

SUPPORTING INFORMATION

REACTION MECHANISM AND PRODUCT BRANCHING RATIOS OF THE CH + C₃H₄
REACTIONS: A THEORETICAL STUDY

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Input file for RRKM - ME calculations of temperature- and pressure-
dependent rate constants for chemical reactions involving the C₄H₅ PES
using MESS software package

```
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_W8.out
LogOutput                   ME_W8.log
EigenvalueOutput            eigenvalue_W8.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
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OutputTemperatureSize 20
OutputReferenceEnergy[kcal/mol] 0.
Well W1 #B2PLYPD3/cc-pVTZ Opt "CH3-cCCHCH Radical"
Species
RRHO
Geometry[angstrom] 9
C 1.574565 -0.018598 0.014056
C 0.103905 0.029950 -0.016883
C -1.017251 0.714931 0.018128
C -1.128511 -0.734310 -0.132328
H 2.011916 0.974720 0.082804
H 1.944047 -0.510141 -0.886919
H 1.911363 -0.616307 0.861608
H -1.511534 1.665249 0.091467
H -1.552040 -1.465362 0.553203
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
314.2238 334.0125
663.5345 732.6336 938.9274
949.2718 973.0506 1020.2914
1060.1887 1117.7389 1252.9315
1412.4864 1490.2055 1493.2726
1789.0047 3047.9309 3072.5024
3105.4274 3138.2064 3286.7392
ZeroEnergy[kcal/mol] -79.79
ElectronicLevels[1/cm] 1
0 2
End
End
Well W2 #B2PLYPD3/cc-pVTZ Opt "(Cs) CH3-cCCHCH Radical"
Species
RRHO
Geometry[angstrom] 9
C -0.075983 1.548185 0.000000
C 0.431240 0.141789 0.000000
C -0.075983 -1.059117 0.656708
C -0.075983 -1.059117 -0.656708
H 0.269595 2.087220 0.880748
H -1.173436 1.571036 0.000000
H 0.269595 2.087220 -0.880748
H -0.292748 -1.587959 1.566460
H -0.292748 -1.587959 -1.566460
Core RigidRotor
SymmetryFactor 1

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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
338.7268      366.3482
619.2924      756.3104      806.8784
880.9027      964.9706      1048.8080
1060.3631     1093.5163      1370.6619
1405.2284     1488.0122      1500.0048
1647.2968     2981.5130      3088.3918
3123.5839     3257.1927      3300.2510
  ZeroEnergy[kcal/mol]      -76.97
  ElectronicLevels[1/cm]    1
    0    2
End
End
Well      W3  #B2PLYPD3/cc-pVTZ Opt "CH2-cCCHCH2 Radical"
Species
RRHO
  Geometry[angstrom]      9
C -0.422535  -1.177978    0.000000
C  0.000000   0.267815    0.000000
C  0.973664  -0.657780    0.000000
C -0.416108   1.559894    0.000000
H -0.829949  -1.609129    0.910550
H -0.829949  -1.609129   -0.910550
H  2.016466  -0.908312    0.000000
H -1.466227   1.806129    0.000000
H  0.299531   2.368727    0.000000
  Core RigidRotor
  SymmetryFactor          1
End
Frequencies[1/cm]      21
316.3530      351.2962      452.8866
564.6969      729.6087      809.9978
904.9440      995.3530      1044.3803
1045.0435     1081.8068      1118.7921
1205.3532     1469.2961      1509.5307
1583.9070     3068.5386      3134.4660
3166.8764     3264.1549      3295.3387
  ZeroEnergy[kcal/mol]      -91.43
  ElectronicLevels[1/cm]    1
    0    2
End
End
Well      W4  #B2PLYPD3/cc-pVTZ Opt "CH3C(C)CH2 Radical"
Species
RRHO

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      Geometry[angstrom]      9
C -0.535999 -1.203973 0.000000
C 0.000000 0.241460 0.000000
C -1.117633 0.963106 0.000000
C 1.355192 0.551032 0.000000
H -1.626009 -1.236058 0.000000
H -0.181930 -1.708540 0.895144
H -0.181930 -1.708540 -0.895144
H 1.685415 1.576273 0.000000
H 2.095097 -0.232889 0.000000
      Core RigidRotor
      SymmetryFactor      1
      End
      Rotor Hindered
      Group      5 6 7
      Axis      1 2
      Symmetry      3
      Potential[kcal/mol]      2
      0.000
      1.825
      End
      Frequencies[1/cm]      20
206.6867      338.5154
448.5041      466.6253      699.0210
813.8014      968.4443      1022.9828
1053.2250      1209.3953      1389.2773
1468.3861      1489.1840      1498.1337
1528.3350      3056.4568      3127.3221
3159.1690      3183.7647      3288.9494
      ZeroEnergy[kcal/mol]      -59.12
      ElectronicLevels[1/cm]      1
      0 2
      End
      End
      Well      W5 #B2PLYPD3/cc-pVTZ Opt "CH3-cCCCH2 Radical"
      Species
      RRHO
      Geometry[angstrom]      9
C 0.000000 0.276209 0.000000
C 1.277523 0.211531 0.000000
C -1.369988 0.795648 0.000000
C 0.724818 -1.167716 0.000000
H -1.350712 1.884988 0.000000
H -1.914950 0.459080 0.881708
H -1.914950 0.459080 -0.881708
H 0.693249 -1.748590 0.916225
H 0.693249 -1.748590 -0.916225
      Core RigidRotor
      SymmetryFactor      1
      End
      Rotor Hindered
      Group      5 6 7
      Axis      1 3
      Symmetry      3

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        Potential[kcal/mol]      2
        0.000
        1.250
    End
    Frequencies[1/cm]          20
290.9798      295.4826
594.3105      739.2715      939.9627
992.2061      1042.7723      1045.1681
1068.0520      1107.8552      1416.7014
1484.1117      1494.0907      1519.8195
1903.0925      3048.1163      3082.1254
3112.9900      3124.1799      3163.2969
        ZeroEnergy[kcal/mol]      -70.74
        ElectronicLevels[1/cm]      1
        0      2
    End
End
Well      W6      #B2PLYPD3/cc-pVTZ Opt "CH2CHCCH2 Radical"
Species
RRHO
        Geometry[angstrom]      9
C -0.654830      -0.535424      0.000000
C  0.000000      0.638630      0.000000
C -0.052956      -1.789140      0.000000
C  0.632689      1.772647      0.000000
H -1.738502      -0.486088      0.000000
H -0.653367      -2.683775      0.000000
H  1.020750      -1.889181      0.000000
H  0.910851      2.269382      0.923553
H  0.910851      2.269382      -0.923553
        Core      RigidRotor
        SymmetryFactor      1
    End
    Frequencies[1/cm]          21
212.8442      212.9679      511.9051
529.4426      575.5624      750.0959
891.0044      918.3543      953.1291
990.7089      1093.6281      1190.4479
1384.7621      1463.3865      1507.0299
1912.4389      3105.1504      3151.3218
3171.1780      3181.8078      3286.1986
        ZeroEnergy[kcal/mol]      -107.62
        ElectronicLevels[1/cm]      1
        0      2
    End
End
Well      W7      #B2PLYPD3/cc-pVTZ Opt "trans-CH2CHCHCH Radical"
Species
RRHO
        Geometry[angstrom]      9
C  1.182654      1.317879      0.000000
C -0.152787      -0.748354      0.000000
C  0.000000      0.705075      0.000000
C -1.295173      -1.390475      0.000000

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H  2.106737    0.755782    0.000000
H  1.258597    2.394457    0.000000
H  0.772822   -1.328363    0.000000
H -0.913461    1.285149    0.000000
H -1.632862   -2.411773    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
300.5846              514.5649
570.8790              746.5843      800.5108
873.5369              955.3792      956.4737
1043.5686             1186.3517     1261.9800
1331.0330             1459.7710     1665.5862
1779.9472             3055.5553     3161.8324
3186.5197             3253.6923     3275.2089
  ZeroEnergy[kcal/mol]   -97.47
  ElectronicLevels[1/cm]  1
    0    2
  End
End
Well      W8  #B2PLYPD3/cc-pVTZ Opt "CH3CHCCH Radical"
Species
RRHO
  Geometry[angstrom]    9
C -0.707189   -0.418185    0.000000
C -1.323284   -1.470624    0.000000
C  0.000000    0.760907    0.000000
C  1.491862    0.820073    0.000000
H -1.863136   -2.382434    0.000000
H -0.554972    1.689046    0.000000
H  1.861529    1.357993    0.876191
H  1.861529    1.357993   -0.876191
H  1.926711   -0.175626    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

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209.9872	389.9902	
477.4037	551.4595	589.2705
644.8007	871.3160	1013.6311
1106.2251	1154.2445	1396.8294
1414.4490	1489.1600	1505.9999
2045.1073	3028.0601	3071.1731
3143.2033	3187.6033	3485.9022
ZeroEnergy[kcal/mol]		-107.45
ElectronicLevels[1/cm]		1
0	2	
End		
End		
Well W9 #B2PLYPD3/cc-pVTZ Opt "CH3CCCH2 Radical"		
Species		
RRHO		
Geometry[angstrom]		9
C	0.000000 0.514786	0.000000
C	0.021449 1.968202	0.000000
C	-0.008435 -0.706614	0.000000
C	-0.019957 -2.078597	0.000000
H	1.046529 2.341980	0.000000
H	-0.477691 2.367222	0.882566
H	-0.477691 2.367222	-0.882566
H	-0.024744 -2.631546	-0.926419
H	-0.024744 -2.631546	0.926419
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
189.4453	206.1615	
381.7450	419.5992	662.2734
772.4866	1040.8469	1044.4072
1062.2695	1254.8016	1424.7054
1481.4310	1488.9568	1489.3048
2179.1557	3042.7230	3101.0684
3115.3076	3169.4306	3262.5615
ZeroEnergy[kcal/mol]		-110.08
ElectronicLevels[1/cm]		1
0	2	
End		
End		
Well W10 #B2PLYPD3/cc-pVTZ Opt "CH2CH2CCH Radical"		
Species		
RRHO		
Geometry[angstrom]		9
C	0.000000 0.780272	0.000000

