

## **Supporting information**

### **Detailed experimental and kinetic modeling study of 3-carene pyrolysis**

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## Contents

1	Experimental result .....	3
2	Kinetic model.....	3
3	Nomenclature .....	3
4	Sample composition.....	4
5	Tabulated comparsion between simulation results and experimental data .....	5
6	Sensitivity analyses .....	6
7	Optimized Geometries .....	11
7.1	Hydrogen abstraction on 3-carene .....	11
7.2	Hydrogen abstraction on cara-2,4-diene.....	17
7.3	Hydrogen elimination reaction on 3-carene .....	22
7.4	Diels Alder reaction on 3-carene .....	23
7.5	Three membered ring opening reaction on 3-carene through molecule chemistry .....	24
7.6	Three membered ring opening reaction on cara-2,4-diene molecule chemistry .....	32
7.7	C-C $\beta$ -scission reaction.....	37
7.8	Intramolecular hydrogen abstraction reaction on 1,5-p-menthadien-8-yl .....	50
7.9	Intramolecular hydrogen abstraction reaction on 1,3-m-menthadien-8-yl .....	52
7.10	Intramolecular hydrogen abstraction reaction generating 4-isopropylbenzyl radical.....	53

## 1 Experimental result

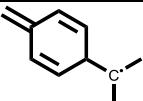
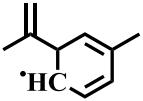
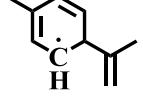
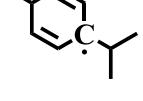
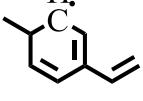
The experimental data acquired for the pyrolysis of 3-carene in the jet-stirred reactor, located in Nancy, France, is provided as a separate Excel spreadsheet.

## 2 Kinetic model

The kinetic model in CHEMKIN format developed for the pyrolysis of 3-carene is provided as a separate text file.

## 3 Nomenclature

Table S. 1: Nomenclature

Name	Identifier	Structure
R1	InChI=1S/C10H13/c1-8(2)10-6-4-9(3)5-7-10/h4-7,10H,3H2,1-2H3	
R2	InChI=1S/C10H13/c1-8(2)10-6-4-5-9(3)7-10/h4-7,10H,1H2,2-3H3	
R3	InChI=1S/C10H13/c1-8(2)10-6-4-9(3)5-7-10/h4-7,10H,1H2,2-3H3	
R4	InChI=1S/C10H15/c1-8(2)10-6-4-9(3)5-7-10/h4-9H,1-3H3	
R5	InChI=1S/C9H11/c1-3-9-6-4-8(2)5-7-9/h3-8H,1H2,2H3	

## 4 Sample composition

The tentatively identified sample composition before and after purification is presented in Table S. 2.

Table S. 2: The weight percentage (wt. %) of the feedstock before and after the purification through vacuum distillation

Species name	Species structure	Before purification (Wt%)	After purification (Wt%)
3-carene		95.90	98.90
C <sub>10</sub> H <sub>16</sub> _1		1.10	0.43
C <sub>10</sub> H <sub>16</sub> _2		0.67	0.56
C <sub>10</sub> H <sub>16</sub> _3		2.16	0.10
C <sub>10</sub> H <sub>14</sub>		0.03	0.00
C <sub>9</sub> H <sub>16</sub>		0.10	0.00
C <sub>9</sub> H <sub>16</sub> _2		0.02	0.00
Sum	-	99.98	99.99

## 5 Tabulated comparsion between simulation results and experimental data

	JSR Experime nt (mol %)	Current model (mol %)	Sharath model <sup>11</sup> (mol %)	JSR Experiment (mol %)	Current model (mol %)	Sharath model <sup>11</sup> (mol %)	
Temperature (K)	850			950			
Hydrogen gas	$2.99 \cdot 10^{-4}$	$3.76 \cdot 10^{-4}$	$2.95 \cdot 10^{-6}$	$1.74 \cdot 10^{-3}$	$2.04 \cdot 10^{-3}$	$9.03 \cdot 10^{-4}$	
Methane	$1.37 \cdot 10^{-4}$	$2.43 \cdot 10^{-5}$	-	$1.04 \cdot 10^{-3}$	$5.87 \cdot 10^{-4}$	-	
Ethylene	$6.37 \cdot 10^{-5}$	$2.38 \cdot 10^{-5}$	$2.76 \cdot 10^{-6}$	$4.52 \cdot 10^{-4}$	$3.03 \cdot 10^{-4}$	$5.57 \cdot 10^{-4}$	
Propylene	$5.46 \cdot 10^{-5}$	$2.85 \cdot 10^{-6}$	-	$1.89 \cdot 10^{-4}$	$1.26 \cdot 10^{-4}$	-	
1,3-Butadiene	$8.14 \cdot 10^{-6}$	$5.78 \cdot 10^{-10}$	$9.77 \cdot 10^{-12}$	$7.06 \cdot 10^{-5}$	$2.90 \cdot 10^{-6}$	$3.42 \cdot 10^{-10}$	
Isoprene	$4.43 \cdot 10^{-5}$	$2.79 \cdot 10^{-7}$	$2.75 \cdot 10^{-6}$	$1.25 \cdot 10^{-4}$	$2.34 \cdot 10^{-5}$	$2.42 \cdot 10^{-4}$	
Benzene	$5.84 \cdot 10^{-6}$	$7.45 \cdot 10^{-8}$	$2.89 \cdot 10^{-9}$	$1.77 \cdot 10^{-4}$	$5.76 \cdot 10^{-5}$	$3.14 \cdot 10^{-6}$	
Toluene	$3.63 \cdot 10^{-5}$	$3.72 \cdot 10^{-5}$	$7.80 \cdot 10^{-9}$	$2.81 \cdot 10^{-4}$	$4.30 \cdot 10^{-4}$	$8.00 \cdot 10^{-6}$	
Styrene	$7.10 \cdot 10^{-6}$	$1.24 \cdot 10^{-10}$	-	$8.74 \cdot 10^{-5}$	$9.73 \cdot 10^{-6}$	-	
Ethylbenzene	$3.53 \cdot 10^{-5}$	$1.03 \cdot 10^{-8}$	$2.26 \cdot 10^{-8}$	$1.25 \cdot 10^{-4}$	$9.48 \cdot 10^{-6}$	$3.22 \cdot 10^{-4}$	
p-Methyl-styrene	$8.87 \cdot 10^{-6}$	$4.66 \cdot 10^{-8}$	-	$1.60 \cdot 10^{-4}$	$1.23 \cdot 10^{-4}$	-	
m-Methyl-styrene	$5.29 \cdot 10^{-6}$	$7.11 \cdot 10^{-8}$	-	$1.28 \cdot 10^{-4}$	$8.36 \cdot 10^{-5}$	-	
p-Cymenene	$2.30 \cdot 10^{-5}$	$2.30 \cdot 10^{-7}$	-	$1.22 \cdot 10^{-4}$	$9.21 \cdot 10^{-5}$	-	
p-Cymene	$1.17 \cdot 10^{-4}$	$3.13 \cdot 10^{-5}$	-	$2.10 \cdot 10^{-4}$	$6.03 \cdot 10^{-4}$	-	
m-Cymene	$1.13 \cdot 10^{-4}$	$2.93 \cdot 10^{-5}$	-	$2.01 \cdot 10^{-4}$	$2.04 \cdot 10^{-4}$	-	
3-Carene	$2.01 \cdot 10^{-3}$	$2.09 \cdot 10^{-3}$	$2.50 \cdot 10^{-3}$	$1.01 \cdot 10^{-4}$	$2.84 \cdot 10^{-4}$	$1.93 \cdot 10^{-3}$	

Table S. 3: Experimental and simulated product yields for 3-carene pyrolysis with the 2565 species and 9331 reactions.

## 6 Sensitivity analyses

The sensitivity analysis study is performed at 900K, 950K, 1000K and 1050K, and the corresponding conversion of 3-carene is 59%, 89%, 97% and 99% to identify which reaction rate coefficients could make the model performance even better. Normalized sensitivity coefficients of the main reactions for 3-carene, p-cymene, m-cymene and toluene are presented in Fig S. 1 to Fig S. 4.

The hydrogen gas elimination reaction, a dominant 3-carene decomposition pathway, is the most sensitive reaction for the consumption of 3-carene, and its importance increases as a function of temperature. 3-carene consumption is also sensitive to hydrogen abstraction reactions generating 3-caren-5-yl and 3-caren-2-yl, and is more sensitive to abstractions by hydrogen radical compared to methyl radical. P-cymene, m-cymene and toluene generation are also found to be sensitive to these hydrogen abstraction reactions. The hydrogen abstraction reaction generating 3-caren-5-yl can be further converted into m-cymene. Its competitive pathway, the hydrogen abstraction reaction generating 3-caren-2-yl will thus inhibit m-cymene generation. Similar phenomenon is also observed for p-cymene. Both reaction pathways help toluene production and thus they have positive sensitivity coefficients. The last sensitive reactions are intramolecular hydrogen abstraction reactions on 1,3-m-menthadien-8-yl and 1,5-p-menthadien-8-yl. These two components can either react through 1,2-intramolecular hydrogen abstraction reactions (reaction#5457&5458) or 1,3-intramolecular reactions (reaction#5596&5597). Decreasing the rate coefficients of the 1,3-intramolecular hydrogen abstraction reactions contributes to the consumption of 3-carene and generation of cymene. This also helps to decrease the over-prediction of toluene at high temperature (>900K). The same effect can be obtained by increasing the rate coefficients of 1,2-intramolecular hydrogen abstraction reactions.

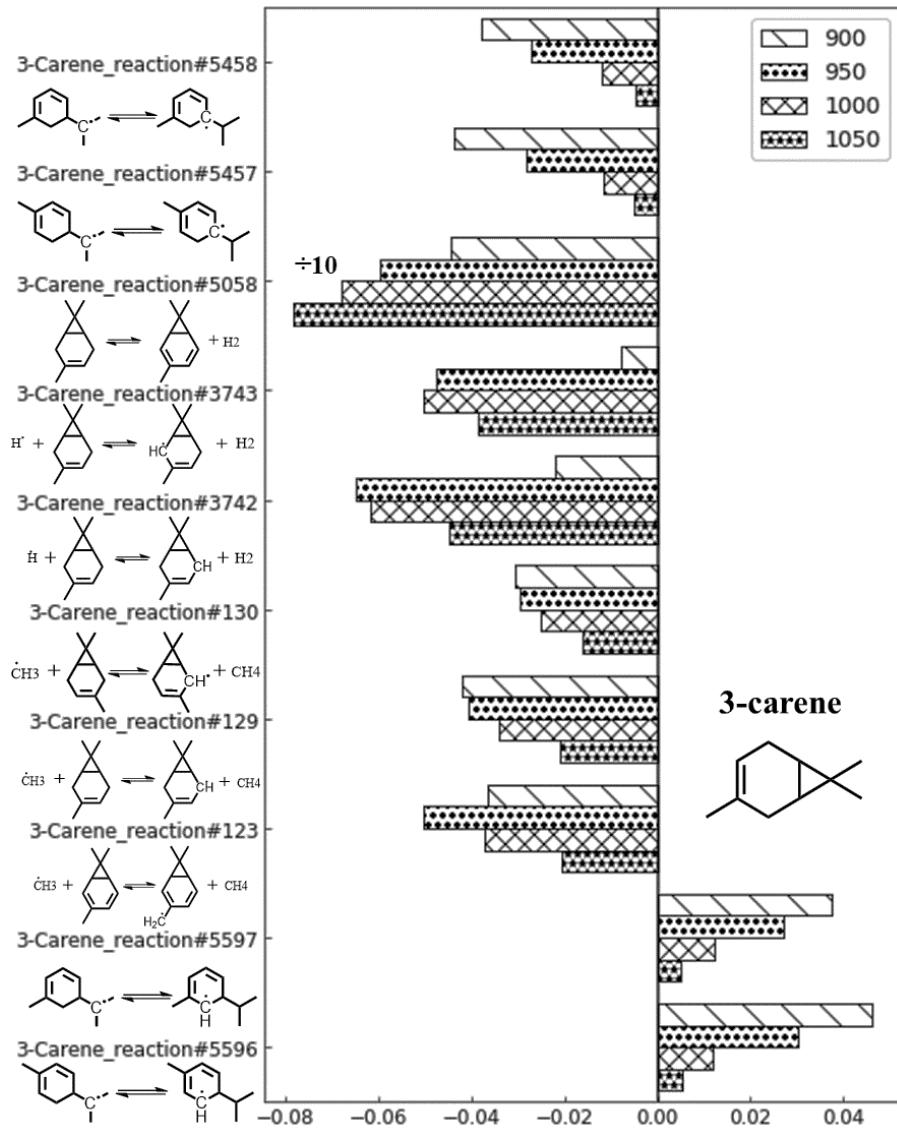


Fig S. 1: Normalized sensitivity coefficients for 3-carene at 900K, 950K, 1000K and 1050K and the corresponding conversion of 3-carene is 59%, 89%, 97% and 99%. (bars filled with slash: 900K, bars filled with circle: 950K, bars filled with cross: 1000K and bars filled with star: 1050K). The reaction and its number in the reaction network are also indicated. The normalized sensitivity coefficients of hydrogen gas elimination of 3-carene are divided by ten.

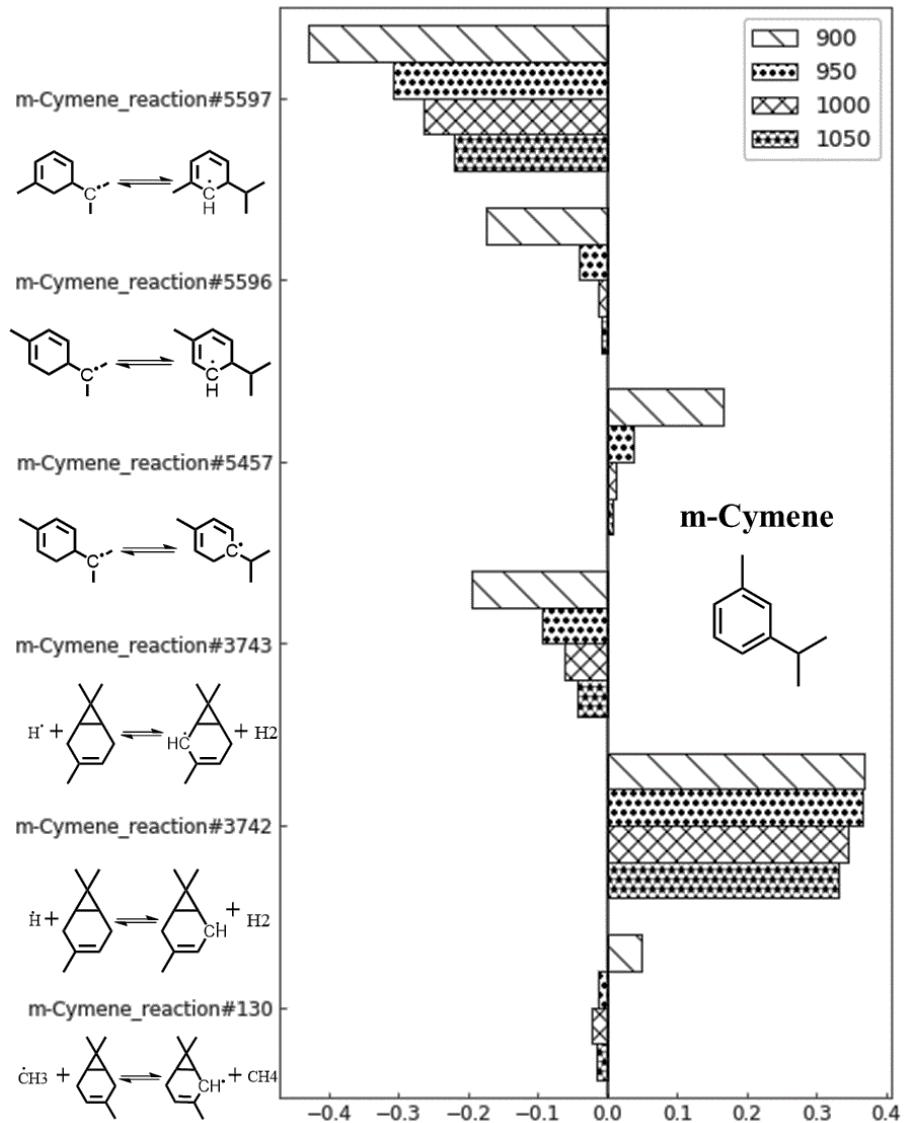


Fig S. 2: Normalized sensitivity coefficients for m-cymene at 900K, 950K, 1000K and 1050K and the corresponding conversion of 3-carene is 59%, 89%, 97% and 99%. (bars filled with slash: 900K, bars filled with circle: 950K, bars filled with cross: 1000K and bars filled with star: 1050K). The reaction and its number in the reaction network are also indicated.

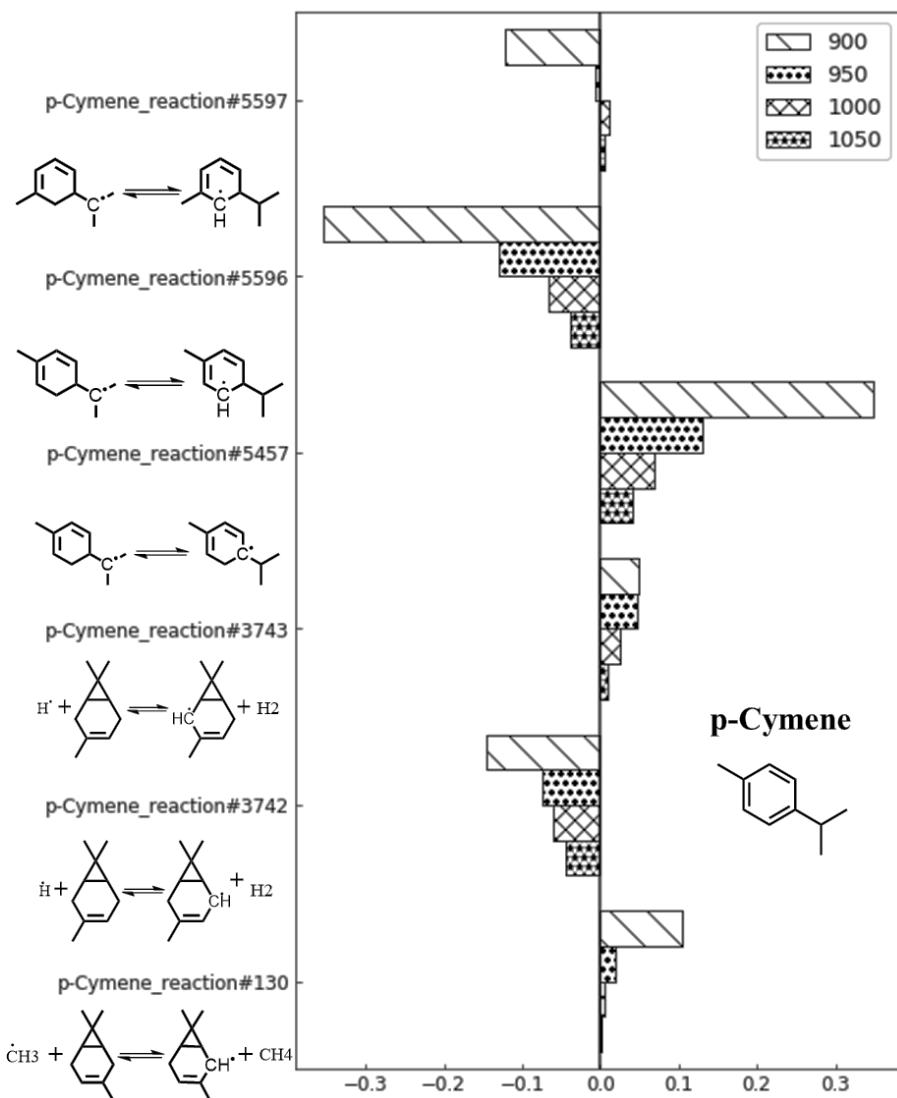


Fig S. 3: Normalized sensitivity coefficients for p-cymene at 900K, 950K, 1000K and 1050K and the corresponding conversion of 3-carene is 59%, 89%, 97% and 99%. (bars filled with slash: 900K, bars filled with circle: 950K, bars filled with cross: 1000K and bars filled with star: 1050K). The reaction and its number in the reaction network are also indicated.

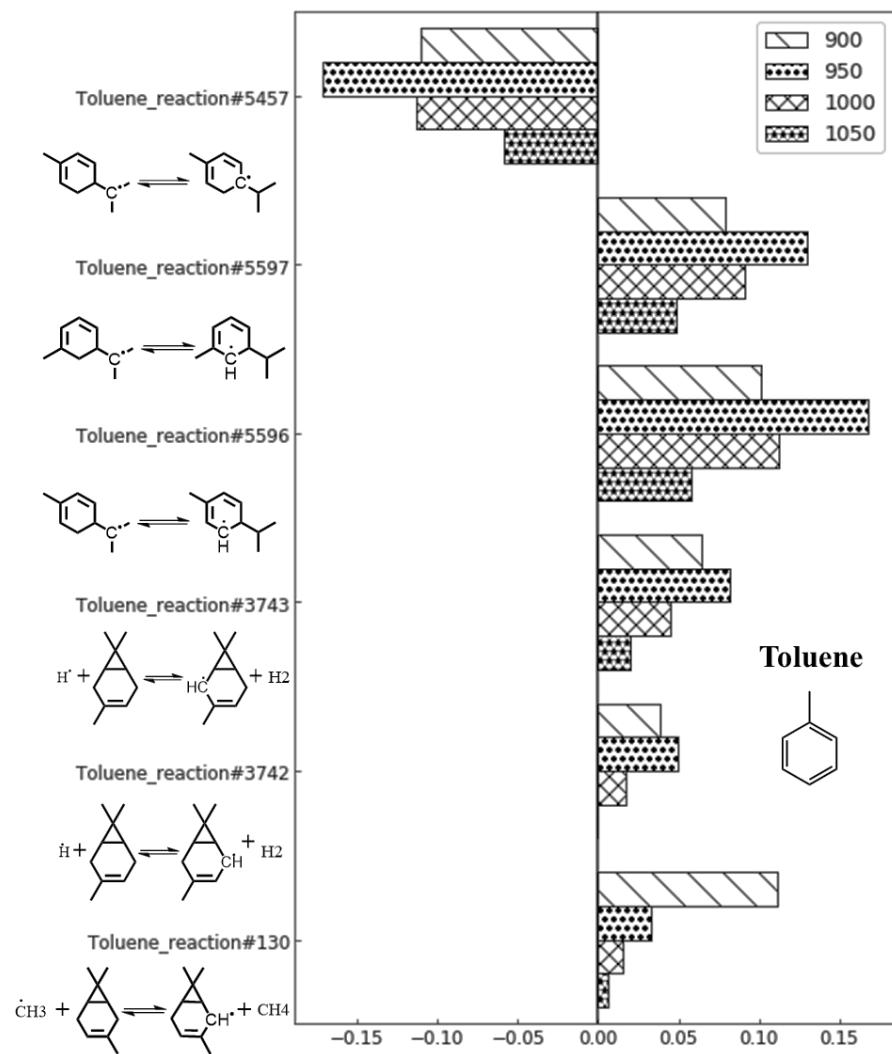


Fig S. 4: Normalized sensitivity coefficients for toluene at 900K, 950K, 1000K and 1050K and the corresponding conversion of 3-carene is 59%, 89%, 97% and 99%. (bars filled with slash: 900K, bars filled with circle: 950K, bars filled with cross: 1000K and bars filled with star: 1050K). The reaction and its number in the reaction network are also indicated.

## 7 Optimized Geometries

Below, the final CBS-QB3 optimized geometries of all the reactants, transition states and products are given in Cartesian Coordinates expressed in Å.

