

# Supplementary Materials: Theoretical Study on the Hydrogenation Mechanisms of Model Compounds of Heavy Oil in a Plasma-Driven Catalytic System

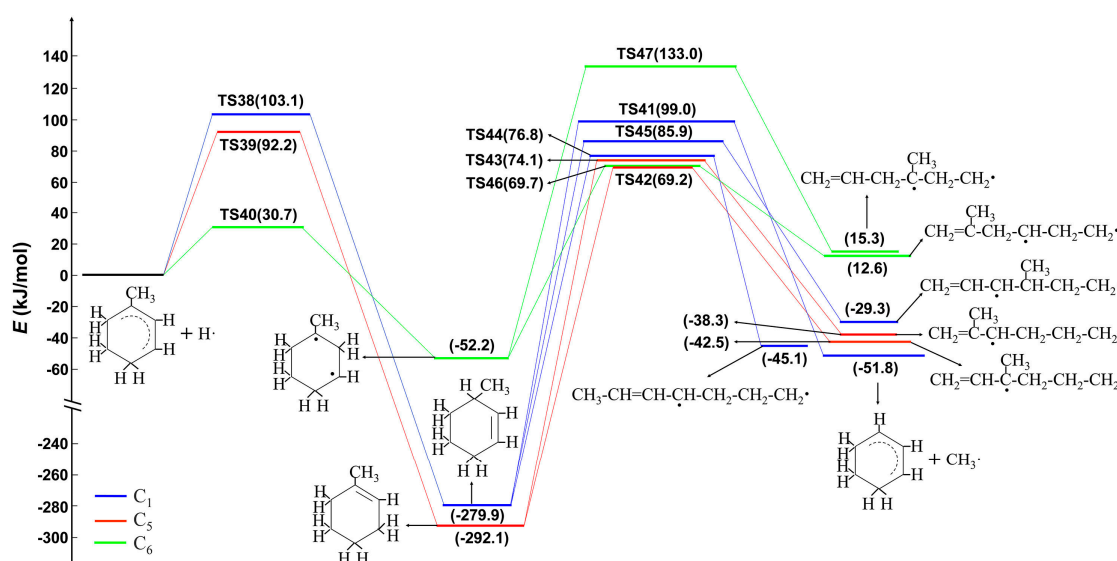
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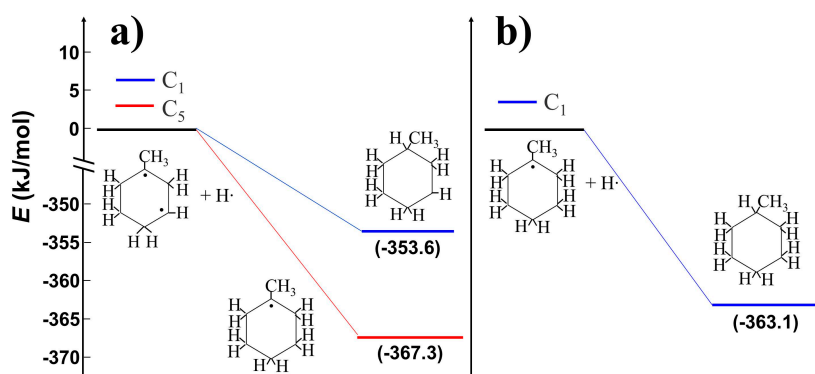
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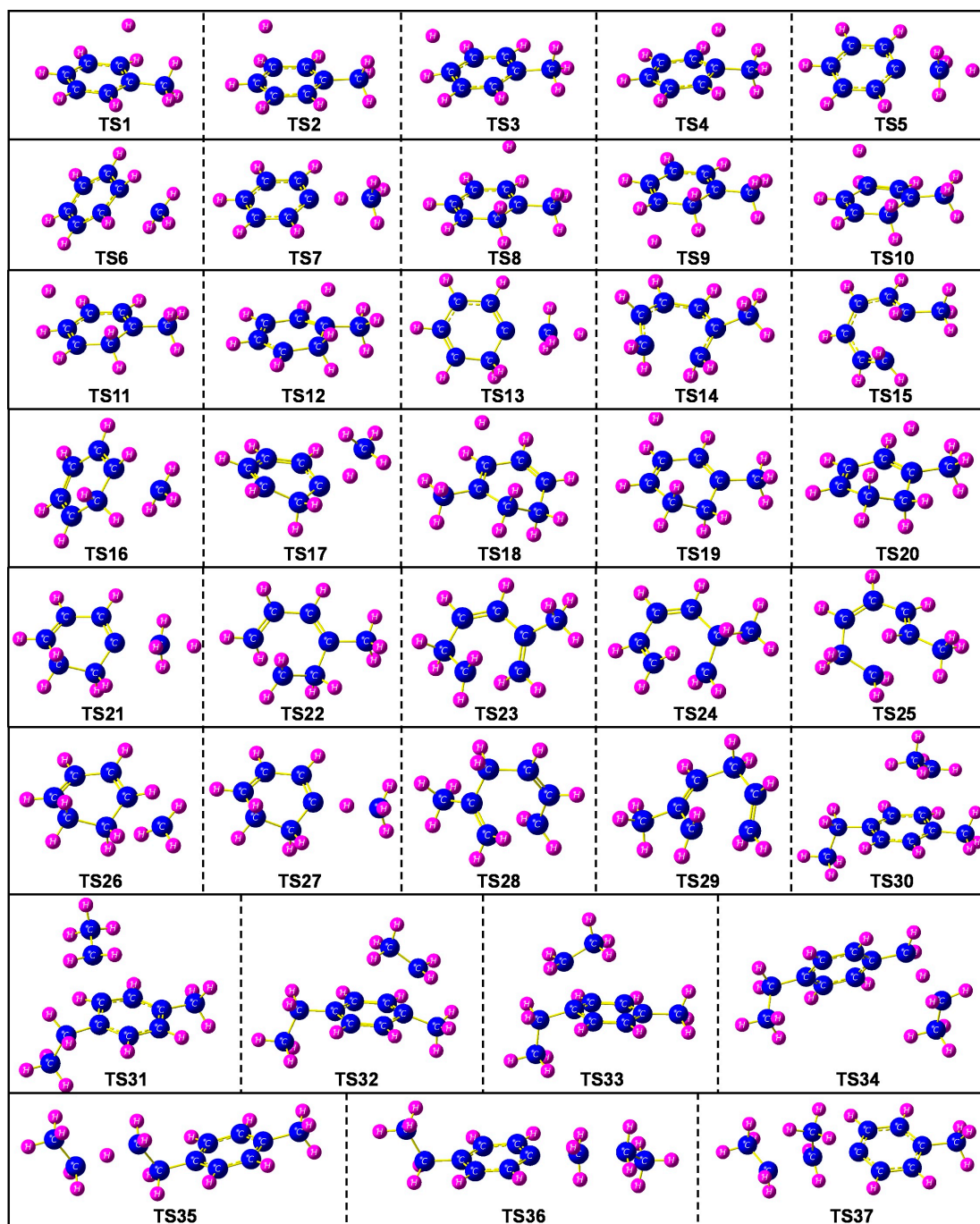
† These authors contributed equally to this work.



**Figure S1.** Energy profiles of hydrogenation and hydrocracking by the fourth H atom for third-generation hydrogenated product.



**Figure S2.** Energy profiles of hydrogenation by the fifth H (a) atom and sixth H (b) atom for fourth-generation and fifth-generation hydrogenated product.

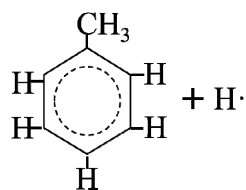


**Figure S3.** The structures of transition state for the model compound hydrogenation in the energy profiles.

**Table S1.** The bond length of transition states for the model compound hydrogenation in the energy profiles.

<b>Transition State</b>	<b>C... H (Å)</b>	<b>C... C (Å)</b>
TS1	1.881	/
TS2	1.843	/
TS3	1.847	/
TS4	1.806	/
TS5	1.419	1.873
TS6	/	2.181
TS7	1.382, 1.300	/
TS8	2.009	/
TS9	1.786	/
TS10	1.606	/
TS11	1.970	/
TS12	1.746	/
TS13	1.426	1.866
TS14	/	2.278
TS15	/	2.271
TS16	/	2.184
TS17	1.278, 1.350	/
TS18	2.097	/
TS19	2.039	/
TS20	2.225	/
TS21	1.422	1.871
TS22	/	2.398
TS23	/	2.390
TS24	/	2.402
TS25	/	2.356
TS26	/	2.402
TS27	1.363, 1.319	/
TS28	/	2.219
TS29	/	2.232
TS30	/	2.176
TS31	/	2.169
TS32	/	2.176
TS33	/	2.177
TS34	1.297, 1.430	/
TS35	1.351, 1.357	/
TS36	/	1.992, 1.957
TS37	/	1.993, 2.032
TS38	1.642	/
TS39	1.678	/
TS40	1.924	/
TS41	/	2.155
TS42	/	2.262
TS43	/	2.263
TS44	/	2.241
TS45	/	2.269
TS46	/	2.314
TS47	/	2.397

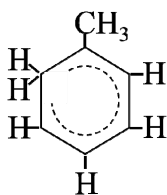
**Table S2.** The Cartesian coordinates of intervening species (reactants, transition states and products) in the energy profiles.



C	-1.93476500	0.00076900	0.01250700
C	-1.23018300	1.20711100	-0.02362000
C	0.16505300	1.20344200	-0.08928200
C	0.88413000	-0.00162200	-0.12248100
C	0.16339500	-1.20541500	-0.08096000
C	-1.23183600	-1.20676600	-0.01524200
H	-3.01531600	0.00171800	0.06615400
H	-1.76466400	2.14791400	0.00355200
H	0.70349300	2.14334100	-0.11227800
H	0.70061500	-2.14615600	-0.09714500
H	-1.76758100	-2.14662500	0.01876200
C	2.39307000	-0.00296300	-0.22344600
H	2.82309400	0.89832800	0.21624000
H	2.82639500	-0.86417300	0.28754800
H	2.72039800	-0.04449100	-1.26682900
H	1.52038100	0.04280800	4.13914400

**TS1:**

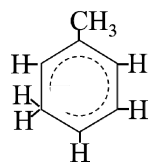
C	1.91839400	0.00861300	-0.02674200
C	1.20737100	-1.18542500	-0.10211500
C	-0.20393100	-1.17610600	-0.05368600
C	-0.91027400	0.05672400	-0.04515100
C	-0.17317800	1.24092100	0.02974200
C	1.22705500	1.22362200	0.04820600
H	3.00009600	-0.00083200	-0.03850300
H	1.73064500	-2.12975500	-0.17118700
H	-0.74619600	-2.08986400	-0.26143800
H	-0.69629300	2.18858700	0.06351500
H	1.77440600	2.15533400	0.10446400
C	-2.41819000	0.06132900	-0.05943200
H	-2.81676400	-0.39221600	0.85337400
H	-2.81309400	1.07503100	-0.12818300
H	-2.81385100	-0.51044500	-0.90256800
H	-0.50243000	-1.67391200	1.73559600



C	-1.92974300	0.03432500	0.00009100
C	-1.28121400	-1.16931500	0.00020600
C	0.22070200	-1.26355200	-0.00021500
C	0.92982800	0.07301300	-0.00005000
C	0.20946400	1.24102000	-0.00019500
C	-1.20947500	1.25812500	-0.00006300
H	-3.01269900	0.06007000	0.00000300
H	-1.84147600	-2.09651400	0.00005600
H	0.56232400	-1.85904700	0.86556700
H	0.74257600	2.18534600	-0.00050300
H	-1.73864800	2.20090900	0.00072600
C	2.43188800	0.04231600	0.00018200
H	2.82076400	-0.48815400	-0.87709800
H	2.85610800	1.04688500	-0.00070700
H	2.82049500	-0.48640500	0.87866500
H	0.56185600	-1.85867800	-0.86643400

**TS2:**

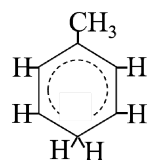
C	1.87939500	0.11537600	-0.08339900
C	1.22444200	-1.13785400	-0.07260700
C	-0.19024400	-1.17800500	-0.10379200
C	-0.94675500	-0.00864000	-0.01568400
C	-0.26965300	1.22496400	0.04659100
C	1.12778300	1.28352200	0.00171800
H	2.95905800	0.15793600	-0.12707300
H	1.78414600	-2.03461100	-0.30198600
H	-0.69026700	-2.13626500	-0.16513600
H	-0.84231400	2.14209300	0.11100400
H	1.62435400	2.24497400	0.02050500
C	-2.45825600	-0.05503900	0.01314000
H	-2.83060000	-1.04240100	-0.26137200
H	-2.84098000	0.17517800	1.01148400
H	-2.89415800	0.67093500	-0.67645500
H	1.53048900	-1.64378200	1.67323400



C	1.90202300	0.14891600	0.00001500
C	1.27337200	-1.21725900	-0.00000900
C	-0.23172200	-1.18608600	-0.00003000
C	-0.95603000	-0.02356000	-0.00001700
C	-0.27513700	1.23447900	-0.00002100
C	1.14151700	1.28669500	0.00001300
H	2.98349000	0.20842200	0.00007000
H	1.63663200	-1.79826400	-0.86567000
H	-0.74610900	-2.14060400	0.00000200
H	-0.84919700	2.15199600	-0.00015300
H	1.62866400	2.25459400	0.00004300
C	-2.46958800	-0.03794200	0.00002900
H	-2.85811800	-1.05659900	-0.00002100
H	-2.86922800	0.47355700	0.87983500
H	-2.86930200	0.47366600	-0.87968100
H	1.63656700	-1.79823200	0.86569000

**TS3:**

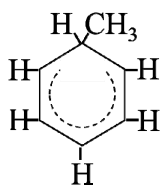
C	1.86933700	0.00000000	-0.03716000
C	1.14738600	-1.21608100	-0.08446200
C	-0.24205600	-1.20789000	-0.04542000
C	-0.96354700	0.00000400	-0.00952300
C	-0.24205400	1.20789400	-0.04541600
C	1.14739100	1.21608200	-0.08446100
H	2.93256400	-0.00000300	-0.23382100
H	1.68376000	-2.15476300	-0.12269300
H	-0.78314600	-2.14623400	-0.05618400
H	-0.78314000	2.14624000	-0.05617500
H	1.68376600	2.15476200	-0.12269100
C	-2.47210100	-0.00000100	0.06911000
H	-2.89730600	-0.88246600	-0.41165700
H	-2.81379400	-0.00027500	1.10899800
H	-2.89727600	0.88273100	-0.41118800
H	2.40843700	-0.00003700	1.72940100



C	-1.95895100	-0.00393100	0.01133800
C	-1.13043000	1.25319300	-0.00038100
C	0.23684300	1.22378600	-0.01016900
C	0.97658200	0.00589900	-0.01231800
C	0.24150400	-1.21975700	-0.01021100
C	-1.12285000	-1.25623900	-0.00044300
H	-2.65510700	-0.00659300	-0.84508000
H	-1.65520100	2.20096700	-0.00273000
H	0.78627100	2.15888800	-0.01847800
H	0.79624200	-2.15194700	-0.01867400
H	-1.64306000	-2.20665600	-0.00290300
C	2.48193700	0.00064900	0.01167300
H	2.88915300	0.97399000	-0.26664500
H	2.87201700	-0.24128100	1.00788700
H	2.89360200	-0.74236900	-0.67703400
H	-2.63172200	-0.00660300	0.88672200