```

C -0.591076    1.829798    0.000000
C  0.701953   -0.499872    0.000000
C -0.206294   -1.683808    0.000000
H -1.107851    2.754987    0.000000
H  1.370432   -0.537037    0.868333
H  1.370432   -0.537037   -0.868333
H  0.215136   -2.676073    0.000000
H -1.275649   -1.563184    0.000000
  Core    RigidRotor
  SymmetryFactor      1
End
Rotor      Hindered
  Group      8 9
  Axis      3 4
  Symmetry    2
  Potential[kcal/mol]  2
    0.000
    0.550
End
  Frequencies[1/cm]      20
206.0709      315.9536
434.2894      526.9684      649.2201
662.9345      843.3317      889.3416
1053.0794     1098.7592     1206.9809
1356.7492     1463.2245     1473.5670
2192.9600     2997.0338     3009.0416
3184.0079     3301.6123     3491.3326
  ZeroEnergy[kcal/mol]      -94.78
  ElectronicLevels[1/cm]    1
    0    2
End
End
Bimolecular      R1    #B2PLYPD3/cc-pVTZ Opt "METHYLACETYLENE and CH
Radical"
  Fragment      C3H4
  RRHO
  Geometry[angstrom]      7
C  0.000000    0.000000   -1.239467
C  0.000000    0.000000    0.217304
C  0.000000    0.000000    1.421732
H  0.000000    1.017925   -1.626250
H -0.881549   -0.508963   -1.626250
H  0.881549   -0.508963   -1.626250
H  0.000000    0.000000    2.481332
  Core    RigidRotor
  SymmetryFactor      3
End
  Frequencies[1/cm]      15
336.8798      336.8811      651.6012
651.6029      944.8666      1065.7321
1065.7325     1425.9436      1494.6113
1494.6144     2195.6126      3057.9875
3124.8822     3124.8839      3492.8257
  ZeroEnergy[kcal/mol]      0.0

