

# Elucidating the Chemical Dynamics of the Elementary Reactions of the 1-Propynyl Radical ( $\text{CH}_3\text{CC}; \text{X}^2\text{A}_1$ ) with Methylacetylene ( $\text{H}_3\text{CCCH}; \text{X}^1\text{A}_1$ ) and Allene ( $\text{H}_2\text{CCCH}_2; \text{X}^1\text{A}_1$ )

Chao He,<sup>a</sup> Long Zhao,<sup>a</sup> Aaron M. Thomas,<sup>a</sup> Alexander N. Morozov,<sup>b</sup> Alexander M. Mebel,<sup>b,\*</sup>  
Ralf I. Kaiser,<sup>a,\*</sup>

<sup>a</sup> *Department of Chemistry, University of Hawaii 'i at Manoa, Honolulu, Hawaii 96822, USA*

<sup>b</sup> *Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, USA*

## Supporting Information

Optimized Cartesian coordinates and vibrational frequencies for all intermediates, transition states, reactants and products involved in the reactions of the propynyl radical with  $\text{C}_3\text{H}_4$  isomers methylacetylene and allene. The data are given in the format of an input file for the MESS package.

---

\* Corresponding Authors:  
Prof. Ralf I. Kaiser: [ralfk@hawaii.edu](mailto:ralfk@hawaii.edu)  
Prof. Alexander M. Mebel: [mebela@fiu.edu](mailto:mebela@fiu.edu)

```

Well   i1
Species
RRHO
Geometry[angstrom] 13
C      1.878499143663   0.074320087220  -0.010846664302
C      0.696827601612   0.316555020683  -0.029020431809
C      3.301037729715   -0.237961370886  0.013259181454
C      -0.684425450577   0.660458600370  -0.056379556163
C      -1.696053305814  -0.184193036577  0.033154555633
C      -3.162143547967  -0.152325248443  0.037323999303
H      3.904240649576   0.653756523986  -0.181515851973
H      3.554336825321  -0.984945508498  -0.745449153612
H      3.601702205406  -0.638125762626  0.986659880389
H      -0.911902822882   1.729462671664  -0.162086863646
H      -3.576432272136  -0.739820781698  -0.788654936126
H      -3.532698580222   0.879650860293  -0.063576467307
H      -3.567660175695  -0.565013055486  0.966984308081

```

```

Core RigidRotor
SymmetryFactor 1.0
End

```

```

Frequencies[1/cm] 33
35.7730      97.0023      121.9173
191.7035     248.9584     251.9076
353.1394     423.7221     493.1980
779.4265     788.9218     940.9038
1041.9837    1050.2681    1050.9349
1057.2879    1196.8857    1293.1013
1395.7622    1416.4735    1450.6500
1472.4331    1478.5188    1479.9298
1727.4004    2337.2804    2962.8300
2996.6655    3017.7072    3044.4150
3066.0778    3071.3489    3076.5515

```

```

ZeroEnergy[kcal/mol] -60.1
ElectronicLevels[1/cm] 1
0 2
End
End

```

```

!-----
!-----c6h7_i2-----
Well   i2

```

```

Species
RRHO
Geometry[angstrom] 13
C      0.023171620331   0.000168588094  0.016676507866

```

C	0.003368154470	-0.006717807747	1.473474874582
C	-0.014087631878	-0.012438214196	2.680607794569
C	-0.053937479750	-0.019344903535	4.109066847061
C	1.021320538016	-0.015476739701	4.879540319046
C	2.483507843895	-0.004814714313	4.765324153608
H	-0.992384863217	-0.003949495308	-0.389686583153
H	0.543111650683	-0.878601862153	-0.377059929053
H	0.532661523767	0.888646371920	-0.368845797715
H	-1.041170937486	-0.028323588091	4.570693574620
H	2.913049901392	0.878497338869	5.249123905794
H	2.788972986049	0.002170348165	3.708897974919
H	2.925290693550	-0.886502322022	5.240995357911

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 33

8.4520	88.4468	104.6886
184.4378	226.3479	334.3562
373.2888	438.9542	568.7975
765.9380	806.0515	919.6624
1041.2495	1048.8050	1050.9366
1054.4730	1182.1608	1305.0697
1389.9509	1416.1599	1454.6234
1466.3820	1478.4592	1479.5816
1710.1607	2326.1343	2976.7631
3018.9900	3049.2868	3068.1205
3072.3753	3078.4952	3095.8441

ZeroEnergy[kcal/mol] -60.4

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c6h7\_i3-----

Well i3

Species

RRHO

Geometry[angstrom] 13

C	-1.277718118822	0.045903691276	0.106852857632
C	-0.072370423869	0.068814920642	0.065014990407
C	-2.733805105716	0.023603819728	0.130340307141
C	1.358986762243	0.083016317514	0.080763280134
C	2.060262242515	0.309467182135	-1.015770185569
C	2.027906800906	-0.176489429165	1.427061264601

H	-3.110523490910	-0.180980578309	1.136692238684
H	-3.125888866838	-0.749175097798	-0.537878713021
H	-3.146873162556	0.983801679717	-0.193431857149
H	3.106366028860	0.374201509685	-1.277716880488
H	3.114930340823	-0.145997253826	1.339876273121
H	1.731406918247	-1.157066614826	1.809891341556
H	1.710422078949	0.575988868170	2.154373085030

