

Direct observation of *para*-xylylene as the decomposition product of the *meta*-xylyl radical using VUV synchrotron radiation

SUPPORTING INFORMATION

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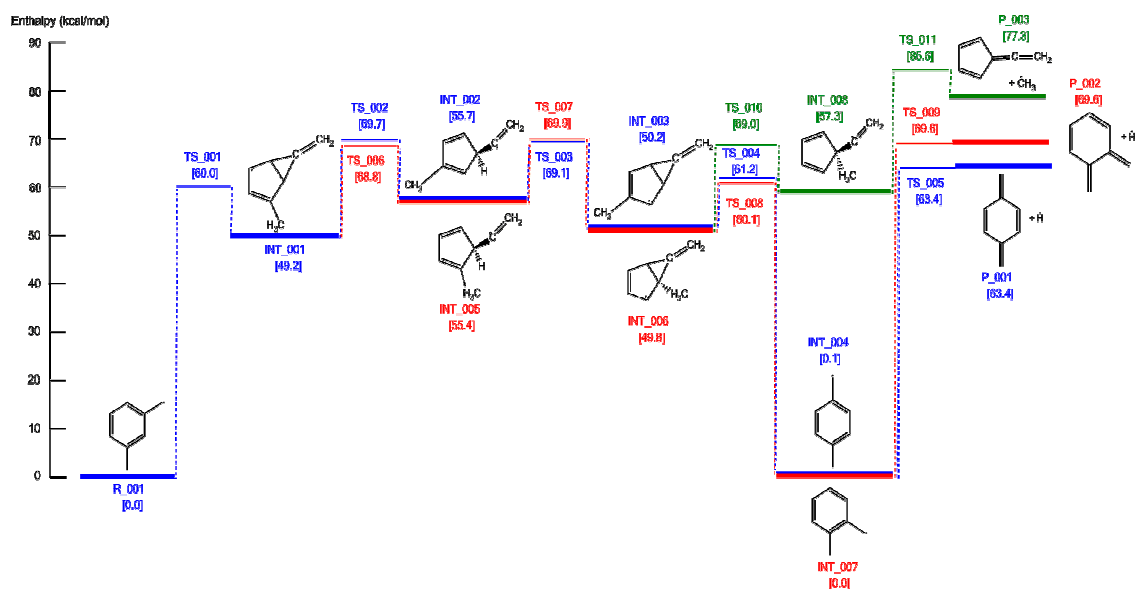


Figure S1. Energy diagram for isomerization and decomposition of the *m*-xylyl radical.

Energies are 298 K enthalpies calculated at the G4 level of theory. Blue pathway indicates isomerization to *p*-xylyl, red pathway indicates isomerization to *o*-xylyl, green pathway indicates dissociation to fulvenallene + CH₃

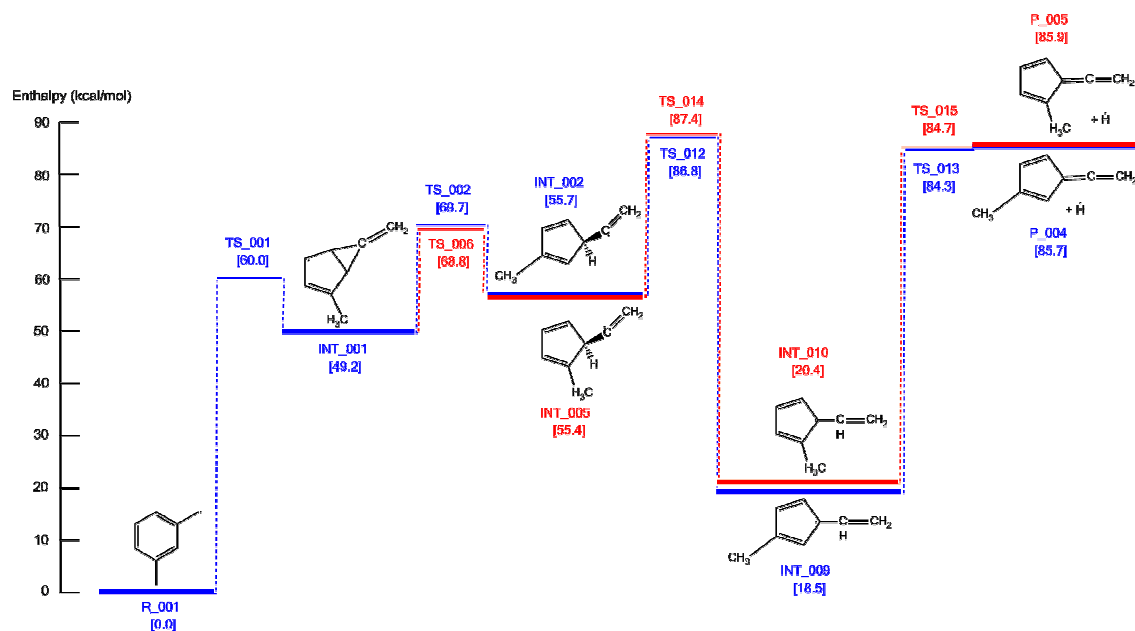


Figure S2. Energy diagram for isomerization and decomposition of the *m*-xylyl radical. Energies are 298 K enthalpies calculated at the G4 level of theory. Blue (red) pathway indicates dissociation to 3 (2)-methylfulvenallene.

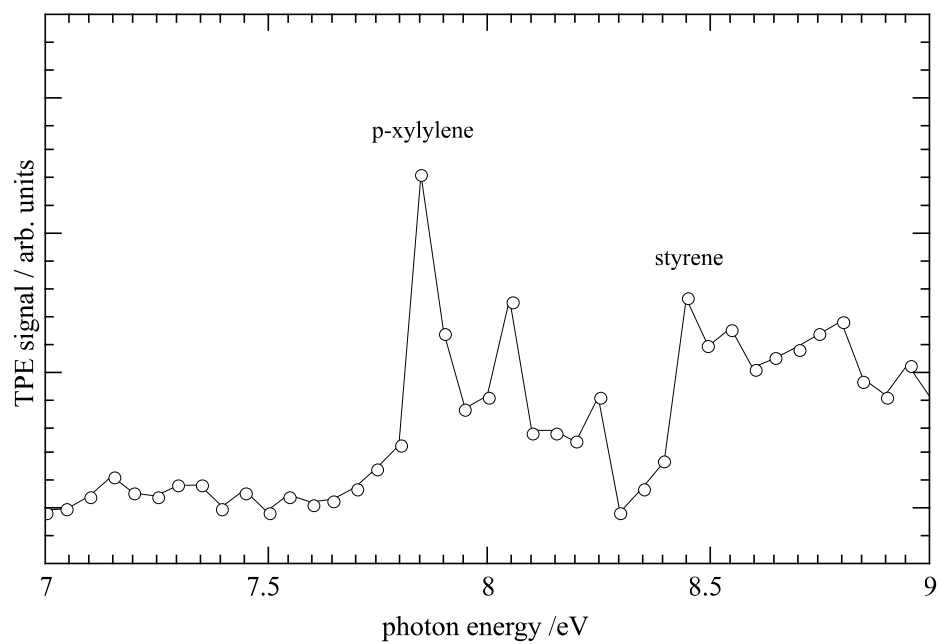


Figure S3. Threshold photoelectron spectrum of the pyrolysis products of *m*-xylyl bromide, showing the presence of *p*-xylylene and styrene.