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        ElectronicLevels[1/cm]          1
            0      1
        End
    Fragment          CH
    RRHO
        Geometry[angstrom]              2
    C 0.000000      0.000000      0.159796
    H 0.000000      0.000000     -0.958776
        Core      RigidRotor
        SymmetryFactor                  1
        End
        Frequencies[1/cm]              1
2874.2920
        ZeroEnergy[kcal/mol]            0.0
        ElectronicLevels[1/cm]          1
            0      2
        End
        GroundEnergy[kcal/mol]          0.000
        End
    Bimolecular      P1      #B2PLYPD3/cc-pVTZ Opt "CH2-cCCHCH and H atom"
    Fragment          C4H4
    RRHO
        Geometry[angstrom]              8
    C 0.000000      0.000000      1.588537
    C 0.000000      0.000000      0.261668
    C 0.000000      0.658999     -1.017098
    C 0.000000     -0.658999     -1.017098
    H 0.000000      0.926834      2.140205
    H 0.000000     -0.926834      2.140205
    H 0.000000      1.568988     -1.588236
    H 0.000000     -1.568988     -1.588236
        Core      RigidRotor
        SymmetryFactor                  2
        End
        Frequencies[1/cm]              18
359.0829              428.5653              682.4520
720.4138              773.8916              843.1552
855.7114              907.7896              1029.3208
1073.5315             1131.3617              1469.4490
1589.5101             1828.1847              3172.6021
3259.9178             3263.6528              3304.0112
        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]          -40.87
        End

```

Bimolecular P2 #B2PLYPD3/cc-pVTZ Opt "1,2,3-Butatriene and H
atom"

Fragment C4H4
RRHO
Geometry[angstrom] 8
C 0.000000 0.000000 0.632552
C 0.000000 0.000000 1.947496
C 0.000000 0.000000 -0.632552
C 0.000000 0.000000 -1.947496
H 0.000000 0.925038 2.508319
H 0.000000 -0.925038 2.508319
H 0.000000 -0.925038 -2.508319
H 0.000000 0.925038 -2.508319
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm] 18
223.3208 229.1549 350.4551
563.5647 780.5227 888.0036
892.5820 897.7558 1027.5560
1050.2275 1419.7775 1480.0316
1672.8603 2188.9914 3143.2235
3145.6077 3224.5403 3224.8276
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] -56.47
End

Bimolecular P3 #B2PLYPD3/cc-pVTZ Opt "VINYLACETYLENE and H
atom"

Fragment C4H4
RRHO
Geometry[angstrom] 8
C 0.000000 -0.741237 0.000000
C 0.467377 -1.854921 0.000000
C -0.586270 0.554659 0.000000
C 0.114458 1.691920 0.000000
H 0.887616 -2.828096 0.000000
H -1.668491 0.590644 0.000000
H -0.386727 2.647773 0.000000
H 1.194212 1.687161 0.000000
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 18
221.0621 315.4571 552.7771
633.2188 663.4921 704.2700

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894.6024          962.3414          1016.8582
1116.9444          1329.1809          1455.2800
1667.2045          2171.8658          3169.7045
3177.5528          3266.7087          3487.1773
  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      #B2PLYPD3/cc-pVTZ Opt "ETHYNE and VINYL Radical"
Fragment      C2H2
RRHO
  Geometry[angstrom]          4
C 0.000000      0.000000      0.601007
C 0.000000      0.000000      -0.601007
H 0.000000      0.000000      1.661449
H 0.000000      0.000000      -1.661449
  Core      RigidRotor
  SymmetryFactor          4
  End
  Frequencies[1/cm]          7
630.3370          630.3370          763.9792
763.9792          2028.6511          3435.8695
3533.6490
  ZeroEnergy[kcal/mol]          0.0
  ElectronicLevels[1/cm]          1
    0      1
  End
Fragment      C2H3
RRHO
  Geometry[angstrom]          5
C 0.048714      -0.585127      0.000000
C 0.048714      0.718163      0.000000
H -0.879122      -1.154924      0.000000
H 0.966045      -1.161353      0.000000
H -0.671493      1.518064      0.000000
  Core      RigidRotor
  SymmetryFactor          1
  End
  Frequencies[1/cm]          9
720.4599          830.9837          937.3528
1064.6896          1407.0877          1671.7477
3078.8623          3178.7563          3266.3189
  ZeroEnergy[kcal/mol]          0.0
  ElectronicLevels[1/cm]          1
    0      2
  End

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GroundEnergy[kcal/mol]      -59.83
End
Barrier      B1      W1      W2
RRHO
Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "CH3-cCCHCH
Conformational Change"
C -1.574332      -0.042797      0.081382
C -0.146005      0.008072      -0.305579
C  1.183850      -0.655187      -0.036442
C  0.992833      0.685330      0.025745
H -1.682539      -0.349423      1.129052
H -2.128004      -0.759961      -0.522546
H -2.041336      0.934735      -0.033077
H  1.699977      -1.428024      0.506124
H  1.413819      1.630167      0.329816
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]      967.0785
WellDepth[kcal/mol]      7.22
WellDepth[kcal/mol]      4.41
End
Frequencies[1/cm]      19
312.1275
340.1757      701.0146      840.1649
908.5556      941.6651      1023.4920
1079.0739      1134.1765      1258.4213
1408.9953      1481.3118      1503.1756
1648.7700      2987.8976      3081.6123
3120.0537      3226.9724      3258.3780
ZeroEnergy[kcal/mol]      -72.57
ElectronicLevels[1/cm]      1
0 2
End
Barrier      B2      W1      W4
RRHO
Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "CH3-cCCHCH to
CH3C(C)CH2 1,2 H Shift + Ring Open"
C -1.521225      -0.063841      -0.015283
C -0.051996      0.047061      0.052667
C  0.884962      1.018559      -0.062884
C  1.077789      -0.755551      0.121077
H -1.975472      0.912918      -0.160003
H -1.902872      -0.497605      0.908548
H -1.818926      -0.723246      -0.829853

