

```

TemperatureList[K]          150. 300.
PressureList[atm]          0.0395
EnergyStepOverTemperature  0.2      #Ratio of
discretization energy step to T
ExcessEnergyOverTemperature 30
ModelEnergyLimit[kcal/mol] 400
WellCutoff                 10
ChemicalEigenvalueMax     0.2
ChemicalEigenvalueMin     1.e-6    #only for direct
diagonalization method
CalculationMethod         direct
RateOutput                ME_2.out
LogOutput                 ME_2.log
EigenvalueOutput         eigenvalue_2.out
!EigenvectorOutput
eigenvector_test.out
!EigenvectorNumber       0
!ReductionNumber        5
Reactant                  #ground energy of bimolecular
species will be used as a reference.
Model
  EnergyRelaxation
    Exponential
      Factor[1/cm]        228      ! Jasper calc N2
      Power              0.86
      ExponentCutoff     15
    End
  CollisionFrequency
    LennardJones
      Epsilons[1/cm]     19.8 44.6 ! N2 , CHCCH3 ! from new
      Jasper calc (Table 3)
      Sigmas[angstrom]   3.38 3.31 ! N2 , CHCCH3 ! from new
      Jasper calc (Table 3)
      Masses[amu]        28.0 53.039 ! N2 , C4H5
    End
  OutputTemperatureStep[K] 100
  OutputTemperatureSize 20
  OutputReferenceEnergy[kcal/mol] 0.
  Well      W1  #B3LYP/6-311++G** Opt "CH3-cCCHCH Radical"
  Species
  RRHO
  Geometry[angstrom]      9
  C  1.576510  -0.018205  0.013142
  C  0.102945   0.029891 -0.012686
  C -1.019041   0.717040  0.019782
  C -1.128436  -0.735239 -0.132139
  H  2.018158   0.977601  0.084828
  H  1.944659  -0.507728 -0.895012
  H  1.920773  -0.623398  0.857986
  H -1.516177   1.670744  0.080971
  H -1.559283  -1.478133  0.542633
  Core  RigidRotor

```

```

SymmetryFactor          0.5
End
Rotor      Hindered
Group              5 6 7
Axis              1 2
Symmetry          3
Potential[kcal/mol] 2
0.000
1.150
End
Frequencies[1/cm]      20
316.3653      335.8899
638.6461      722.5896      917.9652
930.2849      949.9261      1004.3027
1047.6311     1099.2115     1235.9895
1400.0178     1474.2780     1478.3963
1787.3572     3018.0420     3037.0149
3067.5513     3103.8498     3257.8266
ZeroEnergy[kcal/mol]  -80.116
ElectronicLevels[1/cm] 1
0 2
End
End
Well      W2  #B3LYP/6-311++G** Opt "(Cs) CH3-cCCHCH Radical"
Species
RRHO
Geometry[angstrom]    9
C -0.074782    1.556531    0.000000
C  0.421384    0.142806    0.000000
C -0.074782   -1.064904    0.657038
C -0.074782   -1.064904   -0.657038
H  0.276789    2.095569    0.883637
H -1.177292    1.593512    0.000000
H  0.276789    2.095569   -0.883637
H -0.279261   -1.600911    1.569894
H -0.279261   -1.600911   -1.569894
Core      RigidRotor
SymmetryFactor          1
End
Rotor      Hindered
Group              5 6 7
Axis              1 2
Symmetry          3
Potential[kcal/mol] 2
0.000
1.500
End
Frequencies[1/cm]      20
334.8574      361.9318
625.4486      694.9622      794.4139
883.9509      952.5738      1028.7529
1045.7942     1079.1594     1359.2222

```

1393.9878	1471.8363	1484.4287
1657.9737	2937.1678	3054.8467
3089.2865	3225.7908	3271.0818

ZeroEnergy[kcal/mol] -77.243

ElectronicLevels[1/cm] 1

0 2

End

End

Well W3 #B3LYP/6-311++G** Opt "CH2-cCCHCH2 Radical"

Species

RRHO

Geometry[angstrom] 9

C -0.424894 -1.180230 0.000000

C 0.000000 0.269353 0.000000

C 0.974967 -0.662523 0.000000

C -0.414277 1.565513 0.000000

H -0.836016 -1.614950 0.912932

H -0.836016 -1.614950 -0.912932

H 2.020476 -0.917979 0.000000

H -1.467301 1.817699 0.000000

H 0.304076 2.377510 0.000000

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 21

315.4716	350.6035	441.7687
----------	----------	----------

558.3739	722.3862	799.5981
----------	----------	----------

895.7237	980.7297	1028.4213
----------	----------	-----------

1029.9585	1067.6974	1112.3745
-----------	-----------	-----------

1185.8364	1453.8077	1490.0671
-----------	-----------	-----------

1600.9669	3029.2798	3090.6290
-----------	-----------	-----------

3135.3566	3228.9839	3264.9175
-----------	-----------	-----------

ZeroEnergy[kcal/mol] -91.657

ElectronicLevels[1/cm] 1

0 2

End

End

Well W4 #B3LYP/6-311++G** Opt "CH2-cCHCHCH Radical"

Species

RRHO

Geometry[angstrom] 9

C -0.335035 -0.950339 0.643666

C -0.335035 0.441614 0.000000

C -0.335035 -0.950339 -0.643666

C 0.864981 1.260652 0.000000

H -0.266275 -1.470903 1.584684

H -1.275489 0.992086 0.000000

H -0.266275 -1.470903 -1.584684

H 1.845255 0.798298 0.000000

H 0.803528 2.341896 0.000000

Core RigidRotor

SymmetryFactor 1

```

End
Frequencies[1/cm]      21
286.4283              362.2694              396.6316
553.6366              615.3398              691.3933
838.1501              841.7830              967.0046
986.5456              1051.4253             1108.0800
1130.1807             1373.8292             1462.7248
1724.1177             3078.6888             3135.8016
3227.8742             3239.9230             3277.7611
ZeroEnergy[kcal/mol]      -79.000
ElectronicLevels[1/cm]    1
  0  2
End
End
Well      W5  #B3LYP/6-311++G** Opt "CH3-cCCCH2 Radical"
Species
RRHO
Geometry[angstrom]      9
  C  0.000000      0.279300      0.000000
  C  1.275817      0.206733      0.000000
  C -1.369876      0.804423      0.000000
  C  0.726506     -1.176829      0.000000
  H -1.346236      1.898169      0.000000
  H -1.921258      0.471916      0.884767
  H -1.921258      0.471916     -0.884767
  H  0.697035     -1.761882      0.918946
  H  0.697035     -1.761882     -0.918946
Core  RigidRotor
SymmetryFactor          1
End
Rotor      Hindered
Group                5 6 7
Axis                 1 3
Symmetry             3
Potential[kcal/mol]  2
  0.000
  1.250
End
Frequencies[1/cm]      20
289.6688              295.6853              926.4699
570.1280              724.4801              1033.5480
977.9986              1031.7810             1405.5847
1052.4646             1094.9523             1503.9052
1468.3356             1479.3312             3046.7697
1910.1765             3018.0251             3125.4046
3075.0491             3086.5095
ZeroEnergy[kcal/mol]      -71.000
ElectronicLevels[1/cm]    1
  0  2
End
End
Well      W6  #B3LYP/6-311++G** Opt "CH2CHCCH2 Radical"

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```

Species
RRHO
  Geometry[angstrom]      9
  C -0.827314      0.167573      0.000000
  C  0.306036     -0.564329      0.000000
  C -0.896531      1.560034      0.000000
  C  1.394859     -1.273860      0.000000
  H -1.762812     -0.390817      0.000000
  H -1.854766      2.061929      0.000000
  H  0.000000      2.166561      0.000000
  H  1.877645     -1.587091     -0.925202
  H  1.877645     -1.587091      0.925202
  Core  RigidRotor
  SymmetryFactor          1
  End
  Frequencies[1/cm]      21
  207.5694      214.5638      494.5195
  524.9947      573.4053      746.1885
  886.5188      906.4059      935.5398
  979.9697     1089.6216     1193.4881
  1376.0036     1447.6999     1491.8031
  1904.1125     3068.3432     3111.7825
  3127.7334     3150.8865     3251.6498
  ZeroEnergy[kcal/mol]    -107.822
  ElectronicLevels[1/cm]  1
  0  2
  End
End
Well      W7  #B3LYP/6-311++G** Opt "trans-CH2CHCHCH Radical"
Species
RRHO
  Geometry[angstrom]      9
  C  1.772919      0.143298      0.000000
  C -0.689934      0.331140      0.000000
  C  0.561582     -0.423810      0.000000
  C -1.899069     -0.190262      0.000000
  H  1.895995      1.221785      0.000000
  H  2.676608     -0.453840      0.000000
  H -0.592481      1.423716      0.000000
  H  0.469363     -1.506050      0.000000
  H -2.922470      0.152195      0.000000
  Core  RigidRotor
  SymmetryFactor          1
  End
  Rotor      Hindered
  Group              1 5 6 8
  Axis                2 3
  Symmetry            1
  Potential[kcal/mol]  2
  0.000
  2.830
  End