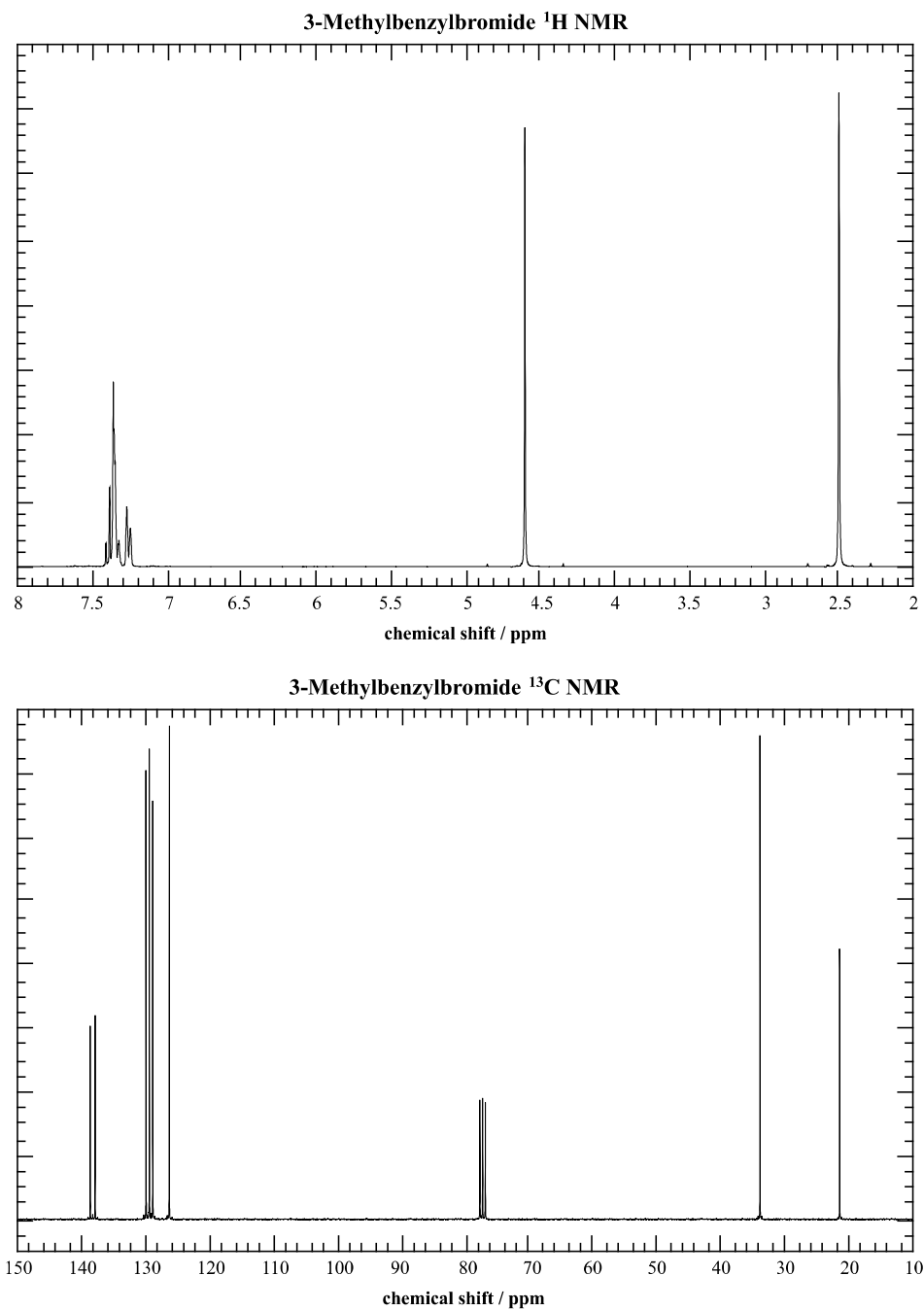


Figure S4. ^1H and ^{13}C NMR spectra of the 3-methylbenzylbromide (*m*-xylyl bromide) precursor.

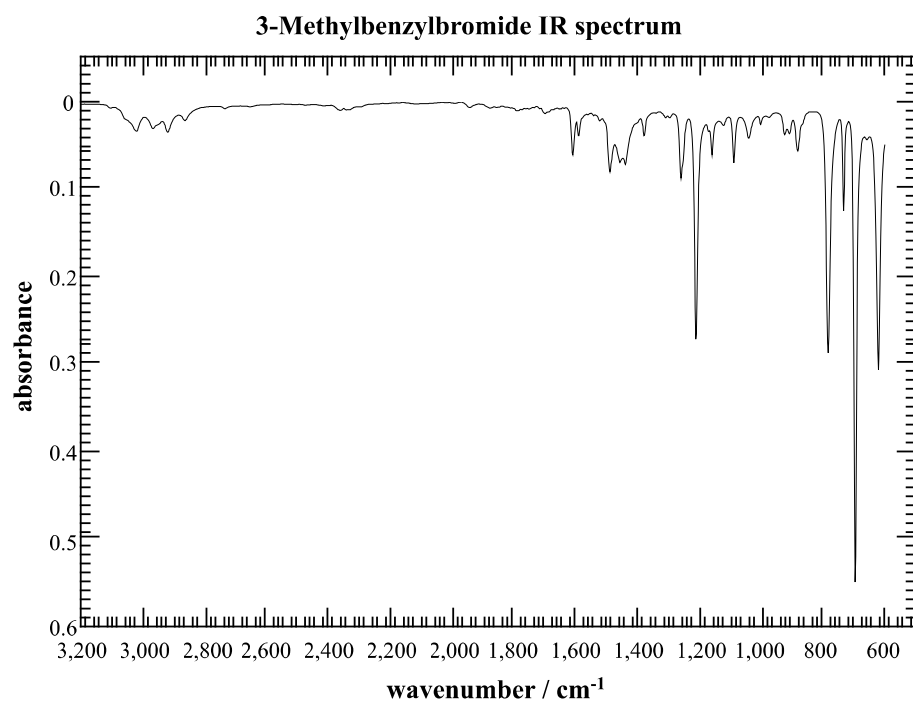
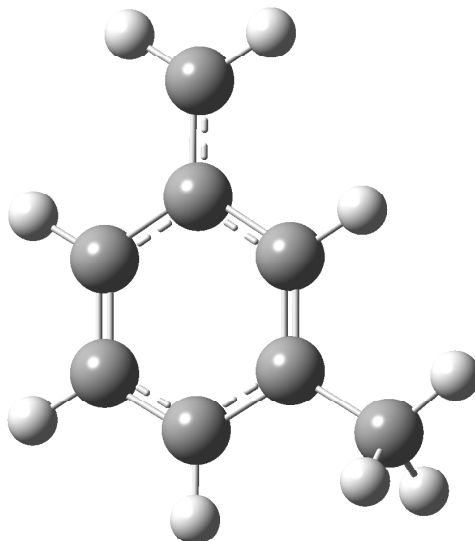


Figure S5. Infrared spectrum of 3-methyl benzylbromide (*m*-xylyl bromide).

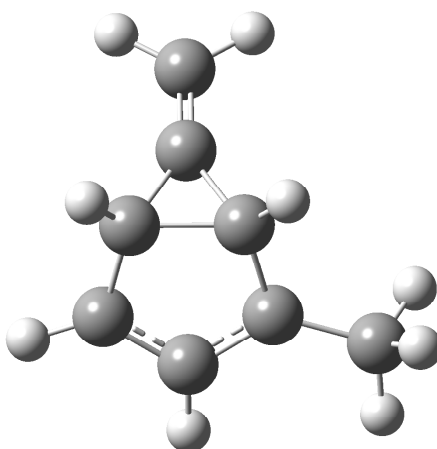
Co-Ordinates for optimised geometries on *m*-methylbenzyl energy surface.