### 7.1 Hydrogen abstraction on 3-carene

#### Reactant

##### 3-carene

C	-0.001324	0.015524	0.012511
H	-0.010965	0.015306	1.105895
H	1.045400	0.024543	-0.311576
H	-0.461413	0.951147	-0.324712
C	-0.737004	-1.188840	-0.551901
C	-0.745470	-1.223020	-2.069694
H	0.278923	-1.243875	-2.457504
H	-1.270886	-2.089517	-2.471640
H	-1.225541	-0.323406	-2.470328
H	-2.148136	-1.112335	1.137828
H	-0.050655	-2.402590	1.154331
C	-0.642963	-2.475479	0.247165
C	-1.936100	-1.680726	0.237142
C	-3.178846	-2.255920	-0.422914
C	-0.595763	-3.847982	-0.404595
H	-0.312863	-4.584775	0.358340
H	0.210871	-3.891431	-1.150691
H	-3.970991	-2.327839	0.334074
H	-3.572796	-1.556386	-1.175121
C	-3.027852	-3.618441	-1.059878
C	-4.270694	-4.160945	-1.716290
H	-4.099790	-5.147653	-2.151524
H	-5.093448	-4.244296	-0.996084
H	-4.619434	-3.492703	-2.512843
C	-1.881986	-4.302102	-1.040438
H	-1.850909	-5.280932	-1.514854

#### Products

##### 3-caren-1-yl

C	-3.155521	-0.693287	0.413764
C	1.417234	-0.205983	1.570792
C	3.042075	-0.507592	-0.366060
C	-1.499352	1.140775	0.099338
C	-0.193637	1.778364	-0.304337
C	-0.831012	-1.191078	-0.530811
C	-1.810329	-0.154844	0.003612

C	0.847797	0.802264	-0.839305
C	0.515937	-0.632549	-0.832016
C	1.611182	-0.209810	0.063165
H	-3.652508	-1.192176	-0.426741
H	-3.054835	-1.442817	1.207698
H	-3.813874	0.099189	0.775789
H	0.394865	0.045400	1.857766
H	1.650039	-1.191140	1.989545
H	2.090714	0.516335	2.045738
H	3.139531	-0.504589	-1.453840
H	3.737040	0.232324	0.045725
H	3.351696	-1.495537	-0.008145
H	-2.250756	1.823872	0.490841
H	-0.401413	2.527180	-1.079071
H	0.211236	2.352069	0.542091
H	-0.761415	-2.027334	0.178477
H	-1.262027	-1.623132	-1.446546
H	1.459627	1.192846	-1.650432

##### 3-caren-4-yl

C	-3.238299	-0.583133	-0.289511
C	1.196448	-0.436150	-1.596368
C	2.983621	-0.494239	0.199702
C	-1.451016	1.160769	-0.219690
C	-0.171594	1.862133	0.003508
C	-0.882807	-1.060380	0.651267
C	-1.854618	-0.067041	0.017608
C	0.874050	0.928134	0.634435
C	0.509117	-0.514354	0.948368
C	1.528822	-0.203824	-0.133167
H	-3.861697	0.194316	-0.732486
H	-3.193365	-1.428850	-0.985549
H	-3.731182	-0.944430	0.620546
H	0.156020	-0.216011	-1.835869
H	1.827610	0.191121	-2.235176
H	1.391444	-1.478380	-1.871491
H	3.655260	0.144592	-0.384435
H	3.195542	-0.321154	1.258132
H	3.237195	-1.536283	-0.024932
H	0.206666	2.287905	-0.935248
H	-0.331618	2.712473	0.676399
H	-1.329469	-1.412660	1.589691
H	-0.818535	-1.948898	0.006918
H	1.512006	1.427246	1.357988
H	0.935145	-0.909582	1.865771

##### 3-caren-5-yl

C	3.148394	-0.658984	0.311773
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C	-3.026179	-0.399645	-0.138683	H	-0.999396	-0.812410	1.946732
C	-1.198272	-0.352713	1.618951				
C	1.467883	1.218622	0.142022				
C	0.224656	1.757271	-0.167480				
C	0.816976	-1.087235	-0.647641				
C	1.795264	-0.116659	-0.034945				
C	-0.868788	0.926911	-0.687239				
C	-0.580908	-0.548738	-0.931651				
C	-1.554211	-0.169520	0.157086				
H	3.077550	-1.474057	1.044612				
H	3.648581	-1.083651	-0.569451				
H	3.799676	0.112359	0.728469				
H	-3.322251	-1.420818	0.127284				
H	-3.251434	-0.253718	-1.198465				
H	-3.655067	0.288814	0.436001				
H	-1.806736	0.307971	2.245106				
H	-0.151447	-0.135810	1.827706				
H	-1.401775	-1.382650	1.933251				
H	2.230796	1.881493	0.542869				
H	0.048663	2.818746	-0.033385				
H	0.753638	-1.985675	-0.013584				
H	1.245527	-1.447798	-1.594200				
H	-1.535985	1.423678	-1.386111				
H	-1.037837	-0.974602	-1.820150				

### 3-caren-6-yl

C	3.105630	-0.831286	-0.327395
C	-1.429625	-0.410170	-1.515971
C	-3.080753	-0.219013	0.412439
C	1.551407	1.105111	-0.238257
C	0.260215	1.837659	0.061895
C	0.772850	-1.104465	0.662447
C	1.785938	-0.186424	0.009883
C	-0.791582	0.938430	0.613055
C	-0.563250	-0.460664	1.013416
C	-1.635475	-0.077557	-0.047141
H	3.797130	-0.121591	-0.785852
H	3.583866	-1.242377	0.569640
H	2.968436	-1.669738	-1.020588
H	-2.016546	0.266143	-2.146801
H	-1.764841	-1.430728	-1.732949
H	-0.385060	-0.324966	-1.819990
H	-3.442677	-1.241659	0.259678
H	-3.730547	0.456064	-0.154914
H	-3.187742	0.030516	1.470266
H	2.338186	1.703761	-0.692913
H	0.474729	2.637519	0.786285
H	-0.094720	2.352527	-0.840832
H	0.623542	-1.987299	0.023049
H	1.222630	-1.498043	1.583080

### 3-caren-8-yl

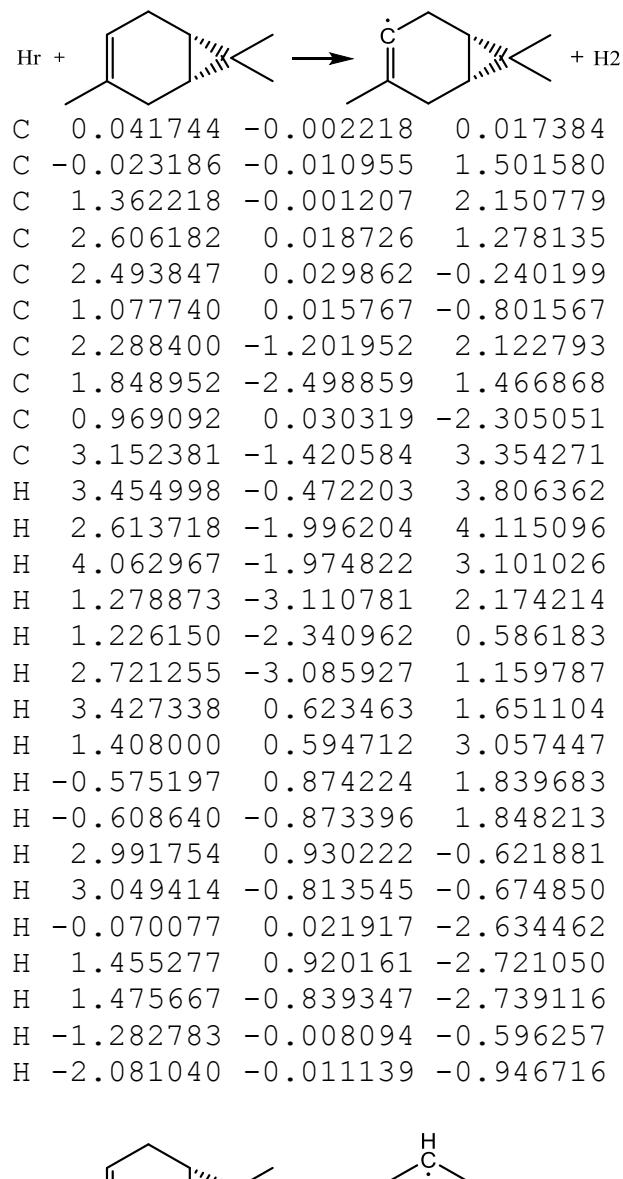
C	0.037551	-0.000312	0.041082
C	0.015706	0.031873	1.545196
C	1.381338	0.028650	2.206948
C	2.623902	0.053609	1.367480
C	2.527712	0.080053	-0.146905
C	1.131768	0.019863	-0.722765
C	2.295969	-1.216511	2.185003
C	3.142826	-1.438784	3.430107
C	1.058101	-0.005320	-2.227100
C	1.864329	-2.432797	1.511083
H	1.247301	-2.409518	0.624040
H	2.160279	-3.397946	1.902156
H	4.056925	-1.990005	3.187271
H	3.437181	-0.491067	3.888145
H	2.591222	-2.014795	4.179934
H	3.464203	0.614420	1.765913
H	1.421872	0.574434	3.144852
H	-0.520740	0.935361	1.863819
H	-0.586563	-0.807896	1.918401
H	3.001064	1.003321	-0.507128
H	3.125672	-0.736055	-0.576733
H	0.025344	-0.035881	-2.580173
H	1.540345	0.878789	-2.661095
H	1.583394	-0.878471	-2.632186
H	-0.936447	-0.035576	-0.442499

### 3-caren-10-yl

C	-3.083313	-0.756494	-0.368313
C	2.978127	-0.408886	0.111674
C	1.136188	-0.326756	-1.624421
C	-1.560924	1.113676	-0.179168
C	-0.277122	1.792799	0.183104
C	-0.842296	-1.160887	0.663301
C	-1.854462	-0.225964	0.012341
C	0.823970	0.883643	0.702596
C	0.538981	-0.587139	0.935711
C	1.502077	-0.166853	-0.159362
H	-3.314058	-1.805724	-0.226887
H	-3.847193	-0.132300	-0.816739
H	3.216905	-0.286789	1.171633
H	3.270383	-1.423624	-0.180746
H	3.601955	0.292497	-0.453608
H	0.080874	-0.143733	-1.824334
H	1.718496	0.367129	-2.240595
H	1.370140	-1.340387	-1.967895

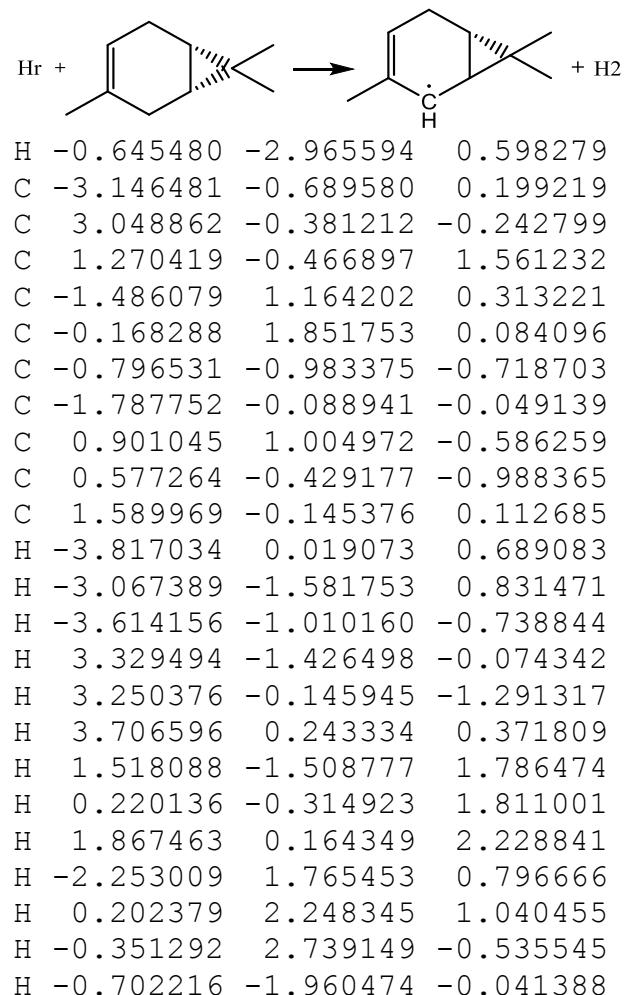
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 H -0.761073 -2.070137 0.055380  
 H 1.473912 1.362591 1.428899  
 H 1.015995 -1.025650 1.807526

### Transition states

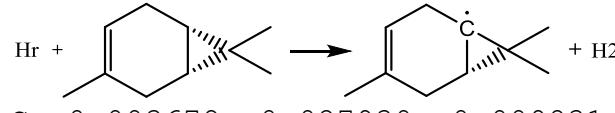


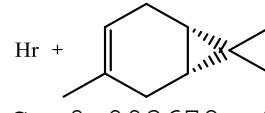
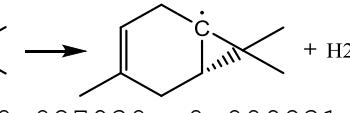
H -1.884897 -2.813574 -0.325345  
 C 0.274331 0.655361 3.232454  
 C -0.323138 0.590053 -2.961567  
 C -1.777106 0.436806 -0.890696  
 C 0.136146 -1.144576 1.520668

C 0.200352 -1.733026 0.155947  
 C 0.733527 1.168084 0.777898  
 C 0.358121 0.140929 1.820244  
 C 0.557631 -0.795186 -0.967790  
 C 0.831030 0.670735 -0.655105  
 C -0.383122 0.289742 -1.472838  
 H 1.227474 1.094994 3.549593  
 H 0.013996 -0.137279 3.936451  
 H -0.478725 1.447999 3.317492  
 H -0.975425 -0.085965 -3.524758  
 H 0.691478 0.479338 -3.353664  
 H -0.650150 1.615570 -3.166124  
 H -2.477027 -0.234855 -1.397282  
 H -2.141356 1.460124 -1.034469  
 H -1.819663 0.214468 0.175859  
 H -0.111340 -1.833791 2.324757  
 H -0.848753 -2.236442 -0.072119  
 H 0.857036 -2.609799 0.148888  
 H 1.703443 1.594006 1.066226  
 H 0.027783 2.009462 0.842717  
 H 1.181801 -1.242699 -1.734420  
 H 1.638180 1.126143 -1.220926

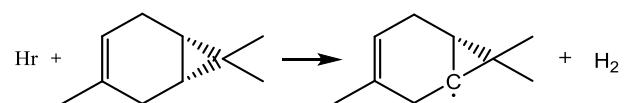


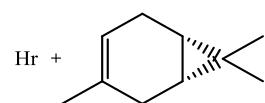
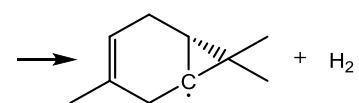
H -1.227633 -1.407920 -1.632050  
 H 1.524935 1.555642 -1.283596  
 H 1.012285 -0.771456 -1.921847



Hr +  →  + H<sub>2</sub>

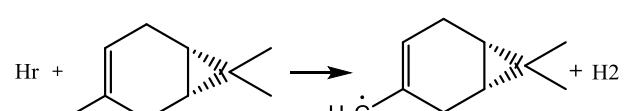
C -0.003678 0.027930 0.009831  
 C 0.001274 0.013690 1.519290  
 C 1.378665 -0.048975 2.116987  
 C 2.614638 0.012660 1.288153  
 C 2.489606 0.038759 -0.228378  
 C 1.077811 0.033598 -0.772995  
 C 2.298978 -1.225695 2.145739  
 C 1.872600 -2.532274 1.497048  
 C 0.972246 0.051438 -2.275862  
 C 3.177142 -1.422953 3.373160  
 H 3.469942 -0.469592 3.817455  
 H 2.647621 -1.999083 4.139506  
 H 4.088385 -1.971445 3.112204  
 H 1.295830 -3.138838 2.203260  
 H 1.258840 -2.379564 0.608527  
 H 2.750991 -3.118773 1.206040  
 H 3.439682 0.605784 1.675804  
 H 1.419128 0.727839 3.257723  
 H -0.499560 0.923692 1.878566  
 H -0.617618 -0.817505 1.883580  
 H 2.989886 0.941235 -0.602552  
 H 3.047680 -0.797822 -0.674156  
 H -0.067775 0.052924 -2.607890  
 H 1.465005 0.936700 -2.695061  
 H 1.469649 -0.821147 -2.715754  
 H -0.987303 0.036769 -0.455102  
 H 1.414628 1.278384 3.981069

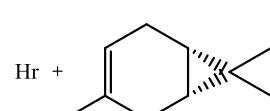
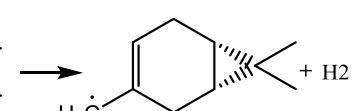


Hr +  →  + H<sub>2</sub>

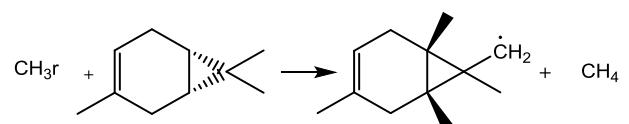
C 0.012996 0.018008 0.000405  
 C 0.007926 0.014880 1.506672  
 C 1.386693 0.002069 2.150731  
 C 2.588902 -0.031878 1.272247  
 C 2.505788 0.046819 -0.226113  
 C 1.094597 0.037579 -0.781955  
 C 2.319110 -1.222586 2.133447  
 C 1.873959 -2.529632 1.498414  
 C 0.999224 0.056637 -2.284958  
 C 3.176016 -1.420094 3.375790  
 H 3.480843 -0.466658 3.811682  
 H 2.627540 -1.983500 4.138039  
 H 4.084793 -1.981582 3.133910

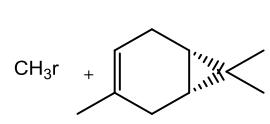
H 1.313235 -3.133092 2.220622  
 H 1.240752 -2.377553 0.623591  
 H 2.743066 -3.119017 1.187430  
 H 3.634216 0.754332 1.709167  
 H 1.458688 0.586572 3.064922  
 H -0.528505 0.908159 1.850754  
 H -0.592293 -0.832457 1.868253  
 H 2.996697 0.972429 -0.559279  
 H 3.082726 -0.765679 -0.689566  
 H -0.039014 0.057431 -2.622903  
 H 1.493566 0.943110 -2.699625  
 H 1.500070 -0.814867 -2.723044  
 H -0.967673 0.016202 -0.470877  
 H 4.308149 1.313709 1.957463



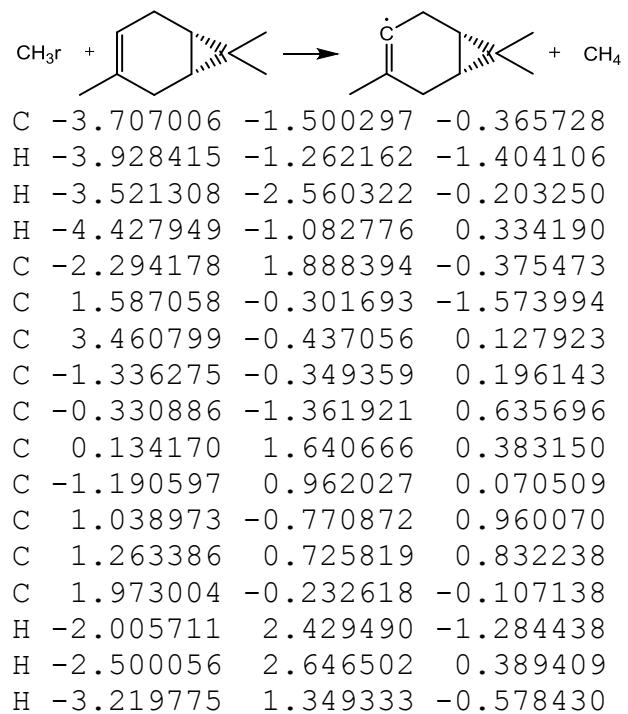
Hr +  →  + H<sub>2</sub>

H -4.611552 0.613825 -1.083396  
 C -2.969756 -0.734352 -0.167331  
 C -6.259410 -1.492504 5.021981  
 C -6.614447 -1.391056 2.515004  
 C -3.791323 -2.702626 1.058695  
 C -4.319675 -3.471152 2.236259  
 C -3.633198 -0.512279 2.266830  
 C -3.471085 -1.399060 1.052378  
 C -4.525879 -2.659179 3.503820  
 C -4.184555 -1.179991 3.516267  
 C -5.628626 -1.626311 3.645710  
 H -3.867999 -0.020100 -0.640710  
 H -2.715548 -1.410625 -0.983462  
 H -2.175937 -0.004102 0.005447  
 H -7.075178 -2.212364 5.151877  
 H -6.675447 -0.489390 5.167390  
 H -5.529942 -1.669001 5.817095  
 H -7.050420 -0.389142 2.590121  
 H -6.162424 -1.482647 1.527047  
 H -7.439578 -2.109366 2.572066  
 H -3.651525 -3.275768 0.144691  
 H -5.252301 -3.976054 1.944940  
 H -3.617249 -4.286491 2.453845  
 H -2.648988 -0.089647 2.505084  
 H -4.252135 0.352617 1.986142  
 H -4.295115 -3.205083 4.413495  
 H -3.743233 -0.806004 4.435192

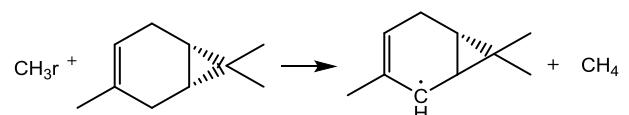
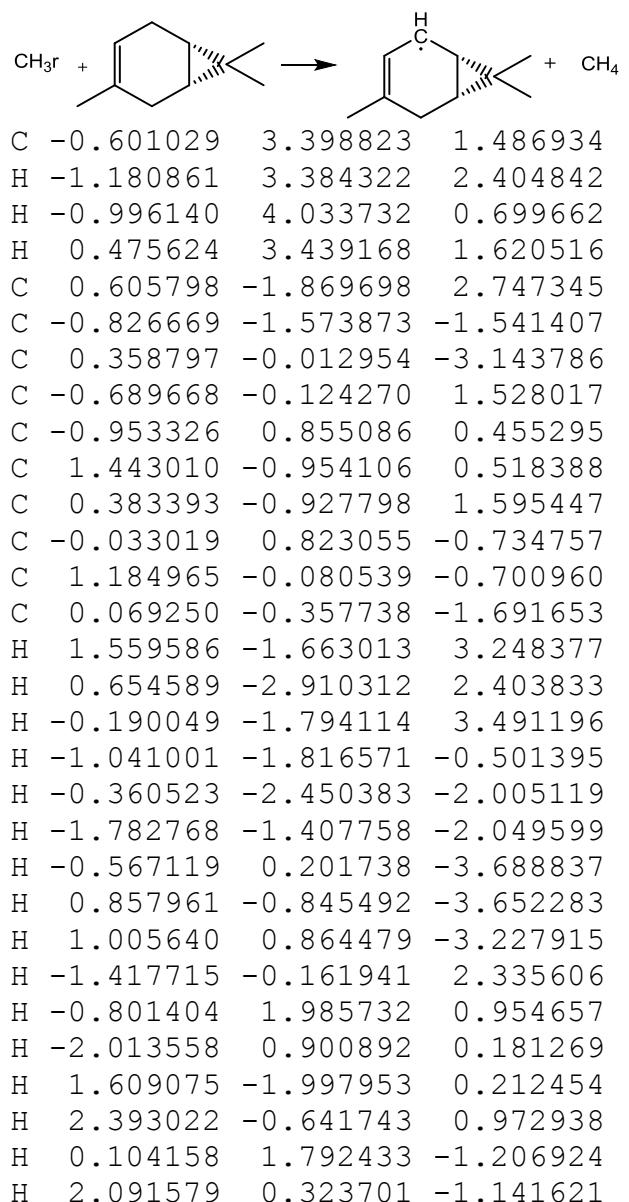


CH<sub>3</sub>r +  →  + CH<sub>4</sub>

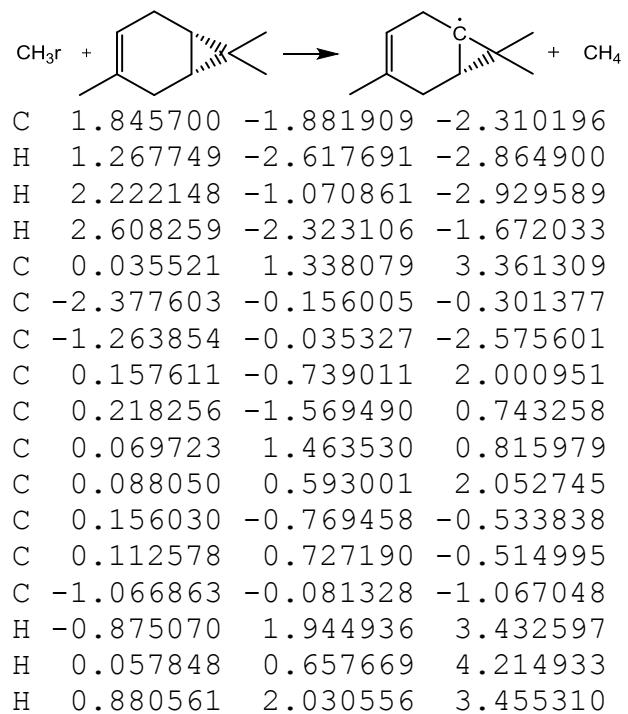
C -2.014547 0.462748 1.113690  
 H -1.196829 -0.083801 1.577323  
 H -2.164731 1.457574 1.526287  
 H -2.930329 -0.115853 1.018738  
 C -4.765018 3.525758 -2.607369  
 C -1.183540 0.931123 -1.433010  
 C -1.167541 -1.510100 -2.078319  
 C -2.840410 2.629635 -3.902290  
 C -1.873221 1.588897 -4.397421  
 C -4.117703 1.067897 -2.426783  
 C -3.834894 2.421379 -3.037096  
 C -2.055493 0.202872 -3.803872  
 C -3.173759 -0.057233 -2.819905  
 C -1.730741 -0.122490 -2.342804  
 H -4.725179 3.674699 -1.521669  
 H -5.806107 3.282362 -2.851272  
 H -4.516465 4.473273 -3.089664  
 H -1.591933 0.690681 -0.211097  
 H -1.528651 1.945814 -1.621002  
 H -0.096063 0.897895 -1.333239  
 H -1.392680 -1.837377 -1.057929  
 H -0.078867 -1.520881 -2.199894  
 H -1.587012 -2.249484 -2.765725  
 H -2.701412 3.630258 -4.306583  
 H -0.845243 1.942303 -4.234299  
 H -1.978172 1.514086 -5.487728  
 H -4.152381 1.172933 -1.332896  
 H -5.137396 0.778642 -2.714116  
 H -1.830905 -0.603646 -4.495632  
 H -3.661113 -1.024395 -2.899695



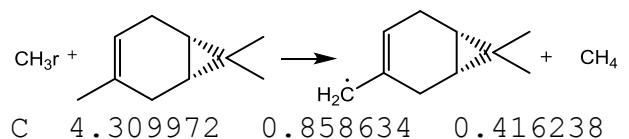
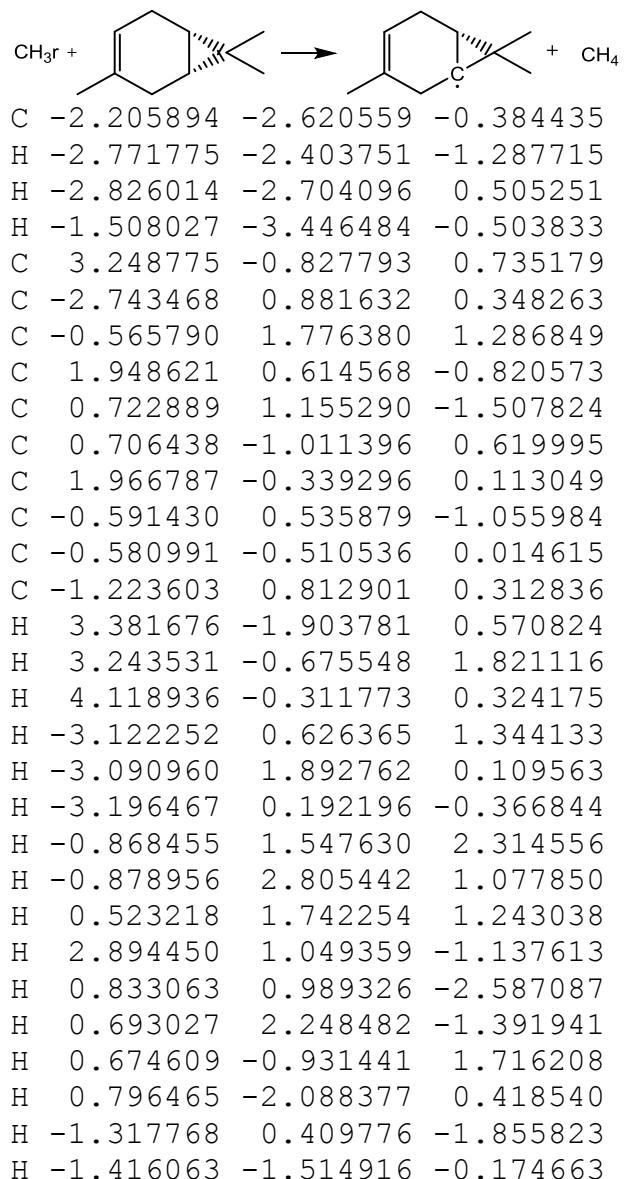
H 1.864773 -1.273471 -1.996581  
 H 0.518865 -0.159420 -1.738034  
 H 2.120156 0.465276 -2.146433  
 H 4.049330 0.327391 -0.391694  
 H 3.787181 -1.415577 -0.241685  
 H 3.710296 -0.382929 1.191124  
 H -2.542867 -0.897202 -0.093264  
 H -0.239946 -2.150214 -0.124975  
 H -0.711928 -1.868253 1.531477  
 H 0.441321 2.229126 -0.493836  
 H -0.050181 2.380657 1.172738  
 H 1.532122 -1.255061 1.797980  
 H 1.902485 1.170205 1.589546



C -2.755842 2.390300 0.395006  
 H -2.201697 3.322021 0.334104  
 H -3.518165 2.255604 -0.366425  
 H -3.050509 2.092441 1.396702  
 C 0.311063 0.479438 1.875473  
 C 0.911823 -1.300167 -2.228402  
 C -0.487781 -0.450668 -4.158844  
 C 1.467861 1.338992 -0.156542  
 C 1.620929 1.682834 -1.613207  
 C -0.859974 0.532871 -0.375717  
 C 0.372821 0.801611 0.404028  
 C 0.449724 1.288362 -2.500980  
 C -0.795886 0.696854 -1.869497  
 C 0.079057 -0.156856 -2.778903  
 H -0.498922 1.032159 2.365035  
 H 0.107340 -0.585598 2.036093  
 H 1.245859 0.727208 2.382273  
 H 1.322860 -1.089518 -1.241993  
 H 0.306996 -2.210442 -2.153441  
 H 1.747501 -1.520316 -2.901921  
 H 0.315334 -0.641636 -4.879483  
 H -1.133023 -1.335973 -4.138670  
 H -1.081611 0.386135 -4.536460  
 H 2.331733 1.543204 0.472134  
 H 1.770116 2.767529 -1.699026  
 H 2.553815 1.240051 -1.991493  
 H -1.700956 1.375275 0.011053  
 H -1.352998 -0.395833 -0.064654  
 H 0.286869 1.966305 -3.333628  
 H -1.743224 0.991103 -2.313932



