

```

TemperatureList[K]          300.0
!TemperatureList[K]        600.0 700.0 800.0 900.0 1000.0
1100.0 1200.0 1300.0 1400.0 1500.0 1600.0 1700.0 1800.0 1900.0
2000.0
PressureList[bar]          0.006666
!PressureList[bar]        !Pressure values for
combustion relevance
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          low-eigenvalue
!RateOutput                one_path.out
!LogOutput                 one_path.log
EigenvalueOutput           eigenvalue.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
!      Factor[1/cm]         125 ! SJK guess
!      Power                0.85
      ExponentCutoff       15
    End
  CollisionFrequency
    LennardJones
      Epsilons[1/cm]       19.8 44.2 ! N2 , C3H6 ! from new
Jasper calc (Table 3)
      Sigmas[angstrom]     3.38 3.43 ! N2 , C3H6 ! from new
Jasper calc (Table 3)
      Masses[amu]          28.0 42.08 ! N2 , C3H6
    End
  OutputTemperatureStep[K] 100
  OutputTemperatureSize    20
  OutputReferenceEnergy[kcal/mol] 0.
  Well                    W1 # c, RingCHCH2CHCH3
  Species
    RRHO
      Geometry[angstrom]   11
      C                    -1.511409 -0.458336 -0.634109
      C                    -0.022377 -0.171071 -0.629292
      C                    0.798012 -0.191060 0.672850

```

H	-1.705496	-1.534645	-0.683648
H	-1.999939	0.010314	-1.494101
H	-1.988335	-0.072402	0.271174
H	0.512398	-0.575606	-1.488348
H	1.792794	-0.626930	0.617901
H	0.288737	-0.383175	1.615627
C	0.520057	1.061701	-0.044818
H	0.032464	1.971792	0.277879
Core RigidRotor			
	SymmetryFactor	0.5	
End			
Rotor	Hindered	! rotating group comment	
Group		4 5 6	
Axis		1 2	
Symmetry		3	
Potential[kcal/mol]		2	
0.000			
2.248			
End			
	Frequencies[1/cm]	26	
322.4728			
356.4751			
608.1744			
772.7725			
818.8177			
880.9805			
898.7730			
996.5987			
1033.7253			
1072.0626			
1091.7644			
1122.3118			
1169.9048			
1246.4673			
1382.4972			
1410.8235			
1470.2333			
1491.3639			
1500.1104			
3015.5065			
3071.8029			
3072.3375			
3073.7343			
3091.3248			
3143.0669			
3194.2782			
	ZeroEnergy[kcal/mol]	-82.6	
	ElectronicLevels[1/cm]	1	
	0	2	
End			
End			
Well	W2	# c,transRingCHCH2CHCH3	

```

Species
RRHO
  Geometry[angstrom] 11
  C      -1.403937   -0.688525   -0.680394
  C      0.079819    -0.364663   -0.702717
  C      0.883513    -0.398364    0.606556
  C      0.606354     0.864024   -0.093325
  H     -1.571743    -1.768599   -0.730765
  H     -1.915870    -0.225240   -1.529332
  H     -1.870299    -0.312479    0.233772
  H      0.595859    -0.723604   -1.593709
  H      1.895197    -0.798575    0.607920
  H      0.322831    -0.630015    1.510218
  H      1.250060     1.652250   -0.457660
  Core   RigidRotor
  SymmetryFactor      0.5
  End
  Rotor   Hindered   ! rotating group comment
  Group   5 6 7
  Axis    1 2
  Symmetry 3
  Potential[kcal/mol] 2
0.000
2.594
  End
  Frequencies[1/cm] 26
323.3364
368.1702
593.5136
749.9985
812.3095
864.3427
919.4193
1004.9157
1041.9632
1075.2949
1086.3359
1136.7610
1161.1702
1241.7373
1383.9467
1410.2078
1469.8796
1492.1894
1501.0582
3019.3827
3070.5803
3072.2206
3078.2476
3095.4598
3140.5923
3202.0588

```

```

ZeroEnergy[kcal/mol]          -82.4
ElectronicLevels[1/cm]       1
    0    2
End
End
Well          W3  # d,CH2CHCHCH3
Species
RRHO
Geometry[angstrom]    11
C          -1.802980    0.277358    0.596890
C          -0.312303    0.242497    0.510743
C           0.402907   -0.278869   -0.555652
C           1.781134   -0.319959   -0.653299
H          -2.167766   -0.269738    1.475713
H          -2.175738    1.304482    0.700723
H          -2.268972   -0.161130   -0.289009
H           0.243672    0.657876    1.348774
H          -0.172609   -0.689886   -1.384624
H           2.273097   -0.743734   -1.519170
H           2.411917    0.072287    0.136968
Core   RigidRotor
SymmetryFactor              1
End
Rotor   Hindered
Group                    5 6 7
Axis                      1 2
Symmetry                   3
Potential[kcal/mol]       2
0.000
1.147
End
Frequencies[1/cm]        26
216.3678
287.6954
506.5313
543.9350
737.2242
788.4678
882.1335
992.4870
994.1745
1027.2971
1138.9972
1207.2207
1283.5768
1343.6443
1411.5510
1473.9929
1475.5345
1509.9907
1526.2504
2992.6948

```

```

3025.0860
3085.8595
3110.4156
3130.5984
3137.8243
3232.1749
      ZeroEnergy[kcal/mol]          -112.4
      ElectronicLevels[1/cm]        1
      0      2
End
End
Well      W4 # d,cisCH2CHCHCH3
Species
RRHO
  Geometry[angstrom]      11
  C      -1.912859      0.026356      0.679408
  C      -0.429938      -0.049478      0.508094
  C      0.247265      -0.583438      -0.581796
  C      -0.301103      -1.147466      -1.718036
  H      -2.231230      -0.509112      1.582473
  H      -2.240242      1.065620      0.807225
  H      -2.459263      -0.393077      -0.166186
  H      0.168120      0.354584      1.319812
  H      1.333600      -0.550917      -0.528845
  H      0.333776      -1.532436      -2.505627
  H      -1.370672      -1.227924      -1.868288
Core  RigidRotor
      SymmetryFactor          1
End
Rotor  Hindered
      Group          5 6 7
      Axis          1 2
      Symmetry          3
      Potential[kcal/mol]    2
0.000
0.172
      End
      Frequencies[1/cm]      26
287.9243
293.8882
538.1241
574.6382
696.2150
783.2922
876.1939
990.9523
1020.7025
1024.9868
1085.2119
1200.9428
1242.5011
1399.5724

```

1435.1478  
1456.9343  
1477.4886  
1515.5524  
1526.0020  
3001.3122  
3034.0315  
3106.9939  
3123.4048  
3146.4752  
3153.8230  
3235.1832

ZeroEnergy[kcal/mol] -111.7  
ElectronicLevels[1/cm] 1  
0 2

End

End

Well W5 # e, (CH2)2CCH3

Species

RRHO

Geometry[angstrom] 11  
C -1.422100 0.143820 -0.280117  
C 0.067806 -0.146304 -0.286515  
C 0.705638 -0.396524 -1.493065  
C 0.766910 -0.134904 0.911954  
H -1.606626 1.216938 -0.392201  
H -1.885322 -0.174556 0.656143  
H -1.930116 -0.365839 -1.101510  
H 1.772837 -0.580932 -1.532203  
H 0.161062 -0.415549 -2.429249  
H 1.835721 -0.312435 0.936044  
H 0.270251 0.050662 1.856550

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered

Group 5 6 7

Axis 1 2

Symmetry 6

Potential[kcal/mol] 2

0.000

0.007

End

Frequencies[1/cm] 26

409.8813  
433.6667  
482.6836  
539.7693  
553.6714  
765.8925  
794.5709  
848.1959

970.4361  
1021.8536  
1044.4608  
1057.4609  
1331.4075  
1371.0407  
1415.8814  
1481.1875  
1495.9709  
1497.9662  
1529.7311  
3028.7822  
3085.0172  
3105.8990  
3133.4808  
3141.0958  
3228.5112  
3230.7984

ZeroEnergy[kcal/mol] -111.9  
ElectronicLevels[1/cm] 1  
0 2

End

End

Well W6 # f,CH2CH2CHCH2

Species

RRHO

Geometry[angstrom] 11

C	-0.969616	0.047544	0.297405
C	0.520069	0.220903	0.135458
C	1.300241	-0.542064	-0.623842
C	-1.378999	-0.247412	1.704222
H	-1.305136	-0.758210	-0.377102
H	-1.482964	0.954510	-0.047610
H	0.962802	1.033016	0.709103
H	2.368528	-0.371011	-0.694792
H	0.897391	-1.366075	-1.205675
H	-2.329558	0.094661	2.094244
H	-0.782868	-0.912962	2.316762

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 27

99.4024  
130.5537  
325.4173  
421.0547  
492.0300  
659.3540  
796.2665  
897.3514  
945.6614  
1028.0377

```

1046.7376
1072.7178
1114.6959
1239.8907
1318.3528
1335.5343
1444.8532
1457.3254
1463.2299
1703.4685
2936.8047
3011.5207
3120.3374
3128.6234
3135.2906
3207.2040
3240.6849
      ZeroEnergy[kcal/mol]          -95.9
      ElectronicLevels[1/cm]       1
      0      2
End
End
Well      W7 # g, RingCH2CH2CCH3
Species
RRHO
      Geometry[angstrom]      11
      C      -1.393884      -0.742595      -0.748181
      C      0.038943      -0.404970      -0.583381
      C      0.957950      -0.465575      0.560022
      C      0.742807      0.835529      -0.235011
      H      -1.554543      -1.824534      -0.756240
      H      -1.802533      -0.324727      -1.672769
      H      -1.990689      -0.332638      0.084147
      H      1.921590      -0.956773      0.449539
      H      0.546740      -0.532485      1.566642
      H      0.186624      1.645315      0.235905
      H      1.568789      1.176804      -0.854173
Core      RigidRotor
      SymmetryFactor          1
End
Rotor      Hindered
      Group          5 6 7
      Axis          1 2
      Symmetry          3
      Potential[kcal/mol]    2
0.000
1.350
      End
      Frequencies[1/cm]      26
244.5021
324.1997
705.8771

```



749.9325  
834.3105  
913.8904  
923.8468  
988.7147  
1020.8467  
1065.3168  
1125.3060  
1136.1843  
1156.8028  
1382.3654  
1414.8918  
1452.5116  
1469.7833  
1483.0069  
1504.1858  
2942.7288  
3044.8953  
3067.1291  
3067.7921  
3083.5783  
3132.7009  
3145.7397

ZeroEnergy[kcal/mol] -85.4  
ElectronicLevels[1/cm] 1  
0 2

End

End

Well W8 # h, RingCH2CH2CHCH2

Species

RRHO

Geometry[angstrom] 11  
C -1.363756 -0.687814 -0.733641  
C 0.052554 -0.385420 -0.606286  
C 0.735344 -0.379122 0.766704  
C 1.055646 -1.471933 -0.200522  
H -1.835892 -1.408253 -0.075989  
H -1.973853 -0.203065 -1.483390  
H 0.437571 0.347651 -1.307043  
H 0.112387 -0.615134 1.621253  
H 1.477283 0.389764 0.948364  
H 2.020929 -1.465047 -0.693312  
H 0.653135 -2.460029 -0.011625

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered

Group 5 6

Axis 1 2

Symmetry 2

Potential[kcal/mol] 2

0.000

```

3.253
      End
      Frequencies[1/cm]          26
333.7082
372.1769
492.6063
762.3433
781.0072
804.9918
848.7879
927.1847
1019.8732
1039.1171
1063.4650
1115.9953
1200.4479
1205.7330
1214.6991
1384.1285
1466.4723
1472.7138
1497.8387
3116.7021
3120.9396
3141.2256
3144.3878
3196.1394
3213.2934
3245.4194
      ZeroEnergy[kcal/mol]      -92.6
      ElectronicLevels[1/cm]    1
          0  2
      End
      End
      Well      W9  # i,CH3CCHCH3
      Species
      RRHO
      Geometry[angstrom]      11
      C      -1.914801      0.034409      0.533397
      C      -0.408457      0.038218      0.469450
      C      0.322211      -0.203217      -0.590541
      C      1.732217      -0.281648      -0.997181
      H      -2.273426      -0.703438      1.259163
      H      -2.294956      1.010330      0.854058
      H      -2.349024      -0.201005      -0.439417
      H      0.108241      0.267483      1.411687
      H      1.985570      -1.275635      -1.379703
      H      2.397984      -0.071823      -0.145046
      H      1.964004      0.441557      -1.785701
      Core      RigidRotor
      SymmetryFactor          1
      End

```

```

      Frequencies[1/cm]          27
154.0812
192.8277
214.9769
245.7676
462.9518
736.7885
839.7891
986.4223
1045.6319
1062.0191
1064.3695
1112.4859
1292.2576
1397.4259
1405.5934
1455.6087
1476.9695
1485.5487
1490.6018
1773.4779
2957.2901
2988.1482
3015.0148
3042.8378
3059.2674
3066.7288
3108.5501
      ZeroEnergy[kcal/mol]      -91.8
      ElectronicLevels[1/cm]    1
          0      2
End
End
Well      W10 # i,cisCH3CCHCH3
Species
RRHO
      Geometry[angstrom]      11
      C      -1.884994      -0.008259      0.690818
      C      -0.406638      0.330732      0.651610
      C      0.396942      0.165200      -0.370837
      C      0.412520      -0.316378      -1.759758
      H      -2.093100      -0.739247      1.479259
      H      -2.480326      0.883868      0.912129
      H      -2.233936      -0.422643      -0.256891
      H      -0.000345      0.749803      1.573599
      H      -0.581625      -0.665322      -2.079669
      H      1.110208      -1.150958      -1.883699
      H      0.722631      0.473675      -2.451352
Core      RigidRotor
      SymmetryFactor          1
End
Rotor      Hindered

