Mechanism and Kinetics of the Oxidation of 1,3-Butadien-1-yl (*n*-C_4H_5): A Theoretical Study

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Supplementary Information

Content

- **Figure S1** – Graph of the overall PES for the *n*-C_4H_5 + O_2 reaction. The upper part (in terms of relative energy) accessed in the entrance channel is encompassed in a blue rectangle.
- **Figure S2** – Complete potential energy diagram for the *n*-C_4H_5 + O_2 reaction. Relative energies calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.
- **Figure S3** – The graph of the first part of the highly exoergic region of the PES for the *n*-C_4H_5 + O_2 reaction. Relative energies calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.
- **Figure S4** – The graph of the second part of the highly exoergic region of the PES for the *n*-C_4H_5 + O_2 reaction. Relative energies calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.
- **Figure S5** – Pressure- and temperature-dependent channel specific rate constants and relative yields for various products: hollow blue squares – *trans*-1-oxo-*n*-butadienyl + O (**p1**), solid blue squares – stabilization in w1, hollow red circles – *cis*-1-oxo-*n*-butadienyl + O (**p2**), solid red circles – stabilization in w1, hollow green triangles – acrolein + HCO (**p6**), solid green triangles – 3-oxopropyl + CO (**p9**), magenta stars – interconversion of reactants, navy rhombi – furan + OH (**p3**), cyan plus signs – 2(5H)-furanone + H (**p7**), cyan cross symbols – 2(3H)-furanone + H (**p8**), violet right-pointing triangles – ketene + c-C_2H_3O (**p4**), violet left-pointing triangles – ketene + vinoxy (**p5**). A – 0.1 atm, B – 10 atm.
- Input file for MESS calculations for the C_4H_5 + O_2 reaction.
- Input file for MESS calculations for the C_4H_5O secondary reaction.

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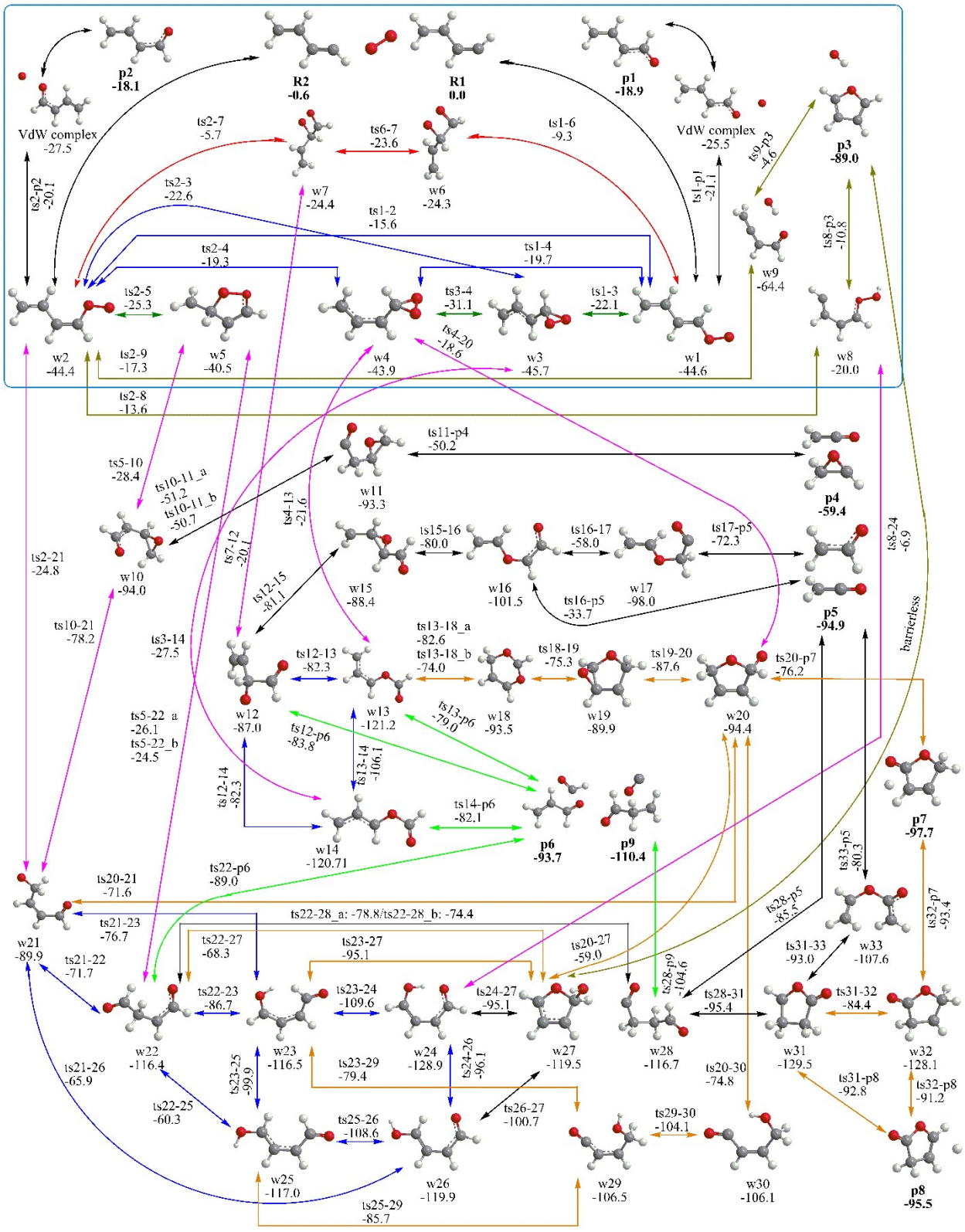

Figure S1. Graph of the overall PES for the *n*-C_4H_5 + O_2 reaction. The upper part (in terms of relative energy) accessed in the entrance channel is encompassed in a blue rectangle. Relative energies calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.

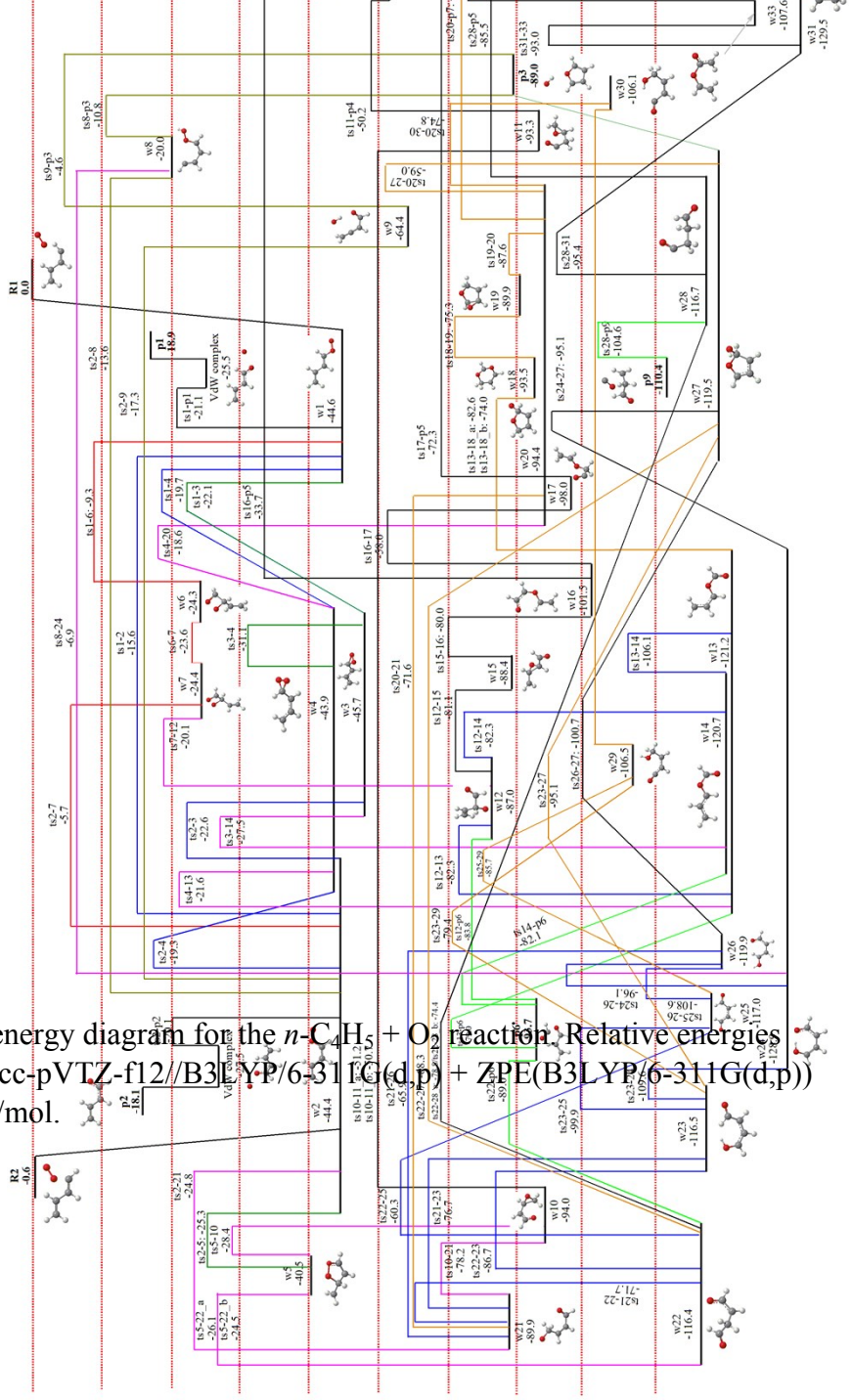

Figure S2. Complete potential energy diagram for the *n*-C_4H_5 + O_2 reaction. Relative energies calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.

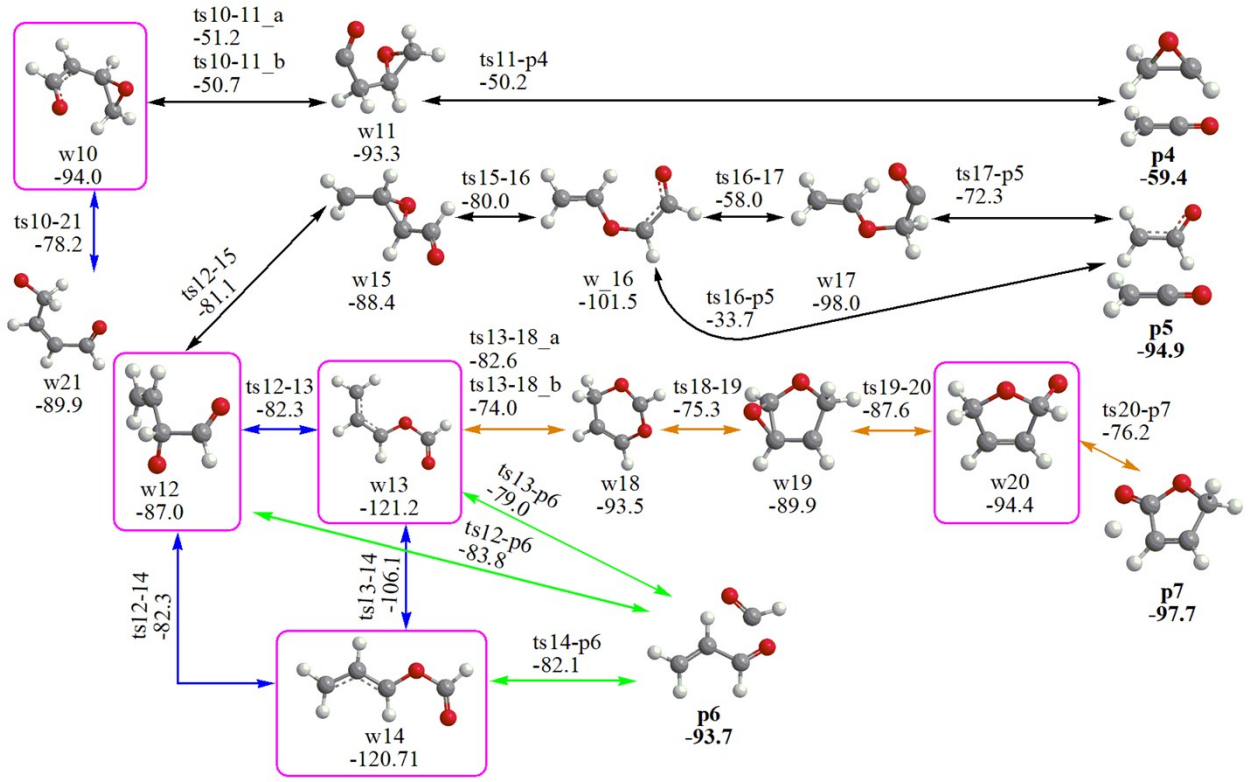

Figure S3. The graph of the first part of the highly exoergic region of the PES for the *n*-C_4H_5 + O_2 reaction. Relative energies calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.

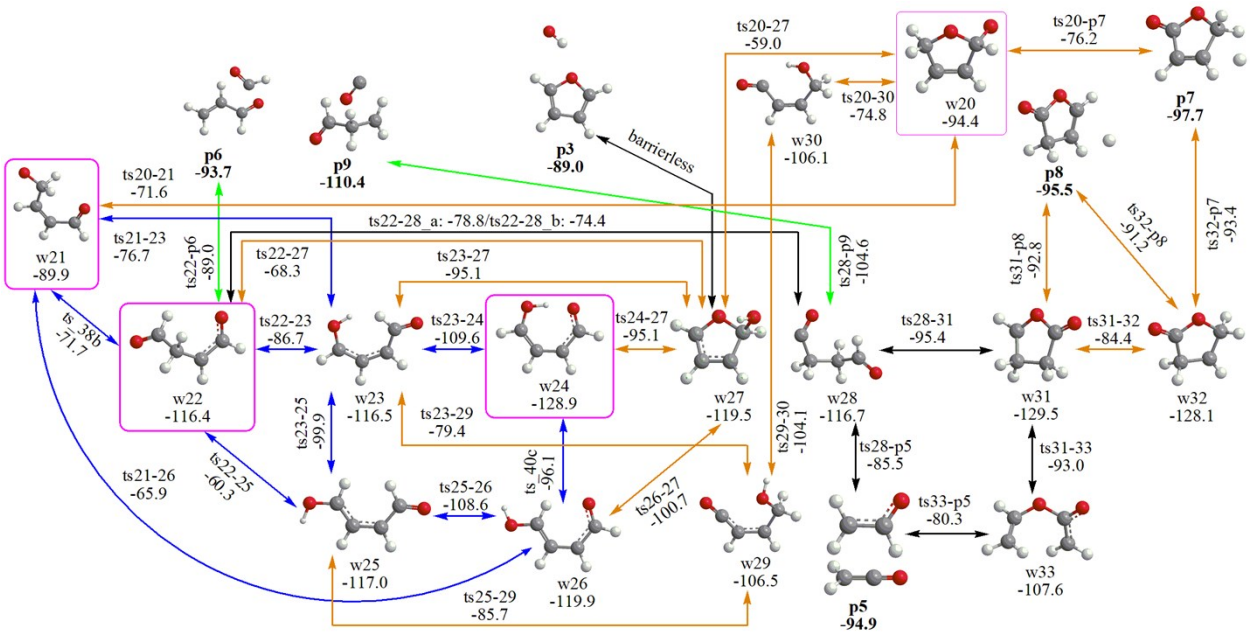

Figure S4. The graph of the second part of the highly exoergic region of the PES for the *n*-C_4H_5 + O_2 reaction. Relative energies calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.