H -2.234036 -0.171786 0.779411  
 H -3.013380 0.702387 -0.545690  
 H -2.931781 -1.059346 -0.578685  
 H -0.311609 0.029021 -3.105785  
 H -1.869140 0.831888 -2.861319  
 H -1.782375 -0.933559 -2.928708  
 H 0.177927 -1.298349 2.934309  
 H 1.154906 -2.144326 0.755779  
 H -0.579148 -2.325441 0.764931  
 H -0.806535 2.127379 0.860787  
 H 0.934666 2.137676 0.868345  
 H 0.953732 -1.297533 -1.443860  
 H 0.686364 1.241925 -1.282538



H 5.217561 0.573903 -0.108672  
 H 4.243330 0.495455 1.437895  
 H 4.018634 1.896955 0.285201  
 C 2.394133 -0.607722 -0.882614  
 C 0.009620 1.964866 2.029045  
 C -2.231544 2.882734 1.282366  
 C 0.401973 -1.079247 0.487317  
 C -0.961439 -0.831203 1.068049  
 C 0.440620 1.003189 -0.904148  
 C 1.040952 -0.287692 -0.389983  
 C -1.633883 0.457752 0.624082  
 C -0.930651 1.373554 -0.361329  
 C -1.157805 1.828540 1.068274  
 H 3.254852 0.101927 -0.270859  
 H 2.573447 -0.334111 -1.924874  
 H 2.718091 -1.629385 -0.682127  
 H 0.778652 1.207864 1.873824  
 H 0.480884 2.947967 1.921415  
 H -0.335895 1.882706 3.065446  
 H -2.644783 2.823090 2.295448  
 H -3.058725 2.761146 0.577786  
 H -1.824723 3.891297 1.148286  
 H 0.892351 -1.995266 0.810331  
 H -1.609826 -1.673390 0.791919  
 H -0.899785 -0.874664 2.165536  
 H 0.369571 0.923284 -1.996288  
 H 1.156628 1.818454 -0.726363  
 H -2.709211 0.368805 0.502440  
 H -1.569353 1.855815 -1.095356

## 7.2 Hydrogen abstraction on cara-2,4-diene

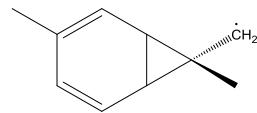
### Reactant

#### Cara-2,4-diene

C 0.239024 0.314700 -0.010679  
 C 0.371274 0.542956 1.425891  
 C 1.377705 -0.365355 -0.727297  
 C -0.632060 1.048533 2.169433  
 H 1.275911 0.192178 1.913802  
 C -1.878104 1.553257 1.577556  
 H -0.554979 1.048920 3.252533  
 C -2.035909 1.315877 0.036590  
 H -2.765500 1.446853 2.195160  
 C -0.922741 0.620261 -0.628138  
 C -1.920975 2.718461 0.603027  
 H -1.080865 0.306064 -1.656175  
 H 1.127426 -0.572271 -1.769636  
 H 2.279300 0.257451 -0.715321

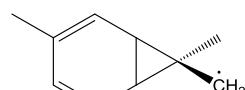
H 1.640443 -1.313122 -0.244533  
 C -0.691788 3.562558 0.345323  
 C -3.213197 3.518388 0.616495  
 H -3.026941 1.055538 -0.325069  
 H -0.771342 4.056890 -0.628651  
 H -0.600470 4.340898 1.110285  
 H 0.226572 2.978377 0.350413  
 H -3.367902 4.023453 -0.343069  
 H -4.081658 2.880609 0.801471  
 H -3.189053 4.285485 1.398025

### Products



2,4-caradien-8-yl

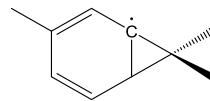
C 0.247189 0.290589 -0.000537  
 C 0.368097 0.567856 1.429525  
 C 1.404138 -0.381781 -0.692610  
 C -0.647210 1.088806 2.146011  
 H 1.280671 0.261868 1.932100  
 C -1.902389 1.524242 1.522431  
 H -0.569934 1.161084 3.226258  
 C -2.044308 1.243132 0.022753  
 H -2.788702 1.451259 2.143103  
 C -0.914088 0.567109 -0.632590  
 C -1.954595 2.712350 0.514791  
 H -1.055693 0.250117 -1.661702  
 H 1.170034 -0.609551 -1.734205  
 H 2.295590 0.255461 -0.678709  
 H 1.675139 -1.317168 -0.190708  
 C -0.711924 3.534394 0.239903  
 C -3.204888 3.454993 0.498651  
 H -3.027682 0.977039 -0.350340  
 H -0.770858 3.977770 -0.758600  
 H -0.632659 4.346778 0.968456  
 H 0.201730 2.946361 0.292619  
 H -3.208262 4.522015 0.320730  
 H -4.153070 2.959981 0.670551



2,4-caradien-8-yl

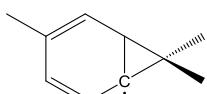
C 0.214482 0.352017 -0.044484  
 C 0.359679 0.558226 1.396276  
 C 1.355994 -0.294526 -0.785483  
 C -0.638604 1.049707 2.153472  
 H 1.277380 0.220265 1.868174

C -1.897080 1.531668 1.569771  
 H -0.544181 1.069415 3.234508  
 C -2.064484 1.324468 0.059185  
 H -2.776968 1.436627 2.199199  
 C -0.952846 0.665413 -0.644436  
 C -1.959674 2.763970 0.623002  
 H -1.112210 0.401061 -1.685683  
 H 1.104819 -0.469767 -1.833296  
 H 2.252401 0.335063 -0.754454  
 H 1.627297 -1.255096 -0.333655  
 C -0.786352 3.580131 0.377754  
 C -3.278981 3.520649 0.672534  
 H -3.058071 1.086458 -0.309949  
 H 0.202525 3.152570 0.305667  
 H -0.894028 4.651940 0.274227  
 H -3.465166 4.034587 -0.275592  
 H -4.121722 2.850698 0.860025  
 H -3.265579 4.271760 1.468475



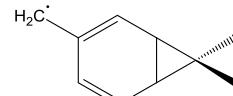
2,4-caradien-1-yl

C 0.280588 0.210376 0.023113  
 C 0.424788 0.463649 1.447439  
 C 1.339270 -0.594360 -0.681317  
 C -0.499745 1.137891 2.170606  
 C -1.735115 1.630305 1.540637  
 C -1.805669 1.452806 0.066793  
 C -0.790009 0.761242 -0.638010  
 C -1.916004 2.845243 0.539610  
 H 1.150411 -0.648111 -1.755261  
 H 2.335563 -0.163831 -0.531337  
 H 1.376281 -1.620237 -0.296063  
 C -0.766110 3.801480 0.293819  
 C -3.282107 3.506955 0.610882  
 H -0.858340 4.264802 -0.694606  
 H -0.765509 4.604835 1.038628  
 H 0.197084 3.291255 0.338546  
 H -3.507913 4.001549 -0.340042  
 H -4.070949 2.775728 0.797941  
 H -3.313141 4.265073 1.400444  
 H 1.307344 0.070332 1.944172  
 H -0.382381 1.232212 3.246462  
 H -0.846241 0.686198 -1.722124  
 H -2.637625 1.505731 2.139538



2,4-caradien-6-yl

C 0.281730 0.183866 -0.006976  
 C 0.384457 0.375959 1.428725  
 C 1.382416 -0.578725 -0.699804  
 C -0.530729 1.134484 2.112715  
 C -1.680365 1.621434 1.451388  
 C -1.891565 1.360239 0.007816  
 C -0.790600 0.671709 -0.685224  
 C -1.925649 2.822199 0.633220  
 H 1.196870 -0.664677 -1.771959  
 H 2.350871 -0.086046 -0.561138  
 H 1.477317 -1.589044 -0.287666  
 C -0.783140 3.783980 0.375985  
 C -3.303456 3.462443 0.629476  
 H -2.889215 1.097167 -0.345028  
 H -0.949077 4.340356 -0.552958  
 H -0.703951 4.513035 1.189921  
 H 0.170972 3.260920 0.296659  
 H -3.503406 3.962611 -0.323828  
 H -4.087939 2.724427 0.807892  
 H -3.368879 4.213686 1.424030  
 H 1.244034 -0.040087 1.945177  
 H -0.358534 1.382592 3.157220  
 H -0.895009 0.459213 -1.746049

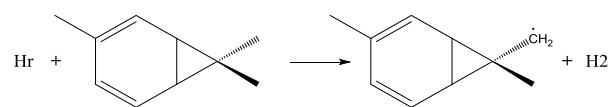


2,4-caradien-10-yl

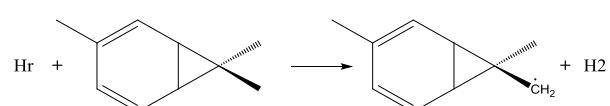
C 0.275513 0.370801 -0.062668  
 C 0.405367 0.594379 1.386734  
 C 1.320346 -0.203368 -0.768732  
 C -0.577945 1.124741 2.128810  
 C -1.845829 1.614659 1.551554  
 C -2.035302 1.379723 0.037346  
 C -0.948495 0.700081 -0.669088  
 C -1.909994 2.800997 0.603644  
 H 1.238016 -0.399937 -1.830817  
 H 2.248216 -0.472703 -0.279569  
 C -0.684354 3.640354 0.314154  
 C -3.201258 3.599256 0.638579  
 H -0.779319 4.121980 -0.664476  
 H -0.581590 4.429668 1.066454  
 H 0.235303 3.057846 0.312731  
 H -3.373565 4.104369 -0.317753  
 H -4.066001 2.961832 0.841154  
 H -3.161438 4.367088 1.418930  
 H 1.321246 0.256563 1.861124

H	-0.465206	1.187725	3.207138
H	-1.115588	0.406986	-1.700583
H	-2.720021	1.490430	2.184408
H	-3.036181	1.131613	-0.304536

### Transition states

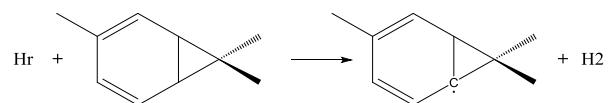


C	0.234626	0.307032	0.000027
C	0.365884	0.567388	1.431652
C	1.377646	-0.378566	-0.702782
C	-0.635700	1.095390	2.160560
H	1.273701	0.235906	1.926669
C	-1.885930	1.571016	1.549967
H	-0.555302	1.142861	3.241886
C	-2.044130	1.290791	0.035058
H	-2.771317	1.487495	2.173322
C	-0.927426	0.599133	-0.624598
C	-1.925119	2.734022	0.562137
H	-1.080454	0.279071	-1.651224
H	1.132707	-0.600456	-1.743170
H	2.277138	0.247250	-0.694353
H	1.640579	-1.318599	-0.205441
C	-0.690381	3.562579	0.281254
C	-3.193860	3.514042	0.561098
H	-3.033520	1.030672	-0.327209
H	-0.773710	4.041977	-0.699354
H	-0.589575	4.350002	1.034758
H	0.222070	2.970004	0.288968
H	-3.291041	4.234560	-0.252305
H	-4.105415	2.932631	0.701535
H	-3.193024	4.298432	1.633564
H	-3.197373	4.857093	2.422112

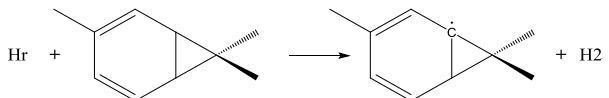


C	0.237838	0.309942	-0.006082
C	0.380271	0.585818	1.422188
C	1.376792	-0.381150	-0.710445
C	-0.619302	1.109287	2.156653
H	1.296036	0.268021	1.911517
C	-1.880386	1.569697	1.555242
H	-0.527908	1.167254	3.236526
C	-2.040730	1.291613	0.039294
H	-2.761102	1.475033	2.183811

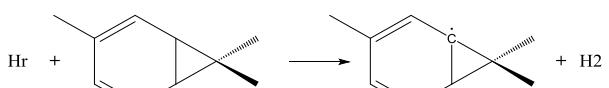
C	-0.929207	0.593105	-0.623289
C	-1.941395	2.732739	0.570176
H	-1.090974	0.263535	-1.645519
H	1.125022	-0.611951	-1.747293
H	2.276236	0.244718	-0.713265
H	1.643225	-1.317002	-0.207050
C	-0.739448	3.560932	0.303213
C	-3.246779	3.511022	0.569284
H	-3.032825	1.034910	-0.320889
H	-0.869151	4.297589	-0.490381
H	-0.546464	4.333074	1.376717
H	0.207577	3.034970	0.228334
H	-3.411427	3.994487	-0.399258
H	-4.102716	2.861392	0.768655
H	-3.231318	4.291186	1.337135
H	-0.410294	4.875247	2.152145



C	0.235290	0.278279	-0.009049
C	0.355610	0.497201	1.427494
C	1.365317	-0.424729	-0.716318
C	-0.628531	1.068380	2.156794
H	1.252268	0.138361	1.924447
C	-1.839054	1.572408	1.530871
H	-0.540586	1.136706	3.237125
C	-2.011281	1.328530	0.029886
H	-2.911092	1.411968	2.313349
C	-0.906959	0.630824	-0.643007
C	-1.934487	2.754616	0.616054
H	-1.058676	0.334179	-1.677168
H	1.132461	-0.597507	-1.768642
H	2.287606	0.164721	-0.667411
H	1.581429	-1.392482	-0.250962
C	-0.718962	3.626544	0.379297
C	-3.250927	3.514557	0.593241
H	-3.005471	1.082242	-0.335762
H	-0.815238	4.157409	-0.573560
H	-0.629840	4.375746	1.172798
H	0.205212	3.050397	0.353770
H	-3.396252	4.003419	-0.375485
H	-4.102779	2.856750	0.775694
H	-3.257585	4.290086	1.366221
H	-3.661163	1.293238	2.886468

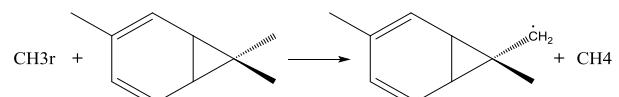


C	0.230408	0.275847	-0.000526
C	0.368409	0.503881	1.433371
C	1.353851	-0.422852	-0.721304
C	-0.616508	1.052890	2.173999
H	1.266306	0.136856	1.921304
C	-1.854370	1.559650	1.570064
H	-0.536449	1.065632	3.256822
C	-1.983981	1.349140	0.059621
H	-2.747265	1.460091	2.182595
C	-0.910380	0.650778	-0.629431
C	-1.936686	2.748954	0.587095
H	-1.054069	0.410311	-1.679477
H	1.112200	-0.590303	-1.772388
H	2.277741	0.164190	-0.674987
H	1.570829	-1.393652	-0.262236
C	-0.725131	3.616485	0.315931
C	-3.244838	3.520875	0.648700
H	-3.185917	0.995891	-0.403940
H	-0.811613	4.088701	-0.668140
H	-0.654307	4.412377	1.064652
H	0.204022	3.048162	0.336595
H	-3.424320	4.041872	-0.297507
H	-4.096408	2.862945	0.831834
H	-3.212933	4.271152	1.445340
H	-4.035808	0.733131	-0.745315

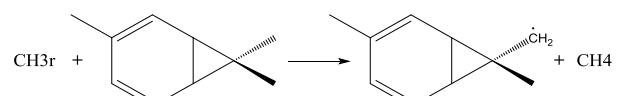


C	0.237108	0.275470	0.034817
C	0.331713	0.490223	1.477668
C	1.368541	-0.369112	-0.662975
C	-0.683821	1.008041	2.193641
H	1.216776	0.121795	1.986758
C	-1.904848	1.538189	1.569981
H	-0.637251	1.003380	3.278311
C	-2.024653	1.314981	0.025157
H	-2.811567	1.437661	2.159677
C	-0.907629	0.611341	-0.615651
C	-1.898884	2.713945	0.609979
H	-1.039393	0.309429	-1.650751
H	1.127005	-0.743863	-1.657760
H	2.255186	0.457654	-0.876850
H	1.893634	-1.123393	-0.074022
C	-0.648275	3.537591	0.391127
C	-3.177091	3.535723	0.590110

H	-3.009315	1.079055	-0.368370
H	-0.690212	4.034666	-0.583478
H	-0.569523	4.313094	1.160181
H	0.261600	2.941146	0.423615
H	-3.294535	4.048277	-0.370515
H	-4.061711	2.912912	0.747274
H	-3.160425	4.298061	1.376288
H	3.079072	1.135285	-1.107901

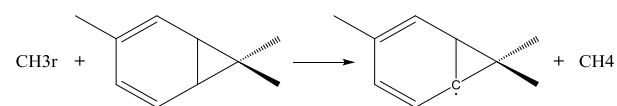


C	0.232131	0.333789	0.017941
C	0.388880	0.639814	1.437931
C	1.365856	-0.367714	-0.684717
C	-0.603063	1.182248	2.169647
H	1.307191	0.327127	1.926002
C	-1.867058	1.635347	1.570476
H	-0.503430	1.255879	3.248179
C	-2.052628	1.306837	0.063290
H	-2.740542	1.560773	2.211837
C	-0.944367	0.597060	-0.592002
C	-1.937933	2.761171	0.544857
H	-1.115825	0.238984	-1.603227
H	1.101173	-0.626174	-1.711828
H	2.260997	0.263714	-0.716465
H	1.646016	-1.288942	-0.162031
C	-0.714319	3.586968	0.209781
C	-3.216467	3.538385	0.546156
H	-3.047160	1.026006	-0.268871
H	-0.826210	4.037605	-0.781733
H	-0.595751	4.396806	0.936329
H	0.201357	2.998984	0.209417
H	-3.344611	4.182655	-0.326607
H	-4.111662	2.940597	0.726065
H	-3.208354	4.381389	1.552632
C	-3.236864	5.276701	2.637771
H	-2.691803	4.768412	3.429587
H	-2.744198	6.174846	2.273117
H	-4.294242	5.414334	2.851460



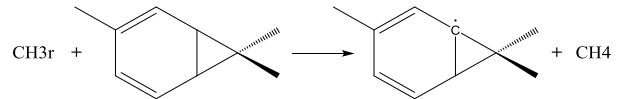
C	0.264745	0.374255	-0.003450
C	0.425329	0.670751	1.418395
C	1.413376	-0.284274	-0.723538
C	-0.577810	1.166886	2.167171

H 1.359435 0.386088 1.893523  
 C -1.864008 1.582624 1.587395  
 H -0.469300 1.229693 3.245518  
 C -2.047015 1.275503 0.074417  
 H -2.728528 1.463587 2.234447  
 C -0.925182 0.604915 -0.598702  
 C -1.983032 2.722415 0.583306  
 H -1.095983 0.252120 -1.611837  
 H 1.147232 -0.540105 -1.750954  
 H 2.288080 0.375012 -0.756718  
 H 1.726878 -1.201828 -0.213416  
 C -0.814588 3.595485 0.276583  
 C -3.316843 3.452051 0.595679  
 H -3.036303 0.973214 -0.257634  
 H -0.990086 4.269137 -0.564821  
 H -0.621598 4.410158 1.289078  
 H 0.140427 3.085659 0.181346  
 H -3.516388 3.912258 -0.377761  
 H -4.144966 2.775120 0.821265  
 H -3.318546 4.245993 1.349344  
 C -0.373100 5.275903 2.363379  
 H 0.673410 5.549606 2.252639  
 H -1.059392 6.108058 2.224755  
 H -0.577465 4.680048 3.249513

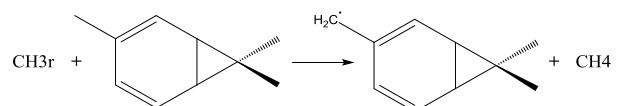
CH3r +  + CH4

C 0.206505 0.289293 0.020129  
 C 0.298182 0.522127 1.457415  
 C 1.346737 -0.427539 -0.656473  
 C -0.700882 1.099146 2.159603  
 H 1.180168 0.158648 1.977059  
 C -1.904379 1.607647 1.513647  
 H -0.635807 1.163623 3.242284  
 C -2.033819 1.355886 0.000750  
 H -2.968167 1.451250 2.259700  
 C -0.920152 0.640964 -0.639905  
 C -1.945316 2.779358 0.573043  
 H -1.051347 0.335751 -1.674616  
 H 1.132436 -0.614244 -1.710502  
 H 2.270563 0.158981 -0.599347  
 H 1.551137 -1.389592 -0.173930  
 C -0.707826 3.625086 0.354337  
 C -3.241219 3.572275 0.508317  
 H -3.020624 1.116038 -0.389569  
 H -0.767517 4.140268 -0.610308  
 H -0.626639 4.387388 1.136449  
 H 0.206424 3.033337 0.364844  
 H -3.342727 4.064281 -0.464766

H -4.115416 2.936072 0.659187  
 H -3.256325 4.349542 1.279768  
 C -4.054485 1.220888 3.109406  
 H -3.678091 0.495675 3.827408  
 H -4.293819 2.187156 3.547204  
 H -4.837274 0.825637 2.465984



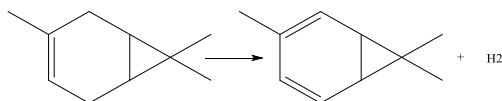
C 0.199064 0.376958 -0.166291  
 C 0.381646 0.453892 1.279289  
 C 1.308843 -0.221070 -0.992036  
 C -0.588312 0.898012 2.104198  
 H 1.301438 0.055321 1.696950  
 C -1.853390 1.445265 1.598679  
 H -0.472170 0.796772 3.179264  
 C -2.044659 1.385586 0.072312  
 H -2.721202 1.269788 2.230572  
 C -0.971175 0.784860 -0.712629  
 C -1.972441 2.723253 0.750320  
 H -1.146504 0.638703 -1.775669  
 H 1.032573 -0.286172 -2.046120  
 H 2.222972 0.378611 -0.918497  
 H 1.561299 -1.228533 -0.642892  
 C -0.772885 3.622770 0.534603  
 C -3.275931 3.484394 0.934374  
 H -3.226887 1.053106 -0.378480  
 H -0.894624 4.199828 -0.388192  
 H -0.677069 4.332569 1.363171  
 H 0.158086 3.062478 0.460423  
 H -3.494191 4.091737 0.049509  
 H -4.120942 2.811833 1.093280  
 H -3.210754 4.158204 1.795195  
 C -4.449473 0.622008 -0.906103  
 H -4.841041 1.467323 -1.467175  
 H -4.180829 -0.229438 -1.527365  
 H -5.052627 0.353040 -0.041855



C 0.221793 0.816101 -0.565761  
 C -0.104812 0.238410 0.738319  
 C 1.457653 0.372819 -1.239571  
 C -1.273338 0.479015 1.361436  
 H 0.591206 -0.480651 1.159492  
 C -2.255975 1.450000 0.857768  
 H -1.536460 -0.083389 2.252208

C	-1.928971	2.075459	-0.537193	H	0.202008	5.253440	3.171112
H	-3.295182	1.215818	1.071095	H	1.953365	5.278889	3.410604
C	-0.687515	1.621002	-1.178023	H	1.272672	5.636433	1.817466
C	-1.955402	2.932732	0.718545	H	0.381554	2.129037	-0.079363
H	-0.523065	1.921892	-2.208862	H	-1.164252	1.639980	0.555327
H	1.291696	-0.781067	-1.731130				
H	1.741655	0.978935	-2.099764				
H	2.306317	0.223404	-0.569560				
C	-0.681780	3.526167	1.280237				
C	-3.160497	3.849095	0.849609				
H	-2.762629	2.245431	-1.213076				
H	-0.439334	4.458623	0.759751				
H	-0.809887	3.758568	2.342746				
H	0.171592	2.857450	1.183728				
H	-2.989089	4.794523	0.323846				
H	-4.062479	3.393627	0.432207				
H	-3.359468	4.082512	1.901152				
C	1.142628	-2.115149	-2.350309				
H	0.846914	-2.742283	-1.514228				
H	0.365008	-1.947204	-3.089732				
H	2.125197	-2.331743	-2.759676				

### 7.3 Hydrogen elimination reaction on 3-carene



#### Reactant

C	0.391022	-0.611885	0.151875
C	0.451013	0.441109	1.227730
C	0.961943	0.190977	2.434855
C	1.056857	1.172103	3.572060
C	0.528390	2.565602	3.272868
H	0.029800	3.033598	4.116357
C	-0.057402	2.872103	1.906538
H	-0.920027	3.531732	1.899744
C	1.237882	3.531516	2.342111
C	2.555241	3.148286	1.691956
C	1.159974	5.005191	2.706075
C	-0.114691	1.788722	0.841651
H	0.945094	-0.295927	-0.740220
H	-0.642310	-0.790070	-0.169138
H	0.808820	-1.561493	0.492356
H	1.345272	-0.806127	2.642187
H	0.496727	0.763945	4.423304
H	2.099057	1.222744	3.919162
H	2.711553	3.725732	0.774132
H	3.392112	3.372428	2.362490
H	2.609565	2.090318	1.434591

#### Product

C	-4.286287	1.349136	-0.206857
C	-3.019801	0.622004	0.166906
C	-1.889694	1.273386	0.516724
C	-0.630193	0.589640	0.851534
C	0.129685	-0.282184	-0.130602
C	1.633321	-0.338673	0.083087
C	-0.274955	-0.346919	-1.587288
C	-0.697187	-0.972535	0.941602
C	-2.016218	-1.564297	0.679559
C	-3.066384	-0.835320	0.254849
H	-4.158420	2.431713	-0.146493
H	-4.595131	1.103512	-1.229216
H	-5.114960	1.065948	0.451550
H	-1.901439	2.356331	0.603819
H	-0.004897	1.101340	1.578129
H	2.129572	0.495704	-0.424185
H	1.893295	-0.286412	1.143742
H	2.049480	-1.269166	-0.317913
H	0.158127	0.495836	-2.136384
H	0.097333	-1.270919	-2.042197
H	-1.354299	-0.316982	-1.724587
H	-0.115103	-1.456060	1.721132
H	-2.141082	-2.622921	0.886167
H	-4.017769	-1.324182	0.066930

#### Transition state

Two hydrogen atoms on the same side as the three membered ring.

C	-0.030813	0.171598	-0.010297
C	-0.087563	-0.139805	1.464682
C	1.030227	0.037220	2.297341
C	0.826005	0.007793	3.678652
C	-0.094289	-1.070443	4.205832
H	0.454263	-1.945776	4.548583
C	-1.299845	-1.274671	3.320983
H	-1.583232	-2.291131	3.053780
C	-1.495619	-0.915532	4.793005
C	-2.098091	0.392458	5.307206
C	-1.912762	-2.111703	5.642101
C	-1.306375	-0.344070	2.128256
H	0.797609	0.841959	-0.253893
H	-0.959046	0.639278	-0.350402

H	0.102839	-0.742236	-0.599930	C	0.451013	0.441109	1.227730
H	1.940270	0.464928	1.887682	C	0.961943	0.190977	2.434855
H	1.617071	0.354737	4.338535	C	1.056857	1.172103	3.572060
H	-0.407906	1.089375	3.608317	C	0.528390	2.565602	3.272868
H	-2.731436	0.885308	4.566562	H	0.029800	3.033598	4.116357
H	-2.722089	0.182753	6.180523	C	-0.057402	2.872103	1.906538
H	-1.338164	1.113617	5.616056	H	-0.920027	3.531732	1.899744
H	-1.480667	-3.045514	5.272057	C	1.237882	3.531516	2.342111
H	-1.588844	-1.982541	6.680365	C	2.555241	3.148286	1.691956
H	-3.002067	-2.225520	5.643357	C	1.159974	5.005191	2.706075
H	-1.105715	0.959390	3.085968	C	-0.114691	1.788722	0.841651
H	-2.228913	-0.284504	1.554089	H	0.945094	-0.295927	-0.740220

Two hydrogen atoms on the opposite side to the three membered ring.