```

```

      Group          9 10 11
      Axis          4 3
      Symmetry      3
      Potential[kcal/mol] 2
0.000
0.872
      End
      Rotor      Hindered
      Group          5 6 7
      Axis          1 2
      Symmetry      3
      Potential[kcal/mol] 2
0.000
1.455
      End
      Frequencies[1/cm]      25
196.4656
364.5832
528.7885
743.3332
838.3612
986.4060
1017.6611
1044.5857
1050.4457
1093.3040
1310.1531
1388.5483
1404.1159
1458.3807
1473.1978
1482.9056
1492.4224
1765.1979
2960.2392
3014.9716
3041.8282
3062.6196
3066.3423
3076.8338
3104.8464
      ZeroEnergy[kcal/mol]      -91.0
      ElectronicLevels[1/cm]      1
      0 2
      End
      End
      Well      W11 # j, (CH3)2CCH
      Species
      RRHO
      Geometry[angstrom]      11
      C      -1.428168      0.161015      -0.085146
      C      0.090969      0.116633      -0.113312

```

C	0.718869	-0.035550	-1.481421
C	0.807851	0.205080	0.982063
H	-1.795658	0.998346	-0.688790
H	-1.815039	0.271622	0.928693
H	-1.843728	-0.756885	-0.515642
H	0.375894	-0.959156	-1.961061
H	0.423911	0.793819	-2.134016
H	0.634440	0.314509	2.043014
H	1.806958	-0.059408	-1.421155
Core	RigidRotor		
	SymmetryFactor	1	
End			
Frequencies[1/cm]		27	
163.9563			
203.3987			
362.3305			
399.3136			
429.8068			
675.6769			
789.5365			
858.6194			
956.7198			
965.1432			
1090.3574			
1094.5720			
1192.9569			
1391.6610			
1408.8477			
1474.7402			
1480.6186			
1485.2165			
1492.3408			
1692.9854			
3009.1666			
3013.9142			
3057.6600			
3060.8367			
3109.5875			
3117.9674			
3226.0835			
ZeroEnergy[kcal/mol]		-89.1	
ElectronicLevels[1/cm]		1	
	0	2	
End			
End			
Well	W12	# 1,CH3CH2CCH2	
Species			
RRHO			
Geometry[angstrom]		11	
C	0.741729	-1.615181	-0.134588
C	-1.087978	1.415267	0.803851
C	-0.913119	0.246164	0.243202

C	-0.036705	-0.428418	-0.728726
H	1.381472	-1.287528	0.687983
H	0.057835	-2.373875	0.252613
H	1.372747	-2.080144	-0.896115
H	-0.446957	2.269018	0.559433
H	-0.638164	-0.776054	-1.577266
H	0.671409	0.311747	-1.138560
H	-1.871776	1.602412	1.533197
Core	RigidRotor		
	SymmetryFactor	0.5	
End			
Rotor	Hindered		
	Group	5 6 7	
	Axis	1 4	
	Symmetry	3	
	Potential[kcal/mol]	2	
0.000			
2.867			
End			
	Frequencies[1/cm]	26	
111.2114			
288.2074			
369.5472			
554.8667			
782.9378			
832.6321			
884.7038			
956.5897			
1019.5413			
1088.6138			
1123.7766			
1272.5289			
1332.5629			
1409.4387			
1415.7555			
1458.8306			
1497.2022			
1506.3288			
1740.4964			
2938.5778			
3021.9386			
3023.9828			
3033.2635			
3100.3718			
3103.8589			
3142.5020			
	ZeroEnergy[kcal/mol]	-89.5	
	ElectronicLevels[1/cm]	1	
	0 2		
End			
End			
Well	W13	# m, CH3CH2CHCH	

```

Species
RRHO
  Geometry[angstrom] 11
  C      0.801995   -1.418488   -0.313253
  H      0.763151   -1.600195    0.763766
  H      0.035587   -2.040790   -0.784526
  H      1.776196   -1.752991   -0.680323
  C     -1.004922    1.508813    0.696803
  C     -0.785164    0.558026   -0.173714
  C      0.580148    0.067744   -0.627372
  H     -0.429139    2.190963    1.306458
  H     -1.637103    0.043416   -0.624423
  H      0.661836    0.226460   -1.709703
  H      1.361399    0.672887   -0.159365
  Core  RigidRotor
  SymmetryFactor      0.5
  End
  Rotor  Hindered
  Group      2 3 4
  Axis      1 7
  Symmetry    3
  Potential[kcal/mol] 2
0.000
3.005
  End
  Frequencies[1/cm] 27
106.4550
231.6061
328.8447
396.4855
682.2545
782.0299
820.5957
872.3123
899.6433
1015.2767
1083.3722
1117.9746
1259.6852
1292.4506
1339.2559
1410.2658
1483.8680
1497.6777
1505.9750
1666.7966
3011.2291
3024.5740
3057.5027
3073.4643
3089.4893
3096.1791

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3223.9562
  ZeroEnergy[kcal/mol]          -85.7
  ElectronicLevels[1/cm]       1
    0 2
End
End
Well      W14 # m,cisCH3CH2CHCH
Species
RRHO
  Geometry[angstrom]          11
  C      0.743594 -1.494677 -0.114830
  C     -1.165756  1.367189  0.880365
  C     -0.892174  0.437540  0.002904
  C      0.488129 -0.011329 -0.419894
  H      0.683752 -1.687587  0.959290
  H      0.006956 -2.134048 -0.610623
  H      1.735354 -1.798199 -0.460615
  H     -2.036930  1.828846  1.320529
  H     -1.725546 -0.092042 -0.477985
  H      0.596241  0.158489 -1.498195
  H      1.236531  0.611125  0.076611
Core  RigidRotor
  SymmetryFactor              0.5
End
Rotor  Hindered
  Group                      5 6 7
  Axis                       1 4
  Symmetry                   3
  Potential[kcal/mol]        2
0.000
3.014
End
  Frequencies[1/cm]          27
110.3832
232.6069
331.9427
419.3853
652.0049
765.1187
794.8623
833.9997
907.4093
1020.6361
1089.3981
1132.6474
1254.5078
1294.8469
1346.5150
1410.3129
1485.2865
1498.5121
1506.8283

```



1676.5060  
2996.3736  
3012.6803  
3024.2940  
3066.9793  
3090.1572  
3096.4023  
3237.9720

ZeroEnergy[kcal/mol] -86.1  
ElectronicLevels[1/cm] 1  
0 2

End

End

Well W15 # n,4-Ring

Species

RRHO

Geometry[angstrom] 11

C	-0.779330	0.394396	-0.450582
C	-0.284130	1.793151	-0.219138
C	0.826155	1.375522	0.701817
C	0.358250	-0.104133	0.501223
H	-1.800074	0.183818	-0.103400
H	-0.713363	0.027576	-1.483971
H	-0.611061	2.758670	-0.585688
H	0.758688	1.747503	1.733260
H	1.845126	1.591096	0.352493
H	1.096105	-0.750031	0.023166
H	0.004451	-0.592801	1.410169

Core RigidRotor

SymmetryFactor 2

End

Frequencies[1/cm] 27

83.3601  
258.2074  
742.3935  
747.6210  
796.1328  
901.1663  
903.8622  
966.9823  
1000.3822  
1008.4628  
1036.0019  
1182.1408  
1206.3598  
1214.9697  
1246.8337  
1280.9984  
1309.1125  
1457.7879  
1465.6151  
1497.7175

```

2974.6560
2978.7061
2992.8655
2996.9816
3060.7058
3109.7557
3181.9251
    ZeroEnergy[kcal/mol]          -91.3
    ElectronicLevels[1/cm]        1
      0  2
End
End
Bimolecular      R1  # C3H6+CH
Fragment         C3H6
RRHO
  Geometry[angstrom]      9
  C      -1.467054  -0.247836   0.585542
  C       0.030549  -0.187355   0.515967
  C       0.757529  -0.389660  -0.578479
  H      -1.884113   0.706052   0.927272
  H      -1.797463  -1.008392   1.301790
  H      -1.904859  -0.482538  -0.387548
  H       0.541521   0.042396   1.449634
  H       1.839990  -0.331251  -0.561519
  H       0.295414  -0.621647  -1.533696
  Core      RigidRotor
  SymmetryFactor          1
  End
  Frequencies[1/cm]      21
204.3804          425.7634          590.6356
923.8042          940.5952          948.6235
1029.0335         1070.7181         1189.1812
1327.6604         1408.8905         1448.7188
1481.0539         1494.9488         1713.0513
3012.1903         3055.8298         3090.9901
3119.2670         3126.4358         3207.0111
    ZeroEnergy[kcal/mol]          0.
    ElectronicLevels[1/cm]        1
      0  1
End
Fragment         CH
RRHO
  Geometry[angstrom]      2
  C      -0.564023   0.000000   0.000000
  H       0.564008   0.000000   0.000000
  Core      RigidRotor
  SymmetryFactor          1
  End
  Frequencies[1/cm]      1
2804.9231
    ZeroEnergy[kcal/mol]          0.
    ElectronicLevels[1/cm]        1

```

```

0 2
End
GroundEnergy[kcal/mol] 0.0
End
Bimolecular P1 # cCHCHCH2 + CH3
Fragment cCHCHCH2
RRHO
Geometry[angstrom] 7
C -0.267210 -0.733767 -0.734416
C -0.061611 -0.390586 0.720955
C -0.096730 0.519845 -0.482374
H -0.437873 -1.525611 -1.443085
H 0.892370 -0.616521 1.199430
H -0.910282 -0.412916 1.406032
H -0.021456 1.536506 -0.827471
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 15
605.9288 786.7510 870.3403
922.5376 1015.4220 1031.7665
1069.1808 1110.4418 1153.8656
1520.9837 1733.3226 3031.5182
3094.1620 3246.1606 3293.3466
ZeroEnergy[kcal/mol] 0.
ElectronicLevels[1/cm] 1
0 1
End
Fragment CH3
RRHO
Geometry[angstrom] 4
C 0.010526 0.085155 0.194783
H -0.044537 0.239428 -0.873182
H -0.153501 0.913041 0.869378
H 0.229627 -0.897005 0.588148
Core RigidRotor
SymmetryFactor 6
End
Frequencies[1/cm] 6
505.1400 1403.0741 1403.0813
3103.6554 3282.6758 3282.6811
ZeroEnergy[kcal/mol] 0. #Always 0.
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -44.1 # Relative energy of R1
End
Bimolecular P2 # CH3cCCHCH2 + H
Fragment CH3cCCHCH2
RRHO
Geometry[angstrom] 10
C -1.287957 -0.792819 -0.870005

```

```

C          -0.063025   -0.189822   -0.308172
C          1.086780   -0.432738    0.640542
C          0.784500    0.780029   -0.207291
H          -1.051985   -1.728523   -1.387702
H          -1.781655   -0.118900   -1.574062
H          -1.993697   -1.042562   -0.070758
H          1.893821   -1.109865    0.351351
H          0.915861   -0.397511    1.718965
H          1.113039    1.766503   -0.486179
Core      RigidRotor
SymmetryFactor      1
End
Frequencies[1/cm]      24
159.9815      297.8095      322.7140
674.7119      736.1955      940.1772
975.2382      986.8635     1050.8003
1062.9951     1081.1975     1120.0040
1189.6337     1405.8360     1477.8137
1482.6766     1522.8184     1861.7349
3014.5922     3017.1218     3065.5568
3073.5821     3095.6097     3264.6958
ZeroEnergy[kcal/mol]      0.
ElectronicLevels[1/cm]      1
  0      1
End
Fragment      H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]      1
  0      2
End
GroundEnergy[kcal/mol]      -37.4
End
Bimolecular      P3      # CH3cCHCHCH + H
Fragment      CH3cCHCHCH
RRHO
Geometry[angstrom]      10
C          -0.877172   -0.756511   -0.781228
C          0.602679   -0.475047   -0.577156
C          1.210788   -0.337816    0.796901
C          1.093104    0.763869    0.130828
H          -1.074258   -1.833677   -0.814535
H          -1.234990   -0.328973   -1.724316
H          -1.472267   -0.329168    0.030701
H          1.232068   -0.887506   -1.370565
H          1.507874   -0.849597    1.697057
H          1.221416    1.832027    0.075757
Core      RigidRotor
SymmetryFactor      1
End
Frequencies[1/cm]      24
185.1911      365.2391      415.0320

```

619.6281	778.1304	834.1557
873.8252	952.0605	1007.7305
1038.3741	1093.8122	1118.5912
1222.2257	1396.5581	1407.2658
1490.7716	1497.1179	1718.7233
3008.4136	3029.1559	3061.6253
3085.5981	3233.9498	3280.3784

ZeroEnergy[kcal/mol] 0.

ElectronicLevels[1/cm] 1

0 1

End

Fragment H

Atom

Mass[amu] 1

ElectronicLevels[1/cm] 1

0 2

End

GroundEnergy[kcal/mol] -34.2

End

Bimolecular P4 # CH2cCCH2CH2 + H

Fragment CH2cCCH2CH2

RRHO

Geometry[angstrom] 10

C -1.226968 -0.762452 -0.921303

C -0.161949 -0.237044 -0.348967

C 0.954145 -0.390761 0.590351

C 0.738762 0.911629 -0.204459

H -1.553808 -1.770859 -0.688544

H -1.812875 -0.204323 -1.644554

H 1.792246 -1.021413 0.309102

H 0.747862 -0.371990 1.656337

H 0.391260 1.784327 0.340401

H 1.435653 1.134848 -1.006800

Core RigidRotor

SymmetryFactor 2

End

Frequencies[1/cm] 24

291.2813	356.4422	619.7969
----------	----------	----------

740.7685	755.5492	899.5309
----------	----------	----------

918.6445	959.1209	1034.1931
----------	----------	-----------

1062.6957	1070.4355	1096.4386
-----------	-----------	-----------

1139.8256	1165.3201	1443.1569
-----------	-----------	-----------

1448.6896	1483.3411	1834.4032
-----------	-----------	-----------

3097.4361	3098.5396	3119.4951
-----------	-----------	-----------

3168.1115	3181.1843	3199.0308
-----------	-----------	-----------

ZeroEnergy[kcal/mol] 0.

