	2.368040	1.809940	0.000000
1	0	2.740544	-1.228788	0.000000
1	0	6.625213	0.511659	0.000000

Frequencies

41.3854	76.2752	88.7572
168.4440	199.8460	207.9519
315.0984	326.0922	395.6476
412.6149	419.9192	476.7744
495.1764	562.1622	615.5683
624.2264	626.0156	679.6003
715.0217	745.3753	755.6125
809.7724	820.0342	855.1418
871.4554	891.8096	938.0962
952.7129	962.0506	967.4890
970.9169	990.9841	1035.1887
1094.4578	1141.3337	1148.6789
1158.1166	1208.3136	1238.6626
1262.5411	1288.6255	1318.6665
1341.8769	1349.1121	1384.2579

1437.0368		1465.5309		1501.3434
1599.7722		1625.6737		1649.1397
1669.6653		2194.1225		3013.9382
3036.0703		3141.2986		3151.6874
3158.5500		3174.4784		3175.7091
3190.6567		3213.9080		3477.9449

5-(but-3-en-1-ynyl)-1H-indene [P5] C₁₃H₁₀, C_s, 1A'

6	0	0.303343	-1.795813	0.000000
6	0	-1.095489	-1.975727	0.000000
6	0	-1.943454	-0.878223	0.000000
6	0	-1.395967	0.403623	0.000000
6	0	0.000000	0.597514	0.000000
6	0	0.856020	-0.521038	0.000000
6	0	0.933153	-3.119804	0.000000
6	0	-0.015056	-4.072134	0.000000
6	0	-1.393805	-3.455595	0.000000
6	0	0.539274	1.914721	0.000000
6	0	0.988472	3.039716	0.000000
6	0	1.556166	4.338110	0.000000
6	0	0.858632	5.482000	0.000000
1	0	-3.021162	-1.004356	0.000000
1	0	-2.042768	1.272314	0.000000
1	0	1.929423	-0.372552	0.000000
1	0	2.002903	-3.286240	0.000000
1	0	0.156406	-5.140435	0.000000
1	0	-1.977354	-3.759841	0.878198
1	0	-1.977354	-3.759841	-0.878198
1	0	2.643263	4.380334	0.000000
1	0	-0.224864	5.486480	0.000000
1	0	1.363783	6.440033	0.000000

Frequencies

37.3530	59.4502	71.1221
175.7068	182.7313	196.7812
289.6946	333.7955	383.1536
395.7752	410.7592	475.5495
503.5157	557.6953	613.0435
628.7753	691.8118	694.4499
714.7585	747.9352	758.4873
833.3893	850.3109	886.9347

903.9531	936.6605	939.8884
955.5093	963.8808	969.3097
988.0660	1006.8252	1087.6981
1101.8110	1142.8521	1147.9026
1177.0535	1210.6716	1245.4469
1288.7333	1309.7203	1319.5006
1340.1434	1366.4855	1435.7678
1443.8591	1460.9537	1498.7601
1593.9406	1622.9650	1648.3173
1665.3601	2297.3347	3013.9340
3036.1722	3127.7758	3145.4338
3162.7170	3182.7178	3191.6089
3191.9518	3214.5280	3234.7356

Transition states

[i0a] → [i1] C₁₃H₁₁, C₁, ²A

6	0	-1.918514	-0.642900	0.070680
6	0	-1.979738	0.760619	-0.063750
6	0	-0.824051	1.520545	-0.173108
6	0	0.424365	0.874266	-0.149989
6	0	0.429304	-0.496655	-0.015786
6	0	-0.681733	-1.303241	0.096457
6	0	-3.288523	-1.155824	0.162890
6	0	-4.159607	-0.134482	0.090540
6	0	-3.431685	1.179814	-0.059479
6	0	3.653398	-0.736593	-0.560766
6	0	2.818305	-1.551049	0.115993
6	0	4.944715	1.297650	0.477036
6	0	4.343685	0.358145	0.016883
1	0	-0.871830	2.600587	-0.276071
1	0	1.345882	1.439590	-0.232932
1	0	-0.616620	-2.381591	0.200760
1	0	-3.542160	-2.202708	0.272511
1	0	-5.237998	-0.214250	0.131616
1	0	-3.662058	1.867507	0.763976
1	0	-3.716249	1.698239	-0.983774
1	0	3.805176	-0.890670	-1.625858
1	0	2.680924	-1.457307	1.185256
1	0	2.362088	-2.400450	-0.374923
1	0	5.473311	2.119284	0.893837

Frequencies

-109.6636	15.2019	29.2603
40.5122	81.0842	170.6361
195.0712	226.2267	231.5991
360.5137	391.7154	392.1893
420.3817	529.0208	550.7939
558.7483	593.4891	627.1295
676.4546	697.0965	716.9915
736.8666	740.3857	795.7224
814.0946	858.7222	861.5499
894.8322	920.1694	932.4135
956.0537	958.2670	963.7489
982.8647	1040.0645	1086.7855
1112.7856	1127.8259	1148.4564
1168.6988	1207.3232	1239.8583
1288.5305	1305.4199	1323.7831
1375.9126	1417.5433	1435.8496
1438.1322	1460.7758	1565.7523
1607.2372	1620.3709	1632.5060
2183.4535	3014.7392	3037.3693
3140.4843	3151.1902	3155.6490
3156.2324	3174.3537	3189.4352
3212.5363	3248.9910	3476.3532

[i1] → [P4] C₁₃H₁₁, C₁, ²A

6	0	1.686442	-0.680660	-0.004812
6	0	2.081387	0.671087	-0.016296
6	0	1.126626	1.676784	0.040374
6	0	-0.222118	1.332433	0.102107
6	0	-0.635524	-0.012187	0.103672
6	0	0.339688	-1.022499	0.059095
6	0	2.893875	-1.509784	-0.064915
6	0	3.981614	-0.721559	-0.111096
6	0	3.587721	0.736294	-0.085083
6	0	-3.117917	0.387790	-0.127201
6	0	-2.049861	-0.408998	0.145737
6	0	-5.602515	-0.436095	-0.186966
6	0	-4.452029	-0.072849	-0.154735
1	0	1.417086	2.722299	0.044049
1	0	0.033863	-2.063734	0.071129
1	0	2.891619	-2.592428	-0.070084

1	0	5.009017	-1.057209	-0.159997
1	0	3.938510	1.270120	-0.977473
1	0	4.019319	1.260490	0.777025
1	0	-2.973051	1.444969	-0.329088
1	0	-2.235063	-1.473401	0.252181
1	0	-2.231605	-0.506665	2.238469
1	0	-6.612290	-0.764464	-0.212435
1	0	-0.961744	2.121492	0.166942

Frequencies

-538.5765		44.0429		77.4099
88.1213		159.3538		195.1057
217.9353		253.6778		299.1060
332.2775		354.6217		392.0713
397.0214		425.5673		466.1593
509.0859		568.4400		617.0577
624.2837		641.2482		678.7256
714.3188		747.6876		757.5920
799.1498		823.3815		849.3989
858.4636		901.7426		937.3464
947.9218		959.8336		962.6260
967.2444		987.9288		1042.7024
1091.2570		1137.9889		1147.4307
1174.6545		1205.5228		1239.0032
1255.8334		1296.6812		1307.4904
1324.9283		1349.6044		1381.3411
1435.4606		1457.0248		1500.4902
1599.5349		1610.2254		1630.6342
1651.5953		2181.8667		3014.1504
3036.4826		3146.7262		3158.0723
3160.8743		3163.5316		3184.5352
3191.3738		3214.5962		3476.6721

[i1] → [i3] C₁₃H₁₁, C₁, ²A

6	0	1.140650	-0.598237	-0.096614
6	0	2.080590	0.439259	0.124588
6	0	1.672301	1.762066	0.233801
6	0	0.313890	2.083666	0.126956
6	0	-0.627191	1.071815	-0.088985
6	0	-0.188845	-0.239760	-0.193369
6	0	1.864121	-1.869682	-0.169445

6	0	3.179754	-1.648928	-0.004059
6	0	3.458234	-0.178760	0.198511
6	0	-2.132678	1.213347	-0.210347
6	0	-2.636938	-0.179661	-0.650159
6	0	-3.713635	-0.774432	0.070793
6	0	-4.601176	-1.298814	0.699059
1	0	2.400167	2.549706	0.399877
1	0	-0.004511	3.118277	0.210374
1	0	1.390805	-2.829202	-0.331064
1	0	3.955394	-2.403283	-0.009591
1	0	4.130634	0.217819	-0.572810
1	0	3.945645	0.013140	1.162823
1	0	-2.575081	1.489168	0.751011
1	0	-2.421438	1.985341	-0.930043
1	0	-2.750806	-0.275601	-1.731796
1	0	-1.537385	-0.801906	-0.441086
1	0	-5.387893	-1.754722	1.247936

Frequencies

-1645.5757	43.9178	92.2740
130.3900	184.5110	215.7462
246.3150	284.2900	375.8955
394.2850	421.4506	451.4411
485.3748	522.0465	550.6351
585.0681	602.6033	620.2243
666.0268	698.6040	751.7665
754.9918	807.6594	810.2291
848.6737	856.3503	930.8772
932.0978	954.4627	958.3130
963.4025	990.6142	1021.7421
1070.5103	1082.3830	1133.7964
1145.5522	1162.5318	1186.7676
1216.5669	1231.1964	1256.7963
1291.4096	1297.1294	1335.9358
1359.2127	1376.0061	1434.8172
1448.9873	1453.6786	1485.4127
1584.5872	1616.7976	1642.3407
1660.9132	2167.5609	3013.2733
3036.4271	3036.4499	3065.9734
3083.2292	3150.3559	3168.5322
3195.3308	3217.1730	3475.7960

[i3] → [i4] C₁₃H₁₁, C₁, ²A

6	0	1.013715	-0.479919	-0.154852
6	0	1.766222	0.699026	0.076662
6	0	1.133123	1.928566	0.152531
6	0	-0.255738	1.994371	-0.004871
6	0	-1.026959	0.843734	-0.241344
6	0	-0.350398	-0.367976	-0.315195
6	0	1.941913	-1.615604	-0.172815
6	0	3.196632	-1.180741	0.032965
6	0	3.222933	0.319039	0.210969
6	0	-2.527071	0.941929	-0.442552
6	0	-3.346645	-0.029898	0.452576
6	0	-2.804553	-1.376847	0.298782
6	0	-1.885057	-2.129032	0.015546
1	0	1.698522	2.836331	0.336174
1	0	-0.753576	2.958079	0.052011
1	0	1.644054	-2.643772	-0.332512
1	0	4.084841	-1.797608	0.069107
1	0	3.848828	0.807618	-0.546642
1	0	3.636004	0.606448	1.186186
1	0	-2.860891	1.965613	-0.252692
1	0	-2.766682	0.712258	-1.486245
1	0	-3.279994	0.270775	1.504144
1	0	-4.403599	0.017597	0.172796
1	0	-1.316202	-3.013225	-0.152738