```

```

      Frequencies[1/cm]          20
301.3181          512.7427
561.4622          724.1572          783.2255
860.3522          940.3697          947.1496
1024.8261         1173.3624         1249.7289
1316.3091         1442.4047         1625.2797
1677.7834         3016.5265         3132.8973
3153.6957         3222.1380         3248.6993
      ZeroEnergy[kcal/mol]          -97.985
      ElectronicLevels[1/cm]          1
      0 2
      End
      End
      Well          W8  #B3LYP/6-311++G** Opt "CH3CHCCH Radical"
      Species
      RRHO
      Geometry[angstrom]          9
      C 0.000000    0.822516    0.000000
      C -0.583071   1.897353    0.000000
      C 0.647459   -0.387066    0.000000
      C -0.056719  -1.709103    0.000000
      H -1.085749   2.833165    0.000000
      H 1.733760   -0.383467    0.000000
      H 0.223166   -2.302767    0.879106
      H 0.223166   -2.302767   -0.879106
      H -1.140360  -1.586362    0.000000
      Core  RigidRotor
      SymmetryFactor          1
      End
      Rotor      Hindered
      Group          7 8 9
      Axis          3 4
      Symmetry          3
      Potential[kcal/mol]    2
      0.000
      0.450
      End
      Frequencies[1/cm]          20
212.6467          387.7892
442.8521          553.6165          601.3266
652.2967          866.9814          1006.0116
1097.6863         1150.6208         1386.8143
1403.1215         1474.9563         1492.8113
2010.5044         2997.7198         3033.3146
3110.4941         3146.6048         3468.7438
      ZeroEnergy[kcal/mol]          -107.616
      ElectronicLevels[1/cm]          1
      0 2
      End
      End
      Well          W9  #B3LYP/6-311++G** Opt "CH2CCCH3 Radical"
      Species

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```

RRHO
Geometry[angstrom]      9
  C  0.000000    0.515437    0.000000
  C  0.028408    1.968747    0.000000
  C -0.011346   -0.709665    0.000000
  C -0.026179   -2.078030    0.000000
  H  1.058882    2.342574    0.000000
  H -0.469577    2.375368    0.885628
  H -0.469577    2.375368   -0.885628
  H -0.032512   -2.636122   -0.928729
  H -0.032512   -2.636122    0.928729
Core   RigidRotor
SymmetryFactor          1
End
Rotor   Hindered
Group                    5 6 7
Axis                    1 2
Symmetry                 3
Potential[kcal/mol]     2
  0.000
  0.001
End
Frequencies[1/cm]      20
178.8159    206.1511
388.7345    421.1299    679.4289
771.5723    1029.5846    1029.8240
1051.4246   1261.2193    1413.3594
1464.0542   1471.8983    1472.6387
2144.7784   3007.0208    3056.4019
3073.4766   3133.1803    3220.6395
ZeroEnergy[kcal/mol]   -110.276
ElectronicLevels[1/cm] 1
  0  2
End
End
Well      W10  #B3LYP/6-311++G** Opt "CH2CH2CCH Radical"
Species
RRHO
Geometry[angstrom]      9
  C  0.000000    0.784443    0.000000
  C -0.575056    1.840110    0.000000
  C  0.692632   -0.502235    0.000000
  C -0.213894   -1.692896    0.000000
  H -1.081688    2.773927    0.000000
  H  1.366830   -0.541836    0.870276
  H  1.366830   -0.541836   -0.870276
  H  0.214496   -2.687206    0.000000
  H -1.288558   -1.579579    0.000000
Core   RigidRotor
SymmetryFactor          1
End
Rotor   Hindered

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```

Group                8 9
Axis                 3 4
Symmetry             2
Potential[kcal/mol] 2
0.000
0.550
End
Frequencies[1/cm]   20
209.2577            319.1324
451.7039            527.9737            664.3708
687.4020            835.5476            875.6804
1045.0359           1082.8359           1196.2074
1344.0266           1445.3477           1453.8062
2219.7546           2957.9343           2961.8863
3148.9866           3264.9721           3477.9062
ZeroEnergy[kcal/mol] -94.737
ElectronicLevels[1/cm] 1
0 2
End
End
Well                W11 #B3LYP/6-311++G** Opt "CH3C(C)CH2 Radical"
Species
RRHO
Geometry[angstrom] 9
C -0.562363 -1.204845 0.000000
C 0.000000 0.233641 0.000000
C -1.087796 1.012987 0.000000
C 1.363675 0.522983 0.000000
H -1.656165 -1.220615 0.000000
H -0.217608 -1.720259 0.897845
H -0.217608 -1.720259 -0.897845
H 1.713869 1.546028 0.000000
H 2.096413 -0.273486 0.000000
Core RigidRotor
SymmetryFactor      1
End
Rotor Hindered
Group                5 6 7
Axis                 1 2
Symmetry             3
Potential[kcal/mol] 2
0.000
1.800
End
Frequencies[1/cm]   20
204.6531            343.3366
438.3927            458.7791            686.4519
809.1989            963.1627            1013.1989
1037.0125           1206.4558           1380.5613
1453.0860           1478.6720           1479.0139
1509.8888           3032.0025           3096.9496
3124.5799           3151.5759           3253.4681

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ZeroEnergy[kcal/mol]          -59.406
ElectronicLevels[1/cm]       1
  0  2
End
End
Well      W12  #B3LYP/6-311++G** Opt "cCH2CHCCH2 Radical"
Species
RRHO
Geometry[angstrom]          9
  C  1.098076  -0.114005  0.000000
  C  0.000000   0.958835  0.000000
  C  0.176959  -1.070701  0.000000
  C -1.064185  -0.203213  0.000000
  H  2.176911  -0.062410  0.000000
  H -0.032756  1.581450  0.898461
  H -0.032756  1.581450 -0.898461
  H -1.688247  -0.262992 -0.893269
  H -1.688247  -0.262992  0.893269
Core  RigidRotor
SymmetryFactor                1
End
Frequencies[1/cm]            21
323.3342          709.0644          821.1196
834.4976          865.8761          888.8255
997.9521          1028.5952         1061.7206
1121.7626         1152.3970         1188.9574
1224.1049         1460.1494         1479.5231
1604.7006         3023.2279         3060.8907
3082.3791         3111.4854         3228.0052
ZeroEnergy[kcal/mol]          -86.235
ElectronicLevels[1/cm]       1
  0  2
End
End
Well      W13  #B3LYP/6-311++G** Opt "cCH2CHCHCH Radical"
Species
RRHO
Geometry[angstrom]          9
  C  0.000000   0.000000   1.056603
  C  0.000000   1.018947  -0.089611
  C  0.000000   0.000000  -1.045308
  C  0.000000  -1.018947  -0.089611
  H  0.891229   0.000000   1.692580
  H -0.891229   0.000000   1.692580
  H  0.000000   2.099509  -0.124464
  H  0.000000   0.000000  -2.128671
  H  0.000000  -2.099509  -0.124464
Core  RigidRotor
SymmetryFactor                2
End
Frequencies[1/cm]            21
386.0086          540.7944          556.7434

```

866.2998	900.9091	910.9441
927.5324	957.7312	1002.3195
1079.0431	1171.3986	1186.3194
1221.1520	1326.5413	1432.3772
1482.9757	3025.1440	3062.6786
3183.0223	3212.7474	3225.2350