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 33

31.1842	115.8319	147.3710
182.5187	305.1917	348.3289
348.4363	553.0021	553.5498
638.5390	660.6732	856.5890
967.5613	1032.2400	1050.1226
1055.0547	1059.8408	1248.4345
1394.2265	1416.3709	1477.4492
1478.8605	1479.0607	1483.2348
1647.8530	2334.7959	3020.2215
3026.9940	3075.3148	3079.3695
3087.5248	3115.3635	3232.1491

ZeroEnergy[kcal/mol] -56.6

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c6h7\_i4-----

Well i4

Species

RRHO

Geometry[angstrom] 13

C	0.020530470173	-0.001117242222	-0.004022817950
C	-0.000469804751	0.004652232006	1.452237984514
C	-0.010515933945	0.009373846780	2.659451697727
C	-0.045879066072	0.015173783288	4.092583266645
C	-1.407729367578	0.029050828278	4.759910914882
C	1.083516167364	0.008433705116	4.780241906969
H	-0.994017570716	0.005738355423	-0.412979578979
H	0.529724839747	-0.890655823392	-0.387351030424
H	0.544405880842	0.876869057887	-0.394141957861
H	2.141227059647	-0.001192206586	4.561787369560
H	-1.304237549999	0.032361694972	5.845419864211

H	-1.985987603394	-0.849625173591	4.460137361889
H	-1.971329519889	0.914882917283	4.453358019063

Core RigidRotor  
SymmetryFactor 1.0  
End

Frequencies[1/cm] 33

31.3800	113.7297	149.4791
182.4024	300.5503	348.3634
349.2910	529.2800	538.4827
662.3445	678.7620	830.4258
1002.2180	1047.3370	1053.7582
1054.2969	1059.4362	1254.9205
1401.7389	1416.3864	1478.2514
1478.7526	1480.7448	1481.9631
1639.8176	2323.3657	3019.8273
3028.4955	3074.8243	3079.0856
3084.6962	3120.9765	3236.7588

ZeroEnergy[kcal/mol] -57.0

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c6h7\_i5-----

Well i5

Species

RRHO

Geometry[angstrom] 13

C	2.588340293379	-0.465418673579	0.006710185677
C	1.515240788040	0.540565792229	0.049861209986
C	0.227924996570	0.677017411625	0.043635736033
C	-0.991253136490	1.472972511361	0.073862240343
C	-1.165321782479	0.175482848962	0.001726041129
C	-2.053875304011	-1.000774705092	-0.071397459998
H	3.242539926351	-0.334870877858	-0.862820782176
H	2.169839640537	-1.482752678108	-0.052855189538
H	3.223881368242	-0.430342358681	0.898876794816
H	-1.428196876284	2.458820828398	0.122652027848
H	-1.848359870568	-1.573422307075	-0.981144878741
H	-3.106805009681	-0.709104167373	-0.066735061605
H	-1.866941033606	-1.668576624846	0.775301136853

Core RigidRotor  
SymmetryFactor 1.0  
End

Frequencies[1/cm] 33

112.0501	117.6767	135.9239
187.6721	262.2818	288.7270
461.6761	493.1371	634.6647
745.3713	753.8956	951.2658
985.3987	1033.1357	1045.0396
1051.9461	1110.1456	1174.2203
1397.9729	1403.9710	1458.5241
1473.2560	1478.1590	1486.4928
1726.3058	1897.0678	2952.7157
3021.6969	3023.5445	3042.0855
3076.4427	3098.5260	3231.1066

ZeroEnergy[kcal/mol] -37.4

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c6h7\_i7-----

Well i7

Species

RRHO

Geometry[angstrom] 13

C	0.460232104219	0.004116193754	-0.270558641163
C	-0.066231695487	0.013051960986	1.081209458693
C	-0.487572562989	0.020214452796	2.240376460279
C	-0.990517006123	0.026280992600	3.460647295436
C	-1.295988422818	0.039368097803	4.734221423089
C	-2.692784720848	0.005893445520	5.305449853039
H	1.554660775035	-0.063836545747	-0.277449781809
H	0.072464851413	-0.847036268395	-0.840797837100
H	0.181938706838	0.917173767654	-0.807559099195
H	-0.486029476760	0.077698670811	5.469390880592
H	-3.444959044153	-0.031599873376	4.516799968484
H	-2.823095866769	-0.867837408162	5.953562984293
H	-2.878068636096	0.892219514087	5.922323037291

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 33

17.2758	43.1626	114.7958
140.7434	171.8383	304.8717
368.9529	418.2412	513.5602
660.0272	718.6464	930.9224

```

1026.8514      1039.9276      1047.4995
1071.9997      1161.6909      1348.1503
1398.7755      1411.0922      1466.4532
1471.2040      1482.0511      1489.3971
1861.0439      2100.5802      2999.3184
3012.2194      3035.7138      3048.1187
3057.7995      3062.6398      3116.0203
ZeroEnergy[kcal/mol] -67.6
ElectronicLevels[1/cm]  1
0 2
End
End
!-----
!-----h_c6h6_p1-----
Bimolecular  p1
Fragment      c6h6
RRHO
Geometry[angstrom] 12
C              3.365282791149  -0.082133147797  -0.000000425991
C              1.911503033387  -0.089067631603  -0.000002755194
C              0.701537927149  -0.093855808742  -0.000003351954
C             -0.663329431652  -0.098558409645  -0.000003086570
C             -1.873328598624  -0.102370304170  -0.000002041362
C             -3.327084109973  -0.105074359874   0.000000047691
H              3.753865194419   0.941037877485  -0.000802317328
H              3.761494812858  -0.591476117645  -0.883941195488
H              3.761483380429  -0.590085894401   0.884744242769
H             -3.719923374624  -0.616413786012  -0.884271570167
H             -3.722357628034   0.915488985963  -0.000143209520
H             -3.719921996485  -0.616164403559   0.884416948828
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 30
26.3687      101.1890      101.3171
243.0578      243.1346      367.8221
367.8513      549.4967      549.5602
559.7189      954.1470      1045.0958
1045.1381      1050.3274      1050.4187
1292.1423      1411.8773      1419.1732
1475.3576      1475.4099      1475.4177
1475.4694      2268.7841      2371.7555
3017.0258      3017.5361      3074.1746
3074.4319      3074.4806      3074.6329