R_001 (m-methylbenzyl)



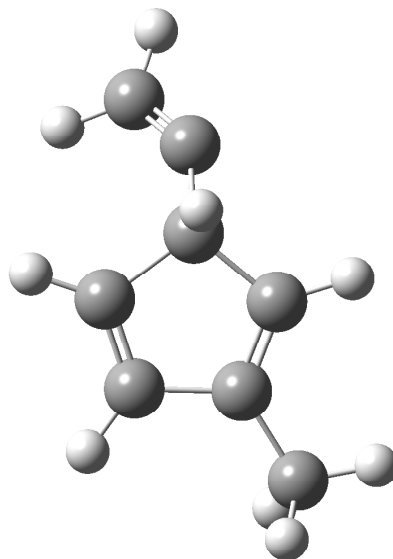
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C	-0.01399500	-0.98417600	-0.00004000
C	1.27578400	-0.37844200	-0.00000600
C	1.32838600	1.04305700	0.00003100
C	0.16530000	1.79100900	0.00002600
H	-1.98889200	1.76424900	-0.00002600
H	-0.07272400	-2.06929600	-0.00007900
H	2.29700600	1.53296600	0.00004900
H	0.22153600	2.87508000	0.00003600
C	2.44434800	-1.15355800	-0.00001500
H	3.42389800	-0.69037800	0.00001100
H	2.39930700	-2.23621300	-0.00004500
C	-2.53518000	-0.90378500	0.00002400
H	-3.12072500	-0.61418200	-0.87996600
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H	-3.11986900	-0.61576500	0.88111300

INT_001



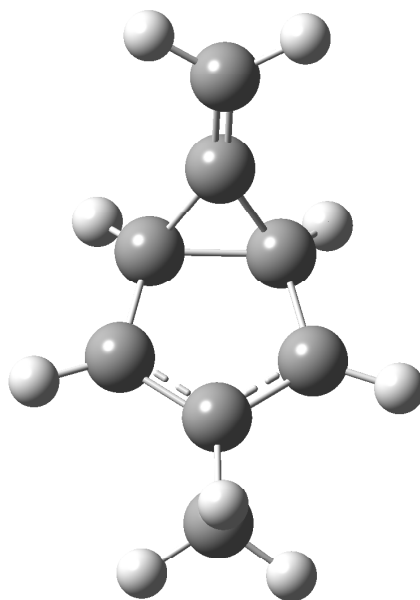
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C	1.36966900	-0.43409000	0.03260100
C	0.96534300	0.85458300	0.63815400
C	0.11694500	1.75276900	-0.19172800
H	-1.84050700	1.53595100	-1.15648000
H	0.06799600	-1.00001200	1.73199400
H	1.57278100	1.25687000	1.44489600
H	0.42288600	2.73876900	-0.51439100
C	2.27753700	-1.12199400	-0.62387600
H	3.17832800	-0.65202800	-1.00863200
H	2.16169100	-2.18619100	-0.80965000
C	-2.26165400	-1.14446100	-0.07855200
H	-1.94603300	-2.04985000	-0.61623800
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INT_002



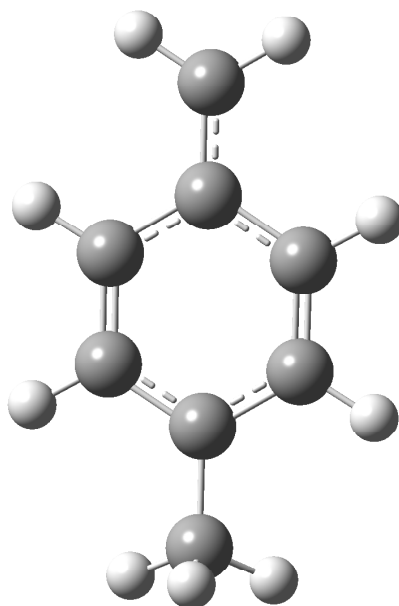
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C	1.99982200	-0.61088900	0.11318600
C	0.36494200	1.29457500	0.31404800
C	-0.89753800	1.24610800	-0.13807200
H	1.01925600	2.15378400	0.36627700
H	-1.47327400	2.08281000	-0.51790200
C	2.91541900	-0.27822300	-0.76038900
H	2.91598000	0.69224700	-1.26497600
H	3.72468700	-0.95177700	-1.03413700
C	-2.80281500	-0.52387100	-0.46187400
H	-2.97652200	-1.59250500	-0.31235600
H	-3.56452100	0.02684800	0.10344400
H	-2.97207000	-0.29703100	-1.52153800
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INT_003



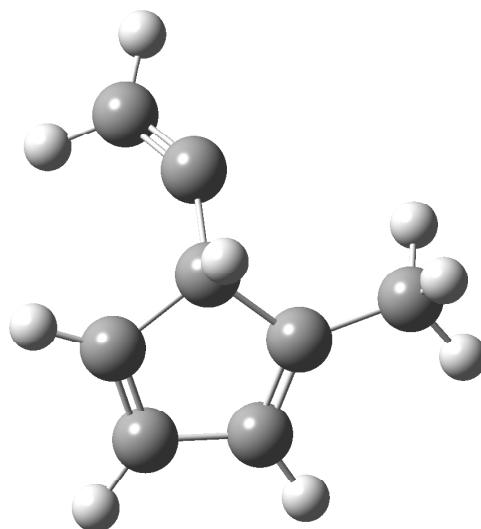
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C	1.61873600	0.00001300	0.13392100
C	0.75175000	-0.77840600	-0.78130400
C	-0.59929300	-1.14219500	-0.28092000
H	1.22578800	-1.36090000	-1.56715000
H	-0.92934700	-2.16271800	-0.13215500
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H	2.98875100	-0.92576900	1.42581300
H	2.98877300	0.92563800	1.42591400
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H	-2.66564700	0.00024100	1.72594900
H	-3.28278400	0.88556800	0.33037200
H	-3.28257500	-0.88589800	0.33079000
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INT_004



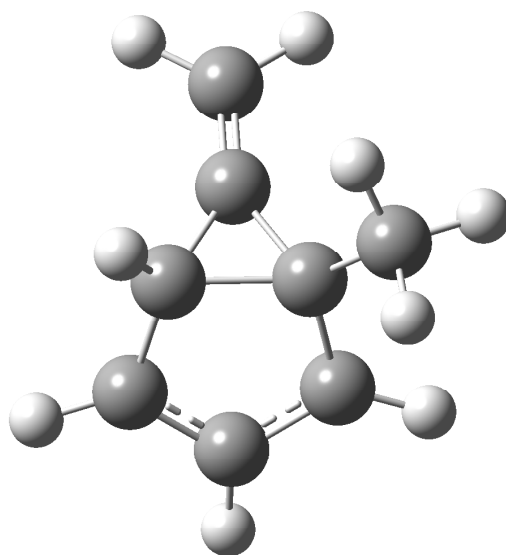
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C	0.75141400	-1.21162400	-0.00212500
C	1.50055500	-0.00009900	0.00336100
C	0.75328700	1.21172500	-0.00166300
H	-1.16750500	2.14641700	-0.01638400
H	1.28753400	-2.15590200	-0.00427700
H	-1.16946100	-2.14430300	-0.01727300
H	1.29014900	2.15555900	-0.00342200
C	2.90182100	-0.00137300	0.00890300
H	3.46182300	-0.92901600	0.01117300
H	3.46344800	0.92529000	0.01158600
C	-2.86024300	-0.00035600	0.01263000
H	-3.26932100	-0.83138300	-0.57067000
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INT_005