**TS4:**

C	-1.92635300	0.00000000	-0.03503300
C	-1.22173700	1.21105700	-0.03259500
C	0.16808500	1.21530000	-0.00083400
C	0.90326900	0.00000000	0.08855700
C	0.16808500	-1.21530000	-0.00083400
C	-1.22173700	-1.21105700	-0.03259500
H	-3.00771900	0.00000000	-0.05837600
H	-1.76114900	2.14873300	-0.06527300
H	0.70856400	2.15341800	-0.00579400
H	0.70856300	-2.15341800	-0.00579400
H	-1.76114900	-2.14873300	-0.06527300
C	2.40407000	0.00000000	-0.15474500
H	2.87693700	0.88157600	0.27760700
H	2.87693700	-0.88157700	0.27760600
H	2.60998500	0.00000100	-1.22898200
H	1.10694200	-0.00000100	1.88275600

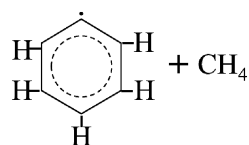


C	-1.86253400	0.00000000	0.23650300
C	-1.16775200	-1.22626200	0.06126900
C	0.16001700	-1.25388200	-0.26738500
C	0.98255500	0.00000000	-0.44677900
C	0.16001800	1.25388100	-0.26738600
C	-1.16775100	1.22626300	0.06126800
H	-2.91179600	0.00000100	0.49652900
H	-1.70573800	-2.15784500	0.18998200
H	0.67134100	-2.20066100	-0.39929600
H	0.67134200	2.20066100	-0.39929200
H	-1.70573800	2.15784600	0.18998000
C	2.22713300	0.00000000	0.49331300
H	2.84187400	-0.88503900	0.31604900
H	2.84187200	0.88504100	0.31605000
H	1.91341400	-0.00000100	1.53763000
H	1.39331700	-0.00000100	-1.47245700

**TS5:**

C	-2.01814300	0.00001000	0.01053300
C	-1.31894500	-1.21116000	0.00340000
C	0.08233300	-1.21272600	-0.01120700
C	0.76479500	-0.00001100	-0.01950100
C	0.08235100	1.21271400	-0.01120800
C	-1.31892600	1.21116900	0.00340200
H	-3.09997800	0.00001800	0.02105000
H	-1.85916200	-2.14954300	0.00809800
H	0.62335700	-2.15189100	-0.01628500
H	0.62338900	2.15187100	-0.01629500
H	-1.85912900	2.14956100	0.00810200
C	2.63786800	0.00000000	0.01100800
H	2.69480200	-0.93732200	-0.53010000
H	2.69474100	0.93740200	-0.52996200
H	2.65738700	-0.00007400	1.09466600
H	4.05659900	-0.00000400	0.04217000

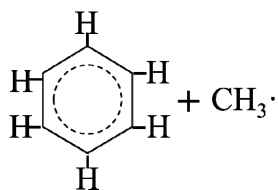




C	-2.44033000	-0.00081500	-0.04367700
C	-1.74758600	-1.21660600	-0.01687600
C	-0.34193500	-1.22676500	0.03771400
C	0.28856400	0.00081700	0.06206900
C	-0.34341900	1.22764000	0.03766800
C	-1.74905000	1.21581200	-0.01695000
H	-3.52125300	-0.00146500	-0.08548400
H	-2.28925700	-2.15348500	-0.03787700
H	0.20698000	-2.15816300	0.05900100
H	0.20439500	2.15968700	0.05902500
H	-2.29184700	2.15203800	-0.03797500
C	4.56921300	0.00008700	-0.03156300
H	4.91799200	-0.88280700	-0.56553900
H	4.92318900	0.89494900	-0.54166500
H	4.95681700	-0.01470100	0.98615000
H	3.48024400	0.00293200	-0.00594000

**TS6:**

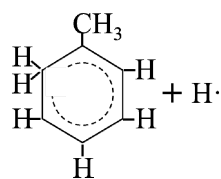
C	1.13025900	1.21509200	0.12255000
C	-0.10328600	1.22359000	-0.51413500
C	-0.80095100	0.00007800	-0.75426200
C	-0.10343700	-1.22351500	-0.51419800
C	1.13011000	-1.21517600	0.12250400
C	1.74746100	-0.00008800	0.46421300
H	1.63093600	2.15022200	0.33886600
H	-0.56497100	2.16069300	-0.79685500
H	-1.61543800	0.00013400	-1.46691700
H	-0.56524000	-2.16055900	-0.79693600
H	1.63067400	-2.15037300	0.33879100
H	2.71058300	-0.00015800	0.95659400
C	-2.30919800	0.00002300	0.82077000
H	-1.67388700	-0.00044100	1.69643200
H	-2.84896400	0.91899500	0.62301100
H	-2.84943600	-0.91853300	0.62235000



C	2.37033000	0.00011500	0.03110600
C	1.67115800	1.21085200	0.01203400
C	0.27341600	1.21042600	-0.02616800
C	-0.42633300	-0.00011300	-0.04525100
C	0.27361300	-1.21053800	-0.02616100
C	1.67135600	-1.21073700	0.01204100
H	3.45211400	0.00020300	0.06051600
H	2.21196200	2.14813600	0.02682900
H	-0.26759100	2.14760600	-0.04086200
H	-0.26724100	-2.14780600	-0.04085100
H	2.21231200	-2.14793200	0.02683900
C	-4.53270800	-0.00000500	0.03260000
H	-4.59851200	0.93596700	-0.50143300
H	-4.59870600	-0.93341600	-0.50587200
H	-4.44062400	-0.00256300	1.10825700
H	-1.50871600	-0.00020100	-0.07462800

TS7:

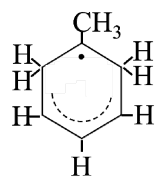
C	-2.13200100	0.00053500	-0.00103400
C	-1.43538500	1.21370000	-0.00031700
C	-0.03297900	1.21745700	0.00102200
C	0.63624600	-0.00053700	0.00167000
C	-0.03394800	-1.21804900	0.00101900
C	-1.43631400	-1.21320400	-0.00031100
H	-3.21401100	0.00095400	-0.00216400
H	-1.97736200	2.15090100	-0.00088000
H	0.51118700	2.15347100	0.00172700
H	0.50959500	-2.15444400	0.00168700
H	-1.97903600	-2.14997600	-0.00086400
C	3.31821600	-0.00034200	-0.00077000
H	3.61623700	-0.20186500	1.02459800
H	3.60727300	-0.78607800	-0.69377300
H	3.60464300	0.99127000	-0.34152000
H	2.01846800	-0.00159200	0.00351000



C	-1.87245200	0.04089800	-0.17026400
C	-1.22702800	-1.16558300	-0.13807900
C	0.27116900	-1.26314900	-0.03893600
C	0.98211600	0.07198500	0.00575400
C	0.26587600	1.24181800	-0.03455000
C	-1.15028900	1.26288800	-0.12084400
H	-2.95244400	0.06940700	-0.24592400
H	-1.78848800	-2.09098800	-0.17983300
H	0.55261500	-1.85674800	0.84964100
H	0.80023500	2.18474000	0.00048700
H	-1.67651100	2.20680600	-0.14897600
C	2.48126400	0.03740200	0.09694600
H	2.92120600	-0.49127000	-0.75692600
H	2.90725100	1.04081600	0.12518300
H	2.81455600	-0.49504800	0.99561600
H	0.66770400	-1.86141900	-0.87862100
H	-2.75005200	-0.06386200	2.63919900

**TS8:**

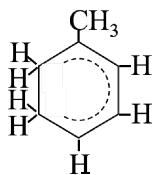
C	-1.93791500	0.01843000	-0.05244000
C	-1.29963200	-1.18928100	0.02686700
C	0.20122900	-1.29749900	0.07247500
C	0.92585100	0.02230400	-0.05411000
C	0.21312300	1.21353200	-0.05875600
C	-1.21299400	1.23494900	-0.09768400
H	-3.02004800	0.05062500	-0.08434900
H	-1.86883400	-2.11013600	0.06268800
H	0.51284500	-1.79470200	1.01016500
H	0.75129400	2.13975100	-0.21936100
H	-1.73309300	2.18078600	-0.15029500
C	2.42458200	-0.01794300	-0.08647100
H	2.78993300	-0.63834700	-0.91252700
H	2.85409800	0.97798500	-0.19735900
H	2.82995800	-0.45578900	0.83421200
H	0.55568700	-1.98741600	-0.71166400
H	0.44269300	1.73029000	1.86921000



C	-1.93594100	0.00001300	-0.08027400
C	-1.27540400	-1.22001400	-0.02087000
C	0.21965600	-1.30844700	0.10876600
C	0.94023600	0.00000200	-0.07007400
C	0.21973100	1.30842100	0.10875200
C	-1.27542200	1.22003300	-0.02083900
H	-3.01647700	-0.00001800	-0.17134700
H	-1.83685400	-2.14552400	-0.05429400
H	0.47167100	-1.75016300	1.09625000
H	0.61401300	2.04460400	-0.60835100
H	-1.83677200	2.14559700	-0.05428600
C	2.43737300	-0.00001400	-0.09425400
H	2.83337300	-0.88425300	-0.60155900
H	2.83336900	0.88413300	-0.60173400
H	2.87056000	0.00010500	0.92014500
H	0.61403000	-2.04462400	-0.60829900
H	0.47170900	1.75017200	1.09622400

**TS9:**

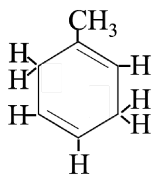
C	1.89608300	0.13111000	-0.11151900
C	1.30170800	-1.10096000	-0.04677000
C	-0.20827000	-1.24508100	-0.08107400
C	-0.95964100	0.05684800	-0.01968800
C	-0.27219500	1.27444200	0.04965900
C	1.11366100	1.35052500	0.01326700
H	2.97275300	0.20634200	-0.19554100
H	1.50769800	-1.55334700	1.66856300
H	-0.49953700	-1.80049500	-0.98887400
H	-0.85100300	2.18806200	0.12665700
H	1.61647900	2.30608000	0.05818400
C	-2.45735900	-0.01872200	0.00219800
H	-2.81669900	-0.57947900	0.87436200
H	-2.91306100	0.97155600	0.03164400
H	-2.84655700	-0.54114100	-0.88006800
H	-0.53694200	-1.90054100	0.74510300
H	1.88295500	-1.98601400	-0.27646400



C	1.91573800	0.14913700	0.01993900
C	1.24005400	-1.17777200	-0.25242700
C	-0.20667500	-1.20617400	0.28423100
C	-0.96345000	0.08612800	0.00973900
C	-0.27384100	1.24259000	-0.05525300
C	1.18554200	1.27524400	0.08945200
H	2.99605000	0.17679500	0.09638100
H	1.81154800	-2.00141100	0.18124800
H	-0.74309100	-2.05759100	-0.14250900
H	-0.79692000	2.18166700	-0.19590200
H	1.66403300	2.23585300	0.23751200
C	-2.46252400	0.00727900	-0.08019600
H	-2.88730600	-0.44567400	0.82308500
H	-2.91190000	0.99316300	-0.20549400
H	-2.77928400	-0.61883200	-0.92088000
H	-0.19217300	-1.36976500	1.37206300
H	1.22997300	-1.35279600	-1.33841500

**TS10:**

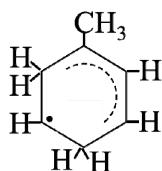
C	1.89688600	0.08309000	0.02140500
C	1.21686300	1.23934000	-0.00539200
C	-0.28882500	1.29665800	-0.06862500
C	-0.96890600	-0.03677700	0.02805500
C	-0.16627600	-1.24933500	-0.22034100
C	1.20394400	-1.22408400	-0.02475900
H	2.97708000	0.07744200	0.08835100
H	1.74555100	2.18539400	0.00549300
H	-0.67069000	1.96700000	0.71694400
H	-0.67732600	-2.18285300	-0.42155800
H	1.78948200	-2.09322500	-0.30131500
C	-2.45884500	-0.09850200	0.10585500
H	-2.86140400	0.66596900	0.77753000
H	-2.93256400	0.07274800	-0.87620100
H	-2.80642400	-1.07211700	0.45763600
H	-0.58158800	1.81566500	-1.00839200
H	1.40883500	-1.49837200	1.54431800



C	-1.91109000	0.11409600	-0.00001700
C	-1.20377400	1.24584200	-0.00005300
C	0.30398200	1.28524400	0.00006900
C	0.95465500	-0.08513100	0.00000500
C	0.22843600	-1.21008800	0.00002200
C	-1.27961100	-1.25501400	0.00002500
H	-2.99527800	0.15317500	-0.00005600
H	-1.71499400	2.20294200	-0.00012100
H	0.66074100	1.85663000	-0.86922200
H	0.73793600	-2.16916800	-0.00000800
H	-1.63476700	-1.82637100	0.86931200
C	2.46348300	-0.09314200	-0.00004400
H	2.86191300	0.42513800	0.87871800
H	2.86022500	-1.10890200	-0.00029700
H	2.86187300	0.42557000	-0.87856600
H	0.66059300	1.85646400	0.86953700
H	-1.63472800	-1.82632400	-0.86933500

**TS11:**

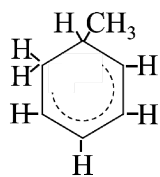
C	-1.89061100	0.03266100	-0.07037800
C	-1.22321300	-1.18095700	-0.11789700
C	0.27212700	-1.26578000	-0.00200000
C	0.97679900	0.07409700	-0.00084300
C	0.25343900	1.24090600	-0.03859800
C	-1.16192600	1.25982800	-0.07700300
H	-2.95969700	0.05624300	-0.23599900
H	-1.78026400	-2.10688000	-0.18654400
H	0.54725900	-1.82058800	0.91463400
H	0.78542200	2.18564500	-0.04102400
H	-1.69281300	2.20094700	-0.09572200
C	2.47780100	0.04821900	0.04817200
H	2.89607400	-0.49142200	-0.80958300
H	2.89913100	1.05383800	0.04987500
H	2.83847200	-0.46901600	0.94508700
H	0.67814700	-1.89526500	-0.81161200
H	-2.43822000	0.03265100	1.82216900



C	-1.98739300	0.03251800	0.05822800
C	-1.19214200	-1.22364500	-0.13079000
C	0.29208200	-1.27389000	0.07062700
C	0.98431900	0.06722700	0.00087000
C	0.23496400	1.24217200	-0.03377900
C	-1.15166500	1.28203900	-0.00427700
H	-2.79370600	0.08149400	-0.68823600
H	-1.72212700	-2.15393800	-0.29957600
H	0.53497200	-1.74308900	1.04673500
H	0.77333400	2.18374700	-0.07965600
H	-1.66554100	2.23525600	-0.01635100
C	2.48536800	0.06855400	-0.00926100
H	2.88310800	-0.46257000	-0.88297200
H	2.88772700	1.08228400	-0.02456300
H	2.89497400	-0.44042900	0.87214600
H	0.74434700	-1.95939800	-0.66220100
H	-2.53027900	0.00678900	1.02497400