```

```

ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -29.6
End
!-----h_c6h6_p2-----
Bimolecular p2
Fragment c6h6
RRHO
Geometry[angstrom] 12
C 0.150120910350 -0.133919606128 0.136790290630
C -0.064684559278 0.047704199998 1.565759812384
C -0.227707913937 0.194410805890 2.751732697033
C -0.474394428237 0.381793641474 4.141138032770
C 0.419881803061 0.213615995648 5.089386826860
C 1.289833251628 0.052474574405 6.041112801728
H -0.788741484923 -0.041897732866 -0.416992531595
H 0.569093241308 -1.122007153769 -0.076635500473
H 0.844978462846 0.614476031856 -0.256608800732
H -1.479689982319 0.686547614976 4.430301835534
H 1.423715873944 -0.908617365306 6.530156703433
H 1.919647821608 0.871293994095 6.378235832817
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 30
21.0342 94.5615 185.5476
249.5812 312.2358 379.8395
396.3276 550.9486 632.9859
802.3123 880.4000 886.8631
1007.1400 1050.4531 1054.6103
1069.5490 1206.8981 1365.1171
1416.2125 1471.3985 1477.9697
1479.4105 2039.5849 2340.1376
3019.6284 3073.9383 3079.2288
3104.3026 3108.0959 3177.2074
ZeroEnergy[kcal/mol] 0.0

```



```

ElectronicLevels[1/cm]  1
0 1
End
Fragment  H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]  1
0 2
End
GroundEnergy[kcal/mol] -23.6
End
!-----ch3_c5h4_p3-----
Bimolecular p3
Fragment  c5h4
RRHO
Geometry[angstrom] 9
C          -2.511175000000  0.000355000000  0.000154000000
C          -1.058306000000 -0.000440000000 -0.000158000000
C          0.151032000000 -0.000518000000 -0.000251000000
C          1.515731000000 -0.000213000000 -0.000120000000
C          2.723235000000  0.000346000000  0.000161000000
H          -2.903515000000 -0.876384000000 -0.523818000000
H          -2.902536000000 -0.014751000000  1.021800000000
H          -2.902292000000  0.892999000000 -0.497195000000
H          3.785238000000  0.000959000000  0.000504000000
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 21
147.8630    147.8866    335.2890
335.2965    539.8279    539.8339
643.5649    643.5729    680.7778
1047.6789   1047.7507   1183.1184
1414.3444   1473.7509   1473.7920
2167.2954   2351.2830   3020.9561
3079.9650   3079.9838   3478.6182
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm]  1
0 1
End
Fragment  ch3
RRHO
Geometry[angstrom] 4
C, 0, 0., 0.0000001995, 0.

```

H, 0, 0., 1.0804553795, 0.  
 H, 0, 0.9357017515, -0.5402277895, 0.  
 H, 0, -0.9357017515, -0.5402277895, 0.  
 Core RigidRotor  
 SymmetryFactor 6  
 End  
 Frequencies[1/cm] 6  
 505.1501            1403.0831            1403.0885  
 3103.6402           3282.6573            3282.6683  
 ZeroEnergy[kcal/mol] 0.0  
 ElectronicLevels[1/cm] 1  
 0 2  
 End  
 GroundEnergy[kcal/mol] -36.3  
 End  
 !-----h\_c6h6\_p4-----  
 Bimolecular p4  
 Fragment c6h6  
 RRHO  
 Geometry[angstrom] 12  
 C, 0, -0.759696, 0., 0.  
 C, 0, 0.12596, 1.178158, 0.  
 C, 0, 0.12596, -1.178158, 0.  
 C, 0, 1.402657, 0.737542, 0.  
 C, 0, 1.402657, -0.737542, 0.  
 C, 0, -2.100626, 0., 0.  
 H, 0, -0.218274, 2.202502, 0.  
 H, 0, -0.218274, -2.202502, 0.  
 H, 0, 2.294557, 1.34981, 0.  
 H, 0, 2.294557, -1.34981, 0.  
 H, 0, -2.667015, -0.924873, 0.  
 H, 0, -2.667015, 0.924873, 0.  
 Core RigidRotor  
 SymmetryFactor 2  
 End  
 Frequencies[1/cm] 30  
 208.9659            344.4463            492.6127  
 636.8016            679.7937            691.3194  
 779.2379            790.9522            807.8704  
 909.0420            929.8510            943.5150  
 962.0616            962.1712            999.7109  
 1102.3399           1104.8600           1252.7553  
 1334.2716           1368.3560           1452.5919  
 1531.9813           1616.7669           1699.6352

```

3135.3788      3196.5225      3206.3028
3220.5810      3223.6554      3229.6272
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment      H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -66.0
End
!-----h_c6h6_p5-----
Bimolecular p5
Fragment      c6h6
RRHO
Geometry[angstrom] 12
C      0.      0.      0.
C      0.      0.      1.47153
C      0.78173  0.      2.5034
C      2.10193  0.      3.17532
C      3.56938  0.      3.01702
C      1.03514  0.      3.9375
H      -0.50203  -0.88218 -0.41332
H      -0.502   0.8822  -0.41332
H      0.61428  0.      4.93152
H      3.88801  -0.87956 2.44899
H      4.07726  0.      3.98439
H      3.88801  0.87957  2.449
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 30
130.0531      135.3324      190.8871
263.0030      319.8387      437.2043
556.4633      633.7750      686.1637
751.9313      768.3806      884.7891
982.5922      1009.6810     1041.1961
1047.1792     1133.4582     1358.9142
1403.2113     1473.2691     1477.7809
1521.1988     1795.8244     2102.2295
3026.7295     3076.1934     3080.1691