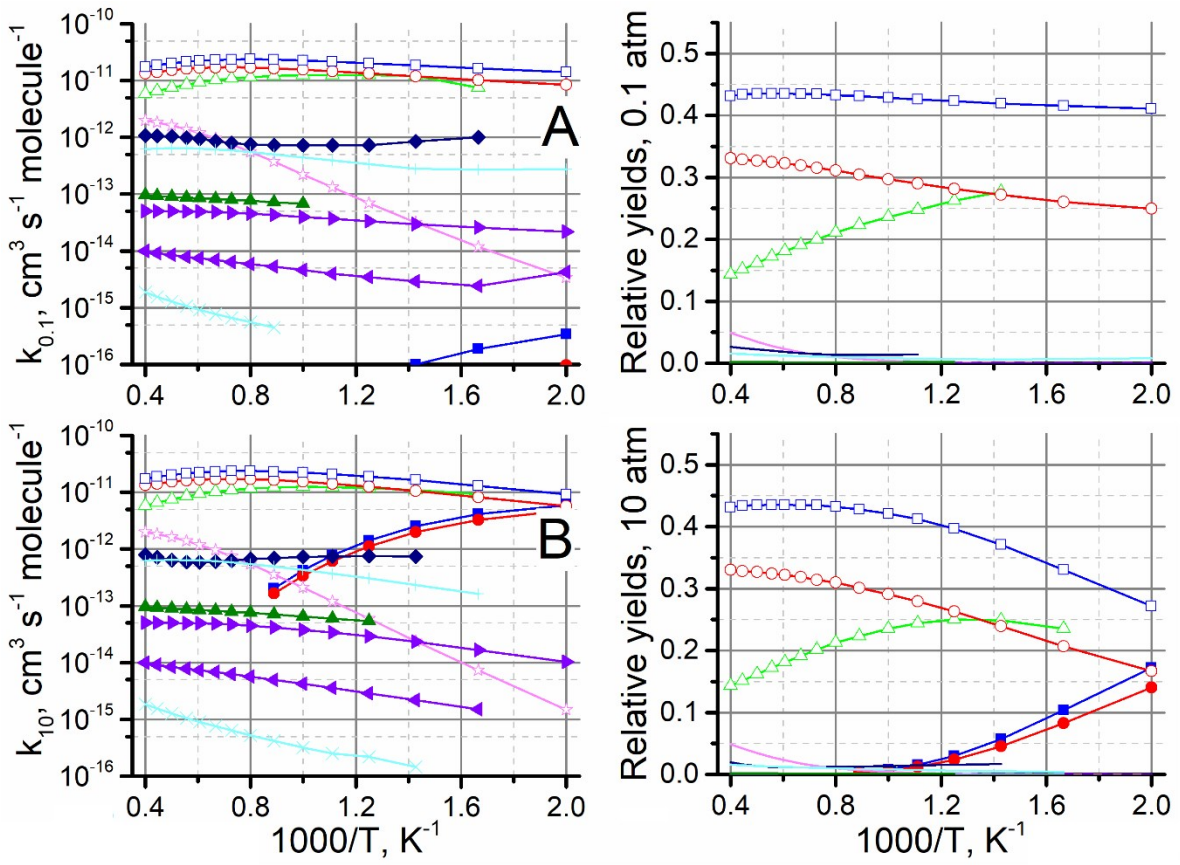

Figure S5. Pressure- and temperature-dependent channel specific rate constants and relative yields for various products: hollow blue squares – *trans*-1-oxo-*n*-butadienyl + O (**p1**), solid blue squares – stabilization in w1, hollow red circles – *cis*-1-oxo-*n*-butadienyl + O (**p2**), solid red circles – stabilization in w1, hollow green triangles – acrolein + HCO (**p6**), solid green triangles – 3-oxopropyl + CO (**p9**), magenta stars – interconversion of reactants, navy rhombi – furan + OH (**p3**), cyan plus signs – 2(5H)-furanone + H (**p7**), cyan cross symbols – 2(3H)-furanone + H (**p8**), violet right-pointing triangles – ketene + c-C_2H_3O (**p4**), violet left-pointing triangles – ketene + vinoxy (**p5**). A – 0.1 atm, B – 10 atm.

Input file for MESS calculations for the $C_4H_5 + O_2$ reaction.

```
TemperatureList[K]                500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650.
1800. 2000. 2250. 2500.
PressureList[atm]                 0.01 0.1 1.0 10. 100.
EnergyStepOverTemperature         0.2         #Ratio of discretization energy step to T
ExcessEnergyOverTemperature       100
ModelEnergyLimit[kcal/mol]          600
WellCutoff                      10
ChemicalEigenvalueMax             0.2
ChemicalEigenvalueMin             1.e-6       #only for direct diagonalization method
CalculationMethod               direct
EigenvalueOutput                                eigenvalue.out
Reactant       #ground energy of bimolecular species will be used as a reference.
Model
 EnergyRelaxation
  Exponential
   Factor[1/cm]              333    ! Jasper-Hansen H + fulvene paper
   Power                          0.7
   ExponentCutoff                 15
  End
 CollisionFrequency
  LennardJones
    Epsilons[1/cm]         68.0  285.2
    Sigmas[angstrom]       3.610  5.18
Masses[amu]           28.  85.
End
OutputTemperatureStep[K]  100
OutputTemperatureSize  20
OutputReferenceEnergy[kcal/mol]  0.
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Species
RRHO
Geometry[angstrom]   11
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C  -2.598302444   0.4697455332   0.3273629504
C  -1.4406525199   -0.3950053191   0.3442075738
C  -0.175469695   0.0470320288   0.3531588396
O  -4.8974559682   0.8959427082   0.3028318556
O  -6.0939400436   0.3165070692   0.2955759358
H  -4.1680550119   -1.0329368604   0.3228213231
H  -2.4464120283   1.5451301149   0.321441141
H  -1.6292838288   -1.4659606249   0.3497300937
H  0.6625302376   -0.6385266878   0.3657652584
H  0.0551608827   1.1071875376   0.3481073302
    Core                          MultiRotor
#7 1 5 6 s 11 30.
#1 2 3 9 s 11 30.
      SymmetryFactor  1
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      InternalRotation
            Group                  6
            Axis                  1 5
            Symmetry                1
            MassExpansionSize           11
            GridSize                100
      End
      InternalRotation
            Group                  4 9 10 11
            Axis                  2 3
            Symmetry                1
            MassExpansionSize           11
            GridSize                100
      End
    End

Frequencies[1/cm]  25
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592.2483            663.1303            873.0738
933.5932            952.8360            968.0069
1034.4387           1054.1506           1140.0961
1212.2619           1278.0809           1298.7967
1328.9127           1455.4997           1631.5780
1666.4882           3136.3909           3142.2025
3164.8523           3201.4757           3229.3136
ZeroEnergy[kcal/mol] -44.6
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!-------well_ip02------------
Well       ip02
Species
RRHO
Geometry[angstrom]   11
C  1.1720559808   0.213020049   0.0112399072
C  -0.1445700139   -0.4214886359   0.0160532605
C  -1.3264147461   0.3048548279   -0.0053157307
C  -2.5907845341   -0.245633174   -0.0018312636
O  2.1975440612   -0.4119121644   -0.7166560014
O  2.1884397515   -0.3823164569   0.7758412702
H  1.1975759739   1.3029477145   -0.0101896447
H  -0.1504383421   -1.5063515054   0.0375006978
H  -1.2467108717   1.3906007256   -0.0264023692
H  -3.4760310331   0.376462805   -0.0193878628
H  -2.7339372264   -1.3200341855   0.0186617368
Core  RigidRotor
SymmetryFactor  1.0
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Rotor     Hindered     #101.8929
Group                5 6 7
Axis                1 2
Symmetry              1
Potential[kcal/mol]    12
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1.775726638 3.615584756 5.571720401 4.579941494 1.509411568
End

Frequencies[1/cm]  26
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429.6141            434.4371            485.9655
556.6572            778.6678            815.9636
822.4007            838.9775            966.8036
1003.4204            1144.5973            1167.2594
1198.1710            1258.2082            1276.9668
1290.9423            1428.5446            1509.5377
1526.3939            3101.7444            3125.1045
3143.9372            3175.8960            3241.3131
ZeroEnergy[kcal/mol] -45.7
ElectronicLevels[1/cm]        1
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End
End
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Species
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C  0.2004191538   -0.1213189184   0.0345873619
C  -1.0942835788   0.3169796471   0.2387362767
C  -2.211198306   -0.4804205981   0.1185888045
O  2.8328451018   -0.7464387997   -0.3142390333
O  1.2253949249   0.7858282895   0.1894706623
H  3.1733707158   1.2143315544   0.1557563154
H  0.4917786366   -1.1254943049   -0.2389892101
H  -1.2144612867   1.3622142745   0.5108974122
H  -3.2018852463   -0.0822952771   0.2904537389
H  -2.1326504075   -1.5273228475   -0.1510132297
     Core                              MultiRotor
#2 6 1 5 s 11 30.
#1 6 2 3 s 11 30.
       SymmetryFactor  1.0
       InterpolationEnergyMax[kcal/mol]        100
       PotentialEnergySurface[kcal/mol]        /home/dporfirev/C4H5+O2/kin/dat/w_04_double.dat
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             Group                        5 7
             Axis                        1 6
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            GridSize                 100
        End
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            Group                    1 5 7
            Axis                     2 6
            Symmetry                 1
            MassExpansionSize        11
            GridSize                 100
        End
    End

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548.5385            722.3508         790.2352
795.0002            941.2725         986.3060
1007.9148           1080.2072        1170.7229
1202.7975           1283.6351        1343.3875
1403.6633           1496.5731        1525.3490
1808.0702           3064.1969        3146.0242
3152.3896           3221.5908        3243.5643
ZeroEnergy[kcal/mol] -120.7
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!-------well_ip04b------------
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Species
RRHO
Geometry[angstrom]   11
C  1.6126900067   0.3889252754   -0.5529081649
C  -0.325874532   -0.3951292739   0.5281695205
C  -1.7055163538   -0.4342608745   0.6207396561
C  -2.5971219186   0.2178891633   -0.2029072426
O  2.3711089623   -0.1843983543   0.1716144485
O  0.2542663361   0.356690411   -0.4697397264
H  1.8863876687   1.0312038332   -1.3986076918
H  0.3574582768   -0.9134378297   1.1836046166
H  -2.0900881957   -1.0466304365   1.4309812794
H  -3.6638014474   0.1248600264   -0.0494317246
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#2 6 1 5 s 11 30.
#1 6 2 3 s 11 30.
      SymmetryFactor  1.0
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/home/dporfirev/C4H5+O2/kin/dat/w_04b_double.dat
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            Group                 5 7
            Axis                1 6
            Symmetry              1
            MassExpansionSize          11
            GridSize              100
      End
      InternalRotation
            Group                 1 5 7
            Axis                2 6
            Symmetry              1
            MassExpansionSize          11
            GridSize              100
      End
    End

Frequencies[1/cm]  25
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280.3018          398.0124          551.0692
598.8605          692.3072          795.9398
801.4885          966.0566          968.9462
1012.4249          1045.0402          1156.6464
1201.4947          1231.6911          1395.9855
1418.4712          1483.6872          1518.4739
1812.0294          3062.7013          3154.9844
3159.0603          3238.0541          3252.3040
ZeroEnergy[kcal/mol] -121.2
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
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Well       ip06
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RRHO
Geometry[angstrom]   11
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C  -0.0767147855   -0.3437160843   5.78077E-5
C  -1.365493622   0.3163922152   6.17079E-5
C  -2.5307644245   -0.3442264035   3.211951E-4
O  1.1941919165   1.6388802017   -4.764369E-4
O  2.4398570178   2.1023876356   -6.978825E-4
H  2.0862921916   -0.2178640164   -1.931111E-4
H  -0.0601655686   -1.4287762571   2.732981E-4
H  -1.3635106704   1.401602426   -1.582221E-4
H  -3.4779530072   0.1807399948   3.170368E-4
H  -2.5697395423   -1.4288901159   5.452985E-4
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#7 1 5 6 s 11 30.
#1 2 3 9 s 11 30.
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            Axis                   1 5
            Symmetry                 1
            MassExpansionSize          11
            GridSize                 100
      End
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            Group                  4 9 10 11
            Axis                   2 3
            Symmetry                 1
            MassExpansionSize          11
            GridSize                 100
      End
    End

Frequencies[1/cm]  25
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679.4890          723.1262          814.3155
916.9646          941.0317          957.8008
1003.1249          1038.1458          1144.7553
1198.1719          1242.3237          1322.5533
1370.2918          1459.4581          1629.1265
1673.6341          3135.8689          3163.3945
3174.0062          3217.5169          3226.8046
ZeroEnergy[kcal/mol] -44.4
ElectronicLevels[1/cm]      1
0  2
End
End
!---------------------------------
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Species
RRHO
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C  0.6853636026   -0.6143855712   -0.4389904639
C  -0.5270295754   -0.4109987486   0.4083089781
C  -1.7685065894   -0.5503991525   -0.0483180054
O  2.6374820424   -0.3621760683   0.2509941608
O  1.6864584821   -1.4918521358   0.2148038224
H  1.7057273058   1.495971034   -0.1950795919
H  0.4214675771   -1.0258509924   -1.4193615154
H  -0.3358336988   -0.1139025849   1.4358180742
H  -2.6311229511   -0.364425253   0.5807584966
H  -1.9655863249   -0.8527051475   -1.0723202762
Core  RigidRotor
SymmetryFactor  0.5
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```
End

Rotor     Hindered     #102.9823
Group                4 9 10 11
Axis                 2 3
Symmetry             1
Potential[kcal/mol]    12
0 1.167544343 3.699984796 3.327746107 1.163528282 1.361382056 2.987510407
3.103223175 2.440824052 2.661519175 3.110000279 1.197037294
End

Frequencies[1/cm]  26
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353.5078            441.3013            645.0477
693.5158            846.0572            877.1307
886.5998            955.8461            971.4993
1025.6772           1054.6226           1133.7341
1162.9903           1214.4096           1286.0519
1312.1365           1338.1115           1454.1480
1696.1994           3028.1978           3131.5130
3154.1540           3172.4441           3218.8757
ZeroEnergy[kcal/mol] -24.3
ElectronicLevels[1/cm]       1
0  2
End
End
!----------------------------------
!-------well_ip07b------------
Well       ip07b
Species
RRHO
Geometry[angstrom]   11
C  -1.0021391421   0.9526662007   0.3383671222
C  0.1154453848   0.2208307854   -0.3310452526
C  1.3592141991   -0.0915433867   0.4296291149
C  2.5800641454   0.0821224238   -0.0681498625
O  -1.892447932   -0.0853437045   0.1336531646
O  -0.8083625579   -0.9372523368   -0.393772591
H  -1.3631646015   1.9694796191   0.2353469079
H  0.3488334161   0.557544804   -1.3502041704
H  1.2093423517   -0.4656898549   1.4379554529
H  2.7343301076   0.4538146571   -1.0765883984
H  3.4683566289   -0.1356772071   0.5131615125
Core  RigidRotor
SymmetryFactor  0.5
End

Rotor     Hindered     #103.4867
Group                4 9 10 11
Axis                 2 3
Symmetry             1
Potential[kcal/mol]    12
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0 1.216992099 3.562748448 2.953311134 1.808482638 2.348705644 2.971948169
1.968685837 1.499496916 3.123428984 3.523215344 1.11433153
End

Frequencies[1/cm] 26
162.5423 309.9469
355.2478 460.7328 615.0740
682.3496 858.3547 871.4456
900.5777 948.9669 975.7334
1026.5924 1037.7784 1140.6036
1174.9688 1228.3430 1298.4324
1308.5151 1335.9966 1457.4412
1701.7125 2989.0329 3131.5745
3160.8981 3176.6734 3219.0186
ZeroEnergy[kcal/mol] -24.4
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
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Well ip10min2
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RRHO
Geometry[angstrom] 11
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C 0.7452934615 0.8189165885 -0.0449406353
C 1.6107477576 -0.351761157 -0.0252732197
C 2.9271852735 -0.3244001517 -0.0646218379
O -1.2394247801 -0.3827545211 0.3502598312
O -2.520397078 -0.3556667334 -0.3623709701
H -1.2282915199 1.6585336159 0.0176809163
H 1.2097021332 1.7935508774 -0.1379841626
H 1.1044180507 -1.3211926969 0.014970816
H -3.0968277158 -0.6710227208 0.3480040021
H 3.7356250646 -1.0395469961 -0.0726039578
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
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215.7135 341.2174 386.8267
471.3893 662.9884 690.6029
787.5389 810.2314 858.2643
896.8852 948.6516 1018.4902
1150.1747 1240.0603 1263.6446
1386.1529 1404.9162 1627.6060
1680.9772 3047.0502 3174.2617
3193.9006 3244.6004 3775.8704
ZeroEnergy[kcal/mol] -20.0
ElectronicLevels[1/cm] 1
0 2

End
End
!---------------------------------
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Well ip12_oh
Species
RRHO
Geometry[angstrom] 11
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C -0.5109837901 0.9182554545 0.1337699543
C -1.5043064139 0.0654696735 0.0251008547
C -2.4263117593 -0.8431760961 -0.0823640011
O 1.2857422124 -0.6760060302 0.1535998865
O -0.7397247685 -2.7963842346 -0.0899333303
H 1.632055666 1.2988940067 0.2860102447
H -0.696505788 1.9877878173 0.1827084964
H 0.0523842581 -2.2238054102 -0.0091461295
H -2.7668206412 -1.1849359252 -1.0536911989
H -2.8797143149 -1.2891609117 0.7961276996
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 27
28.9455 107.2150 137.6821
188.3084 188.3910 372.3547
421.7847 481.4756 523.3482
615.5810 785.2540 860.1386
883.3730 911.1980 985.9281
1026.8553 1122.6523 1352.4962
1422.3357 1451.0900 1747.0913
2010.8262 2930.1154 3136.8040
3147.1907 3214.9187 3593.0585
ZeroEnergy[kcal/mol] -64.4
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------well_ip15min------------
Well ip15min
Species
RRHO
Geometry[angstrom] 11
C -1.5062991437 0.0898181847 -0.2659035501
C -0.1809861648 0.0883201968 0.4163297918
C 1.0598132975 -0.0592940508 -0.4425874767
C 2.2470136965 -0.7097207863 0.0611457462
O 0.6694874977 1.1929127607 0.147437012
O -2.4524867266 -0.5506812923 0.1164474337
H -1.543360837 0.7278712362 -1.1757023203
H -0.1616769432 -0.3104840835 1.4273618648
H 0.886667388 -0.1072567514 -1.5160052178