**TS12:**

C	-1.95592500	0.04062700	-0.03018300
C	-1.28475200	-1.18183700	-0.05390700
C	0.20808100	-1.26920400	0.00240500
C	0.91970800	0.07876400	0.10137300
C	0.19243200	1.23919800	-0.03356600
C	-1.26270700	1.24422000	-0.01364600
H	-3.03893200	0.04787200	-0.03526100
H	-1.84387900	-2.10879500	-0.07903900
H	0.52160900	-1.90517700	0.84847000
H	0.71427700	2.18766900	-0.07961000
H	-1.78958700	2.18799500	-0.01146200
C	2.41620700	0.05264100	-0.13660800
H	2.62688500	-0.19377500	-1.18300300
H	2.87189500	1.01851800	0.08185500
H	2.90525000	-0.70049300	0.48387900
H	0.59427200	-1.80096100	-0.88407200
H	1.03994200	0.04069100	1.84303700

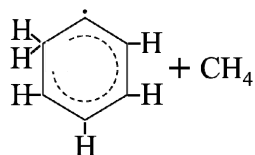


C	1.93266800	0.03670900	-0.04108400
C	1.31814700	-1.15848700	-0.03454500
C	-0.17938900	-1.24769800	0.17541500
C	-0.92838300	-0.00663100	-0.36589400
C	-0.18052500	1.26671700	-0.00582900
C	1.15787900	1.27347600	0.11935800
H	3.00834400	0.10846900	-0.14433500
H	1.88531800	-2.07806200	-0.11707400
H	-0.58356300	-2.14935700	-0.29046800
H	-0.75290000	2.18359200	0.08523400
H	1.69021600	2.19392800	0.32610000
C	-2.39344200	0.01757700	0.10103200
H	-2.45243500	0.07763800	1.19067300
H	-2.92440200	0.87820500	-0.31247100
H	-2.92086600	-0.88455200	-0.21660800
H	-0.38045400	-1.34380800	1.25418800
H	-0.93099100	-0.07603500	-1.46596300

**TS13:**

C	2.04017500	0.03638000	-0.00003800
C	1.39772900	-1.17061700	-0.00002300
C	-0.11103200	-1.27349700	0.00004600
C	-0.78089800	0.06672000	0.00005400
C	-0.09814900	1.24749100	0.00003700
C	1.32379100	1.26595200	0.00000000
H	3.12313900	0.06264900	-0.00008300
H	1.96203900	-2.09567700	-0.00005000
H	-0.44909700	-1.86761000	-0.86724500
H	-0.63712800	2.18945800	0.00004700
H	1.85584500	2.20748100	-0.00000900
C	-2.64651700	0.03635100	-0.00005100
H	-2.68722900	-0.50903100	0.93652500
H	-2.70991300	1.11833700	-0.00034900
H	-2.68718100	-0.50952000	-0.93635300
H	-0.44900800	-1.86757200	0.86739900
H	-4.07206400	0.01880300	-0.00002700

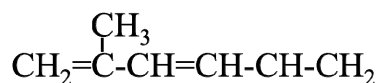




C	2.45418600	0.03203900	0.01812600
C	1.81911100	-1.16548800	-0.07589800
C	0.33559800	-1.21384200	0.05059700
C	-0.46845100	0.06269700	0.03454700
C	0.30739600	1.24753900	-0.09897200
C	1.68619600	1.24355700	0.06608700
H	3.53373200	0.09867900	-0.00284000
H	2.37276500	-2.08044500	-0.25637700
H	-0.10481500	-1.91254300	-0.67712100
H	-0.20340100	2.19477200	-0.22295700
H	2.21864700	2.17994800	0.20046200
C	-4.46758000	-0.00210800	-0.00142100
H	-4.88847600	0.68836100	0.72948200
H	-4.80465800	0.28056200	-0.99885600
H	-3.37891800	0.03508000	0.04385200
H	0.06653600	-1.69781800	1.00517000
H	-4.81015500	-1.01295700	0.22077900

**TS14:**

C	-1.86105300	0.31060900	0.36180400
C	-1.74575400	-1.07284600	0.16537700
C	0.44341300	-1.31049500	-0.41797700
C	1.05157900	-0.06304200	-0.19796000
C	0.35213200	1.13364100	-0.41504000
C	-1.02514400	1.29770700	-0.17256900
H	-2.55359900	0.65233100	1.12950600
H	-1.81411700	-1.48156600	-0.82559100
H	0.90233000	-2.19980100	0.00526000
H	0.92950700	2.05090500	-0.47541400
H	-1.36717000	2.32531000	-0.09992300
C	2.41654900	0.00269800	0.46913100
H	3.13107800	-0.68669300	0.01693200
H	2.83277500	1.00942900	0.41251400
H	2.33860900	-0.25396500	1.53146600
H	-0.02144600	-1.47541100	-1.37313500
H	-2.16829600	-1.73017200	0.92178900



C	-2.08986300	0.08003900	-0.05027600
C	-1.99656400	-1.02825700	0.69489000
C	1.04536400	-1.11053700	-1.01142100
C	1.17568900	-0.05656100	-0.19377900
C	0.25430400	1.10614900	-0.21884500
C	-1.09243700	1.15331100	-0.19723600
H	-3.02682300	0.26913400	-0.56896500
H	-1.10858200	-1.26898200	1.26337100
H	1.75569600	-1.92806000	-0.99471900
H	0.76665600	2.06581700	-0.26028100
H	-1.53397300	2.14200600	-0.29786000
C	2.33946500	0.07227200	0.76883100
H	3.01302300	-0.78169000	0.69667700
H	2.91833100	0.97887200	0.56560600
H	1.98927200	0.14651400	1.80228900
H	0.22697300	-1.18950900	-1.71353300
H	-2.81631000	-1.73259800	0.75442700

**TS15:**

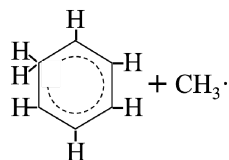
C	1.90064600	-0.33757800	0.00385000
C	1.54814800	0.98758200	-0.24999700
C	0.35955000	1.59905600	0.18029000
C	-1.15961100	-0.08095100	0.34719600
C	-0.41792500	-1.22402800	-0.01000500
C	0.96138100	-1.38473900	0.11698700
H	2.92233500	-0.63809600	-0.20326900
H	2.17476600	1.52577700	-0.95872100
H	0.15188600	1.62759100	1.23507700
H	-0.93893100	-2.00017200	-0.57053400
H	1.35747500	-2.38682900	-0.01250800
C	-2.52023700	0.17645500	-0.26510800
H	-2.54028900	-0.08530100	-1.32355700
H	-3.30003100	-0.40483500	0.24129900
H	-2.79741100	1.22781900	-0.17613400
H	0.01769600	2.48687900	-0.34554600
H	-1.07921100	0.23239300	1.37461500



C	1.63919900	-0.87226200	-0.19412800
C	2.00110200	0.54982200	-0.31979200
C	1.60620600	1.56430400	0.46001300
C	-1.44354400	0.11551600	-0.33854100
C	-0.87023600	-0.88580600	0.34526200
C	0.46712500	-1.45932200	0.12891100
H	2.46969500	-1.54694800	-0.38867900
H	2.73220300	0.75891700	-1.09793200
H	0.91019200	1.42582300	1.27666800
H	-1.46702100	-1.39673800	1.09913600
H	0.49692100	-2.54114800	0.23871800
C	-2.83707100	0.62435800	-0.10731700
H	-3.34269500	0.06989100	0.68515300
H	-2.82997400	1.68275100	0.17426500
H	-3.44502600	0.54783800	-1.01428200
H	1.97612500	2.56918700	0.30143500
H	-0.87710000	0.61076000	-1.12092300

**TS16:**

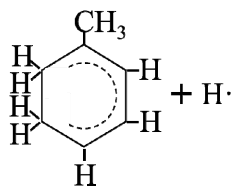
C	-1.74064000	0.01191300	0.49997900
C	-1.09275400	1.22145700	0.18733500
C	0.19560600	1.25304000	-0.57868200
C	0.83537800	-0.11945600	-0.75739900
C	0.07054400	-1.25798800	-0.58314300
C	-1.20906600	-1.20719700	0.12806100
H	-2.67688100	0.04563100	1.04395500
H	-1.53031100	2.16519800	0.48741100
H	0.02079400	1.67627300	-1.58481600
H	0.45681100	-2.22038300	-0.89380200
H	-1.72395800	-2.12992900	0.35783000
C	2.23549200	-0.08346900	0.91805300
H	1.54879600	0.14476500	1.72320600
H	2.64061300	-1.08714700	0.90898200
H	2.92013900	0.70589600	0.62853800
H	0.90071000	1.95534900	-0.11614500
H	1.67592300	-0.16544800	-1.44038000



C	2.38647900	0.01493100	0.00342500
C	1.72109300	-1.18049800	0.00156700
C	0.21664100	-1.25653000	-0.00285700
C	-0.45129600	0.09358400	-0.00480300
C	0.26838100	1.25720700	-0.00280900
C	1.68939900	1.25318500	0.00130700
H	3.46987400	0.02262600	0.00657700
H	2.27083000	-2.11397800	0.00322400
H	-0.12795800	-1.84744800	-0.86936200
H	-0.25354800	2.20667300	-0.00436500
H	2.23652100	2.18554600	0.00283600
C	-4.54155800	0.02058200	0.00356400
H	-4.52219500	0.55410200	0.94189500
H	-4.54095000	0.56613100	-0.92802800
H	-4.59929200	-1.05748600	-0.00281500
H	-0.13308300	-1.84751400	0.86154000
H	-1.53503300	0.11658900	-0.00786800

**TS17:**

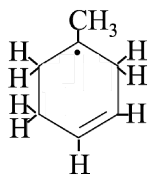
C	1.86055000	0.06075600	-0.49134900
C	1.27648500	-1.14991000	-0.31300000
C	0.06141500	-1.25662500	0.56117500
C	-0.71947000	0.02940200	0.77399800
C	-0.09797400	1.24471800	0.39722500
C	1.21716300	1.26625100	-0.03090600
H	2.78284200	0.15324200	-1.05122700
H	1.67308700	-2.04113400	-0.78484400
H	-0.59162400	-2.07604500	0.25389000
H	-0.64870600	2.17139800	0.51162700
H	1.75553800	2.20380900	-0.09650700
C	-2.71039600	-0.00236100	-0.62635700
H	-3.41729100	-0.79300800	-0.38108200
H	-3.15557000	0.98862000	-0.62631300
H	-2.14425000	-0.20619400	-1.52740400
H	0.38613300	-1.54029300	1.57738400
H	-1.96679000	-0.01377900	0.49976000



C	-1.92812500	0.14770600	-0.05235600
C	-1.25250800	-1.17480000	0.23475900
C	0.18761300	-1.21592400	-0.31697100
C	0.95079500	0.07598300	-0.06678800
C	0.26200700	1.23720500	-0.00703600
C	-1.19669300	1.27211300	-0.14088100
H	-3.00883500	0.17649100	-0.12128000
H	-1.83118600	-2.00573000	-0.17441700
H	0.72588100	-2.06330100	0.11472200
H	0.79012900	2.17592700	0.11353600
H	-1.67372400	2.23211300	-0.29588600
C	2.45168200	-0.00088500	-0.01866800
H	2.84922500	-0.43785900	-0.94202300
H	2.90247500	0.98373600	0.10971700
H	2.79212300	-0.63950200	0.80196800
H	0.16180900	-1.39183200	-1.40282500
H	-1.22648300	-1.32646100	1.32419400
H	0.66995800	0.24802700	2.67993300

**TS18:**

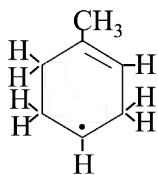
C	1.92330700	0.14933700	-0.03579000
C	1.27471600	-1.20909000	-0.19146800
C	-0.17194800	-1.21923600	0.34792600
C	-0.95281900	0.02405400	-0.03846000
C	-0.28613000	1.20745300	-0.12782800
C	1.17919000	1.26635700	-0.01470500
H	3.00464300	0.20238500	0.00608800
H	1.86128700	-1.97653500	0.31867000
H	-0.69303700	-2.11700800	0.00697300
H	-0.81472000	2.10664700	-0.41890900
H	1.64369800	2.24089700	0.06545300
C	-2.44338900	-0.08994300	-0.16771600
H	-2.88751800	-0.46723900	0.76105400
H	-2.90500500	0.87173700	-0.39287000
H	-2.72157500	-0.79635300	-0.95640100
H	-0.14905200	-1.27674000	1.44660100
H	1.27508000	-1.48522400	-1.25578000
H	-0.75136600	1.92384000	1.78736800



C	1.90699000	0.11896400	-0.08966200
C	1.24830800	-1.23442800	-0.21557500
C	-0.18849200	-1.23003500	0.35825800
C	-0.96486300	-0.01144500	-0.05373400
C	-0.28925800	1.32681500	0.07162800
C	1.22034500	1.25677700	0.05171800
H	2.99123800	0.14762900	-0.12346800
H	1.84813900	-1.99235800	0.29728500
H	-0.71659000	-2.13899600	0.05715600
H	-0.63367100	1.99340000	-0.73237600
H	1.74936500	2.19978700	0.14338600
C	-2.45648300	-0.06237000	-0.16619400
H	-2.95241900	0.04411000	0.81392200
H	-2.84158900	0.74439100	-0.79668600
H	-2.79767800	-1.01184700	-0.58672900
H	-0.11225500	-1.27356400	1.45958400
H	1.21933600	-1.53459000	-1.27026300
H	-0.61316200	1.83637700	0.99955100

**TS19:**

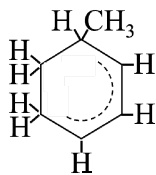
C	-1.88699400	0.00702000	-0.13954200
C	-1.16228700	-1.25225600	0.26775600
C	0.30522100	-1.25207700	-0.21239600
C	0.98875300	0.09453900	-0.02262100
C	0.24953100	1.21996700	-0.02731200
C	-1.21178500	1.18520900	-0.19507600
H	-2.95721300	-0.02755000	-0.29995800
H	-1.67945200	-2.13786300	-0.10684600
H	0.86230100	-2.03311100	0.31170900
H	0.72658500	2.18769900	0.06938600
H	-1.70071400	1.92452300	1.64121400
C	2.48968900	0.09518000	0.07989300
H	2.94265100	-0.40276500	-0.78480600
H	2.89032400	1.10790400	0.13395300
H	2.82740600	-0.45066200	0.96690900
H	0.34804300	-1.51407700	-1.27949600
H	-1.18184400	-1.32786800	1.36551700
H	-1.71085200	2.08827100	-0.52179500