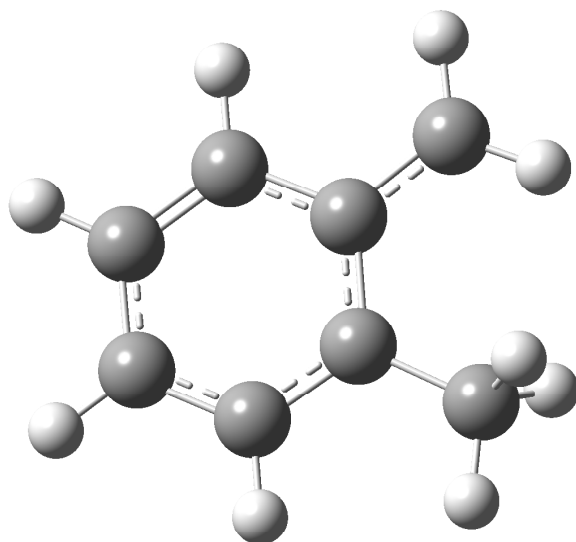
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C	-1.56722600	0.61117400	0.14566000
C	-0.24374100	-1.50963800	0.43360200
C	0.89839400	-1.77024200	-0.22316300
H	-1.00161400	-2.20951500	0.75635200
H	1.25076000	-2.74846700	-0.52799900
C	-2.66052500	0.32829400	-0.51511200
H	-2.88804300	-0.68462000	-0.85918300
H	-3.40043000	1.08727400	-0.76006700
H	2.58110700	-0.45804400	-0.97515600
C	1.28600100	1.97434200	0.01067300
H	1.39078300	2.38211200	1.02443400
H	2.22680300	2.14625000	-0.51928100
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INT_006



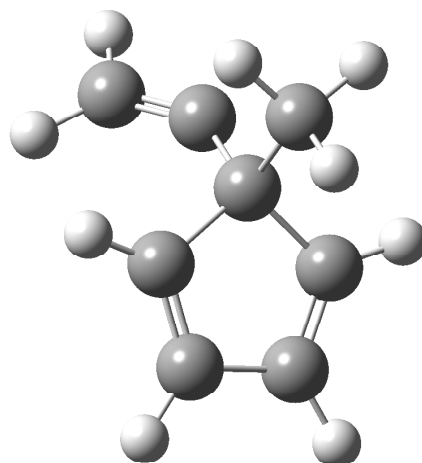
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C	-0.90271100	-0.70342400	-0.08233100
C	0.13101800	-0.51704700	0.96691900
C	1.53149200	-0.85381900	0.59984900
H	2.90224900	-0.15367300	-0.96423500
H	-0.18923300	-0.53443300	2.00605400
H	2.11107700	-1.62933500	1.08275400
C	-1.82687900	-1.48098400	-0.60206000
H	-1.98150000	-2.49632500	-0.24760000
H	-2.46861300	-1.14120700	-1.41037900
H	0.98401300	1.51660000	-1.67817000
C	-1.10094100	1.84041100	0.40355900
H	-0.47812400	2.59251900	0.89932200
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INT_007



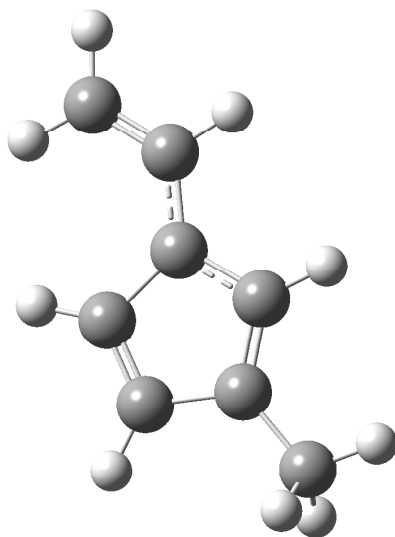
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C	0.88918700	1.32215300	-0.00002700
C	1.99052100	0.48973700	-0.00004400
C	1.81258100	-0.89704100	-0.00003100
H	0.38806300	-2.50623400	0.00001200
H	1.02062100	2.40006800	-0.00003700
H	2.99026400	0.91151900	-0.00006600
H	2.67041600	-1.56076200	-0.00004500
C	-1.52878100	1.69044000	0.00001400
H	-1.36578100	2.76191100	0.00000100
H	-2.55401900	1.34607700	0.00003300
C	-1.98410800	-1.23025800	0.00005100
H	-2.56287100	-0.92555400	0.88023400
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H	-1.92554600	-2.32150900	0.00008800

INT_008



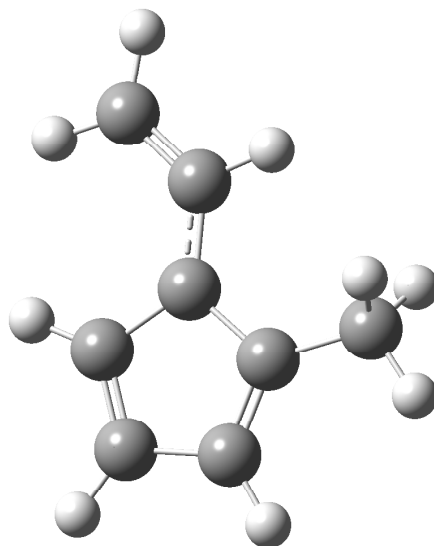
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C	-1.50457900	-0.14905900	-0.45109700
C	0.41939100	-0.41916000	1.08793700
C	1.60491700	-0.88217100	0.65806600
H	-0.05369200	-0.59696800	2.04430600
H	2.28716800	-1.51192400	1.21625300
C	-2.33073700	-1.13750200	-0.21963100
H	-2.14740100	-1.88639100	0.55577600
H	-3.24515100	-1.26900500	-0.79443100
H	0.68658600	0.85522000	-2.05582700
C	-0.43744800	1.89752200	0.48155300
H	-0.85666700	2.50232500	-0.32747600
H	-1.13649300	1.92457500	1.32220200
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H	2.74151500	-0.62238200	-1.28285400

INT_009



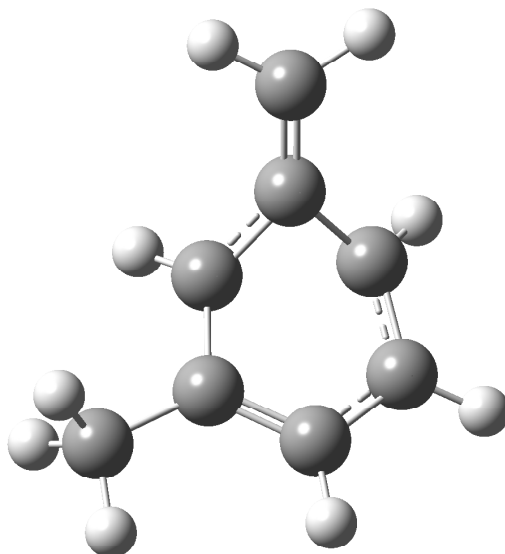
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C	-0.73317200	-0.18353400	-0.00005800
C	-2.05384400	-0.70512800	-0.00010500
C	-0.33157300	1.22795000	0.00004400
C	1.02261400	1.27259400	0.00008800
H	-1.00946900	2.06920800	0.00004800
H	1.64453000	2.15858900	0.00015700
C	-3.20032400	0.01980300	0.00000800
H	-3.19403700	1.10410100	0.00014900
H	-4.17084200	-0.46237300	-0.00003500
C	2.99208200	-0.46217800	0.00008400
H	3.14246400	-1.54473300	-0.00087200
H	3.50353400	-0.04550800	-0.87765300
H	3.50297600	-0.04719200	0.87895700
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INT_010



