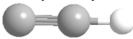
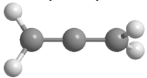
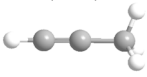
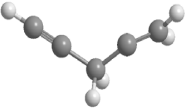
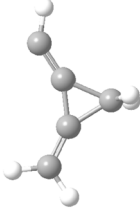
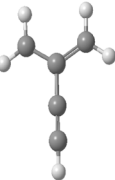
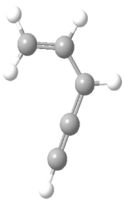
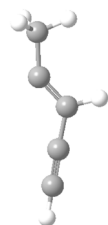


## Electronic Supplementary Information

**Table S1.** B3LYP and CCSD(T) calculated total energies at 0 K, zero-point energy corrections (ZPE), B3LYP/6-311G\*\* optimized Cartesian coordinates, unscaled vibrational frequencies ( $\nu_i$ ), and moments of inertia ( $I_i$ ) of all species involved in the  $C_2H + C_3H_4$  reaction.

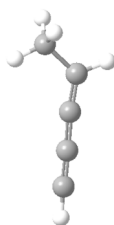
Species, (point group) electronic state	Energies, a.u.	$i$	$I_i$ , a.u.	Cartesian coordinates, angstroms				$\nu_i$ , $cm^{-1}$
				Atom	X	Y	Z	
<b>H (18-21)</b>	ZPE(B3LYP/6-311G**) = 0.0 E(B3LYP/6-311G**) = -0.502155930011 E(CCSD(T)/CC-PVDZ) = -0.499278 E(CCSD(T)/CC-PVTZ) = -0.49980982 E(CCSD(T)/CC-PVQZ) = -0.499946 E(CCSD(T)/CC-PV5Z) = -0.499995 E(CCSD(T)/CBS) = -0.49999							
<b>C<sub>2</sub>H</b> (C <sub>∞v</sub> ) 	ZPE(B3LYP/6-311G**) = 0.014445 E(B3LYP+ZPE) = -76.615013 E(CCSD(T)/CC-PVDZ) = -76.398687 E(CCSD(T)/CC-PVTZ) = -76.46769892 E(CCSD(T)/CC-PVQZ) = -76.4876915 E(CCSD(T)/CC-PV5Z) = -76.4936542 E(CCSD(T)/CBS) = -76.49585	A B C	0.00000 40.54466 40.54466	C H C	0.000000 0.000000 0.000000	0.000000 0.000000 0.000000	-0.473068 -1.536812 0.729203	370, 416, 2089, 3465
<b>CH<sub>2</sub>CCH<sub>2</sub></b> Allene (D <sub>2d</sub> ) 	ZPE(B3LYP/6-311G**) = 0.054873 E(B3LYP+ZPE) = -116.638325 E(CCSD(T)/CC-PVDZ) = -116.314014 E(CCSD(T)/CC-PVTZ) = -116.43338571 E(CCSD(T)/CC-PVQZ) = -116.466524 E(CCSD(T)/CC-PV5Z) = -116.476317 E(CCSD(T)/CBS) = -116.47946	A B C	12.21789 203.15738 203.15833	C C H H C H H	0.000002 1.306511 1.877635 1.877580 -1.306511 -1.877613 -1.877615	0.000014 0.000001 0.662901 -0.662926 -0.000037 -0.639697 0.639851	0.000058 -0.000019 0.639704 -0.639744 -0.000055 0.662927 -0.662796	369, 369, 896, 921, 921, 1055, 1108, 1466, 1508, 2041, 3114, 3116, 3187, 3187
<b>CH<sub>3</sub>CCH</b> Methyl Acetylene (C <sub>3v</sub> ) 	ZPE(B3LYP/6-311G**) = 0.055468 E(B3LYP+ZPE) = -116.635302 E(CCSD(T)/CC-PVDZ) = -116.315233 E(CCSD(T)/CC-PVTZ) = -116.43520449 E(CCSD(T)/CC-PVQZ) = -116.46871 E(CCSD(T)/CBS) = -116.4817	A B C	11.25810 210.15954 210.15977	C H C C H H H	-1.420160 -2.482190 -0.219254 1.238135 1.629948 1.629948 1.629969	-0.000001 -0.000004 0.000001 0.000001 1.011755 -0.386271 -0.625488	0.000001 0.000006 -0.000005 -0.000001 -0.138100 0.945252 -0.807125	339, 340, 666, 943, 1057, 1057, 1417, 1480, 1480, 2231, 3025, 3084, 3084, 3479
<b>HCCCH<sub>2</sub>CCH<sub>2</sub> (1)</b> (C <sub>1</sub> ) 	ZPE(B3LYP/6-311G**) = 0.075116 E(B3LYP+ZPE) = -193.341599 E(CCSD(T)/CC-PVTZ) = -192.99550682	A B C	88.19176 694.82838 747.59397	C C C H C C H H	-2.365351 -1.318329 -0.044912 -0.129227 1.114161 2.246218 2.542024 2.943916	-0.508426 0.077818 0.801351 1.657627 -0.033911 -0.440266 -0.174286 -1.061725	0.041871 0.026158 0.008989 -0.672050 -0.386572 0.125118 1.144727 -0.429228	89, 196, 316, 328, 434, 577, 669, 686, 859, 895, 909, 976, 1046, 1223, 1315, 1412, 1439, 1741, 2231, 2945, 3020, 3033, 3153, 3479