Frequencies

-372.3832	64.8145	90.2484
154.3351	194.0543	206.4422
301.2222	336.5116	359.7025
399.5989	439.3819	463.3781
468.9763	545.2956	585.2869
626.6863	651.3271	699.6645
705.0301	738.0138	749.6857
765.4171	814.6094	848.2439
851.5552	896.7419	928.7326
951.7592	954.0504	958.1540
987.0845	992.5472	1024.0618
1072.9425	1133.5981	1145.7804
1158.6694	1186.0144	1211.0169

1222.2206	1245.3887	1270.8859
1325.5325	1332.2820	1349.5683
1380.0249	1434.2532	1441.0575
1449.2882	1476.0405	1483.8427
1571.3105	1615.9357	1640.6549
2061.7093	3012.3629	3024.3397
3026.1075	3035.2018	3058.7386
3074.2120	3144.5102	3167.3217
3191.7733	3214.5129	3437.9273

[i4] → [i5] C₁₃H₁₁, C₁, 2A

6	0	0.933942	-0.465560	-0.054102
6	0	1.687952	0.716748	0.042150
6	0	1.062600	1.953365	0.084993
6	0	-0.337702	2.006576	0.014344
6	0	-1.104412	0.853193	-0.090538
6	0	-0.480368	-0.430295	-0.119078
6	0	1.858967	-1.598018	-0.051869
6	0	3.126203	-1.149923	0.028696
6	0	3.153415	0.356407	0.096671
6	0	-2.610228	0.925795	-0.278128
6	0	-3.282142	-0.316953	0.261399
6	0	-2.679644	-1.586654	0.175319
6	0	-1.303989	-1.598622	-0.217844
1	0	1.637176	2.869840	0.167841
1	0	-0.833864	2.971896	0.027255
1	0	1.560897	-2.636733	-0.101554
1	0	4.017352	-1.763143	0.046770
1	0	3.718336	0.792799	-0.736865
1	0	3.633639	0.714273	1.016093
1	0	-3.018823	1.830248	0.180888
1	0	-2.835209	0.995258	-1.354533
1	0	-2.862492	-1.005324	1.312077
1	0	-4.304007	-0.229323	0.626408
1	0	-0.860571	-2.536139	-0.536452

Frequencies

-1514.2831	100.1474	110.4142
175.9726	233.3435	240.9282
308.8017	396.8593	421.4278
448.8008	464.9229	490.8814

522.6268	578.8461	609.9493
645.5944	692.1086	705.2015
724.0592	753.9355	796.9331
810.2492	831.7762	846.8874
916.5329	929.0883	946.8859
952.3852	960.9619	963.2822
965.8487	1031.1185	1070.1074
1124.7195	1146.0882	1162.0074
1185.6736	1217.2956	1220.3829
1230.3427	1258.4891	1268.3912
1293.8213	1327.6876	1351.1999
1369.9172	1397.7749	1425.8317
1434.3814	1442.0820	1456.4663
1468.9804	1586.3516	1609.7172
1612.3574	2126.0567	2960.4640
3014.8127	3037.5939	3058.8806
3117.9504	3153.4676	3155.7566
3172.0785	3197.1533	3218.6736

[i5] → [P1] C₁₃H₁₁, C₁, ²A

6	0	-0.935347	-0.472794	0.008611
6	0	-1.685509	0.699979	-0.018330
6	0	-1.065217	1.957974	-0.054203
6	0	0.312547	2.028530	-0.058312
6	0	1.109540	0.857891	-0.031405
6	0	0.485653	-0.431156	-0.001753
6	0	-1.859707	-1.610251	0.041566
6	0	-3.128201	-1.162103	0.036110
6	0	-3.151307	0.344732	-0.002699
6	0	2.539016	0.926755	-0.020114
6	0	1.303767	-1.591066	-0.004095
6	0	2.677199	-1.492006	-0.056023
6	0	3.300481	-0.231769	-0.086590
1	0	-1.659288	2.865650	-0.076053
1	0	0.808393	2.993136	-0.075588
1	0	-1.562141	-2.650159	0.068020
1	0	-4.020614	-1.773079	0.057042
1	0	-3.669342	0.768259	0.867319
1	0	-3.677224	0.723072	-0.888666
1	0	3.010526	1.893275	-0.155857
1	0	2.851658	1.353839	1.880958

1	0	0.835702	-2.568323	0.018081
1	0	3.283722	-2.390324	-0.079474
1	0	4.381137	-0.163638	-0.132365

Frequencies

-638.3681		111.7084		128.7348
220.7028		241.5701		260.6962
277.6307		356.6917		393.2974
434.4268		457.8514		465.6427
514.4098		524.2491		565.6011
612.8697		666.2526		681.5059
725.9719		749.6764		751.3412
805.6751		825.5235		840.7263
880.4402		889.6009		933.4111
952.1503		955.3874		964.0990
968.9362		971.7986		999.0330
1045.3904		1069.7533		1126.4368
1142.6721		1161.0960		1177.9509
1190.5181		1217.7385		1233.6712
1277.9198		1293.0191		1350.8478
1370.0866		1387.0355		1427.1455
1431.3550		1462.6158		1479.7315
1546.5258		1583.4545		1607.7160
1622.4911		1650.4731		3014.2766
3037.1585		3158.0279		3163.3691
3170.2041		3175.8388		3181.2758
3190.5777		3196.3336		3218.1406

[i1] → [i6] C₁₃H₁₁, C₁, 2A

6	0	-1.764769	-0.649610	0.074878
6	0	-1.787172	0.759443	-0.036527
6	0	-0.608915	1.481249	-0.210839
6	0	0.555124	0.733591	-0.259952
6	0	0.620556	-0.648582	-0.156376
6	0	-0.567281	-1.364985	0.015928
6	0	-3.145996	-1.110546	0.245080
6	0	-3.983391	-0.059413	0.241825
6	0	-3.219965	1.231284	0.065053
6	0	2.034902	-1.191619	-0.228670
6	0	2.912861	0.014837	-0.630442
6	0	4.081168	0.293625	0.138545

6	0	5.051817	0.556033	0.806513
1	0	-0.609095	2.562949	-0.299554
1	0	-0.560617	-2.447965	0.100325
1	0	-3.431113	-2.149308	0.355971
1	0	-5.059278	-0.101951	0.349193
1	0	-3.370728	1.913329	0.911275
1	0	-3.540594	1.775508	-0.832176
1	0	2.350369	-1.582414	0.742842
1	0	2.129414	-2.009424	-0.949576
1	0	3.091911	0.078725	-1.705580
1	0	2.015898	0.908553	-0.453251
1	0	5.910203	0.780154	1.390434

Frequencies

-1641.9172	37.1080	99.1695
123.3936	189.8635	230.2908
265.0044	282.7198	359.1145
392.6566	405.4631	420.4879
438.8542	537.1487	591.9319
597.7084	620.0044	646.8268
666.5604	701.7290	747.4383
748.6446	764.1438	841.8613
852.9783	862.4447	886.8031
922.6386	948.9750	953.1576
957.5425	962.3462	1022.4307
1074.3851	1091.2221	1132.2117
1146.5602	1167.7923	1187.0943
1232.0243	1245.0308	1253.8627
1289.2680	1297.1907	1327.0767
1359.0459	1372.3163	1436.3107
1440.5920	1462.4025	1484.2928
1579.3244	1616.9007	1637.7405
1665.9693	2168.6747	3014.9151
3035.8618	3037.6959	3065.4666
3083.1672	3149.8473	3158.2135
3188.4667	3212.1821	3475.9045

[i6] → [i7] C₁₃H₁₁, C₁, 2A

6	0	1.514095	-0.692155	-0.006639
6	0	1.578512	0.713566	-0.066340
6	0	0.415053	1.462997	-0.230257

6	0	-0.768805	0.760069	-0.345418
6	0	-0.891090	-0.623796	-0.287331
6	0	0.292852	-1.358573	-0.112975
6	0	2.876690	-1.201416	0.177391
6	0	3.744502	-0.176213	0.228841
6	0	3.020839	1.141909	0.080551
6	0	-2.228232	-1.322654	-0.443015
6	0	-3.338326	-0.779666	0.500303
6	0	-3.399484	0.673010	0.364024
6	0	-2.878747	1.738212	0.073834
1	0	0.442275	2.548334	-0.268117
1	0	0.251539	-2.443608	-0.067017
1	0	3.129504	-2.251442	0.257596
1	0	4.816106	-0.253863	0.356980
1	0	3.374949	1.706155	-0.791447
1	0	3.172321	1.791414	0.951951
1	0	-2.580344	-1.201486	-1.472963
1	0	-2.107643	-2.395254	-0.267908
1	0	-4.293512	-1.252510	0.251983
1	0	-3.114855	-1.037557	1.541565
1	0	-2.717496	2.778071	-0.090444

Frequencies

-370.4211	58.6623	97.7936
163.0988	196.4580	223.8368
293.7441	337.7523	349.4061
404.8583	411.7495	427.5795
498.3770	519.6255	586.0164
650.5126	655.4083	705.3961
721.6923	737.5220	745.5357
757.3256	849.6264	850.9347
854.4660	881.1555	886.2157
944.2673	946.8017	954.6839
959.5082	995.0562	1025.4245
1089.9494	1137.2587	1145.1529
1172.5261	1185.0150	1209.9712
1233.8840	1254.9061	1272.0687
1322.0755	1326.7896	1348.8996
1372.2422	1424.5750	1436.8734
1463.3758	1476.4795	1483.4579
1567.8202	1610.9074	1637.5400

2065.2732		3014.0397		3024.2521
3025.9979		3036.6838		3058.6611
3073.3324		3141.4262		3143.6684
3187.0481		3211.5512		3435.1164

[i7] → [i8] C₁₃H₁₁, C₁, ²A

6	0	1.467699	-0.724873	0.013931
6	0	1.504350	0.690596	-0.017421
6	0	0.338962	1.416894	-0.082956
6	0	-0.914252	0.747208	-0.119007
6	0	-0.939041	-0.681494	-0.109649
6	0	0.245587	-1.402156	-0.037866
6	0	2.837774	-1.215468	0.089976
6	0	3.695243	-0.175482	0.104882
6	0	2.948417	1.135076	0.038182
6	0	-2.274780	-1.381668	-0.275083
6	0	-3.412263	-0.536921	0.256455
6	0	-3.405789	0.871717	0.203756
6	0	-2.148908	1.463385	-0.159813
1	0	0.350927	2.502614	-0.095977
1	0	0.219274	-2.487813	-0.036080
1	0	3.110902	-2.262612	0.127181
1	0	4.773896	-0.242433	0.156284
1	0	3.234833	1.722706	-0.842983
1	0	3.154620	1.766678	0.911217
1	0	-2.456261	-1.559025	-1.347435
1	0	-2.259951	-2.368039	0.197654
1	0	-4.317385	-1.054876	0.570585
1	0	-3.346527	0.219188	1.327076
1	0	-2.122326	2.522710	-0.399848

Frequencies

-1486.0331	79.6620	125.0895
152.6728	254.8706	260.8908
309.0523	390.7747	406.0754
419.9931	431.5895	478.4532
536.9844	566.1964	631.0846
703.7422	714.4554	723.4795
740.0566	755.0323	777.3139
790.9513	838.2072	862.2334
886.4839	893.5882	935.3381