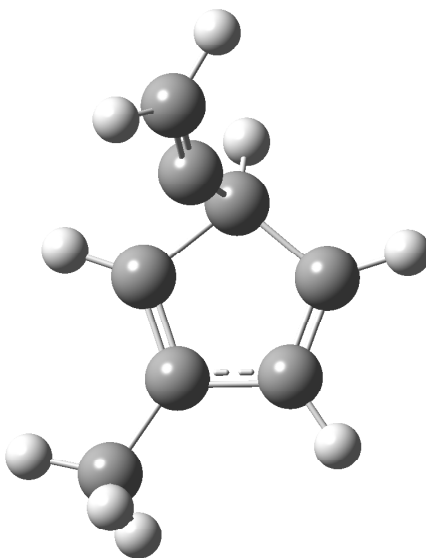
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C	-0.37845100	-0.09286600	-0.00012500
C	-1.62373500	0.58087800	-0.00011400
C	-0.14489100	-1.52376000	0.00019200
C	1.20157700	-1.72117900	-0.00001200
H	2.94457700	-0.26618800	-0.00051500
H	-1.58233900	1.66838600	-0.00022000
H	-0.91116400	-2.28479400	0.00041200
H	1.71413900	-2.67437600	0.00003200
C	-2.85179400	-0.00415200	0.00006700
H	-2.97424800	-1.08151100	0.00021900
H	-3.75757000	0.59086400	0.00007300
C	1.15074700	2.05143000	0.00020900
H	0.71020800	2.53612500	-0.88024500
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H	2.22008500	2.27996300	-0.00054400

TS_001



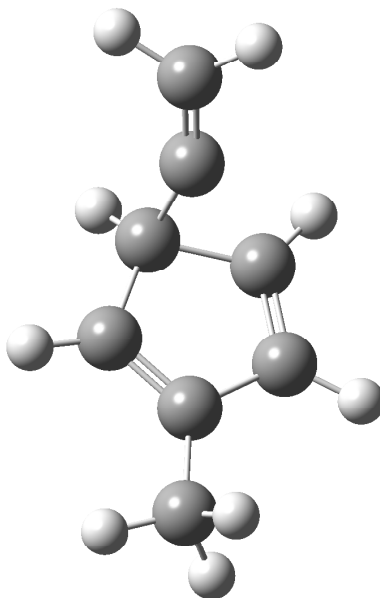
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C	0.07805200	1.77574100	-0.07216300
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C	1.33825300	-0.41690300	-0.03203600
C	0.08583400	-0.66499700	0.63447600
C	-1.16871100	-0.18250000	0.02345800
H	1.89471200	1.39648300	1.06839700
H	0.05420100	-1.29330000	1.52303000
C	2.37072300	-1.10983300	-0.49220000
H	2.32295800	-2.18876000	-0.59529000
H	3.29796100	-0.62013600	-0.77020900
H	-1.95195500	1.60032600	-0.92330200
C	-2.34682800	-1.10095700	-0.06350500
H	-3.22952500	-0.57778000	-0.44097700
H	-2.14983700	-1.95667400	-0.72267000
H	-2.59080600	-1.51993700	0.92181500
H	0.16752900	2.85726500	-0.06966000

TS_002



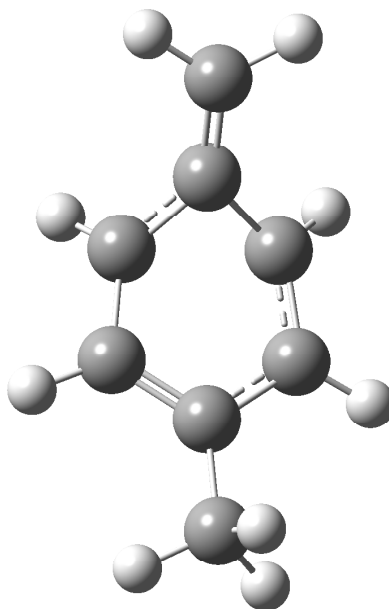
C	-1.06593100	1.15069000	-0.46732600
C	0.15282100	1.61952400	-0.10572400
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C	1.59976500	-0.37242600	-0.08278400
C	-0.16229500	-0.53644000	0.78627500
C	-1.28553500	-0.17877000	0.05926100
H	0.60192000	2.56281900	-0.38389500
H	-1.77678500	1.67389000	-1.09719000
C	2.70628800	-0.87674400	-0.56262900
H	2.73468800	-1.81674100	-1.11101500
H	3.66822600	-0.36312000	-0.45912800
C	-2.48820200	-1.02722000	-0.21069200
H	-3.41706100	-0.48338400	-0.00114500
H	-2.53712500	-1.34131200	-1.26207100
H	-2.48290700	-1.93272800	0.40232900
H	1.33194300	0.94121600	1.65233300
H	-0.03577600	-1.41892500	1.39666600

TS_003



C	-0.82618400	1.20770200	-0.25445900
C	0.43771800	1.28868700	0.29341400
C	0.78086600	-0.04854900	0.92882200
C	1.73339700	-0.12932600	-0.16871100
C	-0.46709400	-0.85127700	0.67990300
C	-1.37579100	-0.10860300	-0.00598900
H	1.07167300	2.15907200	0.37329300
H	-1.31699100	1.98165400	-0.83060600
C	2.81813500	-0.56542600	-0.75116400
H	3.18721400	-0.15477000	-1.68954400
H	3.40683600	-1.38970200	-0.33429000
C	-2.72188900	-0.56157000	-0.48652500
H	-3.51520500	0.10321700	-0.12549300
H	-2.77485000	-0.55302300	-1.58160700
H	-2.94674000	-1.57564500	-0.14648900
H	1.18457000	-0.07371000	1.94837500
H	-0.57145900	-1.88691700	0.97461800

TS_004

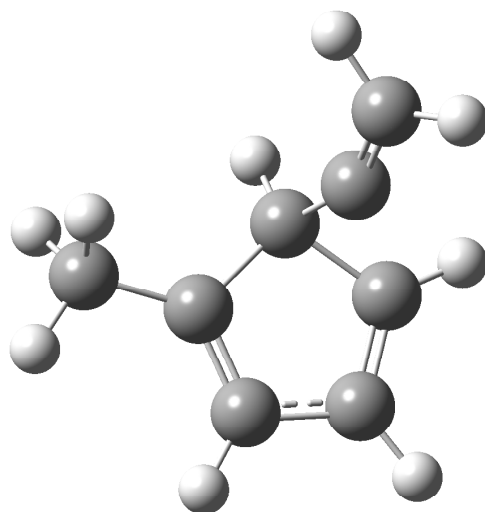


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C	-0.76051700	1.01195900	-0.50923800
C	-1.58324000	-0.03115600	0.13239100
C	-0.76761100	-0.91355300	-0.66012600
C	0.63052300	-1.14212300	-0.25930200
H	1.11186100	2.11902600	-0.39509700
H	-1.28579700	1.74986300	-1.11110000
H	-1.20798700	-1.46820600	-1.48612300
H	1.01699600	-2.15463000	-0.19583700
C	-2.72729600	-0.04811000	0.80022000
H	-3.23258000	-0.98128100	1.02615400
H	-3.19661300	0.87025900	1.13683100
C	2.77689300	-0.02153700	0.54302000
H	2.82935900	0.26080600	1.60169400
H	3.23963700	-1.00757400	0.44264200
H	3.39237400	0.69912100	-0.00846100

TS_005

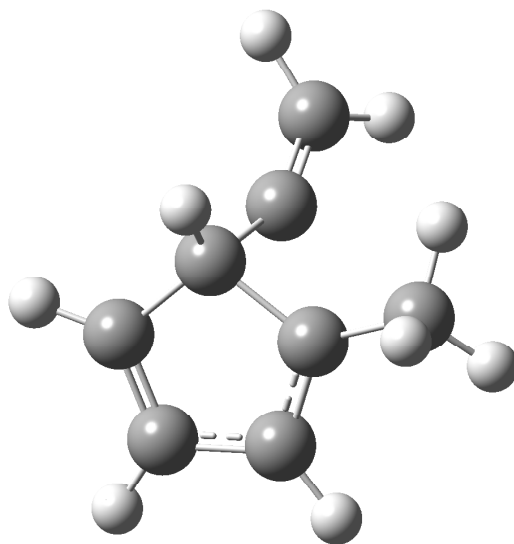
Could not obtain TS structure explicitly. Performed a scan to confirm a barrierless transition structure.