ElectronicLevels[1/cm] 1

0 1

End

Fragment H

Atom

Mass[amu] 1

```

      ElectronicLevels[1/cm]      1
      0      2
    End
    GroundEnergy[kcal/mol]      -48.3
  End
  Bimolecular      P5      # 1,3-BUTADIENE + H
  Fragment      CH2CHCHCH2
  RRHO
  Geometry[angstrom]      10
  C      -1.929395      0.006649      0.623493
  C      -0.595751      -0.043865      0.545373
  C      0.140773      -0.595488      -0.583021
  C      1.474416      -0.646034      -0.661126
  H      -2.433836      0.427268      1.484994
  H      -2.558084      -0.373078      -0.175896
  H      0.002129      0.346696      1.366546
  H      -0.457107      -0.986017      -1.404210
  H      1.978857      -1.066650      -1.522628
  H      2.103105      -0.266327      0.138272
  Core      RigidRotor
  SymmetryFactor      2
  End
  Frequencies[1/cm]      24
  174.4618      297.9563      518.5775
  538.8644      781.0536      899.1049
  935.4825      936.4360      1000.7070
  1003.9076      1057.4740      1226.5958
  1314.7843      1319.8183      1415.4438
  1473.3110      1652.9446      1705.8448
  3121.6929      3130.9346      3134.4849
  3135.0879      3218.7868      3219.2135
  ZeroEnergy[kcal/mol]      0.
  ElectronicLevels[1/cm]      1
  0      1
  End
  Fragment      H
  Atom
  Mass[amu]      1
  ElectronicLevels[1/cm]      1
  0      2
  End
  GroundEnergy[kcal/mol]      -67.8
  End
  Bimolecular      P6      # 1,2-BUTADIENE + H
  Fragment      CH3CHCCH2
  RRHO
  Geometry[angstrom]      10
  C      -1.629402      1.222069      0.127455
  C      -0.239876      0.896607      -0.362785
  C      0.397929      -0.215360      -0.122346
  C      1.032665      -1.328251      0.119976
  H      -1.620589      2.123880      0.748494

```

```

H          -2.043540    0.402854    0.716590
H          -2.302304    1.416616   -0.714200
H           0.260831    1.655187   -0.962972
H           1.668079   -1.440421    0.993791
H           0.951356   -2.184056   -0.544005
Core      RigidRotor
SymmetryFactor      1
End
Frequencies[1/cm]      24
167.2302           211.3757           339.8847
540.8075           572.7933           871.7458
879.2869           896.9413          1021.6269
1059.5654          1091.3001          1149.8597
1361.2886          1407.9900          1471.7299
1485.5359          1504.8476          2056.7958
3017.8638          3064.1379          3103.6283
3109.9377          3119.6110          3179.7902
ZeroEnergy[kcal/mol]      0.
ElectronicLevels[1/cm]      1
  0      1
End
Fragment      H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]      1
  0      2
End
GroundEnergy[kcal/mol]      -55.8
End
Bimolecular      P7      # C2H4 + C2H3
Fragment      C2H4
RRHO
Geometry[angstrom]      6
C          -0.663490    0.000003   -0.001619
C           0.663490   -0.000003   -0.001619
H          -1.234624    0.922530   -0.001619
H          -1.234632   -0.922519   -0.001619
H           1.234624   -0.922530   -0.001619
H           1.234632    0.922519   -0.001619
Core      RigidRotor
SymmetryFactor      4
End
Frequencies[1/cm]      12
834.2930           972.9229           974.1221
1066.8560          1238.5875          1379.4650
1472.0484          1691.5383          3121.2068
3136.3251          3192.3839          3220.8385
ZeroEnergy[kcal/mol]      0.
ElectronicLevels[1/cm]      1
  0      1
End
Fragment      C2H3

```

```

RRHO
  Geometry[angstrom]      5
  C      -0.684229      0.016634      -0.001324
  C      0.616675      0.112803      0.000964
  H      -1.330433      0.899144      -0.005094
  H      -1.194882      -0.944319      0.000376
  H      1.369721      0.887323      0.000220
  Core      RigidRotor
  SymmetryFactor          1
  End
  Frequencies[1/cm]      9
711.9318      819.3915      921.8191
1046.0240      1391.3839      1650.5207
3036.9249      3132.7310      3234.1829
  ZeroEnergy[kcal/mol]      0.      #Always 0.
  ElectronicLevels[1/cm]      1
    0      2
  End
  GroundEnergy[kcal/mol]      -62.7      # Relative energy of R1
  End
Bimolecular      P8      # C2H2 + C2H5
  Fragment      C2H2
  RRHO
  Geometry[angstrom]      4
  C      -0.830252      -0.518579      0.461299
  C      0.367889      -0.518523      0.461208
  H      -1.893100      -0.518628      0.461379
  H      1.430736      -0.518473      0.461128
  Core      RigidRotor
  SymmetryFactor          4
  End
  Frequencies[1/cm]      7
642.1288      642.1288      772.7548
772.7548      2069.5125      3420.8344
3523.7079
  ZeroEnergy[kcal/mol]      0.
  ElectronicLevels[1/cm]      1
    0      1
  End
  Fragment      C2H5
  RRHO
  Geometry[angstrom]      7
  C      -0.777218      -0.264204      -0.000066
  C      0.709984      -0.299398      -0.000078
  H      -1.164879      0.768217      0.000064
  H      -1.196648      -0.750449      0.886051
  H      -1.196658      -0.750237      -0.886292
  H      1.268165      -0.242994      0.926229
  H      1.268156      -0.242912      -0.926385
  Core      RigidRotor
  SymmetryFactor          1
  End

```



```

Frequencies[1/cm]      15
110.6015              477.0683              812.8929
980.4733              1062.3353             1191.6355
1400.9527             1464.8461             1482.5199
1482.9204             2942.1680             3034.0564
3077.4055             3137.9085             3237.5055
ZeroEnergy[kcal/mol]      0.    #Always 0.
ElectronicLevels[1/cm]    1
  0    2
End
GroundEnergy[kcal/mol]    -62.9 # Relative energy of R1
End
Bimolecular      P9    # CH3CH2CCH + H
Fragment         CH3CH2CCH
RRHO
Geometry[angstrom]  10
C      -1.226138    -0.112945    1.340374
C      0.308830     -0.222153    1.310385
C      0.855356     -0.270633   -0.043844
C      1.285809     -0.309207   -1.165155
H      -1.560885     0.792820    0.830635
H      -1.584564     -0.080124    2.372222
H      -1.686021     -0.969476    0.843223
H      0.625965     -1.119038    1.854110
H      0.750057     0.628562    1.841626
H      1.671679     -0.343670   -2.154089
Core      RigidRotor
SymmetryFactor      1
End
Frequencies[1/cm]      24
201.3980             222.2377             359.7333
519.6919             665.1267             673.1279
790.5867             846.8289             1020.4294
1089.8753            1109.5180            1290.3431
1351.5875            1413.1341            1479.6263
1497.0522            1507.6532            2221.6353
3019.8794            3036.0759            3044.8990
3103.7623            3110.3579            3478.4275
ZeroEnergy[kcal/mol]      0.
ElectronicLevels[1/cm]    1
  0    1
End
Fragment      H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]    1
  0    2
End
GroundEnergy[kcal/mol]    -54.6
End
Bimolecular      P10    # CYCLOBUTENE + H
Fragment         CH2CH2CHCH

```

```

RRHO
Geometry[angstrom]      10
C      -0.805173    -0.613224    -0.415522
C      -0.297884     0.798424    -0.177284
C       0.687402     0.417514     0.642752
C       0.353607    -1.061214     0.548971
H      -1.814517    -0.826045    -0.050663
H      -0.718775    -0.985106    -1.440917
H      -0.628845     1.761894    -0.548316
H       1.455456     0.956114     1.186330
H       1.116651    -1.694801     0.086889
H       0.020957    -1.535562     1.477159
Core      RigidRotor
SymmetryFactor          2
End
Frequencies[1/cm]      24
323.8372      650.7409      865.6700
868.0774      886.2401      897.3758
940.6823      997.7991      1039.7296
1099.0384     1129.8877     1169.3048
1214.5744     1235.7818     1317.3938
1469.0744     1488.8901     1635.5762
3027.6032     3033.1384     3063.3419
3078.0210     3162.1413     3193.9712
ZeroEnergy[kcal/mol]      0.
ElectronicLevels[1/cm]    1
  0      1
End
Fragment      H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]    1
  0      2
End
GroundEnergy[kcal/mol]      -56.2
End
Bimolecular      P11      # 2-BUTYNE + H
Fragment      CH3CCCH3
RRHO
Geometry[angstrom]      10
C      -1.828199    -0.089051     0.769208
C      -0.370566    -0.093957     0.711646
C       0.831462    -0.097983     0.664508
C       2.289106    -0.102875     0.607180
H      -2.209015     0.890522     1.075416
H      -2.198554    -0.828791     1.486130
H      -2.263820    -0.324899    -0.206984
H       2.645023    -0.362546    -0.394937
H       2.710477    -0.830097     1.308569
H       2.698614     0.880035     0.861224
Core      RigidRotor
SymmetryFactor          2

```

```

End
Rotor      Hindered      ! rotating group comment
  Group      8 9 10      # atoms in rotating group
excluding the atom on the axis
  Axis      3 4      # rotational axis
  Symmetry      3      #360/angle of rotation to
recover the initial structure
  Potential[kcal/mol]      1      # number of equidistant
point on the potetial energy curve with respect to the rotational
angle
0.013
End
Frequencies[1/cm]      23
202.5118      202.5719
383.2549      383.2865      724.7585
1045.6719      1045.6772      1067.9943
1068.0090      1170.9262      1417.5319
1421.1159      1482.4246      1482.4328
1482.4698      1482.4766      2365.3674
3014.2948      3014.5932      3069.1918
3069.2105      3070.0744      3070.0932
ZeroEnergy[kcal/mol]      0.
ElectronicLevels[1/cm]      1
  0      1
End
Fragment      H
Atom
  Mass[amu]      1
  ElectronicLevels[1/cm]      1
    0      2
End
GroundEnergy[kcal/mol]      -59.7
End
Bimolecular      P12      # ALLENE + CH3
Fragment      CH2CCH2
RRHO
Geometry[angstrom]      7
C      1.008730      -0.438496      0.061354
C      0.999532      -0.539942      -1.237111
C      1.017827      -0.337022      1.359801
H      1.882642      -0.853265      -1.785129
H      0.108495      -0.314357      -1.814633
H      1.291459      0.591254      1.851552
H      0.752019      -1.177276      1.993612
Core      RigidRotor
  SymmetryFactor      4.0
End
Frequencies[1/cm]      15
371.7584      371.7832      866.5943
866.6493      884.9124      1016.8797
1016.8879      1109.3379      1422.4912
1479.5907      2052.4039      3116.7834

```

```

3120.8210          3191.5569          3191.6569
  ZeroEnergy[kcal/mol]          0.
  ElectronicLevels [1/cm]      1
    0    1
  End
Fragment          CH3
RRHO
  Geometry[angstrom]          4
  C          0.010526    0.085155    0.194783
  H          -0.044537    0.239428   -0.873182
  H          -0.153501    0.913041    0.869378
  H          0.229627   -0.897005    0.588148
  Core          RigidRotor
  SymmetryFactor              6
  End
  Frequencies [1/cm]          6
505.1400          1403.0741          1403.0813
3103.6554          3282.6758          3282.6811
  ZeroEnergy[kcal/mol]          0.
  ElectronicLevels [1/cm]      1
    0    2
  End
  GroundEnergy[kcal/mol]       -66.4
  End
Bimolecular      P13    # METHYLACETYLENE + CH3
Fragment          CH3CCH
RRHO
  Geometry[angstrom]          7
  C          0.875790    0.064719   -0.104678
  C          0.927574   -0.079654   -1.553810
  C          0.833114    0.183698    1.089554
  H          0.407512   -0.986092   -1.876107
  H          0.455507    0.773138   -2.049659
  H          1.961476   -0.142470   -1.904626
  H          0.795372    0.288918    2.145685
  Core          RigidRotor
  SymmetryFactor              3.0
  End
  Frequencies [1/cm]          15
339.3075          339.3317          665.9353
665.9357          943.6403          1056.5474
1056.5550         1416.6281          1479.6777
1479.7085         2230.4244          3025.9120
3084.7794         3084.8075          3479.3595
  ZeroEnergy[kcal/mol]          0.
  ElectronicLevels [1/cm]      1
    0    1
  End
Fragment          CH3
RRHO
  Geometry[angstrom]          4
  C          0.010526    0.085155    0.194783

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H          -0.044537    0.239428   -0.873182
H          -0.153501    0.913041    0.869378
H           0.229627   -0.897005    0.588148
Core      RigidRotor
SymmetryFactor      6
End
Frequencies[1/cm]      6
505.1400          1403.0741          1403.0813
3103.6554          3282.6758          3282.6811
ZeroEnergy[kcal/mol]      0.
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol]    -67.4
End
Barrier B1  W1  W2  #  TSa
RRHO
Geometry[angstrom]      11
C          -1.408722   -0.682325   -0.691040
C           0.081474   -0.379605   -0.704639
C           0.898134   -0.392766    0.605951
C           0.625101    0.838568   -0.122463
H          -1.590737   -1.760609   -0.738821
H          -1.910035   -0.217563   -1.545588
H          -1.876055   -0.297117    0.219127
H           0.600939   -0.788387   -1.574496
H           1.898413   -0.825984    0.584897
H           0.362607   -0.596585    1.534195
H           0.740395    1.906057   -0.174626
Core      RigidRotor
SymmetryFactor      0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  480.0649
WellDepth[kcal/mol]      1.6      # relative energy of B1
with respect to W1
WellDepth[kcal/mol]      1.4      # relative energy of B1
with respect to W2
End
Frequencies[1/cm]      26
216.6315
335.2771
373.0150
760.8601
843.5946
847.8470
914.2876
951.7870
1041.1822
1051.1418
1092.3506
1132.3108

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1146.8293
1252.2620
1380.9730
1406.9421
1469.7413
1490.6667
1500.3084
3016.7121
3042.4369
3044.5427
3075.3371
3090.0455
3105.2154
3276.9479
      ZeroEnergy[kcal/mol]      -81.0
      ElectronicLevels[1/cm]    1
      0      2
End
Barrier      B2      W3      W4      #      TSb
RRHO
      Geometry[angstrom]      11
      C      -1.403688      0.195090      1.309838
      C      -0.021302      0.457383      0.806624
      C      0.580544      -0.372171      -0.249896
      C      0.603864      -0.074081      -1.548280
      H      -1.457639      -0.740665      1.891007
      H      -1.755350      0.998756      1.961197
      H      -2.113521      0.081295      0.482952
      H      0.632464      1.100525      1.389838
      H      1.038063      -1.315866      0.066789
      H      1.060751      -0.739370      -2.273057
      H      0.170750      0.846240      -1.926909
      Core      RigidRotor
      SymmetryFactor      0.5
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      244.8855
      WellDepth[kcal/mol]      14.7      # relative energy of
B2 with respect to W3
      WellDepth[kcal/mol]      14.0      # relative energy of
B2 with respect to W4
      End
      Frequencies[1/cm]      26
100.0842
270.8970
307.8498
490.3698
671.1466
859.9769
953.1071
977.8129
1004.0357