```
H  2.7960754267   -1.4035614678   -0.5600492522
H  2.569850509   -0.5350379462   1.0789449687
    Core                        MultiRotor
#2 3 4 10 s 11 30.
#3 2 1 6 s 11 30.

      SymmetryFactor  0.5
      InterpolationEnergyMax[kcal/mol]       100
      PotentialEnergySurface[kcal/mol]       /home/dporfirev/C4H5+O2/kin/dat/w_15_double.dat
      InternalRotation
            Group                  10 11
            Axis                   3 4
            Symmetry                 1
            MassExpansionSize          11
            GridSize                 100
      End
      InternalRotation
            Group                  7 6
            Axis                   1 2
            Symmetry                 1
            MassExpansionSize          11
            GridSize                 100
      End
    End

Frequencies[1/cm]  25
                                          219.7119          252.3153
                                          398.6678          448.7202
522.6533          579.9400          748.0641
800.2091          970.0521          1001.5874
1060.9925         1081.9886         1133.5112
1168.2586         1212.1700         1307.0269
1388.4644         1420.0369         1461.5665
1801.4860         2886.7430         3113.6377
3139.7585         3157.5550         3268.6624
ZeroEnergy[kcal/mol] -88.4
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!-------well_ip16------------
Well       ip16
Species
RRHO
Geometry[angstrom]   11
C  1.747926457   -0.2931206857   0.0733104371
C  0.6139861019   -1.1327315736   -0.1006757666
C  -1.1213863127   0.5150269645   -0.022771475
C  -2.4274309136   0.7417469892   -0.0830370551
O  -0.6763142431   -0.7935617388   -0.1467135768
O  1.7536625143   0.9359573982   0.2179468269
```

```
H  2.6955598868   -0.8650564777   0.0692317469
H  0.7451700013   -2.2014224684   -0.2173697922
H  -0.3429848054   1.2514301442   0.115409688
H  -2.7987811372   1.7525713938   0.0108672022
H  -3.1355855493   -0.0649709456   -0.2247922353
    Core                          MultiRotor
#1 2 5 3 s 11 30.
#2 5 3 4 s 11 30.
      SymmetryFactor  0.5
      InterpolationEnergyMax[kcal/mol]       100
      PotentialEnergySurface[kcal/mol]       /home/dporfirev/C4H5+O2/kin/dat/w_16_double.dat
      InternalRotation
            Group                  3 4 9 10 11
            Axis                   2 5
            Symmetry                  1
            MassExpansionSize            11
            GridSize                100
      End
      InternalRotation
            Group                  4 9 10 11
            Axis                   3 5
            Symmetry                  1
            MassExpansionSize            11
            GridSize                100
      End
    End

Frequencies[1/cm]  25
                                                                                213.4153
313.2291            419.7356            485.6828
674.2775            731.9848            836.3877
876.9385            899.3349            937.6239
1007.9356           1013.0822           1128.6090
1312.8650           1341.9754           1411.0284
1415.2723           1496.8901           1589.0439
1684.7878           2927.2558           3161.2435
3200.9506           3225.7943           3259.5860
ZeroEnergy[kcal/mol] -101.5
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!-------well_ip19min------------
Well       ip19min
Species
RRHO
Geometry[angstrom]   11
C  -1.4841357748   0.1527749256   -0.1238253439
C  -0.0158156853   0.4700249967   0.4090765729
C  0.9164502907   -0.7096595896   0.3042800689
C  2.1222118686   -0.6234444555   -0.2436831813
```

```
O  0.3602331328   1.6312130151   -0.1255921491
O  -1.8588426109   -0.9428943978   -0.3983412174
H  -2.1025594653   1.0661360298   -0.1962253785
H  -0.3044748108   0.6357285588   1.4784081281
H  0.5418775026   -1.6475275544   0.7031059832
H  2.778803072   -1.4829922939   -0.3053410321
H  2.4798934804   0.3169817651   -0.6473614507
    Core                        MultiRotor
#1 2 3 4 s 11 30.
#3 2 1 6 s 11 30.
      SymmetryFactor  0.5
      InterpolationEnergyMax[kcal/mol]       100
      PotentialEnergySurface[kcal/mol]
/home/dporfirev/C4H5+O2/kin/dat/w_19min_double.dat
      InternalRotation
            Group                 4 9 10 11
            Axis                  2 3
            Symmetry                 1
            MassExpansionSize           11
            GridSize                100
      End
      InternalRotation
            Group                 6 7
            Axis                  1 2
            Symmetry                 1
            MassExpansionSize           11
            GridSize                100
      End
   End

Frequencies[1/cm]  25
                                                                    218.4602
297.1918          390.7364          490.9458
609.1032          704.8361          710.8368
788.3814          957.9824          980.3285
1021.9205          1042.2108          1075.4723
1172.6131          1291.4035          1315.8061
1352.0623          1435.6384          1700.6088
1840.2325          2770.4240          2948.2066
3140.3182          3161.8917          3230.3854
ZeroEnergy[kcal/mol] -87.0
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!-------w_21min------------
Well       ip21min
Species
RRHO
Geometry[angstrom]   11
C  1.3618161892   -0.2151189238   -0.3676866229
```

```
C  0.4738395106   0.7274434794   0.4636982337
C  -1.6916851946   0.1190014845   -0.2685036173
C  -1.6583232131   -1.1367300033   0.1747107705
O  -0.7272805019   1.0775731253   -0.1753562846
O  2.4003049977   -0.6530187305   -0.0209207411
H  0.3007068112   0.265303773   1.4445776193
H  1.0369470786   1.6536938552   0.597443812
H  -2.5551446236   0.5288545706   -0.778701166
H  -2.5247550802   -1.7638604789   0.0159563672
H  -0.813086974   -1.5851651516   0.677788629
    Core                        MultiRotor
#6 1 2 5 s 11 30.
#2 5 3 4 s 11 30.
      SymmetryFactor  0.5
      InterpolationEnergyMax[kcal/mol]       100
      PotentialEnergySurface[kcal/mol]
/home/dporfirev/C4H5+O2/kin/dat/w_21min_double.dat
      InternalRotation
           Group                  6
           Axis                  1 2
           Symmetry                 1
           MassExpansionSize           11
           GridSize                100
      End
      InternalRotation
           Group                  4 9 10 11
           Axis                  5 3
           Symmetry                 1
           MassExpansionSize           11
           GridSize                100
      End
    End

Frequencies[1/cm]  25
                                                                    179.0037
306.6199          358.2571          476.0210
621.5130          711.5282          825.3074
843.6511          850.7484          932.0937
996.1985         1058.8464         1222.5395
1269.1900          1327.4135          1359.5501
1427.2874          1465.6899          1684.5694
1927.3049          3002.4338          3097.8796
3169.2862          3195.6703          3252.1681
ZeroEnergy[kcal/mol] -98.0
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!-------well_ip32------------
Well       ip32
Species
```

RRHO
Geometry[angstrom] 11
C 1.2537004059 0.6764262635 0.4142602055
C -0.1078954569 0.9754865986 0.6973520273
C -1.1960402708 0.0873327326 0.7171402515
C -1.2198209353 -1.2785023186 0.470991458
O 1.7275299752 -0.4447353055 0.1297584818
H 1.9479790307 1.5290856478 0.4537299991
H -0.3168483923 2.0157927997 0.9228842669
H -2.1650792594 0.5116902023 0.9573048074
H -2.1673720238 -1.8064687148 0.5330771786
O -0.2144567666 -2.0550659616 0.1602937191
H 0.6470756933 -1.5010029442 0.1174656048
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 27
161.1641 301.6653 306.1064
325.4863 539.0322 645.8009
708.4369 877.2486 920.8284
928.9020 935.8878 982.6435
1088.3521 1140.3144 1210.9754
1338.0200 1394.1760 1450.0969
1487.3857 1538.1498 1603.4742
1635.6152 2594.4482 3003.8316
3155.2176 3168.0318 3181.8395
ZeroEnergy[kcal/mol] -128.9
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------well_ip33------------
Well ip33
Species
RRHO
Geometry[angstrom] 11
C 1.0523824669 -0.1751493313 -0.720746639
C 0.4958638369 0.8987200785 0.1194719975
C -0.7831370892 0.9412543182 0.5253703033
C -1.8668647833 -0.0585552422 0.2179743006
O 0.4202688514 -1.1278487277 -1.1324030536
O -3.0797760049 0.2328320516 0.7619232063
H 2.1275796046 -0.0670859746 -0.9715375209
H 1.1805151951 1.6887152523 0.4132730384
H -1.1193191728 1.7688165852 1.1454266376
H -1.9869153413 -0.2040889075 -0.873935476
H -1.5721265634 -1.0827391025 0.5212972058
Core RigidRotor
SymmetryFactor 1.0
End

Rotor Hindered #42.5471
Group 6 10 11
Axis 3 4
Symmetry 1
Potential[kcal/mol] 12
0 0.302083117 1.475024042 3.438438798 5.016562666 5.305091576 7.24610424 5.307727116
5.017064674 3.444588392 1.479918617 0.304153898
End

Frequencies[1/cm] 26
165.7531 177.6427
341.7461 383.1473 484.7648
520.0351 740.8903 808.2047
946.6518 1011.6165 1025.8800
1037.5000 1072.5289 1128.8449
1216.2444 1263.9105 1342.9921
1409.1706 1434.8753 1651.8342
1764.8086 2893.4539 2903.9198
2908.0818 3144.1339 3165.3171
ZeroEnergy[kcal/mol] -89.9
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_ip35----------
Well ip35
Species
RRHO
Geometry[angstrom] 11
C 0.1752998791 -1.328410404 0.0599444891
C 0.2840941039 0.9974864626 -0.0260010667
C -1.0456807939 1.081441507 -0.0252627991
C -1.8697161673 -0.1595647788 0.1396799764
O -1.055206706 -1.2451166867 0.6300772508
O 0.9589007562 -0.1884917421 0.0527687567
H 0.7362814487 -2.196659641 0.3832261742
H 0.9619234038 1.8366849614 -0.0968215919
H -1.5326289395 2.0437984854 -0.1112780162
H -2.6489801469 -0.0262728501 0.8929419253
H -2.350178838 -0.4694563135 -0.7974670987
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
159.6045 302.9297 457.3079
539.5714 596.6962 718.4230
815.7943 880.0137 926.6541
933.6133 971.3563 1000.8464
1072.0874 1108.8426 1185.9051
1250.3361 1271.2526 1345.8386
1407.9131 1420.4904 1502.9026

1704.4377 2997.7285 3079.0510
3186.9901 3197.2109 3223.0477
ZeroEnergy[kcal/mol] -93.5
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_ip37----------
Well ip37
Species
RRHO
Geometry[angstrom] 11
C -0.9025546066 -0.9512649287 0.7832056834
C -0.379309865 0.4086467803 0.5491047159
C 0.8316844634 0.2168959245 -0.2146050291
C 0.920121554 -1.2356086667 -0.5701911314
O -1.5950926647 -0.167967107 -0.1533019983
O -0.0435967943 -1.910639339 0.2699974933
H -1.4482389351 -1.3040900004 1.6510364664
H -0.5946694946 1.2749363366 1.1593202598
H 1.4951571459 0.9832371203 -0.5868685748
H 0.6714686192 -1.416383771 -1.6254228263
H 1.9025015775 -1.6803323489 -0.3765870588
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
209.7579 342.0321 448.4495
525.8981 546.3223 778.7431
795.8444 829.6185 907.4511
936.7871 956.9536 1025.7103
1032.8113 1095.8314 1102.2823
1188.3855 1221.2248 1296.5875
1324.1179 1353.2056 1403.2991
1488.0943 2981.0594 3031.5902
3173.0105 3199.8491 3232.3815
ZeroEnergy[kcal/mol] -89.9
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------w_38min----------
Well ip38min
Species
RRHO
Geometry[angstrom] 11
C -1.8370675874 -0.5484391018 0.0286483216
C -0.4212382184 -0.5911297833 0.2185562651
C 1.8571040285 0.4590931764 -0.0739459267
C 0.3912497635 0.6499472313 0.2602273605