952.4739	954.7196	960.2392
963.9352	1042.1518	1091.3783
1117.4094	1149.4421	1165.0706
1182.1277	1223.9093	1231.5165
1236.2206	1254.4142	1271.7909
1298.8792	1318.4409	1347.2174
1354.6686	1389.6225	1435.0051
1439.0749	1454.6281	1463.2424
1492.7071	1552.8453	1606.4407
1628.2968	2122.1677	2959.5309
3016.0159	3038.6245	3053.5199
3111.9196	3138.2947	3152.9454
3156.5882	3190.3441	3213.9244

[i8] → [P2] C₁₃H₁₁, C₁, ²A

6	0	1.468605	0.727764	-0.031980
6	0	1.493551	-0.700491	0.016830
6	0	0.330917	-1.418806	0.039745
6	0	-0.921017	-0.740248	0.013507
6	0	-0.944290	0.691736	-0.028803
6	0	0.274285	1.411934	-0.052512
6	0	2.853567	1.198674	-0.048135
6	0	3.694665	0.150804	-0.011748
6	0	2.936254	-1.155439	0.033522
6	0	-2.212306	1.354964	-0.032287
6	0	-2.151442	-1.446108	0.008930
6	0	-3.390628	0.623504	-0.100282
6	0	-3.357146	-0.781185	-0.057065
1	0	0.338154	-2.504159	0.074617
1	0	0.249857	2.496575	-0.079291
1	0	3.140971	2.241934	-0.083278
1	0	4.775450	0.206365	-0.012763
1	0	3.176502	-1.735315	0.933382
1	0	3.178238	-1.797808	-0.822354
1	0	-2.321931	1.892227	1.866414
1	0	-2.232596	2.428904	-0.177762
1	0	-2.128367	-2.530540	0.041468
1	0	-4.341433	1.140585	-0.157070
1	0	-4.284946	-1.341385	-0.081696

Frequencies

-627.4394		100.7808		131.0957
234.6061		261.0698		273.5486
284.1626		355.4229		403.4864
407.7691		419.4678		428.1362
513.3206		559.8521		576.1645
626.5006		686.0140		732.2410
743.6832		751.6836		760.4405
792.0909		804.8092		858.0692
870.4064		890.1291		902.3627
914.3136		955.8485		957.9191
968.2727		972.8020		997.4677
1044.8681		1074.7111		1119.2089
1154.7801		1163.4725		1173.0817
1179.1870		1242.9325		1250.0622
1267.0137		1280.1541		1346.8745
1373.4261		1376.4289		1429.2370
1444.8037		1471.7435		1476.4855
1532.7180		1597.5965		1621.0673
1633.4966		1673.3742		3013.9616
3035.7807		3153.7969		3158.6335
3162.2506		3167.2946		3176.6528
3189.3852		3190.1128		3212.5394

[i0b] → [i2] C₁₃H₁₁, C₁, 2A

6	0	-1.359446	-0.600415	-0.064351
6	0	-2.303288	0.443957	0.044322
6	0	-1.899826	1.770202	0.084064
6	0	-0.527021	2.068224	0.013203
6	0	0.354875	1.013906	-0.095380
6	0	0.011189	-0.318971	-0.135650
6	0	-2.085480	-1.873874	-0.080096
6	0	-3.406553	-1.643566	0.013212
6	0	-3.686526	-0.162278	0.101565
6	0	2.832144	1.507995	-0.271753
6	0	3.465357	0.533497	0.078402
6	0	4.111904	-0.635052	0.544172
6	0	4.525880	-1.643513	-0.238200
1	0	-2.624699	2.574379	0.170201
1	0	-0.189011	3.098850	0.047493
1	0	0.755077	-1.104428	-0.216537
1	0	-1.611988	-2.844623	-0.156034

1	0	-4.184224	-2.395986	0.025698
1	0	-4.214613	0.096246	1.028087
1	0	-4.324016	0.180085	-0.723393
1	0	2.514314	2.456888	-0.629300
1	0	4.277517	-0.689472	1.617755
1	0	4.383432	-1.623675	-1.312055
1	0	5.018953	-2.508929	0.187011

Frequencies

-190.8335		5.3959		28.7760
39.6296		69.3194		103.7902
192.9840		225.9433		229.6048
334.7460		391.4330		393.1097
421.0761		519.0059		551.5487
559.8212		583.2630		658.3132
669.7645		697.4687		700.3741
739.1137		740.5447		783.0903
821.4257		864.4816		871.1003
898.5864		925.3887		937.7404
954.8031		955.7543		963.2090
1002.5038		1036.9013		1086.1928
1111.8592		1127.5547		1148.2636
1169.3740		1206.6557		1239.0846
1287.8493		1315.4003		1325.1144
1374.7508		1419.2408		1438.8378
1440.8139		1461.8532		1565.3108
1622.1436		1633.1857		1640.8633
2121.7774		3013.9677		3036.4350
3132.5889		3146.0660		3146.3877
3162.0270		3164.6801		3189.2702
3212.1837		3236.8509		3459.2868

[i2] → [P5] C₁₃H₁₁, C₁, ²A

6	0	1.677947	-0.657222	-0.027726
6	0	2.194552	0.651939	0.056560
6	0	1.341732	1.745362	0.029479
6	0	-0.031430	1.533619	-0.082835
6	0	-0.558571	0.231632	-0.161778
6	0	0.309362	-0.875130	-0.137437
6	0	2.802785	-1.595939	0.023072
6	0	3.956016	-0.914515	0.132493

6	0	3.698196	0.573214	0.165049
6	0	-1.973182	0.017716	-0.248942
6	0	-3.127944	-0.341177	-0.084829
6	0	-4.485451	-0.717395	0.001483
6	0	-5.473280	0.081205	0.435455
1	0	1.727870	2.757416	0.091323
1	0	-0.711702	2.375436	-0.114240
1	0	-0.098269	-1.876945	-0.202162
1	0	2.701146	-2.672811	-0.022312
1	0	4.946593	-1.345797	0.190642
1	0	4.199848	1.092888	-0.661093
1	0	4.070583	1.032496	1.089522
1	0	-2.322759	1.143620	-1.887654
1	0	-4.720689	-1.731525	-0.313883
1	0	-5.280578	1.097298	0.757847
1	0	-6.496435	-0.271920	0.471745

Frequencies

-607.9652	32.8488	51.5546
83.8286	109.0690	166.3211
196.0397	203.8607	286.9496
329.3804	391.3791	395.2754
406.1319	442.4512	491.7515
503.8083	563.3899	608.3488
628.9138	688.4372	700.2949
714.8900	747.7058	759.4217
832.7415	850.7859	889.8314
904.6011	936.5387	939.7764
955.6944	963.9269	970.0030
988.7578	1000.1553	1087.4808
1101.3764	1143.2807	1148.1227
1177.7283	1210.5434	1245.2036
1284.0755	1307.0361	1316.2202
1340.7236	1367.6190	1435.4342
1442.8143	1458.7687	1496.9076
1596.1920	1623.2266	1641.4159
1651.7229	2223.1136	3014.5180
3036.9335	3129.5829	3147.1712
3164.0776	3184.0143	3191.8229
3194.3548	3214.7395	3237.9366

Optimized Cartesian Coordinates (Å) and Calculated Vibrational Frequencies (cm⁻¹) for the 6-Indenyl + Vinylacetylene System

Reactants

Vinylacetylene C₄H₄, C_s, ¹A'

6	0	0.735441	0.110182	0.00000
6	0	1.906556	-0.171715	0.00000
6	0	-0.635858	0.488606	0.00000
6	0	-1.659532	-0.371423	0.00000
1	0	2.936402	-0.432190	0.00000
1	0	-0.832528	1.558030	0.00000
1	0	-1.500612	-1.443195	0.00000
1	0	-2.682903	-0.016548	0.00000

Frequencies

224.3116	316.4854	557.7241
647.7553	680.3933	703.5142
892.2781	954.7667	1010.0968
1111.4928	1320.9953	1443.5247
1668.6181	2205.5842	3136.2470
3147.5999	3236.4714	3476.1732

6-indenyl C₉H₇, C_s, ²A'

6	0	-2.128299	0.813777	0.0000
6	0	-2.288651	-0.552933	0.0000
6	0	-1.125228	-1.337803	0.0000
6	0	0.116811	-0.702180	0.0000
6	0	0.214843	0.706135	0.0000
6	0	-0.932098	1.499536	0.0000
6	0	1.477466	-1.249417	0.0000
6	0	2.373217	-0.247733	0.0000
6	0	1.676289	1.092217	0.0000
1	0	-3.269711	-1.014887	0.0000
1	0	-1.198460	-2.420689	0.0000
1	0	-0.881655	2.583568	0.0000
1	0	1.707588	-2.307447	0.0000
1	0	3.449841	-0.355555	0.0000
1	0	1.942889	1.690960	0.880331
1	0	1.943405	1.694453	-0.876938

Frequencies

203.9833	207.9492	390.3342
399.5867	416.9998	533.6907
533.9369	602.1477	696.7671
737.6841	738.2471	804.6383
831.2133	849.7065	861.1688
941.2000	947.5813	955.4983
963.0625	1040.9162	1086.2879
1126.9877	1146.6321	1164.3760
1211.2079	1239.6846	1283.5058
1323.0788	1377.0933	1415.6713
1435.8132	1459.8382	1572.5637
1607.7744	1638.4690	3017.0930
3040.3913	3157.9721	3160.4538
3175.1085	3190.5542	3214.0340

Intermediates

[i'0a] C₁₃H₁₁, C₁, ²A

6	0	2.744945	1.626041	-0.622564
6	0	3.232709	1.267410	0.613511
6	0	2.728734	0.089942	1.187473
6	0	1.773391	-0.646654	0.486497
6	0	1.313441	-0.226226	-0.780414
6	0	1.804385	0.941779	-1.363680
6	0	1.076564	-1.890666	0.829480
6	0	0.232043	-2.228886	-0.160282
6	0	0.289992	-1.218916	-1.281400
1	0	3.976458	1.862678	1.131464
1	0	3.081102	-0.235381	2.161111
1	0	1.465313	1.284903	-2.335657
1	0	1.232380	-2.442365	1.748105
1	0	-0.411669	-3.098249	-0.179531
1	0	0.592332	-1.678666	-2.230560
1	0	-0.685327	-0.749301	-1.458471
6	0	-4.260561	0.401183	0.111168
6	0	-5.158042	-0.399914	0.046951
6	0	-3.227887	1.378843	0.163494
6	0	-2.019672	1.178022	0.701076
1	0	-5.943641	-1.113219	-0.001585

1	0	-3.469009	2.345826	-0.271551
1	0	-1.743423	0.228020	1.142936
1	0	-1.274766	1.964000	0.705878

Frequencies

5.2705		8.8041		12.6339
14.8985		35.1801		58.4345
203.8553		213.2776		225.5546
320.4522		390.3562		400.7407
417.8551		533.9341		534.5839
558.5229		602.7212		645.5557
678.6387		698.0419		705.5244
737.8413		738.0640		804.0267
831.2553		849.6365		861.3244
890.9760		940.1905		948.3580
956.0632		963.8471		967.2626
1011.0912		1039.7825		1085.8749
1110.2121		1126.5417		1150.9256
1164.6425		1210.4702		1240.6720
1284.1193		1320.6098		1323.0283
1377.0490		1415.3917		1435.5743
1445.3289		1458.9868		1571.7576
1606.3040		1637.2110		1666.5173
2204.4138		3019.5875		3044.4094
3135.9639		3149.3887		3157.9740
3161.2903		3175.4084		3190.8802
3214.5692		3239.2806		3477.0804