```

1038.7828  
1101.1754  
1129.7781  
1313.3605  
1345.1139  
1401.6588  
1448.1417  
1472.8881  
1484.4649  
1682.5586  
2943.1027  
3029.0906  
3032.4501  
3087.9717  
3125.2330  
3137.8258  
3208.8936

ZeroEnergy[kcal/mol] -97.7  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B3 W9 W10 # TSc  
RRHO

Geometry[angstrom] 11  
C -1.834543 0.146826 -1.080711  
C -0.479090 0.155497 -0.563153  
C 0.748508 0.145087 -0.136721  
C 2.004462 0.111553 -0.993260  
H -2.566719 -0.209872 -0.339784  
H -1.938629 -0.501580 -1.962380  
H -2.144371 1.154261 -1.379229  
H 0.949479 0.165466 0.944458  
H 2.612328 -0.767286 -0.751643  
H 2.624620 0.994537 -0.803345  
H 1.761706 0.082863 -2.056746

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 268.3697

WellDepth[kcal/mol] 6.0 # relative energy of B3

with respect to W9

WellDepth[kcal/mol] 5.2 # relative energy of B3

with respect to W10

End

Frequencies[1/cm] 26

36.0  
156.1942  
306.3220  
377.1536  
710.1095  
786.6223

984.8860  
1009.4297  
1039.6817  
1048.9666  
1049.4940  
1311.9746  
1391.7858  
1408.9757  
1454.4152  
1471.6584  
1483.3305  
1489.3122  
1846.0646  
2947.4791  
2958.5738  
2982.2735  
3010.3308  
3050.0806  
3058.6865  
3105.8698

ZeroEnergy[kcal/mol] -85.8

ElectronicLevels[1/cm] 1

0 2

End

Barrier B4 W13 W14 # TSd

RRHO

Geometry[angstrom] 11

C -1.783533 -0.081742 -0.762687

C -0.263913 0.129190 -0.809322

C 0.380130 -0.009844 0.562992

C 1.044608 0.903232 1.201688

H -2.034280 -1.064033 -0.351048

H -2.217564 -0.019148 -1.764319

H -2.263362 0.674618 -0.136164

H -0.028453 1.112785 -1.222607

H 0.185218 -0.616690 -1.476915

H 0.229998 -0.996575 1.025266

H 1.592065 1.659295 1.713003

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 702.2153

WellDepth[kcal/mol] 3.6 # relative energy of B4

with respect to W13

WellDepth[kcal/mol] 4.0 # relative energy of B4

with respect to W14

End

Frequencies[1/cm] 26

100.7058

232.6412

339.3739



435.4104  
655.9458  
761.0917  
810.7379  
866.0844  
1013.3796  
1084.3328  
1092.2272  
1259.4315  
1295.6679  
1337.1130  
1409.6136  
1483.3278  
1498.1993  
1505.6975  
1668.4211  
2965.6328  
3010.1634  
3023.5215  
3067.4014  
3089.2668  
3094.8642  
3437.7169

ZeroEnergy[kcal/mol] -82.1  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B5 W1 W3 # TS1a

RRHO

Geometry[angstrom] 11  
C -1.547355 -0.549520 -0.866450  
C -0.064843 -0.322760 -0.744049  
C 1.397852 -0.846996 0.534740  
C 0.584682 0.349734 0.281894  
H -1.782461 -1.618876 -0.840726  
H -1.909668 -0.172609 -1.829861  
H -2.099516 -0.058377 -0.063115  
H 0.526123 -0.676890 -1.586102  
H 2.276695 -1.083797 -0.053992  
H 1.107831 -1.551433 1.306720  
H 0.034576 0.858073 1.067121

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 742.3274

WellDepth[kcal/mol] 20.3 # relative energy of

B5 with respect to W1

WellDepth[kcal/mol] 50.1 # relative energy of

B5 with respect to W3

End

Rotor Hindered

```

Group          5 6 7
Axis          1 2
Symmetry      3
Potential[kcal/mol] 2
  0.000
  0.550
End
Frequencies[1/cm] 25
325.7658
394.4778
591.1639
596.0531
721.3535
790.6671
911.0633
966.7902
1027.5381
1092.6419
1109.2102
1262.6618
1299.3956
1392.5492
1432.1684
1461.9209
1480.5679
1510.2066
3012.9174
3061.6814
3099.4258
3111.1593
3119.1356
3151.8375
3209.7175
ZeroEnergy[kcal/mol] -62.3
ElectronicLevels[1/cm] 1
  0 2
End
Barrier      B6   W2   W4   #   TS1b
RRHO
Geometry[angstrom] 11
C      -1.436622  -0.573798  -0.706464
C      0.030032   -0.301243  -0.815582
C      1.022827   -0.365038   0.922892
C      0.740291    0.660851    0.032948
H      -1.713707   -1.544747   -1.123895
H      -2.005436    0.200143   -1.244070
H      -1.778191   -0.533287    0.333418
H      0.587737   -0.776708   -1.616705
H      2.032165   -0.614258    1.259896
H      0.230383   -0.941159    1.389473
H      1.488110    1.358853   -0.324048
Core      RigidRotor

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SymmetryFactor      0.5
End
Tunneling           Eckart
ImaginaryFrequency[1/cm]  870.2920
WellDepth[kcal/mol]      21.4      # relative energy of
B6 with respect to W2
WellDepth[kcal/mol]      50.7      # relative energy of
B6 with respect to W4
End
Rotor              Hindered
Group              5 6 7
Axis               1 2
Symmetry           3
Potential[kcal/mol] 2
0.000
0.994
End
Frequencies[1/cm]    25
267.2404
371.8992
633.1548
667.5398
775.8650
894.8828
914.8167
969.0443
1003.5086
1090.2525
1154.1712
1247.3466
1315.4797
1372.4427
1408.2023
1479.2064
1481.9929
1514.3610
2968.9946
3036.8214
3051.8665
3088.1200
3139.4898
3155.3143
3173.2408
ZeroEnergy[kcal/mol]      -61.0
ElectronicLevels[1/cm]    1
0 2
End
Barrier             B7  W2  W8  #  TS6
RRHO
Geometry[angstrom]      11
C      -1.304804  -0.446310  -0.538483
C      0.178426   -0.262839  -0.723395

```

C	0.890382	-0.210872	0.607960	
C	0.229334	1.015810	0.073988	
H	-1.676876	-1.307848	0.017830	
H	-1.931868	-0.125227	-1.367370	
H	-1.137372	0.679456	0.259832	
H	0.714737	-0.471012	-1.640828	
H	1.975850	-0.214538	0.568920	
H	0.477730	-0.733206	1.466725	
H	0.655342	1.985108	-0.161209	
Core	RigidRotor			
	SymmetryFactor	0.5		
End				
Tunneling	Eckart			
	ImaginaryFrequency[1/cm]	2117.9341		
	WellDepth[kcal/mol]	37.1	# relative energy of	
B7 with respect to W2				
	WellDepth[kcal/mol]	47.3	# relative energy of	
B7 with respect to W8				
End				
	Frequencies[1/cm]	26		
379.3399				
507.0660				
615.5336				
780.9880				
795.3063				
819.3678				
908.8597				
924.0283				
972.5948				
1038.5328				
1063.6992				
1077.4819				
1102.9183				
1126.9538				
1201.9140				
1301.8969				
1328.2570				
1435.8290				
1484.0994				
1795.3804				
3060.4189				
3091.1598				
3152.3697				
3163.7522				
3168.0684				
3177.1842				
	ZeroEnergy[kcal/mol]	-45.3		
	ElectronicLevels[1/cm]	1		
	0	2		
End				
Barrier	B8	W1	W7	# TS2
RRHO				

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      Geometry[angstrom]      11
      C      -1.404918      -0.707188      -0.717742
      C      0.030561      -0.366840      -0.499895
      C      0.952436      -0.415692      0.675245
      C      0.724081      0.860252      -0.077562
      H      -1.545166      -1.767012      -0.946652
      H      -1.824682      -0.124266      -1.542844
      H      -1.995147      -0.474329      0.180962
      H      0.840850      0.301451      -1.246000
      H      1.906473      -0.935403      0.650550
      H      0.447449      -0.467431      1.637947
      H      0.339109      1.835153      0.197308
      Core      RigidRotor
      SymmetryFactor      0.5
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      1907.5310
      WellDepth[kcal/mol]      43.1      # relative energy of
      B8 with respect to W1
      WellDepth[kcal/mol]      45.9      # relative energy of
      B8 with respect to W7
      End
      Rotor      Hindered
      Group      5 6 7
      Axis      1 2
      Symmetry      3
      Potential[kcal/mol]      2
      0.000
      1.937
      End
      Frequencies[1/cm]      25
      286.5598
      326.2335
      677.3967
      734.0087
      852.9234
      866.9794
      962.4740
      1017.2087
      1054.0822
      1067.4625
      1092.9058
      1120.6381
      1209.3664
      1396.0476
      1431.7268
      1474.5480
      1491.4318
      1530.2166
      2271.9530
      2973.9309
      3052.4990

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3080.7919
3082.8395
3150.0085
3160.5708
      ZeroEnergy[kcal/mol]          -39.5
      ElectronicLevels[1/cm]       1
      0      2
End
Barrier      B9      W7      W8      #      TS4
RRHO
  Geometry[angstrom]              11
  C      -1.165673      -0.753356      -0.909606
  C      -0.285411      -0.038852      0.020576
  C      0.989807      -0.322237      0.700759
  C      0.774739      0.977091      -0.093779
  H      -1.258150      -1.830465      -0.837005
  H      -1.519468      -0.251677      -1.802429
  H      -1.568723      -0.148094      0.189294
  H      1.646935      -1.075313      0.269163
  H      1.055333      -0.240094      1.781277
  H      0.701013      1.900489      0.472314
  H      1.290618      1.077388      -1.047207
  Core      RigidRotor
  SymmetryFactor                  1
End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]        1993.0595
  WellDepth[kcal/mol]              41.9      # relative energy of
B9 with respect to W7
  WellDepth[kcal/mol]              49.1      # relative energy of
B9 with respect to W8
End
  Frequencies[1/cm]                26
267.2127
291.5578
364.3626
720.5004
755.7345
785.0499
855.2272
929.0706
981.9637
1027.9409
1072.6422
1107.8615
1110.2820
1157.2157
1168.4824
1401.6034
1438.1092
1460.0510
1515.3933

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2190.2620
3076.8058
3077.4426
3117.9298
3152.0759
3163.2056
3232.0823
      ZeroEnergy[kcal/mol]          -43.5
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B10      W6      W8      #      TS5
RRHO
  Geometry[angstrom]      11
  C      -1.355839      0.380099      -0.762232
  C      -0.018415      0.699062      -0.616951
  C      0.809138      0.390686      0.589373
  C      1.237044      -0.702915      -0.313536
  H      -1.896226      -0.151864      0.012955
  H      -1.884838      0.597742      -1.681124
  H      0.456965      1.310794      -1.375349
  H      0.237165      0.086712      1.464285
  H      1.564618      1.131179      0.845177
  H      2.105664      -0.594382      -0.947703
  H      0.743744      -1.662661      -0.277112
  Core      RigidRotor
  SymmetryFactor      0.5
End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]      588.9625
  WellDepth[kcal/mol]      12.3      # relative energy of
B10 with respect to W6
  WellDepth[kcal/mol]      9.0      # relative energy of
B10 with respect to W8
End
  Frequencies[1/cm]      26
282.5232
394.3737
493.4607
608.3932
696.0066
736.8709
822.6227
891.7363
912.0241
989.6459
1093.1086
1186.6707
1199.2851
1222.0534
1268.2347
1409.8736