```
O  2.3831341986   -0.605210662   -0.269800408
O  -2.466293532   0.5003459061   -0.1275060638
H  -2.3612859786   -1.521725762   0.0282639285
H  0.0812507026   -1.5460343189   0.3274326849
H  2.443193495   1.4018313938   -0.1147358566
H  0.3587331097   1.0998598769   1.268454711
H  -0.0452549816   1.4259380436   -0.3804370164
    Core                        MultiRotor
#1 2 3 4 s 11 30.
#5 1 2 3 s 11 30.
      SymmetryFactor  0.5
      InterpolationEnergyMax[kcal/mol]       100
      PotentialEnergySurface[kcal/mol]       /home/dporfirev/C4H5+O2/kin/dat/w_91_double.dat
      InternalRotation
            Group                  1 5 7 8
            Axis                   2 3
            Symmetry                  1
            MassExpansionSize            11
            GridSize                100
      End
      InternalRotation
            Group                  5
            Axis                   1 2
            Symmetry                  1
            MassExpansionSize            11
            GridSize                100
      End
    End

Frequencies[1/cm]  25
                                                                                204.8517
 343.6075            381.2557            719.8788
 741.2312            811.4428            833.8840
 887.9814            975.6214           1046.7307
1090.3443           1159.1710           1167.8372
1228.7596           1299.5965           1324.1498
1425.1600           1437.5525           1523.8956
1928.6419           3029.4089           3065.1150
3071.2804           3095.4510           3200.8769
ZeroEnergy[kcal/mol] -116.4
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!-------well_ip39------------
Well       ip39
Species
RRHO
Geometry[angstrom]   11
C  -1.8416337851   0.056628307   0.6975250212
C  -0.5917370762   -0.7817090535   0.4878879286
```

C 1.2053797457 1.0224654727 0.3533313509
C 0.5099228447 -0.1159635593 -0.3650360105
O 2.3929642167 1.06472871 0.5488356806
O -2.07832019 1.1341485295 0.2756537638
H -0.9313818816 -1.7117379001 0.0209831498
H -0.2269248404 -1.0710531277 1.4787574744
H 0.5399456088 1.8398229567 0.7023015652
H 0.053796457 0.2845504141 -1.2777869232
H 1.2677979005 -0.8502117493 -0.6460120008
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
48.7918 74.5519 156.7712
211.7195 313.9396 491.0440
625.8926 770.4676 801.0492
848.2328 958.3245 1044.5266
1076.3686 1186.3719 1231.0666
1318.5754 1331.0430 1422.1916
1444.7878 1459.3652 1814.8186
1922.7233 2899.9994 3030.6404
3045.5936 3076.0502 3098.8106
ZeroEnergy[kcal/mol] -116.7
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_ip40----------
Well ip40
Species
RRHO
Geometry[angstrom] 11
C -1.6953953859 -0.4552551436 -0.0053269881
C -0.7590161732 0.5560559464 0.0045754005
C 0.6437082805 0.5226268448 0.0167669627
C 1.5229108538 -0.6113243837 -0.0978881414
O -1.4963318264 -1.7806865709 0.03658456
O 2.7411314257 -0.540831112 -0.0408266026
H -2.7521232472 -0.2212951794 -0.0407010828
H -1.2060919038 1.5451430923 0.0192115196
H 1.1668356981 1.4694329934 0.1038986688
H -0.5550540497 -1.9826356041 0.1279327036
H 1.0592553281 -1.6121848832 -0.2781510002
Core RigidRotor
SymmetryFactor 0.5
End

#Rotor Hindered #42.5471 NO ROT
#Group 10
#Axis 1 5
#Symmetry 1

#Potential[kcal/mol] 12
#0 1.455382992 4.680719534 6.18153422 4.002946426 1.192581976 0.250376326
1.675387854 4.643633717 6.194084412 4.002256165 0.925074638
#End

Frequencies[1/cm] 27
90.7942 160.5444 213.6022
318.4548 393.1225 518.7247
551.6597 746.8661 783.1304
856.5766 941.1398 962.8762
979.6791 1101.6528 1202.6623
1254.5341 1377.7143 1381.7974
1456.9337 1500.5740 1567.8853
1661.0026 2786.5047 3155.9266
3174.2904 3204.8009 3739.7412
ZeroEnergy[kcal/mol] -116.5
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------w_45_min----------
Well ip45min
Species
RRHO
Geometry[angstrom] 11
C -1.886125 -0.027812 -1.9E-5
C -0.93303 1.055981 -3.0E-6
C 0.460762 0.922385 6.0E-6
C 1.143778 -0.26983 5.5E-5
O -1.610711 -1.225711 2.2E-5
O 2.493606 -0.25852 -2.7E-5
H -2.94788 0.29134 -6.5E-5
H -1.346804 2.058998 -6.0E-6
H 1.066422 1.824645 3.8E-5
H 2.823006 -1.162663 2.8E-5
H 0.629784 -1.222816 -1.91E-4
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 27
188.9058 194.9691 196.7045
325.9418 408.0604 443.9224
508.7803 727.1262 833.1649
864.6243 953.5339 961.6553
986.9086 1115.4414 1192.8398
1248.7234 1310.6986 1378.4470
1424.4870 1486.6836 1599.5533
1662.2719 2904.5892 3148.8868
3172.7702 3205.5738 3844.6097
ZeroEnergy[kcal/mol] -119.9
ElectronicLevels[1/cm] 1

0 2
End
End
!---------------------------------
!-------well_ip48------------
Well ip48
Species
RRHO
Geometry[angstrom] 11
C 1.4435921095 -0.4111902579 0.2131342675
C 1.2696893955 0.9638154158 0.1536322433
C -0.0289688683 1.2109772096 -0.2532911165
C -0.7241002943 -0.1049813585 -0.442364218
O 0.3206001462 -1.0891605057 -0.1253103535
O -1.8567126338 -0.3154645663 0.3468868774
H 2.2976100718 -1.0088413291 0.4906840036
H 2.0282293444 1.6935561512 0.3955187143
H -0.5102004145 2.161643642 -0.4226159719
H -1.0468843649 -0.3221231681 -1.4646921668
H -1.6553914915 0.0051127671 1.2350367204
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
157.5392 345.9479 442.9520
521.8083 544.7344 625.7365
659.6365 756.0203 815.4828
873.8974 882.9133 979.0738
1026.6705 1079.4320 1123.5775
1176.0859 1261.8420 1297.4609
1350.1127 1398.7782 1442.8096
1496.0969 3050.8561 3223.6087
3241.8494 3255.5222 3783.9804
ZeroEnergy[kcal/mol] -119.5
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------well_ip49min------------
Well ip49min
Species
RRHO
Geometry[angstrom] 11
C 1.6370225642 -0.1820218814 -0.2646377238
C 0.9318896753 1.0900018463 0.0714075452
C -0.4788938814 1.1681007217 0.0978930513
C -1.3561769043 0.1629211848 -0.0412564531
O 0.9183864594 -1.3337767233 0.1912913672
O -2.2039884303 -0.6269244314 -0.139935114
H 1.7123858363 -0.3266599898 -1.3513142297
H 1.4971093915 2.005836267 0.1809887323

H -0.9657336329 2.126321573 0.2560283616
H 2.6628916327 -0.1674216158 0.1269390068
H 0.8787032893 -1.2859339509 1.1533594562
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
94.2317 140.8555 238.5934
298.1916 382.0582 444.1084
477.7018 543.6183 681.8514
761.4980 886.6829 977.4150
994.9289 1067.4673 1160.5803
1189.7489 1357.8836 1383.3715
1398.8781 1427.3054 1495.6487
2183.8384 2979.2134 3005.5244
3155.3106 3202.3932 3802.5047
ZeroEnergy[kcal/mol] -106.5
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------well_ip52------------
Well ip52
Species
RRHO
Geometry[angstrom] 11
C 0.7662043432 0.3319931878 -0.348159005
C -0.5003888307 1.1301861564 -0.0305814727
C -1.4863897832 0.2806967455 0.2201786874
C -1.0144441844 -1.1348720272 0.0408184464
O 1.6988071337 0.585074954 0.5864194971
O 0.3287364923 -1.0212264479 -0.432497808
H 1.2131698421 0.6052066454 -1.3245915158
H -0.4984279531 2.2081563346 0.028711314
H -2.4961366175 0.5389159864 0.5132917392
H -1.0528087773 -1.6998950578 0.9819933386
H -1.6031376651 -1.6820464772 -0.7042472213
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
78.0740 255.8173 424.7914
521.9921 702.3418 737.1022
791.9039 850.1315 925.1205
950.4527 963.3601 1035.9501
1062.7063 1082.0498 1109.8380
1130.1841 1200.2253 1278.5789
1320.0737 1371.7323 1512.2013
1673.2180 2888.8278 2996.1085
3033.3561 3200.1707 3240.8819
ZeroEnergy[kcal/mol] -94.4

ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------well_ip54------------
Well ip54
Species
RRHO
Geometry[angstrom] 11
C -1.2486421015 0.154051801 0.0489173671
C -0.1857931376 1.1572428526 -0.0777870225
C 1.1186029566 0.8495694145 -0.0426273017
C 1.7617009011 -0.495501683 0.1066628637
O -2.4244350889 0.3019673462 0.0084146687
O 0.9524591379 -1.6311521732 -0.057053557
H 0.0611745206 -1.4311047718 0.2737979183
H -0.5120226218 2.191477693 -0.1799751056
H 1.8316412142 1.6696400047 -0.0989736515
H 2.57026655 -0.5647238816 -0.6310464532
H 2.2615536693 -0.4896466024 1.0935362739
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
103.3898 168.9695 191.9955
319.0366 365.7818 428.8615
488.8905 713.1766 754.9286
866.4615 957.2055 992.5958
1043.3774 1124.0935 1219.3204
1251.8445 1350.7737 1386.6266
1443.6531 1479.3757 1668.0448
1890.2917 2917.1984 3027.4701
3107.7295 3145.9203 3611.7250
ZeroEnergy[kcal/mol] -106.1
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------well_ip55------------
Well ip55
Species
RRHO
Geometry[angstrom] 11
C 1.4738646462 -0.3778459182 0.0471667143
C 0.6622299924 0.6952458125 -0.2290392453
C -0.7395641932 0.7394403522 -0.1814488816
C -1.6217727132 -0.3455652406 0.1716060484
O 2.8199396041 -0.3575700026 -0.0165885421
O -2.8408237142 -0.2437465767 0.194395362
H 1.1103475442 -1.3519043592 0.3451854217

H 1.166446866 1.6175450505 -0.5182954655
H -1.2370404836 1.6705271833 -0.4303208681
H -1.1446659452 -1.3135797042 0.4323457851
H 3.1232553965 0.5197634031 -0.2838473289
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 27
137.6939 141.2491 163.5575
333.0167 375.9490 441.8860
498.8528 716.1402 771.9234
849.5271 945.9298 990.3048
1011.7607 1151.1356 1196.1174
1284.0511 1306.0476 1368.2703
1426.3621 1481.4486 1580.3201
1667.6450 2880.4250 3107.3616
3178.7171 3215.5701 3785.4303
ZeroEnergy[kcal/mol] -117.0
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_ip57----------
Well ip57
Species
RRHO
Geometry[angstrom] 11
C -1.4699033386 -0.3708767319 -0.0323527868
C -0.7093906216 0.6604291552 -0.3115187611
C 0.8033574562 0.6935407575 -0.2338117201
C 1.4268826346 -0.6304635634 0.2163397692
O -2.1580067134 -1.2788123275 0.2123210133
O 2.7863771868 -0.6228507464 0.2931569301
H -1.2448886797 1.5511047212 -0.6218711332
H 1.2201901211 0.9537049898 -1.2126596625
H 1.0356513419 -0.9470230074 1.2049959878
H 1.1316354621 -1.4652725775 -0.4519224604
H 1.1228921506 1.4771163303 0.4615248237
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 27
24.9709 114.3900 133.9512
301.0381 403.9669 444.9545
504.1943 555.4833 713.6298
861.4554 902.3642 1047.6428
1074.1154 1135.2813 1152.4668
1277.7697 1289.8987 1360.2966
1398.0039 1421.6671 1499.3132
2210.4673 2881.7144 2889.7922
3023.7729 3054.6550 3171.2219

ZeroEnergy[kcal/mol] -89.0
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------well_ip58------------
Well ip58
Species
RRHO
Geometry[angstrom] 11
C -0.790156983 -0.0344432141 -0.0302135821
C -0.0045436256 1.2765308626 -0.0964074122
C 1.407360989 0.8371250377 -0.0189217053
C 1.4508239585 -0.6493906613 0.0856472915
O -1.9748421039 -0.1844556546 -0.0581569978
O 0.0772759059 -1.0836063247 0.0712209916
H -0.3289002956 1.9292983589 0.7254338426
H 2.2818859513 1.4702523008 -0.0340942109
H 1.9699045465 -1.1346011217 -0.7516436503
H 1.9126939189 -1.0121067585 1.0135513298
H -0.271183262 1.8063191747 -1.021095897
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 27
113.8279 172.4703 317.8671
490.5722 556.5316 666.6607
748.9471 830.2718 898.6873
944.9386 975.2154 1004.0521
1080.0958 1128.6506 1149.8581
1187.7247 1280.8068 1338.9907
1389.1923 1440.0267 1501.0372
1872.5565 2985.8135 2993.7664
3003.1616 3006.6701 3228.8641
ZeroEnergy[kcal/mol] -128.1
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------well_ip59------------
!Well ip59
!Species
!RRHO
!Geometry[angstrom] 10
!C 0.9786472844 -0.5637620664 -4.692984E-4
!C 0.1513352858 0.6696510538 5.876041E-4
!C -1.1341645053 0.326257936 -0.0012692234
!C -1.2381735439 -1.1699006119 -0.0036800097
!O 2.1678791532 -0.6940626976 5.50118E-4
!O 0.1115491199 -1.6376838649 -0.0030225788

!H 0.5915639602 1.655069861 0.0025609367
!H -1.9959213623 0.9804057594 -0.0011523098
!H -1.7515574457 -1.5572064742 0.882895663
!H -1.7497459463 -1.5544728952 -0.8924899017
!Core RigidRotor
!SymmetryFactor 1.0
!End
!Frequencies[1/cm] 24
!206.1178 349.2708 495.3627
!674.3232 695.5232 792.4523
!818.6784 871.1496 945.7783
!969.4283 1028.7098 1055.8265
!1109.3958 1141.4276 1203.3793
!1348.7949 1365.4456 1491.1856
!1659.8195 1861.8092 3028.9005
!3059.9728 3209.8465 3248.4305
!ZeroEnergy[kcal/mol] -97.7
!ElectronicLevels[1/cm] 1
!0 1
!End
!End
!----------
!-------well_ip60----------
Well ip60
Species
RRHO
Geometry[angstrom] 11
C -1.3646809917 -0.1346104134 0.2334976371
C -5.21857E-4 0.5566513163 0.2478277577
C 0.8357231488 0.2492218872 -0.953212993
C 1.7894166952 -0.4656376852 -0.0571141661
O -2.3748332861 0.4029446953 -0.1325827813
O 0.954172296 -0.1349320783 1.0919457583
H -1.3263459444 -1.1951146094 0.563026616
H -0.134210054 1.6124214985 0.5195484446
H 0.731401624 0.4139282946 -2.0143637723
H 1.8868546113 -1.5521160732 -0.1929937579
H 2.7964177579 -0.0346148323 0.034918257
Core RigidRotor
SymmetryFactor 0.5
End

Rotor Hindered #89.8043
Group 5 7
Axis 1 2
Symmetry 1
Potential[kcal/mol] 12
0 0.601091436 1.379077826 2.577621143 4.096257102 3.928963045 2.274220256
2.221948707 4.043420794 4.781121068 2.59770145 0.782755463
End

Frequencies[1/cm] 26

139.7139 195.4804
277.4316 397.5964 478.9827
860.7914 900.7388 920.5687
928.1046 982.2532 1004.9526
1029.4361 1087.9143 1108.8346
1206.6534 1254.3009 1260.2728
1327.5023 1374.7576 1495.3556
1810.9958 2891.6416 2970.6079
2995.3313 2997.2524 3243.9213
ZeroEnergy[kcal/mol] -82.9
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_ip67----------
Well ip67
Species
RRHO
Geometry[angstrom] 11
C -0.7938556228 -0.0817843352 0.0227168155
C -0.059011968 1.2450973567 -0.113875434
C 1.4137872407 -0.5881484804 -0.1625547967
C 1.419969621 0.8872431904 0.0996961466
O 0.1398435921 -1.1025620135 -0.0221119807
O -1.9606053599 -0.2984588031 0.1330273219
H -0.4656747156 1.9702993727 0.5895979878
H -0.24944086 1.6196791949 -1.1240313612
H 2.2013635098 -1.2962765356 0.0497281783
H 1.7291492776 1.1100590896 1.1321695972
H 2.100858285 1.4295259635 -0.5602804747
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 27
126.9987 243.3678 487.4718
497.7015 542.5972 673.9295
741.7409 803.4775 848.0036
946.1488 1004.4680 1023.8501
1115.0150 1139.9047 1163.6260
1222.0333 1281.9072 1323.6219
1363.2844 1461.3467 1488.2816
1884.1837 2962.9354 3055.7857
3071.3417 3125.3935 3222.7585
ZeroEnergy[kcal/mol] -129.5
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_ip68----------
Well ip68