TS_006



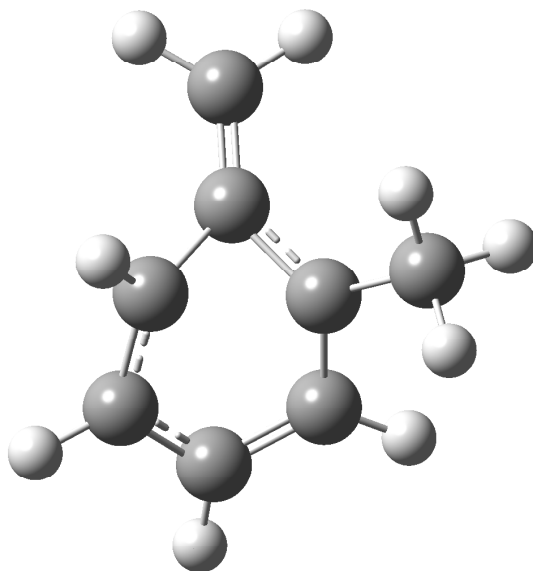
C	0.29034800	-0.07558600	0.79730800
C	0.41034800	1.41460400	0.52509500
C	-0.65416700	1.80486600	-0.26407100
C	-0.98369500	-0.45339700	0.07206200
C	-1.48958500	0.66150400	-0.52027400
C	1.45391100	-0.15677300	-0.06907600
C	2.54272400	-0.73440700	-0.50451700
H	3.22057800	-0.25548200	-1.20899300
H	2.82349000	-1.74717800	-0.19582000
H	1.16484700	2.03839700	0.98008000
H	0.38987000	-0.45280800	1.82341000
H	-0.80844900	2.79425700	-0.67326300
H	-2.38173500	0.68086200	-1.13579400
C	-1.49299700	-1.85420200	0.02486800
H	-2.40984100	-1.92340900	-0.56698900
H	-0.75157100	-2.53119300	-0.41988700
H	-1.70851000	-2.24309300	1.02888500

TS_007



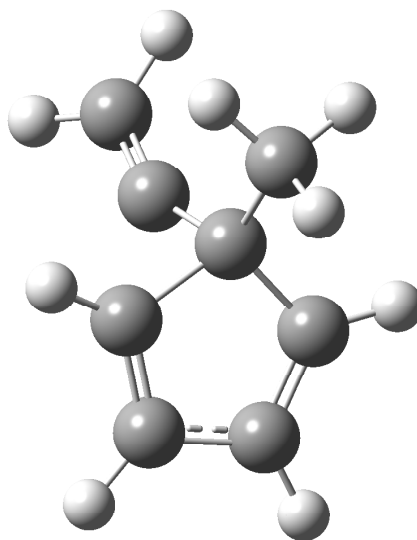
C	1.39028500	0.59185600	-0.64882100
C	1.86716200	-0.73311000	-0.36620100
C	1.03014300	-1.36073500	0.49976500
C	-1.18148700	-0.53725000	-0.14493000
C	-0.11135200	-0.44061200	0.83886600
C	0.22147000	0.83008800	0.06144700
H	2.74929400	-1.17330200	-0.81539900
H	1.85066300	1.28974900	-1.33636900
C	-2.36199800	-0.93502600	-0.54122900
H	-2.81299100	-0.59859700	-1.47327700
H	-2.95382200	-1.65356800	0.03586500
C	-0.45944000	2.14903200	0.27433600
H	-0.00194800	2.68535600	1.11636300
H	-0.37154500	2.78809600	-0.60948700
H	-1.52180600	2.02552300	0.49802700
H	1.09085000	-2.38176200	0.84945000
H	-0.39739300	-0.36695800	1.89542700

TS_008



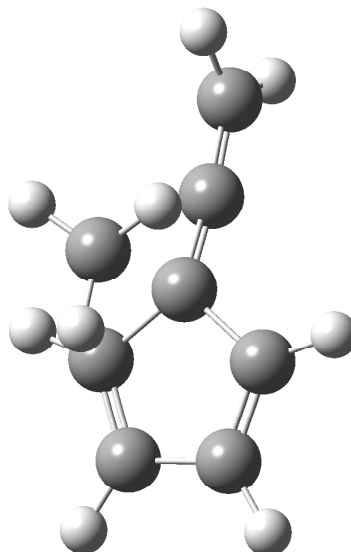
C	1.96775100	0.13186300	-0.45717000
C	1.61154300	-0.89830000	0.45201800
C	0.23143300	-0.99539200	0.77273300
C	-0.83335900	-0.68388800	-0.19851800
C	-0.34655600	0.66100100	-0.02332300
C	0.93678600	0.99880500	-0.67725300
H	2.95411600	0.23522000	-0.89106900
H	2.34567600	-1.50575100	0.97063800
H	-0.08088200	-1.44782400	1.71109200
H	1.00522600	1.89323000	-1.28821200
C	-1.91565200	-1.30808400	-0.64259000
H	-2.66547200	-0.78887800	-1.23050000
H	-2.08635100	-2.35844800	-0.43110100
C	-1.18996200	1.74156600	0.59668900
H	-0.59767200	2.40797400	1.23239200
H	-1.63954000	2.36273100	-0.19230300
H	-2.00700700	1.31632200	1.18354500

TS_010



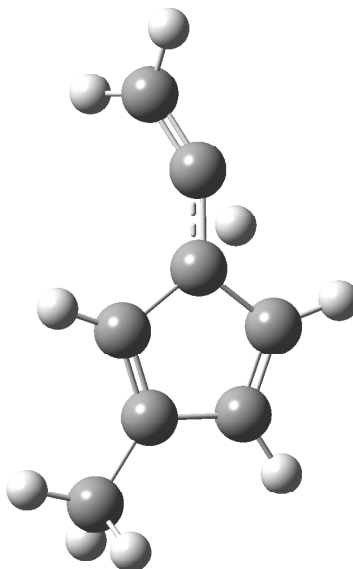
C	0.81036800	0.48524500	-1.07141200
C	1.89024700	-0.23748800	-0.68562800
C	1.68753800	-0.76365300	0.64192400
C	-1.11662300	-0.64389900	-0.09238100
C	0.45647800	-0.34545800	1.10093300
C	-0.22425000	0.50132800	0.03112900
H	2.76727100	-0.42867000	-1.29221800
H	0.65226700	0.97451100	-2.02310600
C	-2.24744300	-1.23258500	-0.37799700
H	-3.04628100	-0.72165000	-0.92587200
H	-2.45318700	-2.26858400	-0.11272000
C	-0.82289500	1.86140900	0.39569600
H	-0.03186200	2.55514900	0.69697000
H	-1.35125400	2.29056000	-0.46166200
H	-1.53634300	1.76294300	1.21842100
H	2.36823700	-1.42319700	1.16332400
H	0.03063700	-0.49045200	2.08328000