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1455.3911
1491.8876
1512.7856
3075.3246
3134.4823
3138.0468
3157.4211
3167.4548
3228.7512
3270.2172
      ZeroEnergy[kcal/mol]          -83.6
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B11      W5      W7      #      TS3
RRHO
  Geometry[angstrom]      11
  C      -1.365022      -0.614929      -0.652331
  C      0.076131      -0.286306      -0.456568
  C      0.873281      -0.647530      0.615498
  C      0.653169      1.062620      -0.422482
  H      -1.553235      -1.678366      -0.483798
  H      -1.687716      -0.364739      -1.667459
  H      -2.012942      -0.047596      0.034727
  H      1.955065      -0.591733      0.562650
  H      0.472557      -1.054633      1.550853
  H      0.167582      1.840143      0.159713
  H      1.598134      1.306857      -0.894289
  Core      RigidRotor
  SymmetryFactor      0.5
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]      975.5912
  WellDepth[kcal/mol]      49.4      # relative energy of
B11 with respect to W5
  WellDepth[kcal/mol]      22.9      # relative energy of
B11 with respect to W7
End
Rotor      Hindered
  Group      5 6 7
  Axis      1 2
  Symmetry      3
  Potential[kcal/mol]      2
  0.000
  0.772
End
Frequencies[1/cm]      25
269.7222
355.6421
590.1017
628.7328
702.1333

```



842.1892  
906.4569  
943.4099  
965.8342  
1016.7921  
1076.6901  
1271.2256  
1392.1147  
1424.0451  
1438.4236  
1477.4279  
1484.4038  
1534.8463  
2956.3976  
3019.9958  
3046.0350  
3090.1435  
3103.3261  
3163.2646  
3202.9498

ZeroEnergy[kcal/mol] -62.5  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B12 W3 W6 # TS9a

RRHO

Geometry[angstrom] 11  
C -0.853518 -0.037454 -0.085508  
C 0.578686 -0.057095 -0.237711  
C 1.241103 -0.079613 -1.412822  
C -1.555824 0.200272 1.207621  
H -1.295285 -0.993719 0.596055  
H -1.461067 0.048227 -0.981087  
H 1.158810 -0.060220 0.684221  
H 2.322759 -0.104400 -1.447545  
H 0.716821 -0.069208 -2.362830  
H -2.615433 0.405103 1.205491  
H -0.983850 0.312905 2.117839

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1848.9299

WellDepth[kcal/mol] 48.9 # relative energy of

B12 with respect to W3

WellDepth[kcal/mol] 32.4 # relative energy of

B12 with respect to W6

End

Frequencies[1/cm] 26

165.4258  
277.2911  
382.8278

493.3906  
610.8949  
637.0372  
835.2993  
854.3655  
869.0823  
980.0098  
993.5217  
1139.4294  
1227.6380  
1236.1769  
1306.3956  
1349.2693  
1429.1129  
1474.7125  
1626.0045  
2186.2201  
3114.2320  
3133.7188  
3152.4529  
3158.5288  
3222.9456  
3279.3098

ZeroEnergy[kcal/mol] -63.5  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B13 W4 W6 # TS9b

RRHO

Geometry[angstrom] 11  
C -1.325767 0.415894 1.028936  
C 0.146841 0.274373 0.941768  
C 0.854164 -0.392331 -0.127283  
C 0.308810 -0.939291 -1.234081  
H -0.515306 -0.469287 1.699076  
H -1.751170 1.132700 1.715450  
H -1.969619 -0.118176 0.346644  
H 0.719946 0.924974 1.593651  
H 1.929950 -0.464715 0.010182  
H 0.924214 -1.449606 -1.964280  
H -0.752674 -0.882727 -1.446797

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 1827.5493  
WellDepth[kcal/mol] 47.2  
WellDepth[kcal/mol] 31.4

End

Frequencies[1/cm] 26

207.8329  
276.4788

418.6200  
560.4889  
623.8704  
633.6426  
834.4202  
849.2498  
869.8146  
980.4379  
1024.4908  
1077.7092  
1194.0859  
1244.3931  
1318.7729  
1403.4872  
1454.0499  
1460.1456  
1613.7644  
2196.0510  
3134.9662  
3141.6541  
3163.0559  
3168.8288  
3224.0165  
3283.1984

ZeroEnergy[kcal/mol] -64.5  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B14 W3 W9

Union

RRHO

Geometry[angstrom] 11  
C -1.605168 0.245487 0.914797  
C -0.258133 0.002120 0.339340  
C 0.305670 -0.359536 -0.802623  
C 1.753317 -0.326100 -0.397907  
H -1.797980 -0.417114 1.763995  
H -1.700747 1.273781 1.276501  
H -2.384829 0.073210 0.161738  
H -0.131279 -0.611689 -1.764372  
H 2.275532 -1.272689 -0.257609  
H 2.376837 0.489070 -0.765524  
H 1.087853 0.057851 0.801108

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 2185.6168

WellDepth[kcal/mol] 61.5

WellDepth[kcal/mol] 40.9

End

Frequencies[1/cm] 26

156.5684  
235.0935  
300.0669  
468.0591  
598.1379  
811.8646  
900.0914  
959.6759  
1034.4041  
1037.3578  
1050.7859  
1065.7765  
1127.6563  
1234.5816  
1391.5854  
1430.2473  
1462.3632  
1479.0055  
1729.3960  
1811.3068  
2995.5436  
3055.0035  
3062.3082  
3073.9777  
3144.6629  
3153.6971

ZeroEnergy[kcal/mol] -50.9  
ElectronicLevels[1/cm] 1  
0 2

End

RRHO

Geometry[angstrom] 11  
C -1.872959 0.085511 0.602524  
C -0.394668 -0.161176 0.705205  
C 0.418014 -0.464777 -0.301459  
C 1.780299 -0.340199 -0.705342  
H -2.438176 -0.628157 1.213654  
H -2.132670 1.086159 0.967150  
H -2.215499 -0.002122 -0.430189  
H 0.033732 -0.144893 1.713269  
H 0.742328 -0.003560 -1.473385  
H 2.232419 -1.139999 -1.282712  
H 2.445299 0.416730 -0.286417

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 1936.3637  
WellDepth[kcal/mol] 64.2  
WellDepth[kcal/mol] 43.6

End

Rotor Hindered

```

Group          5 6 7
Axis           1 2
Symmetry       3
Potential[kcal/mol] 2
0.000
1.409
End
Frequencies[1/cm] 25
234.1161
243.3596
401.8274
515.5619
788.1017
838.5336
886.9904
1009.1427
1052.4433
1099.3007
1118.7709
1138.7484
1307.6556
1406.3617
1445.6558
1481.3919
1489.0401
1700.5115
2157.6710
3004.0922
3029.9166
3044.1066
3050.8918
3101.5376
3181.1364
ZeroEnergy[kcal/mol] -48.2
ElectronicLevels[1/cm] 1
0 2
End
End
Barrier      B15   W4   W10   #   TS7b
RRHO
Geometry[angstrom] 11
C      -1.393344   0.360775   1.189262
C      -0.006880  -0.232099   1.106787
C       0.633305  -0.470971  -0.034554
C       0.381864  -0.817123  -1.397506
H      -1.396588   1.282667   1.780395
H      -1.789276   0.590629   0.197622
H      -2.087825  -0.333106   1.679461
H       0.497839  -0.420960   2.051716
H       1.269782  -1.438653  -0.623267
H       1.016942  -0.398232  -2.171122
H      -0.536869  -1.312469  -1.715926

```

```

Core      RigidRotor
  SymmetryFactor      0.5
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]      1945.0400
  WellDepth[kcal/mol]           64.0
  WellDepth[kcal/mol]           43.3
End
Rotor      Hindered
  Group                5 6 7
  Axis                 1 2
  Symmetry              3
  Potential[kcal/mol]   2
  0.000
  1.399
End
Frequencies[1/cm]      25
196.7777
338.8921
395.2230
569.5364
790.3931
831.7166
886.6092
1023.1058
1034.3343
1062.5629
1093.4261
1127.0576
1347.2041
1398.5995
1444.7844
1480.9273
1490.8682
1680.6322
2167.7390
3000.9248
3048.3299
3049.5596
3092.9281
3122.8516
3181.3272
  ZeroEnergy[kcal/mol]           -47.7
  ElectronicLevels[1/cm]        1
    0    2
End
Barrier      B16    W3    W12    #    TS10a
RRHO
  Geometry[angstrom]            11
  C          1.141315           -1.601514           -0.066941
  C          -0.919013           1.479130            0.902911
  C          -0.508278           0.269822            0.524126

```

C	0.399349	-0.331705	-0.394085
H	2.119378	-1.364438	0.369076
H	0.593529	-2.192132	0.671899
H	1.317484	-2.213625	-0.955624
H	-0.233023	2.328090	0.890601
H	-1.911938	1.658465	1.298915
H	-0.910117	-0.619372	-0.329735
H	0.750332	0.249174	-1.252475
Core	RigidRotor		
	SymmetryFactor	0.5	
End			
Tunneling	Eckart		
	ImaginaryFrequency[1/cm]	1875.0570	
	WellDepth[kcal/mol]	64.8	
	WellDepth[kcal/mol]	41.9	
End			
Rotor	Hindered		
	Group	5 6 7	
	Axis	1 4	
	Symmetry	3	
	Potential[kcal/mol]	2	
	0.000		
	2.067		
End			
	Frequencies[1/cm]	25	
186.4561			
281.4754			
454.2411			
630.2033			
782.5756			
820.5085			
882.2351			
999.0995			
1025.9217			
1096.2759			
1125.8288			
1146.3834			
1317.3952			
1410.1846			
1439.6041			
1479.7459			
1497.7327			
1638.8130			
2150.6585			
3006.9762			
3036.4489			
3060.2949			
3063.0516			
3096.6883			
3181.5440			
	ZeroEnergy[kcal/mol]	-47.6	
	ElectronicLevels[1/cm]	1	

0 2

```
End
Barrier      B17   W4   W12   #   TS10b
RRHO
  Geometry[angstrom]      11
  C      -1.386286      0.444867      1.156576
  C       0.100139      0.289601      0.937758
  C       0.685896     -0.334037     -0.197758
  C       0.332601     -1.103530     -1.228610
  H      -1.789302     -0.450729      1.646715
  H      -1.614479      1.302718      1.793303
  H      -1.907491      0.557035      0.202976
  H       0.753573      0.450456      1.792616
  H       0.811206      0.948258      0.014414
  H       0.852218     -1.073049     -2.179539
  H      -0.445678     -1.860712     -1.121041
  Core      RigidRotor
  SymmetryFactor      0.5
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]      1871.0311
  WellDepth[kcal/mol]           63.1
  WellDepth[kcal/mol]           40.9
End
Rotor      Hindered
  Group                        5 6 7
  Axis                          1 2
  Symmetry                       3
  Potential[kcal/mol]            2
  0.000
  1.448
End
Frequencies[1/cm]      25
189.8608
385.9732
498.8431
514.0339
764.4177
807.8896
865.9081
1011.4240
1029.7103
1075.1146
1127.4428
1175.3527
1371.0173
1398.3079
1441.9101
1481.2329
1489.4833
1634.4482
2129.2323
```



```

3001.6514
3066.1835
3067.5242
3102.6435
3127.9301
3178.8840
      ZeroEnergy[kcal/mol]      -48.6
      ElectronicLevels[1/cm]    1
        0  2
End
Barrier      B18   W3   W14   #   TS11
RRHO
  Geometry[angstrom]      11
  C      -1.908576      0.006376      0.643679
  C      -0.403169      -0.027841      0.543981
  C       0.257529      -0.608452      -0.679307
  C       0.763557      0.498031      -1.197087
  H      -2.312139      -1.000872      0.817618
  H      -2.240853      0.641202      1.468828
  H      -2.354468      0.379384      -0.282602
  H       0.130365      -0.186902      1.483596
  H       0.285728      -1.640656      -1.015330
  H       1.351225      0.777281      -2.068764
  H       0.173325      1.113228      -0.045086
  Core      RigidRotor
    SymmetryFactor      0.5
  End
  Tunneling      Eckart
    ImaginaryFrequency[1/cm]  2150.7966
    WellDepth[kcal/mol]      64.0
    WellDepth[kcal/mol]      37.7
  End
  Rotor      Hindered
    Group              5 6 7
    Axis               1 2
    Symmetry           3
    Potential[kcal/mol] 2
    0.000
    2.052
  End
  Frequencies[1/cm]    25
221.2289
367.0563
634.3493
670.9189
818.3027
855.0214
903.3399
944.2637
1042.9594
1085.7024
1107.3008

```

1160.4294  
1221.4552  
1333.4892  
1401.8065  
1485.0715  
1488.4846  
1628.7773  
1818.1076  
2989.6395  
3057.5812  
3071.1666  
3097.2233  
3122.3779  
3167.5797

ZeroEnergy[kcal/mol] -48.4  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B19 W6 W12 # TS13

RRHO

Geometry[angstrom] 11  
C 0.884974 -1.509727 -0.106824  
C -1.071654 1.115165 0.894551  
C -0.085470 0.323307 0.516418  
C 0.582950 -0.140816 -0.739782  
H 1.923505 -1.792787 0.044184  
H 0.408207 -0.876773 1.051344  
H 0.206265 -2.325103 -0.339793  
H -1.539328 1.808746 0.194288  
H -1.442570 1.125893 1.913421  
H -0.046306 -0.159641 -1.633510  
H 1.492078 0.422163 -0.968966

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 2115.0491

WellDepth[kcal/mol] 46.0

WellDepth[kcal/mol] 39.6

End

Frequencies[1/cm] 26

96.4930  
338.0929  
362.2057  
597.7159  
627.0002  
788.0135  
876.2714  
895.8924  
944.8162  
992.8272  
1048.9675

1109.2845  
1197.7362  
1224.1422  
1245.6691  
1414.0211  
1431.3746  
1474.5784  
1711.0677  
1815.8106  
3036.9931  
3073.9557  
3076.8306  
3096.2793  
3182.8903  
3200.3243

ZeroEnergy[kcal/mol] -49.9  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B20 W6 W14 # TS14

RRHO

Geometry[angstrom] 11  
C -0.559576 0.366624 -0.621417  
C 0.924449 0.427656 -0.932138  
C 1.630880 -0.535437 -0.363545  
C -0.717928 -0.855722 0.289774  
H -1.149313 0.273008 -1.540424  
H -0.896631 1.288606 -0.134106  
H 1.341340 1.205320 -1.568652  
H 2.682493 -0.791392 -0.367649  
H -1.250477 -1.708702 -0.125959  
H -0.989758 -0.660720 1.325198  
H 0.576390 -1.174967 0.287782

Core RigidRotor  
SymmetryFactor 1

End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 1804.9642  
WellDepth[kcal/mol] 28.0  
WellDepth[kcal/mol] 18.2

End

Frequencies[1/cm] 26

172.2652  
463.1852  
609.1283  
653.4764  
728.5135  
840.0633  
880.8656  
918.2002  
944.7176  
1015.4036

1066.2033  
1084.0011  
1225.8531  
1247.6784  
1255.2213  
1302.2546  
1453.3241  
1489.1165  
1637.8381  
1690.3320  
3016.6327  
3039.8996  
3090.9215  
3128.6845  
3168.2773  
3206.5685

ZeroEnergy[kcal/mol] -67.9  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B21 W6 W15 # TS15

RRHO

Geometry[angstrom] 11  
C -1.035995 -0.189216 -0.929678  
C -0.503463 0.877972 -0.205910  
C 0.793769 0.349888 0.350831  
C 0.279723 -1.089389 0.473349  
H -2.107754 -0.296192 -1.095227  
H -0.431830 -0.694904 -1.677771  
H -1.110100 1.623501 0.293732  
H 1.117116 0.821768 1.285000  
H 1.634621 0.410799 -0.351350  
H 0.878322 -1.920264 0.102423  
H -0.320720 -1.306927 1.350603

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 836.0458  
WellDepth[kcal/mol] 33.8  
WellDepth[kcal/mol] 29.2

End

Frequencies[1/cm] 26

253.2215  
515.4139  
565.0405  
658.3553  
781.9534  
817.9309  
896.4247  
939.8865  
950.5058