C	-1.90032900	-0.02201200	-0.16282600
C	-1.17400700	-1.25366300	0.27613500
C	0.29388900	-1.25504700	-0.21428900
C	0.97617000	0.08860200	-0.02399800
C	0.27189600	1.22503400	0.07286800
C	-1.23530200	1.31224600	-0.01876400
H	-2.95091200	-0.06655700	-0.42337800
H	-1.68798400	-2.15468000	-0.06625500
H	0.85638900	-2.03068400	0.31584400
H	0.79734900	2.16575500	0.20875100
H	-1.61727900	1.84331100	0.87260400
C	2.48460500	0.06618500	0.02655600
H	2.90186800	-0.38949800	-0.87788300
H	2.90049000	1.07025700	0.11898900
H	2.84389700	-0.52921300	0.87251300
H	0.32592300	-1.53041300	-1.27583000
H	-1.15744800	-1.31194800	1.37821100
H	-1.51381800	1.96560200	-0.85765900

**TS20:**

C	-1.93005400	0.15701600	-0.05183100
C	-1.26703800	-1.17686200	0.20440400
C	0.18710400	-1.20705400	-0.30798000
C	0.94854200	0.07426300	-0.00277200
C	0.25768600	1.24543600	0.03282100
C	-1.19397000	1.28339100	-0.10828900
H	-3.01024300	0.19424500	-0.12531200
H	-1.83896500	-1.98933900	-0.24939700
H	0.71122700	-2.06819600	0.11133700
H	0.78944500	2.18129300	0.15759200
H	-1.67003400	2.24721500	-0.23987300
C	2.45338200	0.01161100	-0.03289800
H	2.80202900	-0.28767900	-1.02854300
H	2.90081500	0.97744500	0.20330300
H	2.83933800	-0.72483800	0.67471900
H	0.19138300	-1.34487200	-1.39973000
H	-1.26952600	-1.36674000	1.28741200
H	0.82061700	-0.14534100	2.20776900

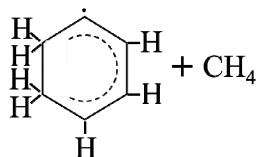


C	-1.92034500	0.18407400	-0.08470300
C	-1.31826900	-1.17546700	0.15537700
C	0.17364700	-1.21165700	-0.23958200
C	0.97055300	-0.03018200	0.36583200
C	0.25404800	1.27396400	0.10141300
C	-1.12013000	1.32099700	-0.11299800
H	-2.99169300	0.26683100	-0.22000500
H	-1.86951400	-1.94078400	-0.39916600
H	0.62429400	-2.15892200	0.06739100
H	0.83608100	2.18860800	0.10287000
H	-1.58638600	2.28282000	-0.29654100
C	2.42278200	-0.00466600	-0.14630200
H	2.44776700	0.13030900	-1.23042400
H	2.98546700	0.81467500	0.30741100
H	2.93825000	-0.93791000	0.09139200
H	0.25245600	-1.15559400	-1.33036900
H	-1.42135700	-1.44787200	1.21654700
H	1.01091900	-0.18453500	1.45666900

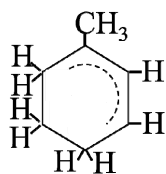
**TS21:**

C	2.02706400	0.14606000	0.01592500
C	1.35039700	-1.18334000	-0.25439400
C	-0.10426000	-1.21640900	0.28167000
C	-0.81410400	0.08572000	0.02086300
C	-0.16076000	1.25065500	-0.05344600
C	1.30727800	1.27909400	0.08291900
H	3.10748300	0.16772800	0.09227800
H	1.92140600	-2.00675000	0.18049400
H	-0.64301100	-2.05679500	-0.16450500
H	-0.68612900	2.18955100	-0.19227500
H	1.79115900	2.23734600	0.23048200
C	-2.68204500	0.01182000	-0.06637600
H	-2.75391200	-0.44779400	0.91335000
H	-2.76081100	1.08811600	-0.16765500
H	-2.65997300	-0.61796000	-0.94837700
H	-0.09509100	-1.39943200	1.36601100
H	1.33900200	-1.35836500	-1.33984900
H	-4.10153900	-0.03724700	-0.13291900





C	2.44009200	0.13338400	0.05074800
C	1.76417000	-1.19430700	-0.23788900
C	0.27565700	-1.22616000	0.23638300
C	-0.35048300	0.09863400	-0.03445800
C	0.26740200	1.27258100	-0.09114500
C	1.74064700	1.28048400	0.08631800
H	3.51747100	0.14022700	0.16404200
H	2.30601000	-2.01976900	0.22848400
H	-0.24920800	-2.04233000	-0.26321800
H	-0.25387900	2.20945100	-0.24029600
H	2.23104300	2.23326200	0.24378100
C	-4.63960000	0.00991800	-0.01848200
H	-4.96749000	-0.23492200	0.99092800
H	-5.06096900	0.97003500	-0.31329000
H	-3.55217500	0.06700300	-0.04391000
H	0.22581100	-1.43259300	1.31314200
H	1.79600700	-1.37572200	-1.32084800
H	-4.97992800	-0.76185100	-0.70766800

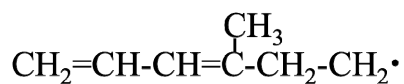


C	1.93024400	0.09141200	0.18623500
C	1.19297000	-1.16020600	-0.33442200
C	-0.24913300	-1.23611400	0.20877400
C	-1.00383700	0.06190000	0.01894700
C	-0.29064900	1.25754100	-0.08051000
C	1.09491800	1.33157200	0.00321500
H	2.89228300	0.19881700	-0.32360900
H	1.74482200	-2.06512500	-0.06937300
H	-0.78729400	-2.05594100	-0.27890900
H	-0.85124900	2.17718000	-0.21671300
H	1.59040400	2.29329500	-0.04719700
C	-2.50336000	0.01118800	-0.01738100
H	-2.91322300	-0.43139800	0.89929000
H	-2.93984500	1.00480000	-0.12987700
H	-2.86535400	-0.61043300	-0.84555500
H	-0.22446300	-1.49366000	1.27872600

H	1.15436800	-1.11541800	-1.42689000
H	2.17263100	-0.04587400	1.25095300

**TS22:**

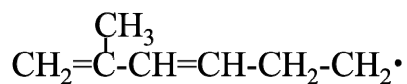
C	-2.03659800	-0.32790900	0.49829600
C	-0.93098200	1.57498200	-0.45358700
C	0.41397100	1.28132600	0.15533100
C	0.94588300	-0.14750200	0.02997500
C	0.16767800	-1.24241000	-0.15584700
C	-1.28273700	-1.24020400	-0.18216200
H	-3.10767600	-0.26821400	0.35063500
H	-1.53062800	2.37839700	-0.04312700
H	1.16671800	1.93836100	-0.30868700
H	0.66443800	-2.18878400	-0.35215800
H	-1.76939000	-1.92358300	-0.87216100
C	2.45058700	-0.26172500	0.08103200
H	2.84586200	0.16624600	1.00919800
H	2.77920700	-1.29975000	0.02699100
H	2.92190700	0.28859400	-0.74066200
H	0.41204500	1.57065700	1.21454900
H	-1.09114700	1.34305700	-1.49860100
H	-1.65815300	0.17566400	1.37579200



C	-2.37247000	0.58366200	-0.13187300
C	1.05694200	1.91613700	-0.40252900
C	0.76506200	0.88601000	0.64906800
C	0.64122100	-0.52767000	0.10944400
C	-0.53299900	-1.15315100	-0.11859600
C	-1.90237500	-0.65754500	0.06719100
H	-3.41481600	0.81818100	0.04264000
H	1.47666100	2.87642000	-0.13076300
H	1.56439100	0.90753400	1.40176300
H	-0.47837800	-2.18772700	-0.44933400
H	-2.61384800	-1.42124800	0.37407500
C	1.95547400	-1.22752300	-0.14890000
H	2.53850800	-1.32120400	0.77363700
H	1.81017200	-2.22605200	-0.56140400
H	2.57029700	-0.65528500	-0.85050500
H	-0.15360500	1.15032000	1.19259300
H	0.78887400	1.74783800	-1.43725000
H	-1.75338600	1.39169900	-0.49828300

TS23:

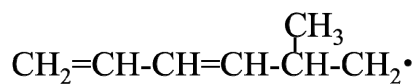
C	-1.99174600	0.08097300	0.06976300
C	-1.38142900	-1.19843400	0.57791700
C	0.55965400	-1.11412200	-0.81438300
C	1.08947700	0.01152700	-0.24430800
C	0.29218500	1.23564200	-0.18783900
C	-1.05350200	1.26841600	-0.08204400
H	-2.79653100	0.39599300	0.75195800
H	-1.80352200	-2.14613000	0.26668000
H	1.07977500	-2.06300200	-0.76063300
H	0.83138300	2.17951800	-0.17433900
H	-1.54077200	2.23840400	-0.05890200
C	2.41123600	0.00170000	0.48725200
H	2.93948500	-0.94209300	0.35022800
H	3.06147300	0.80422100	0.12371600
H	2.28078700	0.16684400	1.56225200
H	-0.22652200	-1.05184800	-1.55176500
H	-0.88407200	-1.19023500	1.53957900
H	-2.49674000	-0.10587900	-0.88691400



C	-2.06406100	0.06409000	-0.17376200
C	-1.83183000	-1.01483000	0.83933900
C	0.92342400	-1.16967300	-0.90549800
C	1.18117600	-0.05951800	-0.19600200
C	0.29289800	1.12355700	-0.17440800
C	-1.04980500	1.19412800	-0.18211000
H	-3.05455200	0.51626700	-0.00451200
H	-2.26925900	-1.99608900	0.71064300
H	1.60655600	-2.00996400	-0.90296600
H	0.82461400	2.07164100	-0.12391500
H	-1.48043200	2.19104200	-0.18331000
C	2.45244900	0.08024500	0.61747100
H	3.08699600	-0.80068400	0.52244100
H	3.03124600	0.95126000	0.29436000
H	2.22643300	0.22564400	1.67782300
H	0.03959600	-1.27079000	-1.51845500
H	-1.29316000	-0.80725400	1.75327000
H	-2.14354700	-0.37905300	-1.17556400

TS24:

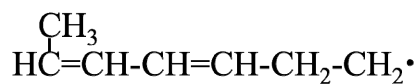
C	1.97985400	0.22791700	0.25107200
C	1.82368700	-0.96995500	-0.38544800
C	-0.41961800	-1.32337800	0.39566000
C	-1.03836200	-0.15597000	-0.33850800
C	-0.27661100	1.15732600	-0.19282600
C	1.03438700	1.31888700	0.09830100
H	2.75920700	0.33980800	0.99890200
H	2.45771500	-1.81519500	-0.14838200
H	-0.60537900	-2.32773400	0.03269600
H	-0.88866100	2.04903300	-0.29271400
H	1.39695900	2.32545100	0.28429200
C	-2.51101000	0.04729000	0.11903000
H	-2.55034400	0.30345000	1.17966500
H	-2.98193500	0.85633700	-0.44607700
H	-3.09487200	-0.86089600	-0.03612300
H	-0.23361900	-1.22345800	1.45820800
H	1.26592100	-1.04932600	-1.30697200
H	-1.07895900	-0.41016900	-1.40717800



C	2.14352600	-0.29397400	0.22028100
C	2.20646700	1.03015600	0.42400600
C	-1.46123800	1.26944800	-0.78822000
C	-1.03468000	0.19945700	0.18083100
C	-0.21260000	-0.84638100	-0.55911600
C	1.11883400	-1.04323300	-0.51908000
H	2.95641300	-0.90494700	0.60643300
H	3.01906800	1.47174900	0.98638900
H	-2.41797900	1.20542400	-1.29307500
H	-0.80325600	-1.51811100	-1.17707800
H	1.50348800	-1.89558300	-1.07363600
C	-2.24693900	-0.46004800	0.87199600
H	-2.89631100	-0.94502000	0.13778200
H	-1.92288400	-1.21661600	1.58840500
H	-2.83835000	0.28744300	1.40362500
H	-0.75704100	2.01696700	-1.13033800
H	1.47645700	1.71718800	0.01732000
H	-0.39983100	0.64896000	0.94997800

TS25:

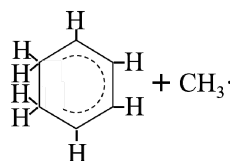
C	-1.83394000	-0.47263600	-0.15519800
C	-1.57510500	1.02452400	-0.20763800
C	-0.32850200	1.49765700	0.49592100
C	1.14510100	-0.12615000	-0.36532800
C	0.50877000	-1.18976200	0.22460200
C	-0.91234900	-1.43583300	0.07531500
H	-2.87269100	-0.76741600	-0.26369100
H	-2.45367500	1.52128800	0.23141100
H	0.16515500	2.39541000	0.14192200
H	1.05519400	-1.80472400	0.93529700
H	-1.25988400	-2.45567500	0.21205100
C	2.58408400	0.23319100	-0.09844600
H	2.95328300	-0.24273500	0.81145000
H	3.23040000	-0.07682900	-0.92642700
H	2.71004900	1.31244900	0.01506300
H	-0.21978400	1.28098600	1.55154300
H	-1.55715300	1.36113600	-1.25255100
H	0.72075400	0.29016400	-1.27143800



C	-1.46556400	0.96769400	0.01399500
C	-1.75544200	-0.39165600	0.60420100
C	-2.18158300	-1.41526700	-0.40732600
C	1.46519300	-0.32141700	-0.16551100
C	1.07467300	0.95096400	0.01853100
C	-0.25995200	1.52014400	-0.21438800
H	-2.34343100	1.55587800	-0.23671900
H	-2.54499300	-0.28868000	1.35974300
H	-2.75573100	-2.28279200	-0.10713100
H	1.82680500	1.66952000	0.34025100
H	-0.25177700	2.54018000	-0.59059700
C	2.85556900	-0.83340300	0.08624600
H	3.51529900	-0.04302000	0.44826500
H	2.85518600	-1.63657800	0.83006300
H	3.29688000	-1.25156200	-0.82399500
H	-1.87819600	-1.33330400	-1.44253600
H	-0.87116400	-0.74455200	1.15571300
H	0.75375400	-1.04744200	-0.54755000

TS26:

C	-1.79521800	0.32482900	-0.50387500
C	-1.48564600	-1.06634000	0.00685000
C	0.03555600	-1.30168200	0.13527700
C	0.75163800	-0.10471000	0.75699700
C	0.20636400	1.14685600	0.61896800
C	-0.98519900	1.35905300	-0.18285400
H	-2.70894200	0.48469100	-1.06342000
H	-1.91962400	-1.82641500	-0.64636100
H	0.22577900	-2.20252400	0.72253800
H	0.68249800	2.00163600	1.08313200
H	-1.23858100	2.36899700	-0.48254400
C	2.69019700	-0.00119100	-0.65754000
H	2.16462300	0.23642800	-1.57164300
H	3.26192300	0.78874600	-0.18956300
H	3.03750100	-1.01780800	-0.52404300
H	0.44380600	-1.49188600	-0.86264500
H	-1.96652700	-1.19577700	0.98774600
H	1.51139300	-0.28697900	1.50386400