```

```

H 1.909647    0.319828    0.098105
H 1.450448   -1.489266   -0.590265
  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] 873.5263
    WellDepth[kcal/mol]      35.25
    WellDepth[kcal/mol]      14.59
  End
  Frequencies[1/cm]      19
358.8641
377.4710          627.9552          843.1739
889.8560          905.6994          947.3524
1041.1494         1090.3750         1296.4444
1419.8659         1495.6350         1498.0056
1689.8930         2323.3200         3059.2279
3100.4187         3119.8601         3149.0094
  ZeroEnergy[kcal/mol]      -44.54
  ElectronicLevels[1/cm]    1
    0    2
  End
  Barrier      B3    W1    W7
  RRHO
    Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "CH3-cCCHCH to
CH2CHCHCH 1,2 H Shift + Ring Open"
C 0.815620   -0.531062    0.130360
C 1.565664    0.542770   -0.015689
C -0.562539   -0.580004   -0.375832
C -1.425619    0.406674    0.091776
H 1.250108   -1.457657    0.489907
H 1.444356    1.513885   -0.467416
H -1.503879   -0.775636    0.544796
H -2.430529    0.472639   -0.312797
H -1.118812    1.216507    0.761822
  Core      RigidRotor
    SymmetryFactor    0.5
  End
  Tunneling      Eckart
    ImaginaryFrequency[1/cm] 1103.6477
    WellDepth[kcal/mol]      55.69
    WellDepth[kcal/mol]      73.38
  End
  Frequencies[1/cm]      20
190.4871          322.2645
425.0135          643.7339          719.2240

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857.3654          917.3905          977.7308
1064.1440         1112.0170         1263.2182
1315.1188         1401.4741         1522.1766
1611.9748         2211.9213         3012.0001
3146.0575         3162.1410         3247.6482
  ZeroEnergy[kcal/mol]          -24.09
  ElectronicLevels[1/cm]        1
    0    2
  End
Barrier          B4    W1    W8
RRHO
  Geometry[angstrom]          9          #B2PLYPD3/cc-pVTZ Opt "CH3-cCCHCH to
CH3CHCCH 1,2 H Shift + Ring Open"
C  0.734578   -0.219636   0.082994
C  1.936904    0.264366   0.062297
C -0.533879   -0.589796  -0.306877
C -1.665404    0.302533   0.059579
H  0.396877   -0.850329   0.997839
H  2.673006    0.674945  -0.596995
H -2.571509   -0.249843   0.296997
H -1.464239    1.071055   0.808288
H -1.867330    0.809371  -0.894090
  Core          RigidRotor
  SymmetryFactor          0.5
  End
Rotor          Hindered
  Group                      7 8 9
  Axis                      3 4
  Symmetry                    3
  Potential[kcal/mol]        2
    0.000
    0.860
  End
Tunneling          Eckart
  ImaginaryFrequency[1/cm]    307.5251
  WellDepth[kcal/mol]         56.42
  WellDepth[kcal/mol]         84.08
  End
  Frequencies[1/cm]          19
212.0829
371.1863          472.4323          636.0844
672.7984          761.5385          832.6410
994.7400          1082.3278         1229.0378
1371.4787         1438.8511         1508.2367
1745.9929         2533.9194         3002.4477
3068.4338         3128.7613         3338.6277
  ZeroEnergy[kcal/mol]          -23.36
  ElectronicLevels[1/cm]        1
    0    2
  End
Barrier          B5    W3    W6
RRHO
  Geometry[angstrom]          9          #B2PLYPD3/cc-pVTZ Opt "CH2-cCCHCH2 to
CH2CHCCH2 Ring Open"

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```

C -1.095120    0.249774    0.000000
C  0.000000   -0.431728    0.000000
C -0.152400    1.373761    0.000000
C  1.053777   -1.295105    0.000000
H -2.161321    0.088101    0.000000
H  0.137797    1.851213   -0.925104
H  0.137797    1.851213    0.925104
H  1.524091   -1.585370   -0.927369
H  1.524091   -1.585370    0.927369
  Core      RigidRotor
  SymmetryFactor    1
End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]    663.4559
  WellDepth[kcal/mol]    16.15
  WellDepth[kcal/mol]    32.34
End
  Frequencies[1/cm]    20
112.1772            293.8053
321.6417            638.3697            643.7203
761.6960            809.0552            944.8562
1022.6557           1069.1116           1111.0864
1210.8291           1455.3381           1491.2195
1904.1126           3130.0407           3163.2203
3214.5531           3232.0140           3255.1438
  ZeroEnergy[kcal/mol]    -75.28
  ElectronicLevels[1/cm]    1
  0    2
End
Barrier      B6    W3    W4
RRHO
  Geometry[angstrom]    9      #B2PLYPD3/cc-pVTZ Opt "CH2-cCCHCH2 to
CH3C(C)CH2 1,2 H Shift + Ring Open"
C  0.194941   -1.229508    0.000000
C  0.000000    0.230705    0.000000
C -1.309169   -0.155897    0.000000
C  0.772474    1.358436    0.000000
H -1.103472   -1.437695    0.000000
H  0.499433   -1.708447    0.923023
H  0.499433   -1.708447   -0.923023
H  0.306692    2.331399    0.000000
H  1.848439    1.300776    0.000000
  Core      RigidRotor
  SymmetryFactor    1
End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]    811.8982
  WellDepth[kcal/mol]    39.45
  WellDepth[kcal/mol]    7.141
End
  Frequencies[1/cm]    20
375.9693            395.1234
523.7870            684.8551            720.5846
775.1551            913.4627            1028.1900