<b>CH<sub>2</sub>CCH<sub>2</sub>CCH (2)</b> (C <sub>s</sub> )	ZPE(B3LYP/6-311G**) = 0.075371	A	154.79121	H	-3.292194	-1.027136	0.053979	228, 292, 440, 473, 528, 672,
	E(B3LYP+ZPE) = -193.329691	B	414.62452	H	0.144756	1.226129	1.009186	703, 759, 792, 797, 816, 1037,
	E(CCS(D)(CC-PVTZ)) = -192.8706069	C	557.26723	C	1.864712	-0.790976	0.000436	1061, 1113, 1219, 1358, 1469,
				C	2.929174	-0.621528	0.001276	1500, 1783, 3142, 3143, 3234,
				C	0.763447	-0.117911	-0.000791	3234, 3246
				C	-0.653852	0.000629	-0.001027	
				C	-1.834567	-0.599390	0.000331	
				H	-2.754445	-0.025221	0.001721	
				H	-1.912396	-1.680414	-0.000044	
				C	0.096972	1.276890	0.000247	
				H	0.158070	1.854831	0.919553	
				H	0.159329	1.856887	-0.917688	
				H				
<b>HCCC(CH<sub>2</sub>)<sub>2</sub> (3)</b> (C <sub>2v</sub> )	ZPE(B3LYP/6-311G**) = 0.075198	A	172.72704	C	2.172908	0.000045	-0.001555	192, 265, 405, 526, 542, 571,
	E(B3LYP+ZPE) = -193.382714	B	438.31183	C	0.970003	-0.001116	0.002549	625, 657, 687, 767, 797, 800,
	E(CCS(D)(CC-PVTZ)) = -193.03509924	C	611.03798	C	-0.468552	-0.000015	0.000278	981, 1038, 1292, 1367, 1474,
				C	-1.136488	1.222109	-0.000241	1518, 2212, 3148, 3155, 3255,
				H	-0.595453	2.158006	0.001079	3257, 3477
				C	-1.138116	-1.221315	-0.000101	
				H	-0.598452	-2.158024	-0.000043	
				H	-2.220784	-1.250613	-0.001827	
				H	3.235223	-0.000981	-0.001871	
				H	-2.219064	1.253369	-0.002925	
				C	-2.326649	-0.411202	-0.129762	90, 190, 335, 372, 489, 666,
				C	-1.255792	0.127744	-0.053153	678, 682, 806, 843, 935, 968,
				C	0.055066	0.763763	0.052778	1016, 1206, 1271, 1317, 1464,
<b>HCCCH<sub>2</sub>CHCH (4)</b> (C <sub>1</sub> )	ZPE(B3LYP/6-311G**) = 0.075444	A	91.02892	C	-2.326649	-0.411202	-0.129762	1668, 2222, 3014, 3064, 3107,
	E(B3LYP+ZPE) = -193.336569	B	670.89859	C	-1.255792	0.127744	-0.053153	3236, 3477
	E(CCS(D)(CC-PVTZ)) = -192.99220308	C	704.65729	C	0.055066	0.763763	0.052778	
				H	0.304313	1.262707	-0.887986	
				C	1.159866	-0.229627	0.423064	
				C	2.245624	-0.427191	-0.274200	
				H	2.701276	-0.074222	-1.187797	
				H	-3.274741	-0.884725	-0.202589	
				H	0.013410	1.543497	0.823386	
				H	0.987057	-0.788181	1.342623	
<b>CHCCHCHCH<sub>2</sub> (5)</b> (C <sub>s</sub> )	ZPE(B3LYP/6-311G**) = 0.075850	A	130.93286	C	2.189719	2.189719	0.000000	158, 225, 383, 435, 559, 562,
	E(B3LYP+ZPE) = -193.394519	B	530.92725	H	3.087318	3.087318	0.000000	651, 667, 736, 863, 943, 997,
	E(CCS(D)(CC-PVTZ)) = -193.04363509	C	661.86011	C	1.167048	1.167048	0.000000	1037, 1159, 1260, 1415, 1434,
				C	0.000000	0.000000	0.000000	1544, 2104, 3143, 3146, 3164,
				H	0.120051	0.120051	0.000000	3240, 3471
				C	-1.309155	-1.309155	0.000000	
				H	-2.114271	-2.114271	0.000000	
				C	-1.638382	-1.638382	0.000000	
				H	-2.673087	-2.673087	0.000000	
				H	-0.875400	-0.875400	0.000000	
				C	2.618037	-0.254102	-0.000165	148, 154, 199, 328, 409, 526,
				C	1.458463	0.070739	0.000131	626, 684, 789, 889, 1042,
				C	0.104738	0.511669	-0.000252	1046, 1059, 1284, 1397, 1451,
<b>CHCCHCCH<sub>3</sub> (6)</b> (C <sub>s</sub> )	ZPE(B3LYP/6-311G**) = 0.075191	A	40.27641	C	-2.417319	-0.161949	0.000401	1471, 1727, 2206, 2966, 3009,
	E(B3LYP+ZPE) = -193.352873	B	812.27235	C				
	E(CCS(D)(CC-PVTZ)) = -193.00374491	C	841.34594	C				



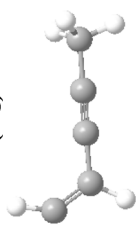
**CHCCCHCH<sub>3</sub> (7)**  
(C<sub>s</sub>)

ZPE(B3LYP/6-311G**) = 0.074183	A	47.69908	-2.731697	0.893098	0.001892	3048, 3070, 3478
E(B3LYP+ZPE) = -193.371149	B	805.87018	-2.852785	-0.642014	-0.881971	
E(CCSD(T)/CC-PVTZ) = -193.01445218	C	842.40451	-2.851289	-0.644147	0.882316	
			3.635758	-0.557674	0.001956	
			-0.045599	1.598469	0.000546	
			2.669314	-0.207850	0.000349	54, 144, 226, 292, 379, 440,
			1.457646	0.013512	-0.000077	512, 610, 721, 788, 1035,
			0.154860	0.214972	-0.001572	1048, 1087, 1324, 1399, 1482,
			-1.112963	0.539260	0.000338	1487, 1810, 2010, 3016, 3046,
			-2.269943	-0.429323	0.000225	3063, 3120, 3469
			-1.925628	-1.463697	-0.001322	
			-2.900626	-0.271043	0.881681	
			-2.902385	-0.268972	-0.879594	
			3.717227	-0.379286	0.001744	
			-1.382060	1.599571	0.001919	



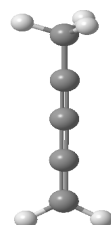
**CHCHCCCH<sub>3</sub> (8)**  
(C<sub>1</sub>)

ZPE(B3LYP/6-311G**) = 0.075493	A	51.97354	-2.472756	0.159901	-0.000048	29, 139, 194, 313, 388, 501,
E(B3LYP+ZPE) = -193.350468	B	805.72700	-2.773300	0.796914	-0.837438	694, 718, 873, 911, 1050,
E(CCSD(T)/CC-PVTZ) = -193.00216449	C	846.45706	-3.016444	-0.785306	-0.085878	1054, 1178, 1268, 1416, 1478,
			-1.033433	-0.061081	-0.000112	1478, 1623, 2330, 3020, 3075,
			0.160479	-0.236549	0.000103	3081, 3087, 3237
			1.568754	-0.469596	0.000007	
			1.892762	-1.511266	-0.000069	
			2.476585	0.487705	-0.000023	
			2.495092	1.567891	0.000052	
			-2.795878	0.6494890	0.923768	



**CH<sub>2</sub>CCCCCH<sub>3</sub> (9)**  
(C<sub>1</sub>)

ZPE(B3LYP/6-311G**) = 0.073725	A	17.41919	2.606751	0.004845	0.000011	26, 56, 136, 143, 324, 358,
E(B3LYP+ZPE) = -193.378718	B	924.78311	3.003110	-0.480185	0.898428	550, 675, 871, 980, 1027,
E(CCSD(T)/CC-PVTZ) = -193.01947811	C	930.95599	3.002317	1.027154	-0.028634	1039, 1142, 1411, 1444, 1465,
			1.156707	-0.009818	-0.000198	1471, 1859, 2101, 3000, 3049,
			-0.077120	-0.002344	-0.000034	3057, 3064, 3114
			-1.394209	0.002666	-0.000018	
			-2.700866	0.001581	0.000010	
			-3.280050	0.925357	0.000074	
			3.005384	-0.530542	-0.868576	
			-3.278347	-0.923363	0.000080	

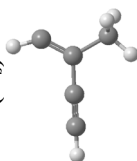


**HCCCHCCH<sub>3</sub> (10)**  
(C<sub>s</sub>)

ZPE(B3LYP/6-311G**) = 0.075191	A	40.27641	2.618037	-0.254102	-0.000165	148, 154, 199, 328, 409, 526,
E(B3LYP+ZPE) = -193.352873	B	812.27235	1.458463	0.070739	0.000131	626, 684, 789, 889, 1042,
E(CCSD(T)/CC-PVTZ) = -193.00374491	C	841.34594	0.104738	0.511669	-0.000252	1046, 1059, 1284, 1397, 1451,
			-0.956317	-0.274313	-0.000904	1471, 1727, 2206, 2966, 3009,
			-2.417319	-0.161949	0.000401	3048, 3070, 3478
			-2.731697	0.893098	0.001892	
			-2.852785	-0.642014	-0.881971	
			-2.851289	-0.644147	0.882316	
			3.635758	-0.557674	0.001956	
			-0.045599	1.598469	0.000546	

### HCCC(CH)CH<sub>3</sub> (11)

(C<sub>s</sub>)



ZPE(B3LYP/6-311G\*\*) = 0.075097  
E(B3LYP+ZPE) = -193.34202  
E(CCSD(T)/CC-PVTZ) = -192.99616215

C 184.90177  
C 437.53394  
C 611.18936

0.606730  
0.337147  
0.000000  
0.972514  
2.051922  
-1.476434  
-1.718437  
-1.718437  
-2.103331  
0.848539