[i'0b] C₁₃H₁₁, C₁, ²A

6	0	0.480082	1.174534	-1.006946
6	0	0.945590	2.061147	-0.062555
6	0	2.059456	1.666345	0.694582
6	0	2.630693	0.416664	0.452890
6	0	2.106325	-0.446602	-0.533489
6	0	1.000597	-0.070100	-1.294874
6	0	2.929827	-1.713424	-0.559235
6	0	3.778139	-0.251858	1.074360
6	0	3.962001	-1.459060	0.513429
1	0	0.479132	3.026677	0.097837

1	0	2.464098	2.328795	1.452916
1	0	0.580686	-0.715192	-2.059615
1	0	3.391554	-1.884564	-1.539657
1	0	2.324022	-2.602032	-0.342385
1	0	4.377018	0.178363	1.867133
1	0	4.733650	-2.171489	0.773373
6	0	-4.301008	0.076774	-0.134725
6	0	-3.128791	0.338025	-0.233197
6	0	-5.693033	-0.205055	-0.056273
6	0	-6.260173	-0.981924	0.872644
1	0	-2.091074	0.563197	-0.313018
1	0	-6.314534	0.258289	-0.819004
1	0	-5.673323	-1.459696	1.648118
1	0	-7.329458	-1.155141	0.874636

Frequencies

4.7957	10.3917	23.4269
26.8851	38.7854	45.7249
204.9249	209.9256	227.8717
319.4738	390.8357	399.9875
417.4479	532.4227	533.9520
557.4302	602.7955	685.7646
697.0593	707.7880	711.2152
737.1602	737.8890	805.1172
831.0875	850.3346	861.4806
892.8139	941.4296	948.1416
950.8394	955.4319	964.3578
1010.9656	1040.4816	1087.6101
1112.1895	1127.8530	1147.9292
1164.7131	1211.4775	1240.2545
1284.3417	1321.6397	1323.6159
1377.8444	1415.8392	1436.0538
1443.7181	1459.7364	1571.7985
1607.7415	1637.8788	1668.5122
2201.2739	3018.3592	3041.8088
3134.0508	3146.6616	3160.0672
3163.5759	3176.8744	3192.3610
3215.6521	3235.4416	3440.0874

[i'1] C₁₃H₁₁, C₁, ²A

6	0	-0.638895	0.793055	0.329057
6	0	0.159078	1.907800	0.051368
6	0	1.531535	1.786684	-0.172985
6	0	2.110861	0.522116	-0.117005
6	0	1.314622	-0.608545	0.161403
6	0	-0.045440	-0.479299	0.379477
6	0	3.493671	0.073585	-0.299016
6	0	3.562486	-1.260065	-0.143958
6	0	2.199364	-1.833845	0.163172
1	0	-0.301616	2.889894	0.014452
1	0	2.130437	2.666159	-0.384262
1	0	-0.660741	-1.349421	0.588545
1	0	4.324206	0.730878	-0.524336
1	0	4.456491	-1.864593	-0.222286
1	0	1.887221	-2.570176	-0.588064
1	0	2.183635	-2.353117	1.129677
6	0	-3.938089	-0.601289	-0.336426
6	0	-4.809479	-1.435514	-0.141030
6	0	-2.957242	0.334894	-0.543104
6	0	-2.134164	0.942773	0.562788
1	0	-5.570077	-2.158258	0.023321
1	0	-2.751176	0.656834	-1.559609
1	0	-2.416410	0.486271	1.515537
1	0	-2.371815	2.011423	0.644577

Frequencies

23.6445	23.8233	94.5785
168.3237	203.5572	213.9530
276.2101	316.5430	388.6711
418.5183	424.2851	433.5893
438.2408	482.4253	544.0570
597.8043	603.4986	641.5882
645.6714	708.5937	748.4552
759.8523	782.7126	840.6684
861.2846	878.5015	895.0264
935.3559	952.2138	954.4476
958.4002	965.3205	1024.5447
1090.2584	1134.9266	1143.9661
1148.2151	1149.4065	1187.8073
1217.5877	1241.4358	1251.3015

1292.6574		1313.4736		1341.5832
1390.5438		1400.8730		1437.3998
1459.3096		1475.1130		1501.9624
1596.5743		1635.0247		1655.6407
2013.3248		2999.5471		3015.9488
3038.5915		3064.8789		3151.1323
3154.1947		3155.5427		3173.2923
3189.6919		3213.3833		3468.1783

[i'2] C₁₃H₁₁, C₁, ²A

6	0	-0.589723	-0.414471	-0.102889
6	0	-0.454919	0.983694	-0.162366
6	0	0.793392	1.592725	-0.123566
6	0	1.934917	0.794590	-0.023301
6	0	1.811908	-0.606951	0.037806
6	0	0.566043	-1.208797	-0.000896
6	0	-1.910233	-1.074338	-0.145881
6	0	-3.079634	-0.498238	-0.251908
6	0	-4.297447	0.068779	-0.372655
6	0	-5.115066	0.477825	0.679419
6	0	3.193776	-1.209348	0.142146
6	0	3.357638	1.133029	0.037730
6	0	4.088255	0.007665	0.131634
1	0	-1.349414	1.591978	-0.238697
1	0	0.873888	2.673580	-0.170158
1	0	0.468558	-2.289589	0.045396
1	0	-1.882723	-2.165330	-0.080966
1	0	-4.667609	0.218270	-1.387832
1	0	-4.804841	0.357340	1.709425
1	0	-6.080002	0.926396	0.483829
1	0	3.319560	-1.799472	1.058670
1	0	5.167087	-0.048127	0.192447
1	0	3.747077	2.143081	0.009854
1	0	3.414969	-1.885112	-0.693611

Frequencies

31.9882	54.6577	117.2573
154.0167	210.8505	226.6823
230.7652	319.3666	353.9436

405.7995	428.2069	436.6876
521.0910	551.0885	577.0795
589.1075	642.3180	705.8815
746.1904	754.8140	757.7987
761.8484	814.0805	850.6277
862.0220	896.0742	900.9807
938.8955	952.5244	953.8104
960.2115	966.2129	970.5335
1080.5592	1094.3078	1136.8253
1148.1659	1163.3470	1191.0530
1216.0221	1242.9464	1249.8832
1292.1893	1312.9005	1341.5538
1388.4105	1405.0701	1436.4361
1468.7124	1490.4305	1504.5509
1588.6987	1631.8635	1650.1515
1886.0799	3015.7372	3038.6180
3055.3633	3093.4399	3149.6803
3151.5406	3162.2827	3179.1096
3190.2459	3214.0194	3250.3651

[i'3] C₁₃H₁₁, C₁, ²A

6	0	-0.615405	0.427330	0.390174
6	0	-0.004591	1.665464	0.115389
6	0	1.365584	1.772737	-0.129996
6	0	2.157621	0.626583	-0.107124
6	0	1.574265	-0.639494	0.164105
6	0	0.230824	-0.669198	0.394043
6	0	-2.101782	0.307552	0.638726
6	0	-2.849535	-0.324399	-0.562548
6	0	-4.286118	-0.446892	-0.334583
6	0	-5.465858	-0.534877	-0.122651
6	0	2.655463	-1.693456	0.129566
6	0	3.592654	0.419244	-0.317986
6	0	3.890888	-0.884981	-0.188188
1	0	-0.623019	2.558304	0.102798
1	0	1.804637	2.743293	-0.333259
1	0	-2.523949	1.294705	0.841724
1	0	-2.284484	-0.307178	1.524218
1	0	-2.424787	-1.312748	-0.767993

1	0	-2.671488	0.280526	-1.458278
1	0	-6.509517	-0.617695	0.056439
1	0	2.743476	-2.221217	1.086817
1	0	4.294008	1.212690	-0.544275
1	0	4.873746	-1.325249	-0.291592
1	0	2.457311	-2.459108	-0.630169

Frequencies

31.9384		60.1176		60.9704
150.3215		190.8421		207.9293
271.2505		315.6089		352.9353
409.3885		428.5989		441.1015
467.7241		546.5038		596.6534
615.9279		664.2990		674.9666
698.7931		739.8925		749.9524
770.1786		781.7585		829.5392
864.1248		936.1354		936.2343
942.3440		955.4232		960.5673
972.0895		1010.6958		1025.9925
1080.4498		1135.8307		1145.2354
1157.8669		1180.9622		1231.9352
1246.1061		1270.0616		1291.8041
1300.7239		1325.1323		1367.6936
1381.5240		1431.9733		1442.7619
1453.8008		1477.3817		1498.3153
1559.0903		1621.5515		1646.9214
2220.4737		3023.0232		3024.1811
3046.8028		3046.9628		3052.9629
3090.9981		3149.4133		3175.7474
3190.3127		3214.5109		3477.8598

[i'4] C₁₃H₁₁, C₁, ²A

6	0	-1.105284	0.826312	0.103122
6	0	-0.366487	2.004448	0.012188
6	0	1.028870	1.992792	-0.060194
6	0	1.685086	0.766371	-0.036668
6	0	0.951896	-0.434941	0.050664
6	0	-0.437632	-0.423841	0.118043
6	0	1.921656	-1.594876	0.037054

6	0	3.109313	0.428357	-0.100122
6	0	3.262415	-0.906059	-0.057938
6	0	-2.612415	0.852463	0.274413
6	0	-3.320892	-0.353332	-0.395587
6	0	-2.543131	-1.572760	-0.080261
6	0	-1.248794	-1.662650	0.167089
1	0	-0.892073	2.954341	0.002165
1	0	1.582328	2.922455	-0.134245
1	0	1.749737	-2.268238	-0.812522
1	0	1.846650	-2.214025	0.940479
1	0	3.906169	1.158257	-0.170114
1	0	4.202420	-1.441208	-0.085645
1	0	-3.027351	1.788024	-0.110807
1	0	-2.840175	0.821658	1.348297
1	0	-3.367513	-0.225167	-1.485651
1	0	-4.353775	-0.419874	-0.041280
1	0	-0.754018	-2.609927	0.358505

Frequencies

98.8177	128.7097	190.5629
228.7212	233.2451	306.7168
367.6071	411.5570	424.2886
465.9665	486.1856	516.8100
560.4868	619.3816	630.6970
711.7920	715.6887	744.1591
770.0540	826.9381	833.7547
838.0439	863.8812	902.2676
943.4000	945.5059	954.4662
962.2105	972.3019	974.9567
1019.7509	1039.4270	1114.2120
1147.0753	1159.8280	1175.7902
1197.7037	1215.5080	1241.9594
1246.7396	1258.2967	1290.5740
1320.3742	1327.6739	1364.2490
1396.2555	1436.6032	1450.9033
1466.0018	1475.7394	1482.6522
1600.0623	1633.7190	1637.1772
1685.2989	2993.4583	3002.3948
3009.8781	3031.6508	3056.2825
3064.2787	3151.5606	3153.2098
3175.7776	3189.6038	3213.6517