C	0.187228	0.336944	0.123454
C	-0.059111	-0.079006	1.550405
C	1.380229	0.192485	1.029779
C	2.241788	-1.011976	1.238725
C	1.711742	-2.336424	0.879089
C	2.624615	-3.413536	0.371510
C	0.463319	-2.558919	1.326729
H	0.031483	-3.550487	1.355814
C	-0.142238	-1.471660	2.095947
H	3.308006	-0.857878	1.082694
H	2.040590	-1.103630	2.324556
H	0.698875	-1.354974	2.826306
H	-1.056928	-1.707935	2.638065
H	-0.519095	0.664057	2.198004
H	1.860268	1.114205	1.337224
H	2.148202	-4.391839	0.468700
H	2.890792	-3.268653	-0.678179
H	3.562626	-3.434757	0.938131
C	-0.183019	1.794059	-0.128462
C	-0.088336	-0.524512	-1.089565
H	-1.246452	1.884706	-0.373128
H	0.014995	2.425976	0.741256
H	0.390486	2.194722	-0.970867
H	-1.144187	-0.438702	-1.374373
H	0.507605	-0.166725	-1.942029
H	0.133200	-1.575792	-0.940666

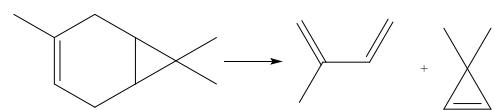
C	0.451013	0.441109	1.227730
C	0.961943	0.190977	2.434855
C	1.056857	1.172103	3.572060
C	0.528390	2.565602	3.272868
H	0.029800	3.033598	4.116357
C	-0.057402	2.872103	1.906538
H	-0.920027	3.531732	1.899744
C	1.237882	3.531516	2.342111
C	2.555241	3.148286	1.691956
C	1.159974	5.005191	2.706075
C	-0.114691	1.788722	0.841651
H	0.945094	-0.295927	-0.740220
H	-0.642310	-0.790070	-0.169138
H	0.808820	-1.561493	0.492356
H	1.345272	-0.806127	2.642187
H	0.496727	0.763945	4.423304
H	2.099057	1.222744	3.919162
H	2.711553	3.725732	0.774132
H	3.392112	3.372428	2.362490
H	2.609565	2.090318	1.434591
H	0.202008	5.253440	3.171112
H	1.953365	5.278889	3.410604
H	1.272672	5.636433	1.817466
H	0.381554	2.129037	-0.079363
H	-1.164252	1.639980	0.555327

### Product

#### Isoprene

C	1.378152	1.350658	-0.133250
C	0.503576	0.368012	0.126941
C	0.849683	-0.771467	1.052246
C	-1.790694	-0.516396	-0.329517
C	-0.824047	0.391463	-0.497560
H	-2.744783	-0.417563	-0.833462
H	1.125911	2.168760	-0.799393
H	2.367416	1.366485	0.309699
H	1.861858	-0.664049	1.444502
H	0.157380	-0.815284	1.899175
H	0.783930	-1.733527	0.533965
H	-1.668728	-1.383161	0.310013
H	-1.012004	1.238338	-1.153860

### 7.4 Diels Alder reaction on 3-carene



#### Reactant

C	0.391022	-0.611885	0.151875
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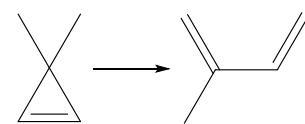
#### 3,3-diemethyl-cyclopropene

C	1.158983	-1.155717	4.564101
C	1.562138	-0.853905	3.124306
C	3.071527	-0.745317	2.933024
C	0.692471	-1.331003	1.984513
C	0.632786	-0.062610	2.233672
H	1.512992	-0.372649	5.244723

H	1.594725	-2.102095	4.905062
H	0.073707	-1.226632	4.664069
H	3.572790	-1.677753	3.217739
H	3.323520	-0.528921	1.892583
H	3.491470	0.051643	3.557735
H	0.370870	-2.174438	1.395175
H	0.225811	0.908069	2.000689

### Transition state

C	-0.679437	-0.624177	0.399771
C	0.498596	0.140665	0.963979
C	0.960892	-0.209156	2.262103
C	1.864379	0.524460	2.984297
C	0.641123	2.546563	3.097123
H	0.193170	2.260462	4.035641
C	0.222132	2.865518	1.857407
H	-0.721078	2.964971	1.343104
C	1.192677	3.824393	2.509019
C	2.642454	3.945714	2.052315
C	0.654463	5.156290	3.030987
C	0.967242	1.268715	0.332812
H	-1.542369	-0.592741	1.073946
H	-0.423907	-1.679138	0.256221
H	-0.990109	-0.224870	-0.567427
H	0.420486	-1.000164	2.777808
H	2.080476	0.258815	4.012975
H	2.597223	1.161001	2.512679
H	2.732701	4.689463	1.252664
H	3.278353	4.276614	2.881060
H	3.054356	3.009275	1.677365
H	-0.385545	5.067696	3.353627
H	1.245124	5.510347	3.883767
H	0.705144	5.930517	2.256696
H	1.939870	1.679229	0.554089
H	0.542819	1.577925	-0.616200

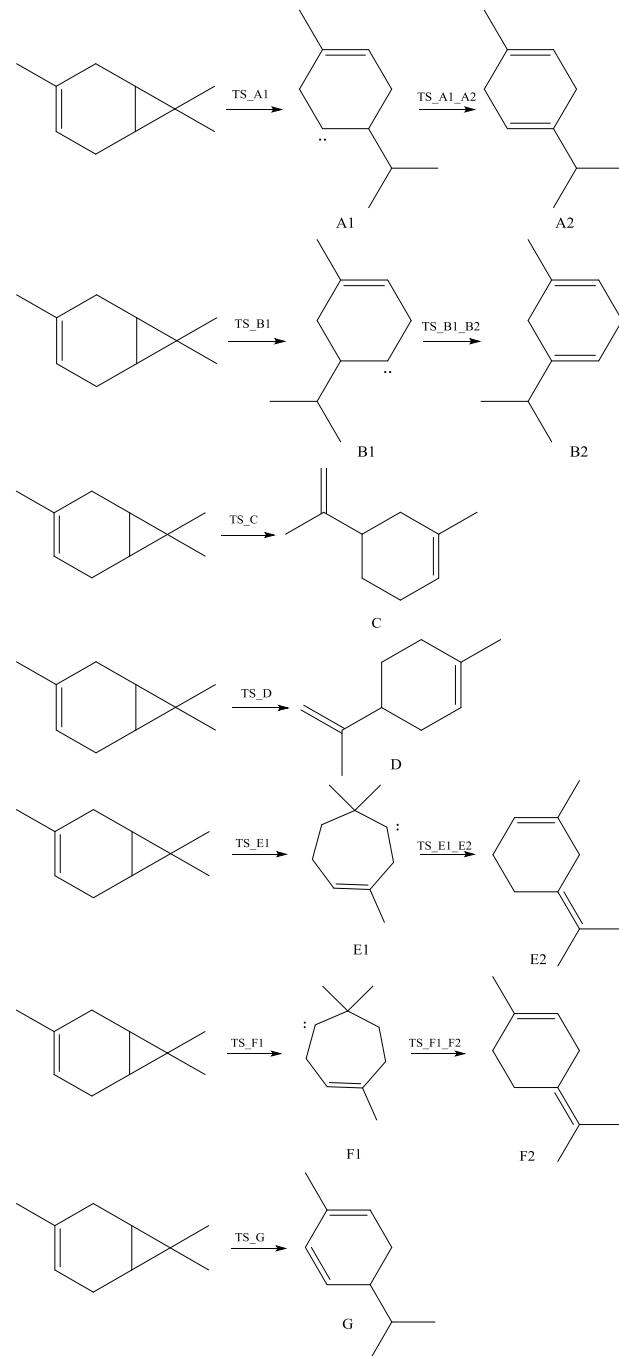


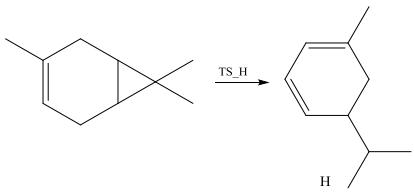
### Transition state

C	1.756018	1.346532	-0.059740
C	1.521850	-0.096039	-0.151636
C	2.203153	-1.091459	0.754511
C	-0.045137	0.106638	-0.110887
C	0.547530	-0.444631	-1.224861
H	0.222210	1.425348	0.009654
H	1.672385	1.922445	-0.982464
H	2.451715	1.769828	0.669890
H	2.322075	-0.701142	1.771905

H	1.622284	-2.014091	0.797953
H	3.198369	-1.348362	0.378070
H	-0.470518	-0.152737	0.843692
H	0.516716	-0.010981	-2.222457

## 7.5 Three membered ring opening reaction on 3-carene through molecule chemistry





### Reactant

#### 3-carene:

C 0.391022 -0.611885 0.151875  
 C 0.451013 0.441109 1.227730  
 C 0.961943 0.190977 2.434855  
 C 1.056857 1.172103 3.572060  
 C 0.528390 2.565602 3.272868  
 H 0.029800 3.033598 4.116357  
 C -0.057402 2.872103 1.906538  
 H -0.920027 3.531732 1.899744  
 C 1.237882 3.531516 2.342111  
 C 2.555241 3.148286 1.691956  
 C 1.159974 5.005191 2.706075  
 C -0.114691 1.788722 0.841651  
 H 0.945094 -0.295927 -0.740220  
 H -0.642310 -0.790070 -0.169138  
 H 0.808820 -1.561493 0.492356  
 H 1.345272 -0.806127 2.642187  
 H 0.496727 0.763945 4.423304  
 H 2.099057 1.222744 3.919162  
 H 2.711553 3.725732 0.774132  
 H 3.392112 3.372428 2.362490  
 H 2.609565 2.090318 1.434591  
 H 0.202008 5.253440 3.171112  
 H 1.953365 5.278889 3.410604  
 H 1.272672 5.636433 1.817466  
 H 0.381554 2.129037 -0.079363  
 H -1.164252 1.639980 0.555327

### Products

#### A1:

C 0.632027 0.333141 -0.093151  
 C 1.865728 -0.453173 0.364586  
 C 0.452581 1.606657 0.746279  
 C -0.648831 -0.544769 -0.057535  
 C -1.003744 -1.065665 1.271664  
 H -0.366089 -1.546046 -0.470141  
 C -1.793559 -0.020925 -0.960623  
 C -2.412962 -1.517203 1.403705  
 H 0.786557 0.631923 -1.138210  
 H 2.055592 -1.310531 -0.289463  
 H 2.757557 0.180059 0.352167  
 H 1.720200 -0.830444 1.379353

H -0.397921 2.206074 0.409056  
 H 0.289205 1.343118 1.795786  
 H 1.342699 2.239456 0.689271  
 H -2.814164 -0.736112 2.083392  
 C -3.292831 -1.640506 0.172918  
 H -1.430807 0.083780 -1.988271  
 C -2.992970 -0.928947 -0.915376  
 H -2.070776 0.992313 -0.639187  
 H -3.622804 -0.991245 -1.799128  
 H -2.459912 -2.415866 2.033070  
 C -4.474923 -2.564721 0.264144  
 H -5.049491 -2.576361 -0.664660  
 H -4.157298 -3.591230 0.482065  
 H -5.148075 -2.267096 1.077239

#### A2:

C 0.617737 0.369921 0.281097  
 C 0.548595 1.464152 1.363404  
 C 0.917866 0.986486 -1.098525  
 C -0.622718 -0.510716 0.265644  
 C -0.540737 -1.816826 0.527809  
 H 0.431886 -2.248604 0.755218  
 C -1.952878 0.133427 -0.055484  
 C -1.704630 -2.767826 0.536323  
 H 1.459251 -0.285150 0.534342  
 H 0.346853 1.033043 2.347465  
 H 1.496859 2.006965 1.419048  
 H -0.234602 2.196993 1.148300  
 H 0.980128 0.214588 -1.870021  
 H 0.146945 1.702501 -1.398095  
 H 1.871116 1.523011 -1.078053  
 H -1.770248 -3.266424 1.516221  
 C -3.030280 -2.122674 0.215402  
 H -1.897991 0.628936 -1.035679  
 C -3.117132 -0.818626 -0.047051  
 H -2.149452 0.951245 0.652928  
 H -4.089815 -0.387581 -0.274497  
 H -1.518568 -3.589460 -0.173193  
 C -4.227997 -3.033537 0.211446  
 H -5.145537 -2.492769 -0.029457  
 H -4.106313 -3.841701 -0.519789  
 H -4.361427 -3.513494 1.188427

#### B1:

C 0.523281 0.345803 0.033861  
 C 1.707868 -0.619490 -0.086783  
 C 0.696141 1.275983 1.243655  
 C -0.828866 -0.414858 0.107906  
 C -0.960956 -1.340549 1.241811  
 H -0.775259 -1.244850 -0.643858  
 C -2.051897 0.448274 -0.291621  
 C -2.363933 -1.707189 1.557031

H	0.494682	0.965418	-0.872025	C	1.224081	1.247524	3.415058
H	1.639695	-1.219620	-1.000087	C	-0.044416	2.093544	3.249232
H	2.654096	-0.071586	-0.117291	H	-0.915373	1.493503	3.536154
H	1.727358	-1.303895	0.764119	C	-0.198617	2.558610	1.788423
H	-0.117626	2.002446	1.324969	C	-0.326642	1.325406	0.868624
H	0.721790	0.687914	2.166228	H	1.197494	-0.383569	-0.825951
H	1.631405	1.838262	1.172522	H	-0.103999	-1.313749	-0.097854
H	-2.476947	-1.141164	2.508622	H	1.566997	-1.585789	0.423597
C	-3.466310	-1.350863	0.589271	H	2.107478	-0.563091	2.481504
H	-1.885134	0.883279	-1.283363	H	1.210021	0.741051	4.387337
C	-3.339220	-0.344077	-0.277778	H	2.108757	1.899964	3.438558
H	-2.134435	1.300425	0.396662	H	-0.213727	1.642541	-0.175113
C	-4.418759	0.064158	-1.240348	H	-1.336482	0.898061	0.937081
H	-2.423998	-2.747147	1.898615	C	-1.327594	3.554737	1.584922
H	-4.379051	-1.940868	0.618435	C	-2.712981	3.164228	2.041598
H	-5.309572	-0.558741	-1.135041	C	-1.096033	4.741959	1.021356
H	-4.712465	1.108481	-1.079973	H	-1.891090	5.463079	0.862095
H	-4.069480	-0.006266	-2.277159	H	-0.101376	5.033321	0.699888

### B2:

C	-0.006152	0.008258	0.008726
C	0.024696	0.021365	1.549035
C	1.423599	-0.014067	-0.564840
C	-0.845384	1.140195	-0.565637
C	-1.939995	0.885337	-1.285454
H	-2.228417	-0.149337	-1.458713
C	-0.400827	2.561130	-0.295692
C	-2.827949	1.935114	-1.890533
H	-0.493719	-0.924088	-0.298280
H	-0.986853	0.025451	1.963382
H	0.542667	-0.864585	1.928152
H	0.552401	0.897917	1.936298
H	1.409505	-0.035642	-1.657666
H	1.999698	0.861460	-0.251211
H	1.961476	-0.900308	-0.215279
H	-3.858863	1.802370	-1.527784
C	-2.366729	3.336135	-1.609054
H	0.627626	2.704305	-0.659406
C	-1.280709	3.633497	-0.895593
H	-0.330207	2.728821	0.789390
C	-0.848485	5.051301	-0.633277
H	-2.899876	1.777863	-2.977773
H	-2.969614	4.142036	-2.021313
H	-1.527178	5.771649	-1.094473
H	-0.810217	5.259408	0.442838
H	0.160007	5.234913	-1.023173

### C:

C	0.851019	-0.819763	0.118444
C	0.683705	0.239535	1.175646
C	1.378607	0.227576	2.316503

### D:

H	1.171580	0.026979	-0.416445
C	0.925110	0.554608	0.503028
C	0.801444	-0.141766	1.636226
C	0.475177	0.546155	2.942700
C	0.740457	2.054946	2.901442
H	0.356664	2.531309	3.807920
C	0.138083	2.713660	1.635500
C	0.757856	2.049261	0.389268
C	0.953149	-1.638378	1.686645
H	-0.576971	0.353324	3.193251
H	1.061211	0.091456	3.750670
H	1.741651	2.501855	0.202848
H	0.157063	2.288912	-0.494795
C	-1.385558	2.725374	1.678354
C	-1.991477	3.753890	2.604365
C	-2.158606	1.908887	0.960514
H	-3.240381	1.959115	1.029507
H	-1.748553	1.162887	0.290999
H	-3.081704	3.702069	2.601159
H	-1.651336	3.620630	3.636795
H	-1.696199	4.766650	2.306038
H	1.822488	2.227989	2.891682
H	0.451138	3.765525	1.639401
H	0.045371	-2.110989	2.081018
H	1.151655	-2.058844	0.698405
H	1.772539	-1.930633	2.354179

**E1:**

C -0.590929 -2.714309 -1.752365  
 C -0.394787 -1.563624 -0.789380  
 C 0.017426 -1.801783 0.459417  
 C 0.313086 -0.871246 1.604318  
 C -0.184533 0.571520 1.538965  
 H 0.161570 1.094507 2.437438  
 C -0.735722 1.098603 -0.754183  
 H -1.280358 0.589233 1.589977  
 C 0.262246 1.423291 0.303569  
 C 1.720394 1.125182 -0.123487  
 C 0.146208 2.918175 0.671974  
 C -0.748259 -0.221066 -1.422421  
 H 0.030348 -2.589299 -2.647326  
 H -1.629755 -2.767377 -2.097878  
 H -0.336861 -3.671919 -1.294698  
 H 0.206328 -2.845823 0.706346  
 H -0.102047 -1.322790 2.514421  
 H 1.399777 -0.874500 1.767834  
 H 1.994220 1.751694 -0.977127  
 H 2.409376 1.365442 0.692208  
 H 1.871174 0.082337 -0.404613  
 H -0.865118 3.150586 1.014283  
 H 0.853934 3.187295 1.463667  
 H 0.349604 3.543504 -0.200934  
 H -0.039736 -0.048734 -2.261225  
 H -1.707784 -0.346237 -1.942870

**E2:**

C 0.271379 0.236230 0.162652  
 C 0.359882 0.737975 1.396439  
 C 1.485275 -0.100716 -0.661817  
 C -0.834401 1.045812 2.258256  
 H 1.342801 0.931194 1.820525  
 C -2.101019 0.343944 1.736993  
 H -0.636389 0.733709 3.290644  
 H -1.000444 2.131133 2.299155  
 C -2.256836 0.538920 0.245276  
 H -1.994908 -0.732144 1.932134  
 H -2.972768 0.676911 2.298246  
 C -1.065629 -0.020961 -0.511050  
 C -3.310522 1.129255 -0.346517  
 H -1.183433 -1.109800 -0.639233  
 H -1.010977 0.383920 -1.524233  
 H 1.472639 -1.153778 -0.968165  
 H 1.515573 0.492569 -1.583593  
 H 2.410098 0.080419 -0.110279  
 C -3.468101 1.281069 -1.843445  
 C -4.491398 1.709288 0.399613  
 H -3.480315 2.340877 -2.126269

H -2.692402 0.787763 -2.425880  
 H -4.431546 0.866430 -2.163097  
 H -5.407591 1.153417 0.164851  
 H -4.375070 1.716477 1.481476  
 H -4.668040 2.742818 0.079127

**F1:**

C -0.695027 -2.689836 -1.737890  
 C -0.435963 -1.557751 -0.768877  
 C 0.127096 -1.814541 0.416067  
 C 0.491600 -0.919825 1.584635  
 C 0.270137 0.539597 1.672038  
 H -1.778243 0.821261 0.336894  
 C -0.954832 0.986853 -0.369157  
 H -1.248660 1.859674 -0.962719  
 C 0.319114 1.388951 0.447404  
 C 1.625968 1.199269 -0.361338  
 C 0.194615 2.873843 0.851303  
 C -0.838169 -0.206975 -1.315545  
 H -0.203646 -2.501854 -2.699987  
 H -1.766345 -2.788846 -1.948112  
 H -0.333886 -3.645529 -1.354359  
 H 0.357221 -2.858986 0.624226  
 H 0.112364 -1.395851 2.499411  
 H 1.592728 -0.974074 1.727996  
 H 1.611768 1.830728 -1.255146  
 H 2.484896 1.506531 0.241837  
 H 1.781508 0.165651 -0.672532  
 H -0.739030 3.046300 1.392351  
 H 1.015497 3.158522 1.514130  
 H 0.215051 3.527692 -0.027463  
 H -0.144556 0.038843 -2.131635  
 H -1.810867 -0.326526 -1.810413

**F2:**

C 0.120355 -0.155411 0.117440  
 C 0.350216 0.393114 1.312343  
 H 0.959966 -0.531610 -0.463515  
 C -0.791783 0.899360 2.163040  
 C 1.734967 0.541877 1.883404  
 C -2.148506 0.328103 1.715378  
 H -0.609120 0.636861 3.212755  
 H -0.816773 1.997303 2.129179  
 C -2.334242 0.453149 0.219485  
 H -2.166102 -0.739696 1.974021  
 H -2.954308 0.795998 2.279232  
 C -1.238107 -0.279520 -0.534091  
 C -3.338178 1.120389 -0.376586  
 H -1.496029 -1.348079 -0.618282  
 H -1.154378 0.079336 -1.562206  
 C -3.530383 1.196608 -1.875079

C	-4.421740	1.870988	0.364928	H	0.451743	-0.960396	2.504065
H	-3.442022	2.232473	-2.225116	H	1.147514	0.638227	4.308352
H	-2.829877	0.589075	-2.444714	H	1.675273	2.162139	0.546458
H	-4.541953	0.867299	-2.140933	H	0.105605	2.282447	-0.211641
H	-5.399957	1.403440	0.197523	C	-1.393078	3.148652	1.941798
H	-4.263719	1.934786	1.439705	C	-1.789505	3.991067	3.164258
H	-4.500378	2.894863	-0.019200	C	-1.935521	3.811586	0.666438
H	1.835487	-0.009073	2.826163	H	-1.862188	2.162607	2.046009
H	2.498993	0.178885	1.192641	H	-3.012940	3.979700	0.752478
H	1.954371	1.592161	2.110624	H	-1.462087	4.786182	0.501674

### G:

H	0.436336	-0.254841	-0.219065
C	0.590660	0.413171	0.623537
C	0.771910	-0.081558	1.857465
C	1.020106	0.864745	2.957610
C	0.772199	2.175289	2.831239
H	0.950553	2.845161	3.665860
C	0.176304	2.743266	1.557169
C	0.673284	1.897655	0.364241
C	0.759812	-1.553569	2.172364
H	1.404604	0.469254	3.893952
H	1.726511	2.155789	0.173231
H	0.135791	2.159826	-0.549410
C	-1.378653	2.845805	1.659489
C	-1.811630	3.615898	2.916909
C	-1.997918	3.503230	0.416935
H	-1.767285	1.823320	1.738781
H	-3.082497	3.588177	0.531009
H	-1.601555	4.514565	0.271240
H	-1.813114	2.936132	-0.497503
H	-2.901557	3.692357	2.965136
H	-1.474650	3.127009	3.832948
H	-1.410389	4.636126	2.909322
H	0.548809	3.766815	1.422412
H	1.713378	-1.868871	2.611470
H	-0.020253	-1.796753	2.902505
H	0.584984	-2.152339	1.276298

### H:

C	0.155324	-0.386018	-0.160074
C	0.401230	0.526737	1.004706
C	0.530983	0.097174	2.270318
C	0.819549	1.036983	3.353274
C	0.677538	2.359328	3.184498
H	0.885576	3.041906	4.001196
C	0.151521	2.922848	1.878197
C	0.600059	2.002768	0.721756
H	0.947858	-0.283541	-0.912177
H	-0.785574	-0.138515	-0.666176
H	0.111718	-1.432915	0.147928

H	0.451743	-0.960396	2.504065
H	1.147514	0.638227	4.308352
H	1.675273	2.162139	0.546458
H	0.105605	2.282447	-0.211641
C	-1.393078	3.148652	1.941798
C	-1.789505	3.991067	3.164258
C	-1.935521	3.811586	0.666438
H	-1.862188	2.162607	2.046009
H	-3.012940	3.979700	0.752478
H	-1.462087	4.786182	0.501674
H	-1.774334	3.206377	-0.227989
H	-2.870822	4.153714	3.185314
H	-1.509832	3.507382	4.101889
H	-1.309123	4.976075	3.133631
H	0.603644	3.909238	1.712580

### Transition state

#### TS\_A1(only this is used in the calculation)

C	0.309121	0.054373	0.122664
C	-0.131974	0.597503	1.473458
C	1.602484	0.658538	-0.420348
C	-0.755233	-0.139538	-0.981974
C	-0.371916	-1.563001	-0.701825
H	-0.383351	0.233883	-1.938070
C	-2.177795	0.377014	-0.738850
C	-1.331916	-2.299682	0.225113
H	0.651008	-1.089235	0.222234
H	-1.005982	0.080274	1.866989
H	0.680125	0.508089	2.200114
H	-0.383366	1.660899	1.390607
H	1.939312	0.104199	-1.298689
H	1.433597	1.699580	-0.714661
H	2.399633	0.639127	0.328493
H	-0.798876	-2.650630	1.119619
C	-2.658753	-1.679693	0.612389
H	-2.677399	0.460832	-1.713023
C	-3.022574	-0.478712	0.162002
H	-2.146347	1.405205	-0.353118
H	-3.997765	-0.079733	0.433858
H	-1.538185	-3.237422	-0.315371
C	-3.547189	-2.520190	1.489773
H	-4.496437	-2.022744	1.701081
H	-3.765766	-3.485613	1.017838
H	-3.059024	-2.745200	2.445958

#### TS\_A1\_A2:

C	0.530952	0.544829	-0.025554
C	1.795867	-0.116122	0.532170
C	0.370999	1.970374	0.535428
C	-0.758206	-0.249033	0.264034

C -0.919339 -0.894380 1.505083  
 H -0.386091 -1.432478 0.336928  
 C -1.899468 -0.003553 -0.726424  
 C -2.285551 -1.490835 1.743409  
 H 0.633815 0.621210 -1.115531  
 H 1.963890 -1.099792 0.082285  
 H 2.670158 0.504062 0.316255  
 H 1.712537 -0.256350 1.610491  
 H -0.504589 2.481115 0.125842  
 H 0.266332 1.932544 1.623336  
 H 1.248914 2.575944 0.295077  
 H -2.723126 -0.813362 2.496991  
 C -3.243328 -1.645717 0.578445  
 H -1.518248 -0.044792 -1.753404  
 C -3.046656 -0.959153 -0.548013  
 H -2.239786 1.032348 -0.587469  
 H -3.733181 -1.071026 -1.383400  
 H -2.187266 -2.440624 2.282872  
 C -4.390048 -2.601022 0.763551  
 H -5.032351 -2.640206 -0.119127  
 H -4.027254 -3.614872 0.968813  
 H -5.007342 -2.311200 1.622291