```

973.6141
1007.4523
1104.0827
1191.4937
1235.2250
1272.5593
1369.8378
1446.9681
1483.2367
1531.2793
3000.9417
3033.7930
3080.3077
3087.2825
3150.7936
3184.6153
3195.4415
      ZeroEnergy[kcal/mol]          -62.1
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B22      W12      W13      #      TS12
RRHO
      Geometry[angstrom]           11
      C      1.009474      -1.619353      -0.141312
      C      -0.762542      1.502582      0.829284
      C      -0.510240      0.359642      0.280281
      C      0.265303      -0.414161      -0.732844
      H      1.726289      -1.300666      0.619081
      H      0.309702      -2.315536      0.327299
      H      1.555117      -2.155435      -0.921829
      H      -0.529738      2.569815      0.818468
      H      -1.445090      0.463932      1.164940
      H      -0.423135      -0.753509      -1.514160
      H      0.976097      0.273974      -1.213911
      Core      RigidRotor
      SymmetryFactor      0.5
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      2106.5150
      WellDepth[kcal/mol]           47.5
      WellDepth[kcal/mol]           43.7
      End
      Rotor      Hindered
      Group                        5 6 7
      Axis                        1 4
      Symmetry                      3
      Potential[kcal/mol]           2
      0.000
      2.900
      End
      Frequencies[1/cm]            25

```

89.1047  
211.7282  
330.6430  
424.1091  
626.8350  
789.0015  
800.8445  
851.1056  
1010.6462  
1081.4292  
1088.2414  
1275.2354  
1326.8380  
1411.2029  
1465.8063  
1496.7678  
1505.6432  
1847.9939  
2347.3872  
2973.7746  
3031.9084  
3036.5491  
3042.1784  
3098.8452  
3101.7881

ZeroEnergy[kcal/mol] -42.0

ElectronicLevels[1/cm] 1

0 2

End

Barrier B23 W5 W11 # TS16

RRHO

Geometry[angstrom] 11

C	-1.499350	-0.322680	0.044870
C	-0.007092	-0.367612	0.069136
C	0.939895	-0.509561	-1.097013
C	0.895291	-0.303192	1.037808
H	-1.852622	0.513469	-0.568716
H	-1.915709	-0.213146	1.048425
H	-1.908041	-1.236385	-0.400719
H	1.012764	-1.482366	-1.584613
H	1.070680	0.346313	-1.760178
H	1.830168	-0.433824	-0.014452
H	0.904665	-0.199498	2.120976

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 2169.3076

WellDepth[kcal/mol] 61.2

WellDepth[kcal/mol] 38.4

End

Rotor Hindered

```

Group          5 6 7
Axis           1 2
Symmetry       3
Potential[kcal/mol] 2

0.000
1.693
End
Frequencies[1/cm] 25
340.8762
370.8366
462.1443
598.9028
683.5186
860.7180
932.2439
975.9095
982.2690
1013.1448
1082.5974
1109.9841
1254.7713
1406.7713
1423.7473
1478.8864
1482.6307
1687.7145
1852.5845
3013.6354
3051.1127
3059.2143
3099.2245
3127.5482
3142.9512
ZeroEnergy[kcal/mol] -50.7
ElectronicLevels[1/cm] 1
0 2
End
Barrier      B24   W5   W12   #   TS18
RRHO
Geometry[angstrom] 11
C      -0.002354  -2.221955   0.914984
C       0.381319  -0.740326  -0.073647
C       0.865784  -0.659783  -1.324773
C       0.889125  -0.597163   1.223189
H      -0.975193  -2.101550   1.379599
H       0.677877  -2.783560   1.574009
H      -0.078510  -2.815133   0.001439
H       1.685477   0.019541  -1.558428
H       0.413712  -1.188012  -2.157414
H       1.963712  -0.595436   1.440196
H       0.251426  -0.238261   2.024065
Core      RigidRotor

```

```

SymmetryFactor      0.5
End
Tunneling           Eckart
ImaginaryFrequency[1/cm]  1034.4633
WellDepth[kcal/mol]      79.3
WellDepth[kcal/mol]      56.9
End
Frequencies[1/cm]      26
194.2267
316.5572
329.1120
488.2273
623.0496
730.2596
773.4616
818.6293
948.4609
979.5285
1002.2736
1060.4038
1126.1845
1298.0456
1424.4023
1432.1905
1476.1053
1487.4548
1595.1706
2930.8259
2999.5708
3049.6440
3075.7720
3162.6080
3173.7799
3178.6626
ZeroEnergy[kcal/mol]    -32.6
ElectronicLevels[1/cm]  1
0 2
End
Barrier              B25   W10   W11   #   TS17
RRHO
Geometry[angstrom]    11
C                   -1.346791   0.227144   -0.116588
C                    0.009466   -0.403378   -0.031213
C                    1.239844   -0.231275   -1.253819
C                    1.170108   -0.154083    0.529576
H                   -1.306968   1.323791   -0.187690
H                   -1.885600   -0.025739    0.800952
H                   -1.934295   -0.159733   -0.952674
H                    1.610111   -1.197962   -1.572463
H                    0.520515    0.175125   -1.980112
H                    1.531425    0.754438    1.035637
H                    2.049658    0.515611   -1.248706

```



```

Core      RigidRotor
  SymmetryFactor    0.5
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]    520.1272
  WellDepth[kcal/mol]        61.8
  WellDepth[kcal/mol]        59.9
End
Rotor      Hindered
  Group                5 6 7
  Axis                 1 2
  Symmetry              3
  Potential[kcal/mol]   2
0.000
0.764
End
  Frequencies[1/cm]      25
279.2827
303.2839
367.8621
594.8060
718.6412
815.5055
897.5214
915.8393
995.7023
1024.8119
1072.7143
1324.1654
1388.5651
1448.6176
1460.4762
1469.5088
1486.4018
1731.9871
2937.5200
2948.2834
2964.3881
2973.7052
3063.8848
3093.5034
3180.8720
  ZeroEnergy[kcal/mol]      -29.2
  ElectronicLevels[1/cm]    1
    0    2
End
Barrier      B26    W2    P1    #    TS22
RRHO
  Geometry[angstrom]      11
  C      -1.530002    -0.846357    -0.649909
  C      0.843916    -0.395342    -0.639687
  C      1.157377    -0.044950    0.798973

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C          1.102609    0.865436   -0.388920
H          -1.736757   -0.723326   -1.704817
H          -1.844196   -0.058366    0.020867
H          -1.464679   -1.851936   -0.254914
H           0.914369   -1.188979   -1.361925
H           2.128748   -0.297009    1.228854
H           0.344485   -0.057135    1.526316
H           1.262015    1.866599   -0.749171
Core      RigidRotor
SymmetryFactor    0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]    387.5568
WellDepth[kcal/mol]        44.7
WellDepth[kcal/mol]        6.4
End
Rotor      Hindered      ! rotating group comment
Group                        5 6 7      # atoms in rotating group
excluding the atom on the axis
Axis                        1 2      # rotational axis
Symmetry                      3      #360/angle of rotation to
recover the initial structure
Potential[kcal/mol]          2      # number of
0.00
0.36
End
Frequencies[1/cm]          25
158.7822
197.9484
424.8199
437.1403
590.4809
703.1874
790.4803
824.5894
916.4159
1005.1865
1035.5469
1066.5871
1088.0729
1152.6421
1411.4057
1415.2412
1496.2611
1602.7502
3027.9071
3087.9852
3092.3366
3249.2902
3257.9058
3261.9247
3284.8569

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ZeroEnergy[kcal/mol]          -37.7
ElectronicLevels[1/cm]       1
    0    2
End
Barrier      B27    W2    P2    #    TS21
RRHO
  Geometry[angstrom]         11
  C      -1.499822   -0.760968   -0.746572
  C      -0.207921   -0.204044   -0.281003
  C       0.894067   -0.407444    0.738264
  C       0.556443    0.827237   -0.049077
  H      -1.383773   -1.779860   -1.121267
  H      -1.939672   -0.142990   -1.532388
  H      -2.199013   -0.799420    0.096744
  H       0.829127   -0.818802   -1.981099
  H       1.760731   -1.012611    0.472765
  H       0.646608   -0.437413    1.802077
  H       0.796624    1.861999   -0.224406
  Core      RigidRotor
  SymmetryFactor             0.5
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]   517.5842
  WellDepth[kcal/mol]        48.4
  WellDepth[kcal/mol]        3.4
End
Rotor      Hindered
  Group                               5 6 7
  Axis                               1 2
  Symmetry                             3
  Potential[kcal/mol]                2
0.000
1.630
End
  Frequencies[1/cm]           25
253.3991
342.0295
362.4703
410.0496
677.1463
716.7325
939.3588
958.7990
1001.4077
1040.6909
1068.9077
1086.4137
1105.3847
1183.2256
1405.3583
1475.5550
1487.3768

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1511.8817
1787.5092
3019.4717
3026.0341
3079.9408
3094.2766
3108.1366
3262.6134
      ZeroEnergy[kcal/mol]          -34.0
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B28      W2      P3      #      TS20a
RRHO
      Geometry[angstrom]           11
      C      -1.509472      -0.710591      -0.780224
      C      -0.027207      -0.431846      -0.592020
      C      0.599136      -0.303936      0.777427
      C      0.462741      0.804186      0.113650
      H      -1.705934      -1.787476      -0.817471
      H      -1.876045      -0.277712      -1.717265
      H      -2.096871      -0.288104      0.039748
      H      0.595312      -0.842791      -1.389937
      H      2.769638      -0.937589      0.357979
      H      0.820995      -0.799136      1.707313
      H      0.567205      1.875593      0.072463
      Core      RigidRotor
      SymmetryFactor      0.5
End
Tunneling      Eckart
      ImaginaryFrequency[1/cm]      288.3258
      WellDepth[kcal/mol]           49.6
      WellDepth[kcal/mol]           1.4
End
Rotor      Hindered
      Group                        5 6 7
      Axis                          1 2
      Symmetry                       3
      Potential[kcal/mol]            2
0.000
1.723
      End
      Frequencies[1/cm]            25
145.2543
222.5021
368.7475
421.6912
631.7412
779.1287
834.5512
863.9886
951.0462

```

1012.1674  
1036.2838  
1093.7782  
1118.6753  
1220.2286  
1393.7548  
1407.3388  
1491.0016  
1496.7026  
1677.7751  
3010.6957  
3042.4555  
3064.9699  
3087.0102  
3237.6953  
3281.0837

ZeroEnergy[kcal/mol] -32.8  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B29 W1 P3 # TS20b

RRHO

Geometry[angstrom] 11  
C -1.407969 -0.781081 -0.647735  
C 0.038306 -0.330790 -0.770950  
C 0.992361 -0.327945 0.400017  
C 0.592407 0.840716 -0.007082  
H -1.501214 -1.858992 -0.817485  
H -2.040128 -0.275480 -1.385504  
H -1.800834 -0.560341 0.348136  
H 0.461777 -0.522989 -1.761439  
H 1.667960 -0.912571 1.000172  
H -0.243902 -0.735790 2.240222  
H 0.624283 1.913049 0.090285

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 354.6104  
WellDepth[kcal/mol] 50.3  
WellDepth[kcal/mol] 2.1

End

Frequencies[1/cm] 26

172.4410  
199.9827  
267.0659  
377.0881  
435.9504  
636.7656  
774.9604  
828.5399  
861.5155

```

950.4314
1001.6887
1039.1069
1092.2606
1120.3743
1222.0814
1390.5915
1404.7925
1487.5712
1496.2246
1668.8302
3011.3531
3022.3676
3066.2615
3090.3591
3239.6659
3282.3380
      ZeroEnergy[kcal/mol]      -32.1
      ElectronicLevels[1/cm]    1
      0      2
End
Barrier      B30      W7      P2      #      TS23a
RRHO
      Geometry[angstrom]      11
      C      -1.421005      -0.695951      -0.746267
      C      -0.115580      -0.214974      -0.228529
      C      1.039644      -0.430500      0.360432
      C      0.761988      1.000809      -0.072737
      H      -1.513034      -1.781148      -0.636005
      H      -1.524998      -0.434344      -1.806316
      H      -2.243533      -0.212316      -0.204722
      H      1.814353      -1.130566      0.630460
      H      0.704491      -0.246008      2.346320
      H      0.537052      1.745131      0.694800
      H      1.256500      1.409133      -0.958265
      Core      RigidRotor
      SymmetryFactor      0.5
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      724.7959
      WellDepth[kcal/mol]      51.1
      WellDepth[kcal/mol]      3.1
      End
      Frequencies[1/cm]      26
137.1268
204.2352
302.7424
334.9441
404.3180
685.2052
795.9387
945.2808

```

```

984.0766
1010.1758
1061.9791
1092.6568
1098.1845
1127.7627
1223.1689
1428.3492
1500.7055
1508.6759
1542.9007
1795.9063
3049.7155
3074.9509
3114.2857
3139.8995
3144.2945
3301.2491
      ZeroEnergy[kcal/mol]          -34.3
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B31      W7      P4      #      TS24a
RRHO
      Geometry[angstrom]      11
      C      -1.222195      -0.705557      -0.819219
      C      -0.085574      -0.208262      -0.312351
      C      1.015493      -0.351095      0.653936
      C      0.799380      0.955709      -0.143568
      H      -1.512299      -1.734772      -0.623996
      H      -1.772305      -0.162556      -1.583473
      H      -2.635100      -0.139949      0.490477
      H      1.872642      -0.964354      0.384229
      H      0.775434      -0.339414      1.715268
      H      0.418418      1.819408      0.397803
      H      1.517021      1.186035      -0.928090
      Core      RigidRotor
      SymmetryFactor      1
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      744.2981
      WellDepth[kcal/mol]      40.5
      WellDepth[kcal/mol]      3.4
      End
      Frequencies[1/cm]      26
203.1952
243.7320
356.7761
384.6024
705.3229
746.8091
768.4905

```