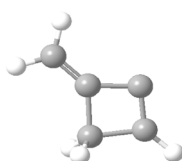
-2.071418  
-0.896757  
0.495810  
1.390987  
1.392526  
0.878336  
1.472235  
1.472235  
-0.013036  
-3.105709

0.000000  
0.000000  
0.000000  
0.000000  
0.000000  
0.000000  
0.883862  
-0.883862  
0.000000  
0.000000

171, 179, 271, 369, 532, 539,  
643, 678, 692, 771, 853, 1029,  
1053, 1194, 1404, 1481, 1482,  
1642, 2191, 3031, 3089, 3124,  
3242, 3476

### CH<sub>2</sub>CCCHCH<sub>2</sub> (12)

(C<sub>s</sub>)



ZPE(B3LYP/6-311G\*\*) = 0.078256  
E(B3LYP+ZPE) = -193.34283  
E(CCSD(T)/CC-PVTZ) = -193.00216744

A 123.22462  
B 369.83729  
C 481.36137

0.000132  
-0.000202  
-0.000230  
-0.083550  
-0.000019  
0.901971  
0.000014  
0.000016  
-0.000035  
-0.901094  
-0.000122

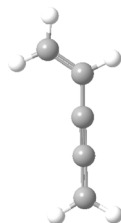
-0.044439  
0.897963  
-0.083550  
0.970073  
1.588447  
-0.228937  
-1.082677  
-0.956071  
1.589700  
-0.302864

0.000132  
-0.000202  
-0.000230  
-0.083550  
-0.000019  
0.901971  
0.000014  
0.000016  
-0.000035  
-0.901094  
-0.000122

219, 350, 525, 714, 715, 771,  
837, 891, 899, 955, 981, 1086,  
1099, 1180, 1219, 1432, 1459,  
1563, 1740, 3023, 3085, 3140,  
3224, 3243

### CH<sub>2</sub>CCCHCH<sub>2</sub> (13)

(C<sub>s</sub>)



ZPE(B3LYP/6-311G\*\*) = 0.075347  
E(B3LYP+ZPE) = -193.395824  
E(CCSD(T)/CC-PVTZ) = -193.03902804

A 46.81254  
B 793.15635  
C 839.96877

-2.566363  
-2.966951  
-3.271326  
-1.236092  
-0.014198  
1.355027  
1.654973  
2.319247  
3.367615  
2.069961

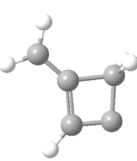
0.178257  
1.185527  
-0.645291  
-0.042967  
-0.235980  
-0.487221  
-1.533577  
0.467164  
0.196571  
1.521248

-0.000250  
0.000372  
-0.000475  
0.000839  
-0.000688  
-0.000019  
0.000644  
-0.000013  
0.000483  
-0.000240

143, 178, 312, 330, 447, 536,  
645, 749, 769, 893, 978, 1031,  
1067, 1284, 1314, 1435, 1492,  
1568, 2047, 3122, 3131, 3147,  
3215, 3242

### CH<sub>2</sub>CCHCCH<sub>2</sub> (14)

(C<sub>s</sub>)



ZPE(B3LYP/6-311G\*\*) = 0.078278  
E(B3LYP+ZPE) = -193.341591  
E(CCSD(T)/CC-PVTZ) = -192.63246835

A 150.84209  
B 326.46169  
C 465.73102

1.790073  
2.373878  
0.459008  
-0.618607  
-0.653868  
-1.528814  
-0.576232  
-0.545485  
2.326826  
-0.653918

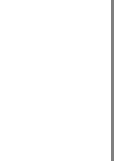
0.003270  
0.916533  
0.035917  
-1.072974  
-1.693831  
0.149237  
1.091317  
2.170652  
-0.938055  
-1.695897

0.000089  
-0.000198  
-0.000265  
0.000182  
0.897510  
-0.000484  
0.000213  
0.000532  
-0.000576  
-0.895680

209, 351, 461, 692, 711, 828,  
841, 876, 907, 999, 1059,  
1125, 1148, 1215, 1436, 1470,  
1558, 1711, 3059, 3109, 3137,  
3224, 3235

### CH<sub>2</sub>CCHCCH<sub>2</sub> (15)

(C<sub>s</sub>)



ZPE(B3LYP/6-311G\*\*) = 0.073680  
E(B3LYP+ZPE) = -193.568438  
E(CCSD(T)/CC-PVTZ) = -192.40831791

A 74.21263  
B 739.56529  
C 789.16665

-2.371748  
-2.882372  
-1.207599  
-0.000320  
1.211277  
2.370167  
2.892596

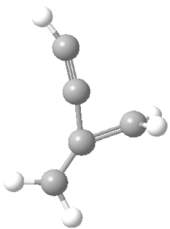
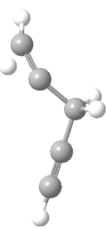
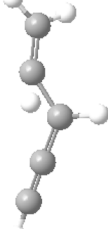
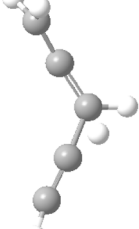
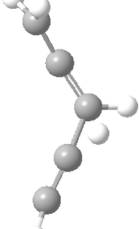
-0.437567  
-0.692966  
0.135452  
0.755923  
0.143743  
-0.439846  
-0.704762

0.002227  
0.931639  
-0.008520  
0.000286  
0.007565  
-0.002098  
0.917902

122, 134, 154, 351, 435, 497,  
611, 868, 893, 895, 945, 975,  
979, 1042, 1330, 1437, 1453,  
1874, 1929, 3053, 3057, 3088,  
3109, 3110