```

```

3109.8419      3135.7499      3254.8241
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment      H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -0.3
End
!-----c6h7_ts1-----
Barrier      ts1 i1 p1
RRHO
Geometry[angstrom] 13
C              3.354293504966  -0.121488179749  -0.000050158050
C              1.904068959251  -0.021295986502  -0.000020929817
C              0.698188845679   0.056456956350   0.000000509466
C             -0.671442041734   0.164796021452   0.000029943495
C             -1.864891837133  -0.106889130134  -0.000060582671
C             -3.314268644208  -0.159007668911  -0.000083488482
H              3.815385066118   0.870810580530  -0.000696209761
H              3.711347243113  -0.658425913917  -0.884137440805
H              3.711456326673  -0.657322182143   0.884662790423
H             -0.767794875019   2.045746845129   0.000619797839
H             -3.692917746631  -0.679157179767  -0.885121474553
H             -3.732864785865   0.854746603198   0.000249684710
H             -3.692925015193  -0.679741765526   0.884607558208
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 779.5039
WellDepth[kcal/mol] 36.3
WellDepth[kcal/mol] 5.8
End
Frequencies[1/cm] 32
9.5222          82.4220
98.1990         121.0375      219.4061
242.6997        356.7129      379.7984
494.0327        523.4174      524.8826
630.2406        955.4922      1032.6297

```

```

1048.1794      1049.6430      1051.3682
1281.8939      1408.3274      1416.3536
1466.6094      1471.9500      1474.9213
1475.0661      2190.7028      2347.3999
3006.6320      3019.4471      3062.4890
3076.9987      3077.9574      3077.9833
ZeroEnergy[kcal/mol] -23.8
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c6h7_ts2-----
Barrier  ts2 i1 i5
RRHO
Geometry[angstrom] 13
C          0.005362241942  0.093981437319  0.157797125675
C          -0.027733322788 -0.363469594707  1.543697802639
C          -0.002314163632 -0.282467053334  2.793355420465
C          0.133900719161  0.772145908671  4.186936531538
C          0.285851341276  2.046366825613  4.905950951979
C          -0.011175272132 -0.525535481482  4.196225135863
H          0.835811749107  -0.353341715303 -0.399077066214
H          0.127901702048  1.185578416392  0.105972367720
H          -0.918295931954 -0.155353059835 -0.375625050389
H          -0.098432365694 -1.382615899792  4.857844397956
H          1.222551389555  2.538307227077  4.625518423981
H          0.283529003677  1.899084408805  5.994087488110
H          -0.525852091985  2.733966580100  4.648270470834
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling  Eckart
ImaginaryFrequency[1/cm] 630.2406
WellDepth[kcal/mol] 28.9
WellDepth[kcal/mol] 6.2
End
Frequencies[1/cm] 32
82.3594      105.5250
122.1335      198.4387      224.3082
240.1000      418.0151      423.7397
711.5693      778.0967      870.9375
1013.0451      1037.2757      1041.1812
1055.3997      1091.7651      1250.0055
1394.2660      1408.9592      1463.4319

```

```

1467.1878      1470.4554      1480.3277
1792.2566      1988.8616      2972.9807
2987.6951      3032.6021      3053.0536
3057.5721      3072.1124      3134.1232
ZeroEnergy[kcal/mol] -31.2
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c6h7_ts3-----
Barrier  ts3 i1 p2
RRHO
Geometry[angstrom] 13
C          0.242224968454 -0.240058858005  0.269187706748
C          -0.017080324716  0.042236198094  1.674008521886
C          -0.217281895777  0.268840451313  2.841422879656
C          -0.499095074357  0.559921871799  4.206458748191
C          0.277342294480  0.236769076892  5.214223015574
C          1.074306468056 -0.100233302853  6.196898414738
H          -0.688673362579 -0.272863796823 -0.304432336759
H          0.744965172086 -1.204216773736  0.149133211792
H          0.882386313170  0.527804053837 -0.176153653794
H          -1.428092312051  1.088978912196  4.419814715182
H          2.716138676854 -1.088032461528  5.302634857032
H          0.929095041533 -1.025248942789  6.747059981838
H          1.814117018220  0.593853574102  6.584633940206
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling  Eckart
ImaginaryFrequency[1/cm] 428.063
WellDepth[kcal/mol] 39.3
WellDepth[kcal/mol] 2.8
End
Frequencies[1/cm] 32
18.0043      85.9595
154.1788      210.2840      252.2244
303.2514      323.9833      400.6462
408.0093      550.9847      676.1447
796.9069      887.0370      900.0315
1013.3272      1050.4432      1053.8759
1059.2785      1204.3406      1356.5699
1416.1685      1465.4872      1477.5033
1479.0971      2000.9822      2340.3094