[i'5] C₁₃H₁₁, C_s, ²A”

6	0	-1.082887	0.886308	0.000097
6	0	-0.299492	2.040466	-0.000059
6	0	1.094027	1.988497	-0.000146
6	0	1.713264	0.736865	-0.000077
6	0	0.945043	-0.435712	0.000051
6	0	-0.460343	-0.395133	0.000113
6	0	1.877074	-1.624496	-0.000051
6	0	3.130285	0.360469	-0.000025
6	0	3.242014	-0.978607	0.000115
6	0	-2.594920	1.002139	0.000222
1	0	-0.793733	3.007714	-0.000087
1	0	1.678427	2.901986	-0.000285
1	0	1.731525	-2.267502	0.877847
1	0	3.949753	1.068350	-0.000009
1	0	4.165453	-1.542576	0.000413
1	0	-2.915612	1.600324	-0.867813
1	0	-2.915609	1.599603	0.868769
6	0	-3.326804	-0.303940	-0.000135
6	0	-2.669768	-1.504206	-0.000188
6	0	-1.266611	-1.581590	0.000093
1	0	-4.410951	-0.272645	-0.000250
1	0	-0.781413	-2.549819	0.000100
1	0	-3.244786	-2.424905	-0.000340
1	0	1.731645	-2.266890	-0.878407

Frequencies

82.9856	108.4550	178.8092
233.4622	239.3658	293.3270
419.0093	421.0676	452.8672
463.3513	496.9249	519.2376
603.3887	613.7911	660.3440
662.0740	704.9687	728.8582
737.4980	780.6106	824.3068
833.3454	861.7936	927.0441
937.4934	941.1819	953.4729
955.6621	960.7784	964.7030
976.6067	1028.6003	1098.3921

1124.8098		1145.2385		1167.1394
1176.7355		1199.7010		1221.9212
1246.9332		1252.5082		1270.2439
1301.0872		1346.9644		1381.4239
1398.4420		1431.7417		1437.0816
1442.2514		1446.9794		1494.0362
1557.2710		1592.6302		1618.2668
1633.2851		2951.2607		2951.6549
3008.6595		3030.0161		3148.0728
3152.0162		3172.3823		3174.8543
3189.4499		3190.2378		3213.3358

[i'6] C₁₃H₁₁, C₁, ²A

6	0	0.617913	0.200906	0.450625
6	0	-0.299833	-0.866500	0.354095
6	0	-1.640138	-0.610328	0.105265
6	0	-2.115019	0.707876	-0.055848
6	0	-1.229196	1.791959	0.032537
6	0	0.081490	1.462419	0.277738
6	0	2.091091	-0.033103	0.695663
6	0	2.922379	0.040692	-0.610519
6	0	-3.558814	0.652346	-0.298263
6	0	-2.807741	-1.559786	-0.034503
6	0	-3.968368	-0.628167	-0.290123
1	0	0.057085	-1.885049	0.485106
1	0	-1.563728	2.817420	-0.083205
1	0	2.239071	-1.013629	1.155420
1	0	2.476193	0.711384	1.396705
1	0	2.538783	-0.695084	-1.325745
1	0	-4.185050	1.520932	-0.457613
1	0	-2.962223	-2.161735	0.869800
1	0	-4.982805	-0.972537	-0.442222
6	0	4.346603	-0.191308	-0.389601
6	0	5.513925	-0.386718	-0.180785
1	0	6.547687	-0.556490	-0.005627
1	0	2.777427	1.023467	-1.071509
1	0	-2.668195	-2.270402	-0.858800

Frequencies

25.8431	57.3841	61.2326
150.4037	193.6023	221.0979
264.8165	310.7814	351.9270
405.7647	420.1755	426.8974
458.5394	541.3332	604.9030
632.1354	664.0326	674.8147
700.5551	736.1332	745.7583
769.1288	774.9769	856.1377
863.5578	878.8840	914.5507
948.7008	956.2888	962.3493
967.4658	1010.8347	1017.1614
1087.5626	1137.1018	1148.3659
1163.3402	1187.1676	1238.0468
1251.3096	1271.9201	1287.9306
1298.1511	1325.6616	1365.8980
1377.1622	1418.0305	1436.6072
1462.4677	1475.9026	1496.2747
1558.8046	1620.6860	1637.1746
2220.4503	3016.2355	3024.2577
3039.1109	3047.9661	3053.1029
3091.9113	3141.1791	3164.8304
3192.4204	3215.0765	3477.5654

[i'7] C₁₃H₁₁, C₁, ²A

6	0	-0.324347	1.452644	-0.059578
6	0	2.278400	-1.330190	-0.290050
6	0	-0.251294	-1.358528	-0.065929
6	0	-1.466325	-0.689906	-0.005539
6	0	-1.505571	0.716234	-0.006791
6	0	0.901756	0.780699	-0.113598
6	0	2.184269	1.522661	-0.125391
6	0	3.299427	0.860106	0.120893
6	0	3.445346	-0.585219	0.407887
6	0	0.941008	-0.633429	-0.123782
6	0	-2.880814	-1.215180	0.065399
6	0	-2.908913	1.134676	0.058801
6	0	-3.703659	0.051224	0.099442
1	0	-0.343339	2.537963	-0.050478
1	0	2.507952	-1.383374	-1.362757

1	0	2.223626	-2.360133	0.073725
1	0	-0.217430	-2.444482	-0.074358
1	0	2.160235	2.596784	-0.287215
1	0	4.401181	-0.982718	0.054197
1	0	3.418473	-0.744104	1.494683
1	0	-3.048976	-1.832398	0.957021
1	0	-3.238627	2.166045	0.072021
1	0	-4.784471	0.055667	0.150003
1	0	-3.134324	-1.843990	-0.797429

Frequencies

92.0760		124.7938		185.4197
255.5855		260.2380		307.5575
374.9967		397.1141		411.6938
422.1987		444.8280		522.6197
559.9496		638.6087		702.9477
719.7022		732.2053		754.3984
764.2783		779.5866		827.2894
864.3767		888.2202		892.8556
901.4110		929.7722		950.3812
955.3634		961.1661		974.2373
1021.0479		1065.6523		1112.8233
1146.5939		1172.0623		1178.7444
1196.6383		1212.2832		1236.4590
1244.3973		1275.1210		1297.0727
1320.2537		1328.4259		1361.1778
1376.1516		1436.7478		1453.8789
1467.7899		1477.0521		1499.9975
1578.1871		1625.3395		1650.3908
1688.1367		2992.2147		3001.2099
3014.4879		3036.6303		3055.9846
3063.3621		3142.8713		3147.9092
3159.9683		3189.3827		3213.5981

[i'8] C₁₃H₁₁, C_s, ²A''

6	0	0.311771	1.436537	0.000032
6	0	-2.222472	-1.452586	0.000091
6	0	0.297226	-1.374786	0.000061
6	0	1.496646	-0.681711	0.000159

6	0	1.503174	0.731145	0.000127
6	0	-0.918988	0.740838	0.000027
6	0	-2.166527	1.449208	-0.000045
6	0	-3.392867	0.764534	-0.000116
6	0	-3.455434	-0.602561	-0.000071
6	0	-0.916824	-0.681417	0.000053
6	0	2.924304	-1.174419	-0.000139
6	0	2.899469	1.177861	0.000080
6	0	3.717954	0.111866	-0.000153
1	0	0.305668	2.522023	-0.000014
1	0	-2.245192	-2.130912	0.868530
1	0	-2.245109	-2.131161	-0.868152
1	0	0.288880	-2.461783	0.000035
1	0	-2.149113	2.532982	-0.000078
1	0	-4.313885	1.339026	-0.000208
1	0	-4.414914	-1.108170	-0.000116
1	0	3.150385	-1.792416	-0.878675
1	0	3.150936	-1.792860	0.877913
1	0	4.799669	0.140480	-0.000119
1	0	3.208075	2.215751	0.000243

Frequencies

72.2141	116.5805	165.3467
254.3218	259.6955	310.1044
400.6193	405.7825	419.8417
425.5202	492.3428	559.5826
585.4616	635.3246	661.3105
709.3075	723.3503	746.6234
749.2109	776.8984	784.8426
859.9822	882.2178	890.5191
899.0744	938.0228	950.3026
955.7335	955.7675	963.1191
964.5835	1046.5286	1103.5171
1127.9455	1147.8607	1169.3633
1180.2847	1200.9499	1222.6510
1242.0134	1256.7794	1269.3929
1312.4356	1346.6626	1357.8798
1390.6820	1437.0080	1438.9281
1445.9265	1460.3952	1499.6899
1555.2448	1581.1370	1622.4995

1646.3857		2945.9360		2947.5565
3010.6828		3031.8721		3142.1595
3151.5327		3159.7944		3170.7215
3182.0276		3189.4014		3213.1242

Products

1H-cyclopenta-[b]naphthalene [P2] C₁₃H₁₀, C_s, 1A'

6	0	-3.4297275383	0.6926828295	0.0039083678
6	0	0.2561865651	-1.4034018581	-0.0085023831
6	0	-3.4192071452	-0.7206557811	-6.487593E-4
6	0	1.4301622887	-0.6884204437	-0.0080385742
6	0	0.2375332283	1.4304945887	5.892895E-4
6	0	1.4176697405	0.7420283073	-0.0034772169
6	0	-2.2463676634	1.3923572342	0.0043120379
6	0	-2.2271153712	-1.4039826096	-0.0046946993
6	0	-0.9977522925	0.720531113	2.165193E-4
6	0	-0.9860464949	-0.7144502301	-0.0044032352
6	0	2.8281081359	-1.1220833093	-0.0116269207
6	0	2.8483269174	1.2348432817	-0.004056437
6	0	3.6409965108	-0.0519460444	-0.0095010525
1	0	-4.3754448604	1.222915632	0.0070883174
1	0	0.2599391198	-2.4888289276	-0.0119952953
1	0	-4.3573702871	-1.2643043552	-9.374379E-4
1	0	0.217623734	2.5163608324	0.0041197655
1	0	-2.2529829395	2.477688416	0.0078122976
1	0	-2.2185160279	-2.4892073171	-0.0081914894
1	0	3.1434835396	-2.157922306	-0.0153885217
1	0	3.0748527551	1.8496933954	0.8759822814
1	0	3.072160391	1.8553276045	-0.8808330576
1	0	4.7229266941	-0.0789710526	-0.0107867963

Frequencies

102.2294		134.8645		251.8437
263.5800		278.6570		394.6986
405.8898		417.1671		426.3605
487.3719		559.6989		578.1974
628.8197		686.4746		732.6775
738.6653		751.4693		764.7804
783.4099		806.1723		857.4753
858.7720		890.3014		902.4118

913.7707	955.6878	957.5792
963.1137	970.5211	991.6628
1043.4534	1077.4282	1121.2771
1155.6730	1169.2853	1174.4788
1180.6497	1244.5385	1251.5039
1268.6960	1282.1901	1347.9739
1373.3697	1387.7710	1434.9787
1446.5223	1470.3410	1486.9167
1537.3526	1611.9868	1627.0456
1655.0763	1677.6805	3013.8854
3035.4208	3153.1920	3155.6051
3159.0651	3162.4123	3173.3962
3186.6618	3189.2638	3212.1926