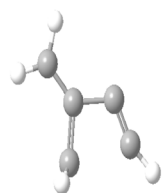


 <b>CH3CCH3 (21)</b> (C <sub>3v</sub> )	E(CCSO(T)/CC-PVQZ) = -192.982539 E(CCSO(T)/CBS) = -193.00419	3.138402 -0.000017 0.000518 -3.138138 0.000067	-1.141487 0.869907 1.529935 -1.141860 1.529532	0.000724 0.000038 -0.875961 -0.000367 0.876324	3013, 3037, 3477, 3478,
 <b>CH3CCH3 (21)</b> (C <sub>3v</sub> )	ZPE(B3LYP/6-311G**) = 0.065682 E(B3LYP+ZPE) = -192.800155 E(CCSO(T)/CC-PVDZ) = -192.755153 E(CCSO(T)/CC-PVTZ) = -192.4454355 E(CCSO(T)/CC-PVQZ) = -192.998799 E(CCSO(T)/CBS) = -193.0198	A B C	11.27539 882.41245 882.41455	-0.001382 -0.817579 0.003766 -0.000120 0.000239 0.001426 -0.129842 1.018489 -0.000386 0.001796 -0.392110	148, 148, 335, 335, 539, 540, 643, 644, 680, 1047, 1048, 1182, 1413, 1473, 1474, 2167, 2351, 3022, 3081, 3083, 3479
 <b>CH3 (22)</b> (D <sub>3h</sub> )	ZPE(B3LYP/6-311G**) = 0.029569 E(B3LYP+ZPE) = -39.853757 E(CCSO(T)/CC-PVDZ) = -39.715785 E(CCSO(T)/CC-PVTZ) = -39.760817 E(CCSO(T)/CC-PVQZ) = -39.772271 E(CCSO(T)/CC-PV5Z) = -39.775614 E(CCSO(T)/CBS) = -39.77618	A B C	6.30449 6.30449 12.60896	0.000000 0.000000 1.080657 -0.540328 -0.540328	501, 1402, 1402, 3108, 3288, 3288
 <b>HC4H (22)</b> (C <sub>∞v</sub> )	ZPE(B3LYP/6-311G**) = 0.037493 E(B3LYP+ZPE) = -153.528449693 E(CCSO(T)/CC-PVDZ) = -153.047959522 E(CCSO(T)/CC-PVTZ) = -153.195968803 E(CCSO(T)/CC-PVQZ) = -153.2379899667 E(CCSO(T)/CC-PV5Z) = -153.250397472 E(CCSO(T)/CBS) = -153.25465	A B C	0.000000 408.53335 408.53335	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 -1.889186 -2.951597	235, 236, 527, 527, 663, 663, 663, 663, 917, 2111, 2285, 3475, 3477
 <b>C2H2 (23)</b> (D <sub>∞h</sub> )	ZPE(B3LYP/6-311G**) = 0.026978 E(B3LYP+ZPE) = -77.354698 E(CCSO(T)/CC-PVDZ) = -77.108671 E(CCSO(T)/CC-PVTZ) = -77.187388 E(CCSO(T)/CC-PVQZ) = -77.20918 E(CCSO(T)/CC-PV5Z) = -77.215664 E(CCSO(T)/CBS) = -77.21752	A B C	0.000000 50.62104 50.62104	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.599026 1.661350 -0.599026 -1.661350	642, 642, 773, 773, 2071, 3420, 3523
 <b>C3H3 (23)</b> (C <sub>2v</sub> )	ZPE(B3LYP/6-311G**) = 0.040938 E(B3LYP+ZPE) = -116.037356 E(CCSO(T)/CC-PVDZ) = -115.662911 E(CCSO(T)/CC-PVTZ) = -115.777715 E(CCSO(T)/CC-PVQZ) = -115.810061 E(CCSO(T)/CC-PV5Z) = -115.819593 E(CCSO(T)/CBS) = -115.82275	A B C	6.22440 188.46833 194.69273	-0.000031 0.929996 -0.929830 -0.000114 -0.000084 -0.000056 -0.000042 0.000445	352, 403, 468, 638, 681, 1031, 1089, 1455, 2013, 3140, 3230, 3469
 <b>TS 1</b> (C <sub>1</sub> )	ZPE(B3LYP/6-311G**) = 0.075117 E(B3LYP+ZPE) = -193.341599 E(CCSO(T)/CC-PVTZ) = -192.99550331	A B C	88.25421 694.68250 747.44558	-0.508112 -1.030182 0.077640 -0.032652 -0.440886 -0.179149 -1.059414 -0.430676 0.801484 1.225108	683i, 135, 190, 317, 355, 489, 509, 689, 853, 907, 938, 957, 1025, 1118, 1193, 1428, 1444, 1765, 1965, 3014, 3043, 3070, 3149, 3410

<b>TS 2</b> <b>(C<sub>s</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.072708	A	161.50255	H	0.129493	1.658787	-0.670313	633i, 208, 245, 312, 390, 419, 611, 678, 768, 796, 850, 916, 950, 1021, 1168, 1417, 1451, 1704, 1904, 3123, 3141, 3228, 3233, 3385
		E(B3LYP+ZPE) = -193.323918							
		E(CCS(D)(T)(CC-PVTZ)) = -192.9694158							
<b>TS 3</b> <b>(C<sub>1</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.068827	A	87.54154	C	-2.358826	-0.498711	0.059510	1612i, 127, 144, 287, 374, 443, 518, 589, 680, 725, 768, 869, 1003, 1013, 1267, 1430, 1466, 1759, 1939, 2034, 3058, 3143, 3149, 3231
		E(B3LYP+ZPE) = -193.265084							
		E(CCS(D)(T)(CC-PVTZ)) = -192.91262339							
<b>TS 4</b> <b>(C<sub>1</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.070135	A	57.91029	C	2.494666	-0.361986	-0.077479	1936i, 130, 211, 313, 374, 504, 588, 658, 697, 822, 871, 914, 1015, 1086, 1127, 1283, 1434, 1686, 2108, 2182, 3058, 3071, 3177, 3476
		E(B3LYP+ZPE) = -193.284176							
		E(CCS(D)(T)(CC-PVTZ)) = -192.92729569							
<b>TS 5</b> <b>(C<sub>1</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.067262	A	81.86631	C	-2.359856	-0.529603	-0.108710	1683i, 126, 179, 326, 359, 425, 559, 614, 645, 753, 896, 902, 954, 993, 1100, 1206, 1340, 1449, 1908, 2044, 3054, 3127, 3133, 3433
		E(B3LYP+ZPE) = -193.274281							
		E(CCS(D)(T)(CC-PVTZ)) = -192.90903759							
<b>TS 6</b> <b>(C<sub>s</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.068305	A	21.09378	C	2.580507	-0.044832	-0.000010	2122i, 22, 137, 140, 228, 289, 369, 477, 583, 662, 851, 1044, 1045, 1141, 1413, 1471, 1475, 1868, 2258, 2316, 3013, 3041, 3066, 3074
		E(B3LYP+ZPE) = -193.288697							
		E(CCS(D)(T)(CC-PVTZ)) = -192.92781170							







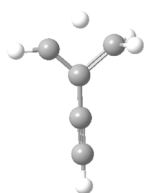
E(CSD(T)/CC-PVQZ) = -193.00753348  
E(CSD(T)/CBS) = -193.00753348

C -0.215373 1.258555 0.000033 1711, 1736, 3107, 3144, 3217,  
H -0.275686 1.817948 -0.928366 3232, 3371  
C -1.743812 -0.359047 -0.000116  
C -0.626783 -0.946300 0.000143  
H -0.276798 1.817178 0.928813  
H -2.808262 -0.245409 -0.000593

**TS 12**  
(C<sub>s</sub>)

ZPE(B3LYP/6-311G\*\*) = 0.069824  
E(B3LYP+ZPE) = -193.285473  
E(CSD(T)/CC-PVTZ) = -192.93245570

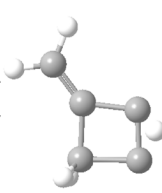
C -2.276147 -0.096972 0.000101 2152i, 185, 236, 461, 511,  
C -1.076117 0.014637 -0.000192 524, 569, 659, 670, 713, 849,  
C 0.335326 0.107221 -0.000243 954, 984, 1047, 1102, 1210,  
C 1.174858 1.141623 -0.000036 1420, 1639, 1857, 2202, 3069,  
H 1.100997 2.226368 0.000792 3145, 3169, 3476  
C 1.355967 -1.005919 0.000121  
H 1.488614 -1.571173 0.921463  
H 1.489602 -1.570591 -0.921451  
H -3.334811 -0.185708 0.000285  
H 2.172274 0.137568 0.000397



**TS 13**  
(C<sub>1</sub>)

ZPE(B3LYP/6-311G\*\*) = 0.07173  
E(B3LYP+ZPE) = -193.246693  
E(CSD(T)/CC-PVTZ) = -192.896689

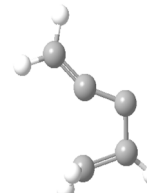
C -1.860758 -0.068880 0.012333 941i, 179, 350, 430, 467, 715,  
H -2.378542 -1.020663 -0.011915 724, 841, 854, 876, 941, 947,  
C -0.539836 -0.015132 -0.027518 1101, 1143, 1156, 1401, 1423,  
C 0.575462 1.005104 0.015570 1438, 1735, 2208, 3063, 3134,  
H 0.662368 1.610343 0.917829 3137, 3224  
C 1.635647 -0.210197 -0.072790  
C 0.561082 -1.051622 -0.100959  
H 1.254861 -0.996569 0.946444  
H -2.461058 0.833034 0.067295  
H 0.692782 1.618214 -0.879470