```

```

3020.4785      3075.3904      3080.6412
3096.8050      3112.3231      3185.4428
ZeroEnergy[kcal/mol] -20.8
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c6h7_ts4-----
Barrier  ts4 i1 i2
RRHO
Geometry[angstrom] 13
C          -0.032351560697   0.032307770558  -0.053291023902
C          -0.049310091122  -0.017232538637   1.402777376185
C          -0.051390605375  -0.062789541737   2.608721092855
C          -0.093944241497  -0.100064789136   4.040583767687
C          0.873760659105   -0.532513260207   4.811256488284
C          1.950947429138  -1.009900154597   5.652004192010
H          -0.998200336425   0.360979923822  -0.448322970783
H          0.185150982030  -0.951619888909  -0.480458127210
H          0.730427012511   0.727912918699  -0.417143276098
H          -1.027323592794   0.270961161800   4.485456825696
H          2.880687078786  -0.461664347375   5.454495111618
H          2.152517964395  -2.071923526739   5.466459942925
H          1.735719294760  -0.904276726465   6.727226602375
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling  Eckart
ImaginaryFrequency[1/cm] 274.4071
WellDepth[kcal/mol] 6.0
WellDepth[kcal/mol] 6.3
End
Frequencies[1/cm] 32
12.7785      20.4842
104.9059     194.1049     288.0033
302.9418     388.8273     493.8290
734.4959     788.0058     898.2066
992.0213     1026.0294    1050.5272
1054.6605    1183.1481    1307.5790
1404.2166    1416.6554    1449.0422
1467.1882    1479.0772    1479.8759
1805.2506    2329.2743    2942.5693
2973.2913    3007.6455    3017.2529
3042.8643    3070.2944    3075.8048

```

```

ZeroEnergy[kcal/mol] -54.1
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c6h7_ts5-----
Barrier  ts5 i2 p1
RRHO
Geometry[angstrom] 13
C          0.937899811208  -0.069673071546  -0.547251029879
C          0.240324905137  -0.034116117508   0.727627255079
C         -0.344172889993  -0.006298639147   1.784878853286
C         -0.991989001131   0.031602352964   2.995880069819
C         -1.849905242966  -0.050612096206   3.864992101927
C         -2.669107988353  -0.062998994271   5.061722196449
H          1.980528917636   0.241612558812  -0.431963365151
H          0.933410660904  -1.078989810543  -0.969935787918
H          0.465678825949   0.599769428953  -1.272686669059
H          0.463969279749   0.623980299917   4.033442661336
H         -3.523196124193   0.614102502408   4.965335371672
H         -3.055532901166  -1.065653214888   5.268080436243
H         -2.081079254488   0.257274804387   5.930380905674
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling  Eckart
ImaginaryFrequency[1/cm] 779.5028
WellDepth[kcal/mol] 36.6
WellDepth[kcal/mol] 5.8
End
Frequencies[1/cm] 32
9.9344      82.4287
98.2007     121.0391     219.4076
242.7016    356.7140     379.7997
494.0324    523.4174     524.8821
630.2405    955.4922     1032.6304
1048.1821   1049.6461    1051.3693
1281.8939   1408.3281    1416.3552
1466.6097   1471.9503    1474.9221
1475.0669   2190.7029    2347.3998
3006.6300   3019.4364    3062.4870
3076.9875   3077.9461    3077.9812
ZeroEnergy[kcal/mol] -23.8
ElectronicLevels[1/cm] 1

```



```

0 2
End
!-----
!-----c6h7_ts6-----
Barrier   ts6 i2 p2
RRHO
Geometry[angstrom] 13
C          0.741284984780  -0.265963713463  -0.471130811468
C          0.311887324536  -0.086279610557   0.908702498877
C         -0.057501539418   0.060729482165   2.047257730548
C         -0.439907254428   0.241921913270   3.406270856735
C         -1.673155392835   0.192986264655   3.852227779125
C         -2.874511963394   0.158671333095   4.369877588683
H          1.832503114683  -0.285061872549  -0.543957339890
H          0.361367749574  -1.205934559480  -0.882688196155
H          0.377542728041   0.547341723537  -1.106543145543
H          0.356096605022   0.435616772168   4.126335146251
H         -3.507016157649   1.041432297987   4.383789264174
H         -3.328838555427  -0.778902882071   4.676580570544
H         -2.575814642002   0.524821850303   6.463893058623
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling   Eckart
ImaginaryFrequency[1/cm] 378.8881
WellDepth[kcal/mol] 39.4
WellDepth[kcal/mol] 2.6
End
Frequencies[1/cm] 32
25.3556      88.5696
137.4811     207.9261     227.8246
277.8806     345.1087     393.7190
405.4454     554.3722     665.3622
796.7644     888.2273     896.2704
1012.0606    1050.3457    1053.9685
1057.4672    1203.3553    1359.8352
1416.1683    1465.7906    1477.7697
1478.9620    2004.3944    2340.6499
3020.5827    3075.4060    3080.6664
3092.0302    3111.7082    3184.6656
ZeroEnergy[kcal/mol] -21.0
ElectronicLevels[1/cm] 1
0 2
End