1H-cyclopenta[*a*]naphthalene [P3] C₁₃H₁₀, C_s, ¹A'

6	0	3.3589805782	-0.1589532841	-0.0052741521
6	0	-0.8626124942	-0.4592216299	0.0061451685
6	0	2.7512244302	-1.4362419127	-0.0057558711
6	0	-1.6304316353	0.7002778521	0.0104255245
6	0	0.3504445096	2.0582620245	0.0073112859
6	0	-1.0208972146	1.9753841923	0.0110703316
6	0	2.58240266	0.9743296087	-0.0010636067
6	0	1.3828455855	-1.5556845697	-0.0020600345
6	0	1.1658232353	0.8928735063	0.0028576508
6	0	0.5497812064	-0.4047593755	0.0022898527
6	0	-3.0471181043	0.3231433831	0.013518318
6	0	-1.786615793	-1.65287093	0.0068930735
6	0	-3.1559300206	-1.0165005908	0.0115352725
1	0	4.4401442599	-0.0787740034	-0.00823888
1	0	3.372925776	-2.3247255603	-0.0090822067
1	0	0.8378607683	3.0277237362	0.0077226495
1	0	-1.6280620211	2.8741736402	0.0144845493
1	0	3.0467756867	1.9552584003	-6.703734E-4
1	0	0.9246806356	-2.5385591873	-0.0024656456
1	0	-3.8673579721	1.0301984874	0.0178637838
1	0	-1.6405804813	-2.2929696258	-0.8725833972
1	0	-1.6357579267	-2.2952054346	0.8839587431
1	0	-4.0761106684	-1.5851637269	0.0138329637

Frequencies

111.6057		140.7443		235.7064
237.2840		257.3698		398.3460
432.9203		435.8184		465.2515
517.6631		520.4055		551.8391
616.8391		670.8841		681.8888
717.6433		751.4780		760.5919
787.6060		828.8756		839.7089
870.5955		872.9566		937.1401
954.7419		955.4339		959.8592
969.6851		982.2343		991.7663
1043.6091		1060.8926		1117.9424
1144.2864		1166.9366		1179.2631
1185.6203		1233.5150		1244.7639
1263.9305		1288.3090		1363.9889
1378.3244		1398.4726		1416.6215
1434.3888		1470.0882		1487.4172
1552.8699		1587.7715		1621.6410
1637.3459		1664.1362		3014.2828
3037.1636		3156.0941		3158.7295
3163.7980		3176.1937		3177.0078
3187.4191		3190.5460		3215.9190

(E)-6-(but-1-en-3-yn-1-yl)-1H-indene [P6] C₁₃H₁₀, C_s, ¹A'				
6	0	0.658422	0.002137	-0.000145
6	0	-0.333062	-1.001011	-0.000143
6	0	-1.671187	-0.654180	-0.000142
6	0	-2.061256	0.699443	-0.000058
6	0	-1.092378	1.705594	-0.000073
6	0	0.250089	1.351307	-0.000143
6	0	2.059853	-0.409915	-0.000089
6	0	3.149735	0.385262	0.000017
6	0	4.478748	-0.104334	0.000114
6	0	5.622901	-0.486474	0.000202
6	0	-2.913241	-1.514276	-0.000025
6	0	-3.522593	0.756479	0.000219
6	0	-4.024269	-0.491967	0.000230
1	0	-0.030281	-2.043898	-0.000161
1	0	-1.378963	2.751727	-0.000027
1	0	0.996816	2.136433	-0.000181

1	0	2.226999	-1.483733	-0.000084
1	0	3.044791	1.466577	0.000039
1	0	6.626958	-0.832507	0.000178
1	0	-2.962498	-2.169866	-0.878511
1	0	-5.073510	-0.755979	0.000486
1	0	-4.098727	1.673175	0.000358
1	0	-2.962149	-2.170312	0.878117

Frequencies

42.9157		81.1724		90.2873
164.2416		209.8993		219.8334
298.4934		310.0383		394.9551
409.1366		428.1513		468.5369
508.4610		571.6992		601.4583
614.5102		640.2369		679.4867
706.5788		755.5357		762.8297
800.5242		835.2791		859.1374
866.5909		897.7669		942.0719
951.5885		955.8052		958.4509
966.9996		991.1371		1038.9222
1087.9708		1136.8482		1148.3601
1171.7773		1223.1273		1248.5745
1253.0242		1296.5698		1319.7943
1331.0501		1349.6969		1394.3906
1434.8369		1461.0457		1502.5962
1585.2607		1629.4557		1645.8185
1667.2320		2192.8918		3016.8829
3039.8340		3142.1278		3150.1471
3155.8150		3165.8536		3186.5309
3191.6192		3214.8150		3477.4300

6-(but-3-ene-1-yn-1-yl)-1H-indene [P7] C₁₃H₁₀, C_s, 1A'

6	0	0.000000	0.596652	0.000000
6	0	-1.403233	0.458704	0.000000
6	0	-2.003296	-0.794917	0.000000
6	0	-1.194987	-1.932143	0.000000
6	0	0.210395	-1.804947	0.000000
6	0	0.809532	-0.560823	0.000000
6	0	-1.525249	-3.356975	0.000000

6	0	-0.393951	-4.084901	0.000000
6	0	0.820091	-3.187491	0.000000
6	0	0.594552	1.887587	0.000000
6	0	1.093335	2.992125	0.000000
6	0	1.716364	4.264321	0.000000
6	0	1.069568	5.437977	0.000000
1	0	-2.012758	1.354195	0.000000
1	0	-3.084455	-0.880668	0.000000
1	0	1.888285	-0.452540	0.000000
1	0	-2.534048	-3.750159	0.000000
1	0	-0.333014	-5.165156	0.000000
1	0	1.454615	-3.359469	0.878356
1	0	1.454615	-3.359469	-0.878356
1	0	2.804309	4.259342	0.000000
1	0	1.616405	6.372836	0.000000
1	0	-0.012673	5.490068	0.000000

Frequencies

49.4975	61.8250	99.5978
166.9944	179.4692	210.0654
265.5520	339.4232	382.5588
384.4054	413.2267	450.3929
504.8386	549.3600	601.3854
609.9153	666.9862	688.8452
734.2738	755.7113	765.9189
844.7839	850.7163	885.5887
910.3171	955.6141	958.1626
971.7304	974.9741	990.9467
1004.3592	1014.1815	1082.8126
1106.8265	1151.4599	1160.9645
1175.0731	1254.4709	1258.8153
1305.8460	1308.0270	1321.0875
1354.1131	1400.9547	1417.5866
1440.9764	1480.3506	1494.9988
1529.5659	1543.8819	1589.7353
1656.5463	2203.1157	3028.2172
3053.4078	3154.9652	3159.7361
3195.6641	3199.6786	3210.9945
3213.9335	3230.7234	3256.3990

Transition states**[i'0a] → [i'1] C₁₃H₁₁, C₁, 2A**

6	0	0.406341	1.019195	-0.020563
6	0	-0.456152	2.089097	-0.125601
6	0	-1.832856	1.818014	-0.143156
6	0	-2.259093	0.492997	-0.053191
6	0	-1.329257	-0.563798	0.054075
6	0	0.040491	-0.308296	0.073048
6	0	-2.086074	-1.869930	0.133793
6	0	-3.605883	-0.086464	-0.046042
6	0	-3.527338	-1.423922	0.059296
1	0	-0.096695	3.110389	-0.195005
1	0	-2.547796	2.630664	-0.225168
1	0	0.775565	-1.102683	0.153826
1	0	-1.873220	-2.412988	1.063119
1	0	-1.824156	-2.548237	-0.687832
1	0	-4.518183	0.492660	-0.116202
1	0	-4.362864	-2.110797	0.089118
6	0	2.995815	1.386340	-0.100857
6	0	3.559567	0.371230	0.584905
6	0	3.929718	-0.871260	0.012075
6	0	4.254174	-1.940356	-0.443456
1	0	2.782223	2.327664	0.387904
1	0	2.857549	1.336403	-1.172951
1	0	3.728126	0.475393	1.653518
1	0	4.542729	-2.875549	-0.856289

Frequencies

-113.3941	18.4857	27.5133
40.3811	82.1787	170.5188
208.3829	213.6230	228.6298
360.2825	392.8758	401.5502
419.1716	528.7428	538.8661
558.6717	596.4474	627.2607
676.7173	697.9841	716.5019
738.3783	739.1932	805.4931
816.8815	859.2324	865.8132
894.5821	919.7666	937.1123
949.6328	955.1935	962.7010
983.0918	1038.9387	1086.5286

1112.3847	1128.7959	1147.1311
1163.7998	1212.7900	1240.5866
1286.1258	1305.7734	1323.4779
1379.3522	1416.7530	1435.6563
1435.8432	1462.6200	1572.0874
1607.1395	1609.6393	1638.7644
2183.5377	3017.2211	3040.1994
3141.5758	3153.4599	3157.0484
3161.1594	3169.2609	3189.6384
3213.3975	3249.8688	3476.1110

[i'1] → [P6] C₁₃H₁₁, C₁, ²A

6	0	0.630327	0.006657	0.088311
6	0	-0.357166	-0.997610	0.049038
6	0	-1.694077	-0.650586	-0.006263
6	0	-2.084393	0.703159	-0.015663
6	0	-1.117594	1.709238	0.034456
6	0	0.224502	1.354294	0.087696
6	0	2.038555	-0.402613	0.125053
6	0	3.120020	0.392649	-0.103709
6	0	4.447378	-0.084608	-0.140595
6	0	5.593204	-0.462435	-0.178999
6	0	-2.934426	-1.511101	-0.060781
6	0	-3.544784	0.759510	-0.075011
6	0	-4.045078	-0.489103	-0.102092
1	0	-0.054313	-2.040322	0.060517
1	0	-1.404250	2.755283	0.037923
1	0	0.970538	2.138173	0.142845
1	0	2.212739	-1.472504	0.186381
1	0	2.991793	1.460044	-0.257026
1	0	6.598650	-0.803297	-0.210455
1	0	2.206555	-0.590582	2.201397
1	0	-2.947367	-2.163923	-0.942532
1	0	-5.093240	-0.753672	-0.146477
1	0	-4.120934	1.675976	-0.093807
1	0	-3.018986	-2.169875	0.812582

Frequencies

-550.8601 44.7638 76.7265

88.3748	154.3240	209.4789
218.4651	246.7741	300.1233
326.2414	350.6162	395.0462
414.8763	427.8223	464.8793
509.2824	571.5536	602.8318
614.7294	639.9177	678.3105
707.1886	755.7185	763.8421
799.2602	835.0222	847.3893
866.2537	893.4282	941.0866
951.6845	956.7442	958.4368
967.4268	989.0394	1043.1460
1088.2101	1136.3718	1148.4223
1170.2539	1220.5100	1245.7586
1251.7061	1293.4800	1309.7227
1320.4497	1343.9226	1393.9498
1434.8190	1458.5413	1501.1457
1584.3468	1611.8045	1630.8272
1651.1334	2180.1707	3017.2296
3040.2281	3147.3651	3154.1508
3160.4300	3166.3092	3185.6363
3191.9592	3215.1432	3476.2192