```

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1030.3939          1118.8631          1144.6988
1246.3022          1451.6302          1474.9706
1533.9334          2226.5669          3106.0876
3180.0558          3206.3149          3280.5969
  ZeroEnergy[kcal/mol]          -51.98
  ElectronicLevels[1/cm]          1
    0    2
  End
Barrier          B7    W4    W5
RRHO
  Geometry[angstrom]          9          #B2PLYPD3/cc-pVTZ Opt "CH3C(C)CH2
CH3c-CCCH2 Ring Close"
C -0.012599      0.168037      0.113802
C  0.827227      1.174364     -0.104173
C -1.469249     -0.118487      0.002168
C  1.071895     -0.755982      0.023961
H -2.021930      0.776420     -0.269681
H -1.847670     -0.492559      0.952788
H -1.645425     -0.889380     -0.747876
H  2.022173     -0.604015      0.506710
H  0.989207     -1.598061     -0.656493
  Core          RigidRotor
  SymmetryFactor          0.5
  End
  Tunneling          Eckart
  ImaginaryFrequency[1/cm]          128.8621
  WellDepth[kcal/mol]          0.90
  WellDepth[kcal/mol]          12.52
  End
  Frequencies[1/cm]          20
139.0081          337.1742
374.1443          600.6977          789.1710
842.0886          929.3175          990.9895
1055.8364          1214.7757          1412.5543
1455.6063          1490.8558          1499.9508
1649.3602          3056.9285          3118.7669
3119.8742          3153.1063          3267.6242
  ZeroEnergy[kcal/mol]          -58.23
  ElectronicLevels[1/cm]          1
    0    2
  End
Barrier          B8    W4    W9
RRHO
  Geometry[angstrom]          9          #B2PLYPD3/cc-pVTZ Opt "CH3C(C)CH2 to
CH3CCCH2 1,2 CH3 Shift"
C -0.425877     -1.277265      0.000000
C  0.000000      0.464293      0.000000
C -1.283063      0.332400      0.000000
C  1.290316      0.919262      0.000000
H -0.862448     -1.688571      0.899496
H  0.644208     -1.489797      0.000000
H -0.862448     -1.688571     -0.899496
H  1.458727      1.983390      0.000000
H  2.133706      0.251406      0.000000

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Core      RigidRotor
SymmetryFactor      1
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] 339.7657
WellDepth[kcal/mol] 58.87
WellDepth[kcal/mol] 7.919
End
Frequencies[1/cm]      19
364.6548
367.3928          422.2075          603.4468
639.9742          932.7971          956.9320
1037.9542         1055.4551         1325.2236
1456.9522         1467.7428         1493.6412
1742.7253         3063.7639         3163.1941
3197.8332         3226.7302         3300.9980
ZeroEnergy[kcal/mol] -51.20
ElectronicLevels[1/cm] 1
0 2
End
Barrier      B9      W5      W9
RRHO
Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "CH3-cCCCH2 to
CH3CCCH2 Ring Open"
C 0.000000      0.437191      0.000000
C 1.153792      -0.043564      0.000000
C -1.292643      1.095995      0.000000
C 0.749548      -1.471572      0.000000
H -1.118993      2.173722      0.000000
H -1.870417      0.848075      0.888735
H -1.870417      0.848075      -0.888735
H 0.597824      -1.989084      0.932611
H 0.597824      -1.989084      -0.932611
Core      RigidRotor
SymmetryFactor      1
End
Rotor      Hindered
Group              5 6 7
Axis              1 3
Symmetry          3
Potential[kcal/mol] 2
0.000
0.860
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 570.9739

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WellDepth[kcal/mol]      7.31
WellDepth[kcal/mol]      46.65
End
Frequencies[1/cm]       19
281.5064
285.0833          335.3668          516.6338
886.3516          983.8397          1029.9924
1074.3556         1104.3932          1408.0513
1443.3938         1468.5316          1495.5902
1983.8743         3050.3062          3116.7692
3129.9145         3170.7884          3288.4380
ZeroEnergy[kcal/mol]     -63.43
ElectronicLevels[1/cm]   1
0 2
End
Barrier      B10    W6    W7
Union
RRHO
Geometry[angstrom]      9          #B2PLYPD3/cc-pVTZ Opt "CH2CHCCH2 to
CH2CHCHCH 1,3 H Shift"
C -0.342834   -0.909875   0.000000
C  0.894153   -1.400972   0.000000
C  0.000000    0.499073   0.000000
C -0.522914    1.708903   0.000000
H -1.308556   -1.395606   0.000000
H  1.359761   -2.378580   0.000000
H  1.289131   -0.046608   0.000000
H  0.089423    2.597289   0.000000
H -1.600187    1.840724   0.000000
Core      RigidRotor
SymmetryFactor      1
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  2297.0774
WellDepth[kcal/mol]      55.47
WellDepth[kcal/mol]      45.37
End
Frequencies[1/cm]       20
194.0988          327.2112
544.6541          653.3852          729.8000
880.3601          892.7418          937.3680
955.4016          1081.4701          1108.0392
1237.0565         1439.5874          1646.6650
1790.3380         1911.1363          3124.4427
3177.1122         3217.2961          3235.8402
ZeroEnergy[kcal/mol]     -52.15
ElectronicLevels[1/cm]   1
0 2
End
RRHO
Geometry[angstrom]      9          #B2PLYPD3/cc-pVTZ Opt "CH2CHCCH2 to
CH2CHCHCH 1,2 H Shift"
C -0.679218    0.206420    0.118713
C -1.870834   -0.267634   -0.030672