```

```

!-----
!-----c6h7_ts7-----
Barrier   ts7 i2 i7
RRHO
Geometry[angstrom] 13
C          0.422706923951   0.003014457968  -0.266939534954
C          -0.001661664404   0.008967690210   1.123279523428
C          -0.387897005325   0.013074021437   2.276177623345
C          -0.654991065893   0.021845037643   3.623532448428
C          -1.350270337173   0.018750144257   4.720115738293
C          -2.730306132048  -0.004717365423   5.279359550508
H          1.511993420195  -0.070793489337  -0.354197928261
H          -0.013193542439  -0.842519542714  -0.808844539566
H          0.109494759931   0.919816590097  -0.776694918556
H          -0.027849942415   0.046712074705   4.731751175173
H          -3.470193791245  -0.029141493101   4.468229563155
H          -2.877633998404  -0.882807802385   5.913875201775
H          -2.915231622163   0.879592672329   5.895116098127
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 2126.3321
WellDepth[kcal/mol] 44.0
WellDepth[kcal/mol] 51.2
End
Frequencies[1/cm] 32
27.8427      92.5598
92.8846      165.9388      222.0702
231.1318     344.6875      368.5189
500.8543     514.9602      605.6092
906.4785     1018.6937     1027.2336
1045.1882    1046.6280     1197.6318
1383.1343    1413.9266     1463.0376
1472.3711    1474.1325     1476.4766
1926.1053    2251.5267     2297.4948
2988.5167    3010.1890     3061.9862
3069.3443    3069.4679     3087.0302
ZeroEnergy[kcal/mol] -16.4
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c6h7_ts8-----

```

```

Barrier  ts8 i5 p5
RRHO
Geometry[angstrom] 13
C          2.783347388050  -0.508547709310  -0.008159203588
C          1.388628867642  -0.101243973772   0.014040537096
C          0.159924750851   0.250982197304  -0.024757432657
C          -0.935660688452   1.239216872217  -0.080879743422
C          -1.294426973798  -0.020708613075  -0.006144896051
C          -2.357708368839  -1.044171120759   0.061846445114
H          3.394433768961   0.144607707131  -0.648445930568
H          2.911487282405  -1.528161960533  -0.403100929124
H          3.234362526738  -0.494244669834   0.991170622855
H          -1.238840132939   2.275586534611  -0.136538255697
H          -2.266350526418  -1.739426960621  -0.778451097923
H          -3.352873413692  -0.592895173233   0.042343239762
H          -2.253230480511  -1.635170130124   0.977077644197

```

```

Core RigidRotor
SymmetryFactor 1.0
End

```

```

Tunneling  Eckart
ImaginaryFrequency[1/cm] 225.6606
WellDepth[kcal/mol] 37.4
WellDepth[kcal/mol] 0.3
End

```

```

Frequencies[1/cm] 32
50.9591      127.0049
153.2694     167.0699     229.1650
436.1490     450.8477     590.3705
651.4307     733.0367     935.8315
961.0249     993.5301    1042.7202
1050.2464    1093.9333    1180.0507
1398.9359    1411.8712    1468.2097
1472.1462    1472.6873    1478.2593
1758.4312    1938.5305    2949.9970
2975.4189    3020.5117    3027.1838
3076.3555    3095.8414    3202.4000

```

```

ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End

```

```

!-----
!-----c6h7_ts9-----

```

```

Barrier  ts9 i7 p3
RRHO

```

```

Geometry[angstrom] 13
C      0.      0.      0.
C      0.      0.      1.4507
C      0.02807  0.      2.68377
C      0.0023   -0.00246  4.00338
C      0.17976  0.00537  5.30104
C      -1.34157 -0.07356  6.74649
H      1.0182   -0.04978  -0.40401
H      -0.55513 -0.85739  -0.39587
H      -0.46826  0.9084   -0.39376
H      1.20063  0.05702  5.69237
H      -2.32803 -0.12341  6.28436
H      -1.21427 -0.94943  7.39231
H      -1.30396  0.80948  7.39399
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 383.54
WellDepth[kcal/mol] 38.1
WellDepth[kcal/mol] 6.8
End
Frequencies[1/cm] 32
20.2998      30.7871
68.4182      149.0064      179.3176
335.1022     337.9133      405.1173
434.2015     497.1515      539.1824
625.0096     661.1257      684.0507
766.3374     1044.5088     1046.5764
1183.3311    1408.8048     1413.5738
1416.6533    1472.4251     1473.6290
2063.3872    2294.2366     3016.8723
3073.1543    3076.3751     3095.5436
3259.2311    3270.9656     3433.9041
ZeroEnergy[kcal/mol] -29.5
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c6h7_ts10-----
Barrier ts10 i7 p1
RRHO
Geometry[angstrom] 13
C      0.161854183164  0.010854868521  -0.070225675459