[i'1] → [i'3] C₁₃H₁₁, C₁, ²A

6	0	0.617962	1.086964	0.085449
6	0	-0.319592	2.102321	-0.127175
6	0	-1.677078	1.790198	-0.233984
6	0	-2.091788	0.461194	-0.127309
6	0	-1.151990	-0.577908	0.090861
6	0	0.170024	-0.225525	0.186256
6	0	2.123797	1.218604	0.207476
6	0	2.619194	-0.176987	0.649011
6	0	3.694456	-0.778401	-0.068155
6	0	4.580515	-1.309000	-0.693383
1	0	0.004424	3.135631	-0.207546
1	0	2.418006	1.989319	0.926494
1	0	2.569986	1.489985	-0.753599
1	0	2.728201	-0.274009	1.731075
1	0	5.366502	-1.769621	-1.239402
6	0	-1.887614	-1.894209	0.163315
6	0	-3.422747	-0.148896	-0.198176

6	0	-3.326397	-1.479759	-0.035706
1	0	-1.549845	-2.594507	-0.610340
1	0	-4.338225	0.406997	-0.359000
1	0	-4.148881	-2.182625	-0.042313
1	0	1.514847	-0.793382	0.435508
1	0	-2.403714	2.578852	-0.397120
1	0	-1.733746	-2.398214	1.125365

Frequencies

-1655.8707		43.5849		92.3763
127.0059		191.8201		221.8022
244.8249		268.6024		376.8399
412.9522		417.8839		448.6821
477.6263		523.1360		552.1824
579.4151		606.5165		619.6509
666.2445		698.7910		740.9696
753.0693		797.5705		823.8335
849.5110		878.4443		926.3330
936.5521		947.8141		952.7900
961.3806		979.6255		1022.2011
1071.5288		1080.8521		1132.6694
1145.1457		1162.3032		1186.0599
1222.6447		1233.4991		1257.5861
1286.9638		1296.2665		1328.1858
1359.4360		1386.8449		1432.7136
1446.5877		1453.8015		1484.5675
1579.1141		1623.1824		1642.8757
1658.2534		2167.3807		3020.7595
3035.5741		3044.1915		3064.8050
3083.3695		3151.6279		3173.4396
3188.9584		3214.2651		3474.9971

[i'3] → [i'4] C₁₃H₁₁, C₁, ²A

6	0	-1.025413	0.852585	0.240589
6	0	-0.266797	2.011048	0.003195
6	0	1.119690	1.963485	-0.155694
6	0	1.768299	0.733536	-0.081382
6	0	1.024974	-0.451838	0.150222
6	0	-0.330573	-0.353195	0.312223

6	0	1.978462	-1.625175	0.167990
6	0	3.179282	0.361818	-0.211921
6	0	3.317113	-0.968213	-0.073416
6	0	-2.525567	0.930062	0.443928
6	0	-3.333030	-0.052345	-0.451502
6	0	-2.772502	-1.392089	-0.299804
6	0	-1.843352	-2.132237	-0.015749
1	0	-0.776745	2.968647	-0.052840
1	0	1.677533	2.875276	-0.339329
1	0	1.738684	-2.360533	-0.610435
1	0	1.951897	-2.162298	1.124164
1	0	3.980449	1.067572	-0.394276
1	0	4.246646	-1.519829	-0.123855
1	0	-2.873642	1.949224	0.255309
1	0	-2.762286	0.696176	1.487603
1	0	-3.271694	0.250576	-1.502695
1	0	-4.390305	-0.020150	-0.170616
1	0	-1.264053	-3.009327	0.154908

Frequencies

-373.7169	67.7407	87.6671
154.1190	194.0981	213.3771
292.3277	333.4670	356.6857
417.0651	441.7102	456.2145
466.9709	540.7529	590.2310
622.1669	654.0723	700.0999
705.1641	732.4491	749.9930
764.7393	827.6891	840.9211
868.3238	888.9210	937.8949
940.1318	952.3074	959.5071
978.8036	990.6930	1022.8894
1075.1608	1132.1344	1142.8863
1157.0764	1186.4386	1211.6879
1235.5455	1239.3208	1272.0639
1312.0145	1325.8333	1366.5078
1384.9988	1431.1158	1439.4519
1450.1166	1474.9854	1483.2586
1564.1641	1621.2159	1640.0736
2060.6455	3015.0372	3023.1789
3026.4607	3038.9392	3059.5241
3074.5486	3144.4834	3173.4392

3186.7479 3212.1283 3436.5647

[i'4] → [i'5] C₁₃H₁₁, C₁, ²A

6	0	-1.098967	0.852862	0.102409
6	0	-0.347331	2.020315	0.000228
6	0	1.048312	1.989629	-0.072644
6	0	1.690183	0.753356	-0.039360
6	0	0.943925	-0.435594	0.051944
6	0	-0.452033	-0.415838	0.122794
6	0	1.895913	-1.607333	0.039637
6	0	3.110942	0.398280	-0.101641
6	0	3.246266	-0.938120	-0.057199
6	0	-2.613207	0.905424	0.275546
6	0	-3.243995	-0.316917	-0.364097
6	0	-2.542192	-1.540345	-0.313141
6	0	-1.281570	-1.611268	0.225851
1	0	-0.859320	2.977628	-0.013162
1	0	1.613131	2.911807	-0.153495
1	0	1.811639	-2.224605	0.943778
1	0	1.708610	-2.279640	-0.807339
1	0	3.916930	1.117846	-0.174090
1	0	4.179127	-1.485669	-0.084550
1	0	-3.025262	1.821693	-0.155776
1	0	-2.853123	0.937136	1.348366
1	0	-4.067448	-0.202934	-1.065467
1	0	-3.691495	-1.370558	0.309788
1	0	-0.870262	-2.529408	0.629981

Frequencies

-1702.0983	102.1524	114.6402
189.2373	233.2466	245.3597
297.9707	404.5305	422.7118
449.2976	465.5399	477.5297
534.4221	598.6358	618.4442
639.8195	685.3965	713.0623
733.7070	743.8985	785.3794
818.6939	830.9579	840.7420
912.9372	931.3530	940.3265
946.1616	953.9384	961.3533
987.2645	1027.9886	1083.7413

1115.9028		1143.7859		1159.6523
1184.3475		1200.6438		1218.6546
1240.7777		1245.7015		1265.3637
1287.2341		1315.0646		1346.3750
1374.9890		1397.5565		1430.0217
1437.9586		1448.1227		1461.0650
1491.3126		1593.6316		1620.3219
1633.5640		2086.2271		2977.3810
3010.2040		3032.5131		3062.1033
3128.6210		3152.4791		3165.0551
3176.1361		3189.4268		3213.4805

[i'5] → [P3] C₁₃H₁₁, C₁, ²A

6	0	-1.108136	0.863708	-0.032745
6	0	-0.323453	2.043966	-0.058341
6	0	1.051515	1.992333	-0.053534
6	0	1.688986	0.733356	-0.018241
6	0	0.946190	-0.443031	0.006933
6	0	-0.466228	-0.418204	-0.003164
6	0	1.896012	-1.615880	0.040033
6	0	3.113512	0.387086	-0.001936
6	0	3.250721	-0.949416	0.031917
6	0	-2.537559	0.914776	-0.020457
1	0	-0.831911	3.002222	-0.075332
1	0	1.637232	2.904890	-0.074129
1	0	1.756640	-2.239570	0.932275
1	0	3.918238	1.111393	-0.014922
1	0	4.182925	-1.497686	0.051515
1	0	-3.021132	1.875378	-0.156652
1	0	-2.855940	1.334971	1.877631
6	0	-3.285494	-0.253078	-0.085654
6	0	-2.645950	-1.506126	-0.054974
6	0	-1.272415	-1.589590	-0.004438
1	0	-4.366871	-0.198399	-0.130114
1	0	-0.790481	-2.560608	0.018444
1	0	-3.242225	-2.411444	-0.077290
1	0	1.767322	-2.280555	-0.823823

Frequencies

-649.8645	109.0848	136.2622
226.7618	236.0127	252.1176
276.0125	352.0434	408.5551
434.3317	450.0075	465.9904
518.3310	537.6427	551.7296
616.6457	667.7983	681.4303
717.0251	749.0600	764.9057
795.8234	832.6098	839.5166
869.0842	883.0763	938.0351
955.7167	955.9607	964.9243
973.6390	981.1450	998.9466
1045.3275	1057.6205	1116.7689
1144.4799	1160.5928	1178.5283
1184.2764	1229.6508	1245.0675
1263.1922	1282.9418	1362.0693
1370.8056	1396.0496	1413.1785
1433.7977	1463.4314	1481.1701
1543.8592	1584.0924	1609.9530
1626.5058	1652.1148	3014.2360
3037.1605	3160.2662	3162.8406
3169.3373	3178.4429	3180.1201
3190.9237	3192.3202	3217.1715

[i'1] → [i'6] C₁₃H₁₁, C₁, 2A

6	0	0.615207	-0.631116	-0.161097
6	0	-0.583236	-1.336860	0.009724
6	0	-1.768505	-0.616654	0.070487
6	0	-1.781923	0.792915	-0.036868
6	0	-0.591000	1.510180	-0.209544
6	0	0.561613	0.751736	-0.260407
6	0	2.023357	-1.188302	-0.236209
6	0	2.913465	0.011714	-0.631061
6	0	4.082140	0.276540	0.142024
6	0	5.053246	0.527422	0.813794
6	0	-3.190712	-1.096673	0.246416
6	0	-3.172267	1.245951	0.064150
6	0	-3.984941	0.187391	0.224741
1	0	-0.582576	-2.420681	0.090450
1	0	-0.585383	2.591749	-0.293812

1	0	2.110357	-2.002524	-0.962422
1	0	2.336202	-1.588790	0.732441
1	0	3.095403	0.078748	-1.705487
1	0	5.911959	0.741571	1.400984
1	0	-3.327959	-1.643747	1.187713
1	0	-3.479842	2.282998	0.014429
1	0	-5.061664	0.220955	0.326557
1	0	2.023493	0.913648	-0.452225
1	0	-3.498657	-1.779392	-0.555524

Frequencies

-1648.8339	37.1813	99.5563
120.4714	192.8081	242.3887
261.1453	269.8259	357.6819
405.1807	406.7156	416.8302
437.7187	537.5411	590.6784
595.2044	619.0683	650.5508
666.3570	700.5708	741.8589
748.2476	763.1976	840.7919
861.2056	869.9739	880.9881
916.2022	950.7165	953.2179
959.0968	961.9232	1022.2984
1074.4359	1085.5542	1129.1109
1150.1364	1177.9794	1186.9236
1234.4315	1242.5718	1264.3713
1279.9205	1299.2946	1324.9840
1360.5340	1376.1166	1434.6317
1438.3183	1464.4948	1484.3004
1573.6403	1625.2815	1633.0300
1666.1448	2168.7638	3015.5854
3034.1725	3038.1856	3063.8142
3083.9765	3144.9524	3164.7618
3189.7879	3213.3134	3475.0806

[i'6] → [i'7] C₁₃H₁₁, C₁, ²A

6	0	0.882775	-0.611385	-0.286359
6	0	-0.314563	-1.331619	-0.114147
6	0	-1.522006	-0.656073	-0.008759