#### TS\_B1(only this is used in the calculation)

C 0.300878 0.045553 0.129034  
 C -0.140068 0.581924 1.482697  
 C 1.587057 0.661647 -0.417503  
 C -0.764747 -0.158570 -0.971873  
 C -0.366275 -1.578912 -0.693964  
 H -0.399895 0.219514 -1.928974  
 C -2.190548 0.348990 -0.726353  
 C -1.321432 -2.320789 0.233833  
 H 0.653371 -1.096077 0.225684  
 H -1.001890 0.049185 1.882428  
 H 0.678112 0.504611 2.203898  
 H -0.407732 1.641603 1.402473  
 H 1.925599 0.111468 -1.297806  
 H 1.408353 1.701671 -0.709775  
 H 2.386968 0.648030 0.328498  
 H -0.784504 -2.672772 1.124618  
 C -2.636400 -1.688146 0.614262  
 H -2.696050 0.422254 -1.698677  
 C -3.047904 -0.494862 0.184657  
 H -2.164206 1.381188 -0.349184  
 C -4.390415 0.081845 0.545648  
 H -1.526435 -3.256125 -0.310412  
 H -3.294267 -2.278414 1.250709  
 H -4.963400 -0.597974 1.179728  
 H -4.281358 1.035158 1.076695  
 H -4.983549 0.291112 -0.352740

#### TS\_B1\_B2

C 0.513952 0.532889 -0.026090  
 C 1.782585 -0.126395 0.524996  
 C 0.362222 1.962964 0.525868  
 C -0.774537 -0.255326 0.281180  
 C -0.920291 -0.905989 1.520755  
 H -0.400728 -1.441532 0.351885  
 C -1.926025 -0.000088 -0.696581  
 C -2.285418 -1.500187 1.769040  
 H 0.607412 0.601415 -1.117536  
 H 1.943521 -1.114648 0.082726  
 H 2.656028 0.489641 0.294217  
 H 1.710121 -0.256764 1.605274  
 H -0.514616 2.473925 0.119224  
 H 0.265580 1.933244 1.614770  
 H 1.240234 2.563945 0.274729  
 H -2.707755 -0.828528 2.536576  
 C -3.237273 -1.629479 0.606082  
 H -1.552471 -0.025715 -1.727795  
 C -3.084107 -0.956507 -0.535112  
 H -2.273021 1.031276 -0.541957  
 C -4.025911 -1.074421 -1.701504  
 H -2.186119 -2.456185 2.295289  
 H -4.073563 -2.316761 0.715373  
 H -4.840665 -1.769784 -1.489668  
 H -4.465937 -0.101952 -1.953645  
 H -3.501993 -1.422934 -2.599611

#### TB\_C:

C 0.310380 -0.456438 -0.102446  
 C 0.412605 0.490523 1.064613  
 C 0.791727 0.086075 2.278554  
 C 0.958021 0.991622 3.471811  
 C 0.298054 2.331507 3.342011  
 H -0.342929 2.691346 4.136125  
 C 0.131472 2.896684 1.950447  
 H -0.690215 3.610983 1.899000  
 C 1.410718 3.628655 2.250935  
 C 2.723183 3.135909 1.893061  
 C 1.274476 5.066938 2.693160  
 C 0.043918 1.925204 0.765995  
 H 0.969688 -0.146496 -0.922162  
 H -0.707868 -0.473086 -0.509622  
 H 0.578793 -1.476054 0.181704  
 H 1.054940 -0.959394 2.426508  
 H 0.604163 0.497051 4.381495  
 H 2.063465 1.093660 3.617598  
 H 1.959818 2.933393 3.140564  
 H 2.846697 2.244403 1.297341  
 H 3.592554 3.673528 2.241861  
 H 0.377508 5.220474 3.295657

H	2.141824	5.397835	3.268773
H	1.209812	5.694556	1.797369
H	0.662525	2.292376	-0.064201
H	-0.984096	1.937130	0.381679

#### TB\_D:

H	0.169949	-0.476230	0.040916
C	0.333191	0.246506	0.837949
C	0.838819	-0.176392	1.998317
C	1.139610	0.784157	3.130207
C	0.451632	2.112313	3.050381
H	-0.107007	2.476234	3.902639
C	0.136669	2.658011	1.676880
H	-0.695816	3.360867	1.701325
C	1.430417	3.408608	1.837768
C	2.703572	2.924145	1.349051
C	1.322881	4.850629	2.275392
C	-0.054222	1.665861	0.521512
C	1.210444	-1.614258	2.240596
H	0.920190	0.316199	4.095128
H	2.254192	0.900710	3.117555
H	2.079009	2.731399	2.671291
H	2.771892	2.032601	0.744568
H	3.599087	3.473773	1.599142
H	0.491669	5.001424	2.966431
H	2.241172	5.198659	2.753718
H	1.157212	5.466306	1.384311
H	0.498069	2.013015	-0.361867
H	-1.109303	1.678184	0.221379
H	0.630025	-2.035679	3.070104
H	1.039199	-2.232592	1.356668
H	2.267159	-1.704278	2.519970

#### TS\_E1:

C	0.361509	-0.588051	0.166788
C	0.443488	0.513997	1.195162
C	0.889694	0.268222	2.429053
C	1.029591	1.245661	3.565599
C	0.473279	2.632945	3.312807
H	0.277157	3.210349	4.216767
C	-0.132303	3.118355	1.535589
H	-0.627060	2.574397	2.906954
C	1.123422	3.530859	2.225050
C	2.502560	3.107821	1.710797
C	1.130874	5.011686	2.623618
C	-0.067712	1.856432	0.695811
H	0.970470	-0.349467	-0.713144
H	-0.666665	-0.717637	-0.189374
H	0.705036	-1.543255	0.568721
H	1.202140	-0.746328	2.666419
H	0.523518	0.828132	4.444880

H	2.088905	1.318171	3.848786
H	2.749885	3.691003	0.818266
H	3.276960	3.319647	2.454820
H	2.563439	2.052471	1.449024
H	0.144910	5.317308	2.978536
H	1.871822	5.211704	3.406398
H	1.375779	5.634751	1.758014
H	0.545223	2.156724	-0.172773
H	-1.064684	1.672512	0.275275

#### TS\_E1\_E2:

C	-0.430624	-2.657157	-1.760727
C	-0.351927	-1.555305	-0.732127
C	0.115462	-1.798837	0.496048
C	0.233778	-0.804294	1.619209
C	-0.566396	0.470776	1.413972
H	-0.435995	1.203642	2.203595
C	-0.879788	1.040695	-0.354653
H	-1.630116	0.248168	1.372050
C	0.345611	1.524025	0.106102
C	1.734231	1.034424	-0.291213
C	0.386157	2.923313	0.704903
C	-0.881528	-0.213832	-1.215709
H	0.177067	-2.417447	-2.641216
H	-1.458917	-2.786896	-2.116811
H	-0.086564	-3.612834	-1.359401
H	0.453542	-2.806040	0.730238
H	-0.138391	-1.271624	2.541241
H	1.291754	-0.588272	1.816267
H	2.082222	1.664084	-1.117754
H	2.455778	1.157761	0.521847
H	1.744856	-0.000676	-0.625260
H	-0.613665	3.239358	1.000916
H	1.078929	3.003106	1.550347
H	0.737954	3.614474	-0.068872
H	-0.335102	0.051728	-2.136835
H	-1.908526	-0.399681	-1.560244

#### TS\_F1:

C	0.298930	-0.582028	0.234020
C	0.444916	0.495018	1.279574
C	1.007038	0.246432	2.464514
C	1.206522	1.182355	3.635753
C	0.760107	2.632406	3.630365
H	-0.607744	2.543772	2.907969
C	-0.099997	2.930329	1.919935
H	-0.783752	3.752588	1.706733
C	1.237533	3.470536	2.491791
C	2.512189	3.124366	1.717075
C	1.179466	4.974236	2.786385
C	-0.082616	1.848329	0.857796

H	0.809465	-0.300562	-0.694806	H	-1.206435	3.388885	1.925210
H	-0.754578	-0.743141	-0.023570	C	1.363097	3.568459	2.385075
H	0.714346	-1.532504	0.573489	C	2.478415	3.036327	1.541084
H	1.341682	-0.771248	2.658172	C	1.302871	5.036354	2.698246
H	0.772733	0.688562	4.514406	C	-0.374762	1.552249	0.984576
H	2.286871	1.241173	3.857536	H	0.919184	-0.287607	-0.721349
H	2.581192	3.714044	0.797428	H	-0.509139	-1.064943	-0.043646
H	3.385568	3.379059	2.325464	H	1.096890	-1.527055	0.531646
H	2.585908	2.070533	1.452140	H	1.703750	-0.624445	2.605679
H	0.276833	5.219216	3.349210	H	0.332160	0.872442	4.349183
H	2.037571	5.273327	3.396005	H	1.983655	1.360849	4.060977
H	1.197167	5.564157	1.862544	H	3.163063	3.837419	1.253416
H	0.492094	2.193391	-0.013280	H	3.047288	2.244527	2.045618
H	-1.108185	1.714023	0.491184	H	2.120791	2.565138	0.603349

#### TS\_F2:

H	-0.359082	-2.623701	-1.779601
C	-0.331066	-1.819744	-1.044948
C	0.095821	-2.124209	0.184095
C	0.166651	-1.114478	1.306682
C	-0.635147	0.156661	1.079037
H	-0.543415	0.879814	1.882999
C	-0.883046	0.752084	-0.691112
H	-1.694020	-0.075475	0.993570
C	0.320809	1.235481	-0.175957
C	1.725950	0.759234	-0.529129
C	0.330759	2.624485	0.447294
C	-0.835660	-0.491733	-1.566072
C	0.555585	-3.513830	0.546126
H	-0.230668	-1.582413	2.218501
H	1.217822	-0.895800	1.534713
H	2.103329	1.407024	-1.328283
H	2.415002	0.868276	0.313674
H	1.753217	-0.268297	-0.885242
H	-0.681198	2.930363	0.711009
H	0.991110	2.693574	1.319234
H	0.707077	3.330447	-0.301133
H	-0.236356	-0.222057	-2.452289
H	-1.840568	-0.677910	-1.969732
H	1.584442	-3.503637	0.926366
H	-0.067192	-3.943358	1.340097
H	0.520563	-4.185891	-0.313500

#### TS\_G:

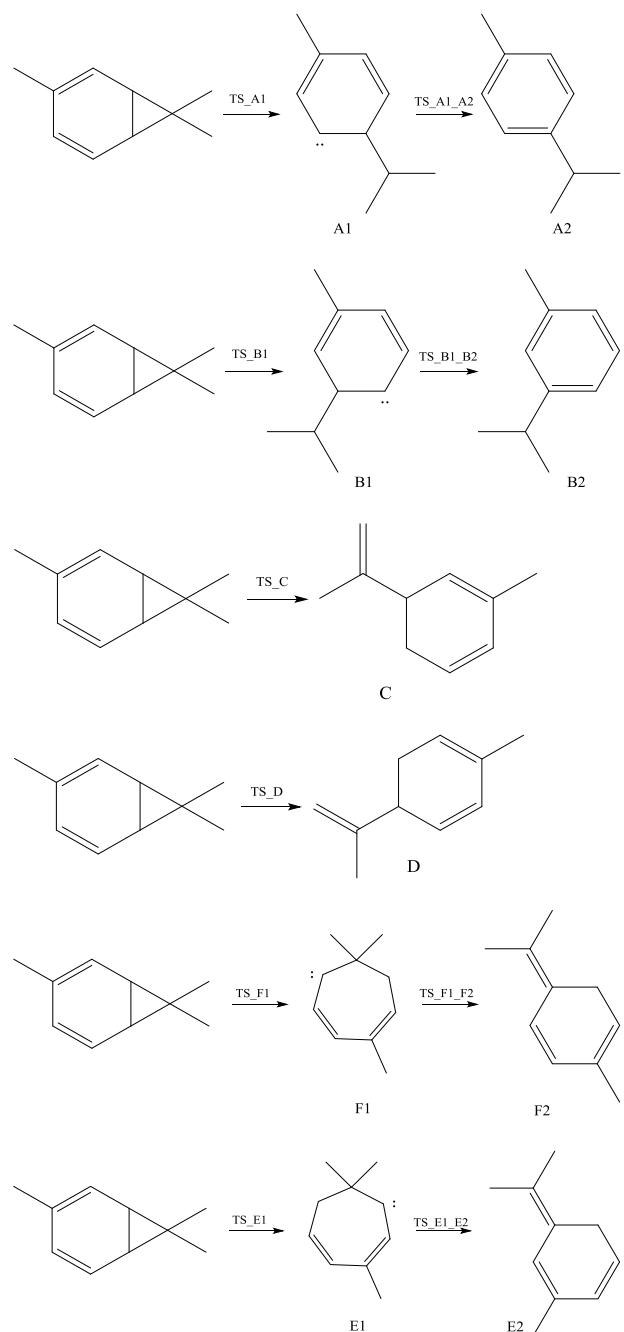
C	0.487124	-0.682734	0.204509
C	0.411576	0.383432	1.273528
C	1.089295	0.255632	2.443592
C	1.007885	1.247968	3.568319
C	0.488333	2.635240	3.154925
H	0.017560	3.131787	4.005475
C	-0.386445	2.681996	1.936180

H	-1.206435	3.388885	1.925210
C	1.363097	3.568459	2.385075
C	2.478415	3.036327	1.541084
C	1.302871	5.036354	2.698246
C	-0.374762	1.552249	0.984576
H	0.919184	-0.287607	-0.721349
H	-0.509139	-1.064943	-0.043646
H	1.096890	-1.527055	0.531646
H	1.703750	-0.624445	2.605679
H	0.332160	0.872442	4.349183
H	1.983655	1.360849	4.060977
H	3.163063	3.837419	1.253416
H	3.047288	2.244527	2.045618
H	2.120791	2.565138	0.603349
H	0.299988	5.344431	3.010917
H	1.983596	5.299349	3.524407
H	1.589368	5.651658	1.840168
H	0.276562	2.796659	0.895640
H	-0.994432	1.624363	0.101106

#### TS\_H:

H	-0.021863	0.086995	0.007821
C	-0.028028	0.068435	1.094433
C	1.157374	0.010671	1.754846
C	1.209256	-0.056485	3.259011
C	-0.080001	0.364439	3.984516
H	-0.148387	-0.143971	4.948201
C	-1.359352	0.244460	3.207687
H	-2.254443	-0.049063	3.741038
C	-0.437866	1.809742	4.098224
C	0.053056	2.792510	3.082352
C	-1.065204	2.301550	5.370896
C	-1.305532	0.147835	1.737053
C	2.475265	-0.060928	1.035037
H	1.434623	-1.087205	3.566738
H	2.047667	0.546168	3.640088
H	-0.086652	3.816942	3.434739
H	1.111146	2.647381	2.831285
H	-0.477101	2.710979	2.110872
H	-1.686513	1.532715	5.841833
H	-0.302521	2.585895	6.114665
H	-1.693157	3.182427	5.206202
H	-1.588748	1.264186	2.534613
H	-2.235074	0.092994	1.188921
H	3.143480	0.760380	1.326829
H	3.013055	-0.990598	1.266255
H	2.342991	-0.015861	-0.048604

## 7.6 Three membered ring opening reaction on cara-2,4-diene molecule chemistry



### Reactant

cara-2,4-diene:

C	-4.286287	1.349136	-0.206857
C	-3.019801	0.622004	0.166906
C	-1.889694	1.273386	0.516724
C	-0.630193	0.589640	0.851534
C	0.129685	-0.282184	-0.130602

C	1.633321	-0.338673	0.083087
C	-0.274955	-0.346919	-1.587288
C	-0.697187	-0.972535	0.941602
C	-2.016218	-1.564297	0.679559
C	-3.066384	-0.835320	0.254849
H	-4.158420	2.431713	-0.146493
H	-4.595131	1.103512	-1.229216
H	-5.114960	1.065948	0.451550
H	-1.901439	2.356331	0.603819
H	-0.004897	1.101340	1.578129
H	2.129572	0.495704	-0.424185
H	1.893295	-0.286412	1.143742
H	2.049480	-1.269166	-0.317913
H	0.158127	0.495836	-2.136384
H	0.097333	-1.270919	-2.042197
H	-1.354299	-0.316982	-1.724587
H	-0.115103	-1.456060	1.721132
H	-2.141082	-2.622921	0.886167
H	-4.017769	-1.324182	0.066930

### Products

#### A1:

C	0.564349	0.288943	-0.096229
C	1.894473	-0.140822	0.527885
C	-0.161611	1.317607	0.778633
C	-0.358704	-0.951795	-0.366127
C	-0.712041	-1.695673	0.867619
H	0.303658	-1.681213	-0.886227
C	-1.468278	-0.671027	-1.325289
C	-1.996127	-2.224925	0.969908
H	0.769469	0.747568	-1.072062
H	2.466329	-0.778736	-0.153959
H	2.508334	0.733063	0.764608
H	1.716020	-0.704705	1.445664
H	-1.102428	1.640158	0.323479
H	-0.386519	0.885895	1.758313
H	0.459603	2.204590	0.932046
H	-2.243757	-2.914700	1.776720
C	-3.041990	-1.664702	0.231695
H	-1.231529	-0.302519	-2.321044
C	-2.744407	-0.955347	-0.982629
H	-3.565740	-0.711410	-1.649526
C	-4.468127	-1.782353	0.683582
H	-5.137683	-1.947261	-0.165451
H	-4.593350	-2.596283	1.400740
H	-4.795671	-0.856324	1.171530

#### A2:

C	0.620489	0.372443	0.265822
C	0.572529	1.423737	1.389392

C	0.876460	1.033841	-1.100593	C	0.075228	0.040391	1.541150
C	-0.625345	-0.501491	0.250485	C	1.418945	-0.011018	-0.612544
C	-0.537790	-1.877568	0.468985	C	-0.835599	1.153219	-0.550604
H	0.434135	-2.326166	0.651124	C	-1.999141	0.888045	-1.276020
C	-1.897457	0.035737	0.014418	H	-2.301768	-0.140657	-1.444290
C	-1.672143	-2.688217	0.454485	C	-0.470152	2.490798	-0.353642
H	1.469143	-0.289619	0.473069	C	-2.770068	1.930066	-1.788589
H	0.427341	0.952251	2.364552	H	-0.490820	-0.918587	-0.285684
H	1.504095	1.996785	1.422437	H	-0.925616	0.022177	1.979675
H	-0.247537	2.131428	1.235764	H	0.628965	-0.824659	1.918386
H	0.947062	0.285416	-1.893805	H	0.580809	0.941325	1.901014
H	0.069699	1.724147	-1.364392	H	1.372122	-0.065909	-1.702998
H	1.810145	1.604192	-1.085090	H	1.983466	0.887860	-0.347728
H	-1.567070	-3.755133	0.625655	H	1.982806	-0.876245	-0.251038
C	-2.939043	-2.151335	0.221828	C	-2.389197	3.250951	-1.581785
H	-2.009844	1.100203	-0.164111	H	0.432603	2.720329	0.204722
C	-3.028768	-0.772055	-0.000210	C	-1.230009	3.548813	-0.856056
H	-4.000108	-0.324635	-0.189078	C	-0.826669	4.982474	-0.603109
C	-4.175242	-3.018434	0.227809	H	-3.668885	1.708818	-2.354159
H	-4.842816	-2.767541	-0.601116	H	-2.991837	4.058030	-1.986353
H	-3.919153	-4.076839	0.145172	H	-1.014315	5.609645	-1.478462
H	-4.745559	-2.888312	1.154023	H	-1.394666	5.409874	0.230546
				H	0.233436	5.060835	-0.352294

B1:

C	0.512716	0.215623	-0.080807
C	1.831620	-0.501598	0.221813
C	0.153543	1.220959	1.018337
C	-0.644553	-0.821217	-0.311060
C	-0.935828	-1.640018	0.890269
H	-0.240605	-1.523606	-1.067863
C	-1.880972	-0.208230	-0.910059
C	-2.199338	-1.917039	1.318724
H	0.625745	0.762665	-1.025487
H	2.129583	-1.156139	-0.603446
H	2.636269	0.221121	0.384487
H	1.736906	-1.116998	1.120306
H	-0.776561	1.747977	0.790280
H	0.026823	0.710219	1.977389
H	0.945287	1.966668	1.133652
H	-2.388464	-2.656641	2.092606
C	-3.252533	-1.093908	0.860807
H	-1.785643	0.265577	-1.884544
C	-3.100490	-0.284158	-0.305852
C	-4.315273	0.417963	-0.867683
H	-4.194929	-1.068258	1.401598
H	-5.123441	-0.288752	-1.078721
H	-4.704459	1.150640	-0.153211
H	-4.075940	0.946542	-1.791996

B2:

C	0.008324	0.013352	0.003434
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C	0.075228	0.040391	1.541150
C	1.418945	-0.011018	-0.612544
C	-0.835599	1.153219	-0.550604
C	-1.999141	0.888045	-1.276020
H	-2.301768	-0.140657	-1.444290
C	-0.470152	2.490798	-0.353642
C	-2.770068	1.930066	-1.788589
H	-0.490820	-0.918587	-0.285684
H	-0.925616	0.022177	1.979675
H	0.628965	-0.824659	1.918386
H	0.580809	0.941325	1.901014
H	1.372122	-0.065909	-1.702998
H	1.983466	0.887860	-0.347728
H	1.982806	-0.876245	-0.251038
C	-2.389197	3.250951	-1.581785
H	0.432603	2.720329	0.204722
C	-1.230009	3.548813	-0.856056
C	-0.826669	4.982474	-0.603109
H	-3.668885	1.708818	-2.354159
H	-2.991837	4.058030	-1.986353
H	-1.014315	5.609645	-1.478462
H	-1.394666	5.409874	0.230546
H	0.233436	5.060835	-0.352294

C:

C	0.671140	-0.860463	0.167130
C	0.592190	0.306033	1.116266
C	1.330622	0.213604	2.386901
C	1.104332	1.073684	3.387039
C	0.059960	2.152452	3.248446
H	-0.897650	1.751981	3.613450
C	-0.080961	2.620162	1.782933
C	-0.096974	1.425413	0.844219
H	0.092219	-0.678124	-0.740181
H	0.293900	-1.776574	0.635075
H	1.708916	-1.058224	-0.124831
H	2.050883	-0.590920	2.504001
H	1.624917	0.971983	4.334052
H	-0.611536	1.535401	-0.106256
C	-1.267718	3.546692	1.572684
C	-2.645691	2.984025	1.820891
C	-1.089369	4.805826	1.170022
H	-1.927185	5.475914	1.007574
H	-0.098591	5.208937	0.988119
H	-3.419697	3.705085	1.552338
H	-2.808645	2.068485	1.242844
H	-2.786864	2.716003	2.873229
H	0.294970	3.011375	3.882965
H	0.823689	3.200132	1.542699

D:

H 1.932073 1.584610 -0.132950  
 C 1.326041 1.461053 0.760540  
 C 0.941384 0.092285 1.146728  
 C 0.369006 -0.106844 2.342368  
 C 0.160945 1.017190 3.325948  
 H -0.721290 0.828521 3.945934  
 C 0.048273 2.426258 2.681947  
 C 0.935032 2.535340 1.455790  
 C 1.219592 -1.019262 0.169983  
 H 0.091179 -1.109958 2.654245  
 H 1.200888 3.534720 1.125377  
 C -1.385128 2.839817 2.348052  
 C -2.170960 1.975594 1.394862  
 C -1.909403 3.942241 2.887487  
 H -2.922182 4.259687 2.661502  
 H -1.345297 4.564615 3.574571  
 H -3.154905 2.405433 1.197508  
 H -1.644063 1.862598 0.443000  
 H -2.311635 0.967193 1.796263  
 H 1.013269 1.023174 4.020965  
 H 0.406620 3.151575 3.418420  
 H 0.703818 -0.849160 -0.781901  
 H 2.289925 -1.082829 -0.057529  
 H 0.898588 -1.986191 0.562170

### E1:

C -0.819538 -2.733520 -1.749160  
 C -0.528733 -1.599172 -0.798767  
 C 0.300599 -1.847665 0.318442  
 C 0.667236 -0.995420 1.330508  
 C 0.185794 0.402571 1.529912  
 H 0.696794 0.846959 2.390567  
 C -0.455111 0.870317 -0.836412  
 H -0.886787 0.398601 1.765789  
 C 0.350655 1.367339 0.294211  
 C 1.832681 1.481098 -0.129865  
 C -0.170373 2.764247 0.712164  
 C -1.000921 -0.293015 -1.206720  
 H -1.859300 -2.698821 -2.091651  
 H -0.642676 -3.704875 -1.283104  
 H -0.191252 -2.676427 -2.647514  
 H 0.694157 -2.859655 0.385014  
 H 1.342654 -1.390974 2.082675  
 H 1.936334 2.164591 -0.975360  
 H 2.431793 1.864933 0.702323  
 H 2.235081 0.509633 -0.422041  
 H -1.219578 2.719023 1.014755  
 H 0.414800 3.144016 1.554969  
 H -0.085084 3.470611 -0.115874  
 H -1.735373 -0.285047 -2.013326

### E2:

C 0.275230 0.230579 0.076432  
 C 0.345379 0.186486 1.537900  
 C 1.525884 -0.084323 -0.698786  
 C -0.720888 0.453289 2.298753  
 H 1.294701 -0.071066 1.998425  
 C -2.057649 0.814887 1.717671  
 H -0.648394 0.415219 3.381512  
 C -2.119016 0.857116 0.191179  
 H -2.810353 0.110039 2.102963  
 H -2.369395 1.786183 2.131497  
 C -0.891655 0.547507 -0.528816  
 C -3.289524 1.174576 -0.418476  
 H -0.914121 0.572085 -1.611559  
 H 1.889019 -1.093112 -0.469666  
 H 1.358475 -0.021497 -1.775724  
 H 2.335772 0.607823 -0.439873  
 C -3.496011 1.254552 -1.908948  
 C -4.518447 1.482553 0.404719  
 H -3.839865 2.256428 -2.194861  
 H -2.605253 1.033069 -2.493829  
 H -4.282091 0.557379 -2.224876  
 H -4.802547 0.639434 1.047304  
 H -4.359221 2.338072 1.073514  
 H -5.375616 1.716092 -0.229668

### F1:

C -0.660531 -2.763583 -1.691597  
 C -0.538616 -1.558586 -0.775507  
 C -0.226896 -1.831026 0.583163  
 C 0.231323 -0.926537 1.595491  
 C 0.702820 0.310899 1.364379  
 H -1.626539 0.930785 0.206871  
 C -0.799286 0.970801 -0.513730  
 H -1.010280 1.801476 -1.194992  
 C 0.484113 1.334959 0.326208  
 C 1.732234 1.444840 -0.578162  
 C 0.227921 2.698683 1.014709  
 C -0.742407 -0.302906 -1.291176  
 H -0.995346 -2.474900 -2.689401  
 H -1.381224 -3.484687 -1.293109  
 H 0.296052 -3.285974 -1.793135  
 H -0.195265 -2.882202 0.861979  
 H 0.378867 -1.356158 2.585731  
 H 1.576933 2.215318 -1.340501  
 H 2.610135 1.713761 0.013148  
 H 1.935982 0.499288 -1.083987  
 H -0.650774 2.654530 1.662970  
 H 1.086338 2.990762 1.622671  
 H 0.059187 3.470372 0.257813  
 H -0.932977 -0.229077 -2.357760

F2:

C	0.225289	0.261163	-0.009634
C	0.392704	0.305701	1.443689
H	1.091377	0.012785	-0.615475
C	-0.664981	0.610833	2.208709
C	1.755085	0.004340	2.011072
C	-2.029954	0.913620	1.654532
H	-0.561783	0.649242	3.289801
C	-2.159292	0.855056	0.133219
H	-2.756448	0.225568	2.113918
H	-2.343190	1.906094	2.013919
C	-0.955229	0.515661	-0.609699
C	-3.356631	1.114058	-0.451007
H	-1.008423	0.465026	-1.689825
C	-3.619201	1.090842	-1.934349
C	-4.557763	1.458744	0.397309
H	-3.988656	2.066889	-2.272506
H	-2.747580	0.841551	-2.536658
H	-4.406153	0.364394	-2.172014
H	-4.801342	0.655357	1.103995
H	-4.384535	2.357469	1.002679
H	-5.442609	1.638909	-0.216001
H	1.758324	0.067586	3.100920
H	2.085712	-1.001127	1.727359
H	2.504883	0.705154	1.627101