**TS 14**  
(C<sub>1</sub>)

ZPE(B3LYP/6-311G\*\*) = 0.074465  
E(B3LYP+ZPE) = -193.301102  
E(CSD(T)/CC-PVDZ) = -192.76351055  
E(CSD(T)/CC-PVTZ) = -192.95052295  
E(CSD(T)/CC-PVQZ) = -193.00443295  
E(CSD(T)/CBS) = -193.02627

C 1.998726 0.171867 -0.085620 682i, 208, 264, 515, 531, 604,  
H 2.320809 1.196109 0.052090 713, 819, 835, 851, 965, 987,  
C 0.748560 -0.191293 0.099829 1019, 1126, 1263, 1416, 1455,  
C -1.063626 0.994006 0.020964 1523, 1797, 3075, 3123, 3186,  
H -1.335456 1.729675 -0.737722 3198, 3215  
C -1.460051 -0.404611 -0.094692  
C -0.299050 -1.062667 0.136555  
H 2.74657 -0.557174 -0.390455  
H -0.854602 1.388310 1.007905  
H -2.422761 -0.800734 -0.394028



**TS 15**  
(C<sub>1</sub>)

ZPE(B3LYP/6-311G\*\*) = 0.074698  
E(B3LYP+ZPE) = -193.298423  
E(CSD(T)/CC-PVTZ) = -192.94847058

C 1.878758 -0.329586 -0.075733 638i, 219, 283, 406, 579, 656,  
H 2.627868 0.307357 -0.544214 702, 815, 870, 918, 961, 1011,  
C 0.664089 0.129587 0.142020 1038, 1134, 1270, 1422, 1478,  
C -1.179516 -0.983960 0.035942 1511, 1758, 3094, 3094, 3175,  
H -1.087354 -1.301227 1.070703 3195, 3200  
C -1.393827 0.366367 -0.232371  
C -0.311540 1.134753 0.076281  
H -0.214096 2.195820 0.266797  
H 2.179510 -1.333730 0.195287  
H -1.453713 -1.771187 -0.665405

**TS 16**  
**(C<sub>1</sub>)**

ZPE(B3LYP/6-311G\*\*) = 0.071515  
E(B3LYP+ZPE) = -193.259869  
E(CCSD(T)/CC-PVTZ) = -192.9106839

A 130.36624  
B 358.14053  
C 481.03667

C 1.860319  
H 2.476132  
C 0.527203  
C -0.627028  
H -1.408461  
C -1.637400  
C -0.498831  
H -0.468989  
H 2.366149  
H -0.710411

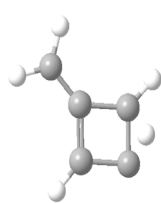
0.020885  
0.037863  
-0.031417  
-0.055842  
0.949009  
-0.062226  
-0.009860  
0.027460  
0.045727  
-0.229300

-0.066162  
0.826078  
0.017086  
-0.954280  
-0.758413  
0.088934  
1.054934  
2.137110  
-1.024264  
-2.023578

-0.576070  
-0.300226  
-0.013847  
0.021556  
-0.032601  
-0.789094  
0.662657  
1.049823  
1.156714

0.052075  
0.434838  
0.036033  
-0.178784  
-0.001360  
0.071153  
-0.488090  
-0.315014  
-0.182406

2093i, 199, 341, 453, 654,  
708, 719, 806, 861, 912, 920,  
946, 1073, 1160, 1202, 1263,  
1293, 1438, 1681, 2039, 3139,  
3161, 3195, 3227



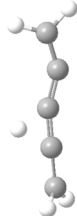
**TS 17**  
**(C<sub>1</sub>)**

ZPE(B3LYP/6-311G\*\*) = 0.068384  
E(B3LYP+ZPE) = -193.28886  
E(CCSD(T)/CC-PVTZ) = -192.91833706

A 23.25507  
B 862.07388  
C 874.49871

C 2.581159  
H 3.362945  
C 1.315894  
C 0.032321  
C -1.254093  
C -2.585847  
H -3.123527  
H -3.152109  
H 2.905970  
H -0.529877

1612i, 127, 144, 287, 374,  
443, 518, 589, 680, 725, 768,  
869, 1003, 1013, 1267, 1430,  
1466, 1759, 1939, 2034, 3058,  
3143, 3149, 3231



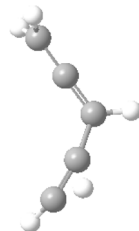
**TS 18**  
**(C<sub>1</sub>)**

ZPE(B3LYP/6-311G\*\*) = 0.068079  
E(B3LYP+ZPE) = -193.280253  
E(CCSD(T)/CC-PVTZ) = -192.918796

A 91.33058  
B 686.67776  
C 750.65042

C 2.279424  
H 2.743234  
C 1.268156  
C -0.004758  
C -1.154719  
C -2.285842  
H -2.772683  
H -2.790106  
H 2.211326  
H -0.005341

2093i, 91, 183, 277, 281, 314,  
504, 606, 647, 823, 861, 879,  
914, 1003, 1099, 1328, 1458,  
1886, 1994, 2319, 3038, 3094,  
3124, 3161



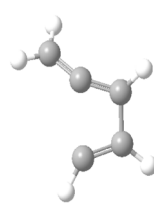
**TS 19**  
**(C<sub>1</sub>)**

ZPE(B3LYP/6-311G\*\*) = 0.073879  
E(B3LYP+ZPE) = -193.314200  
E(CCSD(T)/CC-PVTZ) = -192.96311109

A 141.53011  
B 418.37554  
C 543.13004

C -1.973096  
H -2.621665  
C -0.742695  
C 0.312195  
C 1.466643  
C 1.069182  
H -2.368345  
H 2.415410  
H 1.485836  
H 0.295388

674i, 241, 270, 448, 583, 640,  
719, 766, 839, 856, 899, 989,  
1024, 1043, 1218, 1332, 1439,  
1515, 1828, 3109, 3130, 3158,  
3190, 3194



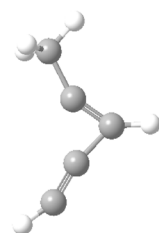
**TS 20**  
**(C<sub>s</sub>)**

ZPE(B3LYP/6-311G\*\*) = 0.072673  
E(B3LYP+ZPE) = -193.311422  
E(CCSD(T)/CC-PVTZ) = -192.95670401

A 123.82773  
B 530.00290  
C 642.68166

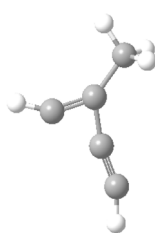
C -2.137536  
H -2.701422  
C -1.099533  
C 0.663410  
C -0.128419  
H -0.129143  
C 1.998852  
H 2.129339

667i, 128, 185, 228, 388, 426,  
513, 517, 781, 870, 946, 1036,  
1042, 1167, 1396, 1462, 1469,  
1791, 1886, 2991, 3061, 3076,  
3136, 3404



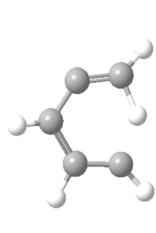
**TS 21**  
( $C_s$ )

ZPE(B3LYP/6-311G**) = 0.072473	A	159.25289	-2.022918	-0.618418	-0.000092	710i, 138, 227, 249, 419, 460,
E(B3LYP+ZPE) = -193.310158	B	441.32817	-3.087719	-0.653871	0.001331	507, 550, 646, 728, 777, 979,
E(CCS(D)(T)(CC-PVTZ)) = -192.957026	C	589.39571	-0.881320	-0.116934	-0.000233	1044, 1191, 1401, 1475, 1482,
			0.518590	0.158859	-0.000270	1734, 1912, 3032, 3090, 3119,
			0.059243	1.380793	0.000043	3235, 3416
			0.251556	2.443051	0.000470	
			1.762271	-0.662222	0.000125	
			1.786803	-1.308707	0.881780	
			1.787148	-1.309220	-0.881141	
			2.647019	-0.023715	0.000120	