TS_011



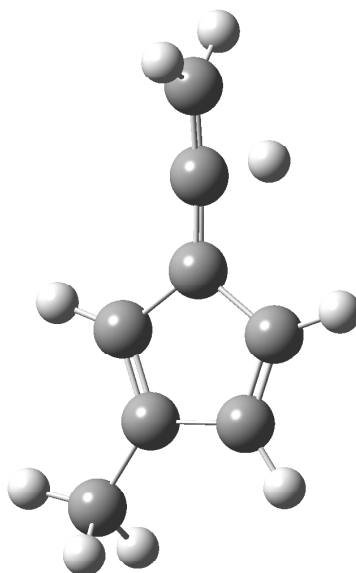
C	-0.64935500	-0.25764700	-1.17988300
C	-1.90743800	-0.46252600	-0.73142900
C	-1.90743200	-0.46250800	0.73145500
C	-0.64934600	-0.25761900	1.17989400
H	-0.29922000	-0.21913800	-2.20086800
H	-2.78834800	-0.59859400	-1.34546900
H	-2.78833800	-0.59856200	1.34550500
H	-0.29920400	-0.21908600	2.20087600
C	0.24321700	-0.11353900	0.00000000
C	1.53281900	-0.51464600	0.00000000
C	2.81844200	-0.69133500	-0.00000200
H	3.27152600	-1.68156400	0.00000800
H	3.51291600	0.15120500	-0.00001500
C	0.27745000	2.12354800	-0.00002700
H	-0.78647400	2.32475400	-0.00002500
H	0.81350300	2.32931800	0.91969700
H	0.81349500	2.32929500	-0.91976000

TS_012



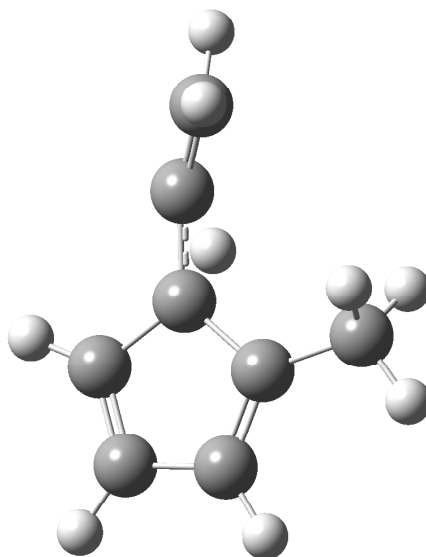
C	-1.27119100	1.20928000	0.14372700
C	-1.47363500	-0.23602600	0.00823200
C	-0.26186000	-0.82801600	-0.16896600
C	0.76679300	0.22535600	-0.16404200
C	0.04833300	1.49952200	0.03594700
H	-0.05114800	-1.87921500	-0.30221400
H	-2.07159300	1.92342500	0.29118100
C	2.18563100	0.06561300	-0.14198300
C	3.21247600	-0.65805300	0.24750500
H	4.17813000	-0.62212100	-0.24884700
H	3.14788500	-1.29427100	1.13431100
H	1.41561400	0.39786600	-1.24479800
H	0.53189200	2.46407000	0.08932400
C	-2.81208300	-0.90460500	0.05334500
H	-3.32382900	-0.70920300	1.00374200
H	-3.47167000	-0.53141100	-0.74018700
H	-2.72206600	-1.98756800	-0.06510600

TS_013



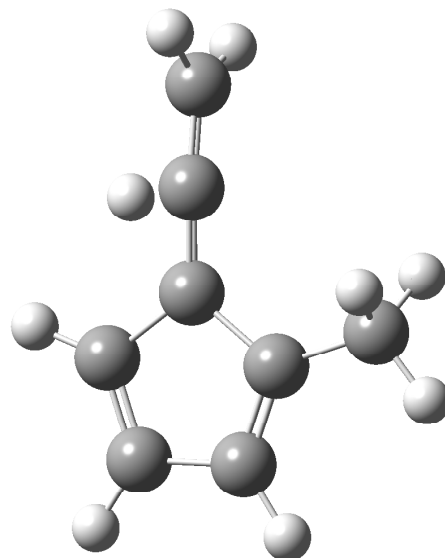
C	-0.35274700	-0.89013600	0.00453600
C	-1.52084400	-0.20240900	-0.01051000
C	-1.20727300	1.24048100	-0.02763600
C	0.13187500	1.41499700	-0.02355200
C	0.74978400	0.07819500	-0.01225700
H	-1.95636400	2.02245000	-0.04513700
H	0.68897300	2.33993600	-0.03059900
H	-0.21969200	-1.96207100	0.02124900
C	2.05031700	-0.18608400	0.01154300
H	2.12330500	-0.10881800	2.18400000
C	3.30938000	-0.44786100	-0.18132400
H	4.01147400	-0.57827400	0.63466900
H	3.69872900	-0.54500700	-1.19271400
C	-2.90977500	-0.75492100	-0.01479300
H	-3.48025100	-0.40213000	0.85358300
H	-3.46441800	-0.43188200	-0.90477100
H	-2.90605900	-1.84776800	0.00367700

TS_014



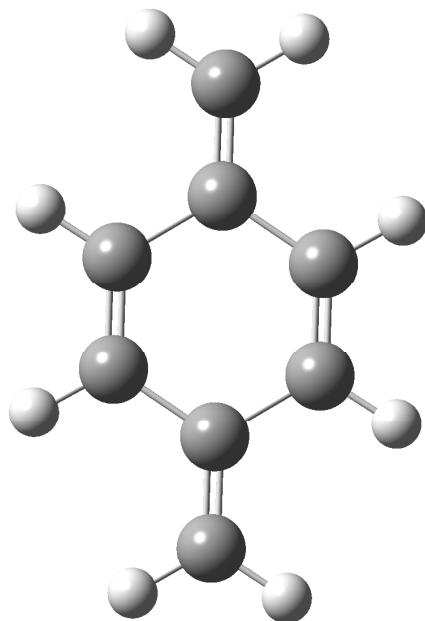
C	-2.03452300	-0.89737800	-0.12879000
C	-1.81470600	0.54280100	-0.12386400
C	-0.49146700	0.81682900	0.02910100
C	0.19525200	-0.49570500	0.14581900
C	-0.84748500	-1.53332500	0.03736200
H	-3.00111600	-1.37157600	-0.23539900
C	1.60303100	-0.73747500	0.16161000
C	2.80912500	-0.42082500	-0.25291400
H	3.70649400	-0.68448200	0.30036700
H	2.96563200	0.08137900	-1.21142700
H	0.76223400	-0.72396600	1.25854800
H	-0.65178200	-2.59453600	0.08099900
C	0.19412200	2.14306400	0.08560900
H	0.78229400	2.26432700	1.00376400
H	0.89155700	2.28106900	-0.74953900
H	-0.53749300	2.95484700	0.04767600
H	-2.59790800	1.28503000	-0.21858000

TS_015



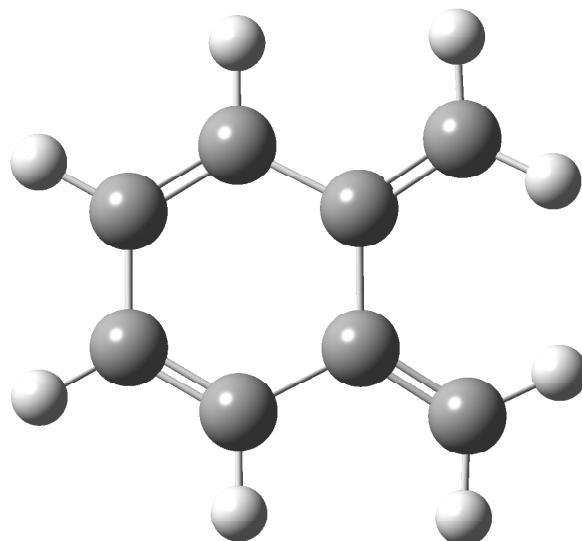
C	0.64262900	0.78015800	-0.01993700
C	1.90260100	0.28326500	-0.03299500
C	1.86111600	-1.18449800	-0.02083400
C	0.57317600	-1.59469900	0.00135600
C	-0.26920800	-0.38915700	-0.00837000
H	2.73544600	-1.82219800	-0.03291300
H	0.18917100	-2.60351400	0.01427500
C	-1.59483600	-0.35002100	0.01659800
H	-1.63429900	-0.10958300	2.16400000
C	-2.88116400	-0.32590200	-0.17498200
H	-3.59376800	-0.29076600	0.64140000
H	-3.28257700	-0.34218500	-1.18603600
H	2.81114100	0.87209100	-0.05177900
C	0.19300700	2.20461100	-0.01351400
H	-0.45625200	2.42986400	-0.86813200
H	-0.38300600	2.44182800	0.88919700
H	1.05021500	2.88192100	-0.05394200