Transition state

TS\_A1:

C	0.365472	0.060899	0.120270
C	0.033806	0.520097	1.522271
C	1.618281	0.648584	-0.516122
C	-0.805950	-0.066961	-0.897591
C	-0.447925	-1.513464	-0.655813
H	-0.514870	0.328606	-1.873036
C	-2.158589	0.412855	-0.498985
C	-1.357262	-2.183766	0.278629
H	0.677303	-1.128031	0.104529
H	-0.745252	-0.094717	1.975591
H	0.921866	0.468796	2.158125
H	-0.323684	1.556360	1.516313
H	1.865168	0.112844	-1.435376
H	1.454784	1.702343	-0.768317
H	2.475174	0.585506	0.160737
H	-1.083625	-3.188999	0.592591
C	-2.591101	-1.718418	0.609141
H	-2.466928	1.406652	-0.811037
C	-2.992604	-0.372920	0.197241
H	-3.986054	-0.025967	0.465108
C	-3.595449	-2.551151	1.357644

H	-4.491736	-2.722398	0.750032
H	-3.183297	-3.521948	1.637422
H	-3.925788	-2.039321	2.268372

TS\_A1\_A2:

C	0.571834	0.505928	-0.034389
C	1.820822	0.096019	0.751329
C	0.160846	1.948809	0.288196
C	-0.619589	-0.439939	0.220085
C	-0.942259	-0.833597	1.598878
H	-0.202035	-1.506386	0.318679
C	-1.612062	-0.546199	-0.859004
C	-2.203891	-1.513041	1.695821
H	0.806409	0.449669	-1.107488
H	2.169508	-0.899412	0.455407
H	2.635865	0.801481	0.568620
H	1.601832	0.065371	1.819994
H	-0.712791	2.260539	-0.292057
H	-0.091401	2.036922	1.349049
H	0.974650	2.644767	0.069371
H	-2.492910	-1.879239	2.680980
C	-3.118307	-1.663314	0.675237
H	-1.378412	-0.148267	-1.842920
C	-2.801207	-1.156245	-0.629705
H	-3.530063	-1.260899	-1.427208
C	-4.447711	-2.336945	0.885225
H	-4.590093	-2.622211	1.928709
H	-5.267838	-1.675775	0.589631
H	-4.528094	-3.239821	0.268670

TS\_B1:

C	0.350811	0.076131	0.096898
C	-0.034841	0.766750	1.386702
C	1.597204	0.593090	-0.610932
C	-0.798071	-0.259528	-0.907144
C	-0.396362	-1.625403	-0.421825
H	-0.490483	-0.023495	-1.928112
C	-2.174243	0.242618	-0.627393
C	-1.309698	-2.153452	0.599587
H	0.701976	-1.070329	0.306558
H	-0.810568	0.219268	1.924093
H	0.834784	0.859541	2.043074
H	-0.420219	1.772290	1.182914
H	1.881498	-0.081268	-1.421450
H	1.402329	1.581782	-1.040719
H	2.440947	0.677835	0.079962
H	-1.017905	-3.071399	1.103560
C	-2.560105	-1.669332	0.789741
H	-2.487952	1.165430	-1.108665
C	-3.027725	-0.433454	0.162092
C	-4.436817	0.020409	0.436028

H -3.264424 -2.216187 1.413160  
 H -4.669338 0.944846 -0.095836  
 H -5.159764 -0.742365 0.126415  
 H -4.596874 0.193853 1.505902

H -1.525489 3.213921 4.130472  
 H -1.889466 0.221634 6.352457  
 H -2.073545 1.982478 6.281197  
 H -3.304643 0.942975 5.563990  
 H -1.923057 -0.820700 1.698478

#### TS\_B1\_B2:

C 0.499114 0.621590 0.016374  
 C 1.833469 0.076493 0.535311  
 C 0.116172 1.926951 0.733591  
 C -0.658310 -0.384822 0.164438  
 C -0.813690 -1.096971 1.436609  
 H -0.215235 -1.470294 0.068307  
 C -1.744201 -0.276418 -0.810936  
 C -2.066766 -1.808699 1.504907  
 H 0.609377 0.840968 -1.053759  
 H 2.155281 -0.799476 -0.037555  
 H 2.614722 0.836860 0.450211  
 H 1.738750 -0.225251 1.579360  
 H -0.821417 2.339052 0.348431  
 H -0.010321 1.740095 1.803468  
 H 0.894451 2.684226 0.604742  
 H -2.265680 -2.389132 2.403510  
 C -3.046083 -1.752137 0.546400  
 H -1.606300 0.353078 -1.687120  
 C -2.907795 -0.967458 -0.642722  
 C -4.035616 -0.919669 -1.641790  
 H -3.972371 -2.307387 0.684984  
 H -3.810137 -0.239376 -2.464926  
 H -4.227450 -1.910988 -2.064854  
 H -4.964605 -0.586248 -1.169128

#### TS\_D:

H -0.003605 -0.424316 0.246747  
 C 0.207319 0.349816 0.981526  
 C 0.945701 -0.026396 2.165843  
 C 0.834435 0.809968 3.269572  
 C 0.318414 2.104429 3.181638  
 H 0.084815 2.688503 4.062378  
 C 0.024744 2.676228 1.794126  
 H -0.738207 3.458072 1.810610  
 C 1.403110 3.318283 1.679400  
 C 2.443130 2.665234 0.957569  
 C 1.554186 4.726771 2.189961  
 C -0.311894 1.586426 0.808589  
 C 1.570241 -1.395278 2.255251  
 H 1.171254 0.451917 4.239535  
 H 2.111962 2.510829 2.340501  
 H 2.217789 1.805613 0.344988  
 H 3.463582 3.015996 1.049715  
 H 0.917315 4.909944 3.055957  
 H 2.585246 4.967681 2.459285  
 H 1.250851 5.411516 1.387921  
 H -1.000831 1.801004 -0.000481  
 H 2.422501 -1.508965 1.574408  
 H 1.933177 -1.597764 3.266180  
 H 0.854236 -2.185489 1.995062

#### TS\_C:

C 0.066566 0.178037 0.115895  
 C -0.024350 0.143891 1.621925  
 C 1.120182 0.569498 2.390771  
 C 1.237053 0.164562 3.717188  
 C 0.152371 -0.343462 4.424202  
 H 0.257785 -0.791517 5.400569  
 C -1.224450 -0.293078 3.758709  
 H -1.902790 -1.051653 4.152416  
 C -1.594556 1.030390 4.381967  
 C -1.361510 2.248228 3.652929  
 C -2.220512 1.051211 5.730696  
 C -1.123562 -0.346940 2.254726  
 H -0.850433 -0.182245 -0.354825  
 H 0.901051 -0.435653 -0.239521  
 H 0.250381 1.198406 -0.238947  
 H 1.977656 0.988467 1.871846  
 H 2.200318 0.255841 4.215519  
 H -0.436037 1.975335 4.062570  
 H -1.208418 2.185177 2.587910

#### TS\_E1:

C 0.305245 -0.622310 0.188215  
 C 0.464468 0.552882 1.119794  
 C 1.167107 0.290435 2.385205  
 C 1.220135 1.176681 3.396817  
 C 0.731330 2.546378 3.292670  
 H 0.275206 2.979389 4.243843  
 C -0.197718 2.945664 1.773381  
 H -0.698912 2.732809 2.502071  
 C 1.137310 3.532958 2.258600  
 C 2.425331 3.285478 1.512079  
 C 0.983402 4.983555 2.687441  
 C -0.139421 1.722374 0.872215  
 H -0.251482 -1.430040 0.680092  
 H 1.273879 -1.037855 -0.104352  
 H -0.232656 -0.345845 -0.714653  
 H 1.572386 -0.705159 2.534740  
 H 1.636321 0.875181 4.357100  
 H 2.462922 3.894559 0.599344

H	3.274278	3.569151	2.136938
H	2.564450	2.243032	1.214088
H	0.029961	5.137258	3.192433
H	1.792439	5.276357	3.371486
H	1.001053	5.642300	1.820279
H	-0.801936	1.781761	0.013027

#### TS\_E1\_E2:

C	-1.775098	-2.581557	-1.774891
C	-0.775212	-1.804281	-0.954349
C	-0.060679	-2.402664	0.111524
C	0.694118	-1.662677	0.995786
C	0.395967	-0.278943	1.119136
H	1.047505	0.307497	1.781572
C	0.620854	0.170840	-0.541843
H	-0.659403	0.008006	1.268002
C	0.820495	1.449485	-0.167409
C	2.147219	1.892855	0.389664
C	-0.322136	2.409741	-0.136364
C	-0.334003	-0.526739	-1.306187
H	0.019193	-3.488528	0.144367
H	1.537839	-2.077842	1.537336
H	2.598094	2.565648	-0.355143
H	2.061439	2.462907	1.322364
H	2.824750	1.047450	0.519480
H	-0.302140	3.077670	0.729931
H	-0.269915	3.044944	-1.036523
H	-1.277024	1.877712	-0.176702
H	-0.564524	-0.138246	-2.318349
H	-1.806143	-2.238836	-2.809477
H	-1.537250	-3.650969	-1.779294
H	-2.791988	-2.485571	-1.372222

#### TS\_F1:

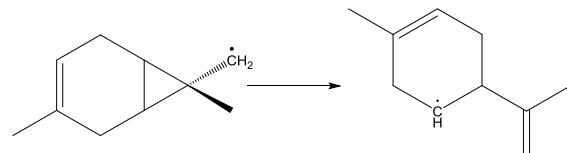
C	0.314277	-0.585724	0.213825
C	0.391158	0.555309	1.195046
C	0.916580	0.261021	2.524221
C	1.093218	1.171402	3.533479
C	0.851008	2.582855	3.663445
H	-0.882053	2.579583	2.304517
C	-0.097891	2.948178	1.808771
H	-0.545214	3.884750	1.305372
C	1.266539	3.433205	2.504722
C	2.564326	3.107159	1.744675
C	1.198816	4.938768	2.806668
C	-0.047623	1.778735	0.845921
H	-0.121530	-0.273034	-0.733240
H	-0.285259	-1.408391	0.618930
H	1.310431	-0.999200	0.006753
H	1.081296	-0.784704	2.756403

H	1.415539	0.763440	4.495123
H	2.660799	3.699150	0.830911
H	3.417191	3.361855	2.389297
H	2.648888	2.054357	1.485441
H	0.268994	5.185894	3.313247
H	2.022086	5.223687	3.468880
H	1.284484	5.533576	1.889988
H	-0.477402	1.929192	-0.137823

#### TS\_F1\_F2:

H	-1.586830	-2.428810	-1.474800
C	-0.876560	-1.837640	-0.906040
C	-0.206850	-2.400370	0.216710
C	0.597430	-1.591400	0.998600
C	0.404540	-0.128080	1.079020
H	1.083430	0.331030	1.793210
C	0.623790	0.093480	-0.841290
H	-0.636790	0.166620	1.242320
C	0.767250	1.301260	-0.189480
C	2.149730	1.828480	0.160870
C	-0.342450	2.344690	-0.141220
C	-0.418610	-0.623990	-1.423310
C	-0.265560	-3.896290	0.451130
H	1.360030	-2.022840	1.641220
H	2.482630	2.529960	-0.615890
H	2.150430	2.373280	1.114190
H	2.873300	1.010120	0.202750
H	-1.327600	1.875390	-0.220790
H	-0.296150	2.932830	0.793440
H	-0.232750	3.046470	-0.978750
H	-0.742570	-0.299750	-2.412630
H	0.085080	-4.460370	-0.422540
H	0.342920	-4.190210	1.302530
H	-1.296420	-4.219910	0.659740

## 7.7 C-C $\beta$ -scission reaction



#### Reactant

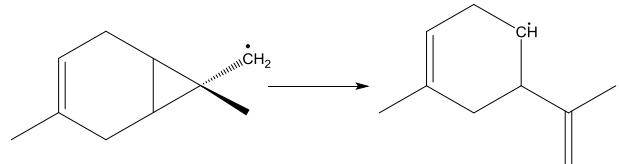
C	0.405273	-0.583088	0.118189
C	0.454907	0.441160	1.221655
C	0.952419	0.160470	2.427716
C	1.036001	1.115494	3.587584
C	0.488302	2.507093	3.317740
H	-0.003232	2.961547	4.171228

C	-0.075213	2.844154	1.969325	C	0.445863	0.410286	1.210815
H	-0.927408	3.515300	1.958951	C	0.968089	0.196025	2.416226
C	1.237315	3.519895	2.423425	C	0.996924	1.203745	3.543828
C	2.554976	3.126304	1.775196	C	0.497008	2.644108	3.124545
C	1.145764	4.924342	2.812430	H	-0.032105	3.051300	3.999379
C	-0.102738	1.800115	0.865184	C	-0.569350	2.534998	1.971909
H	0.967802	-0.243865	-0.759876	H	-1.090819	3.526392	1.818794
H	-0.624903	-0.752801	-0.216995	C	1.650346	3.722511	2.832944
H	0.820138	-1.541103	0.437904	C	2.621569	3.157256	1.788309
H	1.333262	-0.841283	2.615532	C	1.280701	4.913258	2.870415
H	0.478201	0.685076	4.429388	C	-0.226393	1.711386	0.827384
H	2.076033	1.172373	3.938972	H	0.969000	-0.256071	-0.771952
H	2.723777	3.717299	0.869572	H	-0.573747	-0.862484	-0.190976
H	3.387164	3.324972	2.457726	H	0.934103	-1.546190	0.441152
H	2.593761	2.072733	1.499988	H	1.406425	-0.775714	2.629690
H	0.250797	5.314008	3.282826	H	0.364126	0.833651	4.361836
H	1.969729	5.604736	2.640216	H	2.009297	1.263583	3.959648
H	0.414386	2.173577	-0.030652	H	2.964426	3.938971	1.111398
H	-1.145592	1.663572	0.549617	H	3.508076	2.806722	2.365178

### Product

C	1.299383	-0.924422	1.512859
C	0.736953	0.393648	1.973265
C	0.429024	0.636833	3.249007
C	-0.158476	1.923015	3.766235
C	0.025791	3.146266	2.829670
H	-0.815397	3.826242	3.002156
C	0.001026	2.743741	1.384044
H	-0.236040	3.505626	0.648515
C	1.282741	3.961611	3.161955
C	1.179784	5.249644	3.496550
C	2.621133	3.271421	3.083008
C	0.529573	1.435613	0.898866
H	2.280709	-0.792947	1.041297
H	0.650898	-1.389586	0.760731
H	1.412918	-1.625211	2.342423
H	0.579584	-0.151977	3.983320
H	-1.233437	1.774906	3.934767
H	0.259673	2.153687	4.752418
H	2.054725	5.848901	3.726722
H	0.218021	5.749037	3.551595
H	2.660923	2.397642	3.740255
H	2.821764	2.908040	2.070178
H	3.427531	3.951046	3.365412
H	1.484006	1.579479	0.357567
H	-0.143061	1.024813	0.128277

C	0.445863	0.410286	1.210815
C	0.968089	0.196025	2.416226
C	0.996924	1.203745	3.543828
C	0.497008	2.644108	3.124545
H	-0.032105	3.051300	3.999379
C	-0.569350	2.534998	1.971909
H	-1.090819	3.526392	1.818794
C	1.650346	3.722511	2.832944
C	2.621569	3.157256	1.788309
C	1.280701	4.913258	2.870415
C	-0.226393	1.711386	0.827384
H	0.969000	-0.256071	-0.771952
H	-0.573747	-0.862484	-0.190976
H	0.934103	-1.546190	0.441152
H	1.406425	-0.775714	2.629690
H	0.364126	0.833651	4.361836
H	2.009297	1.263583	3.959648
H	2.964426	3.938971	1.111398
H	3.508076	2.806722	2.365178
H	2.277102	2.287215	1.208048
H	0.490402	5.251849	3.534019
H	1.835151	5.695707	2.363050
H	0.396770	2.200919	0.021970
H	-1.175945	1.465650	0.280767



### Reactant

C	0.405273	-0.583088	0.118189
C	0.454907	0.441160	1.221655
C	0.952419	0.160470	2.427716
C	1.036001	1.115494	3.587584
C	0.488302	2.507093	3.317740
H	-0.003232	2.961547	4.171228
C	-0.075213	2.844154	1.969325
H	-0.927408	3.515300	1.958951
C	1.237315	3.519895	2.423425
C	2.554976	3.126304	1.775196
C	1.145764	4.924342	2.812430
C	-0.102738	1.800115	0.865184
H	0.967802	-0.243865	-0.759876
H	-0.624903	-0.752801	-0.216995
H	0.820138	-1.541103	0.437904
H	1.333262	-0.841283	2.615532
H	0.478201	0.685076	4.429388
H	2.076033	1.172373	3.938972
H	2.723777	3.717299	0.869572

### Transition state

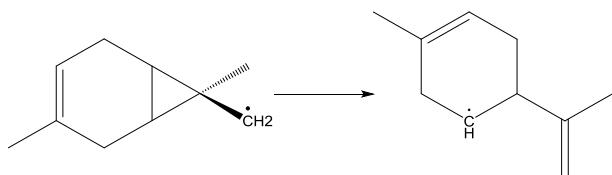
C	0.449082	-0.626318	0.125863
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H	3.387164	3.324972	2.457726
H	2.593761	2.072733	1.499988
H	0.250797	5.314008	3.282826
H	1.969729	5.604736	2.640216
H	0.414386	2.173577	-0.030652
H	-1.145592	1.663572	0.549617

### Product

C	0.560516	-0.252196	-0.042671
C	0.469811	0.517849	1.248273
C	0.895089	0.014088	2.408655
C	0.798145	0.726435	3.729802
C	0.225865	2.100481	3.641164
H	0.071306	2.656557	4.560065
C	0.095429	2.840558	2.342259
H	-0.763569	3.515398	2.425595
C	1.305124	3.752668	2.096704
C	2.648951	3.107225	1.869982
C	1.159518	5.079439	2.102370
C	-0.179388	1.880829	1.154905
H	1.178331	0.278887	-0.776647
H	-0.429817	-0.372538	-0.498246
H	0.987336	-1.245972	0.107908
H	1.335623	-0.980007	2.427374
H	0.201622	0.118674	4.429471
H	1.798930	0.753874	4.200263
H	2.629283	2.430377	1.010430
H	3.418764	3.861139	1.694206
H	2.951686	2.505164	2.732251
H	0.193967	5.546043	2.267983
H	2.001893	5.744534	1.942226
H	0.120970	2.368028	0.219667
H	-1.264456	1.734547	1.068849

H	0.872134	-1.484931	0.373483
H	1.352041	-0.862616	2.585864
H	0.458490	0.566056	4.464017
H	2.023519	1.143272	3.978913
H	2.648345	3.330214	0.658156
H	3.389744	3.613312	2.232703
H	2.682337	2.039248	1.851998
H	0.228336	5.417390	2.961628
H	2.076799	5.519036	2.899122
H	0.314141	2.207661	0.004794
H	-1.194177	1.665079	0.685601



### Reactant

C	0.483780	-0.579938	0.180455
C	0.497407	0.473180	1.257408
C	1.031280	0.250534	2.460162
C	1.081014	1.237003	3.595252
C	0.512924	2.608157	3.278999
H	0.048042	3.102876	4.126523
C	-0.093995	2.879048	1.934598
H	-0.948537	3.549001	1.917127
C	1.226486	3.585176	2.317918
C	2.476740	3.203066	1.677115
C	1.109611	5.061980	2.667550
C	-0.144155	1.788583	0.880366
H	1.017741	-0.235633	-0.713282
H	-0.541070	-0.807987	-0.136142
H	0.948969	-1.508360	0.517822
H	1.469064	-0.724222	2.665011
H	0.522020	0.817946	4.442294
H	2.116403	1.330349	3.950921
H	3.229238	3.954901	1.475782
H	2.687627	2.181807	1.393060
H	0.150979	5.285882	3.142432
H	1.903003	5.363532	3.358845
H	1.190559	5.683470	1.770005
H	0.305434	2.148603	-0.055899
H	-1.196825	1.592018	0.636467

### Transition state

C	0.456710	-0.517830	0.083300
C	0.462872	0.457673	1.230866
C	0.944455	0.134181	2.433068
C	0.982366	1.050287	3.626638
C	0.361019	2.394942	3.394968
H	-0.019924	2.937587	4.248761
C	-0.038207	2.857494	2.041063
H	-0.905771	3.517032	2.036398
C	1.237270	3.635240	2.256735
C	2.558314	3.114745	1.728865
C	1.174099	4.951008	2.710360
C	-0.133314	1.813341	0.926681
H	1.040783	-0.134898	-0.762010
H	-0.561462	-0.682433	-0.289122

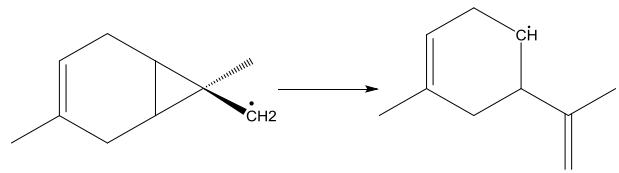
### Product

C	1.299383	-0.924422	1.512859
C	0.736953	0.393648	1.973265
C	0.429024	0.636833	3.249007
C	-0.158476	1.923015	3.766235

C	0.025791	3.146266	2.829670
H	-0.815397	3.826242	3.002156
C	0.001026	2.743741	1.384044
H	-0.236040	3.505626	0.648515
C	1.282741	3.961611	3.161955
C	1.179784	5.249644	3.496550
C	2.621133	3.271421	3.083008
C	0.529573	1.435613	0.898866
H	2.280709	-0.792947	1.041297
H	0.650898	-1.389586	0.760731
H	1.412918	-1.625211	2.342423
H	0.579584	-0.151977	3.983320
H	-1.233437	1.774906	3.934767
H	0.259673	2.153687	4.752418
H	2.054725	5.848901	3.726722
H	0.218021	5.749037	3.551595
H	2.660923	2.397642	3.740255
H	2.821764	2.908040	2.070178
H	3.427531	3.951046	3.365412
H	1.484006	1.579479	0.357567
H	-0.143061	1.024813	0.128277

### Transition state

C	0.471239	-0.603621	0.174755
C	0.474808	0.454050	1.250230
C	1.037418	0.251740	2.443295
C	1.081690	1.242466	3.574513
C	0.535392	2.623251	3.257391
H	0.072835	3.099280	4.119634
C	-0.155049	2.837874	1.955893
H	-0.977631	3.548643	1.935509
C	1.306415	3.593926	2.397329
C	2.503579	3.221425	1.693656
C	1.158248	5.075649	2.728538
C	-0.191747	1.760217	0.887501
H	0.971616	-0.241667	-0.730439
H	-0.551190	-0.871421	-0.115815
H	0.979336	-1.511629	0.504704
H	1.503073	-0.708953	2.645316
H	0.505400	0.831609	4.414047
H	2.110919	1.332002	3.945797
H	3.083238	3.982269	1.182678
H	2.794889	2.189841	1.560779
H	0.128272	5.327519	2.993467
H	1.796177	5.357004	3.573677
H	1.442461	5.697139	1.875061
H	0.259923	2.138443	-0.041728
H	-1.242762	1.554658	0.627992



### Reactant

C	0.483780	-0.579938	0.180455
C	0.497407	0.473180	1.257408
C	1.031280	0.250534	2.460162
C	1.081014	1.237003	3.595252
C	0.512924	2.608157	3.278999
H	0.048042	3.102876	4.126523
C	-0.093995	2.879048	1.934598
H	-0.948537	3.549001	1.917127
C	1.226486	3.585176	2.317918
C	2.476740	3.203066	1.677115
C	1.109611	5.061980	2.667550
C	-0.144155	1.788583	0.880366
H	1.017741	-0.235633	-0.713282
H	-0.541070	-0.807987	-0.136142
H	0.948969	-1.508360	0.517822
H	1.469064	-0.724222	2.665011
H	0.522020	0.817946	4.442294
H	2.116403	1.330349	3.950921
H	3.229238	3.954901	1.475782
H	2.687627	2.181807	1.393060
H	0.150979	5.285882	3.142432
H	1.903003	5.363532	3.358845
H	1.190559	5.683470	1.770005
H	0.305434	2.148603	-0.055899
H	-1.196825	1.592018	0.636467

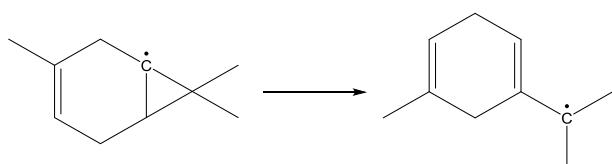
### Product

C	0.560516	-0.252196	-0.042671
C	0.469811	0.517849	1.248273
C	0.895089	0.014088	2.408655
C	0.798145	0.726435	3.729802
C	0.225865	2.100481	3.641164
H	0.071306	2.656557	4.560065
C	0.095429	2.840558	2.342259
H	-0.763569	3.515398	2.425595
C	1.305124	3.752668	2.096704
C	2.648951	3.107225	1.869982
C	1.159518	5.079439	2.102370
C	-0.179388	1.880829	1.154905
H	1.178331	0.278887	-0.776647
H	-0.429817	-0.372538	-0.498246
H	0.987336	-1.245972	0.107908
H	1.335623	-0.980007	2.427374

H	0.201622	0.118674	4.429471	C	0.068048	2.818734	1.886167
H	1.798930	0.753874	4.200263	C	1.276776	3.548164	2.318055
H	2.629283	2.430377	1.010430	C	2.635954	3.205442	1.729817
H	3.418764	3.861139	1.694206	C	1.129443	5.016573	2.695829
H	2.951686	2.505164	2.732251	C	-0.125175	1.782925	0.834076
H	0.193967	5.546043	2.267983	H	0.895289	-0.334274	-0.750276
H	2.001893	5.744534	1.942226	H	-0.696958	-0.794895	-0.164037
H	0.120970	2.368028	0.219667	H	0.744424	-1.592482	0.488447
H	-1.264456	1.734547	1.068849	H	1.332372	-0.827655	2.625547

Transition state

C	0.517116	-0.561248	0.171474	H	3.437963	3.474624	2.426381
C	0.502890	0.466172	1.272736	H	2.732243	2.143819	1.496821
C	1.008378	0.217984	2.482535	H	0.140823	5.222765	3.111651
C	1.022935	1.188384	3.631396	H	1.883392	5.309338	3.434662
C	0.373557	2.506900	3.340925	H	1.257634	5.653610	1.813974
H	0.026374	3.099956	4.176530	H	0.317512	2.101733	-0.119627
C	-0.035663	2.891121	1.964707	H	-1.199939	1.664771	0.629355
H	-0.898887	3.556085	1.924875				
C	1.251121	3.663061	2.125340				
C	2.478165	3.223206	1.645149				
C	1.116639	5.101560	2.588162	C	0.456906	-0.820017	0.260513
C	-0.141763	1.785858	0.915166	C	0.505814	0.150509	1.410732
H	1.077708	-0.198740	-0.698422	C	0.122584	-0.183698	2.642227
H	-0.499085	-0.777539	-0.179673	C	0.157788	0.755617	3.810678
H	0.968776	-1.499227	0.500672	C	0.666291	2.122563	3.475920
H	1.454509	-0.754616	2.677432	H	0.704712	2.828011	4.297927
H	0.511767	0.730715	4.490811	C	1.076993	2.526401	2.219950
H	2.062416	1.329987	3.967694	C	1.545627	3.833557	1.977436
H	3.363741	3.832161	1.781608	C	2.001080	4.311882	0.628302
H	2.606363	2.251594	1.188037	C	1.619026	4.853780	3.084772
H	0.276846	5.239524	3.273081	C	1.019807	1.528541	1.069290
H	2.022491	5.444624	3.094221	H	1.452485	-0.965491	-0.175867
H	0.946269	5.757764	1.726683	H	-0.186014	-0.445371	-0.545125
H	0.275945	2.147290	-0.033840	H	0.077139	-1.795059	0.572268
H	-1.204878	1.598419	0.713472	H	-0.240059	-1.190838	2.833812