6	0	-1.572641	0.750346	-0.066247
6	0	-0.393859	1.491420	-0.227504
6	0	0.777213	0.774001	-0.340091
6	0	2.209504	-1.327681	-0.445691
6	0	3.329254	-0.802183	0.496532
6	0	3.409517	0.649866	0.363318
6	0	2.900545	1.721836	0.076764
6	0	-2.926896	-1.181240	0.178637
6	0	-2.970780	1.166446	0.076307
6	0	-3.753680	0.082411	0.216000
1	0	-0.282655	-2.417615	-0.070838
1	0	-0.411942	2.576606	-0.262238
1	0	2.562490	-1.208900	-1.475830
1	0	2.075255	-2.399201	-0.273225
1	0	3.104445	-1.059306	1.537689
1	0	4.277335	-1.287435	0.244833
1	0	2.751637	2.764121	-0.084054
1	0	-3.235466	-1.844087	-0.639708
1	0	-4.828714	0.084827	0.339389
1	0	-3.305546	2.196266	0.067812
1	0	-3.033138	-1.762143	1.103611

Frequencies

-371.1766	58.7457	95.2251
161.4240	199.4533	230.9795
285.8891	331.5506	344.9162
411.6843	419.7120	425.4316
496.9919	520.6460	588.1381
645.5849	654.9161	702.5513
719.6811	734.7236	748.2708
756.3946	846.6244	863.3109
865.0956	872.4077	880.9606
942.9689	949.4356	955.2494
960.0361	994.5564	1024.4209
1086.1181	1133.9804	1147.6143
1178.9876	1184.9164	1211.2631
1241.5694	1250.0753	1275.5114
1309.2303	1325.8932	1358.7606
1374.2458	1418.5436	1438.1731
1464.6137	1476.0175	1482.5991
1560.5585	1622.7017	1630.7185

2064.4971		3014.1004		3023.2278
3026.1145		3036.3787		3059.1801
3072.7530		3137.2304		3149.1335
3188.7764		3212.6303		3434.3959

[i'7] → [i'8] C₁₃H₁₁, C₁, ²A

6	0	0.311260	1.446584	0.062741
6	0	-2.263707	-1.380652	0.290440
6	0	0.266822	-1.368928	0.058743
6	0	1.473723	-0.685349	-0.001306
6	0	1.496638	0.724263	0.008201
6	0	-0.917709	0.764568	0.118871
6	0	-2.196676	1.461516	0.184739
6	0	-3.288784	0.828010	-0.357712
6	0	-3.368901	-0.581613	-0.373886
6	0	-0.931674	-0.657294	0.125719
6	0	2.893494	-1.194202	-0.076901
6	0	2.896068	1.156762	-0.054800
6	0	3.701989	0.082171	-0.102920
1	0	0.317599	2.531880	0.055297
1	0	-2.475713	-1.505469	1.362533
1	0	-2.214343	-2.389848	-0.128012
1	0	0.246998	-2.455297	0.065621
1	0	-2.236571	2.479331	0.557794
1	0	-4.048016	-1.068690	-1.070170
1	0	-4.246243	0.173313	0.272252
1	0	3.067284	-1.803904	-0.972914
1	0	3.155894	-1.826240	0.781214
1	0	4.782702	0.098405	-0.153699
1	0	3.215157	2.191512	-0.061483

Frequencies

-1698.5896	87.4406	124.5489
180.0663	257.6109	264.0195
315.3241	389.8565	405.3956
420.9263	432.8105	474.2866
539.3852	581.3885	639.7339
695.7748	716.0506	726.1078
746.9276	753.5358	764.9202

794.6612		819.2762		863.3797
886.2314		897.3286		923.5662
950.2851		953.5942		962.2635
983.7204		1049.2621		1093.9787
1114.3151		1147.0502		1171.4577
1183.2557		1205.3236		1212.4667
1241.7652		1256.1860		1263.3152
1297.2202		1311.5154		1341.8216
1356.7053		1393.2140		1437.1287
1439.5055		1456.3033		1462.3975
1499.6460		1572.9985		1622.3062
1643.0072		2086.7235		2975.2679
3011.6965		3033.1724		3058.8066
3126.5124		3146.8734		3159.2539
3163.3609		3189.5857		3213.5459

[i'8] → [P2] C₁₃H₁₁, C₁, ²A

6	0	0.306443	-1.447926	0.038574
6	0	-2.189494	1.363598	-0.029912
6	0	0.298743	1.383293	-0.051854
6	0	1.477741	0.689375	-0.032034
6	0	1.484610	-0.738771	0.016763
6	0	-0.931161	-0.752378	0.012451
6	0	-2.175382	-1.438557	0.008344
6	0	-3.368997	-0.753684	-0.056331
6	0	-3.380829	0.651541	-0.098810
6	0	-0.934298	0.679357	-0.029098
6	0	2.909397	1.176694	-0.047917
6	0	2.880673	-1.178386	0.034894
6	0	3.697434	-0.111871	-0.000432
1	0	0.304139	-2.532695	0.072808
1	0	-2.191834	2.437422	-0.178423
1	0	-2.290047	1.901264	1.856005
1	0	0.283795	2.468731	-0.077864
1	0	-2.169830	-2.523139	0.040272
1	0	-4.305860	-1.298773	-0.080866
1	0	-4.323117	1.183893	-0.155058
1	0	3.135542	1.825931	0.807069
1	0	3.137134	1.760619	-0.948552

1	0	3.191588	-2.214453	0.072225
1	0	4.779215	-0.142502	0.004550

Frequencies

-645.0918	101.2422	130.2764
245.6886	254.3178	260.9959
299.4987	354.7090	405.6628
406.9748	422.3041	426.1855
514.8715	561.6630	576.5665
626.5405	685.1844	732.1514
737.3089	752.2663	769.2219
789.0469	805.1457	857.4916
871.7685	889.7710	903.5553
914.3863	955.6264	957.3250
968.9253	974.2894	998.3680
1044.6468	1074.4091	1118.8989
1155.3329	1163.4957	1174.1717
1178.6142	1241.9891	1250.3140
1267.3796	1279.2591	1347.7605
1371.2412	1378.2204	1428.5712
1444.0594	1471.3515	1477.4004
1531.9252	1601.6605	1616.0670
1635.5296	1673.3176	3014.5358
3036.4261	3156.7875	3159.3180
3163.2972	3168.0065	3177.4607
3190.5855	3192.3979	3214.4504

[i'0b] → [i'2] C₁₃H₁₁, C₁, ²A

6	0	0.400138	0.673747	-0.443520
6	0	-0.162512	1.799852	0.119935
6	0	-1.512743	1.743678	0.495318
6	0	-2.220037	0.559256	0.288357
6	0	-1.595374	-0.568008	-0.287218
6	0	-0.254428	-0.523165	-0.663119
6	0	-2.605978	-1.688872	-0.379347
6	0	-3.613793	0.206720	0.576159
6	0	-3.850651	-1.063057	0.205029
1	0	0.414825	2.705315	0.273608
1	0	-1.992758	2.609364	0.941081

1	0	0.246581	-1.379902	-1.102588
1	0	-2.290185	-2.575453	0.184730
1	0	-2.761675	-2.019458	-1.413981
1	0	-4.332808	0.882109	1.022943
1	0	-4.791093	-1.589814	0.299385
6	0	3.515031	0.344272	-0.362586
6	0	2.784601	0.837461	-1.198468
6	0	4.287520	-0.211396	0.683131
6	0	4.649735	-1.500375	0.764635
1	0	2.373108	1.303814	-2.060300
1	0	4.599477	0.481204	1.461401
1	0	4.359654	-2.220193	0.008721
1	0	5.245824	-1.857666	1.595162

Frequencies

-203.5712	7.3180	22.5071
42.5542	70.9564	94.0173
207.6720	212.0170	230.2228
327.0747	390.7843	401.9622
416.3824	514.9294	542.3213
560.6472	581.6200	655.2967
670.0161	695.6261	698.8091
739.5462	740.2313	810.0079
825.4836	858.4625	860.0148
898.2581	936.6737	940.5438
948.5848	954.4234	962.3420
1001.2358	1036.8395	1086.2055
1111.4508	1128.5597	1146.2689
1162.6472	1212.0909	1240.3110
1284.9521	1315.3752	1323.1054
1379.5263	1414.9446	1436.2530
1440.9206	1461.8999	1573.2990
1607.9560	1638.0638	1642.0100
2114.6607	3016.0327	3038.8642
3134.7230	3147.9290	3153.4457
3157.1970	3169.8613	3188.6101
3212.7845	3238.0522	3458.1101

[i'2] → [P7] C₁₃H₁₁, C₁, ²A

6	0	0.550161	0.289052	0.152209
6	0	0.001253	1.581664	0.047246
6	0	-1.371703	1.772490	-0.064810
6	0	-2.210453	0.658196	-0.070332
6	0	-1.667999	-0.640016	0.038288
6	0	-0.305264	-0.831844	0.152346
6	0	1.969962	0.130976	0.239251
6	0	3.178543	0.171262	0.070421
6	0	4.586512	0.178545	-0.019651
6	0	5.334072	-0.871190	-0.396168
6	0	-2.799910	-1.640110	0.008724
6	0	-3.665124	0.539047	-0.170694
6	0	-4.017633	-0.758344	-0.127661
1	0	0.670573	2.433266	0.053039
1	0	-1.776486	2.775364	-0.145541
1	0	0.120675	-1.824112	0.245528
1	0	5.076504	1.113755	0.242380
1	0	4.884996	-1.819759	-0.664626
1	0	6.413672	-0.796641	-0.438032
1	0	2.029886	-1.002366	1.905683
1	0	-5.026745	-1.145064	-0.180901
1	0	-4.341517	1.379214	-0.264513
1	0	-2.836687	-2.248921	0.920724
1	0	-2.709366	-2.343096	-0.828753

Frequencies

-605.8972	35.6488	51.7989
81.5356	111.3311	166.0192
206.2708	212.0337	273.7931
323.1901	377.5899	392.0719
423.4483	442.3074	493.2497
518.4797	578.9379	602.5160
611.0373	688.3089	695.7077
708.8680	756.8853	764.6486
844.0301	858.4447	882.4161
895.1164	934.8838	953.5361
955.9479	960.7000	969.2156
985.9091	999.2884	1085.1686
1101.8650	1145.1500	1149.2547
1167.7527	1224.6463	1250.7957
1285.2932	1312.6973	1315.3150

1316.2182	1386.0351	1434.7910
1443.8598	1458.8433	1500.3501
1581.4227	1627.8658	1640.1227
1652.5376	2218.0056	3017.8049
3040.9107	3130.2133	3147.8757
3169.3382	3180.7336	3191.9565
3192.7422	3215.5611	3238.6665

References

1. R. B. Miller and J. M. Frincke, *J. Org. Chem.*, 1980, **45**, 5312-5315.
2. A. Hasan Howlader, K. Diaz, A. M. Mebel, R. I. Kaiser and S. F. Wnuk, *Tetrahedron Lett.*, 2020, DOI: <https://doi.org/10.1016/j.tetlet.2020.152427>, 152427.