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```

C 0.694426    0.491684   -0.108249
C 1.685121   -0.404529    0.028056
H -1.588407    0.606394    0.898992
H -2.513739   -0.738789   -0.772485
H 0.928792    1.521804   -0.345889
H 2.713759   -0.112204   -0.114676
H 1.482626   -1.432848    0.286964
  Core      RigidRotor
  SymmetryFactor    0.5
End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]    2063.0644
  WellDepth[kcal/mol]        55.08
  WellDepth[kcal/mol]        44.98
End
  Frequencies[1/cm]          20
157.1935                    228.7549
266.7639                    446.8634          631.1893
667.1998                    835.0239          880.8308
902.8561                    996.4446          1091.4979
1317.6593                   1440.1345          1621.4324
1893.6352                   2358.9592          3063.2698
3169.9807                   3177.4342          3267.1322
  ZeroEnergy[kcal/mol]        -52.54
  ElectronicLevels[1/cm]      1
  0    2
End
End
Barrier      B11    W6    W8
RRHO
  Geometry[angstrom]          9      #B2PLYPD3/cc-pVTZ Opt "CH2CHCCH2 to
CH3CHCCH 1,4 H Shift"
C 0.746117    0.634017    0.199126
C 1.451154   -0.379800   -0.130518
C -0.644907    0.695947   -0.024981
C -1.237157   -0.576694    0.020074
H 2.420739   -0.825683   -0.015551
H -1.154992    1.575313   -0.388791
H -1.015022   -1.215339    0.865964
H 0.102028   -1.073281   -0.481086
H -2.243992   -0.701827   -0.362739
  Core      RigidRotor
  SymmetryFactor    0.5
End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]    2542.9925
  WellDepth[kcal/mol]        69.03
  WellDepth[kcal/mol]        67.70
End
  Frequencies[1/cm]          20
347.5896                    425.0541
566.3511                    635.7334          731.6441
793.3404                    863.9644          969.9861
996.6529                    1122.1849          1154.8916

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1210.4494          1394.5782          1421.3347
1520.2733          1729.2661          3126.1397
3197.7448          3221.6635          3310.4043
  ZeroEnergy[kcal/mol]          -38.55
  ElectronicLevels[1/cm]          1
    0    2
  End
  Barrier          B12    W6    W9
  RRHO
    Geometry[angstrom]          9          #B2PLYPD3/cc-pVTZ Opt "CH2CHCCH2 to
CH3CCCH2 1,2 H Shift"
C  0.000000    0.563103    0.000000
C -0.354478    1.952527    0.000000
C  0.064472   -0.693901    0.000000
C  0.215356   -2.015123    0.000000
H  0.931270    1.369146    0.000000
H -0.512239    2.461828    0.936295
H -0.512239    2.461828   -0.936295
H  0.270554   -2.566218   -0.926650
H  0.270554   -2.566218    0.926650
  Core          RigidRotor
  SymmetryFactor          1
  End
  Tunneling          Eckart
    ImaginaryFrequency[1/cm]    1986.6095
    WellDepth[kcal/mol]        52.86
    WellDepth[kcal/mol]        55.32
  End
  Frequencies[1/cm]          20
64.3141          229.4695
301.7928          434.5985          498.2267
647.6562          736.5555          827.1632
925.2580          1017.4287          1033.1577
1348.9533          1435.5430          1495.8796
2096.6572          2259.2657          3165.9741
3172.4987          3252.0642          3289.6772
  ZeroEnergy[kcal/mol]          -54.76
  ElectronicLevels[1/cm]          1
    0    2
  End
  Barrier          B13    W7    W10
  RRHO
    Geometry[angstrom]          9          #B2PLYPD3/cc-pVTZ Opt "CH2CHCHCH to
CH2CH2CCH 1,2 H Shift"
C -0.747109    0.133298    0.015315
C -1.915828   -0.240442   -0.116025
C  0.642587    0.481281   -0.073478
C  1.689338   -0.409047   -0.011361
H -2.915868   -0.446287    0.180306
H -0.157031    0.642493    1.134370
H  0.836375    1.523801   -0.291753
H  2.703631   -0.047478   -0.047255
H  1.518965   -1.463065    0.137630
  Core          RigidRotor

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SymmetryFactor      0.5
End
Tunneling           Eckart
ImaginaryFrequency[1/cm]      1800.2035
WellDepth[kcal/mol]           48.42
WellDepth[kcal/mol]           45.72
End
Frequencies[1/cm]           20
205.4430                   343.5568
462.3973                   546.5594           625.0260
643.2996                   748.2349           777.2553
881.0051                   1033.7333          1113.9316
1194.3899                  1351.6454          1423.5877
1553.1672                  2030.4861          3174.7123
3184.5151                  3286.5295          3437.6334
ZeroEnergy[kcal/mol]        -49.06
ElectronicLevels[1/cm]      1
0      2
End
Barrier              B14      W8      W10
RRHO
Geometry[angstrom]          9           #B2PLYPD3/cc-pVTZ Opt "CH3CHCCH to
CH2CH2CCH 1,2 H Shift"
C -0.796641      0.145911      -0.019837
C -1.952099      -0.214631      -0.009814
C  0.554027      0.549985      -0.001540
C  1.674432      -0.430574      -0.045132
H -2.965588      -0.523601      -0.011745
H  1.185731      0.205600      1.029396
H  0.790578      1.575573      -0.242819
H  2.660401      -0.079108      -0.293430
H  1.450570      -1.482602      -0.023464
Core      RigidRotor
SymmetryFactor      0.5
End
Tunneling           Eckart
ImaginaryFrequency[1/cm]      1908.6887
WellDepth[kcal/mol]           46.28
WellDepth[kcal/mol]           33.61
End
Frequencies[1/cm]           20
204.8167                   304.5348
485.9095                   524.8749           538.7077
662.8592                   676.0422           779.3420
867.3047                   1082.3344          1172.8101
1251.3112                  1378.2883          1438.9681
2165.7988                  2223.2396          3191.1510
3199.9596                  3318.9322          3491.0634
ZeroEnergy[kcal/mol]        -61.17
ElectronicLevels[1/cm]      1
0      2
End
Barrier              B15      W2      P1
RRHO