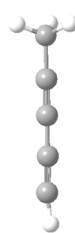
**TS 22**  
( $C_1$ )

ZPE(B3LYP/6-311G**) = 0.070741	A	190.66106	-1.061477	-1.068328	-0.003118	125i, 255, 360, 442, 529,
E(B3LYP+ZPE) = -193.295704	B	306.89863	-1.203290	0.265334	-0.066167	622, 666, 704, 786, 852, 890,
E(CCS(D)(T)(CC-PVTZ)) = -192.941906	C	492.15912	-0.079047	1.175357	-0.006375	948, 1024, 1148, 1218, 1337,
			1.138143	0.564597	-0.059488	1358, 1488, 1765, 1906, 3097,
			1.459107	-0.679905	0.067838	3185, 3236, 3238
			-1.753961	-1.895582	-0.060411	
			-2.199066	0.698042	0.038392	
			-0.239944	2.208548	0.275441	
			0.510712	-1.226841	0.586866	
			2.161651	-1.326494	-0.436431	



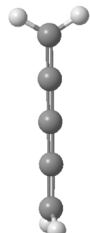
**TS A**  
( $C_s$ )

ZPE(B3LYP/6-311G**) = 0.066205	A	28.04697	-2.601986	0.061610	-0.000065	349i, 17, 132, 148, 234, 337,
E(B3LYP+ZPE) = -193.301336	B	917.30124	-2.981133	0.320379	0.993055	353, 527, 539, 633, 681, 697,
E(CCS(D)(T)(CC-PVTZ)) = -192.94211051	C	934.07103	-3.041591	-0.897620	-0.289725	1046, 1047, 1185, 1414, 1472,
			-1.151606	-0.011249	0.000257	1473, 2138, 2334, 3021, 3080,
			0.057200	-0.071356	0.000169	3081, 3473
			1.416395	-0.142979	0.000031	
			2.628666	-0.158016	-0.000121	
			3.678491	-0.319343	-0.000230	
			-2.955068	0.820528	-0.704703	
			3.207289	2.007997	-0.000018	



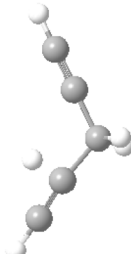
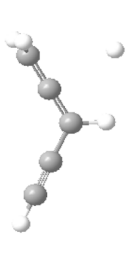
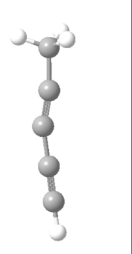
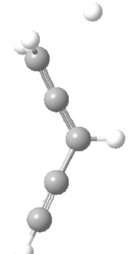
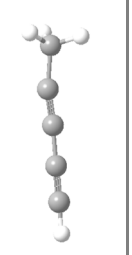
**TS B**  
( $C_s$ )

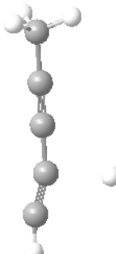
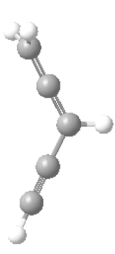
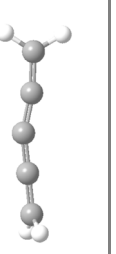
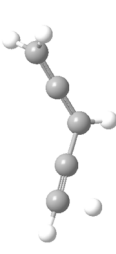

ZPE(B3LYP/6-311G**) = 0.064471	A	29.12588	2.504624	-0.167582	0.000097	25i, 7, 15, 152, 153, 335, 335,
E(B3LYP+ZPE) = -193.298109	B	906.33884	3.058530	-0.236363	-0.931922	541, 541, 698, 754, 852, 852,
E(CCS(D)(T)(CC-PVTZ)) = -192.74088721	C	922.96136	3.210866	2.000366	-0.000145	1006, 1007, 1323, 1432, 1511,
			1.180925	-0.126315	0.000128	1955, 2228, 3113, 3114,
			-0.092692	-0.058128	-0.000284	3187, 3187
			-1.376869	0.000420	-0.000106	
			-2.688260	0.065946	0.000085	
			-3.293900	-0.836864	-0.000744	
			3.058563	-0.238083	0.931975	
			-3.200431	1.024902	0.001312	



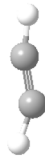

**TS C**

ZPE(B3LYP/6-311G**) = 0.066832	A	101.69504	-2.291140	-0.539909	-0.072525	650i, 96, 160, 321, 347, 407,
E(B3LYP+ZPE) = -193.273502	B	668.21254	-1.265411	0.080781	-0.034406	

<b>(C<sub>1</sub>)</b> 	E(CCS(D)(CC-PVTZ)) = -192.92133116		C	729.44174	C	-0.027965	0.862885	0.001477	459, 562, 656, 674, 691, 694, 900, 935, 997, 1242, 1340, 1456, 2146, 2236, 3022, 3051, 3466, 3478	
	<b>TS D</b> <b>(C<sub>1</sub>)</b> 	ZPE(B3LYP/6-311G**) = 0.062052		A	181.40117	C	-2.541540	0.316583	-0.191139	569i, 94, 150, 324, 363, 393, 429, 608, 631, 651, 689, 870, 897, 953, 1003, 1130, 1352, 1459, 1987, 2197, 3117, 3119, 3203, 3476
		E(B3LYP+ZPE) = -193.226775		B	788.98902	C	-1.420594	-0.076005	0.055095	
		E(CCS(D)(CC-PVTZ)) = -192.9253509		C	929.76742	C	-0.148054	-0.516164	0.364191	
						H	-0.078715	-1.332367	1.127366	
<b>TS E</b> <b>(C<sub>s</sub>)</b> 	ZPE(B3LYP/6-311G**) = 0.066708		A	29.31110,	C	2.707186	-0.152710	0.000006	780i, 85, 140, 162, 308, 342, 488, 525, 560, 653, 654, 707, 1033, 1050, 1175, 1409, 1466, 1470, 2138, 2278, 3010, 3067, 3082, 3478	
	E(B3LYP+ZPE) = -193.294969		B	875.44956,	C	1.508559	-0.020480	-0.000002		
	E(CCS(D)(CC-PVTZ)) = -192.93576183		C	893.47955	C	0.143907	0.142060	-0.000005		
	E(CCS(D)(CC-PVDZ)) = -192.74456623				C	-1.056710	-0.090125	-0.000025		
	E(CCS(D)(CC-PVQZ)) = -192.98987297				C	-2.506015	-0.114107	0.000012		
	E(CCS(D)(CBS)) = -193.01123				H	-2.904580	0.907359	-0.000676		
					H	-2.892500	-0.628349	-0.884860		
					H	-2.892469	-0.627150	0.885593		
					H	3.762168	-0.275588	0.000019		
					H	0.145810	2.035908	0.000011		
<b>TS F</b> <b>(C<sub>s</sub>)</b> 	ZPE(B3LYP/6-311G**) = 0.066086		A	69.60471	C	-2.519677	-0.386181	0.000175	408i, 127, 167, 242, 345, 368, 378, 606, 637, 671, 6912, 8867, 899, 943, 1009, 1129, 1346, 1460, 2005, 2211, 3100, 3116, 3190, 3478	
	E(B3LYP+ZPE) = -193.291486		B	750.73793	C	-1.415141	0.092035	0.000022		
	E(CCS(D)(CC-PVTZ)) = -192.931495		C	807.98144	C	-0.131529	0.707399	-0.000094		
	E(CCS(D)(CC-PVDZ)) = -192.74178176				C	1.005651	0.053069	-0.000620		
	E(CCS(D)(CC-PVQZ)) = -192.98565055				C	2.177914	-0.527290	0.000068		
	E(CCS(D)(CBS)) = -193.00729				H	3.591229	1.072050	0.001521		
<b>TS G</b> <b>(C<sub>s</sub>)</b> 	ZPE(B3LYP/6-311G**) = 0.06687		A	29.24966,	C	2.754632	-0.045447	0.000001	523i, 133, 146, 162, 346, 379, 395, 529, 534, 642, 644, 687, 1040, 1055, 1178, 1412, 1471, 1476, 2147, 2288, 3027, 3090, 3092, 3477	
	E(B3LYP+ZPE) = -193.298989		B	885.48922,	C	1.545965	-0.036609	0.000001		
	E(CCS(D)(CC-PVTZ)) = -192.94027766		C	903.51365	C	0.185951	-0.034684	0.000001		
					C	-1.028753	0.046717	-0.000013		
					C	-2.472080	-0.164227	0.000004		
					H	-2.694569	-1.235377	-0.000138		
				H	-2.934348	0.284352	0.883115			
				H	-2.934408	0.284600	-0.882949			
				H	3.816778	-0.051748	0.000004			