ZeroEnergy[kcal/mol] -106.777
ElectronicLevels[1/cm] 1
0 2
End
End
Well W14 #B3LYP/6-311++G** Opt "bicCH2CHCCH2 Radical"
Species
RRHO
Geometry[angstrom] 9
C 0.164646 -0.224584 1.163998
C 0.164646 0.760543 0.000000
C -0.752568 -0.361318 0.000000
C 0.164646 -0.224584 -1.163998
H 0.999488 -0.915374 1.300258
H -0.272733 0.145775 2.086217
H 0.098268 1.838851 0.000000
H 0.999488 -0.915374 -1.300258
H -0.272733 0.145775 -2.086217
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 21
376.4142 675.3582 719.6908
719.8510 893.1071 924.2729
1019.2839 1059.5640 1059.7041
1094.3269 1109.4555 1118.7360
1234.1233 1313.1870 1487.3638
1529.4981 3043.1954 3045.8656
3161.3100 3162.5893 3200.6169
ZeroEnergy[kcal/mol] -69.225
ElectronicLevels[1/cm] 1
0 2
End
End
Well W15 #B3LYP/6-311++G** Opt "bicCH2CHCHCH Radical"
Species
RRHO
Geometry[angstrom] 9
C 0.181482 -1.131384 0.000000
C 0.181482 0.148613 0.784051
C 0.181482 0.148613 -0.784051
C -0.785961 0.907870 0.000000
H -0.729326 -1.727143 0.000000
H 0.977944 0.504397 -1.424525
H -0.878125 1.988060 0.000000
H 0.977944 0.504397 1.424525

```

      H 1.100643  -1.711989  0.000000
      Core RigidRotor
      SymmetryFactor 1
      End
      Frequencies[1/cm] 21
465.2238 698.3243 735.3511
786.5081 854.1848 868.2053
940.6146 993.7167 1045.8355
1112.2451 1136.2757 1168.4136
1209.0757 1257.8894 1358.2609
1504.3616 3072.1469 3156.3797
3167.9328 3183.0572 3198.3669
      ZeroEnergy[kcal/mol] -81.941
      ElectronicLevels[1/cm] 1
      0 2
      End
      End
      Bimolecular R1 #B3LYP/6-311++G** Opt "ALLENE and CH
Radical"
      Fragment C3H4
      RRHO
      Geometry[angstrom] 7
      C 1.303388 0.000000 0.000000
      C 0.000000 0.000000 0.000000
      C -1.303388 0.000000 0.000000
      H 1.867380 0.254572 -0.891885
      H 1.867380 -0.254573 0.891885
      H -1.867380 0.891885 0.254572
      H -1.867380 -0.891885 -0.254572
      Core RigidRotor
      SymmetryFactor 4
      End
      Frequencies[1/cm] 15
373.8097 373.8097 870.2809
870.2809 880.8264 1016.2240
1016.2240 1106.7650 1421.8177
1477.2793 2042.8217 3117.4267
3121.4438 3192.9650 3192.9650
      ZeroEnergy[kcal/mol] 0.0
      ElectronicLevels[1/cm] 1
      0 1
      End
      Fragment CH
      RRHO
      Geometry[angstrom] 2
      C 0.000000 0.000000 0.160908
      H 0.000000 0.000000 -0.965449
      Core RigidRotor
      SymmetryFactor 1
      End
      Frequencies[1/cm] 1
2821.8395

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```

ZeroEnergy[kcal/mol]          0.0
ElectronicLevels[1/cm]       1
    0    2
End
GroundEnergy[kcal/mol]       0.000
End
Bimolecular      P1      #B3LYP/6-311++G** Opt "CH2-cCCHCH and H
atom"
Fragment          C4H4
RRHO
Geometry[angstrom]      8
  C 0.000000      0.000000      1.591806
  C 0.000000      0.000000      0.262146
  C 0.000000      0.658960     -1.019523
  C 0.000000     -0.658960     -1.019523
  H 0.000000      0.928536      2.148479
  H 0.000000     -0.928536      2.148479
  H 0.000000      1.571700     -1.593155
  H 0.000000     -1.571700     -1.593155
Core      RigidRotor
SymmetryFactor          2
End
Frequencies[1/cm]       18
359.1972              427.7133              688.0839
709.3839              773.7595              840.6369
847.1512              913.4615              1017.5185
1060.2192             1116.0775             1452.5690
1594.5855             1818.6741             3141.7878
3225.7666             3234.8745             3276.2024
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]       -40.970
End
Bimolecular      P2      #B3LYP/6-311++G** Opt "1,2,3-Butatriene and
H atom"
Fragment          C4H4
RRHO
Geometry[angstrom]      8
  C 0.000000      0.000000      0.632819
  C 0.000000      0.000000      1.947762
  C 0.000000      0.000000     -0.632819
  C 0.000000      0.000000     -1.947762
  H 0.000000      0.926670      2.513601
  H 0.000000     -0.926670      2.513601

```

```

      H 0.000000   -0.926670   -2.513601
      H 0.000000    0.926670   -2.513601
Core      RigidRotor
SymmetryFactor      4
End
Frequencies[1/cm]      18
225.1685      231.9865      365.2325
573.2232      773.8189      889.0325
892.8795      901.4177      1021.5626
1041.4837     1407.1649     1464.5865
1675.9091     2199.4522     3113.6525
3116.6213     3190.6226     3190.9217
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]     -56.452
End
Bimolecular      P3      #B3LYP/6-311++G** Opt "VINYLACETYLENE and H
atom"
Fragment      C4H4
RRHO
Geometry[angstrom]      8
C -0.735475    0.110858    -0.000257
C -1.907281   -0.172364    0.001255
C  0.635784    0.489009   -0.002243
C  1.660245   -0.371915    0.001109
H -2.937515   -0.432252    0.002634
H  0.832571    1.558346   -0.006823
H  2.683209   -0.015779   -0.000688
H  1.502099   -1.443841    0.005692
Core      RigidRotor
SymmetryFactor      1
End
Frequencies[1/cm]      18
226.0053      321.2321      558.7894
652.3072      686.5280      703.0444
891.7373      955.5827      1006.1866
1110.8356     1320.0519     1442.7542
1662.4875     2198.8555     3136.4083
3146.5920     3235.9393     3476.4080
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]      -64.257
  End
Bimolecular      P4      #B3LYP/6-311++G** Opt "ETHYNE and VINYL
Radical"
  Fragment      C2H2
  RRHO
  Geometry[angstrom]      4
    C 0.000000      0.000000      0.599672
    C 0.000000      0.000000      -0.599672
    H 0.000000      0.000000      1.662782
    H 0.000000      0.000000      -1.662782
  Core      RigidRotor
  SymmetryFactor      4
  End
  Frequencies[1/cm]      7
647.4657      647.4657      772.7188
772.7188      2061.9752      3419.7407
3522.5335
  ZeroEnergy[kcal/mol]      0.0
  ElectronicLevels[1/cm]      1
    0      1
  End
  Fragment      C2H3
  RRHO
  Geometry[angstrom]      5
    C 0.047935      -0.586187      0.000000
    C 0.047935      0.719235      0.000000
    H -0.880592      -1.164300      0.000000
    H 0.968601      -1.166117      0.000000
    H -0.663231      1.532125      0.000000
  Core      RigidRotor
  SymmetryFactor      1
  End
  Frequencies[1/cm]      9
706.8945      816.6562      923.3114
1041.3236      1390.1280      1644.0285
3037.9840      3135.3333      3238.2586
  ZeroEnergy[kcal/mol]      0.0
  ElectronicLevels[1/cm]      1
    0      2
  End
  GroundEnergy[kcal/mol]      -59.849
  End
Bimolecular      P5      #B3LYP/6-311++G** Opt "ETHENE and C2H
Radical"
  Fragment      C2H4
  RRHO

```

```

Geometry[angstrom]      6
  C  0.000000    0.000000    0.664436
  C  0.000000    0.000000   -0.664436
  H  0.000000    0.922779    1.235160
  H  0.000000   -0.922779    1.235160
  H  0.000000   -0.922779   -1.235160
  H  0.000000    0.922779   -1.235160
Core      RigidRotor
SymmetryFactor      4
End
Frequencies[1/cm]     12
834.6604             974.4598             976.5419
1058.4176            1238.0808            1377.3069
1471.5020            1683.5207            3121.7494
3136.1639            3193.5324            3221.9391
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]   1
  0    1
End
Fragment      C2H
RRHO
Geometry[angstrom]      3
  C  0.000000    0.000000   -0.473406
  C  0.000000    0.000000    0.729725
  H  0.000000    0.000000   -1.537914
Core      RigidRotor
SymmetryFactor      1
End
Frequencies[1/cm]     4
316.4955             316.4955             2082.9154
3459.0242
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]   1
  0    2
End
GroundEnergy[kcal/mol]   -37.520
End
Barrier      B1    W1    W2
RRHO
Geometry[angstrom]      9
cCCHCH Conformational Change"
  C -1.580561   -0.041578    0.078141
  C -0.146534    0.013379   -0.295355
  C  1.182769   -0.658881   -0.034741
  C  1.001553    0.686316    0.026896
  H -1.702085   -0.354126    1.128327
  H -2.129832   -0.761422   -0.534627
  H -2.052961    0.937892   -0.038030
  H  1.705656   -1.451741    0.478083
  H  1.435862    1.633984    0.316601
Core      RigidRotor
SymmetryFactor      0.5