P_001 (p-xylylene)



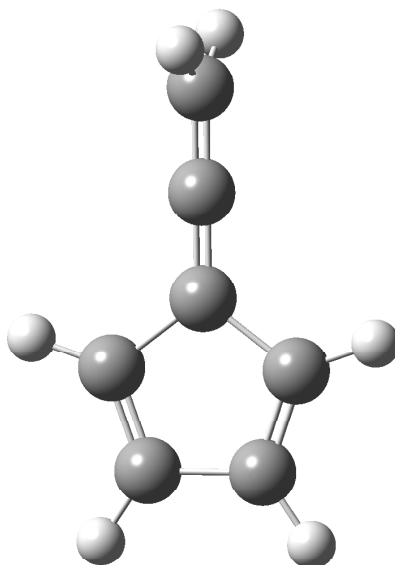
C	-0.08536400	1.40579200	0.00000000
C	1.22613200	0.76612100	0.00000000
C	1.22613200	-0.69304100	0.00000000
C	0.08536400	-1.40579200	0.00000000
C	-1.22613200	-0.76612100	0.00000000
C	-1.22613200	0.69304100	0.00000000
H	-0.11359100	2.49163000	0.00000000
H	0.11359100	-2.49163000	0.00000000
H	2.18954800	-1.19475300	0.00000000
H	-2.18954800	1.19475300	0.00000000
C	-2.37045500	-1.48157800	0.00000000
H	-2.36079700	-2.56596000	0.00000000
H	-3.34123600	-0.99833700	0.00000000
C	2.37045500	1.48157800	0.00000000
H	3.34123600	0.99833700	0.00000000
H	2.36079700	2.56596000	0.00000000

P_002 (o-xylylene)



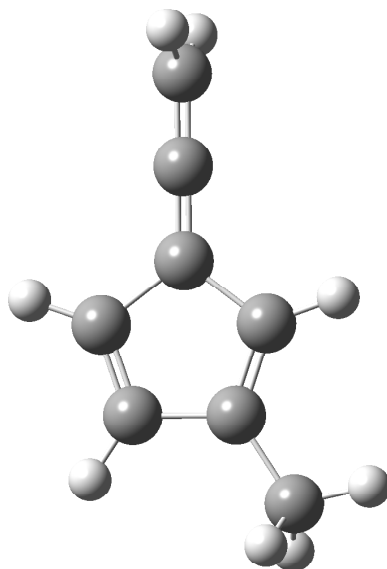
C	0.62034400	-0.74683800	-0.00134400
C	0.62034300	0.74683800	0.00134300
C	-0.67496500	1.40574700	-0.13457400
C	-1.83408700	0.71980000	-0.08534200
C	-1.83408700	-0.71980100	0.08534200
C	-0.67496400	-1.40574700	0.13457300
H	-0.67301300	-2.48712700	0.23173000
H	-2.78368800	1.24001400	-0.15586900
H	-0.67301400	2.48712600	-0.23173200
H	-2.78368800	-1.24001500	0.15587000
C	1.73300900	-1.48946500	-0.17115200
H	1.68550100	-2.57246800	-0.13964200
H	2.70539700	-1.05127200	-0.35999600
C	1.73300800	1.48946600	0.17115300
H	1.68549900	2.57246900	0.13964300
H	2.70539700	1.05127300	0.35999700

P_003 (fulvenallene)



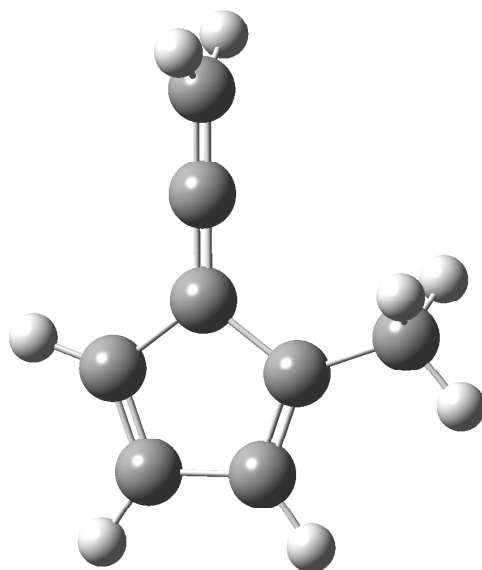
C	-0.59676300	1.17991400	-0.00002000
C	1.60257000	-0.00019000	0.00000100
C	0.28556400	-0.00008300	0.00000000
C	-0.59694300	-1.17994500	0.00002000
C	-1.87367200	-0.73351800	0.00000300
C	-1.87356100	0.73368500	-0.00000800
H	-2.76519100	1.34696800	-0.00001600
H	-0.24351300	-2.20014000	0.00003800
H	-2.76539400	-1.34666600	0.00000800
C	2.89965700	0.00009100	0.00000300
H	3.46808500	0.00008700	-0.92673900
H	3.46808300	-0.00003100	0.92674600
H	-0.24317900	2.20005600	-0.00003600

P_004 (3-methylfulvenallene)



C	-1.48407100	-0.20118100	0.00001500
C	-0.31899600	-0.89287400	-0.00004800
C	0.79057700	0.07261700	0.00003200
C	2.08031700	-0.19289000	-0.00000300
C	0.17269500	1.41129900	-0.00002900
C	-1.16672000	1.23909500	0.00005000
H	0.73065700	2.33591600	-0.00006800
H	-1.91379600	2.02335000	0.00007700
C	3.35180700	-0.45168700	-0.00003700
H	3.90959800	-0.56553500	-0.92645200
H	3.90963600	-0.56555300	0.92635200
C	-2.87518300	-0.75028700	0.00003300
H	-2.87381700	-1.84341600	-0.00011000
H	-3.43727200	-0.41195800	0.87954100
H	-3.43738300	-0.41172500	-0.87931400
H	-0.19017800	-1.96562300	-0.00010300

P_005 (2-methylfulvenallene)



C	1.86947200	0.29652000	-0.00002200
C	0.60458100	0.78087700	0.00000200
C	-0.29804700	-0.39764300	-0.00004800
C	-1.61354300	-0.37262900	-0.00002600
C	0.56169500	-1.59483200	0.00004200
C	1.84437100	-1.16995100	-0.00001700
H	2.77163100	0.89563900	-0.00002200
H	0.18986500	-2.60845500	0.00009200
H	2.72590500	-1.79787600	-0.00001000
C	-2.91095800	-0.34119700	0.00000100
H	-3.47990000	-0.32903200	0.92642700
H	-3.47993700	-0.32905900	-0.92640200
C	0.14469400	2.20241000	0.00003200
H	-0.46975200	2.43097400	-0.87921300
H	-0.46974000	2.43094300	0.87929500
H	0.99832900	2.88553400	0.00003900