```

C	-0.029656463391	0.000441775549	1.369890177347
C	-0.186018752608	-0.008168358136	2.570943994538
C	-0.368569340289	-0.017986838469	3.918523383880
C	-0.457264368073	-0.025152324500	5.132943098105
C	-0.857302999737	-0.040035506296	6.535924004793
H	1.226388600968	0.035506334737	-0.323106542877
H	-0.271677291897	-0.881870753813	-0.531334293916
H	-0.310847775945	0.887438120583	-0.523750040282
H	1.603854843639	0.018820973972	5.547810479220
H	-1.948199975140	-0.064602449889	6.617604677483
H	-0.454485627334	-0.916160018613	7.051142086479
H	-0.493664037850	0.848663182766	7.058692650467

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 470.8111

WellDepth[kcal/mol] 41.0

WellDepth[kcal/mol] 3.0

End

Frequencies[1/cm] 32

18.1137	98.9648	
99.9033	139.1534	252.3376
256.0663	373.9052	378.7743
404.4285	529.5211	532.4778
570.2354	950.2169	1038.9576
1047.1016	1047.8548	1055.5166
1291.5473	1410.4846	1417.0898
1472.1484	1473.6190	1473.8209
1477.1841	2230.5383	2332.4403
3018.2160	3024.1028	3075.7615
3076.7164	3084.9788	3087.2106

ZeroEnergy[kcal/mol] -26.6

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c6h7\_ts11-----

Barrier ts11 i3 p3

RRHO

Geometry[angstrom] 13

C	-0.204918284838	-0.001072726293	0.146950063174
C	-0.047432105591	-0.002258449178	1.592780264945
C	0.104396331829	-0.003236173027	2.791467362597

C	0.248037272326	-0.004264097039	4.165587612412
C	-1.944180447246	0.006825387679	4.709498523589
C	0.926779583769	-0.007953791819	5.197090156125
H	-1.260649934633	-0.044984462083	-0.137001408379
H	0.300195446626	-0.861328689758	-0.302673098305
H	0.223763373782	0.904678779574	-0.292640353935
H	1.203122042473	-0.009597372123	6.225161706460
H	-1.928289850217	0.006256304991	5.791854246715
H	-2.234924556242	-0.915329581225	4.222574046247
H	-2.225293865676	0.932383530927	4.223380879492

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 554.0771

WellDepth[kcal/mol] 32.8

WellDepth[kcal/mol] 12.5

End

Frequencies[1/cm] 32

17.6412	79.6210	
104.7416	150.8713	218.2696
307.4886	336.3872	465.0514
478.7055	514.4979	551.2379
562.8176	651.4903	681.3688
881.8376	1048.0146	1050.4599
1162.4942	1414.4172	1416.8235
1420.5508	1475.1979	1476.1224
1968.2039	2333.8067	3019.9558
3077.6710	3078.0283	3088.8904
3250.4016	3253.0708	3435.3437

ZeroEnergy[kcal/mol] -23.8

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c6h7\_ts11-1-----

Barrier ts11-1 i4 p3

RRHO

Geometry[angstrom] 13

C	-2.939595744077	-0.340686493357	0.001840632860
C	-1.545838092692	0.074840898782	0.003631879167
C	-0.394148180535	0.440233413220	0.005155970822
C	0.931579432870	0.829186233579	0.006723864935
C	1.861693260084	-1.229053160970	-0.010968234376

C	1.823857550227	1.682713306001	0.012547942917
H	-3.028649464141	-1.430176170402	0.048894048186
H	-3.448033433708	-0.001002857445	-0.905634688248
H	-3.474072547118	0.077692453425	0.860117379389
H	2.785288024410	2.139817166008	0.015107542918
H	2.923460351121	-1.018346948122	-0.010231503932
H	1.433794171178	-1.590388414950	-0.937430423833
H	1.435552672396	-1.605575425767	0.910244588236

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 554.0812

WellDepth[kcal/mol] 33.2

WellDepth[kcal/mol] 12.5

End

Frequencies[1/cm] 32

3.4336	79.6264	
104.7859	150.9198	218.3141
307.5283	336.4305	465.0601
478.7103	514.5022	551.2394
562.8189	651.4906	681.3719
881.8400	1048.0912	1050.5568
1162.5016	1414.5017	1416.8233
1420.5511	1475.2204	1476.1989
1968.2030	2333.8061	3019.6652
3077.3255	3077.7512	3088.8913
3250.4023	3253.0718	3435.3413

ZeroEnergy[kcal/mol] -23.8

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----c6h7\_tsi3-----

Barrier tsi3 i3 i4

RRHO

Geometry[angstrom] 13

C	0.018779418164	-0.000780267058	0.017410229531
C	0.020031774940	0.004553750271	1.474024734742
C	0.038640272058	0.008802810024	2.680563350858
C	0.017520009314	0.014160556081	4.118358055786
C	-1.365696790889	0.026055861946	4.764911232469
C	1.130194957037	0.008986729264	4.811540873213
H	-1.001059524312	0.012660084994	-0.378050866371

H	0.517536665461	-0.893101864053	-0.373217776920
H	0.543398473970	0.873654607701	-0.379716740741
H	2.017345565395	0.004988602424	5.399757749742
H	-1.286019419805	0.029442553667	5.852299718830
H	-1.933949362180	-0.854218109259	4.450590253526
H	-1.921752037107	0.911796685572	4.444198185508

Core RigidRotor  
SymmetryFactor 1.0  
End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 722.2746  
WellDepth[kcal/mol] 4.4  
WellDepth[kcal/mol] 4.8  
End