Reactant

C	0.342425	-0.636231	0.147190
C	0.430422	0.418445	1.218419
C	0.955289	0.172751	2.421956
C	1.066210	1.150775	3.564409
C	0.539891	2.547443	3.254635
H	0.037111	3.036046	4.087305

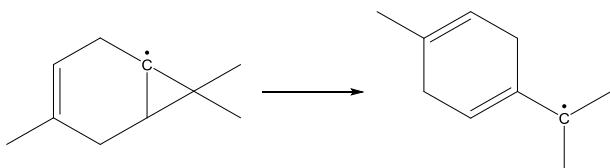
Product

C	0.456906	-0.820017	0.260513
C	0.505814	0.150509	1.410732
C	0.122584	-0.183698	2.642227
C	0.157788	0.755617	3.810678
C	0.666291	2.122563	3.475920
H	0.704712	2.828011	4.297927
C	1.076993	2.526401	2.219950
C	1.545627	3.833557	1.977436
C	2.001080	4.311882	0.628302
C	1.619026	4.853780	3.084772
C	1.019807	1.528541	1.069290
H	1.452485	-0.965491	-0.175867
H	-0.186014	-0.445371	-0.545125
H	0.077139	-1.795059	0.572268
H	-0.240059	-1.190838	2.833812
H	-0.848693	0.832264	4.253771
H	0.769579	0.319308	4.617263
H	1.407513	5.176505	0.300349
H	3.042191	4.660888	0.669439
H	1.938428	3.554783	-0.151853
H	0.636194	5.048397	3.531075
H	2.276940	4.529627	3.900312
H	2.003682	5.806139	2.713649
H	2.019483	1.421428	0.625004
H	0.397764	1.935735	0.259685

Transition state

C	0.342367	-0.652460	0.135218
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C	0.417808	0.332396	1.271273	H	2.665326	2.177154	1.348170
C	0.781496	-0.030048	2.504524	H	0.192496	5.197346	3.236585
C	0.849473	0.896365	3.689204	H	1.943735	5.290138	3.439541
C	0.547326	2.330521	3.341257	H	1.219662	5.663513	1.866931
H	0.484142	3.027454	4.172859	H	0.417463	2.103681	-0.090082
C	0.265323	2.743802	2.043729	H	-1.145685	1.640805	0.522284
C	1.355793	3.732247	2.150116				
C	2.707706	3.435729	1.564941				
C	1.080318	5.130282	2.619760				
C	0.043284	1.763050	0.928434				
H	1.022213	-0.369609	-0.677232				
H	-0.665768	-0.676931	-0.295324				
H	0.599043	-1.663856	0.457488				
H	1.036437	-1.070291	2.694359				
H	0.143187	0.562298	4.465298				
H	1.835917	0.830421	4.172361				
H	2.839445	3.942813	0.595345				
H	3.520348	3.791925	2.211219				
H	2.852799	2.367076	1.393015				
H	0.262496	5.158879	3.345868				
H	1.961002	5.600782	3.068793				
H	0.764358	5.762249	1.774095				
H	0.592690	2.075914	0.030718				
H	-1.015944	1.774465	0.624220				



### Reactant

C	0.367678	-0.644455	0.166812
C	0.439706	0.417955	1.233233
C	0.929465	0.160752	2.449216
C	1.043610	1.161469	3.580429
C	0.614292	2.529525	3.177514
C	-0.037125	2.854216	1.897001
H	-0.890834	3.529581	1.903523
C	1.284307	3.545138	2.340993
C	2.599020	3.224015	1.648858
C	1.147660	5.008316	2.741903
C	-0.098672	1.773633	0.823762
H	0.935042	-0.347497	-0.723275
H	-0.666493	-0.804414	-0.160736
H	0.763619	-1.598925	0.519218
H	1.281170	-0.844653	2.671793
H	0.419476	0.813190	4.416857
H	2.070589	1.169227	3.969333
H	2.727777	3.844410	0.754727
H	3.442929	3.434103	2.314759

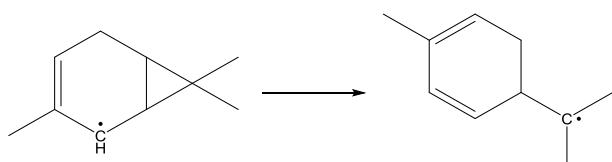
### Product

C	1.059497	-0.540957	0.563773
C	0.631239	0.485891	1.578489
C	0.833326	0.344436	2.896998
C	0.327850	1.362044	3.886425
C	0.237277	2.812009	3.310500
H	-0.526382	3.333783	3.897665
C	-0.234968	2.771545	1.870009
H	-0.686218	3.673329	1.467955
C	1.513538	3.611368	3.458205
C	2.729261	3.277914	2.654682
C	1.685867	4.471162	4.671638
C	-0.038676	1.701938	1.088241
H	1.760489	-0.113846	-0.162351
H	0.199719	-0.910637	-0.006862
H	1.542852	-1.396283	1.039902
H	1.322238	-0.545882	3.282895
H	-0.679110	1.058149	4.209684
H	0.944825	1.362515	4.790354
H	3.372495	4.155874	2.527636
H	3.347254	2.509105	3.149576
H	2.474346	2.891265	1.666218
H	0.738946	4.908594	5.002663
H	2.088090	3.902527	5.528827
H	2.393956	5.286658	4.489481
H	-0.350478	1.725469	0.047397

### Transition state

C	0.142519	-0.878524	0.205141
C	0.317804	0.262310	1.172118
C	0.938706	0.116070	2.345744
C	1.147587	1.214371	3.360679
C	0.662572	2.556814	2.895257
C	-0.072580	2.704263	1.724144
H	-0.602810	3.629754	1.514712
C	1.491332	3.706264	2.483212
C	2.828993	3.480840	1.837177
C	1.140957	5.099437	2.915860
C	-0.276896	1.583231	0.737645
H	0.606536	-0.651948	-0.762333
H	-0.919329	-1.067590	0.005903
H	0.585289	-1.800879	0.586419

H	1.325365	-0.865364	2.613749
H	0.633259	0.932272	4.293337
H	2.209170	1.265964	3.635208
H	3.017668	4.196528	1.026660
H	3.647024	3.613593	2.563691
H	2.921164	2.471733	1.429747
H	0.059497	5.231841	3.014838
H	1.569863	5.310280	3.908774
H	1.523000	5.859044	2.226200
H	0.125955	1.873365	-0.245126
H	-1.356416	1.454561	0.560602



### Reactant

C	0.322114	-0.602858	0.179019
C	0.394102	0.461947	1.254605
C	1.015712	0.190290	2.459172
C	1.097509	1.158833	3.604692
C	0.559630	2.556044	3.319317
H	0.085776	3.026045	4.176002
C	-0.101798	2.821251	1.972369
H	-0.956457	3.492015	1.964701
C	1.224788	3.511653	2.360990
C	2.520303	3.142498	1.666106
C	1.119508	4.989678	2.694989
C	-0.170896	1.717946	1.007948
H	0.966611	-0.352122	-0.669649
H	-0.696517	-0.705149	-0.206376
H	0.636448	-1.576515	0.560281
H	1.439584	-0.795671	2.625305
H	0.537936	0.740391	4.453134
H	2.137069	1.219413	3.961216
H	2.641474	3.727013	0.748238
H	3.374719	3.367452	2.314365
H	2.569748	2.087657	1.398651
H	0.171442	5.225280	3.185932
H	1.928376	5.295261	3.368367
H	1.190569	5.603309	1.790490
H	-0.693988	1.891667	0.072656

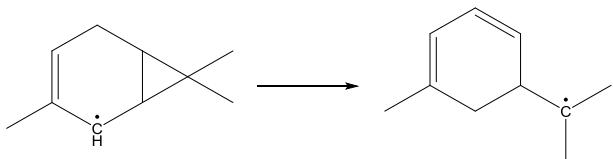
C	0.237277	2.812009	3.310500
H	-0.526382	3.333783	3.897665
C	-0.234968	2.771545	1.870009
H	-0.686218	3.673329	1.467955
C	1.513538	3.611368	3.458205
C	2.729261	3.277914	2.654682
C	1.685867	4.471162	4.671638
C	-0.038676	1.701938	1.088241
H	1.760489	-0.113846	-0.162351
H	0.199719	-0.910637	-0.006862
H	1.542852	-1.396283	1.039902
H	1.322238	-0.545882	3.282895
H	-0.679110	1.058149	4.209684
H	0.944825	1.362515	4.790354
H	3.372495	4.155874	2.527636
H	3.347254	2.509105	3.149576
H	2.474346	2.891265	1.666218
H	0.738946	4.908594	5.002663
H	2.088090	3.902527	5.528827
H	2.393956	5.286658	4.489481
H	-0.350478	1.725469	0.047397

### Transition state

C	0.372400	-0.613319	0.176540
C	0.384349	0.420833	1.276635
C	1.057807	0.219022	2.435985
C	1.039893	1.198344	3.581613
C	0.519792	2.601342	3.223450
H	0.064340	3.071248	4.097439
C	-0.353156	2.664652	1.998289
H	-1.018682	3.511247	1.889010
C	1.381790	3.557771	2.468809
C	2.573975	3.121894	1.675809
C	1.212078	5.026077	2.725871
C	-0.360793	1.640794	1.072587
H	0.786985	-0.208479	-0.753063
H	-0.650323	-0.937291	-0.045435
H	0.953840	-1.495887	0.450449
H	1.597793	-0.710505	2.591378
H	0.403669	0.790276	4.380087
H	2.039958	1.282361	4.026005
H	2.818436	3.854421	0.900667
H	3.462541	3.028367	2.319657
H	2.422833	2.152895	1.198583
H	0.225991	5.262645	3.134371
H	1.954580	5.378332	3.460226
H	1.358542	5.622278	1.819167
H	-0.934878	1.754011	0.158391

### Product

C	1.059497	-0.540957	0.563773
C	0.631239	0.485891	1.578489
C	0.833326	0.344436	2.896998
C	0.327850	1.362044	3.886425



Reactant

C	0.419791	-0.599388	0.134073
C	0.415948	0.459257	1.194496
C	0.854124	0.211362	2.485816
C	0.866531	1.167345	3.494615
C	0.435001	2.549738	3.253893
H	-0.043857	3.039066	4.097451
C	-0.082969	2.896748	1.864160
H	-0.927478	3.578994	1.834745
C	1.211278	3.515114	2.331689
C	2.536375	3.102699	1.722116
C	1.158924	4.981279	2.725107
C	-0.147012	1.802646	0.803856
H	1.021976	-0.295891	-0.732979
H	-0.592568	-0.788047	-0.248761
H	0.819679	-1.544975	0.506566
H	1.204123	-0.790614	2.721558
H	1.192919	0.894232	4.491877
H	2.717675	3.660068	0.796194
H	3.358881	3.329435	2.408319
H	2.581581	2.039162	1.490864
H	0.194805	5.245276	3.167997
H	1.940031	5.220773	3.454640
H	1.311622	5.624861	1.851283
H	0.342588	2.144642	-0.121671
H	-1.200187	1.659078	0.521444

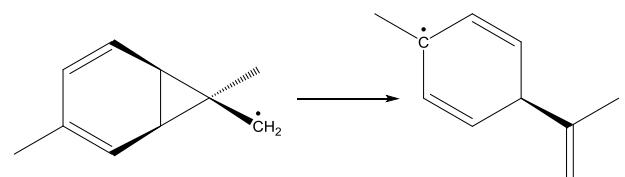
Product

C	0.634648	-0.379240	0.014048
C	0.431347	0.471738	1.233251
C	0.751779	0.071050	2.474063
C	0.507478	0.919448	3.639044
C	0.130934	2.199763	3.510624
H	-0.021544	2.824768	4.384642
C	0.021104	2.862024	2.143795
H	-0.838325	3.541988	2.163412
C	1.250479	3.718654	1.922888
C	2.559694	3.092199	1.557895
C	1.261245	5.106715	2.483719
C	-0.246640	1.810935	1.036049
H	1.301890	0.110914	-0.705684
H	-0.314533	-0.547898	-0.510319
H	1.061236	-1.352333	0.266310
H	1.190726	-0.909468	2.633115
H	0.648081	0.489164	4.625971

H	2.461131	2.357773	0.753528
H	3.282646	3.849668	1.241066
H	3.006588	2.554587	2.409810
H	0.263911	5.557397	2.476566
H	1.615262	5.132870	3.528575
H	1.935400	5.759577	1.918627
H	0.024931	2.235436	0.062902
H	-1.329687	1.625148	0.985444

Transition state

C	0.558871	-0.494822	0.077566
C	0.434793	0.474536	1.215087
C	0.804288	0.172262	2.486731
C	0.656064	1.089678	3.579839
C	0.197679	2.375499	3.377125
H	-0.029719	3.024629	4.212552
C	-0.056108	2.889811	1.985112
H	-0.893077	3.589388	1.933903
C	1.244942	3.601111	2.159523
C	2.541590	3.047522	1.656598
C	1.220817	5.024574	2.632433
C	-0.206268	1.808115	0.901663
H	1.199376	-0.096162	-0.720133
H	-0.417339	-0.695379	-0.384006
H	0.979248	-1.448543	0.403961
H	1.216665	-0.811203	2.695319
H	0.921361	0.764855	4.579763
H	2.645562	3.192974	0.570324
H	3.389502	3.550643	2.129907
H	2.633762	1.975444	1.843609
H	0.295849	5.267720	3.162178
H	2.063146	5.253207	3.293678
H	1.291109	5.718450	1.778893
H	0.176888	2.192988	-0.053185
H	-1.279219	1.635563	0.730930



Reactant

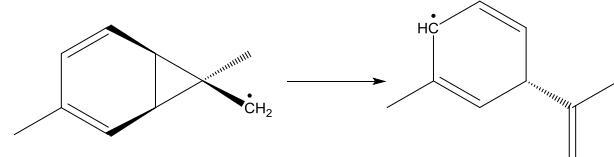
C	-4.219316	1.396273	-0.258028
C	-2.974044	0.651148	0.147236
C	-1.834714	1.282849	0.498938
C	-0.602462	0.568056	0.867554
C	0.186200	-0.309672	-0.136901

C 1.681500 -0.390490 0.133488  
 C -0.195004 -0.373945 -1.534540  
 C -0.695949 -0.959733 0.966731  
 C -2.010866 -1.547536 0.679766  
 C -3.046621 -0.806457 0.244506  
 H -4.069584 2.476912 -0.219214  
 H -4.520475 1.134089 -1.278544  
 H -5.061535 1.144116 0.395832  
 H -1.812442 2.367534 0.548275  
 H 0.041118 1.080857 1.576764  
 H 2.207847 0.433714 -0.357826  
 H 1.901714 -0.336953 1.202514  
 H 2.094019 -1.330495 -0.246097  
 H -1.225922 -0.310727 -1.849326  
 H 0.568740 -0.500314 -2.290719  
 H -0.112837 -1.458552 1.735230  
 H -2.138938 -2.609711 0.862329  
 H -3.999861 -1.282925 0.036194

C 0.212850 -0.458028 -0.188780  
 C 1.697721 -0.407997 0.124028  
 C -0.178753 -0.486582 -1.538915  
 C -0.686034 -0.934495 0.941038  
 C -2.012782 -1.531930 0.645099  
 C -3.056559 -0.779777 0.250365  
 H -4.072419 2.508325 -0.190354  
 H -4.490213 1.190263 -1.292156  
 H -5.088434 1.167591 0.362551  
 H -1.816504 2.383186 0.615527  
 H 0.075005 1.086690 1.547516  
 H 2.204591 0.348120 -0.481839  
 H 1.891379 -0.179763 1.174742  
 H 2.159517 -1.377333 -0.092830  
 H -1.195231 -0.704332 -1.834581  
 H 0.521649 -0.184129 -2.307665  
 H -0.137111 -1.441032 1.734506  
 H -2.127413 -2.602077 0.782010  
 H -4.008494 -1.257764 0.036354

### Product

C 0.464828 0.258553 0.058237  
 C -0.481708 -0.881512 -0.355077  
 C -0.168720 -1.398005 -1.737553  
 C 0.085710 -2.710365 -1.995565  
 C 0.070557 -3.706220 -0.979877  
 C -0.236818 -3.291191 0.345748  
 C -0.499374 -1.993843 0.663974  
 H -0.740182 -1.718556 1.685719  
 C 1.926132 -0.087030 0.171953  
 C -0.004823 1.482469 0.299028  
 H -1.486452 -0.424528 -0.379978  
 H -0.158026 -0.669691 -2.542030  
 H 0.301441 -3.015619 -3.016129  
 C 0.403202 -5.138136 -1.288915  
 H -0.269564 -4.043978 1.129024  
 H -0.116146 -5.824979 -0.614919  
 H 0.131607 -5.400486 -2.315059  
 H 1.478641 -5.335203 -1.181190  
 H 2.517524 0.780562 0.469704  
 H 2.082037 -0.883622 0.906644  
 H 2.313108 -0.461872 -0.781142  
 H 0.651402 2.295573 0.591456  
 H -1.061457 1.714108 0.212203



### Reactant

C -4.219316 1.396273 -0.258028  
 C -2.974044 0.651148 0.147236  
 C -1.834714 1.282849 0.498938  
 C -0.602462 0.568056 0.867554  
 C 0.186200 -0.309672 -0.136901  
 C 1.681500 -0.390490 0.133488  
 C -0.195004 -0.373945 -1.534540  
 C -0.695949 -0.959733 0.966731  
 C -2.010866 -1.547536 0.679766  
 C -3.046621 -0.806457 0.244506  
 H -4.069584 2.476912 -0.219214  
 H -4.520475 1.134089 -1.278544  
 H -5.061535 1.144116 0.395832  
 H -1.812442 2.367534 0.548275  
 H 0.041118 1.080857 1.576764  
 H 2.207847 0.433714 -0.357826  
 H 1.901714 -0.336953 1.202514  
 H 2.094019 -1.330495 -0.246097  
 H -1.225922 -0.310727 -1.849326  
 H 0.568740 -0.500314 -2.290719  
 H -0.112837 -1.458552 1.735230  
 H -2.138938 -2.609711 0.862329  
 H -3.999861 -1.282925 0.036194

### Transition state

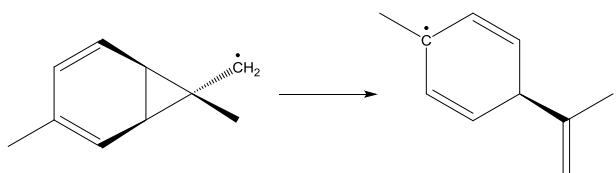
C -4.222249 1.428864 -0.256222  
 C -2.993237 0.675760 0.176173  
 C -1.851569 1.298785 0.571621  
 C -0.665140 0.575695 0.945973

### Product

```

C  1.071874 -0.019804  0.318360
C  0.096620 -1.206111  0.409185
C -0.839335 -1.250417 -0.770924
C -0.977699 -2.363108 -1.546964
C -0.246711 -3.544377 -1.285542
C  0.659283 -3.605575 -0.185838
C  0.824700 -2.511851  0.612540
H  1.510180 -2.554496  1.454010
H -0.507312 -1.010951  1.313105
H -1.411115 -0.352854 -0.982020
H -1.668052 -2.347282 -2.384831
H -0.377410 -4.412905 -1.921070
C  1.413205 -4.888966  0.071561
H  2.069842 -4.799655  0.938886
H  0.723423 -5.719553  0.252579
H  2.027471 -5.163208 -0.792156
C  1.051682  0.952963  1.229275
C  2.032853 -0.026199 -0.841178
H  1.734179  1.794790  1.176376
H  0.352591  0.941755  2.059187
H  2.659087 -0.923997 -0.822766
H  1.494036 -0.041252 -1.794087
H  2.682490  0.850618 -0.823548

```



### Reactant

```

C -4.257648  1.378207 -0.242288
C -3.020280  0.624873  0.171219
C -1.876161  1.249113  0.525900
C -0.653264  0.527698  0.910533
C  0.133170 -0.357308 -0.092958
C  1.566189 -0.444220  0.139302
C -0.290345 -0.423961 -1.546162
C -0.757769 -0.997569  1.014236
C -2.072384 -1.577496  0.715092
C -3.103082 -0.830966  0.272437
H -4.099852  2.457749 -0.206431
H -4.556502  1.114580 -1.263138
H -5.104406  1.134683  0.408865
H -1.847015  2.333786  0.573243
H -0.013050  1.039627  1.621224
H  1.975733 -0.393575  1.140972
H  2.250797 -0.568648 -0.688971
H  0.142331  0.414550 -2.100020
H  0.070836 -1.352484 -1.998301
H -1.370249 -0.387710 -1.672000
H -0.184928 -1.498681  1.786796
H -2.209011 -2.638127  0.900895
H -4.057848 -1.302601  0.060328

```

### Transition state

```

C -4.225879  1.379884 -0.261617
C -2.984404  0.630829  0.149940
C -1.834458  1.264382  0.463512
C -0.596003  0.537970  0.846155
C  0.230857 -0.188800 -0.203276
C  1.699435 -0.388073  0.127018
C -0.163025 -0.284978 -1.549519
C -0.759914 -0.950322  1.044420
C -2.033083 -1.550112  0.751205
C -3.070589 -0.820342  0.272435
H -4.060739  2.458811 -0.268306
H -4.548614  1.079880 -1.264668
H -5.057946  1.164335  0.417408
H -1.794878  2.349308  0.464862
H  0.019563  1.065691  1.574290
H  2.280499  0.473199 -0.219722
H  1.871130 -0.488841  1.201159
H  2.098814 -1.281103 -0.361606
H -1.146985  0.017130 -1.878749
H  0.490575 -0.763826 -2.268296
H -0.086695 -1.472020  1.711520
H -2.150592 -2.613881  0.930136
H -4.016499 -1.301081  0.045864

```

### Product

```

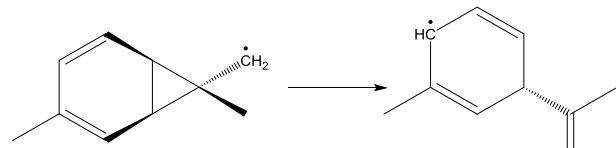
C  0.464828  0.258553  0.058237
C -0.481708 -0.881512 -0.355077
C -0.168720 -1.398005 -1.737553
C  0.085710 -2.710365 -1.995565
C  0.070557 -3.706220 -0.979877
C -0.236818 -3.291191  0.345748
C -0.499374 -1.993843  0.663974
H -0.740182 -1.718556  1.685719
C  1.926132 -0.087030  0.171953
C -0.004823  1.482469  0.299028
H -1.486452 -0.424528 -0.379978
H -0.158026 -0.669691 -2.542030
H  0.301441 -3.015619 -3.016129
C  0.403202 -5.138136 -1.288915
H -0.269564 -4.043978  1.129024
H -0.116146 -5.824979 -0.614919
H  0.131607 -5.400486 -2.315059

```

H 1.478641 -5.335203 -1.181190  
 H 2.517524 0.780562 0.469704  
 H 2.082037 -0.883622 0.906644  
 H 2.313108 -0.461872 -0.781142  
 H 0.651402 2.295573 0.591456  
 H -1.061457 1.714108 0.212203

### Transition state

C -4.246253 1.356634 -0.284554  
 C -3.023409 0.613707 0.182488  
 C -1.890834 1.250958 0.597662  
 C -0.712171 0.544387 1.016659  
 C 0.171715 -0.461896 -0.114107  
 C 1.570389 -0.432864 0.106649  
 C -0.321870 -0.457348 -1.541876  
 C -0.721499 -0.967454 1.006482  
 C -2.041586 -1.578483 0.706618  
 C -3.085651 -0.838786 0.288787  
 H -4.096615 2.437344 -0.244093  
 H -4.504012 1.091916 -1.316708  
 H -5.119202 1.111585 0.331267  
 H -1.869903 2.336222 0.635929  
 H -0.001723 1.054152 1.651518  
 H 1.990211 -0.599731 1.091743  
 H 2.245267 -0.134573 -0.685281  
 H 0.393646 0.064866 -2.181312  
 H -0.423328 -1.483243 -1.911291  
 H -1.290931 0.029785 -1.652456  
 H -0.167029 -1.467911 1.798032  
 H -2.155366 -2.644660 0.872046  
 H -4.034586 -1.323087 0.076569



### Reactant

C -4.257648 1.378207 -0.242288  
 C -3.020280 0.624873 0.171219  
 C -1.876161 1.249113 0.525900  
 C -0.653264 0.527698 0.910533  
 C 0.133170 -0.357308 -0.092958  
 C 1.566189 -0.444220 0.139302  
 C -0.290345 -0.423961 -1.546162  
 C -0.757769 -0.997569 1.014236  
 C -2.072384 -1.577496 0.715092  
 C -3.103082 -0.830966 0.272437

H -4.099852 2.457749 -0.206431  
 H -4.556502 1.114580 -1.263138  
 H -5.104406 1.134683 0.408865  
 H -1.847015 2.333786 0.573243  
 H -0.013050 1.039627 1.621224  
 H 1.975733 -0.393575 1.140972  
 H 2.250797 -0.568648 -0.688971  
 H 0.142331 0.414550 -2.100020  
 H 0.070836 -1.352484 -1.998301  
 H -1.370249 -0.387710 -1.672000  
 H -0.184928 -1.498681 1.786796  
 H -2.209011 -2.638127 0.900895  
 H -4.057848 -1.302601 0.060328

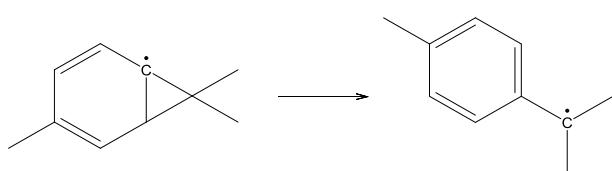
### Product

C 1.071874 -0.019804 0.318360  
 C 0.096620 -1.206111 0.409185  
 C -0.839335 -1.250417 -0.770924  
 C -0.977699 -2.363108 -1.546964  
 C -0.246711 -3.544377 -1.285542  
 C 0.659283 -3.605575 -0.185838  
 C 0.824700 -2.511851 0.612540  
 H 1.510180 -2.554496 1.454010  
 H -0.507312 -1.010951 1.313105  
 H -1.411115 -0.352854 -0.982020  
 H -1.668052 -2.347282 -2.384831  
 H -0.377410 -4.412905 -1.921070  
 C 1.413205 -4.888966 0.071561  
 H 2.069842 -4.799655 0.938886  
 H 0.723423 -5.719553 0.252579  
 H 2.027471 -5.163208 -0.792156  
 C 1.051682 0.952963 1.229275  
 C 2.032853 -0.026199 -0.841178  
 H 1.734179 1.794790 1.176376  
 H 0.352591 0.941755 2.059187  
 H 2.659087 -0.923997 -0.822766  
 H 1.494036 -0.041252 -1.794087  
 H 2.682490 0.850618 -0.823548

### Transition state

C -4.232825 1.388274 -0.254869  
 C -3.005596 0.622305 0.167070  
 C -1.856670 1.239376 0.517040  
 C -0.634193 0.492624 0.911819  
 C 0.180459 -0.266165 -0.123721  
 C 1.563772 -0.456382 0.118703  
 C -0.310412 -0.377043 -1.548174  
 C -0.818766 -0.995157 1.109137  
 C -2.084258 -1.576773 0.761991