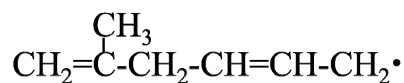
C	2.37019200	0.14506800	0.07374700
C	1.70798300	-1.18223500	-0.23641600
C	0.23526600	-1.21323000	0.22864400
C	-0.48376200	0.08445900	-0.08032500
C	0.19308700	1.24553500	-0.11454200
C	1.64488100	1.27634700	0.10818600
H	3.44540400	0.16842000	0.20645100
H	2.25946500	-2.00625300	0.22134100
H	-0.28105400	-2.05962800	-0.22921800
H	-0.32227100	2.18201400	-0.28958500
H	2.12004200	2.23364400	0.28445600
C	-4.62100400	0.00210000	0.01603900
H	-4.40197500	0.48721200	0.95524500
H	-4.75639000	0.59216300	-0.87782100
H	-4.73421600	-1.07083200	-0.02356400
H	0.19856900	-1.38455500	1.31459900
H	1.75220300	-1.35137900	-1.32242400
H	-1.55963600	0.06093200	-0.21147800

**TS27:**

C	-2.13386400	0.17979500	0.00448500
C	-1.48530600	-1.16528000	0.26858500
C	-0.04136200	-1.23875800	-0.29655400
C	0.69301500	0.05039600	-0.04685400
C	0.07817300	1.23471800	0.03730300
C	-1.39178300	1.29763900	-0.07795400
H	-3.21476700	0.22579500	-0.05459700
H	-2.08460400	-1.97584200	-0.15201200
H	0.48409400	-2.09000400	0.14209300
H	0.63109500	2.15712800	0.17144600
H	-1.85627400	2.26592400	-0.22097500
C	3.37141900	0.00134100	0.08273600
H	3.70434800	-0.43680900	-0.85447700
H	3.65739700	1.04403900	0.19278400
H	3.61538100	-0.60333800	0.95217200
H	-0.07544400	-1.42126400	-1.37972700
H	-1.45731000	-1.33523800	1.35435700
H	2.05433500	0.01050500	0.01845100

**TS28:**

C	1.88432100	-0.02289000	-0.23582700
C	1.22262300	-1.29718200	-0.49111100
C	-0.45212800	-1.01935000	0.93838900
C	-1.02207700	0.05874100	0.29519200
C	-0.23293900	1.35012700	0.14841400
C	1.26682800	1.15438500	0.01470000
H	2.96954000	-0.04397700	-0.15864500
H	1.76662600	-2.20541100	-0.24838100
H	-0.98463800	-1.96248100	0.98271700
H	-0.61553600	1.90166500	-0.72038800
H	1.87461600	2.03356200	0.20016900
C	-2.27252500	-0.07989400	-0.53009900
H	-2.97608200	0.73281700	-0.31999900
H	-2.05487000	-0.02791300	-1.60574100
H	-2.78503800	-1.02277900	-0.33614500
H	0.30502600	-0.87849200	1.69656300
H	0.55175900	-1.40314400	-1.33372800
H	-0.41601800	2.01253300	1.00563100

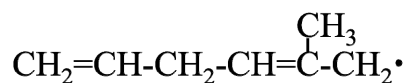


C	2.24981600	-0.24786700	0.25530500
C	2.62970500	0.45323300	-0.87850300
C	-1.32246900	-1.40532900	-0.42831900
C	-1.37220500	-0.12326500	-0.05263000
C	-0.16485300	0.63102000	0.50551500
C	1.01349000	-0.21093100	0.89828300
H	2.99575900	-0.90351200	0.69598800
H	3.62389700	0.34708500	-1.28957800
H	-2.19249700	-1.90907400	-0.83105900
H	0.12782000	1.39583000	-0.22183600
H	0.87401900	-0.84973400	1.76381700
C	-2.63211700	0.70439300	-0.16344800
H	-2.96217100	1.05385200	0.82017400
H	-2.46529500	1.59675700	-0.77544500
H	-3.44732300	0.13637300	-0.61141100
H	-0.41403900	-1.98788100	-0.35478900
H	1.95794800	1.12149800	-1.40051300
H	-0.50632400	1.19127500	1.38743500

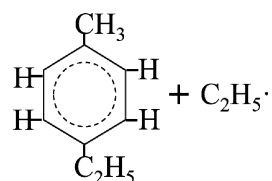
**TS29:**

C	1.94268200	0.04343500	-0.07440900
C	1.44141300	1.13072300	0.59823000
C	-0.45899200	1.23349500	-0.56825400
C	-1.02939600	-0.04882500	-0.13663200
C	-0.29053200	-1.17116700	0.03545300
C	1.21740500	-1.28399000	-0.10842400
H	2.74795400	0.18878300	-0.78677200
H	1.93347700	2.09254000	0.51767200
H	-0.98490100	2.13923700	-0.27708300
H	-0.79519100	-2.07548500	0.36015800
H	1.58466200	-1.94878800	0.68583700
C	-2.50980500	-0.04085300	0.20588200
H	-3.12036900	0.20824800	-0.66631800
H	-2.83790900	-1.00988400	0.58412100
H	-2.72711600	0.71121000	0.97170100
H	0.05386700	1.30742500	-1.51753400
H	0.80050400	1.00993400	1.46093400
H	1.46837600	-1.80013100	-1.04378800





C	2.28214900	0.14296000	0.03343400
C	2.28353500	-0.89702000	-0.80097900
C	-1.46435800	1.17428500	-0.84357800
C	-1.31069600	0.08159200	0.00770500
C	-0.15304600	-0.16596600	0.74838900
C	1.08263900	0.68673100	0.79192100
H	3.20917600	0.68303100	0.21039800
H	3.18710200	-1.21412400	-1.30575600
H	-2.38418300	1.32501300	-1.39300900
H	-0.12286700	-1.06866200	1.35000500
H	0.87346500	1.69939800	0.43206800
C	-2.47314200	-0.89595600	0.13003600
H	-3.36859900	-0.39494100	0.50516500
H	-2.72510600	-1.33160700	-0.83944600
H	-2.23914300	-1.71303000	0.81255800
H	-0.68092000	1.90163500	-1.00046200
H	1.38455100	-1.46209900	-1.01341000
H	1.38404000	0.81563900	1.84031900

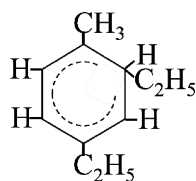


C	0.48277100	0.17803700	0.30213800
C	0.26514600	1.55248300	0.13551800
C	-1.01166600	1.96944700	-0.27321400
C	-2.03130700	1.04597500	-0.50355700
C	-1.81564900	-0.33078500	-0.33300800
C	-0.53974700	-0.74618200	0.07152900
H	1.46146800	-0.17203100	0.60890000
H	-1.20647100	3.02602500	-0.41626700
H	-3.00596000	1.39548100	-0.82401400
H	-0.34118300	-1.80361800	0.20297700
C	1.36665400	2.55904200	0.38475700
H	1.10197900	3.24917300	1.19045600
H	2.29686800	2.06432100	0.66541700
H	1.56630700	3.16251800	-0.50460600
C	-2.93599700	-1.33067200	-0.54463500
H	-3.60621700	-0.96702500	-1.32876200
H	-2.51859900	-2.27400900	-0.90802600

C	-3.75608400	-1.60135000	0.73485900
H	-4.21162500	-0.68188500	1.10777700
H	-4.55411700	-2.32208100	0.54238400
H	-3.12086900	-2.00158700	1.52750100
C	4.58045000	-1.30877500	-0.78705300
C	4.32841900	-1.32090700	0.68297900
H	4.85504100	-0.31463300	-1.14559100
H	5.40437000	-1.98252600	-1.06991100
H	3.70598300	-1.64089400	-1.35274900
H	3.74676000	-2.11131800	1.13990500
H	4.82833200	-0.62378700	1.34272600

**TS30:**

C	0.85981800	-0.00097500	-1.03183300
C	1.25371600	-1.08247700	-0.17346900
C	0.39502500	-1.45438700	0.85711100
C	-0.86627100	-0.86035000	1.01581900
C	-1.32055700	0.11938700	0.10785900
C	-0.47118700	0.50754500	-0.92345400
H	1.35880100	0.08866400	-1.99032400
H	0.69858400	-2.24034700	1.53912200
H	-1.51018700	-1.17886600	1.82665600
H	-0.80920900	1.23950200	-1.64813400
C	2.59131900	-1.75119300	-0.36990900
H	2.74235700	-2.04511900	-1.41241100
H	3.41931400	-1.08485100	-0.10495500
H	2.68163400	-2.64719900	0.24541600
C	-2.72879900	0.67543300	0.21857500
H	-2.97654700	0.82938900	1.27320400
H	-2.77044300	1.65963900	-0.25559600
C	-3.79370700	-0.24061700	-0.42056500
H	-3.79572700	-1.22542200	0.05064400
H	-4.79294900	0.18803800	-0.31503700
H	-3.59463700	-0.38265700	-1.48450700
C	1.85126400	1.93193000	1.06320100
C	2.09676600	1.67171300	-0.39505700
H	2.14446700	1.07963900	1.67893000
H	2.42024500	2.80112000	1.41990300
H	0.79636900	2.13557600	1.25702600
H	1.71180100	2.40639300	-1.09673500
H	3.07180000	1.28044300	-0.67287900

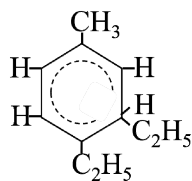


C	-0.97706200	-0.32160100	-0.82511100
C	-1.26665800	1.01655300	-0.16839800
C	-0.30490700	1.64245200	0.58724600
C	0.98884700	1.10253400	0.77751000
C	1.36009500	-0.12886100	0.15678500
C	0.43760100	-0.79717800	-0.60277100
H	-1.12899500	-0.19320600	-1.91366800
H	-0.54181600	2.59524900	1.04878200
H	1.70661200	1.63184800	1.39116800
H	0.71050200	-1.73461800	-1.07787900
C	-2.61867600	1.63429000	-0.40293600
H	-2.85095900	1.68638700	-1.47292200
H	-3.42495400	1.05688000	0.06176500
H	-2.66619800	2.64679700	-0.00027700
C	2.77551800	-0.65236600	0.32783800
H	3.05366700	-0.60454100	1.38574900
H	2.80730300	-1.70818600	0.04706700
C	3.81632700	0.12629100	-0.50270700
H	3.82945100	1.18331400	-0.22964900
H	4.82021500	-0.27452600	-0.34562500
H	3.58658200	0.06181700	-1.56795900
C	-2.03596500	-1.75086900	1.07879800
C	-2.01053100	-1.43488500	-0.42141200
H	-2.31787100	-0.87428600	1.66547600
H	-2.75302400	-2.54549000	1.29629800
H	-1.05446900	-2.07715500	1.42683500
H	-1.75858300	-2.33840800	-0.98573000
H	-3.00499900	-1.13004200	-0.75848000

**TS31:**

C	-1.12442600	0.17600800	0.82128800
C	-1.80481500	-0.84328200	0.16386900
C	-1.08103900	-1.66767700	-0.72422400
C	0.30115600	-1.49893100	-0.89250600
C	0.99937900	-0.48995900	-0.23415300
C	0.24969100	0.45654400	0.54282800
H	-1.65458800	0.80383400	1.52695700
H	-1.59118400	-2.46637700	-1.24891200
H	0.84416900	-2.18669100	-1.53104700

H	0.79135800	1.07712400	1.24870000
C	-3.27977200	-1.08540900	0.40057300
H	-3.47276800	-2.12036500	0.69365500
H	-3.66638600	-0.43837500	1.18889200
H	-3.86479600	-0.89151600	-0.50295400
C	2.50567600	-0.37729400	-0.32898200
H	2.85262900	-0.88283700	-1.23456100
H	2.79360500	0.67393900	-0.43189100
C	3.23912100	-0.97578600	0.89214800
H	3.01534600	-2.03897800	0.99562700
H	4.32099800	-0.86288600	0.79016200
H	2.93427700	-0.48074400	1.81644900
C	-0.48978200	3.30764400	-0.04326700
C	0.13999200	2.16369900	-0.78998900
H	0.09663000	3.59176000	0.83507100
H	-0.57156000	4.20450500	-0.67182800
H	-1.50023400	3.06226700	0.29017500
H	-0.45051500	1.69594200	-1.57013000
H	1.19193100	2.26605800	-1.03987800

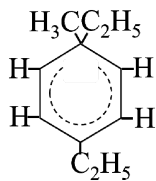


C	-1.21007600	0.89820600	0.50226500
C	-2.22537200	0.05725800	0.13931300
C	-1.90339700	-1.20609800	-0.44328900
C	-0.55459600	-1.59519900	-0.60422200
C	0.50625400	-0.79449800	-0.24905800
C	0.25778300	0.60646900	0.29144400
H	-1.44335700	1.85759800	0.95293700
H	-2.69775900	-1.87751200	-0.74339000
H	-0.34664200	-2.57659100	-1.01749700
H	0.75960200	0.69593800	1.26998500
C	-3.67782200	0.43003100	0.34494600
H	-4.18493700	-0.29383500	0.98868100
H	-3.77508700	1.41338500	0.80599400
H	-4.21867800	0.45085600	-0.60520900
C	1.92673800	-1.29577600	-0.38158400
H	1.91509000	-2.23717300	-0.93763000
H	2.52314500	-0.59910100	-0.98054100
C	2.64333300	-1.52990200	0.96792900
H	2.09439700	-2.25175700	1.57524700

H	3.65054200	-1.91938200	0.80465500
H	2.73460700	-0.60781700	1.54473500
C	2.30215300	2.19742000	-0.16517000
C	0.90832300	1.73193300	-0.61219000
H	3.03571900	1.39057200	-0.18423100
H	2.67115500	2.99298300	-0.81673700
H	2.27175000	2.59254100	0.85367200
H	0.23616300	2.59435700	-0.60766500
H	0.93436300	1.37587000	-1.64530800

**TS32:**

C	-0.59937900	-0.59085600	1.22599400
C	-1.32955200	-0.78667700	0.00386900
C	-0.57323800	-0.60937900	-1.20568700
C	0.71672000	-0.10653400	-1.18675100
C	1.38173700	0.17874700	0.02547700
C	0.69146200	-0.08809000	1.22668100
H	-1.09213900	-0.81437300	2.16510200
H	-1.04652300	-0.84664400	-2.15143700
H	1.23879900	0.05290500	-2.12383100
H	1.19452500	0.08480700	2.17166500
C	-2.48585500	-1.78078700	-0.00086700
H	-2.09967800	-2.80380500	0.01123400
H	-3.12431000	-1.65663900	0.87465700
H	-3.10543000	-1.67043300	-0.89167000
C	2.80993600	0.68184400	0.03471800
H	2.96308000	1.36619600	-0.80535500
H	2.98554300	1.26532200	0.94304700
C	3.85757400	-0.45106500	-0.04507300
H	3.73148800	-1.03482000	-0.95896800
H	4.87218100	-0.04579000	-0.03822300
H	3.75823100	-1.13376700	0.80111000
C	-1.76443300	2.23451300	-0.02764800
C	-2.59368700	0.98366600	-0.02606400
H	-1.11580300	2.28247800	-0.90412200
H	-2.39467600	3.13407300	-0.04114500
H	-1.13356800	2.29635500	0.86085100
H	-3.15990500	0.77383000	0.87763800
H	-3.13952900	0.75801300	-0.93845000