```
Species
RRHO
Geometry[angstrom]   11
C  1.8362219687   0.3197896555   -0.0061304799
C  0.5282271724   -0.3382986155   -0.0046808796
C  -0.7026144715   0.312311081   -0.0016954685
C  -0.9360082971   1.6723800417   5.708845E-4
O  2.8566338886   -0.2893421462   -0.7545193019
O  2.8592070642   -0.2908526218   0.7375199079
H  1.8703115445   1.4070959821   -0.0050218853
H  0.5691285845   -1.4213210583   -0.0062106666
H  -1.577048024   -0.333565874   -0.0010471912
H  -0.1380375306   2.4046032827   1.60548E-4
H  -1.9477428997   2.0561512728   0.0028685326
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  27
68.4246              209.0507              213.8433
401.8202             443.2985              545.5659
570.3503             753.3732              821.4499
825.3767             828.2254              1005.0770
1028.1623            1035.3201             1140.7088
1196.3715            1243.1647             1269.4584
1353.5379            1449.7178             1498.9176
1533.1690            3127.5479             3141.6439
3154.2284            3190.3712             3243.4012
ZeroEnergy[kcal/mol] -43.9
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!-------well_ip69------------
Well       ip69
 Species
  RRHO
   Geometry[angstrom]   11
C  -0.8664418567   0.1152318417   -0.0818421848
C  -0.5723507545   1.4030555155   -0.6564318328
C  1.4339475178   -0.6410683193   -0.128841248
C  2.0071040934   0.2483408299   0.6770215228
O  0.0920459285   -0.8841389885   -0.2588237476
O  -1.9135857359   -0.1768260011   0.4443206052
H  -1.3185624611   2.176058686   -0.5405859549
H  0.3271315564   1.5954634335   -1.2225436073
H  2.0039472593   -1.3233754747   -0.7488681656
H  1.4419417989   0.8955263206   1.3358614512
H  3.0857626539   0.3243061563   0.6971001618
  Core  RigidRotor
    SymmetryFactor  0.5
  End
```

```
 Frequencies[1/cm]  27
    70.2959            140.6876            208.0378
   350.0496            420.5021            525.1306
   582.8831            640.2814            702.0757
   762.3291            829.6679            884.2546
   985.8403            991.9457           1022.2678
  1187.3340           1195.6932           1352.1457
  1434.8951           1457.2136           1674.0883
  1703.8023           3157.3926           3169.9674
  3187.2517           3247.8765           3288.1496
ZeroEnergy[kcal/mol]   -107.6
 ElectronicLevels[1/cm]       1
       0  2
 End
End
!---------------------------------
!-------well_ip94------------
Well       ip94
Species
RRHO
Geometry[angstrom]   11
C  -1.5841695769   0.2609933893   0.0955731291
C  -0.5452569845   1.1055758447   -0.0391858372
C  0.8217312887   0.7014245122   -0.3737153888
C  1.2602242925   -0.6867600239   -0.4267038798
O  -1.5730903257   -1.0748053483   -0.036342456
O  1.6557885251   -0.0487658263   0.6920879538
H  -2.5770182215   0.6275965506   0.3343849091
H  -0.7337308628   2.1606870081   0.1135929584
H  1.4505472294   1.4604832752   -0.830342835
H  -0.6506744337   -1.3616188803   -0.199953539
H  1.9468210694   -1.2389905014   -1.0664490145
Core  RigidRotor
SymmetryFactor  0.5
End

Rotor     Hindered     #111.5652
Group               4 6 9 11
Axis               2 3
Symmetry             1
Potential[kcal/mol]    12
0 1.521208748 0.800576735 1.330006576 3.235125691 4.123553769 3.513488945
3.771269885 5.125372829 6.278923708 4.846633069 1.721698062
End

Frequencies[1/cm]  26
                                        221.5435            277.7497
430.6427            471.8698            609.2110
702.1559            757.4601            780.2100
848.0883            941.6240            978.1414
988.5721           1076.4294           1128.0274
1206.5415           1272.9512           1306.6398
```

1392.5372 1440.8818 1462.1427
1685.8061 3103.4596 3135.8610
3172.8364 3195.6437 3471.8989
ZeroEnergy[kcal/mol] -74.6
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_ip86----------
Well ip86
Species
RRHO
Geometry[angstrom] 11
C 1.0174245031 0.3284400607 0.0585382168
C -0.0856447576 -0.3922968596 -0.0878409319
C -1.273599545 0.5382903332 0.021261107
C -2.1580111362 0.5903276311 -1.170186833
O 0.8300344816 1.6528891068 0.2694989987
O -0.630552237 1.8549608769 0.1822786521
H 2.0600420256 0.0405945877 0.0434728129
H -0.1514312808 -1.4545578136 -0.2538455811
H -1.8580547558 0.3471644968 0.931314284
H -1.7255580463 0.8249541947 -2.1347324949
H -3.2298962517 0.4675183854 -1.0826352306
Core RigidRotor
SymmetryFactor 0.5
End

Rotor Hindered #116.41
Group 10 11
Axis 3 4
Symmetry 1
Potential[kcal/mol] 12
0 0.240524426 0.934863787 1.348769113 1.064695521 0.278865262 0.003890559
0.082266507 0.713039147 1.364519603 1.140310427 0.404931938
End

Frequencies[1/cm] 26
54.2966 296.5648
377.4832 537.9536 560.8039
694.9995 714.1713 792.0098
818.6532 841.3086 890.1664
975.9840 1031.9502 1086.7762
1124.3936 1143.8107 1266.4760
1332.1546 1369.6742 1450.7607
1679.2250 2986.8955 3141.6062
3222.4393 3257.3606 3265.7703
ZeroEnergy[kcal/mol] -40.5
ElectronicLevels[1/cm] 1
0 2
End

```
End
!---------------------------------
!-------w_90min------------
Well       ip90min
 Species
  RRHO
   Geometry[angstrom]   11
C  -1.806606964   0.4177411979   0.065796815
C  -0.4144335676   0.7319665084   -0.0443580615
C  0.6064855573   -0.3020381711   -0.0489196467
C  1.9129206562   -0.099468355   0.6369839166
O  -2.2382384479   -0.7324871364   0.1593285687
O  1.8241740347   0.0106262128   -0.7696391664
H  -2.5006856764   1.278804914   0.0706021729
H  -0.1004301877   1.7675454292   -0.1296371477
H  0.2535344037   -1.3214788415   -0.1634938379
H  2.0991788376   0.8273393317   1.1750164837
H  2.4250223541   -0.9807690901   1.0173479033
  Core  RigidRotor
    SymmetryFactor  0.5
  End

Rotor     Hindered     # 82.2517
Group                 10 11
Axis                 3 4
Symmetry              1
Potential[kcal/mol]    12
0 1.170744642 3.835464116 5.241964111 4.786831405 3.510727903 3.295931371
5.406183371 6.874806815 7.507273731 4.278172132 1.109687959
End

  Frequencies[1/cm]  26
                                                    195.1621             234.5190
    365.6678             436.2328             684.3259
    696.9642             789.8010             868.1910
    901.3486             981.1622            1032.6594
   1088.6396            1138.2123            1166.0642
   1196.6212            1246.4513            1315.4552
   1408.7340            1460.4241            1516.2407
   1589.7337            2936.7090            3074.8109
   3157.8485            3168.5483            3176.4210
ZeroEnergy[kcal/mol]  -94.0
  ElectronicLevels[1/cm]        1
        0  2
 End
End
!---------------------------------
!-------w_91------------
Well       ip91
 Species
  RRHO
   Geometry[angstrom]   11
```

```
C   -1.658029    0.178135    0.120611
C   -0.526243    1.164370   -0.116057
C    0.895223    0.635165   -0.198035
C    1.272465   -0.747815   -0.516581
O   -1.681952   -0.997152    0.010705
O    1.322201   -0.250885    0.831471
H   -0.791583    1.688938   -1.042911
H   -0.592009    1.918334    0.674875
H    1.617825    1.418727   -0.432780
H    0.502084   -1.486778   -0.702123
H    2.241194   -0.934056   -0.974095
     Core                          MultiRotor
#1 2 3 4 s 11 30. 90.9677             149.8987
#5 1 2 3 s 11 30.
       SymmetryFactor  0.5
       InterpolationEnergyMax[kcal/mol]       100
       PotentialEnergySurface[kcal/mol]       /home/dporfirev/C4H5+O2/kin/dat/w_91_double.dat
       InternalRotation
            Group                  1 5 7 8
            Axis                  2 3
            Symmetry                 1
            MassExpansionSize           11
            GridSize                100
       End
       InternalRotation
            Group                  5
            Axis                  1 2
            Symmetry                 1
            MassExpansionSize           11
            GridSize                100
       End
     End

  Frequencies[1/cm]  25
                                                                                204.8517
 343.6075            381.2557            719.8788
 741.2312            811.4428            833.8840
 887.9814            975.6214           1046.7307
1090.3443           1159.1710           1167.8372
1228.7596           1299.5965           1324.1498
1425.1600           1437.5525           1523.8956
1928.6419           3029.4089           3065.1150
3071.2804           3095.4510           3200.8769
ZeroEnergy[kcal/mol]  -93.3
  ElectronicLevels[1/cm]       1
       0  2
 End
End
!---------------------------------
#!-------r_pyr_ip00------------
#Well       pyr_ip00
#Species
```

#RRHO
#Geometry[angstrom] 9
#C -2.2252263104 -0.1329069303 0.7036896199
#C -1.0987044023 0.3811812311 0.2578795059
#C 0.2312750848 -0.2118844585 0.4372002199
#C 1.3571224669 0.3362955855 -0.0285820036
#H -2.5539304092 -1.0012804533 1.2562522939
#H -1.1290731454 1.3234676776 -0.2923591235
#H 0.2738445866 -1.1502800974 0.9836036907
#H 2.3211869874 -0.1334313989 0.1248312137
#H 1.3475521417 1.2723418442 -0.5778084169
#Core RigidRotor
#SymmetryFactor 1.0
#End
#
#Rotor Hindered #165.1774
#Group 1 5 6
#Axis 2 3
#Symmetry 1
#Potential[kcal/mol] 12
#0 1.574421561 5.019637463 5.769072167 3.820215633 3.013175549 3.316764689
3.013175549 3.820152882 5.769009416 5.019825716 1.57435881
#End
#
#Frequencies[1/cm] 20
294.0886 487.6438
#583.3995 723.5481 833.2967
#902.5485 935.2666 937.1869
#1028.2566 1155.6660 1259.7751
#1319.2532 1440.8385 1625.9938
#1673.7751 3084.7801 3133.1800
#3147.5881 3221.3039 3232.9558
#ZeroEnergy[kcal/mol] 0.0
#ElectronicLevels[1/cm] 1
#0 2
#End
#End
#!----------
#!-------r_pyr_2_ip002----------
#Well pyr_2_ip002
#Species
#RRHO
#Geometry[angstrom] 9
#C -2.044365799 0.0263437664 -0.0147296097
#C -0.7947771933 0.4390170602 -0.008671
#C 0.3846267599 -0.424126926 -0.0029983254
#C 1.6407494182 0.0312597549 0.0030234914
#H -3.0315638702 0.4627388193 -0.0204386866
#H -0.5991807975 1.5183144943 -0.0074774447
#H 0.1951593245 -1.4936683173 -0.0039855511
#H 2.4878203197 -0.6437918585 0.0069914263
#H 1.8597468376 1.0944222067 0.0041466998

#Core RigidRotor
#SymmetryFactor 1.0
#End
#
#Rotor Hindered #178.7766
#Group 1 5 6
#Axis 2 3
#Symmetry 1
#Potential[kcal/mol] 12
#0 1.722137319 5.575046201 6.687683455 4.626000697 3.253950979 3.15982454
3.253825477 4.62549869 6.687369701 5.575861964 1.722827579
#End
#
#Frequencies[1/cm] 20
302.0737 513.8392
#564.2009 727.6085 788.0319
#862.4874 937.7054 948.7804
#1031.0575 1174.8099 1252.2328
#1317.1402 1443.7682 1631.3132
#1684.0406 3017.0190 3133.2934
#3153.7978 3221.6888 3245.6689
#ZeroEnergy[kcal/mol] -0.6
#ElectronicLevels[1/cm] 1
#0 2
#End
#End
#!----------
!----------
Bimolecular R1 #
Fragment C12H7
RRHO
Geometry[angstrom] 9
C -2.2252263104 -0.1329069303 0.7036896199
C -1.0987044023 0.3811812311 0.2578795059
C 0.2312750848 -0.2118844585 0.4372002199
C 1.3571224669 0.3362955855 -0.0285820036
H -2.5539304092 -1.0012804533 1.2562522939
H -1.1290731454 1.3234676776 -0.2923591235
H 0.2738445866 -1.1502800974 0.9836036907
H 2.3211869874 -0.1334313989 0.1248312137
H 1.3475521417 1.2723418442 -0.5778084169
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 21
165.1774 294.0886 487.6438
583.3995 723.5481 833.2967
902.5485 935.2666 937.1869
1028.2566 1155.6660 1259.7751
1319.2532 1440.8385 1625.9938
1673.7751 3084.7801 3133.1800
3147.5881 3221.3039 3232.9558