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      Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "(Cs) CH3-
cCCHCH H Loss"
C -0.061968 -1.524415 0.000000
C -0.095817 -0.189043 0.000000
C -0.061968 1.081601 0.660097
C -0.061968 1.081601 -0.660097
H -0.120129 -2.073681 0.925587
H -0.120129 -2.073681 -0.925587
H -0.043185 1.649469 1.571739
H -0.043185 1.649469 -1.571739
H 2.016955 -1.850041 0.000000
      Core      RigidRotor
      SymmetryFactor      1
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      226.9034
      WellDepth[kcal/mol]      37.43
      WellDepth[kcal/mol]      1.32
      End
      Frequencies[1/cm]      20
208.2603      225.5210
360.4405      461.8100      696.2151
764.3986      819.1715      845.5620
867.6196      911.9369      1028.5133
1075.5786      1138.7880      1469.3712
1574.2980      1805.3236      3180.0198
3267.3651      3271.5960      3308.1389
      ZeroEnergy[kcal/mol]      -39.55
      ElectronicLevels[1/cm]      1
      0      2
      End
      Barrier      B16      W3      P1
      RRHO
      Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "CH2-cCCHCH2 H
Loss"
C 1.006031 -0.531801 -0.223341
C -0.309101 0.035325 -0.034595
C 0.916190 0.766312 0.035807
C -1.632259 -0.057153 0.020722
H 1.614454 -1.331273 -0.601748
H 1.427389 1.703582 0.156648
H -2.128120 -0.998274 -0.156873
H -2.235457 0.808698 0.244185
H 1.436571 -1.458835 1.566226
      Core      RigidRotor
      SymmetryFactor      0.5
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      636.8460
      WellDepth[kcal/mol]      53.38
      WellDepth[kcal/mol]      2.82
      End
      Frequencies[1/cm]      20
195.1404      329.2891

```

361.0177	465.6534	698.1858
734.3627	783.6897	838.3653
862.0681	917.8239	1028.4116
1073.2196	1136.0992	1467.3797
1556.5572	1824.3075	3173.5861
3261.9540	3267.0079	3304.6926
ZeroEnergy[kcal/mol]		-38.05
ElectronicLevels[1/cm]		1
0 2		
End		
Barrier	B17 W6 P2	
RRHO		
Geometry[angstrom]	9	#B2PLYPD3/cc-pVTZ Opt "CH2CHCCH2 to
1,2,3-BUTATRIENE H Loss"		
C 0.000000	0.620650	0.000000
C -0.367683	1.879387	0.000000
C -0.039823	-0.662866	0.000000
C 0.178895	-1.947267	0.000000
H 0.352008	2.683172	0.000000
H -1.418624	2.136009	0.000000
H -0.632607	-2.662394	0.000000
H 1.190892	-2.335697	0.000000
H 1.879998	0.839488	0.000000
Core RigidRotor		
SymmetryFactor	1	
End		
Tunneling	Eckart	
ImaginaryFrequency[1/cm]	875.6211	
WellDepth[kcal/mol]	56.71	
WellDepth[kcal/mol]	5.56	
End		
Frequencies[1/cm]	20	
205.6526	225.6808	
306.7953	478.0406	539.3056
600.4231	832.5539	919.9645
941.9965	946.9083	1023.6795
1048.9363	1420.4521	1475.7069
1728.0509	2421.6984	3134.6133
3160.9631	3215.5381	3249.6503
ZeroEnergy[kcal/mol]		-50.91
ElectronicLevels[1/cm]		1
0 2		
End		
Barrier	B18 W6 P3	
RRHO		
Geometry[angstrom]	9	#B2PLYPD3/cc-pVTZ Opt "CH2CHCCH2 to
VINYLACETYLENE H Loss"		
C -0.729973	0.493138	0.076883
C -1.716574	-0.397049	-0.030223
C 0.641599	0.177032	-0.107159
C 1.821309	-0.097394	-0.164680
H -0.956248	1.524316	0.316888
H -2.743611	-0.102182	0.121261
H -1.517586	-1.431111	-0.268659

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H 2.828676 -0.272645 -0.447841
H 2.290605 -0.772740 1.629425
  Core RigidRotor
  SymmetryFactor 0.5
End
  Tunneling Eckart
  ImaginaryFrequency[1/cm] 751.6289
  WellDepth[kcal/mol] 46.72
  WellDepth[kcal/mol] 3.47
End
  Frequencies[1/cm] 20
80.1164 224.1028
252.2023 424.8965 558.0379
662.7909 713.1719 793.5014
900.1511 982.0134 1028.7158
1119.0752 1336.8212 1460.9202
1716.4408 2179.6154 3172.2600
3181.0070 3269.0213 3471.4039
  ZeroEnergy[kcal/mol] -60.90
  ElectronicLevels[1/cm] 1
  0 2
End
Barrier B19 W7 P3
RRHO
  Geometry[angstrom] 9 #B2PLYPD3/cc-pVTZ Opt "CH2CHCHCH to
VINYLACETYLENE H Loss"
C 0.237021 -1.739609 0.000000
C 0.000000 0.720071 0.000000
C -0.494078 -0.624992 0.000000
C 0.002541 1.937971 0.000000
H 1.315932 -1.706775 0.000000
H -0.243765 -2.705690 0.000000
H 1.844532 0.364866 0.000000
H -1.574589 -0.696238 0.000000
H 0.184985 2.983192 0.000000
  Core RigidRotor
  SymmetryFactor 1
End
  Tunneling Eckart
  ImaginaryFrequency[1/cm] 830.0091
  WellDepth[kcal/mol] 39.14
  WellDepth[kcal/mol] 6.04
End
  Frequencies[1/cm] 20
95.3990 322.3444
350.7182 547.8306 573.7646
653.0513 679.6372 717.2377
891.5115 973.7225 1016.8421
1113.4594 1330.2104 1449.5108
1686.4077 2139.0534 3170.2883
3179.4902 3268.3987 3476.8776
  ZeroEnergy[kcal/mol] -58.33
  ElectronicLevels[1/cm] 1
  0 2

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End
Barrier      B20    W7    P4
RRHO
  Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "CH2CHCHCH to
ETHYNE + VINYL C-C Bond Scission"
C -1.675607    0.487607    0.143794
C -0.984841   -0.555462   -0.240229
H -1.203886    1.329974    0.634537
H -2.749844    0.551177   -0.011359
H -1.249343   -1.470332   -0.748064
C  1.234327   -0.507334    0.251195
C  1.761003    0.508962   -0.158532