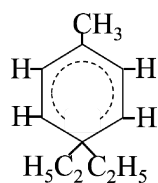


C	-0.57378400	0.24931200	-1.24737500
C	-1.38548600	0.53190100	0.00005000
C	-0.57395600	0.24885800	1.24747800
C	0.73166200	-0.15192900	1.22022400
C	1.44037700	-0.36101000	0.00008300
C	0.73182200	-0.15147100	-1.22009300
H	-1.08026500	0.39316500	-2.19627600
H	-1.08056200	0.39235500	2.19636600
H	1.25426800	-0.32440400	2.15541200
H	1.25456400	-0.32360300	-2.15526900
C	-1.81063100	2.03717100	0.00028300
H	-0.93240800	2.68265400	0.00040800
H	-2.40880300	2.26374600	-0.88581100
H	-2.40883900	2.26346400	0.88642600
C	2.90005600	-0.74490100	0.00007800
H	3.11812800	-1.36220600	0.87695400
H	3.11806200	-1.36246800	-0.87663600
C	3.85241500	0.47486300	-0.00014700
H	3.68761900	1.09689600	0.88162800
H	4.89656200	0.15337900	-0.00016400
H	3.68752100	1.09665600	-0.88207400
C	-2.48420100	-1.84258400	-0.00031000
C	-2.70130600	-0.32495000	-0.00018600
H	-1.92491000	-2.16182900	0.88085700
H	-3.44131800	-2.36899400	-0.00092700
H	-1.92393500	-2.16153200	-0.88096800
H	-3.28865000	-0.03433200	-0.87800700
H	-3.28883800	-0.03451000	0.87756900

**TS33:**

C	1.19264900	-0.49759300	-1.20665700
C	1.91803900	-0.59407400	0.00000900
C	1.19265300	-0.49755200	1.20666800
C	-0.17591600	-0.28474300	1.21515600
C	-0.91300900	-0.07089500	-0.00000300
C	-0.17592300	-0.28479300	-1.21516700
H	1.71790000	-0.61873900	-2.14738900
H	1.71789800	-0.61866500	2.14740600
H	-0.70993900	-0.24854800	2.15792400

H	-0.70995300	-0.24864500	-2.15793200
C	3.41389000	-0.79579500	0.00000400
H	3.74278200	-1.34813800	0.88251400
H	3.74271400	-1.34861900	-0.88223300
H	3.94942600	0.16015100	-0.00028000
C	-2.41610200	-0.36026500	0.00000100
H	-2.87616900	0.10325300	0.87651900
H	-2.87615900	0.10322000	-0.87653900
C	-2.73186500	-1.86897300	0.00002300
H	-2.31158400	-2.35772500	0.88104200
H	-3.81126700	-2.03818400	-0.00001300
H	-2.31151900	-2.35776100	-0.88094500
C	0.22262600	2.76090900	-0.00001200
C	-1.12296600	2.09618500	-0.00001600
H	0.80355800	2.48738100	-0.88271900
H	0.12963200	3.85541400	-0.00003600
H	0.80353200	2.48741900	0.88272300
H	-1.71267800	2.18690700	0.90826800
H	-1.71263000	2.18680900	-0.90834100



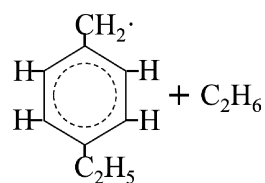
C	1.23824900	-0.02062700	-1.21763200
C	1.97640700	-0.02918500	0.00490600
C	1.23743300	-0.02349900	1.22237500
C	-0.12969300	-0.00600800	1.24727000
C	-0.98639000	0.00910200	-0.00004400
C	-0.12629700	-0.00350900	-1.24521500
H	1.78917300	-0.02964700	-2.15238600
H	1.78623100	-0.03478200	2.15811800
H	-0.65654900	-0.00501200	2.19613200
H	-0.65160100	-0.00049600	-2.19504900
C	3.48162100	-0.01474500	-0.00233800
H	3.88882000	-0.30140100	0.96848500
H	3.88758700	-0.70073500	-0.75087700
H	3.87656800	0.98078000	-0.23892300
C	-1.94786700	-1.23778000	-0.00282300
H	-2.59956300	-1.15691700	0.87382300
H	-2.59589100	-1.15650200	-0.88218400
C	-1.24469100	-2.60023500	-0.00148900
H	-0.61303100	-2.71862600	0.88040300

H	-1.97711600	-3.41073300	-0.00250700
H	-0.61017700	-2.71911500	-0.88127400
C	-1.16648400	2.62538900	0.00018700
C	-1.90991300	1.28448900	-0.00064800
H	-0.53031800	2.72575000	-0.88073100
H	-1.87448300	3.45730100	0.00076200
H	-0.53021600	2.72442100	0.88116100
H	-2.56243200	1.22245000	0.87690100
H	-2.56125600	1.22291400	-0.87913900

**TS34:**

C	0.19029300	-0.32142800	1.32302700
C	0.79970500	-1.01798100	0.25932600
C	-0.00322700	-1.32545000	-0.85838400
C	-1.34552100	-0.95551900	-0.90673500
C	-1.94853800	-0.26017500	0.15417500
C	-1.15303300	0.04584300	1.27011500
H	0.77745800	-0.07818700	2.20041200
H	0.43283300	-1.86776800	-1.68882800
H	-1.93871400	-1.21581100	-1.77575900
H	-1.59517100	0.57094700	2.10886900
C	2.23276800	-1.37012100	0.29233500
H	2.50815800	-2.22503900	-0.32354600
H	2.93139200	-0.41672400	-0.24136400
H	2.66291700	-1.44618900	1.28995700
C	-3.39883700	0.17443300	0.08164800
H	-3.97552700	-0.56923400	-0.47580500
H	-3.82239500	0.20174300	1.08955400
C	-3.58487500	1.55658800	-0.58111500
H	-3.20076700	1.55354600	-1.60305700
H	-4.64089300	1.83390800	-0.61575200
H	-3.04855000	2.32950700	-0.02713000
C	3.55690500	1.83745700	0.07758600
C	3.71815300	0.62957700	-0.81646000
H	3.93749300	1.64606900	1.08371100
H	4.10296500	2.70576300	-0.31205300
H	2.50869800	2.13082100	0.16605000
H	3.26676500	0.70475600	-1.80425600
H	4.71058300	0.18255300	-0.84410800



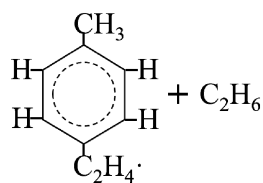


C	-0.40225400	-0.84362300	1.29549300
C	0.16880100	-1.40014100	0.10954200
C	-0.58279900	-1.24993300	-1.09689200
C	-1.80264200	-0.59297900	-1.10703100
C	-2.35324500	-0.04482800	0.06972800
C	-1.62363000	-0.18958400	1.26738300
H	0.13636600	-0.94359400	2.22971000
H	-0.18400200	-1.66456800	-2.01444600
H	-2.35014300	-0.50008600	-2.03766000
H	-2.03147000	0.21749000	2.18516700
C	1.40824700	-2.06724700	0.12914900
H	1.83159700	-2.49032900	-0.77161400
H	4.02442000	0.19365800	-0.59436700
H	1.96890700	-2.18225000	1.04680500
C	-3.66492000	0.70982900	0.03958200
H	-4.32450600	0.26629000	-0.71178700
H	-4.17202000	0.59896200	1.00211300
C	-3.49095400	2.21386300	-0.26837400
H	-3.01796500	2.36077600	-1.24117800
H	-4.45748100	2.72236200	-0.27992500
H	-2.86208900	2.69541800	0.48278100
C	5.46819400	1.40616200	0.50590000
C	4.92332000	0.78334700	-0.78616000
H	5.72990900	0.63831100	1.23731700
H	6.36585300	1.99837100	0.31471100
H	4.73107800	2.06507900	0.96981600
H	4.66291500	1.55157800	-1.51751400
H	5.65992600	0.12333600	-1.24985500

**TS35:**

C	2.46033000	-1.19549900	0.05420400
C	3.15906300	0.01224300	0.20455700
C	2.45160900	1.20602300	0.00293400
C	1.09793300	1.19396000	-0.33915600
C	0.40064600	-0.01314100	-0.49059700
C	1.10779300	-1.20814100	-0.28788400
H	2.98147300	-2.13386000	0.20326200
H	2.96570400	2.15359500	0.11144000
H	0.57773500	2.13237400	-0.49163700

H	0.59439100	-2.15593600	-0.40037500
C	4.63233500	0.02218000	0.54672800
H	4.88616400	-0.78047000	1.24179100
H	5.24995100	-0.11452600	-0.34633000
H	4.92792700	0.96683000	1.00568100
C	-1.08318200	-0.02724800	-0.82537700
H	-1.32160200	0.84118600	-1.44613900
H	-1.30935000	-0.91236800	-1.42695500
C	-1.96770700	-0.02006800	0.41827200
H	-1.89812700	0.88802000	1.01700100
H	-3.25966100	-0.03486300	0.00235800
H	-1.88447200	-0.91331500	1.03722400
C	-5.42946100	0.07184800	0.81459100
H	-5.23943500	1.00250800	1.35464200
H	-5.26457600	-0.75475600	1.50984800
H	-6.49311400	0.06359000	0.55003600
C	-4.54545500	-0.04958100	-0.41157600
H	-4.62342700	-0.99826400	-0.94264600
H	-4.59299900	0.79479600	-1.09938100

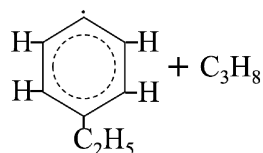


C	2.91521400	-1.14534900	0.03836000
C	3.54297200	0.10506500	0.13698700
C	2.75499700	1.25008400	-0.05389400
C	1.38947100	1.14897100	-0.32422100
C	0.76345000	-0.10193900	-0.41694700
C	1.54935000	-1.24760800	-0.23177600
H	3.50175600	-2.04688900	0.16894200
H	3.21577300	2.22901100	0.00435300
H	0.80614400	2.04993100	-0.47293100
H	1.09169100	-2.22682800	-0.30772400
C	5.01675200	0.21715100	0.45771900
H	5.56502400	-0.66634600	0.12718100
H	5.46498600	1.08813900	-0.02340900
H	5.18231400	0.31953500	1.53461300
C	-0.74047600	-0.21191200	-0.68381100
H	-1.04700000	0.62839800	-1.31311900
H	-0.93182300	-1.12316000	-1.25659100
C	-1.54316900	-0.22381900	0.58520800
H	-1.78251400	0.70262200	1.09162200

H	-4.84630700	-0.46910500	0.17076200
H	-1.71421900	-1.14892000	1.12066000
C	-6.65265600	0.75715400	0.13657200
H	-6.35129500	1.38067600	-0.70804700
H	-6.43136000	1.31229200	1.05082900
H	-7.73621400	0.63062900	0.08239500
C	-5.92979600	-0.59606000	0.11684100
H	-6.23168900	-1.21929600	0.96158800
H	-6.15191400	-1.15111800	-0.79735200

**TS36:**

C	0.21325900	1.30336200	-0.17231600
C	-0.53758000	0.14948400	0.02515500
C	0.06693500	-1.10259200	0.03922700
C	1.45251900	-1.19861000	-0.14624300
C	2.23706700	-0.05143400	-0.34496200
C	1.59829000	1.19899700	-0.35665600
H	-0.26070300	2.27852700	-0.18966000
H	-0.52022000	-2.00229500	0.18592800
H	1.92742100	-2.17357400	-0.14087600
H	2.18690600	2.09579300	-0.51586300
C	-2.51162500	0.30324300	0.23898500
H	-2.51947300	-0.66846000	0.71201500
H	-2.35123700	1.18943600	0.83640200
H	-2.59617500	0.38477100	-0.83504400
C	3.74197700	-0.15848300	-0.50675700
H	3.98719400	-1.08879600	-1.02694500
H	4.09822200	0.65492200	-1.14511300
C	4.50096800	-0.11656300	0.83640300
H	4.18970900	-0.93743400	1.48555800
H	5.57890400	-0.19790600	0.67898700
H	4.30472000	0.81753900	1.36644200
C	-5.12242500	-0.66836000	-0.30812500
C	-4.45167100	0.45534400	0.44965900
H	-6.21447800	-0.63310000	-0.21899600
H	-4.88732600	-0.62650900	-1.37491200
H	-4.80421700	-1.64570300	0.06460000
H	-4.58115700	0.41653700	1.53015200
H	-4.66438200	1.44991300	0.06110500

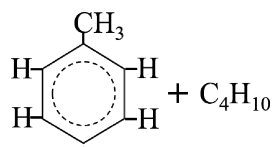


C	0.41754500	1.29904600	-0.11148600
C	-0.24550300	0.09181200	-0.19222400
C	0.36329200	-1.13762500	-0.34059200
C	1.76676400	-1.14844500	-0.41062800
C	2.50672600	0.04359900	-0.33151100
C	1.82068900	1.26084400	-0.18350200
H	-0.10530500	2.23939500	-0.00191800
H	-0.20172600	-2.05740400	-0.40596800
H	2.28468900	-2.09254300	-0.53269800
H	2.38037300	2.18726100	-0.12880200
C	-4.51825300	-0.12545200	-1.13858000
H	-3.43728700	-0.00862100	-1.25148100
H	-5.00086000	0.41926300	-1.95309100
H	-4.75189300	-1.18631200	-1.26282200
C	4.02387600	0.01258000	-0.36916800
H	4.35530900	-0.79894100	-1.02270600
H	4.39553500	0.93890700	-0.81521800
C	4.65964500	-0.16895000	1.02546200
H	4.33238500	-1.10354800	1.48498500
H	5.74943200	-0.18764000	0.95698500
H	4.37533800	0.64640300	1.69340700
C	-4.32269400	-0.35847200	1.40382900
C	-4.98524700	0.38398900	0.23341800
H	-4.55237800	-1.42700400	1.37067600
H	-3.23542800	-0.25215000	1.36853100
H	-4.66573600	0.02564500	2.36709500
H	-4.77032600	1.45439000	0.31487500
H	-6.07317000	0.28534300	0.30803600

**TS37:**

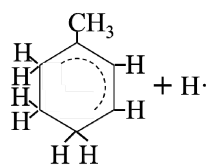
C	2.35951200	-1.13909700	-0.19084700
C	2.97130900	0.12110100	-0.07873000
C	2.14940800	1.25314700	0.02586700
C	0.75208000	1.13443900	0.02224300
C	0.17597400	-0.12551400	-0.08067500
C	0.96517500	-1.26582300	-0.19488000
H	2.97784600	-2.02568700	-0.27860600
H	2.60296100	2.23433400	0.10778000
H	0.13665500	2.02412900	0.10056500