```

923.4412
942.7986
971.7838
1062.8805
1074.4571
1096.5440
1113.1578
1167.6514
1186.1908
1462.3581
1474.9498
1509.1630
1789.5741
3134.9286
3138.4432
3158.5853
3215.4421
3227.7315
3250.1807
      ZeroEnergy[kcal/mol]          -44.9
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B32      W8      P4      #      TS25a
RRHO
      Geometry[angstrom]      11
      C      -1.437070      0.437911      -0.835106
      C      -0.163234      0.384418      -0.410000
      C      0.716102      0.490383      0.775848
      C      1.074210      -0.427629      -0.412742
      H      -2.170365      1.056713      -0.323808
      H      -1.738187      -0.051179      -1.758244
      H      0.541085      1.925953      -1.388408
      H      0.375813      0.022758      1.696551
      H      1.323847      1.380855      0.907636
      H      1.909243      -0.119813      -1.035343
      H      0.970355      -1.501359      -0.276789
      Core      RigidRotor
      SymmetryFactor      1
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      857.3789
      WellDepth[kcal/mol]      49.8
      WellDepth[kcal/mol]      5.5
      End
      Frequencies[1/cm]      26
313.3264
368.3534
391.0822
489.8974
605.1783
753.7886

```



782.6001  
883.5366  
916.7906  
962.6312  
1060.9119  
1081.8884  
1101.8179  
1112.3180  
1156.6244  
1190.3963  
1462.8987  
1478.8690  
1511.8545  
1767.1621  
3148.8206  
3152.6499  
3154.9696  
3233.2705  
3243.9328  
3247.7037

ZeroEnergy[kcal/mol] -42.8  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B33 W3 P5 # TS29a

RRHO

Geometry[angstrom] 11  
C -1.691799 0.134637 0.315498  
C -0.343717 0.112705 0.224656  
C 0.387023 -0.597780 -0.831314  
C 1.724934 -0.640995 -0.909152  
H -2.196900 0.718175 1.079129  
H -2.313072 -0.316718 -0.454808  
H 0.255879 0.617498 0.982035  
H -0.216039 -1.110076 -1.581402  
H 2.231257 -1.175788 -1.707397  
H 2.349954 -0.139692 -0.172858  
H -2.223321 -1.535512 1.499147

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 642.4140

WellDepth[kcal/mol] 47.0

WellDepth[kcal/mol] 2.4

End

Frequencies[1/cm] 26

134.8406  
228.2256  
297.8737  
314.4373  
513.9888

573.9995  
777.9365  
902.1370  
929.2833  
935.3106  
986.9054  
1009.0860  
1046.3338  
1231.1738  
1310.0509  
1324.8631  
1420.9688  
1486.7106  
1630.2949  
1692.1505  
3158.5351  
3163.8195  
3171.6995  
3176.5233  
3253.9804  
3259.7840

ZeroEnergy[kcal/mol] -65.4  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B34 W4 P5 # TS29b

RRHO

Geometry[angstrom] 11  
C -1.189801 0.616125 1.052154  
C 0.135181 0.361370 0.978754  
C 0.803736 -0.227485 -0.201532  
C 0.258407 -1.166603 -0.985690  
H -2.052482 -1.169386 1.706616  
H -1.623169 1.074291 1.936326  
H -1.830667 0.511580 0.180487  
H 0.765403 0.580142 1.840343  
H 1.814437 0.122444 -0.411786  
H 0.789420 -1.557787 -1.848942  
H -0.726558 -1.577565 -0.777076

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 668.1996

WellDepth[kcal/mol] 49.1

WellDepth[kcal/mol] 5.2

End

Frequencies[1/cm] 26

156.8972  
217.2533  
302.9991  
331.4568

490.3564  
642.7066  
764.1628  
892.3195  
945.6361  
947.1402  
1002.2129  
1030.5963  
1072.1772  
1107.2499  
1306.3709  
1340.3742  
1446.2478  
1479.4333  
1643.5026  
1706.7373  
3160.4526  
3165.7336  
3170.5896  
3181.4945  
3255.2382  
3261.5458

ZeroEnergy[kcal/mol] -62.6  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B35 W3 P6 # TS28

RRHO

Geometry[angstrom] 11  
C -1.724093 0.249019 0.431316  
C -0.361577 -0.242657 0.836130  
C 0.657756 -0.398430 0.012215  
C 1.742527 -0.286707 -0.708199  
H -2.469673 -0.547782 0.531665  
H -2.042065 1.071146 1.080665  
H -1.731253 0.597580 -0.601850  
H -0.240662 -0.580744 1.864154  
H 0.050594 -2.204631 -0.636444  
H 2.091388 -1.077947 -1.360361  
H 2.330936 0.625870 -0.666497

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 607.1341  
WellDepth[kcal/mol] 60.5  
WellDepth[kcal/mol] 3.9

End

Rotor Hindered  
Group 5 6 7  
Axis 1 2  
Symmetry 3

```

        Potential[kcal/mol]      2
0.000
1.274
      End
        Frequencies[1/cm]      25
105.8741
226.3176          411.6365          466.5763
565.7345          591.4517          867.0534
876.5128          891.2563          1018.7148
1050.0145         1094.3855          1143.3218
1360.0496         1405.4683          1463.8063
1482.7075         1499.7733          1988.4020
3015.4718         3062.5040          3108.8873
3119.4053         3124.2473          3203.6476
      ZeroEnergy[kcal/mol]      -51.9
      ElectronicLevels[1/cm]    1
        0      2
      End
      Barrier      B36      W6      P5      #      TS31
      RRHO
      Geometry[angstrom]      11
      C      -0.869601      -0.106698      -0.046825
      C      0.564179      0.109235      -0.256562
      C      1.226508      -0.253015      -1.356985
      C      -1.474497      0.034892      1.156744
      H      -1.404567      -0.606471      -0.850261
      H      -1.506181      1.505021      -0.932319
      H      1.101143      0.582534      0.562446
      H      2.292881      -0.090764      -1.456687
      H      0.721012      -0.721867      -2.195385
      H      -2.518218      -0.216075      1.298223
      H      -0.945624      0.452031      2.006968
      Core      RigidRotor
      SymmetryFactor      0.5
      End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      728.8444
      WellDepth[kcal/mol]      33.2
      WellDepth[kcal/mol]      5.1
      End
      Frequencies[1/cm]      26
156.4966
295.4757
352.0251
423.1600
514.0187
550.1653
753.0365
890.2337
900.8089
941.1794
999.2985

```

1007.7799  
1055.8888  
1217.8567  
1294.6729  
1318.8939  
1404.2937  
1469.8586  
1594.8956  
1692.6553  
3128.4830  
3135.2218  
3138.7525  
3142.8310  
3220.2478  
3229.2984

ZeroEnergy[kcal/mol] -62.7  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B37 W6 P7 # TS30

RRHO

Geometry[angstrom] 11  
C -1.107458 -0.212636 -0.128693  
C 1.225130 0.264866 -0.296264  
C 1.793294 0.025037 -1.451729  
C -1.562108 0.078878 1.107535  
H -0.835868 -1.226124 -0.398147  
H -1.226196 0.488391 -0.945999  
H 1.585750 0.648723 0.648260  
H 2.856054 0.212202 -1.623120  
H 1.240925 -0.372086 -2.301154  
H -1.927136 1.068323 1.359794  
H -1.535733 -0.650909 1.909156

Core RigidRotor  
SymmetryFactor 0.5

End

Tunneling Eckart  
ImaginaryFrequency[1/cm] 284.8426  
WellDepth[kcal/mol] 38.1  
WellDepth[kcal/mol] 4.9

End

Rotor Hindered ! rotating group comment  
Group 3 7 8 9 # atoms in rotating group  
excluding the atom on the axis  
Axis 1 2 # rotational axis  
Symmetry 1 #360/angle of rotation to  
recover the initial structure  
Potential[kcal/mol] 4 # number of

0.00  
0.15  
-0.28  
0.15

```

End
Frequencies[1/cm]      25
142.6146
231.5678
237.0144
343.6564
779.7323
828.8617
875.8227
887.9570
920.8363
932.7553
1023.7339
1080.8413
1237.8956
1320.6461
1395.7783
1468.4715
1594.5500
1643.5234
3049.1610
3129.2066
3132.7880
3141.1598
3204.3360
3214.8285
3232.9000
ZeroEnergy[kcal/mol]  -57.8
ElectronicLevels[1/cm]  1
0 2
End
Barrier      B38    W13    P8    #    TS39
RRHO
Geometry[angstrom]  11
C      -1.481410  -0.028726  1.138158
C      0.013344   0.013004  1.169912
C      0.657577  -0.161016 -1.017472
C      1.551563   0.582779 -1.388862
H      -1.897449   0.820207  0.588198
H      -1.907833   0.006353  2.152200
H      -1.856198  -0.948690  0.676878
H      0.546537  -0.867742  1.513640
H      0.494232   0.955793  1.402672
H      -0.070483  -0.927470 -1.171453
H      2.325153   1.307041 -1.483310
Core      RigidRotor
SymmetryFactor      0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  476.8094
WellDepth[kcal/mol]      32.5
WellDepth[kcal/mol]      9.7

```

```

End
Rotor      Hindered      ! rotating group comment
  Group          4 10 11
  Axis           2 3
  Symmetry       2
  Potential[kcal/mol] 5
0.04
0.00
0.13
-0.05
-0.37
End
Rotor      Hindered      ! rotating group comment
  Group          5 6 7
  Axis           1 2
  Symmetry       3
  Potential[kcal/mol] 2
0.000
1.279
End
Frequencies[1/cm] 24
172.1180
255.0741
519.9094
526.0344
649.4712
755.8335
765.0756
814.1248
824.1123
1012.9043
1062.6810
1212.0633
1402.9966
1469.7658
1485.5977
1487.4740
1898.4355
2968.8449
3034.9067
3077.6663
3120.6199
3213.4944
3357.6014
3462.4793
ZeroEnergy[kcal/mol]      -53.2
ElectronicLevels[1/cm]    1
  0 2
End
Barrier      B39  W14  P9  #  TS38
RRHO
Geometry[angstrom] 11

```

C	-1.410073	0.020157	1.027460
C	0.120774	-0.113386	1.063253
C	0.757507	0.107036	-0.243226
C	1.368232	0.559752	-1.187963
H	-1.706442	1.014661	0.687391
H	-1.825615	-0.141218	2.024977
H	-1.845994	-0.715453	0.348490
H	0.398028	-1.104439	1.434492
H	0.542384	0.615070	1.764291
H	0.109719	-1.547248	-1.054234
H	1.865493	0.833445	-2.086634
Core	RigidRotor		
	SymmetryFactor	0.5	
End			
Tunneling	Eckart		
	ImaginaryFrequency[1/cm]	632.3309	
	WellDepth[kcal/mol]	36.3	
	WellDepth[kcal/mol]	4.8	
End			
Rotor	Hindered		
	Group	5 6 7	
	Axis	1 2	
	Symmetry	3	
	Potential[kcal/mol]	2	
0.000			
3.064			
End			
	Frequencies[1/cm]	25	
128.5827			
248.2341			
429.2120			
476.4983			
525.8070			
652.5472			
674.8386			
792.4619			
842.2198			
1019.8652			
1088.2170			
1108.6251			
1289.1542			
1349.5397			
1411.4395			
1477.6327			
1496.1156			
1507.7276			
2132.9171			
3029.2113			
3036.5005			
3061.0356			
3105.4175			
3110.7212			



```

3466.0950
      ZeroEnergy[kcal/mol]          -49.8
      ElectronicLevels[1/cm]       1
      0      2
End
Barrier      B40      W15      P10      #      TS40
RRHO
      Geometry[angstrom]          11
      C      -0.901683      -0.516973      -0.293468
      C      -0.422204      0.740442      -0.234518
      C      0.847437      0.347020      0.493455
      C      0.268980      -1.114505      0.473399
      H      -1.838649      -0.939061      -0.635732
      H      -0.302668      -1.015804      -2.326443
      H      -0.794607      1.695217      -0.587308
      H      0.979910      0.779578      1.489875
      H      1.775809      0.479981      -0.070684
      H      0.872918      -1.850543      -0.062172
      H      0.018919      -1.512422      1.460871
      Core      RigidRotor
      SymmetryFactor      0.5
End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]    339.0266
      WellDepth[kcal/mol]        37.3
      WellDepth[kcal/mol]        2.2
End
      Frequencies[1/cm]          26
213.4612
264.5969
358.4035
669.4227
862.2378
865.0457
888.3836
896.5338
935.2291
995.3122
1033.2845
1097.3949
1127.8995
1170.9367
1215.0910
1236.7850
1316.1673
1465.3259
1484.9558
1583.8257
3028.6981
3041.9288
3066.6450
3088.7646

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3170.7671
3199.4393
      ZeroEnergy[kcal/mol]          -54.0
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B41      W9      P11      #      TS33
RRHO
      Geometry[angstrom]           11
      C      -1.988869      0.166476      0.744462
      C      -0.582901      0.092588      0.339823
      C      0.470906      -0.030341      -0.247975
      C      1.818481      -0.136893      -0.786321
      H      -2.209575      -0.556121      1.534108
      H      -2.236653      1.159913      1.126671
      H      -2.640311      -0.046147      -0.107765
      H      0.192790      0.525664      2.112310
      H      2.010257      -1.137609      -1.184122
      H      2.559830      0.060515      -0.004123
      H      1.983099      0.583537      -1.592756
      Core      RigidRotor
      SymmetryFactor      1.0
End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      532.5075
      WellDepth[kcal/mol]           35.9
      WellDepth[kcal/mol]           3.8
End
      Frequencies[1/cm]      26
68.6896
142.5016
190.6235
210.2150
405.4394
412.0792
509.7491
729.4207
1038.3021
1054.9376
1055.5039
1064.6021
1164.5215
1413.3003
1416.0225
1474.7420
1478.4097
1479.0033
1484.2117
2286.2954
3014.6539
3028.5589
3068.8347