H  1.146026   -1.449408    0.735416
H  2.047748    1.435953   -0.587904
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] 457.1232
    WellDepth[kcal/mol]    44.16
    WellDepth[kcal/mol]    6.53
  End
  Frequencies[1/cm]      19
154.1033
222.1817          336.8551          576.0419
645.1135          764.3561          774.6957
807.4606          884.4081          952.3356
1097.8917         1406.7687         1661.4123
1955.9555         3095.7075         3186.2293
3226.4014         3409.9862         3499.2365
  ZeroEnergy[kcal/mol]      -53.31
  ElectronicLevels[1/cm]    1
    0    2
  End
Barrier      B21    W8    P3
RRHO
  Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "CH3CHCCH to
VINYLACETYLENE H Loss"
C -0.808599    0.122736    0.016070
C -1.968775   -0.208974   -0.002974
C  0.547173    0.544334    0.050258
C  1.583847   -0.252654   -0.242659
H -2.985265   -0.509281   -0.022917
H  0.726166    1.567420    0.355178
H  2.591295    0.133326   -0.241723
H  1.432882   -1.263051   -0.590914

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H  2.113048   -1.161060    1.576205
  Core      RigidRotor
    SymmetryFactor    0.5
  End
  Tunneling      Eckart
    ImaginaryFrequency[1/cm]    590.5234
    WellDepth[kcal/mol]        45.48
    WellDepth[kcal/mol]        2.40
  End
  Frequencies[1/cm]          20
186.2284                229.3650
296.6538                369.8378          554.5182
648.5486                667.5585          743.6047
897.3710                985.8188          1022.8788
1119.4955               1329.5564          1454.9531
1669.0007               2214.4634          3174.5441
3181.5383               3271.6449          3489.3581
  ZeroEnergy[kcal/mol]      -61.97
  ElectronicLevels[1/cm]    1
    0    2
  End
Barrier      B22    W9    P2
RRHO
  Geometry[angstrom]        9          #B2PLYPD3/cc-pVTZ Opt "CH3CCCH2 to
1,2,3-BUTATRIENE H Loss"
C   0.216815    1.848461    0.000000
C   0.000000    0.552949    0.000000
C  -0.182772   -0.699702    0.000000
C  -0.371859   -1.994855    0.000000
H   2.405296    2.042059    0.000000
H   0.263477    2.408490    0.923916
H   0.263477    2.408490   -0.923916
H  -0.452677   -2.550078   -0.924831
H  -0.452677   -2.550078    0.924831
  Core      RigidRotor
    SymmetryFactor    1
  End
  Tunneling      Eckart
    ImaginaryFrequency[1/cm]    586.9437
    WellDepth[kcal/mol]        55.74
    WellDepth[kcal/mol]        2.16
  End
  Frequencies[1/cm]          20
177.6896                220.1818
283.6228                283.6696          352.0359
582.2572                830.5098          910.9588
920.8344                927.0346          1030.4431
1053.3402               1423.7975          1481.9770
1703.5370               2223.2028          3146.0298
3149.5902               3226.9147          3229.4877
  ZeroEnergy[kcal/mol]      -54.31
  ElectronicLevels[1/cm]    1
    0    2
  End

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Barrier      B23    W10    P3
RRHO
  Geometry[angstrom]      9      #B2PLYPD3/cc-pVTZ Opt "CH2CH2CCH to
VINYLACETYLENE H Loss"
C -0.757142    0.085683   -0.054458
C -1.926985   -0.195898    0.015432
C  0.626482    0.433429   -0.166812
C  1.622163   -0.455988    0.027064
H -2.954349   -0.448495    0.081202
H  0.842823    1.377436   -0.649402
H  2.648649   -0.178500   -0.154934
H  1.422605   -1.442794    0.414984
H  0.653166    1.488997    1.380792
  Core      RigidRotor
  SymmetryFactor      0.5
End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]      1002.2149
  WellDepth[kcal/mol]      36.26
  WellDepth[kcal/mol]      5.84
End
  Frequencies[1/cm]      20
218.2788      289.8978
430.7955      458.0921      551.5843
649.1141      671.9862      690.8951
887.9625      937.4046      1047.5385
1113.1876     1312.1325      1448.7650
1618.0451     2212.6653      3176.1100
3180.7534     3276.3193      3490.0879
  ZeroEnergy[kcal/mol]      -58.53
  ElectronicLevels[1/cm]      1
  0    2
End
Barrier      B24    R1    W8
RRHO
  Stoichiometry C4H5
  Core      PhaseSpaceTheory
  FragmentGeometry[angstrom]      7
C  0.000000    0.000000   -1.239467
C  0.000000    0.000000    0.217304
C  0.000000    0.000000    1.421732
H  0.000000    1.017925   -1.626250
H -0.881549   -0.508963   -1.626250
H  0.881549   -0.508963   -1.626250
H  0.000000    0.000000    2.481332
  FragmentGeometry[angstrom]      2
C  0.000000    0.000000    0.159796
H  0.000000    0.000000   -0.958776
  SymmetryFactor      3
  PotentialPrefactor[au]      3.0E0
  PotentialPowerExponent      6.0
End
  Frequencies[1/cm]      16
336.8798      336.8811      651.6012

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651.6029	944.8666	1065.7321
1065.7325	1425.9436	1494.6113
1494.6144	2195.6126	3057.9875
3124.8822	3124.8839	3492.8257
2874.2920		
ElectronicLevels[1/cm]	1	
0 2		
ZeroEnergy[kcal/mol]		0.000
End		
End		