H	0.51410500	-2.24800100	-0.28587900
C	4.47967500	0.24543100	-0.06248500
H	4.79237500	1.28749300	-0.13885100
H	4.90371000	-0.15793300	0.86153700
H	4.93533600	-0.29983900	-0.89226300
C	-1.84839400	-0.30235100	-0.09484500
H	-1.82358600	0.66712600	-0.57411200
H	-1.66929600	-1.18865300	-0.68756500
C	-2.00266000	-0.41772800	1.42610300
H	-1.61836100	0.47205600	1.92515300
H	-3.03984200	-0.54990800	1.73937700
H	-1.43284600	-1.26632200	1.80535400
C	-4.49892400	0.82537200	-0.27791700
C	-3.74629000	-0.41822300	-0.69155400
H	-4.06928500	1.72164700	-0.73332300
H	-5.55041400	0.78209100	-0.58656400
H	-4.49081900	0.96372100	0.80564600
H	-4.07222000	-1.34065800	-0.21391900
H	-3.63750400	-0.54011900	-1.76800800



C	-2.67455000	1.16373300	0.34783700
C	-3.52712400	0.09001100	0.04775400
C	-2.96426400	-1.12524500	-0.38162500
C	-1.57440500	-1.27436200	-0.51280300
C	-0.79431300	-0.17827600	-0.20143900
C	-1.27865500	1.03979300	0.22480200
H	-3.09598600	2.10459700	0.68049700
H	-3.61204300	-1.96209000	-0.61534000
H	-1.14710100	-2.21138000	-0.84304100
H	-0.62782900	1.87122800	0.45898100
C	-5.02878300	0.23013200	0.17927800
H	-5.44163000	-0.52048400	0.85752100
H	-5.30254200	1.21173800	0.56664000
H	-5.52734700	0.10498600	-0.78533800
C	3.44266800	-0.86356200	-0.20739300
H	3.58665300	-1.74841700	-0.83609200
H	2.37027500	-0.63876700	-0.23715700
C	3.85480000	-1.20358100	1.23376200
H	3.31081900	-2.07659600	1.60058900

H	4.92348000	-1.42819700	1.29316500
H	3.64935000	-0.37967500	1.91997100
C	3.97815500	1.66630200	-0.14308600
C	4.22196800	0.31280500	-0.82957000
H	4.51370700	2.46849600	-0.65555400
H	2.91464000	1.92002500	-0.14898400
H	4.31330800	1.66032800	0.89588600
H	5.29347300	0.08229100	-0.81116300
H	3.94578800	0.39541900	-1.88568900

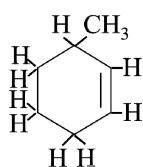


C	1.89588200	0.60128500	0.29222200
C	1.58852800	-0.88831400	0.03255000
C	0.14377400	-1.24911100	0.43700700
C	-0.87225000	-0.28716300	-0.13985200
C	-0.47510700	1.01074500	-0.46556500
C	0.81628800	1.48717800	-0.27225800
H	2.86832800	0.86293600	-0.13535400
H	2.29997100	-1.52259800	0.56655100
H	-0.08647600	-2.27135200	0.11830200
H	-5.56643100	3.55162300	2.50975000
H	-1.21942600	1.68443000	-0.87877600
C	-2.28578600	-0.76424000	-0.30303000
H	-2.71094000	-1.09612700	0.65265800
H	-2.93432400	0.01780700	-0.70083100
H	-2.34433100	-1.62563100	-0.97967000
H	0.06111500	-1.25606400	1.53471000
H	1.71478600	-1.09160300	-1.03504700
H	1.99330900	0.76913900	1.37548700
H	1.05644400	2.51516400	-0.51423000

**TS38:**

C	-1.94014400	0.11498800	-0.25825300
C	-1.24789500	-1.16788800	0.26509200
C	0.22390500	-1.23502500	-0.17641400
C	0.99488600	0.06464100	0.09561500
C	0.32517100	1.26757400	-0.00459800
C	-1.14423400	1.33379900	0.07154000
H	-2.95694800	0.19057800	0.13334000
H	-1.78525400	-2.05226900	-0.08596700

H	0.72653000	-2.06798900	0.31992500
H	0.88692200	2.19494600	0.00867200
H	-1.63168300	2.27950900	0.26737100
C	2.49649100	-0.00455900	-0.10036500
H	2.73380600	-0.27334300	-1.13514900
H	2.97206900	0.95237900	0.11748900
H	2.94424400	-0.76184400	0.54629500
H	0.28215500	-1.43259000	-1.25530100
H	-1.28929200	-1.16957300	1.35767200
H	-2.04181700	0.01945400	-1.35460500
H	0.91018600	-0.12043300	1.72455800

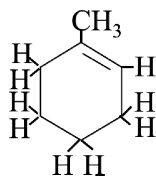


C	1.92157600	0.15190700	0.26252500
C	1.27426600	-1.14589200	-0.25891700
C	-0.19990500	-1.23611200	0.17204200
C	-1.03028200	-0.06014600	-0.38846900
C	-0.28484000	1.25172100	-0.22621600
C	1.01417300	1.34737100	0.07870000
H	2.87347200	0.32920200	-0.24857400
H	1.83155900	-2.01557200	0.09809800
H	-0.63832900	-2.18413100	-0.15168000
H	-0.86955200	2.15701000	-0.36424800
H	1.46384400	2.32779400	0.20200500
C	-2.42656200	0.00619700	0.26149300
H	-2.34366200	0.19395400	1.33477300
H	-3.02830500	0.80730300	-0.17440100
H	-2.96601500	-0.93342800	0.12156800
H	-0.25688300	-1.21762200	1.26672900
H	1.32934000	-1.16196000	-1.35258400
H	2.17386300	0.04190800	1.32548100
H	-1.17988600	-0.23473800	-1.46411500

**TS39:**

C	-1.90392400	0.01125000	-0.22722400
C	-1.15062000	-1.21993600	0.30683700
C	0.30542700	-1.26676400	-0.21260900
C	1.04241700	0.01667100	0.02962300
C	0.27116700	1.27378700	-0.08739400
C	-1.10125900	1.29106500	-0.02026800

H	-2.87818100	0.09476800	0.25782700
H	-1.67589100	-2.13581000	0.02595100
H	0.84230100	-2.10736500	0.23649500
H	0.82211600	2.20781600	-0.09961800
H	-1.61791600	2.23021200	-0.18481700
C	2.53478300	0.05155000	0.06567100
H	2.97134800	0.10668200	-0.94673200
H	2.90663200	0.92383600	0.60969800
H	2.94900800	-0.84410700	0.53458800
H	0.27525500	-1.47599700	-1.29849300
H	-1.13488500	-1.17351700	1.39942800
H	-2.09734600	-0.10571400	-1.30118100
H	-1.35038800	1.33345900	1.63903400



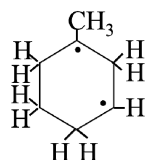
C	1.85669300	-0.01614200	0.34504100
C	1.15801300	-1.21955400	-0.30998600
C	-0.32963100	-1.27003500	0.08402000
C	-1.01305500	0.08519300	0.00569100
C	-0.31126000	1.22405700	-0.08845500
C	1.19890400	1.30225600	-0.10297500
H	2.92204300	-0.00896600	0.10142100
H	1.65260100	-2.15286700	-0.02902300
H	-0.86109300	-1.98051900	-0.55900500
H	-0.84582200	2.16736400	-0.15873400
H	1.53076200	2.12301700	0.54159700
C	-2.52198700	0.06684200	0.04875300
H	-2.88466500	-0.42849900	0.95592700
H	-2.93823900	1.07475300	0.02736600
H	-2.93612900	-0.48895800	-0.79918000
H	-0.43138400	-1.66483600	1.10414400
H	1.24086300	-1.13219400	-1.39868900
H	1.78016700	-0.10752300	1.43391000
H	1.54484000	1.56351700	-1.11227200

**TS40:**

C	1.93892000	0.09865200	0.16154100
C	1.22793200	-1.19764600	-0.28202200
C	-0.21979700	-1.25835800	0.24926600
C	-0.99712500	0.00287900	-0.04343600



C	-0.30643900	1.22873300	-0.13250600
C	1.09726900	1.31086700	-0.12269100
H	2.91095600	0.18401800	-0.33186700
H	1.78930100	-2.07194200	0.05525300
H	-0.73824900	-2.12337800	-0.17600900
H	-0.62922900	1.83768800	1.66355100
H	-0.86997900	2.10856800	-0.42273600
C	-2.49352600	-0.06838100	-0.07979900
H	-2.90091100	-0.38871400	0.88844600
H	-2.94048800	0.89730100	-0.31972200
H	-2.84305300	-0.79782300	-0.81878900
H	-0.20074400	-1.42813800	1.33751100
H	1.20557500	-1.23248100	-1.37517000
H	2.15524100	0.04116700	1.23978600
H	1.57817000	2.27325700	-0.24237700

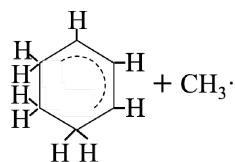


C	1.94169100	0.08174200	0.16457300
C	1.22223400	-1.20399400	-0.30152800
C	-0.22123400	-1.25935800	0.24201300
C	-1.01020200	-0.01730900	-0.07006200
C	-0.33993400	1.32400100	0.09245700
C	1.13986600	1.30609500	-0.15211100
H	2.93553200	0.14526600	-0.28562700
H	1.77941400	-2.08575200	0.02600200
H	-0.73777900	-2.13907000	-0.15428700
H	-0.54087300	1.70113900	1.12648000
H	-0.82494300	2.06681700	-0.55288500
C	-2.50668000	-0.07090400	-0.09182700
H	-2.94006700	0.00224200	0.92057000
H	-2.93199000	0.75406900	-0.67057700
H	-2.87104500	-1.00789500	-0.52065700
H	-0.17103500	-1.41357800	1.33699600
H	1.19529000	-1.22290600	-1.39455300
H	2.11007900	0.00116800	1.25417300
H	1.64297300	2.23686100	-0.38672000

**TS41:**

C	-1.87304200	0.27031200	-0.46472300
C	-1.41401000	-1.06205700	0.17622800

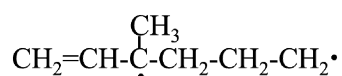
C	0.10931900	-1.26595700	0.00502200
C	0.87764300	-0.11534900	0.66522600
C	0.25529000	1.11994300	0.69551000
C	-0.88388600	1.37861900	-0.21204500
H	-2.87592600	0.53056700	-0.09492800
H	-1.96156000	-1.89625900	-0.26982800
H	0.41969800	-2.21799600	0.44089900
H	0.60975800	1.90593200	1.35398100
H	-0.88976600	2.25229700	-0.85648000
C	2.61133400	0.00649600	-0.60932900
H	2.17619900	0.32655000	-1.54782600
H	3.23364700	0.73669400	-0.10687200
H	2.96448100	-1.01827200	-0.57531500
H	0.33555300	-1.32556400	-1.06384800
H	-1.65036900	-1.05506300	1.24367400
H	-1.99407400	0.13532700	-1.54864000
H	1.53647100	-0.36625800	1.48986000



C	-2.37572000	0.15812800	-0.05817300
C	-1.64972500	-1.12988800	0.38870200
C	-0.27473500	-1.27610600	-0.29929800
C	0.53457900	-0.00886700	-0.19432600
C	-0.08938200	1.22384800	-0.02777400
C	-1.47269500	1.36150100	0.03196500
H	-3.27489300	0.30935300	0.54641200
H	-2.27077500	-2.00519700	0.18511100
H	0.27399400	-2.11652300	0.13587000
H	0.52658400	2.11335600	0.04683300
H	-1.91892400	2.34380500	0.12754100
C	4.62703400	0.00435000	0.12789600
H	4.30879700	0.21838300	1.13701100
H	4.83000000	-1.01340100	-0.16966200
H	4.76783000	0.81050200	-0.57624300
H	-0.42425200	-1.53630400	-1.35810100
H	-1.49690300	-1.08786900	1.47116500
H	-2.73174700	0.03469900	-1.09219300
H	1.61414500	-0.06858800	-0.26769600

TS42:

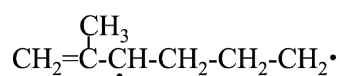
C	2.08808600	-0.08659200	0.26750900
C	1.25123200	-1.19649900	-0.31122800
C	-0.20389600	-1.26219700	0.23256400
C	-1.02693100	-0.01960300	-0.02049100
C	-0.37831100	1.26643100	0.29062100
C	0.77704900	1.65525100	-0.33544300
H	3.01144500	0.17650300	-0.23889000
H	1.72042000	-2.17100700	-0.10846900
H	-0.70703700	-2.13239800	-0.19965000
H	-0.68413600	1.78602000	1.20096100
H	1.31493600	2.53595300	-0.00630100
C	-2.51879900	-0.11702800	-0.13783200
H	-3.01155500	-0.09598400	0.84904000
H	-2.93040800	0.71990600	-0.70705200
H	-2.82612900	-1.04675200	-0.62261400
H	-0.14323800	-1.45741200	1.31865700
H	1.21894000	-1.10583600	-1.40265700
H	2.10996200	0.02562700	1.34671500
H	0.99622200	1.32680800	-1.34393900



C	-2.97020500	-0.35234500	-0.00871100
C	-1.59932200	-0.02075400	-0.50107300
C	-0.55596600	0.13799400	0.63945800
C	0.82899800	0.47848100	0.14201600
C	1.78709700	-0.50181200	-0.14709000
C	1.65243000	-1.87347400	-0.02252100
H	-3.83355100	-0.24659500	-0.65315000
H	-1.62735000	0.89618800	-1.10222100
H	-0.90519400	0.92550300	1.31514500
H	2.74375500	-0.13704300	-0.51314000
H	2.46895100	-2.53541600	-0.27537000
C	1.13663100	1.93745700	-0.06270300
H	1.08238500	2.49070800	0.88282600
H	2.13179800	2.08965000	-0.48201000
H	0.41417200	2.41274300	-0.73676000
H	-0.53920600	-0.78606500	1.22350600
H	-1.23720700	-0.79979000	-1.19052700
H	-3.11897000	-0.80317100	0.96489600
H	0.74243200	-2.33998900	0.33054600

TS43:

C	1.92171600	-0.02374600	0.00631800
C	1.29579300	1.24630800	0.52037300
C	-0.58785900	1.21633200	-0.73385500
C	-1.11301800	0.01491000	-0.32175300
C	-0.30310700	-1.20504500	-0.50788900
C	1.03343500	-1.29217600	0.17854900
H	2.87342200	-0.22139700	0.52195900
H	1.72786400	2.19119600	0.20628100
H	-1.09564900	2.14659100	-0.50647900
H	-0.72964500	-2.09544200	-0.96000000
H	1.58310300	-2.16783700	-0.17550200
C	-2.32702500	-0.07145700	0.57602000
H	-3.05895900	-0.77986600	0.17389300
H	-2.06807900	-0.42898900	1.58010300
H	-2.81934300	0.89725500	0.67666700
H	0.10768400	1.25749500	-1.56192000
H	0.89361900	1.24249500	1.52881200
H	2.17642200	0.09052600	-1.05317700
H	0.88995500	-1.44278700	1.26278500