Frequencies[1/cm] 32

31.4430	114.0529	
144.9136	172.0926	302.6243
348.3774	365.4688	538.9187
556.4359	595.5996	658.8908
948.3156	1032.4502	1050.2187
1050.6063	1055.7449	1216.3478
1390.7300	1416.2429	1478.2955
1478.9833	1479.3696	1480.2774
1645.2332	2327.7524	3019.4369
3025.7126	3074.2315	3078.2315
3084.8459	3121.3269	3435.8852

ZeroEnergy[kcal/mol] -52.2  
ElectronicLevels[1/cm] 1  
0 2  
End

!-----  
!-----c6h7\_ts23-----

Barrier ts23 i3 i5  
RRHO

Geometry[angstrom] 13

C	2.821517516816	-0.487841744900	0.047174428763
C	1.364161026313	-0.544615985066	0.052372390260
C	0.176510110074	-0.162409884931	-0.023155240944
C	-0.900016083151	1.203303676738	-0.281941822817
C	-1.245623772585	-0.035193702301	-0.051792319768
C	-2.405906439357	-0.954672025922	0.115800956424
H	3.172030936587	0.536803102374	-0.143593931562
H	3.250867159621	-1.130087853127	-0.729742115962
H	3.244319090900	-0.804387235381	1.007098085029



H	-1.215802201687	2.219016255275	-0.472704531228
H	-2.368114414563	-1.751679066452	-0.632353161465
H	-3.347576224788	-0.412886588804	0.012226094482
H	-2.373275704181	-1.429525947488	1.100610171431

Core RigidRotor  
SymmetryFactor 1.0  
End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 675.0462  
WellDepth[kcal/mol] 25.0  
WellDepth[kcal/mol] 5.8  
End

Frequencies[1/cm] 32

92.8744	119.2897	
132.5683	158.3022	262.2977
307.5615	444.8677	462.1254
633.7754	657.5418	760.2117
888.5012	1023.4611	1043.6955
1048.2752	1056.3345	1278.6513
1400.2442	1409.1616	1467.6543
1475.5393	1478.8987	1483.9838
1752.2958	2007.6481	2975.4630
3029.5857	3032.6495	3052.5827
3086.1793	3115.4119	3217.3502

ZeroEnergy[kcal/mol] -31.6  
ElectronicLevels[1/cm] 1  
0 2  
End

!-----  
!-----c6h7\_tsa-----

Barrier tsa i1 p4  
RRHO

Geometry[angstrom] 13

C	1.853413806001	0.094186238838	-0.046172040979
C	0.685232890139	0.367383539442	-0.201218453035
C	3.256326405111	-0.251943037799	0.132890823105
C	-0.667974101373	0.737936038563	-0.359128608311
C	-1.717441304021	-0.114350802259	-0.384900715791
C	-3.064789668789	-0.067206020316	0.034498231301
H	3.895210602023	0.631953803604	0.045849554172
H	3.584011532566	-0.975041559369	-0.620987522642
H	3.435100289123	-0.696995844898	1.117199323537
H	-0.871249727965	1.798630273437	-0.535511134104
H	-3.790528012593	-0.724047838668	-0.435948937196

```

H          -3.456377848448   0.716582534192   0.688503438531
H          -2.192802861763  -0.972834324779   0.468273040730
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1827.4491
WellDepth[kcal/mol] 42.6
WellDepth[kcal/mol] 48.5
End
Frequencies[1/cm] 32
28.7984      100.8061
142.2805     228.9166      265.1482
342.8613     429.1444      506.8345
551.8081     794.1817      803.0838
895.5138     1016.4239     1046.8289
1053.8547    1084.4848     1145.0093
1209.9182    1316.8338     1415.3530
1465.7125    1477.1273     1479.1986
1588.8359    2165.2962     2304.5384
3014.0879    3031.4938     3043.3246
3064.8769    3074.5144     3168.7704
ZeroEnergy[kcal/mol] -17.5
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----c6h7_tsa1-----
Barrier tsa1 i2 p4
RRHO
Geometry[angstrom] 13
C          1.853413806001   0.094186238838  -0.046172040979
C          0.685232890139   0.367383539442  -0.201218453035
C          3.256326405111  -0.251943037799   0.132890823105
C          -0.667974101373   0.737936038563  -0.359128608311
C          -1.717441304021  -0.114350802259  -0.384900715791
C          -3.064789668789  -0.067206020316   0.034498231301
H          3.895210602023   0.631953803604   0.045849554172
H          3.584011532566  -0.975041559369  -0.620987522642
H          3.435100289123  -0.696995844898   1.117199323537
H          -0.871249727965   1.798630273437  -0.535511134104
H          -3.790528012593  -0.724047838668  -0.435948937196
H          -3.456377848448   0.716582534192   0.688503438531
H          -2.192802861763  -0.972834324779   0.468273040730

```

```

Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1827.4491
WellDepth[kcal/mol] 42.9
WellDepth[kcal/mol] 48.5
End
Frequencies[1/cm] 32
28.7984      100.8061
142.2805     228.9166      265.1482
342.8613     429.1444      506.8345
551.8081     794.1817      803.0838
895.5138     1016.4239     1046.8289
1053.8547    1084.4848     1145.0093
1209.9182    1316.8338     1415.3530
1465.7125    1477.1273     1479.1986
1588.8359    2165.2962     2304.5384
3014.0879    3031.4938     3043.3246
3064.8769    3074.5144     3168.7704
ZeroEnergy[kcal/mol] -17.5
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```