```

```

End
Rotor      Hindered
  Group          5 6 7
  Axis           1 2
  Symmetry       3
  Potential[kcal/mol] 2
    0.000
    1.200
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm] 801.8451
  WellDepth[kcal/mol]      6.525
  WellDepth[kcal/mol]      3.652
End
Frequencies[1/cm]      19
306.0821
332.5884          686.3283          837.6221
893.2839          923.4354          1009.8152
1065.4587         1123.2869          1245.7127
1398.5334         1465.1782          1487.4012
1637.0086         2942.5357          3045.2880
3084.1529         3197.6477          3232.2470
  ZeroEnergy[kcal/mol]      -73.591
  ElectronicLevels[1/cm]    1
    0  2
End
Barrier      B2  W1  W11
RRHO
  Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH3-
cCCHCH to CH3C(C)CH2 1,3 H Shift + Ring Open"
  C -1.524873  -0.061071  -0.015691
  C -0.050478   0.041229   0.051663
  C  0.888591   1.018669  -0.061557
  C  1.076268  -0.758733   0.120292
  H -1.976209   0.920673  -0.166625
  H -1.911874  -0.487304   0.914528
  H -1.831197  -0.726588  -0.827800
  H  1.917943   0.351680   0.092324
  H  1.464286  -1.499024  -0.580674
Core      RigidRotor
  SymmetryFactor      0.5
End
Rotor      Hindered
  Group          5 6 7
  Axis           1 2
  Symmetry       3
  Potential[kcal/mol] 2
    0.000
    0.860
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm] 873.1951

```



```

WellDepth[kcal/mol]      35.357
WellDepth[kcal/mol]      14.647
End
Frequencies[1/cm]       19
357.2156
378.0134                627.6882                818.6442
870.9085                895.7308                917.1493
1028.1385               1072.5609               1269.7619
1407.8797               1480.2233               1484.0832
1677.6933               2352.8500               3031.2588
3082.2239               3084.5207               3115.9497
ZeroEnergy[kcal/mol]    -44.759
ElectronicLevels[1/cm]  1
  0  2
End
Barrier      B3   W1   W8
RRHO
Geometry[angstrom]    9          #B3LYP/6-311++G** Opt "CH3-
cCCHCH to CH3CHCCH 1,2 H Shift + Ring Open"
  C  0.747878   -0.184289   0.061442
  C  1.963162    0.267285   0.058368
  C -0.523008   -0.584435  -0.252944
  C -1.700482    0.286189   0.036066
  H  0.340322   -0.716775   1.034800
  H  2.804774    0.480011  -0.571523
  H -2.562338   -0.290895   0.378951
  H -1.525307    1.144945   0.694432
  H -1.982753    0.674210  -0.954255
Core      RigidRotor
SymmetryFactor    0.5
End
Rotor      Hindered
Group                7 8 9
Axis                3 4
Symmetry            3
Potential[kcal/mol]  2
  0.000
  1.500
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  426.8301
WellDepth[kcal/mol]      56.446
WellDepth[kcal/mol]      83.946
End
Frequencies[1/cm]       19
191.7574
342.5166                448.9015                539.6803
580.8431                741.5003                835.7859
987.1885                1066.0125               1234.3097
1373.2208               1437.5991               1490.4015
1736.7634               2412.6332               2984.5714
3039.8052               3086.1796               3325.9846

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ZeroEnergy[kcal/mol]          -23.670
ElectronicLevels[1/cm]       1
  0  2
End
Barrier      B4    W1    W7
RRHO
Geometry[angstrom]          9          #B3LYP/6-311++G** Opt "CH3-
cCCHCH to CH2CHCHCH 1,2 H Shift + Ring Open"
  C  0.817955   -0.529767   0.128042
  C  1.592336    0.534936  -0.010051
  C -0.560454   -0.562030  -0.371978
  C -1.449861    0.404488   0.091203
  H  1.241070   -1.469774   0.481090
  H  1.505096    1.511105  -0.467189
  H -1.521336   -0.804383   0.518086
  H -2.451684    0.460325  -0.333224
  H -1.173002    1.216970   0.777941
Core      RigidRotor
SymmetryFactor      0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]    1200.9281
WellDepth[kcal/mol]         55.790
WellDepth[kcal/mol]         73.659
End
Frequencies[1/cm]          20
187.3431                319.6797
409.4994                630.6622                699.7738
835.3726                898.8751                961.1653
1052.3319              1095.1478              1257.4676
1295.1684              1393.5701              1512.7549
1549.1758              2174.6222              2977.5449
3103.6596              3128.1441              3220.3616
ZeroEnergy[kcal/mol]          -24.326
ElectronicLevels[1/cm]       1
  0  2
End
Barrier      B5    W2    W4
RRHO
Geometry[angstrom]          9          #B3LYP/6-311++G** Opt "(Cs) CH3-
cCCHCH to CH2-cCHCHCH 1,2 H Shift"
  C -0.559012    1.505693   0.000000
  C  0.224811    0.265130   0.000000
  C  0.224811   -1.052038   0.653769
  C  0.224811   -1.052038  -0.653769
  H -0.963002    1.877828   0.935293
  H -0.963002    1.877828  -0.935293
  H  0.790792    1.459612   0.000000
  H  0.221340   -1.607875   1.576323
  H  0.221340   -1.607875  -1.576323
Core      RigidRotor
SymmetryFactor      1

```

```

End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]  2028.5243
  WellDepth[kcal/mol]      48.041
  WellDepth[kcal/mol]      49.798
End
Frequencies[1/cm]      20
173.2197              378.8606
410.5654              629.7944              734.1449
734.3915              822.2637              867.6475
980.7724              999.6995              1026.2642
1155.4492             1367.8087             1404.8675
1675.8755             2038.4104             3099.7876
3220.0726             3240.9302             3286.6925
  ZeroEnergy[kcal/mol]     -29.202
  ElectronicLevels[1/cm]   1
  0  2
End
Barrier      B6  W2  P1
RRHO
  Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "(Cs) CH3-
cCCHCH H Loss TS"
  C -0.051087      -1.529281      0.000000
  C -0.105797      -0.183662      0.000000
  C -0.051087      1.087303      0.660552
  C -0.051087      1.087303     -0.660552
  H -0.154500     -2.078818      0.925781
  H -0.154500     -2.078818     -0.925781
  H -0.022829      1.657265      1.574895
  H -0.022829      1.657265     -1.574895
  H  1.909011     -1.926867      0.000000
Core      RigidRotor
  SymmetryFactor      1
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]  570.6625
  WellDepth[kcal/mol]      38.099
  WellDepth[kcal/mol]      1.826
End
Frequencies[1/cm]      20
295.8882              306.6660
362.8296              488.9087              700.9655
781.6398              836.3833              852.4090
857.8178              915.7595              1011.9230
1062.4469             1119.0758             1452.3714
1567.8931             1784.2014             3152.8880
3239.3404             3242.5805             3281.6266
  ZeroEnergy[kcal/mol]     -39.144
  ElectronicLevels[1/cm]   1
  0  2
End
Barrier      B7  W3  W6

```

```

RRHO
  Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH2-
cCCHCH2 Ring Open to CH2CHCCH2"
  C  0.819296    0.759886   -0.003492
  C -0.367213    0.237816   -0.029475
  C  1.241289   -0.645404    0.044436
  C -1.668678   -0.143287   -0.010868
  H  1.280807    1.723569   -0.177153
  H  1.583131   -1.150177   -0.853648
  H  1.369322   -1.160680    0.989997
  H -2.078276   -0.766128   -0.796758
  H -2.303142    0.099349    0.833951
Core      RigidRotor
SymmetryFactor    0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  660.5286
WellDepth[kcal/mol]      16.528
WellDepth[kcal/mol]      32.693
End
Frequencies[1/cm]      20
200.2149          292.8223
337.8619          656.9959          668.7277
736.1080          785.6525          962.3668
1007.6438         1039.3294         1117.9541
1208.7317         1436.4729         1467.1064
1877.3689         3098.4161         3132.9006
3177.5227         3198.3560         3220.5288
ZeroEnergy[kcal/mol]      -75.129
ElectronicLevels[1/cm]    1
  0  2
End
Barrier      B8    W3    W14
RRHO
  Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH2-
cCCHCH2 Bend to bic-CH2CHCCH2"
  C -1.076642   -0.513752   -0.086507
  C  0.181145   -0.140416    0.615240
  C -0.450914    0.859382   -0.227754
  C  1.364362   -0.169695   -0.092848
  H -1.097858   -1.200620   -0.932476
  H -1.973957   -0.536973    0.529589
  H -0.788942    1.885830   -0.137626
  H  2.082253    0.635600    0.030605
  H  1.670793   -0.996949   -0.738883
Core      RigidRotor
SymmetryFactor    0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  862.1432
WellDepth[kcal/mol]      49.639
WellDepth[kcal/mol]      27.207