C -3.101720 -0.829645 0.254602  
 H -4.063289 2.466091 -0.225313  
 H -4.528981 1.119638 -1.274923  
 H -5.083735 1.156849 0.394787  
 H -1.810697 2.323477 0.550354  
 H -0.013879 1.007862 1.642590  
 H 2.003300 -0.234103 1.084072  
 H 2.193049 -0.926028 -0.626266  
 H -0.269714 0.601666 -2.037582  
 H 0.325891 -1.065207 -2.109599  
 H -1.337861 -0.735636 -1.615644  
 H -0.182566 -1.513205 1.812153  
 H -2.223356 -2.639818 0.931060  
 H -4.042695 -1.301480 -0.008517



### Reactant

C -4.412828 1.379776 -0.033973  
 C -3.124875 0.648785 0.248708  
 C -1.943128 1.305332 0.391167  
 C -0.701293 0.590849 0.728609  
 C 0.202025 -0.340880 -0.190886  
 C 1.673253 -0.341378 0.188248  
 C -0.065049 -0.424397 -1.680242  
 C -0.794073 -0.888327 0.746931  
 C -2.034295 -1.536500 0.552050  
 C -3.176359 -0.796110 0.384182  
 H -4.253806 2.456919 -0.110192  
 H -4.863577 1.035861 -0.971211  
 H -5.147349 1.198274 0.757947  
 H -1.927270 2.391736 0.361522  
 H -0.069387 1.093544 1.461403  
 H 2.203607 0.489884 -0.287840  
 H 1.807786 -0.268087 1.269204  
 H 2.143974 -1.273963 -0.141397  
 H 0.472264 0.367448 -2.213439  
 H 0.278520 -1.385261 -2.078976  
 H -1.128628 -0.326917 -1.902737  
 H -2.079444 -2.622014 0.509416  
 H -4.137617 -1.290366 0.282258

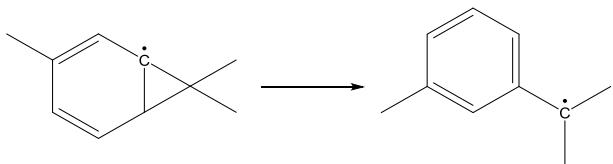
### Product

C 0.655173 0.203102 0.064669  
 C 0.424624 -1.134151 -0.372864  
 C 0.067461 -1.437168 -1.716733

C -0.153642 -2.738191 -2.133771  
 C -0.037998 -3.823641 -1.253124  
 C 0.317857 -3.541883 0.073873  
 C 0.542223 -2.246583 0.506853  
 H 0.817893 -2.083936 1.541302  
 C 1.032314 0.488186 1.491728  
 C 0.527876 1.355202 -0.892650  
 H -0.032062 -0.635405 -2.437725  
 H -0.421429 -2.922775 -3.169946  
 C -0.314505 -5.234228 -1.707750  
 H 0.422243 -4.360653 0.779667  
 H 0.266557 -5.960194 -1.133559  
 H -1.372778 -5.492227 -1.581496  
 H -0.072635 -5.367894 -2.765138  
 H 1.159872 1.558389 1.661081  
 H 0.271706 0.131608 2.198520  
 H 1.971963 -0.003737 1.776126  
 H 0.735145 2.305360 -0.398161  
 H 1.221764 1.266758 -1.738966  
 H -0.478926 1.422514 -1.325417

### Transition state

C -4.537531 1.394580 0.148837  
 C -3.218359 0.680687 0.312766  
 C -2.029997 1.361738 0.345390  
 C -0.762281 0.649806 0.622431  
 C 0.251122 -0.362149 -0.255382  
 C 1.679177 -0.368911 0.275166  
 C 0.136663 -0.526891 -1.757909  
 C -0.852564 -0.799201 0.595896  
 C -2.040004 -1.472378 0.396331  
 C -3.236508 -0.757075 0.411656  
 H -4.399885 2.470044 0.020065  
 H -5.086031 1.012985 -0.719666  
 H -5.176606 1.235587 1.023336  
 H -2.031413 2.447095 0.285570  
 H -0.104171 1.142135 1.356243  
 H 2.296758 0.379027 -0.232848  
 H 1.711469 -0.181251 1.349055  
 H 2.130709 -1.352521 0.098355  
 H 0.782031 0.186053 -2.281876  
 H 0.448226 -1.535866 -2.057351  
 H -0.889641 -0.378725 -2.093416  
 H -2.041196 -2.537110 0.174918  
 H -4.190862 -1.273456 0.368015



Reactant

C	-4.402722	1.379396	-0.003754
C	-3.124655	0.623765	0.241568
C	-1.905519	1.248387	0.343230
C	-0.732474	0.514208	0.645533
C	0.202601	-0.256385	-0.194929
C	1.669896	-0.333758	0.192599
C	-0.061267	-0.365660	-1.683408
C	-0.774455	-0.959086	0.835886
C	-2.081368	-1.584935	0.579441
C	-3.172062	-0.827333	0.317210
H	-4.218328	2.450008	-0.111934
H	-4.908671	1.027158	-0.909509
H	-5.106765	1.243010	0.825668
H	-1.836081	2.319592	0.164902
H	2.221809	0.493666	-0.266343
H	1.802107	-0.259042	1.273752
H	2.120378	-1.270744	-0.151252
H	0.370429	0.491011	-2.212484
H	0.396668	-1.273335	-2.091503
H	-1.129915	-0.392749	-1.900980
H	-0.198427	-1.412128	1.643156
H	-2.185075	-2.659275	0.702659
H	-4.135231	-1.309821	0.176284

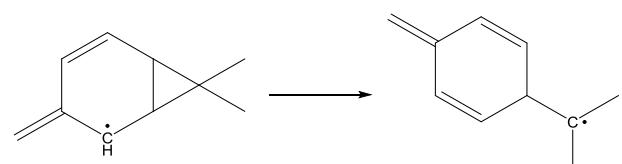
Product

C	1.207922	-0.014419	0.041970
C	0.755355	-1.302788	-0.372459
C	-0.011090	-1.481129	-1.556432
C	-0.442318	-2.739609	-1.943704
C	-0.135796	-3.866964	-1.181603
C	0.619027	-3.737971	-0.004378
C	1.049352	-2.475714	0.380399
H	1.631045	-2.386765	1.290143
H	-0.264687	-0.625318	-2.168701
H	-1.025913	-2.848441	-2.851846
H	-0.480312	-4.846324	-1.497325
C	0.951116	-4.958561	0.821791
H	1.542997	-4.696683	1.701030
H	0.042304	-5.461602	1.166875
H	1.521833	-5.687740	0.238173
C	2.017725	0.148765	1.297874
C	0.884019	1.208682	-0.769956
H	2.281461	1.194016	1.465410

H	1.475206	-0.200212	2.186260
H	1.281892	1.142459	-1.791031
H	-0.198414	1.361709	-0.870278
H	1.300768	2.108003	-0.314193
H	2.952963	-0.425124	1.262717

Transition state

C	-4.459110	1.430814	0.176972
C	-3.224695	0.577427	0.277833
C	-1.927519	1.133283	0.156925
C	-0.837609	0.357203	0.458165
C	0.283311	-0.210233	-0.285923
C	1.669299	-0.276032	0.306037
C	0.184757	-0.318025	-1.785273
C	-0.918278	-1.044471	0.762918
C	-2.214670	-1.655641	0.549731
C	-3.312084	-0.835832	0.377983
H	-4.296415	2.290450	-0.480842
H	-5.311425	0.865371	-0.209147
H	-4.751631	1.831296	1.155973
H	-1.802799	2.125758	-0.271282
H	2.233083	0.623878	0.027291
H	1.643741	-0.313846	1.397309
H	2.227210	-1.141669	-0.064203
H	0.576144	0.587161	-2.269105
H	0.772708	-1.164047	-2.158059
H	-0.851722	-0.442537	-2.103937
H	-0.235438	-1.512227	1.468304
H	-2.339003	-2.731314	0.617631
H	-4.296985	-1.290818	0.310486



Reactant

C	-4.150591	1.367835	-0.315962
C	-3.029657	0.667250	0.099475
C	-1.844039	1.312059	0.490443
C	-0.623385	0.591858	0.855779
C	0.157064	-0.291660	-0.127466
C	1.653638	-0.366754	0.118405
C	-0.220957	-0.333994	-1.592333
C	-0.715523	-0.947562	0.930091
C	-2.035912	-1.532551	0.621609
C	-3.079286	-0.800454	0.204169

H	-4.145029	2.449370	-0.376728
H	-5.064000	0.855058	-0.590745
H	-1.837724	2.394983	0.561417
H	0.003770	1.087193	1.591668
H	2.171962	0.462968	-0.373838
H	1.891375	-0.324680	1.184631
H	2.065629	-1.300519	-0.279671
H	0.225139	0.514148	-2.121813
H	0.158085	-1.252398	-2.053192
H	-1.297295	-0.299404	-1.751636
H	-0.168822	-1.437580	1.730811
H	-2.151526	-2.602857	0.764944
H	-4.026485	-1.282208	-0.016558

C	-3.089283	-0.782766	0.209365
H	-4.232237	2.434450	-0.330950
H	-5.090263	0.819971	-0.615803
H	-1.930950	2.443899	0.687071
H	-0.002491	1.178981	1.570226
H	2.233538	0.367777	-0.449257
H	1.910243	-0.273812	1.171015
H	2.186584	-1.374442	-0.178138
H	0.439517	0.307250	-2.198694
H	-0.065020	-1.383165	-2.111531
H	-1.221575	-0.103773	-1.748197
H	-0.202632	-1.328981	1.734051
H	-2.037755	-2.567789	0.587427
H	-4.011168	-1.298310	-0.042572

### Product

C	0.671800	0.023860	0.345258
C	-0.025477	-1.320966	0.495451
C	-1.043380	-1.521139	-0.606721
C	-1.009237	-2.542609	-1.471473
C	-0.000277	-3.601907	-1.397581
C	0.969336	-3.485166	-0.305045
C	0.958839	-2.464099	0.559975
H	1.697167	-2.416872	1.354879
C	0.176461	1.197366	1.127696
C	1.560240	0.268215	-0.832502
H	-0.566282	-1.287845	1.454267
H	-1.816770	-0.763440	-0.693319
H	-1.754361	-2.615978	-2.258333
C	0.028913	-4.624808	-2.272338
H	1.711416	-4.272462	-0.209768
H	0.777534	-5.405721	-2.204287
H	-0.694948	-4.702907	-3.075355
H	0.952902	1.961754	1.237474
H	-0.677255	1.695375	0.635019
H	-0.163173	0.909188	2.127537
H	2.402475	0.917144	-0.564892
H	1.960805	-0.661662	-1.241657
H	1.025785	0.778755	-1.650556

### Transition state

C	-4.204744	1.351902	-0.289087
C	-3.106032	0.688921	0.156909
C	-1.920410	1.360396	0.631753
C	-0.795678	0.667097	1.041222
C	0.246896	-0.450153	-0.201210
C	1.714227	-0.420537	0.105481
C	-0.177903	-0.397820	-1.633767
C	-0.703670	-0.825889	0.903442
C	-2.002765	-1.483107	0.554748

## 7.8 Intramolecular hydrogen abstraction reaction on 1,5-p-menthadien-8-yl

### Reactant

  
 1,5-p-menthadien-8-yl

C	-0.180428	-0.838681	-0.117983
C	0.007026	-0.677080	1.384579
C	1.140842	-0.192998	1.909276
C	2.306586	0.147781	1.078801
C	2.314006	-0.216923	-0.212141
C	1.188765	-1.010148	-0.826030
H	-0.846677	-0.891077	2.020334
H	1.214934	-0.027550	2.980897
C	3.444514	0.888090	1.730779
H	1.462653	-2.074895	-0.793692
H	4.254248	1.079713	1.023966
H	3.111512	1.850144	2.136422
H	3.855017	0.315866	2.570786
C	-1.024920	0.309611	-0.628441
C	-2.515343	0.186259	-0.559386
C	-0.434375	1.673557	-0.801932
H	-3.002145	0.804531	-1.321489
H	-2.846243	-0.847985	-0.695991
H	-2.918455	0.524070	0.410813
H	-1.098385	2.317115	-1.386796
H	-0.272463	2.174379	0.166614
H	0.540753	1.645532	-1.295480
H	-0.756778	-1.755008	-0.288961
H	3.172530	0.011134	-0.838101
H	1.079759	-0.765740	-1.887959

### Products

1,5-p-menthadien-4-yl

```

C  0.061340  0.025060 -0.091748
C  0.066282  0.230381  1.261138
C  1.252262  0.212844  2.030306
C  2.518380 -0.024473  1.421126
C  2.577314 -0.242105  0.077180
C  1.363027 -0.249218 -0.802333
H -0.869823  0.414183  1.777480
H  1.197154  0.382505  3.099878
C  3.760667 -0.029361  2.279759
H  3.535482 -0.426134 -0.399918
H  1.288221 -1.220137 -1.327641
H  4.656107 -0.222935  1.685976
H  3.891947  0.932103  2.786741
H  3.697871 -0.797204  3.057670
C -1.185053  0.064526 -0.953894
C -2.491651 -0.194190 -0.191387
C -1.280247  1.392879 -1.738566
H -3.329688 -0.258259 -0.890801
H -2.448355 -1.128999  0.372968
H -2.715923  0.615073  0.509788
H -2.130971  1.374757 -2.426420
H -1.415878  2.232926 -1.051077
H -0.380405  1.584164 -2.328044
H -1.077548 -0.738078 -1.698224
H  1.500729  0.470841 -1.628315

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1,5-p-menthadien-3-yl

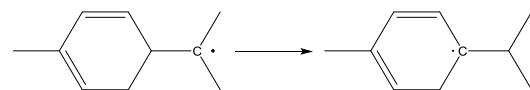
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C -0.114582 -0.738904 -0.078876
C -0.032063 -0.247884  1.340113
C  1.140675  0.125537  1.926541
C  2.387330  0.066433  1.248364
C  2.385263 -0.421932 -0.088723
C  1.243255 -0.806579 -0.720767
H -0.951414 -0.207126  1.914206
H  1.128720  0.473341  2.956248
C  3.658348  0.528736  1.902230
H  3.333193 -0.494487 -0.615604
H  1.289337 -1.183715 -1.738401
H  4.510960 -0.088972  1.604278
H  3.902439  1.563228  1.624673
H  3.582693  0.497379  2.992145
C -1.133660  0.067146 -0.967732
C -2.578902 -0.111669 -0.485925
C -0.761451  1.549574 -1.082498
H -3.277933  0.354297 -1.186328

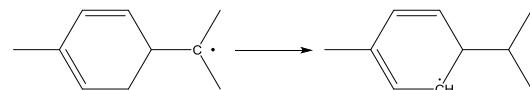
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H -2.845974 -1.169744 -0.402657  
H -2.739425 0.354633 0.490622  
H -1.440236 2.065891 -1.767657  
H -0.824044 2.045891 -0.109586  
H 0.257782 1.676511 -1.455221  
H -1.062615 -0.378502 -1.968600  
H -0.531630 -1.764065 -0.061380

### Transition states



C 0.068010 0.237791 -0.056914  
C 0.063024 0.187805 1.384481  
C 1.222058 0.067166 2.101493  
C 2.511905 -0.021937 1.444367  
C 2.588732 0.191568 0.114516  
C 1.394936 0.602929 -0.711157  
H -0.884352 0.199960 1.910261  
H 1.179010 -0.001460 3.183316  
C 3.722020 -0.362008 2.277335  
H 1.471381 0.159217 -1.708350  
H 4.630553 -0.387337 1.672285  
H 3.866543 0.374920 3.075237  
H 3.608583 -1.337749 2.762186  
C -1.189114 0.291871 -0.868157  
C -2.501506 0.160553 -0.155444  
C -1.207506 0.844371 -2.264254  
H -3.308563 -0.064402 -0.857130  
H -2.487582 -0.628889 0.602617  
H -2.768060 1.092789 0.369681  
H -1.996685 0.378011 -2.861512  
H -1.415907 1.927464 -2.251887  
H -0.264615 0.712779 -2.794923  
H 3.547106 0.138904 -0.393489  
H 1.419534 1.696136 -0.880768  
H -0.362934 -0.819688 -0.563584

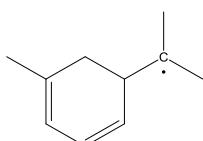


C -0.292769 -0.724435 0.226821  
C 0.031557 -0.161906 1.579592  
C 1.273034 0.241288 1.908132  
C 2.411509 0.107171 1.007879  
C 2.239350 -0.504460 -0.200524  
C 0.947695 -0.946894 -0.668209  
H -0.775160 -0.089793 2.302887  
H 1.456644 0.657322 2.895182

C 3.753599 0.608271 1.470212  
 H 0.922185 -1.841757 -1.288233  
 H 4.532031 0.406197 0.731603  
 H 3.735067 1.689730 1.651666  
 H 4.052044 0.136146 2.413562  
 C -0.944407 0.229831 -0.810434  
 C -2.097138 -0.336306 -1.598507  
 C -0.963782 1.710392 -0.533323  
 H -2.317288 0.268448 -2.482451  
 H -1.898605 -1.361555 -1.926374  
 H -3.011399 -0.367021 -0.985476  
 H -1.159122 2.273634 -1.450117  
 H -1.756304 1.969295 0.185085  
 H -0.020206 2.056065 -0.107332  
 H -0.902080 -1.626871 0.344326  
 H 3.091291 -0.640003 -0.860894  
 H 0.344686 -0.074716 -1.495097

## 7.9 Intramolecular hydrogen abstraction reaction on 1,3-m-menthadien-8-yl

### Reactant

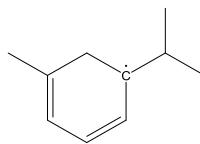


1,3-m-menthadien-8-yl

C 0.007453 -0.283963 0.195214  
 C 0.186290 0.208567 1.626132  
 C 1.411536 0.292424 2.160745  
 C 2.599049 -0.039470 1.374691  
 C 2.537095 -0.127300 0.035749  
 C 1.214172 0.156327 -0.650800  
 H -0.695091 0.448280 2.209989  
 H 1.541893 0.601891 3.193058  
 H 3.544748 -0.178333 1.890203  
 C 3.731098 -0.392281 -0.833186  
 C -1.347196 0.068669 -0.378479  
 C -1.512741 0.635949 -1.752405  
 C -2.545005 -0.580697 0.243594  
 H 3.594192 -1.301355 -1.430660  
 H 3.884223 0.427533 -1.546639  
 H 4.643506 -0.505170 -0.243831  
 H -2.490764 1.115978 -1.858836  
 H -0.749054 1.375451 -2.003722  
 H -1.465686 -0.144631 -2.533289  
 H -2.785801 -1.537451 -0.252837  
 H -2.394955 -0.809110 1.302101  
 H -3.439155 0.046048 0.155922  
 H 1.183224 -0.332981 -1.628696  
 H 0.059238 -1.392710 0.254777

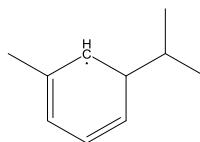
H 1.161769 1.239520 -0.843887

### Products



1,3-m-menthadien-5-yl

C -0.086437 -0.360649 0.348209  
 C 0.184101 -0.988659 1.532178  
 C 1.487742 -1.051375 2.078492  
 C 2.569762 -0.450114 1.393680  
 C 2.398551 0.199579 0.204976  
 C 1.031659 0.297796 -0.423006  
 H -0.632244 -1.457567 2.075017  
 H 1.656611 -1.559474 3.019949  
 H 3.564652 -0.507373 1.826305  
 C 3.528028 0.844509 -0.540254  
 C -1.493337 -0.308624 -0.212627  
 C -1.615435 -1.033902 -1.568256  
 C -2.033017 1.132339 -0.318396  
 H 3.350162 1.918735 -0.681745  
 H 4.478446 0.725637 -0.015943  
 H 3.638518 0.416020 -1.545142  
 H -2.659434 -1.061342 -1.893925  
 H -1.042288 -0.526402 -2.349830  
 H -1.254456 -2.063237 -1.498829  
 H -3.080956 1.125544 -0.632300  
 H -1.970021 1.648698 0.642876  
 H -1.474912 1.718498 -1.054491  
 H 1.078118 -0.116609 -1.446511  
 H 0.793562 1.363191 -0.595539  
 H -2.132532 -0.842869 0.499763

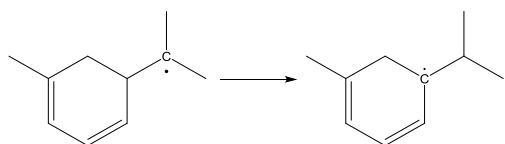


1,3-m-menthadien-6-yl

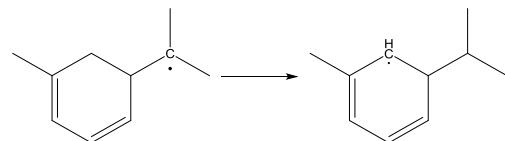
C -0.011379 -1.039583 0.001168  
 C 0.136722 -1.227030 1.483691  
 C 1.216943 -0.765705 2.176368  
 C 2.271791 -0.084136 1.528212  
 C 2.233405 0.126663 0.119289  
 C 1.165457 -0.323488 -0.602438  
 H -0.660797 -1.752451 2.000512  
 H 1.274081 -0.925514 3.248787  
 H 3.118773 0.274593 2.102150  
 C 3.387019 0.841193 -0.544969  
 C -1.397577 -0.385887 -0.359347

C -1.702947 -0.476531 -1.859817  
 C -1.510271 1.056059 0.148347  
 H 3.234433 0.931966 -1.622099  
 H 3.513415 1.848459 -0.135056  
 H 4.327977 0.306420 -0.380030  
 H -2.719704 -0.129980 -2.065932  
 H -1.022984 0.145579 -2.449178  
 H -1.621035 -1.505138 -2.224514  
 H -2.509657 1.456514 -0.045725  
 H -1.323988 1.115744 1.223335  
 H -0.785191 1.705056 -0.351471  
 H 1.157048 -0.175498 -1.677828  
 H -2.149193 -0.989675 0.165719  
 H -0.066069 -2.045242 -0.459268

### Transition states



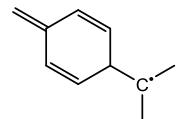
C -0.028790 -0.124050 0.180543  
 C 0.096651 -0.009705 1.613028  
 C 1.325057 0.051629 2.213956  
 C 2.533471 0.019672 1.430461  
 C 2.508020 0.081061 0.081380  
 C 1.191733 0.266843 -0.644488  
 H -0.796254 -0.024209 2.226006  
 H 1.395710 0.096444 3.294512  
 H 3.487186 -0.054771 1.945026  
 C 3.743779 0.080398 -0.768510  
 C -1.352027 -0.268146 -0.505584  
 C -1.549811 0.122274 -1.942041  
 C -2.577165 -0.432019 0.342714  
 H 3.741237 -0.753929 -1.481610  
 H 3.813168 0.998469 -1.368094  
 H 4.649061 0.004776 -0.162466  
 H -0.647772 0.027669 -2.546366  
 H -2.332483 -0.482218 -2.410262  
 H -1.873291 1.174185 -2.017964  
 H -3.418239 -0.801106 -0.249538  
 H -2.420458 -1.128838 1.172065  
 H -2.883730 0.526222 0.793999  
 H 1.219165 -0.296552 -1.583655  
 H 1.100522 1.326405 -0.952595  
 H -0.397823 -1.264694 -0.165483



C -0.150996 -0.679835 0.620611  
 C 0.109252 0.284320 1.740604  
 C 1.281548 0.937551 1.849762  
 C 2.380525 0.709167 0.932464  
 C 2.314299 -0.230538 -0.055514  
 C 1.085847 -0.973054 -0.259119  
 H -0.678423 0.438135 2.471492  
 H 1.433668 1.640338 2.663153  
 H 3.294491 1.277847 1.069559  
 C 3.468087 -0.500840 -0.985738  
 C -0.966053 -0.167524 -0.599297  
 C -1.201381 1.313242 -0.748191  
 C -2.042274 -1.089177 -1.112717  
 H 3.742896 -1.561825 -0.980010  
 H 3.212533 -0.245660 -2.020772  
 H 4.350067 0.077996 -0.704129  
 H -2.000987 1.654832 -0.073894  
 H -0.309073 1.892725 -0.505226  
 H -1.508908 1.556724 -1.768972  
 H -2.376425 -0.802020 -2.113398  
 H -1.701202 -2.128458 -1.150839  
 H -2.922812 -1.064389 -0.452197  
 H 0.323650 -0.474140 -1.257631  
 H -0.608359 -1.590775 1.020987  
 H 1.185492 -2.004643 -0.595906

### 7.10 Intramolecular hydrogen abstraction reaction generating 4-isopropylbenzyl radical

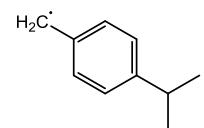
#### Reactant



C -0.119490 -0.596928 -0.054496  
 C 0.112076 -0.335611 1.418334  
 C 1.310665 -0.049141 1.941475  
 C 2.532335 -0.012194 1.134181  
 C 2.367268 -0.322551 -0.288444  
 C 1.175267 -0.597338 -0.831181  
 H -0.765779 -0.362114 2.057391  
 H 1.407134 0.155178 3.003874  
 C 3.733934 0.278549 1.667106  
 H 4.631859 0.297610 1.060266

H	3.845281	0.503995	2.721469	C	0.066650	0.072592	-0.083854
C	-1.126144	0.392907	-0.623924	C	0.080875	-0.043234	1.374063
C	-2.564834	-0.000904	-0.723051	C	1.235772	-0.057677	2.083288
C	-0.770434	1.842954	-0.707777	C	2.538264	0.082877	1.464621
H	-3.093408	0.599374	-1.471047	C	2.520420	0.287722	0.030508
H	-2.683384	-1.056702	-0.986271	C	1.375301	0.304762	-0.694325
H	-3.104025	0.150356	0.228766	H	-0.861829	-0.131919	1.899478
H	-1.225437	2.311605	-1.588317	H	1.194151	-0.160919	3.163045
H	-1.137689	2.406615	0.165691	C	3.698710	0.040726	2.183725
H	0.309650	1.996178	-0.757804	H	1.428890	0.483930	-1.760933
H	-0.572181	-1.595958	-0.154205	H	4.663145	0.154366	1.703599
H	3.261440	-0.330088	-0.904891	H	3.691126	-0.106942	3.256899
H	1.098665	-0.821343	-1.890988	C	-1.207652	0.292518	-0.844414

### Products



C	0.155421	0.178111	-0.197169
C	0.192681	0.755924	1.086172
C	1.335191	0.721683	1.860053
C	2.529677	0.098908	1.393499
C	2.480105	-0.481902	0.094614
C	1.326580	-0.438173	-0.666768
H	-0.694139	1.240669	1.481194
H	1.334340	1.175527	2.845676
C	3.693901	0.060955	2.175230
H	3.368931	-0.965688	-0.296804
H	4.596271	-0.414545	1.811856
H	3.719966	0.506144	3.161904
C	-1.101308	0.215057	-1.049949
C	-2.266375	-0.547659	-0.391556
C	-1.514326	1.655997	-1.404467
H	-3.139041	-0.561654	-1.051390
H	-1.987636	-1.581348	-0.172602
H	-2.568101	-0.076816	0.548658
H	-2.383030	1.654875	-2.069657
H	-1.782341	2.223924	-0.508715
H	-0.701607	2.187464	-1.905647
H	-0.863458	-0.297730	-1.988946
H	1.323446	-0.891233	-1.653572

### Transition states