```
                ZeroEnergy[kcal/mol]       0.0
                ElectronicLevels[1/cm]     1
       0    2
         End
                Fragment       O2
     RRHO
       Geometry[angstrom]     2
O  0.000000    0.000000    0.602812
O  0.000000    0.000000   -0.602812
         Core    RigidRotor
         SymmetryFactor       2.0
   End
           Frequencies[1/cm]   1
         1641.2330
         ZeroEnergy[kcal/mol]         0.0
       ElectronicLevels[1/cm]       1
          0   3
   End
           GroundEnergy[kcal/mol]            0.0
         End
!---------------------------------
Bimolecular      R2    #
    Fragment       C12H7
      RRHO
      Geometry[angstrom]      9
C     1.897962   -0.191368   -0.000092
C     0.690235    0.331319   -0.000056
C    -0.561595   -0.422979   -0.000046
C    -1.772013    0.142834    0.000061
H     2.920223    0.155064    0.000845
H     0.591864    1.423777   -0.000241
H    -0.468457   -1.505173   -0.000037
H    -2.676027   -0.453821    0.000172
H    -1.895133    1.221313    0.000059
         Core    RigidRotor
         SymmetryFactor       1.0
   End
Frequencies[1/cm]       21
 178.7766              302.0739            513.8394
 564.2009              727.6085            788.0309
 862.4874              937.7053            948.7805
1031.0575             1174.8101           1252.2327
1317.1405             1443.7681           1631.3128
1684.0409             3017.0178           3133.2943
3153.7895             3221.6895           3245.6675
                ZeroEnergy[kcal/mol]       0.0
                ElectronicLevels[1/cm]     1
       0    2
         End
Fragment       O2
     RRHO
       Geometry[angstrom]     2
```

```
O  0.000000    0.000000    0.602812
O  0.000000    0.000000   -0.602812
        Core    RigidRotor
        SymmetryFactor       2
   End
Frequencies[1/cm]   1
        1641.2330
        ZeroEnergy[kcal/mol]         0.0
      ElectronicLevels[1/cm]       1
         0   3
   End
   GroundEnergy[kcal/mol]           -0.6
        End
!-------c3h4o_hco_p1_p1------------
Bimolecular   p1_p1
Fragment       c3h4o
RRHO
Geometry[angstrom]   8
C  1.1763676557   -0.0981958161   -1.645765E-4
C  -0.1959960028   0.443454099   -4.497526E-4
C  -1.2578324377   -0.3638529476   -2.999335E-4
O  2.1765649398   0.5801009464   -2.923127E-4
H  1.2330733712   -1.2097907518   1.874479E-4
H  -0.2869410926   1.5252128261   -7.860566E-4
H  -2.2729589485   0.0148249746   -5.061374E-4
H  -1.1384794851   -1.4437153306   3.83213E-5
Core  RigidRotor
SymmetryFactor 1.0
End

Rotor     Hindered     #172.5397
Group               4 5
Axis               1 2
Symmetry             1
Potential[kcal/mol]    12
0 1.611758382 5.889742261 8.767877746 6.080065919 2.809423185 1.619162995
2.809360434 6.079814916 8.767877746 5.890056016 1.611883884
End

Frequencies[1/cm]  17
                                          319.4489            572.3242
612.7740            919.3863            996.5738
1028.5772           1040.5710           1165.6365
1294.9244           1389.4313           1453.1973
1679.7491           1785.2486           2864.7367
3130.2858           3169.7730           3221.9437
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]       1
0  1
End
Fragment       cho
RRHO
```

Geometry[angstrom] 3
C 0.062282 0.584208 0.000000
O 0.062282 -0.589998 0.000000
H -0.871946 1.214739 0.000000
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 3
1110.5094 1941.6774 2624.3441
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] -93.7
End
!-------c4h4o_oh_p2_p2----------
Bimolecular p2_p2
Fragment c4h4o
RRHO
Geometry[angstrom] 9
C -1.0361533866 0.1017501981 0.2098777106
C -0.0550591156 -0.8114228046 0.4266843431
C 1.1162973563 -0.2992447869 -0.224221818
C 0.7503261011 0.8828997843 -0.782823445
O -0.5623059121 1.1446828759 -0.5278817088
H -2.0726957043 0.1613980545 0.4946802511
H -0.1476811598 -1.7331597425 0.9784516615
H 2.0933777947 -0.7532489221 -0.2668729699
H 1.2721110263 1.6239333434 -1.3639430247
Core RigidRotor
SymmetryFactor 2.0
End
Frequencies[1/cm] 21
615.3161 623.2143 734.2602
758.0551 850.3972 883.9850
888.4085 894.9160 1013.6374
1057.8806 1087.0920 1164.1391
1198.7056 1285.0196 1412.2878
1510.2032 1593.2377 3240.5060
3251.3305 3276.3002 3282.8111
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment oh
RRHO
Geometry[angstrom] 2
O 0.000000 0.000000 0.108324
H 0.000000 0.000000 -0.866592
Core RigidRotor
SymmetryFactor 1.0
End

Frequencies[1/cm] 1
3708.5026
ZeroEnergy[kcal/mol]   0.0
ElectronicLevels[1/cm]   1
0 1
End
GroundEnergy[kcal/mol] -89.0
End
!-------c2h3o_c2h2o_p4_p4------------
Bimolecular   p4_p4
Fragment   c2h2o
RRHO
Geometry[angstrom]   5
C   -0.102492   0.000007   -0.000105
C   1.206856   -0.000020   0.000230
O   -1.263828   0.000010   0.000017
H   1.742357   0.937839   -0.000446
H   1.742081   -0.937842   -0.000446
Core RigidRotor
SymmetryFactor 2.0
End
Frequencies[1/cm] 9
 447.1826   562.8840   596.0245
 990.8705   1171.6660   1408.2887
2233.4287   3179.5260   3272.0370
ZeroEnergy[kcal/mol]   0.0
ElectronicLevels[1/cm]   1
0 2
End
Fragment   c2h3o
RRHO
Geometry[angstrom]   6
C 0.5565205051   0.187205527   0.2064879362
C -0.6931384735   -0.3351000549   -0.2341592051
O 1.2844850258   0.8810748601   -0.506173023
H 0.859143845   -0.0596760974   1.242118135
H -1.3116801681   -0.9426707464   0.4160948835
H -1.0283947343   -0.1178534883   -1.2414717265
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 12
451.6646   505.2659   757.2087
975.1475   979.9261   1150.8545
1396.5911   1470.3489   1553.1096
2929.0559   3137.9785   3253.6926
ZeroEnergy[kcal/mol]   0.0
ElectronicLevels[1/cm]   1
0 2
End
GroundEnergy[kcal/mol] -94.9
End

```
!--------------------------------
!-------c2h3o_c2h2o_p4_d_p4_b------------
Bimolecular   p4_p4_db
Fragment      c2h2o
RRHO
Geometry[angstrom]   5
C   -0.102492    0.000007   -0.000105
C    1.206856   -0.000020    0.000230
O   -1.263828    0.000010    0.000017
H    1.742357    0.937839   -0.000446
H    1.742081   -0.937842   -0.000446
Core  RigidRotor
SymmetryFactor 2.0
End
Frequencies[1/cm]  9
 447.1826             562.8840             596.0245
 990.8705            1171.6660            1408.2887
2233.4287            3179.5260            3272.0370
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]       1
0  2
End
Fragment      c2h3o
RRHO
Geometry[angstrom]   6
C   0.594728   -0.567262   -0.160022
C  -0.795293   -0.192373    0.017763
O   0.330907    0.758032    0.031250
H   1.293050   -1.107964    0.474784
H  -1.442462   -0.110680   -0.849998
H  -1.294450   -0.287798    0.978761
Core  RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]  12
 778.9025             803.7333             938.8665
1040.8051            1071.5296            1123.3080
1179.1262            1355.6199            1523.1806
3088.7515            3121.5048            3181.3778
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]       1
0  2
End
GroundEnergy[kcal/mol] -59.4
End
!--------------------------------
!-------c4h4o2_h_p7_p7------------
Bimolecular   p7_p7
Fragment      c4h4o2
RRHO
Geometry[angstrom]   10
C  0.9786472844   -0.5637620664   -4.692984E-4
```

C 0.1513352858 0.6696510538 5.876041E-4
C -1.1341645053 0.326257936 -0.0012692234
C -1.2381735439 -1.1699006119 -0.0036800097
O 2.1678791532 -0.6940626976 5.50118E-4
O 0.1115491199 -1.6376838649 -0.0030225788
H 0.5915639602 1.655069861 0.0025609367
H -1.9959213623 0.9804057594 -0.0011523098
H -1.7515574457 -1.5572064742 0.882895663
H -1.7497459463 -1.5544728952 -0.8924899017
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 24
206.1178 349.2708 495.3627
674.3232 695.5232 792.4523
818.6784 871.1496 945.7783
969.4283 1028.7098 1055.8265
1109.3958 1141.4276 1203.3793
1348.7949 1365.4456 1491.1856
1659.8195 1861.8092 3028.9005
3059.9728 3209.8465 3248.4305
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -97.7
End
!-------c4h5o_o_p8_p8----------w_78
Bimolecular p8_p8
Fragment c4h5o
RRHO
Geometry[angstrom] 10
C -1.7076025385 0.6980471378 0.0478915551
C -0.2851740289 0.5771162743 -0.208766572
C 0.443667883 -0.5621350266 0.1620802819
C 1.7829482561 -0.722739371 -0.0577921128
O -2.3825551767 -0.161058719 0.598313032
H -2.1746257054 1.6439363307 -0.2917108791
H 0.2153642787 1.4043019912 -0.7045820222
H -0.1185742673 -1.35099704 0.6536366567
H 2.3013632403 -1.6230112193 0.2478164764
H 2.3711010587 0.0470556418 -0.546109416
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 24

179.6211 211.7697 271.7239
399.1604 592.0505 751.6503
770.9809 897.6207 922.5424
1003.7469 1038.2769 1057.2528
1213.2861 1285.0173 1350.4177
1418.7240 1472.5911 1536.9545
1671.6960 2912.8662 3137.3301
3154.4099 3163.6807 3233.2056
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment O
Atom
Mass[amu] 16
ElectronicLevels[1/cm] 3
0 5
158.226 3
226.977 1
End
GroundEnergy[kcal/mol] -18.1
End
!-------c4h5o_o_p9_p9----------w_80
Bimolecular p9_p9
Fragment c4h5o
RRHO
Geometry[angstrom] 10
C -1.7660212088 0.4511616452 0.1485942598
C -0.5262921614 -0.283032754 0.2719444163
C 0.6890131261 0.2127286116 -0.2095021744
C 1.889101464 -0.4433250247 -0.1166510588
O -2.8434448382 0.048407224 0.5585886505
H -1.6843072549 1.4374026888 -0.3573619275
H -0.576246353 -1.2511883098 0.7617961249
H 0.6714522504 1.1892652971 -0.6904757802
H 1.960035403 -1.4180474939 0.3531390157
H 2.8016835728 -0.0116228843 -0.5076835263
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 24
147.5053 212.0753 274.1008
468.6102 543.1241 571.5935
819.8044 883.4067 971.2678
991.1643 1021.4055 1149.9104
1226.0426 1284.4263 1289.4898
1417.1920 1488.6333 1528.8451
1672.2147 2879.0023 3128.6752
3142.0369 3165.6147 3237.7196
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2

```
End
   Fragment       O
    Atom
      Mass[amu]   16
      ElectronicLevels[1/cm]       3
         0   5
                          158.226 3
                          226.977 1
   End
GroundEnergy[kcal/mol] -18.9
End
!-------c4h4o2_h_p10_p10------------
Bimolecular   p10_p10
Fragment       c4h4o2
RRHO
Geometry[angstrom]   10
C   0.827587    0.012751    0.000002
C  -0.118546    1.211943    0.000003
C  -1.470998    0.561488   -0.000003
C  -1.284852   -0.754423   -0.000001
O   2.017527   -0.029159   -0.000004
O   0.047737   -1.139164    0.000003
H   0.083391    1.831596    0.879417
H   0.083395    1.831596   -0.879411
H  -2.423116    1.068049   -0.000003
H  -1.984928   -1.575206   -0.000003
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  24
 173.4739            442.6021            492.0179
 570.2659            675.3343            728.0001
 808.3073            841.7840            921.5186
 963.6092            984.5072           1050.7428
1096.8321           1163.8206           1171.8453
1281.5712           1365.7881           1441.0665
1672.6363           1893.3053           3044.2510
3072.7294           3237.6896           3261.6336
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]       1
0  1
End
   Fragment       H
    Atom
      Mass[amu]   1
      ElectronicLevels[1/cm]       1
         0   2
   End
GroundEnergy[kcal/mol] -95.5
End
!--------------------------
!-------c3h5o_co_p12_p12------------
```

```
Bimolecular   p12_p12
Fragment      c3h5o
RRHO
Geometry[angstrom]   9
C        -1.458497   -0.565979    0.000023
C         0.862447    0.434082    0.000039
C        -0.634367    0.667006   -0.000058
O         1.392035   -0.646478   -0.000021
H        -0.977817   -1.534018   -0.000051
H        -2.538385   -0.505015    0.000200
H         1.471152    1.365169    0.000218
H        -0.854380    1.317584    0.864764
H        -0.854345    1.317449   -0.864985
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  21
 149.9839            180.5070            278.4098
 465.1656            663.5154            686.5566
 856.8022            996.4629           1004.1273
1116.7364           1198.4995           1356.2702
1408.2621           1417.3505           1448.9868
1818.6188           2869.8261           2944.8794
2945.9457           3157.3246           3268.9028
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]       1
0  2
End
         Fragment       CO
     RRHO
       Geometry[angstrom]     2
C   0.000000    0.000000   -0.643954
O   0.000000    0.000000    0.482966
         Core    RigidRotor
         SymmetryFactor       1.0
   End