```

```

End
Frequencies[1/cm]      20
366.1842              634.7992
654.8182              808.3494              873.9089
960.5957              981.8888              1000.8858
1037.9683             1060.5492             1130.0319
1246.0304             1387.9896             1495.5033
1517.0722             3054.5963             3057.7706
3136.0437             3149.1980             3179.0663
ZeroEnergy[kcal/mol]  -42.018
ElectronicLevels[1/cm] 1
0 2
End
Barrier      B9   W3   W11
RRHO
Geometry[angstrom]  9          #B3LYP/6-311++G** Opt "CH2-
cCCHCH2 to CH3C(C)CH2 1,3 H Shift + Ring Open TS"
C  0.222332  -1.227871  0.000000
C  0.000000   0.229607  0.000000
C -1.307466  -0.185796  0.000000
C  0.744202   1.379522  0.000000
H -1.097360  -1.454426  0.000000
H  0.532166  -1.707900  0.925354
H  0.532166  -1.707900 -0.925354
H  0.253041   2.344600  0.000000
H  1.825576   1.352854  0.000000
Core      RigidRotor
SymmetryFactor  1
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  818.9190
WellDepth[kcal/mol]      39.505
WellDepth[kcal/mol]      7.254
End
Frequencies[1/cm]      20
377.1812              383.7868
520.9616              677.4303              707.4803
759.1611              908.6953              1013.6754
1018.0150             1090.0169             1126.7598
1228.9267             1442.3456             1466.1473
1538.9386             2230.2691             3076.6931
3148.8425             3174.1571             3245.8760
ZeroEnergy[kcal/mol]  -52.152
ElectronicLevels[1/cm] 1
0 2
End
Barrier      B10  W3   P1
RRHO
Geometry[angstrom]  9          #B3LYP/6-311++G** Opt "CH2-
cCCHCH2 H Loss"
C  0.999740  -0.510767  -0.269873
C -0.319031   0.031081  -0.036727

```

```

C 0.903970 0.775525 0.033351
C -1.642982 -0.075552 0.041496
H 1.617773 -1.317460 -0.626089
H 1.411120 1.714246 0.187816
H -2.138104 -1.019496 -0.146973
H -2.254958 0.780346 0.296335
H 1.713982 -1.479358 1.679425
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 358.1713
WellDepth[kcal/mol] 52.403
WellDepth[kcal/mol] 1.716
End
Frequencies[1/cm] 20
142.4548 249.0661
359.7506 444.9352 683.7688
714.8687 782.9120 836.4923
847.4568 897.6658 1016.3634
1058.7661 1117.7309 1451.1135
1552.0811 1806.8200 3143.4990
3228.7461 3240.3482 3280.1142
ZeroEnergy[kcal/mol] -39.254
ElectronicLevels[1/cm] 1
0 2
End
Barrier B11 W4 P1
RRHO
Geometry[angstrom] 9 #B3LYP/6-311++G** Opt "CH2-
cCHCHCH H Loss Exit Channel"
C -1.041701 -0.656125 -0.066890
C 0.235627 0.000000 0.108472
C -1.041701 0.656125 -0.066890
C 1.574653 0.000000 -0.180242
H -1.593942 -1.578312 -0.137473
H -1.593942 1.578312 -0.137473
H 2.130359 -0.929061 -0.184846
H 2.130359 0.929061 -0.184846
H 0.565901 0.000000 1.877943
Core RigidRotor
SymmetryFactor 1
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1074.6796
WellDepth[kcal/mol] 44.838
WellDepth[kcal/mol] 6.808
End
Frequencies[1/cm] 20
306.4127 462.7371
487.6274 587.2445 658.7179
735.2155 790.8569 839.4915

```

```

872.6448          906.0330          1009.0248
1055.9301         1125.1706         1449.9433
1544.3201         1715.4026         3142.0916
3236.2923         3245.4651         3287.5272
  ZeroEnergy[kcal/mol]          -34.162
  ElectronicLevels[1/cm]        1
    0  2
  End
Barrier          B12   W5   W9
RRHO
  Geometry[angstrom]           9          #B3LYP/6-311++G** Opt "CH3-
cCCCH2 to CH2CCCH3 Ring Open"
  C  0.000000    0.434648    0.000000
  C  1.152929   -0.050950    0.000000
  C -1.286817    1.105596    0.000000
  C  0.739002   -1.475098    0.000000
  H -1.100760    2.186091    0.000000
  H -1.872551    0.867493    0.891848
  H -1.872551    0.867493   -0.891848
  H  0.607588   -2.003124    0.935086
  H  0.607588   -2.003124   -0.935086
Core      RigidRotor
SymmetryFactor      1
End
Rotor      Hindered
  Group                5 6 7
  Axis                1 3
  Symmetry              3
  Potential[kcal/mol]  2
    0.000
    0.790
  End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]  511.4384
  WellDepth[kcal/mol]      7.488
  WellDepth[kcal/mol]      46.764
  End
Frequencies[1/cm]      19
286.3313
290.5758          354.0235          545.9563
883.6172          973.2919          1018.5484
1066.1311         1102.7000         1397.0975
1427.0373         1452.6964         1480.6303
1979.3798         3018.2622         3076.6270
3090.2074         3136.0710         3250.6263
  ZeroEnergy[kcal/mol]          -63.512
  ElectronicLevels[1/cm]        1
    0  2
  End
Barrier          B13   W5   W11
RRHO

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Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH3-
cCCCH2 to CH3C(C)CH2 Ring Open"
  C -0.031402    0.174765    0.117077
  C  0.853122    1.135051   -0.106930
  C -1.488293   -0.117685    0.002453
  C  1.090913   -0.724410    0.016403
  H -2.047638    0.782961   -0.253355
  H -1.868140   -0.513617    0.948903
  H -1.665973   -0.878164   -0.764181
  H  2.000074   -0.653079    0.595039
  H  1.035634   -1.544424   -0.700426
Core      RigidRotor
SymmetryFactor      0.5
End
Rotor      Hindered
Group                5 6 7
Axis                1 3
Symmetry              3
Potential[kcal/mol]  2
  0.000
  0.990
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  279.0681
WellDepth[kcal/mol]      12.526
WellDepth[kcal/mol]      0.932
End
Frequencies[1/cm]      19
337.6812
362.5038                636.5955                789.4380
834.0407                920.2027                975.1719
1042.9192               1180.8847               1399.4964
1439.5420               1474.6512               1483.5658
1664.6859               3026.8380               3080.4616
3082.8433               3118.7926               3232.3569
ZeroEnergy[kcal/mol]    -58.474
ElectronicLevels[1/cm]  1
  0  2
End
Barrier      B14  W5  W14
RRHO
Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH3-
cCCCH2 to bic-CH2CHCCH2 H shift + C-C Scission"
  C  0.002429   -0.070159    0.763000
  C  0.227388    0.916789   -0.229499
  C -1.215407   -0.244922   -0.091365
  C  1.167274   -0.330965   -0.124404
  H -2.132323    0.132890    0.351056
  H -1.288377   -1.177562   -0.651549
  H  2.153256   -0.021590    0.203983
  H  1.152604   -1.151191   -0.840457
  H -0.975261    0.592995   -0.969426

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Core      RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  857.5677
WellDepth[kcal/mol]      49.884
WellDepth[kcal/mol]      48.109
End
Frequencies[1/cm]      20
419.2972      548.0928
621.8660      720.9997      895.5815
917.7200      967.1173      990.8395
1104.8121     1135.8003     1255.6437
1295.2312     1302.5449     1442.5705
1489.9407     2097.2199     3067.8560
3083.0775     3187.9635     3189.9893
ZeroEnergy[kcal/mol]      -21.116
ElectronicLevels[1/cm]    1
  0  2
End
Barrier      B15  W6  W7
Union
RRHO
Geometry[angstrom]      9      #B3LYP/6-311++G** Opt "CH2CHCCH2
to CH2CHCHCH 1,3 H Shift"
  C -0.346499  -0.907411  0.000000
  C  0.890597  -1.415171  0.000000
  C  0.000000   0.499321  0.000000
  C -0.516579   1.718321  0.000000
  H -1.319316  -1.388011  0.000000
  H  1.349035  -2.399822  0.000000
  H  1.298593  -0.053543  0.000000
  H  0.102914   2.606792  0.000000
  H -1.596345   1.864228  0.000000
Core      RigidRotor
SymmetryFactor  1
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  2212.8532
WellDepth[kcal/mol]      55.084
WellDepth[kcal/mol]      45.247
End
Frequencies[1/cm]      20
197.2871      324.8829
522.4710      644.8015      708.9810
860.7034      881.7576      919.7706
941.1881      1054.0044     1093.4402
1220.5030     1422.5025     1573.1840
1704.5896     1872.0168     3090.0245
3149.5190     3184.4938     3200.0889
ZeroEnergy[kcal/mol]      -52.738
ElectronicLevels[1/cm]    1