C	-2.35031000	-0.01418600	-0.37828500
C	-2.51340500	-0.56813300	0.99961100
C	1.78730600	1.26795500	0.56668300
C	1.44486100	0.04300000	0.00577900
C	0.18260800	-0.24260500	-0.52892800
C	-0.99194800	0.68985100	-0.62108800
H	-3.16099400	0.68909000	-0.59872000
H	-1.65174800	-0.88248700	1.57450100
H	2.77593300	1.43647900	0.97229500
H	0.03132400	-1.23176900	-0.95351400
H	-1.02040300	1.14613600	-1.62122900
C	2.51021700	-1.04464400	-0.06227400
H	3.18326900	-0.99459800	0.79475600
H	2.06366700	-2.03960000	-0.07963400
H	3.11875600	-0.94027800	-0.96476700
H	1.09308100	2.09406400	0.62377300
H	-3.49686000	-0.76401900	1.40703700
H	-2.45937900	-0.81693100	-1.12891400
H	-0.89262200	1.51648600	0.08542600

TS44:

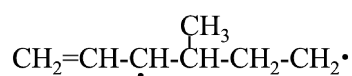
C	-1.92407400	-0.32965300	0.18477800
C	-1.44798500	1.08044200	-0.27130300
C	-0.12583300	1.50281200	0.31412500
C	1.18340500	-0.17958400	-0.37654200
C	0.46858100	-1.21946900	0.17776300
C	-0.94787700	-1.42738500	-0.14301300
H	-2.89993900	-0.54339900	-0.25825600
H	-2.23568800	1.79841700	0.00179100
H	0.38923300	2.33881000	-0.15015100
H	0.88583700	-1.72964500	1.04804900
H	-1.32234100	-2.40267100	-0.43649800
C	2.60197000	0.14482400	0.02674900
H	2.82039800	-0.21576400	1.03341700
H	3.31956700	-0.31882000	-0.65777500
H	2.78706400	1.22036200	0.00714800
H	-0.00641700	1.43928300	1.39172300
H	-1.39260100	1.10063500	-1.36518200
H	-2.08634400	-0.28336800	1.27557800
H	0.89210900	0.16423800	-1.36519400



C	-1.13109300	-0.42280200	0.57216100
C	-2.08595600	0.13021100	-0.52283000
C	-3.25926100	0.87144200	0.02926500
C	1.85548900	0.41730600	0.15810100
C	1.31329100	-0.82120700	-0.16159400
C	-0.00360300	-1.24279600	0.01178300
H	-1.72389000	-1.03994000	1.25748300
H	-2.42375000	-0.71723600	-1.14321300
H	-3.80381000	1.58552100	-0.57501900
H	1.99525900	-1.54760100	-0.59854000
H	-0.25631700	-2.24668500	-0.31508700
C	3.29208700	0.78430200	-0.05975000
H	3.85677400	-0.04179800	-0.49593900
H	3.39294200	1.64665000	-0.72896000
H	3.78464800	1.06570800	0.87820800
H	-3.65843500	0.62931800	1.00692800
H	-1.51511300	0.76935700	-1.20482900
H	-0.75497100	0.41610300	1.16150600
H	1.22093700	1.18187100	0.59464400

TS45:

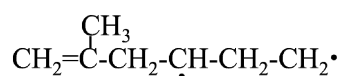
C	-2.06122500	-0.35348200	0.42765800
C	-1.04061700	1.53256700	-0.31480900
C	0.34605600	1.25572100	0.19981700
C	1.00146600	-0.06262200	-0.32634300
C	0.19057800	-1.28755000	0.02815100
C	-1.25840700	-1.27076300	-0.19887800
H	-3.10354500	-0.25032400	0.15144000
H	-1.63450600	2.28345200	0.19682200
H	1.02326500	2.07879900	-0.07599300
H	0.71444000	-2.21178200	0.25400200
H	-1.65478100	-1.81959100	-1.05361500
C	2.45884600	-0.18164700	0.15316700
H	2.50340300	-0.24214300	1.24337600
H	2.93241000	-1.07820300	-0.25257400
H	3.04820300	0.68163700	-0.16264900
H	0.34209000	1.23002400	1.29590500
H	-1.21085700	1.46551300	-1.38438000
H	-1.79826000	0.03752100	1.40259100
H	1.01795300	0.03174900	-1.42750400



C	-2.61850600	0.64461900	-0.75518800
C	2.61191000	0.92893100	-0.31180100
C	1.43425900	0.64676400	0.56267700
C	0.33395600	-0.22844100	-0.11099200
C	-0.88623400	-0.30513300	0.76855800
C	-2.18053800	0.09470300	0.44027400
H	-3.65568500	0.91722700	-0.89203400
H	3.59742300	1.08980800	0.10516100
H	1.75549500	0.16240500	1.49205900
H	-0.72314000	-0.72599100	1.75734200
H	-2.93071300	-0.04356400	1.21421800
C	0.86949500	-1.64439700	-0.42949500
H	1.12483800	-2.17501400	0.49187700
H	0.12067600	-2.23340900	-0.96093300
H	1.76903900	-1.58812100	-1.04509300
H	0.95996700	1.59166900	0.87483300
H	2.47963500	1.10532500	-1.37284800
H	-1.95590400	0.82297100	-1.59133800
H	0.07232000	0.25442900	-1.05744200

TS46:

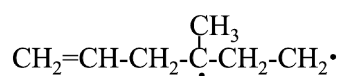
C	-1.92046700	-0.15259600	-0.12929200
C	-1.37582800	1.22274400	-0.47179500
C	0.54642300	1.20744800	0.81688300
C	1.09881100	0.05870700	0.32422800
C	0.35652800	-1.24850600	0.56615900
C	-0.92763000	-1.28021700	-0.22950500
H	-2.78382500	-0.38592200	-0.76883300
H	-1.89356700	2.08820900	-0.07073000
H	0.97219300	2.17658500	0.58766500
H	0.12580200	-1.33574100	1.64108200
H	0.98066800	-2.10740500	0.31129400
C	2.18197600	0.05567200	-0.71921600
H	3.01050700	-0.59860600	-0.42738600
H	1.80947100	-0.32124100	-1.68011000
H	2.58760000	1.05479500	-0.88371300
H	-0.11900500	1.18068800	1.67091900
H	-0.92796800	1.35892300	-1.44972100
H	-2.32608100	-0.11014100	0.89627400
H	-1.19467600	-2.17964900	-0.77150600



C	-1.75539900	-0.48580900	0.21135900
C	-2.99074900	0.25569300	0.60843300
C	2.01885500	-1.13019800	0.61035500
C	1.45685200	-0.07977300	0.00145100
C	0.46811700	-0.25223900	-1.15201200
C	-0.93048900	0.20525400	-0.83265400
H	-2.03181200	-1.50151100	-0.13128500
H	-3.81303100	-0.25321100	1.09416500
H	2.71907000	-1.00870300	1.42791000
H	0.46068700	-1.31356100	-1.43943200
H	0.83905400	0.30122600	-2.02062300
C	1.75219100	1.34605700	0.40357500
H	2.17979900	1.90658500	-0.43416800
H	0.83663700	1.86745700	0.69644200
H	2.45432000	1.39276500	1.23596700
H	1.80132000	-2.14769000	0.30878600
H	-3.03941600	1.33360200	0.52037100
H	-1.11885600	-0.68626800	1.09461100
H	-1.40403900	0.95539700	-1.45579100

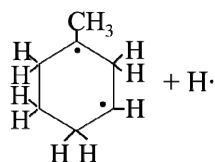
TS47:

C	-1.80299800	-0.34978100	0.77472700
C	-1.03451500	1.58478500	-0.41405000
C	0.36295300	1.32180900	-0.02526500
C	0.92163100	-0.06374700	0.03389000
C	0.15186800	-1.23218600	-0.46844300
C	-1.31620700	-1.24120900	-0.12295700
H	-2.86331700	-0.24682700	0.96276800
H	-1.53241100	2.46640400	-0.03093600
H	0.93788000	1.78774900	-0.86041500
H	0.63677300	-2.15955100	-0.13789500
H	0.20638900	-1.28877300	-1.57388300
C	2.39524900	-0.21515900	0.28110500
H	2.81858900	0.68491200	0.73522700
H	2.59988900	-1.05136700	0.95785800
H	2.97956000	-0.41603400	-0.63325600
H	0.66727200	1.89846000	0.85559200
H	-1.41276400	1.19972100	-1.34910900
H	-1.12092100	0.08099700	1.50456200
H	-1.98482700	-1.78276700	-0.78454900

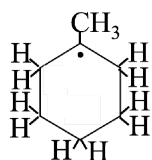


C	-2.88318300	0.41918500	0.18350700
C	2.45822800	1.12974100	-0.16017300
C	1.73090100	0.02866300	0.55085400
C	0.53404300	-0.52974000	-0.18522900
C	-0.51584500	0.41799400	-0.72355400
C	-1.59319000	0.74068500	0.29789200
H	-3.60451900	0.66422500	0.95301100
H	2.98467500	1.89799600	0.39147700
H	2.42289700	-0.80617200	0.75482500
H	-0.99000200	-0.01595400	-1.61037900
H	-0.03163500	1.34944800	-1.03633200
C	0.18025000	-1.97750600	-0.02194400
H	-0.37105600	-2.17069600	0.91203600
H	-0.46131000	-2.32635500	-0.83544200
H	1.07259600	-2.60867800	0.00235600
H	1.43822400	0.38674400	1.55440700
H	2.59051700	1.09269300	-1.23427800
H	-3.26717600	-0.09760700	-0.68926800
H	-1.25043500	1.26023100	1.18946900



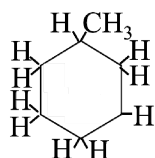


C	-1.90419600	0.29492000	-0.30806000
C	-1.24517900	-1.10233200	-0.34503300
C	0.22717900	-1.00873200	-0.79844000
C	1.02477200	-0.02119200	0.00864600
C	0.39714700	1.30686300	0.35119500
C	-1.09488600	1.26366400	0.49734100
H	-2.92210700	0.22487500	0.08364200
H	-1.80196900	-1.76234200	-1.01551400
H	0.69766500	-1.99580100	-0.75101300
H	0.67139000	2.04732700	-0.44144000
H	0.85776400	1.71702800	1.25863900
C	2.51563900	-0.14586500	0.07472600
H	3.00880600	0.29151100	-0.81050000
H	2.92619500	0.37314900	0.94554400
H	2.83162600	-1.19105100	0.12356900
H	0.24104300	-0.72556100	-1.86846400
H	-1.28525200	-1.54387300	0.65456900
H	-2.00717800	0.64951000	-1.35002900
H	-1.58945800	2.05382000	1.05013800
H	-1.15138200	-3.66254800	5.23860800

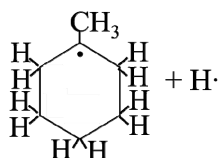


C	1.90038900	0.00000000	0.20480000
C	1.16580600	-1.26864400	-0.26408200
C	-0.30110400	-1.28693700	0.22399100
C	-1.02958700	0.00000700	-0.05658700
C	-0.30109800	1.28694300	0.22399400
C	1.16580700	1.26863600	-0.26408700
H	2.92774800	0.00000400	-0.16974800
H	1.68502800	-2.16327200	0.09029400
H	-0.83533100	-2.13032300	-0.22412200
H	-0.29709600	1.48279000	1.31333500
H	-0.83532000	2.13033000	-0.22412200
C	-2.52596800	-0.00000100	-0.12752100
H	-2.98924500	-0.00003200	0.87449300

H	-2.90619300	0.88509700	-0.64468300
H	-2.90617400	-0.88508000	-0.64473000
H	-0.29709500	-1.48278000	1.31333100
H	1.17880700	-1.30553200	-1.35856700
H	1.96555300	-0.00000200	1.29977200
H	1.17880600	1.30551400	-1.35857300
H	1.68503900	2.16326400	0.09027500

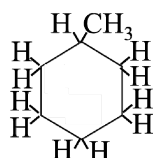


C	1.95755400	0.09786700	0.22095100
C	1.26011400	-1.21083500	-0.22647600
C	-0.21851100	-1.23506200	0.20300600
C	-1.00472800	-0.02233700	-0.34115600
C	-0.32506700	1.30088400	0.10933900
C	1.15144700	1.30661600	-0.14547900
H	2.96328500	0.15566700	-0.20224300
H	1.78898700	-2.07415100	0.18659500
H	-0.69164200	-2.16116800	-0.13756300
H	-0.52559100	1.41907900	1.19064300
H	-0.80881900	2.15106200	-0.37909000
C	-2.48267300	-0.06317800	0.07442300
H	-2.58150100	-0.03523100	1.16351400
H	-3.03200200	0.78942300	-0.33251800
H	-2.96778500	-0.97498000	-0.28212800
H	-0.28107800	-1.23616700	1.29904200
H	1.31943800	-1.29215900	-1.31676200
H	2.09265000	0.05000500	1.31662300
H	1.64830000	2.22419100	-0.43717500
H	-0.95305900	-0.05930000	-1.43659700



C	1.90282000	-0.07957600	0.16231200
C	1.18401500	-1.01627500	-0.82502300
C	-0.30642900	-1.19314200	-0.45433500
C	-1.00857300	0.11471200	-0.20351000
C	-0.28487200	1.14724500	0.61898000
C	1.20461200	1.29033800	0.23153300

H	2.94887000	0.04521800	-0.13092400
H	1.67678400	-1.99194900	-0.85318800
H	-0.82361700	-1.75672500	-1.23694500
H	-0.33585200	0.87336900	1.69015300
H	-0.78818400	2.11566000	0.53938500
C	-2.49878600	0.18989600	-0.33693400
H	-3.01626700	-0.21508500	0.55003400
H	-2.84263200	1.22132600	-0.45239600
H	-2.85725900	-0.38555600	-1.19472500
H	-0.36104900	-1.82545100	0.45241400
H	1.25418700	-0.59473800	-1.83335600
H	1.90869600	-0.53622000	1.15960300
H	1.27379400	1.77711000	-0.74703400
H	1.71280500	1.94199100	0.94752400
H	-0.90699500	-3.38813900	5.95131900



C	1.91257300	-0.00019300	0.28525000
C	1.19830200	-1.27196600	-0.21011700
C	-0.29506700	-1.26729200	0.16964200
C	-1.02358000	-0.00001600	-0.33071400
C	-0.29508000	1.26747500	0.16919300
C	1.19857800	1.27195400	-0.20966100
H	2.95553400	-0.00024000	-0.04371000
H	1.68608200	-2.16200500	0.19732700
H	-0.78808600	-2.15853300	-0.23062600
H	-0.39232300	1.32095000	1.26116100
H	-0.78778800	2.15849500	-0.23195700
C	-2.50565100	-0.00001300	0.07491300
H	-2.61034900	-0.00183700	1.16378500
H	-3.02083900	0.88422300	-0.30840600
H	-3.02163100	-0.88246600	-0.31142600
H	-0.39162400	-1.32001400	1.26171300
H	1.29236700	-1.33580200	-1.30070200
H	1.92987300	-0.00040800	1.38165200
H	1.68624400	2.16164500	0.19868000
H	-0.97126100	-0.00024200	-1.42839000
H	1.29335200	1.33653300	-1.30013000



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