   Frequencies[1/cm]   1
         2220.1208
         ZeroEnergy[kcal/mol]         0.0
      ElectronicLevels[1/cm]       1
         0   1
   End
GroundEnergy[kcal/mol] -110.4
End
!---------------------------
!-------ts_ts01d------------
Barrier     ts01d  ip01  p9_p9
RRHO
Geometry[angstrom]   11
C  -1.1580217625   0.6734058137   5.314521E-4
C  0.2084853914   0.4982954657   -0.1894793279
```

C 1.0383956424 1.4661030061 -0.8202485663
C 2.3759246094 1.3264721793 -0.9705215503
O -1.8466705622 -0.146296188 0.6968587184
O -2.9096242649 -1.1171242403 -0.4189996622
H -1.6543675756 1.5540327844 -0.4248570719
H 0.6507669509 -0.4106289566 0.2082899129
H 0.5547193348 2.3606137341 -1.2059026977
H 2.8968067721 0.4524667172 -0.5944857493
H 2.9712774641 2.0782656844 -1.4734254579
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 507.2889
WellDepth[kcal/mol] 29.2
WellDepth[kcal/mol] 3.5
End
Frequencies[1/cm] 26
60.2758 135.6569
198.7856 224.8952 336.8844
481.3957 528.4094 635.6688
894.1256 939.5360 957.3444
971.8678 1025.8359 1177.0651
1247.0655 1291.1662 1309.7220
1325.4406 1448.6238 1499.1799
1598.7222 3038.8140 3138.5463
3143.4915 3166.5582 3234.6621
ZeroEnergy[kcal/mol] -21.1
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts02a------------
Barrier ts02a ip01 ip02
RRHO
Geometry[angstrom] 11
C 1.5566185233 0.3380801247 -0.0917391183
C 0.3473649788 -0.2946632425 -0.028021244
C -0.8948264125 0.4010125321 0.1328997892
C -2.095760467 -0.2076494897 0.1683526442
O 2.6939833996 -0.3807232293 -0.3428075999
O 2.8038536725 -0.4299346405 1.0921758085
H 1.678584424 1.414184284 -0.0148100359
H 0.3459159801 -1.3756792676 -0.1237254004
H -0.8473192679 1.4828458247 0.2330328019
H -3.0117287758 0.3547395376 0.2992792344
H -2.1866340551 -1.2841104335 0.0695531204
Core RigidRotor
SymmetryFactor 0.5
End

Tunneling Eckart

ImaginaryFrequency[1/cm] 637.4736
WellDepth[kcal/mol] 22.5
WellDepth[kcal/mol] 23.6
End

#Rotor Hindered #165.1774
#Group 4 9 10 11
#Axis 2 3
#Symmetry 1
#Potential[kcal/mol] 12
#0 2.208833757 7.53011508 10.07152892 6.76455338 4.003511184 3.514053704 3.783882828 6.331571763 9.7954247 7.793669108 2.246484332
#End

Frequencies[1/cm] 25
165.1774 194.0766
227.0763 256.6645 470.9910
505.1503 645.7825 804.3735
859.4644 910.4696 942.4562
969.1485 1025.0431 1174.8483
1207.7113 1265.9344 1302.2969
1325.8660 1445.2768 1517.3787
1620.3123 3137.9646 3143.2089
3166.1769 3177.0307 3232.8290
ZeroEnergy[kcal/mol] -22.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts02ab----------
Barrier ts02ab ip01 ip68
RRHO
Geometry[angstrom] 11
C 1.8004529972 0.2719931067 -0.1961067642
C 0.5377759912 -0.246107245 -0.1841009602
C -0.6849705878 0.4928269312 0.0271313153
C -0.8272612305 1.830645628 0.0692944013
O 2.8571979861 -0.5401512686 -0.5155969844
O 2.970388724 -0.7202906567 0.9055513024
H 2.0461152836 1.3126290016 -0.015056011
H 0.4665101 -1.3157177857 -0.3482323705
H -1.5750467033 -0.1171580159 0.1533355191
H -1.7953521791 2.279498031 0.2531453116
H 0.0012916186 2.5124942734 -0.0852597593
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 657.8187
WellDepth[kcal/mol] 24.9
WellDepth[kcal/mol] 24.2
End

Frequencies[1/cm] 26
67.4949 170.7502
202.2934 261.4450 425.2576
595.4216 628.8448 798.7338
854.4311 922.4985 936.1754
1008.0974 1024.0270 1057.3918
1198.2134 1282.5874 1322.5465
1333.3912 1453.0056 1503.7310
1639.9346 3143.8274 3150.0951
3177.8058 3184.4043 3231.7701
ZeroEnergy[kcal/mol] -19.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts02b----------
Barrier ts02b ip02 ip06
RRHO
Geometry[angstrom] 11
C -1.5725602354 0.4749256721 0.0771942889
C -0.4049395207 -0.228335423 0.1949647926
C -0.3017879347 -1.5387543446 0.7702816451
C 0.8666812871 -2.1909366163 0.9103649697
O -2.7499946086 -0.0276272871 0.566978597
O -2.9648123501 -0.4728669283 -0.7874126464
H -1.6230560917 1.4731815254 -0.3426352288
H 0.5020480205 0.2565057625 -0.1543827606
H -1.2276410576 -2.0030015923 1.0918688617
H 1.8064941519 -1.747471698 0.597669552
H 0.9111673392 -3.1839760704 1.3400659286
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 640.187
WellDepth[kcal/mol] 23.1
WellDepth[kcal/mol] 21.8
End

#Rotor Hindered #116.0919
#Group 4 9 10 11
#Axis 2 3
#Symmetry 1
#Potential[kcal/mol] 12
#0 2.215108853 7.781118916 10.78061476 7.228910477 4.267065212 3.896834554
4.336091267 7.034382504 10.7115887 8.076048423 2.284134908
#End

Frequencies[1/cm] 26
116.0919 169.7073
226.5310 317.6988 399.8164
654.8671 703.7163 795.3327

814.7546 921.8286 934.2404
949.4706 1031.2888 1063.4244
1209.0771 1240.7671 1309.0366
1382.0319 1441.4269 1525.9266
1628.6170 3137.3130 3157.2139
3180.2118 3187.1462 3229.9748
ZeroEnergy[kcal/mol] -22.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts02bb----------
Barrier ts02bb ip68 ip06
RRHO
Geometry[angstrom] 11
C 1.6361697053 0.4660496021 -0.1581763763
C 0.2815109174 0.4384464875 0.0209372289
C -0.6304105146 -0.6776946694 -0.0722909841
C -0.3633557699 -1.9211041554 -0.5148571986
O 2.3639721227 -0.6496895352 -0.4833463021
O 2.7073882446 -0.6911862358 0.9153913843
H 2.2032717428 1.3888462397 -0.1038286755
H -0.1631249745 1.4026060977 0.2499999131
H -1.6455037484 -0.4572577502 0.2472132013
H -1.1410785935 -2.675687562 -0.5208762715
H 0.618121868 -2.2033345188 -0.8696609196
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 765.3063
WellDepth[kcal/mol] 24.6
WellDepth[kcal/mol] 25.1
End
Frequencies[1/cm] 26
88.2260 141.3932
234.3096 363.8964 398.6385
617.0479 751.7276 771.9543
807.4551 911.6640 931.3799
969.1101 1022.0173 1093.3076
1114.0079 1260.9750 1339.0733
1381.7922 1459.8631 1504.8068
1637.1717 3139.3925 3153.7714
3159.5550 3180.9127 3254.6297
ZeroEnergy[kcal/mol] -19.3
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts02c----------
Barrier ts02c ip19min ip04b
RRHO

Geometry[angstrom] 11
C -1.6545041424 0.1851767506 0.6412537616
C -0.5053341163 0.2048595679 -0.61278126
C 0.7859821362 -0.383397765 -0.2274147785
C 1.7072675622 0.2903491355 0.4722126885
O -2.8055311833 -0.0338840012 0.4111553528
O -0.8236682518 1.4545260436 -0.2839389582
H -1.1309976215 0.2453352731 1.5967756898
H -0.9852134385 -0.22759641 -1.4972313148
H 0.95683541 -1.4095711834 -0.5404114552
H 2.6527072166 -0.1604079486 0.7481418194
H 1.5339724289 1.3211055375 0.7594104545
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 395.5729
WellDepth[kcal/mol] 4.7
WellDepth[kcal/mol] 38.9
End

Rotor Hindered #117.8985
Group 4 9 10 11
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 2.019388612 7.328433498 7.446593554 6.047058915 3.829251771 1.475275046
1.440385513 4.412396433 7.904236298 5.756584726 1.694401395
End

Frequencies[1/cm] 25
217.9387
272.9802 333.2148 396.2663
572.3071 656.3515 702.7902
888.9435 945.2643 976.0651
1006.4150 1027.0077 1056.7199
1247.3925 1287.7412 1321.5483
1424.4976 1430.5066 1634.7068
1703.4354 3043.1891 3095.1929
3144.2099 3158.6156 3237.9913
ZeroEnergy[kcal/mol] -82.3
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts04gmin----------
Barrier ts04gmin ip19min ip04
RRHO
Geometry[angstrom] 11
C -1.1269396144 -0.1700934599 0.5037563292
C 0.0589469638 -0.0216003727 -0.7067773058
C 1.3522446575 -0.6103271119 -0.3288661904

C 2.2345432789 0.0243511811 0.4527532932
O -2.2645565479 -0.3954794295 0.2195404998
O -0.3004662186 1.1893900545 -0.2879323546
H -0.6343527209 -0.1765326082 1.4774162443
H -0.3828656701 -0.3907624676 -1.6384855513
H 1.5581919986 -1.6032865435 -0.7184796536
H 3.1821445052 -0.4260681786 0.7217229712
H 2.0266333679 1.0239109361 0.8169237181
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 395.4736
WellDepth[kcal/mol] 4.7
WellDepth[kcal/mol] 38.4
End

Rotor Hindered #117.8900
Group 4 9 10 11
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 2.02058088 7.329312011 7.446217048 6.046556907 3.82849876 1.474835789 1.44082477
4.41352595 7.904612803 5.755392458 1.693522882
End

Frequencies[1/cm] 25
217.9445
273.0034 333.2248 396.2289
572.3002 656.3508 702.7689
888.9192 945.2934 976.0412
1006.4042 1026.9941 1056.7165
1247.3807 1287.7294 1321.5379
1424.5020 1430.4771 1634.6918
1703.5725 3043.1665 3095.2058
3144.2249 3158.6518 3238.0287
ZeroEnergy[kcal/mol] -82.3
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts04i------------
Barrier ts04i ip04 ip04b
RRHO
Geometry[angstrom] 11
C 2.5540337836 0.3120426383 0.0393532871
C 0.2634864702 -0.1878107692 -0.1950769242
C -1.1021693099 0.3429390242 -0.118505039
C -1.8442479231 0.6487327857 -1.1803471917
O 2.893446938 -0.8312176428 0.135300873
O 1.274052557 0.749893563 -0.11463958
H 3.2138240137 1.1878653616 0.0593374559

H 0.5444840442 -1.2043673471 0.0461995228
H -1.5264268796 0.4801543671 0.8794598643
H -2.8523664385 1.0332040321 -1.0709906834
H -1.4676132556 0.5223239872 -2.1895795848
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 207.8306
WellDepth[kcal/mol] 14.6
WellDepth[kcal/mol] 15.1
End
Frequencies[1/cm] 26
67.1577 206.2883
295.5029 309.7088 400.7017
535.2538 665.4103 785.0458
975.1367 981.7460 999.0828
1006.1560 1033.5092 1115.4016
1166.0268 1315.4849 1361.5326
1401.6342 1451.6339 1690.7043
1804.0934 3059.8469 3061.8504
3134.3467 3203.4263 3220.5805
ZeroEnergy[kcal/mol] -106.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts06a----------
Barrier ts06a ip01 ip06
RRHO
Geometry[angstrom] 11
C 1.2168993986 0.2926953411 0.0351199597
C -0.0975854693 -0.3523947873 0.0019883006
C -1.294184768 0.353223838 0.0046098459
C -2.5428287466 -0.2340591106 -0.0057566117
O 1.8039229034 0.5551245972 -1.0563766314
O 3.0265201024 1.1320734612 -1.0244232934
H 1.7621495533 0.554383849 0.9428364419
H -0.1154780003 -1.4409329617 4.947456E-4
H -1.2386516492 1.4390275079 0.0091116305
H -3.4441066951 0.3645096634 -0.0099920363
H -2.6562066294 -1.3122223982 -0.0157513513
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 337.6075
WellDepth[kcal/mol] 29.0
WellDepth[kcal/mol] 28.8
End
Frequencies[1/cm] 26
123.6001 147.5029

344.1247 369.6512 413.8534
525.2490 633.9521 708.0474
834.0264 882.3991 952.3573
981.7526 999.5736 1102.5914
1201.9572 1275.7601 1302.4682
1341.9219 1466.5982 1491.9282
1516.9122 3111.7262 3120.9809
3144.0717 3145.8551 3243.7521
ZeroEnergy[kcal/mol] -15.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts06b----------
Barrier ts06b ip06 ip07b
RRHO
Geometry[angstrom] 11
C 1.703236021 0.527953212 -0.0641556193
C 0.5547295581 -0.3196263488 -0.1222231671
C 0.190691652 -1.108454339 -1.2997455033
C -1.0639842276 -1.4987077381 -1.5402870617
O 2.7441644559 -0.2890526439 0.0039075503
O 1.9490517196 -1.4756137817 0.4321212032
H 1.8081052784 1.5552923718 0.2638126921
H -0.2937247122 -0.0602673657 0.5149465949
H 0.9927323369 -1.3424495294 -1.9903851418
H -1.873104616 -1.2704476282 -0.8539572715
H -1.3191564662 -2.0616072091 -2.4297422758
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 649.1911
WellDepth[kcal/mol] 38.7
WellDepth[kcal/mol] 18.7
End

Rotor Hindered #141.7383
Group 4 9 10 11
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 2.216301121 6.668042405 5.997422906 3.484246998 4.154615493 5.322097086
5.228598157 6.157375101 8.149906302 7.892501868 2.452056474
End

Frequencies[1/cm] 25
172.3341
318.8355 332.0093 421.5613
597.6599 674.9573 748.2279
807.1847 918.5497 944.7044
982.2914 1032.4115 1103.9421

1180.4651 1210.3416 1313.3811
1365.1719 1413.4360 1468.5726
1671.9483 3083.9188 3135.5133
3179.9670 3180.6969 3225.6294
ZeroEnergy[kcal/mol] -5.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_06d----------
Barrier ts06d ip06 p8_p8
RRHO
Geometry[angstrom] 11
C -1.1767402457 0.5765602462 0.6042634528
C 0.1187574623 0.614362124 0.0905826908
C 0.9515758058 -0.5353976207 -0.0282538156
C 2.2130733771 -0.4898555676 -0.5108469147
O -1.6815815112 -0.4861742001 1.1061093014
O -2.8222717558 -1.2420511588 -0.0926893799
H -1.7776422699 1.4917307773 0.6037847882
H 0.5148926792 1.5797021113 -0.2127387381
H 0.5206102993 -1.4810681912 0.2834076764
H 2.8153742944 -1.3851610087 -0.6038061106
H 2.6670998644 0.4447434883 -0.8238619507
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 508.0528
WellDepth[kcal/mol] 29.1
WellDepth[kcal/mol] 2.8
End
Frequencies[1/cm] 26
48.5368 161.6563
207.8369 220.9490 374.4600
404.3878 653.8453 728.5936
843.8552 939.6512 946.0926
982.1627 1041.3971 1105.5136
1205.7476 1263.1831 1308.5661
1395.2691 1446.3909 1514.9216
1607.1125 3058.3292 3137.1896
3157.7536 3176.4128 3231.1583
ZeroEnergy[kcal/mol] -20.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts07a----------
Barrier ts07a ip01 ip07
RRHO
Geometry[angstrom] 11
C -1.4874308458 0.6994223134 0.3577997392

C -0.4131577047 -0.2313058226 0.1984910375
C 0.9430735464 0.1954373016 -0.1266651214
C 1.9970622763 -0.6261081031 -0.0578756958
O -2.4973467882 0.1272982461 -0.2890805555
O -1.6421955855 -0.8500398734 -1.0088624987
H -1.5070134363 1.7613743317 0.5670796764
H -0.482422743 -1.1843950276 0.721048002
H 1.0690563961 1.2129899559 -0.4859341745
H 2.9924686791 -0.299180171 -0.3336526768
H 1.8895182058 -1.656106151 0.2666832676
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 599.4113
WellDepth[kcal/mol] 35.3
WellDepth[kcal/mol] 15.0
End

Rotor Hindered #110.9720
Group 4 9 10 11
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 1.376505037 4.330192677 5.453183839 2.962723778 0.805973317 1.257842973
3.415032691 5.484182813 6.652480167 4.685865112 1.423254501
End

Frequencies[1/cm] 25
201.3432
303.5060 346.4771 446.5954
539.3197 674.2932 734.9595
798.9946 925.9125 975.3162
1007.0699 1043.3404 1146.1498
1165.2854 1230.3271 1290.7113
1324.8039 1424.3826 1483.8293
1668.2861 3092.7851 3137.5434
3151.8299 3193.5375 3227.7788
ZeroEnergy[kcal/mol] -9.3
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts07ba----------
Barrier ts07ba ip07 ip07b
RRHO
Geometry[angstrom] 11
C 1.7563898583 0.5382647488 -0.0026757902
C 0.6672142108 -0.367900613 0.4304075249
C -0.5737569381 -0.4737278803 -0.3956354038
C -1.7977844093 -0.4110903418 0.1208126519
O 2.6538470495 -0.4831178327 -0.2301644071

O 1.6220714024 -1.4713053641 0.153532111
H 1.9899990117 1.5748962283 -0.1673050373
H 0.4225855479 -0.356585345 1.5016240807
H -0.4158555047 -0.5834768338 -1.4645691105
H -1.9569206535 -0.3034711391 1.189515273
H -2.6829845751 -0.4600986274 -0.5024398926
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 494.4793
WellDepth[kcal/mol] 0.7
WellDepth[kcal/mol] 0.8
End

Rotor Hindered #103.6430
Group 4 9 10 11
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 1.282880606 3.628072197 2.972889434 2.101153111 2.698228486 3.119914931
1.976027699 1.683419977 3.479540677 3.594876939 1.125312948
End

Frequencies[1/cm] 25
162.2734
316.7138 356.9512 459.3417
674.3501 843.1866 868.5472
893.7129 948.3053 972.1094
1024.9149 1038.4900 1137.3119
1169.1662 1216.9956 1298.8528
1318.7371 1351.8787 1453.5405
1696.5794 2979.5465 3130.8579
3159.1740 3218.2803 3287.3489
ZeroEnergy[kcal/mol] -23.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts10a----------
Barrier ts10a ip06 ip10min2
RRHO
Geometry[angstrom] 11
C 0.7363494832 0.4725270928 -0.1127847748
C -0.5508557573 0.8318432441 0.085843055
C -1.7410970169 -8.0773E-5 0.0562386555
C -1.77562949 -1.3071135514 -0.1859767163
O 1.283643036 -0.7570087083 -0.2186347854
O 0.6186950544 -1.7683108947 0.5192053886
H 1.5110809117 1.214854786 -0.2760996493
H -0.7152996186 1.9004230826 0.1599266225
H -2.6858972269 0.526003155 0.2160157573

H -0.4122338624 -1.7837865431 0.1760682586
H -2.5738565133 -1.9791548901 -0.4703408117
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 878.2442
WellDepth[kcal/mol] 30.8
WellDepth[kcal/mol] 6.4
End
Frequencies[1/cm] 26
173.1944 210.1966
335.7808 425.7485 515.3971
615.4099 693.5884 763.0779
799.9829 878.2930 905.0013
923.8329 936.1807 949.5597
1110.3566 1163.5324 1290.9791
1339.0238 1437.6145 1520.3733
1596.9879 1649.7055 3064.2050
3169.2131 3188.0838 3217.8790
ZeroEnergy[kcal/mol] -13.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts10b----------
Barrier ts10b ip10min2 p2_p2
RRHO
Geometry[angstrom] 11
C 0.3244361187 0.9179515555 0.013409675
C -0.9856488585 1.196225754 0.127861184
C -1.8828143961 0.0532699819 0.1611115856
C -1.3671530955 -1.1467665922 -0.0029756374
O 0.7090436478 -0.3815149504 -0.0775835188
O 2.3129722725 -0.3386736881 0.1162026563
H 1.1293860486 1.6369439047 -0.0290835645
H -1.3371338185 2.2171256219 0.1786603219
H -2.9498516964 0.2035750502 0.3374764005
H 2.5027719495 -1.0737985702 -0.4841934227
H -1.5763511721 -2.2011430673 -0.01100768
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 687.5154
WellDepth[kcal/mol] 9.2
WellDepth[kcal/mol] 78.2
End

Rotor Hindered #157.4745
Group 10
Axis 5 6

Symmetry 1
Potential[kcal/mol] 12
0 0.116779535 0.015311234 0.172565137 0.982680018 2.549634215 5.048251901
7.335022348 5.762985324 3.149784387 1.306349464 0.333897853
End

Frequencies[1/cm] 25
73.2904
250.4948 320.4623 377.3987
488.8484 531.9971 586.9427
695.7225 719.1278 837.7540
875.9241 897.9705 1002.5638
1042.9054 1187.9078 1218.5969
1232.0199 1379.9160 1580.5887
1650.6868 3073.6615 3210.4215
3234.8991 3299.7818 3787.8175
ZeroEnergy[kcal/mol] -10.8
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts10d----------
Barrier ts10d ip10min2 ip32
RRHO
Geometry[angstrom] 11
C 1.2781489984 0.7566843972 0.3760230463
C -0.019667267 0.9569757161 0.6729646507
C -1.1766973182 0.0505207223 0.6233902357
C -1.2444214412 -1.2099474267 0.2510150395
O 1.9414730981 -0.3191620688 -0.07705711
O 0.8719738757 -1.4889704491 -0.168556307
H 1.9948344943 1.5665116714 0.4947724458
H -0.2403021994 1.9603410742 1.0176151134
H -2.1104143738 0.5170928212 0.9496240151
H -1.995420715 -1.984132052 0.2167647745
H 0.7784718482 -1.5092354059 -1.1339809041
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 789.5021
WellDepth[kcal/mol] 13.1
WellDepth[kcal/mol] 122.0
End
Frequencies[1/cm] 26
123.2542 191.0629
332.3705 380.9464 427.0260
475.6496 510.9488 618.9197
756.3409 775.0296 869.1086
882.3935 918.9190 921.2175
1082.2633 1192.2389 1264.9337
1283.0339 1419.5078 1626.6226

1663.6843 3056.6368 3146.8604
3180.3821 3243.1757 3758.1012
ZeroEnergy[kcal/mol] -6.9
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts12a----------
Barrier ts12a ip06 ip12_oh
RRHO
Geometry[angstrom] 11
C -1.0755815779 0.5210231813 0.0270540735
C 0.2626850014 0.7464290986 -0.0673449321
C 1.1769074877 -0.3369743047 -0.1229877971
C 2.4878845115 -0.4938655166 0.0231773604
O -1.6691941608 -0.6735014628 0.0348659854
O -0.802590577 -1.7808360555 0.1982912573
H -1.8267626677 1.3015266721 0.0051864124
H 0.5865225594 1.7695082919 -0.2420790527
H 0.26910374 -1.3539892524 -0.0961595058
H 2.9939304118 -1.4035876236 -0.2813108268
H 3.1031842718 0.2660559717 0.5051880254
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1584.6495
WellDepth[kcal/mol] 27.1
WellDepth[kcal/mol] 47.1
End
Frequencies[1/cm] 26
154.8708 231.4165
302.1315 439.0260 474.6215
562.2158 628.3419 765.1532
840.4308 889.7910 891.5045
922.4965 948.3000 985.4248
1057.0130 1161.8408 1254.0723
1380.1855 1444.6730 1546.8164
1651.2260 1708.9507 3084.8068
3135.3909 3184.6693 3205.8277
ZeroEnergy[kcal/mol] -17.3
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts12c----------
Barrier ts12c ip12_oh p2_p2
RRHO
Geometry[angstrom] 11
C 0.1628827673 0.7297249905 0.0825041797
C -1.2469243871 1.047649139 0.0719535877
C -2.1007270308 0.0076934057 -0.0649473682

C -2.5205887493 -1.1914727067 -0.3957960423
O 0.6184235382 -0.4062372401 -0.0091372204
O 3.3193838104 0.2987429846 0.1208459633
H 0.8469935579 1.5913575402 0.1759560123
H -1.5883617169 2.0667348582 0.1717204516
H -3.2718258829 0.1168713097 -0.1953780361
H -2.9235441411 -1.904894797 0.3236954227
H 2.4590562342 -0.1798104841 0.0484000497
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 433.577
WellDepth[kcal/mol] 59.8
WellDepth[kcal/mol] 84.4
End
Frequencies[1/cm] 26
50.6714 71.1300
143.6365 249.5574 259.9396
412.4350 497.7486 514.0689
565.5166 691.0352 733.0454
746.7617 861.8106 963.0384
1001.3317 1040.1887 1112.8385
1397.3116 1422.0189 1674.5857
1833.1554 2502.2352 2964.6135
3142.3964 3230.2694 3482.0642
ZeroEnergy[kcal/mol] -4.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts13b2----------
Barrier ts13b2 ip19min ip15min
RRHO
Geometry[angstrom] 11
C 1.476019 0.039262 0.295370
C 0.125694 0.180385 -0.380293
C -1.038822 -0.264882 0.441538
C -2.224211 -0.703425 -0.114281
O -0.564535 1.347089 -0.100736
O 2.388103 -0.592065 -0.166452
H 1.548668 0.580494 1.264137
H 0.151616 -0.150323 -1.423128
H -0.902047 -0.260849 1.515135
H -3.047339 -1.018447 0.514077
H -2.371515 -0.699106 -1.186731
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 500.3515
WellDepth[kcal/mol] 5.9

WellDepth[kcal/mol] 7.3
End

Rotor Hindered #91.5451
Group 6
Axis 1 2
Symmetry 1
Potential[kcal/mol] 12
0 2.195467803 5.861065073 6.084772241 3.64990953 2.136983909 2.067204842 2.950299088
3.873742201 4.056410243 2.160892024 0.226468211
End

Frequencies[1/cm] 25
208.0856
253.4122 368.8652 431.8990
493.2919 521.0576 798.9710
861.9155 950.4948 997.4509
1060.6550 1085.3468 1175.9068
1204.5764 1263.8234 1297.0344
1385.0198 1416.6077 1503.7227
1819.4416 2883.8270 3051.3172
3150.2846 3195.0852 3251.1038
ZeroEnergy[kcal/mol] -81.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts13c----------
Barrier ts13c ip15min ip16
RRHO
Geometry[angstrom] 11
C -1.5519247172 0.1760916643 0.4962483521
C -0.2263881659 0.7403282676 0.2745013226
C 1.005786885 -0.4573038247 -0.1333294545
C 2.286775559 -0.3246026767 0.3563458092
O 0.4285459025 0.5379970457 -0.9349950562
O -2.0720850906 -0.6617631365 -0.2166170645
H -2.0509587769 0.5579468191 1.4111236691
H 0.135554147 1.5571730392 0.8921823151
H 0.4908899541 -1.4124302132 -0.167431732
H 2.7489122204 -1.1432646859 0.8911537853
H 2.8320490827 0.6033127012 0.2409370538
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 593.7641
WellDepth[kcal/mol] 8.4
WellDepth[kcal/mol] 21.5
End
Frequencies[1/cm] 26
125.6895 203.1022

265.0275 332.3573 480.4810
535.5718 773.0672 784.1824
809.8900 887.0270 930.8677
970.6477 1007.9053 1099.2387
1204.0264 1255.4354 1364.3199
1402.8473 1408.5328 1494.9407
1707.2824 2896.7138 3153.4241
3154.7247 3162.1630 3260.4830
ZeroEnergy[kcal/mol] -80.0
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts15a------------
Barrier ts15a ip07b ip19min
RRHO
Geometry[angstrom] 11
C 1.8236119665 -0.0035739576 0.2565725181
C 0.4993412729 -0.5121059966 -0.1959430109
C -0.5958638829 0.4475733854 -0.5307415738
C -1.8409908346 0.3235808 -0.0807074993
O 1.1626310752 -0.9935612399 -1.4386960033
O 2.4794390886 -0.2800306697 -0.8705716123
H 2.3144969495 -0.0840788946 1.2215491714
H 0.1161063141 -1.3493568644 0.4003460173
H -0.3070347365 1.2756566229 -1.1712940653
H -2.6100818393 1.0451303785 -0.3299704816
H -2.1354713734 -0.505025564 0.5561035397
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1345.4159
WellDepth[kcal/mol] 4.3
WellDepth[kcal/mol] 66.9
End

Rotor Hindered #114.8931
Group 4 9 10 11
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 1.377509052 3.651039047 2.71090418 1.940887162 3.170366702 3.775411448 1.962598994
1.469564709 3.499244478 4.301201734 1.40091516
End

Frequencies[1/cm] 25
153.9240
313.8125 369.9303 453.2113
634.4716 680.8465 848.7181
882.1464 919.0759 966.2649
1024.1911 1055.3344 1111.6321