```

```

0 2
End
RRHO
Geometry[angstrom] 9 #B3LYP/6-311++G** Opt "CH2CHCCH2
to CH2CHCHCH 1,2 H Shift"
C -0.680940 0.189989 0.099402
C -1.880727 -0.271033 -0.015824
C 0.687027 0.489235 -0.105636
C 1.699500 -0.399192 0.026199
H -1.550883 0.636065 0.895983
H -2.553587 -0.696072 -0.763710
H 0.911511 1.530555 -0.322553
H 2.727711 -0.085120 -0.100346
H 1.516097 -1.439419 0.265780
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1967.5792
WellDepth[kcal/mol] 55.203
WellDepth[kcal/mol] 45.366
End
Frequencies[1/cm] 20
173.8380 229.4074
272.0019 462.1645 626.2111
645.0894 832.1695 862.1045
874.7974 960.5437 1085.1628
1292.7562 1419.3562 1568.8498
1901.7634 2310.6830 3039.6200
3138.5056 3147.2923 3238.8924
ZeroEnergy[kcal/mol] -52.619
ElectronicLevels[1/cm] 1
0 2
End
Barrier B16 W6 W8
RRHO
Geometry[angstrom] 9 #B3LYP/6-311++G** Opt "CH2CHCCH2
to CH3CHCCH 1,4 H Shift"
C 0.756433 0.651017 0.191438
C 1.430803 -0.397029 -0.127260
C -0.637820 0.705446 -0.026503
C -1.227629 -0.584061 0.016606
H 2.406303 -0.843352 -0.024145
H -1.162759 1.589564 -0.369461
H -1.055673 -1.193936 0.900234
H 0.110765 -1.091537 -0.441384
H -2.229358 -0.712976 -0.390936
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart

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    ImaginaryFrequency[1/cm]      2337.4322
    WellDepth[kcal/mol]           62.415
    WellDepth[kcal/mol]           62.209
  End
    Frequencies[1/cm]            20
  367.6432                        429.0334
  555.1984                        649.3886                723.4721
  784.7777                        854.8586                960.5363
  992.3870                        1114.1110               1153.1757
  1186.7722                       1358.5626               1436.3941
  1505.1826                       1659.3882               3091.8031
  3157.7262                       3187.5123               3273.7446
    ZeroEnergy[kcal/mol]         -45.407
    ElectronicLevels[1/cm]       1
    0 2
  End
  Barrier      B17  W6  W9
  RRHO
  Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH2CHCCH2
  to CH2CCCH3 1,2 H Shift"
  C  0.000000      0.564006      0.000000
  C -0.369135      1.951708      0.000000
  C  0.072544     -0.692757      0.000000
  C  0.227756     -2.016825      0.000000
  H  0.929235      1.387910      0.000000
  H -0.544629      2.460385      0.938343
  H -0.544629      2.460385     -0.938343
  H  0.286519     -2.572735     -0.928392
  H  0.286519     -2.572735      0.928392
  Core      RigidRotor
  SymmetryFactor      1
  End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]      1862.5034
  WellDepth[kcal/mol]           52.957
  WellDepth[kcal/mol]           55.411
  End
    Frequencies[1/cm]            20
  87.6757                        227.0076
  304.8613                       434.3681                501.0222
  660.5518                       733.6757                822.8254
  914.0225                       1011.0485               1023.2152
  1336.8778                      1417.3847               1479.1682
  2090.8086                      2210.3013               3134.4388
  3140.0900                      3216.2678               3254.1683
    ZeroEnergy[kcal/mol]         -54.865
    ElectronicLevels[1/cm]       1
    0 2
  End
  Barrier      B18  W6  W12
  RRHO

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Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH2CHCCH2
to cCH2CHCCH2 Ring Close"
  C  0.819079   -0.653943    0.029901
  C  0.864033    0.806393   -0.057863
  C -0.497078   -0.880271   -0.106233
  C -1.249999    0.287352    0.077269
  H  1.640092   -1.330411    0.232743
  H  1.433156    1.406170    0.657032
  H  0.690915    1.274621   -1.018068
  H -2.037951    0.597955   -0.610308
  H -1.342423    0.694473    1.080163
Core      RigidRotor
SymmetryFactor      0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]      678.9659
WellDepth[kcal/mol]          50.047
WellDepth[kcal/mol]          28.460
End
Frequencies[1/cm]      20
356.8329              593.6446
627.3936              726.1166              855.6959
878.5766              958.3319              987.7272
1035.1642             1086.0037             1173.3049
1270.0101             1458.8301             1490.4189
1571.6842             3058.8218             3082.8387
3168.0898             3186.7433             3201.5556
ZeroEnergy[kcal/mol]      -57.775
ElectronicLevels[1/cm]    1
  0  2
End
Barrier      B19  W6  P2
RRHO
Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH2CHCCH2
to 1,2,3-BUTATRIENE H Loss"
  C  0.000000    0.618898    0.000000
  C -0.295086    1.903914    0.000000
  C -0.052108   -0.659604    0.000000
  C  0.098776   -1.962734    0.000000
  H  0.471132    2.669395    0.000000
  H -1.331806    2.227025    0.000000
  H -0.753388   -2.635312    0.000000
  H  1.089004   -2.411869    0.000000
  H  2.015568    0.747919    0.000000
Core      RigidRotor
SymmetryFactor      1
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]      595.6216
WellDepth[kcal/mol]          55.206
WellDepth[kcal/mol]          3.836
End

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Frequencies[1/cm]      20
180.7641              207.9119
247.5139              432.8101              481.3060
581.0789              754.5510              886.5852
898.9419              905.0895              1010.8874
1032.3004             1402.6130             1457.3074
1670.9354             2122.6286             3106.4546
3125.6898             3184.2103             3212.4030
ZeroEnergy[kcal/mol]  -52.616
ElectronicLevels[1/cm] 1
  0  2
End
Barrier      B20   W6   P3
RRHO
Geometry[angstrom]  9          #B3LYP/6-311++G** Opt "CH2CHCCH2
to VINYLACETYLENE H Loss"
  C -0.726142      0.483483      0.101940
  C -1.731833     -0.390237     -0.039200
  C  0.642213      0.169711     -0.102517
  C  1.819765     -0.078432     -0.224056
  H -2.757322     -0.086669      0.132117
  H -1.554016     -1.419893     -0.325687
  H  2.839446     -0.267385     -0.455651
  H  2.388512     -0.842599      1.841277
  H -0.940638      1.509390      0.390942
Core      RigidRotor
SymmetryFactor      0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  318.0615
WellDepth[kcal/mol]      45.268
WellDepth[kcal/mol]      1.703
End
Frequencies[1/cm]      20
67.0353          197.0600
228.7698          349.1524          560.1248
677.8109          692.8351          705.3310
895.1540          956.6645          1003.6667
1111.3157         1318.5180         1442.1092
1653.5928         2165.4764         3138.0908
3147.6660         3237.8247         3471.6604
ZeroEnergy[kcal/mol]  -62.554
ElectronicLevels[1/cm] 1
  0  2
End
Barrier      B21   W7   W10
RRHO
Geometry[angstrom]  9          #B3LYP/6-311++G** Opt "CH2CHCHCH
to CH2CH2CCH 1,2 H Shift"
  C -0.751264      0.127720      0.012810
  C -1.923633     -0.238510     -0.112963
  C  0.639405      0.479651     -0.069800

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C 1.700861 -0.405224 -0.012655
H -2.929535 -0.444404 0.172712
H -0.151189 0.634493 1.134865
H 0.828228 1.525777 -0.295833
H 2.715028 -0.031826 -0.048939
H 1.545258 -1.465865 0.132839
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1669.2580
WellDepth[kcal/mol] 44.884
WellDepth[kcal/mol] 41.636
End
Frequencies[1/cm] 20
207.1717 348.1235
446.5371 545.0500 612.5052
636.6890 738.3970 768.5243
872.8706 1029.0782 1103.6618
1223.7856 1376.3454 1409.6230
1529.9941 2023.0104 3141.6107
3155.8631 3255.4836 3421.3335
ZeroEnergy[kcal/mol] -53.101
ElectronicLevels[1/cm] 1
0 2
End
Barrier B22 W7 W13
RRHO
Geometry[angstrom] 9 #B3LYP/6-311++G** Opt "CH2CHCHCH
to cCH2CHCHCH Ring Close"
C 1.133511 -0.534376 0.082096
C -0.825639 0.582607 0.115435
C 0.581697 0.753995 -0.055289
C -0.998127 -0.725210 -0.183884
H 0.939310 -1.105630 0.979555
H 2.015990 -0.848141 -0.475141
H -1.572348 1.317558 0.403833
H 1.088026 1.610449 -0.488387
H -1.819630 -1.436333 -0.170007
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 725.8740
WellDepth[kcal/mol] 29.714
WellDepth[kcal/mol] 38.506
End
Frequencies[1/cm] 20
450.8698 598.7157
699.2269 740.9900 768.2683
888.6976 906.0296 934.4775
1011.0054 1055.8263 1177.6414