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3080.1256
3090.1644
3090.4439
      ZeroEnergy[kcal/mol]          -55.9
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B42      W9      P6      #      TS32a
RRHO
  Geometry[angstrom]      11
  C      -1.917081      0.149578      0.644896
  C      -0.427873      0.223203      0.878158
  C      0.487218      0.021062      -0.025964
  C      1.442930      -0.174284      -0.903494
  H      -2.371834      -0.609207      1.289854
  H      -2.393178      1.105764      0.884827
  H      -2.145041      -0.098245      -0.392429
  H      -0.098485      0.465938      1.888590
  H      1.825466      -1.169190      -1.109025
  H      3.277713      0.119572      0.243994
  H      1.803042      0.632310      -1.534477
  Core      RigidRotor
  SymmetryFactor      1.0
End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]      308.8564
  WellDepth[kcal/mol]      38.3
  WellDepth[kcal/mol]      2.3
End
Frequencies[1/cm]      26
166.7723
170.0239
182.5507
268.3326
357.7151
574.8679
586.3380
872.4716
889.2927
897.7444
1025.4296
1059.1106
1085.0942
1142.4339
1354.5617
1407.5685
1468.3788
1485.4744
1501.7369
2028.1411
3020.1758
3067.9395

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3097.4686
3115.6838
3117.9233
3189.3126
      ZeroEnergy[kcal/mol]          -53.5
      ElectronicLevels[1/cm]        1
      0      2
End
Barrier      B43      W10      P6      #      TS32b
RRHO
      Geometry[angstrom]           11
      C      -1.290030      0.165112      1.307708
      C      0.173100      0.419821      1.034483
      C      0.776649      0.170464      -0.092261
      C      1.340309      -0.098089      -1.246729
      H      -1.410549      -0.527582      2.146819
      H      -1.799009      1.095417      1.579608
      H      -1.788183      -0.258991      0.435363
      H      0.759454      0.844741      1.848690
      H      -0.259838      -0.909004      -2.471235
      H      1.840880      -1.045039      -1.423011
      H      1.432891      0.659435      -2.018704
      Core      RigidRotor
      SymmetryFactor      1.0
End
      Tunneling      Eckart
      ImaginaryFrequency[1/cm]      318.0032
      WellDepth[kcal/mol]           37.6
      WellDepth[kcal/mol]           2.4
End
      Rotor      Hindered
      Group                        5 6 7
      Axis                        1 2
      Symmetry                      3
      Potential[kcal/mol]           2
0.000
1.579
      End
      Frequencies[1/cm]            25
164.1922
211.0645
284.9112
343.2710
572.9354
594.8503
875.5677
889.6961
895.4715
1025.1193
1059.2311
1086.4491
1140.4727

```

1352.2939  
1406.6641  
1468.2777  
1485.8735  
1501.2714  
2026.4542  
3020.5893  
3068.4089  
3101.4769  
3115.7858  
3121.1172  
3189.5040

ZeroEnergy[kcal/mol] -53.4  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B44 W10 P13 # TS34a

RRHO

Geometry[angstrom] 11  
C -2.279271 0.003755 0.783157  
H -2.423799 -0.611544 1.662672  
H -2.672592 1.012501 0.810686  
H -2.288087 -0.499882 -0.174295  
C -0.039766 0.485179 1.046878  
C 0.671802 0.111728 0.127274  
C 1.280961 -0.427649 -1.078708  
H -0.231569 0.949188 1.987332  
H 0.528303 -0.885578 -1.731789  
H 2.023131 -1.194416 -0.837453  
H 1.785555 0.356408 -1.651064

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 466.1287  
WellDepth[kcal/mol] 33.7  
WellDepth[kcal/mol] 10.1

End

Rotor Hindered ! rotating group comment (47cm-1)

Group 2 3 4 # atoms in rotating group  
excluding the atom on the axis

Axis 1 5 # rotational axis

Symmetry 3 #360/angle of rotation to

recover the initial structure

Potential[kcal/mol] 2 # number of

0.00

0.14

End

Rotor Hindered ! rotating group comment

Group 9 10 11 # atoms in rotating group  
excluding the atom on the axis

Axis 7 6 # rotational axis

Symmetry 3 #360/angle of rotation to  
recover the initial structure  
Potential[kcal/mol] 2 # number of  
0.00  
0.19

End  
Frequencies[1/cm] 24

115.2523  
342.0265  
344.6450  
464.2959  
489.8115  
657.6998  
729.2264  
833.5715  
937.0965  
1037.2694  
1057.2354  
1411.4473  
1415.7131  
1420.6113  
1473.4407  
1475.3204  
2079.1882  
3004.9301  
3058.8629  
3077.9942  
3086.9931  
3244.1635  
3250.9681  
3402.5544

ZeroEnergy[kcal/mol] -57.3  
ElectronicLevels[1/cm] 1  
0 2

End

Barrier B45 W12 P6 # TS36

RRHO

Geometry[angstrom] 11  
C 0.976817 -1.553466 -0.078150  
C -0.799211 1.546090 0.838872  
C -0.413989 0.515536 0.145046  
C 0.053135 -0.470889 -0.593581  
H 1.460359 -1.249335 0.850770  
H 0.412005 -2.471839 0.112614  
H 1.750515 -1.785770 -0.813033  
H -0.272730 2.495732 0.774488  
H -1.657656 1.501249 1.503280  
H -0.411914 -0.640812 -1.562475  
H 1.405389 0.575225 -1.663542

Core RigidRotor  
SymmetryFactor 0.5

End

```

Tunneling      Eckart
  ImaginaryFrequency[1/cm]    531.0853
  WellDepth[kcal/mol]         37.5
  WellDepth[kcal/mol]         3.8
End
Rotor          Hindered
  Group                    5 6 7
  Axis                      1 2
  Symmetry                  3
  Potential[kcal/mol]       2
0.000
1.463
  End
  Frequencies[1/cm]         25
204.7288
243.4198
376.9917
435.9346
545.4145
576.4700
870.9820
877.1293
922.6398
1004.2603
1055.4478
1092.1278
1138.4043
1355.7000
1408.2759
1459.7055
1488.7591
1500.3802
2006.6238
3027.1541
3085.3938
3099.6797
3114.1885
3128.4330
3170.2044
  ZeroEnergy[kcal/mol]       -52.0
  ElectronicLevels[1/cm]     1
    0    2
End
Barrier        B46   W12   P9   #   TS37a
Union
RRHO
  Geometry[angstrom]         11
  C          0.716403        -1.493821        0.012359
  C          -0.804018         1.635275         0.508954
  C          -0.273508         0.795993        -0.181012
  C          0.376737        -0.296563        -0.896063
  H          1.391862        -1.192529         0.815159

```

H	-0.186928	-1.904440	0.467215
H	1.200027	-2.281821	-0.569788
H	-1.280721	2.482905	0.937693
H	-0.850077	0.807426	2.411768
H	-0.276009	-0.625128	-1.712504
H	1.290945	0.081446	-1.367169
Core	RigidRotor		
	SymmetryFactor	1.0	
End			
Tunneling	Eckart		
	ImaginaryFrequency[1/cm]	463.3738	
	WellDepth[kcal/mol]	37.8	
	WellDepth[kcal/mol]	2.9	
End			
	Frequencies[1/cm]	26	
30.5299			
169.3226			
220.2598			
325.7580			
362.5063			
535.5112			
654.3761			
760.3041			
791.7118			
849.3968			
1013.5233			
1085.6903			
1109.2304			
1288.5635			
1346.1743			
1412.2299			
1478.1951			
1496.4046			
1506.8122			
2167.8788			
3020.1591			
3039.0035			
3046.2952			
3107.8196			
3115.0666			
3463.6050			
	ZeroEnergy[kcal/mol]	-51.7	
	ElectronicLevels[1/cm]	1	
	0	2	
End			
RRHO			
	Geometry[angstrom]	11	
C	0.981952	-1.553835	-0.098784
C	-1.004679	1.258774	0.864777
C	-0.462530	0.481185	0.114530
C	0.283949	-0.374725	-0.800071
H	1.689531	-1.195299	0.651350



H	0.253850	-2.195403	0.401677		
H	1.528356	-2.156967	-0.827735		
H	0.138872	2.982096	0.690032		
H	-1.612463	1.791595	1.554926		
H	-0.396814	-0.750839	-1.571913		
H	1.027433	0.239856	-1.322148		
Core	RigidRotor				
	SymmetryFactor	0.5			
End					
Tunneling	Eckart				
	ImaginaryFrequency[1/cm]	457.5408			
	WellDepth[kcal/mol]	37.9			
	WellDepth[kcal/mol]	3.0			
End					
Frequencies[1/cm]	26				
44.7989					
191.2912					
210.2060					
267.4221					
410.8373					
526.2546					
661.6826					
754.8288					
788.1233					
846.8918					
1020.3324					
1088.3056					
1105.1114					
1286.7554					
1348.9839					
1413.7407					
1473.9316					
1497.5788					
1507.2452					
2169.7134					
3013.6608					
3037.8953					
3041.3886					
3106.2021					
3111.9344					
3463.7408					
	ZeroEnergy[kcal/mol]	-51.6			
	ElectronicLevels[1/cm]	1			
	0	2			
End					
End					
Barrier	B47	W5	P12	#	TS26a
RRHO					
	Geometry[angstrom]	11			
C	-1.252243	-0.019106	0.002747		
C	0.982839	-0.699434	-0.006075		
C	1.181730	-0.863206	-1.292231		

```

C          1.310090   -0.695003   1.288070
H          -1.126543   0.864885  -0.609308
H          -1.493057   0.137888   1.045817
H          -1.664100  -0.902994  -0.467328
H          2.158457  -1.188201  -1.640917
H          0.420292  -0.691842  -2.041362
H          1.637572   0.216262   1.778545
H          1.099973  -1.551767   1.920541
Core      RigidRotor
SymmetryFactor      1.0
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]      508.7009
WellDepth[kcal/mol]           56.5
WellDepth[kcal/mol]           11.0
End
Rotor      Hindered      ! rotating group comment
Group                        5 6 7      # atoms in rotating group
excluding the atom on the axis
Axis                        1 2      # rotational axis
Symmetry                    3      #360/angle of rotation to
recover the initial structure
Potential[kcal/mol]         2
0.00
0.31
End
Frequencies[1/cm]          25
115.4809
223.4491          335.7684          361.0470
471.2638          521.4013          779.8172
799.2631          826.2756          890.4782
1013.4309         1020.4788         1056.4265
1414.9793         1426.5885         1431.3433
1473.9185         1901.3789         3090.0387
3115.6191         3121.1427         3194.3906
3211.7991         3252.4563         3253.3227
ZeroEnergy[kcal/mol]      -55.4
ElectronicLevels[1/cm]    1
0 2
End
Barrier      B48      W11      P13      #      TS27a
RRHO
Geometry[angstrom]        11
C          -1.443360   0.134084  -0.123335
C          0.835332   0.083922   0.000766
C          1.128016  -0.065883  -1.436324
C          1.159683   0.191113   1.177227
H          -1.567881   1.003946  -0.757403
H          -1.737875   0.244261   0.911607
H          -1.618238  -0.834799  -0.575985
H          0.681821  -0.979193  -1.837291
H          0.729846   0.774360  -2.010303

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H          2.208567   -0.110989   -1.593565
H          1.160503    0.295561    2.236085
Core      RigidRotor
          SymmetryFactor    1.0
End
Tunneling      Eckart
          ImaginaryFrequency[1/cm]    508.7457
          WellDepth[kcal/mol]        33.6
          WellDepth[kcal/mol]        11.9
End
Rotor      Hindered      ! rotating group comment
          Group          5 6 7      # atoms in rotating group
excluding the atom on the axis
          Axis          1 2      # rotational axis
          Symmetry      3      #360/angle of rotation to
recover the initial structure
          Potential[kcal/mol]    2
0.00
0.27
End
          Frequencies[1/cm]    25
161.8127
218.9152          326.1483          349.8666
492.4868          529.9903          556.5383
678.7565          846.5162          928.6015
1041.8259         1064.0968         1412.2008
1413.5655         1424.8845         1481.8151
1484.5486         2025.4727         3031.3400
3084.3441         3091.9133         3096.9049
3238.0474         3249.9048         3444.9267
          ZeroEnergy[kcal/mol]    -55.5
          ElectronicLevels[1/cm]    1
          0      2
End
Barrier      B49      R1      W1      # (DOUBLE BOND ADDITION)
RRHO
Stoichiometry C4H7
Core      PhaseSpaceTheory
          FragmentGeometry[angstrom]    9
C          -1.467054   -0.247836    0.585542
C          0.030549   -0.187355    0.515967
C          0.757529   -0.389660   -0.578479
H          -1.884113    0.706052    0.927272
H          -1.797463   -1.008392    1.301790
H          -1.904859   -0.482538   -0.387548
H          0.541521    0.042396    1.449634
H          1.839990   -0.331251   -0.561519
H          0.295414   -0.621647   -1.533696
          FragmentGeometry[angstrom]    2
C          -0.564023    0.000000    0.000000
H          0.564008    0.000000    0.000000
          SymmetryFactor    1

```

PotentialPrefactor[au]		1.0E0
PotentialPowerExponent		6.
End		
Frequencies[1/cm]		22
204.3804	425.7634	590.6356
923.8042	940.5952	948.6235
1029.0335	1070.7181	1189.1812
1327.6604	1408.8905	1448.7188
1481.0539	1494.9488	1713.0513
3012.1903	3055.8298	3090.9901
3119.2670	3126.4358	3207.0111
2804.9231		
ElectronicLevels[1/cm]		1
0	2	
ZeroEnergy[kcal/mol]		0.0
End		
End		