<b>TS H</b> <b>(C<sub>s</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.066571	A	28.21390	H	-1.167738	2.123672	0.000005	861i, 24, 150, 157, 346, 349,
		E(B3LYP+ZPE) = -193.293577	B	885.61895	H	-2.927882	-0.582545	0.884726	466, 531, 544, 613, 648, 705,
		E(CCS(D)(T)(CC-PVTZ)) = -192.93412939	C	902.56663	H	-2.976533	0.949611	-0.000160	1048, 1175, 1414, 1473, 1474,
					C	-1.101070	-0.012778	0.000012	2065, 2344, 3022, 3081, 3082,
			C	0.106447	0.021234	-0.000033	3461		
			C	1.479919	0.073857	0.000017			
			H	1.577770	1.936580	-0.000001			
			C	2.657543	-0.253254	-0.000003			
			H	3.717097	-0.339937	0.000021			
			H	-2.927866	-0.582829	-0.884559			
			C	2.416310	-0.301927	0.074511			
<b>TS I</b> <b>(C<sub>1</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.065230	A	86.56636	H	2.416310	-0.301927	0.074511	3i, 27, 81, 141, 295, 350, 359,
		E(B3LYP+ZPE) = -193.293238	B	747.75705	H	2.963118	-0.621138	-0.808262	606, 625, 642, 693, 883, 884,
		E(CCS(D)(T)(CC-PVTZ)) = -192.93529151	C	818.65408	C	1.212546	0.177385	-0.012424	951, 1004, 1139, 1352, 1465,
					C	0.002031	0.680286	-0.102326	2042, 2208, 3111, 3115, 3183,
			C	-1.192732	-0.091031	-0.043565	3478		
			C	-2.226016	-0.707585	0.000712			
			H	-3.137485	-1.251438	0.040037			
			H	2.915521	-0.406414	1.033705			
			H	-0.109562	1.755877	-0.230322			
			H	-3.904425	1.980347	0.463398			
			C	2.573627	-0.133868	0.000018			
<b>TS J</b> <b>(C<sub>s</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.065456	A	31.81967	C	2.573627	-0.133868	0.000018	737i, 135, 152, 186, 309, 344,
		E(B3LYP+ZPE) = -193.291537	B	852.69972	H	3.160625	0.782259	0.000422	462, 535, 556, 664, 766, 853,
		E(CCS(D)(T)(CC-PVTZ)) = -192.92267825	C	872.12636	C	1.266814	-0.095824	-0.000041	858, 991, 1003, 1317, 1426,
					C	-0.000069	0.151130	0.000031	1504, 1928, 2164, 3100, 3115,
			C	-1.271834	-0.000557	-0.000029	3176, 3190		
			C	-2.570229	-0.150559	0.000011			
			H	-3.130568	-0.216829	-0.927800			
			H	-3.130412	-0.217689	0.927855			
			H	3.118139	-1.073431	-0.000421			
			H	-0.007642	2.103760	0.000000			
			C	-2.344543	-0.458770	-0.044864			
<b>TS K</b> <b>(C<sub>1</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.065638	A	86.34344	C	-2.344543	-0.458770	-0.044864	296i, 60, 141, 200, 310, 360,
		E(B3LYP+ZPE) = -193.292555	B	736.25040	H	-2.787200	-0.950300	0.816951	365, 607, 633, 681, 686, 883,
		E(CCS(D)(T)(CC-PVTZ)) = -192.9325076	C	777.28364	C	-1.196000	0.140589	0.035697	884, 954, 1001, 1138, 1352,
					C	-0.040997	0.764367	0.121846	1462, 2035, 2176, 3111, 3116,
			C	1.215760	0.147692	-0.112849	3183, 3474		
			C	2.307230	-0.350101	-0.256256			
			H	2.821920	-1.072399	1.829400			
			H	3.249652	-0.764582	-0.517875			
			H	-2.899206	-0.495409	-0.978304			
			H	-0.033865	1.820021	0.388386			
			C	-2.620812	-0.029126	0.000098			
<b>TS L</b> <b>(C<sub>s</sub>)</b>		ZPE(B3LYP/6-311G**) = 0.065644	A	31.39458	C	-2.620812	-0.029126	0.000098	503i, 145, 149, 171, 337, 365,
		E(B3LYP+ZPE) = -193.295087	B	865.39902	H	-3.185422	-0.023919	-0.927432	391, 541, 541, 691, 754, 853,
		E(CCS(D)(T)(CC-PVTZ)) = -192.92734667	C	884.40603	H	-3.185115	-0.023604	0.927814	866, 1005, 1008, 1321, 1433,
					C	-1.308597	-0.039587	-0.000115	1508, 1932, 2175, 3115, 3120,
			C	-0.038123	-0.056460	-0.000136	3190, 3205		
			C	1.243327	0.014800	-0.000013			
			H	1.258263	2.202849	0.000018			



(C <sub>s</sub> )	E(CSD(T)/CC-PVTZ) = -192.942732	C	889.73957	C	0.000000	0.861462	0.000000	486, 548, 649, 713, 765, 767, 793, 875, 1029, 1150, 1463, 1836, 1951, 3127, 3208, 3347, 3355, 3455
		C		C	1.341320	-0.831016	0.000000	
		C		C	2.536442	-0.558564	0.000000	
		H		H	-2.980031	-0.155144	0.927759	
		H		H	-2.980031	-0.155144	-0.927759	
		H		H	0.651469	1.710611	0.000000	
		H		H	0.546212	-1.545170	0.000000	
		H		H	3.485114	-0.075527	0.000000	

**Table S2.** RRKM calculated rate constants for individual reaction steps of the  $C_2H + C_3H_4$  reaction on the  $C_5H_5$  potential energy surface at collision energies of 0-5.3 kcal/mol.