```

1264.8682	1399.0518	1473.2899
1521.6930	3099.3492	3132.2527
3160.5383	3169.5042	3207.2067

ZeroEnergy[kcal/mol] -68.271
ElectronicLevels[1/cm] 1
0 2
End
Barrier B23 W7 P3
RRHO
Geometry[angstrom] 9 #B3LYP/6-311++G** Opt "CH2CHCHCH
to VINYLACETYLENE H Loss"
C 0.178907 -1.746574 0.000000
C 0.000000 0.721783 0.000000
C -0.523259 -0.609720 0.000000
C 0.079857 1.935669 0.000000
H 1.262214 -1.745875 0.000000
H -0.326814 -2.704279 0.000000
H 1.958930 0.321340 0.000000
H -1.609833 -0.653529 0.000000
H 0.302480 2.975393 0.000000
Core RigidRotor
SymmetryFactor 1
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 632.1058
WellDepth[kcal/mol] 38.941
WellDepth[kcal/mol] 5.213
End
Frequencies[1/cm] 20
81.2920 315.8706
340.6101 511.8137 541.7440
655.3477 664.2317 711.0505
882.2614 964.7256 1001.6621
1102.0781 1319.2625 1434.8190
1667.5835 2109.1504 3136.2427
3146.3356 3236.8431 3463.5955
ZeroEnergy[kcal/mol] -59.044
ElectronicLevels[1/cm] 1
0 2
End
Barrier B24 W7 P4
RRHO
Geometry[angstrom] 9 #B3LYP/6-311++G** Opt "CH2CHCHCH
to ETHYNE + VINYL C-C Bond Scission"
C -1.958925 0.193803 -0.156042
C -0.921121 -0.533827 0.177822
H -1.877809 1.252636 -0.394717
H -2.964719 -0.228449 -0.214296
H -0.780230 -1.574566 0.433965
C 1.165320 0.536882 0.171487
C 2.081856 -0.185084 -0.166511
H 0.647663 1.411024 0.493524

```

H 2.772316 -0.931288 -0.479009
Core RigidRotor
SymmetryFactor 0.5
End
Rotor Hindered
Group 1 3 4 5
Axis 2 6
Symmetry 1
Potential[kcal/mol] 2
0.000
0.100
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 367.1838
WellDepth[kcal/mol] 44.099
WellDepth[kcal/mol] 5.963
End
Frequencies[1/cm] 19
154.6277
212.1654 271.3079 568.8829
650.0343 758.4773 771.9332
780.0273 871.5214 929.1151
1075.1437 1395.4324 1633.2958
1939.6607 3052.5182 3132.1902
3222.3991 3391.4007 3482.5658
ZeroEnergy[kcal/mol] -53.886
ElectronicLevels[1/cm] 1
0 2
End
Barrier B25 W8 W10
RRHO
Geometry[angstrom] 9 #B3LYP/6-311++G** Opt "CH3CHCCH
to CH2CH2CCH 1,2 H Shift"
C -0.800177 0.138762 -0.020937
C -1.958498 -0.212798 -0.010042
C 0.549333 0.542150 -0.002510
C 1.686236 -0.423643 -0.047141
H -2.976138 -0.516884 -0.008585
H 1.180257 0.214430 1.038665
H 0.777889 1.575479 -0.239605
H 2.672269 -0.055901 -0.289137
H 1.484359 -1.483945 -0.017554
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1851.2494
WellDepth[kcal/mol] 46.399
WellDepth[kcal/mol] 33.520
End
Frequencies[1/cm] 20
208.5447 306.8691

```


488.1773	526.4744	537.1354
660.4024	695.5798	788.9761
863.5750	1074.5609	1166.7762
1236.8028	1372.4366	1423.3447
2144.7353	2188.8748	3159.0529
3161.7931	3287.4948	3476.0985

ZeroEnergy[kcal/mol] -61.217
ElectronicLevels[1/cm] 1
0 2
End
Barrier B26 W8 P3
RRHO
Geometry[angstrom] 9 #QCISD/6-311++G** Opt "CH3CHCCH
to VINYLACETYLENE H Loss"
C -0.816693 0.121643 0.018525
C -1.981749 -0.209880 -0.003961
C 0.554252 0.556233 0.045905
C 1.594917 -0.261637 -0.234985
H -3.002454 -0.516744 -0.022000
H 0.732796 1.586860 0.344857
H 2.608866 0.126142 -0.255188
H 1.433397 -1.275122 -0.590666
H 2.123031 -1.159286 1.570091
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 704.0186
WellDepth[kcal/mol] 45.761
WellDepth[kcal/mol] 2.402
End
Frequencies[1/cm] 20
190.2084 228.2183
307.4900 357.6057 551.0466
634.5383 706.5832 710.7070
888.8068 958.8380 990.9093
1119.1059 1317.2388 1449.3463
1623.2726 2220.3980 3172.6888
3195.0383 3271.3885 3491.9647
ZeroEnergy[kcal/mol] -61.855
ElectronicLevels[1/cm] 1
0 2
End
Barrier B27 W9 W11
RRHO
Geometry[angstrom] 9 #B3LYP/6-311++G** Opt "CH2CCCH3
to CH3C(C)CH2 CH3 Migration"
C 1.206675 -0.616805 0.000001
C -0.327252 0.327886 -0.000003
C 0.680192 1.138472 0.000000
C -1.571019 -0.243312 0.000001
H 1.809908 -0.600544 -0.901966

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H 0.603690 -1.530003 0.000002
H 1.809907 -0.600540 0.901969
H -2.435662 0.406527 0.000007
H -1.719416 -1.312887 -0.000005
Core RigidRotor
SymmetryFactor 1
End
Rotor Hindered
Group 5 6 7
Axis 1 3
Symmetry 3
Potential[kcal/mol] 2
0.000
0.090
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 367.0183
WellDepth[kcal/mol] 58.915
WellDepth[kcal/mol] 8.045
End
Frequencies[1/cm] 19
363.5760
365.5880 415.9257 590.6116
643.8443 917.3413 943.6372
1026.2747 1053.5370 1316.6409
1443.4693 1447.5997 1479.2634
1740.7988 3041.2028 3132.8735
3166.8766 3194.8367 3265.8991
ZeroEnergy[kcal/mol] -51.361
ElectronicLevels[1/cm] 1
0 2
End
Barrier B28 W9 P2
RRHO
Geometry[angstrom] 9 #QCISD/6-311++G** Opt "CH2CCCH3
to 1,2,3-BUTATRIENE H Loss"
C 0.244254 1.858380 0.000000
C 0.000000 0.552976 0.000000
C -0.193357 -0.702754 0.000000
C -0.406035 -2.008924 0.000000
H 2.534195 2.092978 0.000000
H 0.291372 2.416542 0.931062
H 0.291372 2.416542 -0.931062
H -0.493057 -2.562066 -0.931473
H -0.493057 -2.562066 0.931473
Core RigidRotor
SymmetryFactor 1
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 440.9826
WellDepth[kcal/mol] 55.120
WellDepth[kcal/mol] 1.296