Reaction Step	Transition State	Symmetry Factor	Collision Energy, kcal/mol					
			0.00	1.00	2.00	3.00	4.00	5.26
1 → 3	TS 1	1	1.00E+10	1.12E+10	1.25E+10	1.39E+10	1.53E+10	1.72E+10
3 → 1	TS 1	2	2.41E+08	2.85E+08	3.35E+08	3.93E+08	4.57E+08	5.51E+08
1 → 4	TS 3	2	6.96E+05	1.12E+06	1.76E+06	2.69E+06	4.03E+06	6.49E+06
4 → 1	TS 3	1	7.71E+05	1.23E+06	1.92E+06	2.92E+06	4.34E+06	6.95E+06
1 → 5	TS 4	2	2.48E+07	3.28E+07	4.27E+07	5.51E+07	7.03E+07	9.41E+07
5 → 1	TS 4	1	5.99E+04	8.44E+04	1.17E+05	1.61E+05	2.18E+05	3.15E+05
1 → 16	TS 5	2	6.44E+04	1.13E+05	1.90E+05	3.10E+05	4.90E+05	8.42E+05
16 → 1	TS 5	1	2.95E+04	5.17E+04	8.72E+04	1.42E+05	2.26E+05	3.88E+05
1 → 18	TS M	2	2.58E+08	3.37E+08	4.34E+08	5.54E+08	6.99E+08	9.24E+08
1 → 20	TS N	2	6.69E+08	9.11E+08	1.22E+09	1.62E+09	2.11E+09	2.91E+09
2 → 3	TS 2	2	8.93E+05	1.18E+06	1.55E+06	2.00E+06	2.57E+06	3.48E+06
3 → 2	TS 2	3	1.46E+08	1.82E+08	2.26E+08	2.78E+08	3.39E+08	4.31E+08
3 → 11	TS 12	2	1.36E+08	1.63E+08	1.92E+08	2.26E+08	2.64E+08	3.20E+08
11 → 3	TS 12	1	1.11E+11	1.26E+11	1.43E+11	1.61E+11	1.80E+11	2.07E+11
3 → 12	TS 11	1	3.35E+07	4.79E+07	6.72E+07	9.25E+07	1.25E+08	1.80E+08
12 → 3	TS 11	1	1.34E+03	2.13E+03	3.32E+03	5.05E+03	7.55E+03	1.22E+04
4 → 20	TS C	3	2.02E+05	3.06E+05	4.53E+05	6.58E+05	9.37E+05	1.43E+06
5 → 6	TS 8	1	5.12E+05	6.46E+05	8.09E+05	1.00E+06	1.24E+06	1.60E+06
6 → 5	TS 8	2	1.95E+08	2.30E+08	2.71E+08	3.17E+08	3.68E+08	4.42E+08
5 → 18	TS D	1	2.16E+06	2.96E+06	4.02E+06	5.40E+06	7.16E+06	1.01E+07
6 → 7	TS 10	1	2.46E+07	3.30E+07	4.37E+07	5.72E+07	7.39E+07	1.01E+08
7 → 6	TS 10	1	9.11E+05	1.24E+06	1.67E+06	2.22E+06	2.91E+06	4.04E+06
6 → 8	TS 9	1	4.16E+08	5.51E+08	7.21E+08	9.32E+08	1.19E+09	1.61E+09
8 → 6	TS 9	1	1.15E+08	1.52E+08	1.98E+08	2.56E+08	3.27E+08	4.38E+08
6 → 10	TS 20	1	5.24E+09	5.92E+09	6.68E+09	7.46E+09	8.34E+09	9.53E+09
10 → 6	TS 20	1	2.83E+12	2.97E+12	3.10E+12	3.23E+12	3.37E+12	3.54E+12
6 → 18	TS F	3	7.95E+08	1.02E+09	1.28E+09	1.61E+09	2.00E+09	2.59E+09
6 → 21	TS E	1	1.80E+09	2.23E+09	2.75E+09	3.36E+09	4.07E+09	5.13E+09
7 → 21	TS G	1	9.97E+07	1.23E+08	1.51E+08	1.84E+08	2.23E+08	2.81E+08
7 → 22	TS P	1	2.07E+09	2.49E+09	2.97E+09	3.53E+09	4.17E+09	5.09E+09
8 → 9	TS 6	1	1.16E+08	1.53E+08	2.00E+08	2.58E+08	3.29E+08	4.41E+08
9 → 8	TS 6	2	1.13E+06	1.54E+06	2.06E+06	2.72E+06	3.56E+06	4.92E+06
8 → 21	TS H	1	4.14E+09	5.01E+09	6.03E+09	7.20E+09	8.54E+09	1.05E+10
9 → 13	TS 7	3	3.73E+04	5.06E+04	6.78E+04	8.96E+04	1.17E+05	1.62E+05
13 → 9	TS 7	1	2.06E+05	2.81E+05	3.79E+05	5.05E+05	6.65E+05	9.28E+05
9 → 19	TS B	3	6.28E+07	9.40E+07	1.25E+08	1.72E+08	2.33E+08	3.37E+08
9 → 21	TS A	2	2.05E+08	2.52E+08	3.08E+08	3.74E+08	4.51E+08	5.67E+08
10 → 11	TS 21	1	2.82E+12	2.95E+12	3.08E+12	3.21E+12	3.34E+12	3.50E+12
11 → 10	TS 21	1	2.80E+10	3.12E+10	3.46E+10	3.83E+10	4.18E+10	4.75E+10
11 → 22	TS O	1	9.26E+09	1.14E+10	1.39E+10	1.69E+10	2.01E+10	2.51E+10
12 → 13	TS 14	1	9.16E+09	1.04E+10	1.21E+10	1.37E+10	1.56E+10	1.82E+10
13 → 12	TS 14	1	1.90E+06	2.30E+06	2.76E+06	3.30E+06	3.91E+06	4.83E+06
12 → 14	TS 13	1	5.63E-03	4.62E-02	3.79E-01	3.04E+00	2.02E+01	8.23E+01
14 → 12	TS 13	1	5.55E-03	4.55E-02	3.73E-01	2.99E+00	1.98E+01	8.09E+01
13 → 15	TS 17	1	9.03E+03	1.40E+04	2.12E+04	3.16E+04	4.61E+04	7.25E+04
15 → 13	TS 17	2	1.82E+05	2.73E+05	4.00E+05	5.76E+05	8.13E+05	1.23E+06



13 → 19	TS L	1	1.15E+06	1.62E+06	2.24E+06	3.06E+06	4.14E+06	5.94E+06
14 → 15	TS 15	1	3.14E+09	3.68E+09	4.28E+09	4.95E+09	5.70E+09	6.76E+09
15 → 14	TS 15	2	1.33E+07	1.59E+07	1.87E+07	2.20E+07	2.57E+07	3.10E+07
14 → 17	TS 16	2	2.70E+04	4.99E+04	8.79E+04	1.49E+05	2.43E+05	4.31E+05
17 → 14	TS 16	2	1.18E+02	2.30E+02	4.24E+02	7.51E+02	1.28E+03	2.40E+03
15 → 16	TS 18	2	3.07E+05	4.58E+05	6.70E+05	9.62E+05	1.36E+06	2.05E+06
16 → 15	TS 18	1	3.45E+06	5.02E+06	7.16E+06	1.00E+07	1.39E+07	2.04E+07
15 → 18	TS K	4	5.35E+08	6.95E+08	8.89E+08	1.13E+09	1.40E+09	1.89E+09
15 → 19	TS J	1	2.46E+06	3.51E+06	4.92E+06	6.78E+06	9.22E+06	1.33E+07
16 → 17	TS 19	1	5.82E+09	6.32E+09	6.85E+09	7.41E+09	8.00E+09	8.76E+09
17 → 16	TS 19	1	5.36E+08	6.17E+08	7.06E+08	8.06E+08	9.17E+08	1.07E+09
16 → 18	TS I	1	2.27E+08	3.03E+08	3.99E+08	5.20E+08	6.69E+08	9.06E+08
16 → 23	TS Q	1	3.30E+10	3.96E+10	4.72E+10	5.58E+10	6.57E+10	7.98E+10