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End
Frequencies[1/cm]      20
164.5976              223.3846
263.8699              263.9615              338.9707
470.6912              796.9891              828.2531
868.4357              890.5554              1031.3033
1059.7452             1422.3744             1488.9706
1659.0745             2100.1742             3162.1081
3165.4015             3250.7411             3254.3747
ZeroEnergy[kcal/mol]  -55.156
ElectronicLevels[1/cm] 1
0 2
End
Barrier      B29    W10    P3
RRHO
Geometry[angstrom]  9          #B3LYP/6-311++G** Opt "CH2CH2CCH
to VINYLACETYLENE H Loss"
C -0.760672      0.078683      -0.057741
C -1.930849      -0.194607      0.022050
C  0.619684      0.420507      -0.187063
C  1.630237      -0.453574      0.036014
H -2.961929      -0.439121      0.100172
H  0.830917      1.364002      -0.682098
H  2.657572      -0.168071      -0.152234
H  1.444974      -1.437789      0.447772
H  0.678066      1.574919      1.406827
Core      RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  738.3539
WellDepth[kcal/mol]      35.522
WellDepth[kcal/mol]      5.042
End
Frequencies[1/cm]      20
222.2692              282.0389
386.3651              417.4733              555.5649
652.1989              675.9608              691.9739
884.9565              916.7662              1011.1490
1105.3845             1296.2193             1432.2062
1589.5341             2204.4795             3144.5062
3149.6974             3244.5219             3476.4885
ZeroEnergy[kcal/mol]  -59.215
ElectronicLevels[1/cm] 1
0 2
End
Barrier      B30    W10    P5
Variational
RRHO
Geometry[angstrom]  9          #B3LYP/6-311++G** Opt "CH2CH2CCH
to ETHENE + CCH C-C Bond Scission (2.0 Ang)"
C  0.000000      0.994070      0.000000

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C -0.581258    2.053429    0.000000
C  0.807968   -0.835495    0.000000
C -0.269287   -1.771096    0.000000
H -1.063319    3.001647    0.000000
H  1.392059   -0.742838    0.908806
H  1.392059   -0.742838   -0.908806
H -0.732669   -2.080713   -0.927897
H -0.732669   -2.080713    0.927897
Core      RigidRotor
SymmetryFactor  1
End
Frequencies[1/cm]    20
134.0312            213.9538
365.5421            395.5540            670.3935
675.7004            749.4139            788.6990
991.6332            1061.1738           1159.1296
1235.5067           1460.7919           1510.9706
2070.5363           3136.3312           3149.7223
3213.3276           3255.8659           3461.7429
ZeroEnergy[kcal/mol]    -54.389
ElectronicLevels[1/cm]  1
0  2
End
RRHO
Geometry[angstrom]    9          #B3LYP/6-311++G** Opt "CH2CH2CCH
to ETHENE + CCH C-C Bond Scission (2.2 Ang) "
C  0.000000    1.065137    0.000000
C -0.611866    2.110337    0.000000
C  0.852919   -0.962832    0.000000
C -0.274388   -1.769418    0.000000
H -1.096342    3.057828    0.000000
H  1.403891   -0.801663    0.917951
H  1.403891   -0.801663   -0.917951
H -0.755713   -2.056923   -0.926541
H -0.755713   -2.056923    0.926541
Core      RigidRotor
SymmetryFactor  1
End
Frequencies[1/cm]    20
100.3314            156.9515
307.0722            393.7236            645.8713
655.0747            815.3361            861.8800
955.2698            980.9156            1234.7807
1239.7485           1467.0510           1542.5697
2037.5938           3147.6383           3154.8845
3232.4632           3257.0678           3455.6110
ZeroEnergy[kcal/mol]    -42.139
ElectronicLevels[1/cm]  1
0  2
End
RRHO

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Geometry[angstrom]      9          #B3LYP/6-311++G** Opt "CH2CH2CCH
to ETHENE + CCH C-C Bond Scission (2.4 Ang) "
  C  0.000000    1.124818    0.000000
  C -0.614322    2.169527    0.000000
  C  0.893781   -1.102577    0.000000
  C -0.304625   -1.745063    0.000000
  H -1.082022    3.125666    0.000000
  H  1.429632   -0.914716    0.921915
  H  1.429632   -0.914716   -0.921915
  H -0.813122   -1.988229   -0.925362
  H -0.813122   -1.988229    0.925362
Core      RigidRotor
SymmetryFactor      1
End
Frequencies[1/cm]    20
71.6058             105.7703
218.5680            328.7025             616.9551
629.0446            832.0880             936.4089
970.4449            979.2892            1237.6577
1315.3412           1471.4346           1586.5436
2018.8095           3144.6538           3155.6583
3228.7329           3255.1004           3452.8935
ZeroEnergy[kcal/mol]      -41.134
ElectronicLevels[1/cm]    1
  0  2
End
Barrier      B31    W12    W14
RRHO
Geometry[angstrom]      9          #B3LYP/6-311++G** Opt
"cCH2CHCCH2 to bicCH2CHCCH2 H Shift + C-C Bond"
  C -1.115680   -0.179753    0.164963
  C  0.121267   -0.798774   -0.418300
  C -0.107286    0.894361   -0.073428
  C  1.179780   -0.187304    0.228588
  H -1.328744   -0.414608    1.210753
  H -0.070770    1.504179   -0.967814
  H  2.177677   -0.022362   -0.166748
  H  0.761569    0.726254    0.966915
  H -2.008218   -0.164646   -0.454042
Core      RigidRotor
SymmetryFactor      0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]    1406.4205
WellDepth[kcal/mol]      64.856
WellDepth[kcal/mol]      47.846
End
Frequencies[1/cm]    20
373.8881           515.7769
567.8538           792.8244             832.2339
876.2504           952.3196             1018.9092

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1069.7468          1119.6839          1137.9647
1181.2781          1301.7880          1400.2228
1471.3163          2158.8611          3038.1951
3150.0083          3157.6158          3174.3904
  ZeroEnergy[kcal/mol]          -21.379
  ElectronicLevels[1/cm]          1
    0    2
  End
Barrier          B32    W14    W15
RRHO
  Geometry[angstrom]          9          #B3LYP/6-311++G** Opt
"bicCH2CHCCH2 to bicCH2CHCHCH H Shift"
  C  1.117627   -0.039143   0.262810
  C -0.111941   -0.744587  -0.160152
  C  0.125630    0.837422  -0.527760
  C -1.174872   -0.003081   0.368730
  H  1.256065    0.129929   1.327079
  H  2.031180   -0.247982  -0.283579
  H -0.183901   -1.474429  -0.958219
  H -0.649501    1.299103   0.269138
  H -2.192511   -0.010282  -0.016191
Core          RigidRotor
SymmetryFactor          0.5
End
Tunneling          Eckart
  ImaginaryFrequency[1/cm]          892.7885
  WellDepth[kcal/mol]          41.722
  WellDepth[kcal/mol]          54.438
End
Frequencies[1/cm]          20
422.8171          492.5360
650.5782          743.4485          837.6173
885.3722          972.2901          1020.1557
1044.8539          1089.4764          1111.5094
1156.5170          1268.6001          1407.0020
1492.4308          2404.0642          3098.0054
3138.6210          3162.6861          3186.5639
  ZeroEnergy[kcal/mol]          -27.503
  ElectronicLevels[1/cm]          1
    0    2
  End
Barrier          B33    R1    W6
RRHO
Stoichiometry  C4H5
Core          PhaseSpaceTheory
FragmentGeometry[angstrom]          7
  C  1.303388    0.000000    0.000000
  C  0.000000    0.000000    0.000000
  C -1.303388    0.000000    0.000000
  H  1.867380    0.254572   -0.891885
  H  1.867380   -0.254573    0.891885
  H -1.867380    0.891885    0.254572

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      H -1.867380   -0.891885   -0.254572
      FragmentGeometry[angstrom]      2
      C 0.000000    0.000000    0.160908
      H 0.000000    0.000000   -0.965449
      SymmetryFactor                    4
      PotentialPrefactor[au]           3.0E0
      PotentialPowerExponent            6.0
      End
      Frequencies[1/cm]                 16
373.8097                               373.8097           870.2809
870.2809                               880.8264           1016.2240
1016.2240                              1106.7650          1421.8177
1477.2793                              2042.8217          3117.4267
3121.4438                              3192.9650          3192.9650
2821.8395
      ElectronicLevels[1/cm]            1
      0      2
      ZeroEnergy[kcal/mol]              0.000
      End
      End

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