```
1164.6277          1248.1874          1293.1592
1302.8418          1328.9234          1455.0545
1698.7999          3008.2877          3131.7315
3147.9214          3160.2299          3218.9863
ZeroEnergy[kcal/mol]  -20.1
ElectronicLevels[1/cm] 1
0  2
End
!---------------------------------
!-------ts_ts16a------------
Barrier     ts16a  ip16  ip21min
RRHO
Geometry[angstrom]   11
C  1.8622460794   -0.3733944589   0.0045759249
C  0.9084030918   0.6511599787   -0.0758675967
C  -1.0650700767   -0.6778909265   -0.0604153051
C  -2.3846970083   -0.7512816386   0.0235890156
O  -0.4479251689   0.5654677812   -0.0961299298
O  1.8729843961   -1.5832924759   0.1066851054
H  1.8380699472   0.483205116   1.0254633985
H  1.2437029191   1.6577930777   -0.2839870922
H  -0.3963304732   -1.5276702898   -0.112762855
H  -2.8656670482   -1.7191409038   0.037393452
H  -2.9990746582   0.13860574   0.0729548824
     Core                              MultiRotor
#1 2 5 3 s 11 30. 90.9677              149.8987
#2 5 3 4 s 11 30.
       SymmetryFactor  0.5
       InterpolationEnergyMax[kcal/mol]        100
       PotentialEnergySurface[kcal/mol]
/home/dporfirev/C4H5+O2/kin/dat/ts_16a_double.dat
       InternalRotation
            Group                    3 4 9 10 11
            Axis                     2 5
            Symmetry                    1
            MassExpansionSize              11
            GridSize                   100
       End
       InternalRotation
            Group                    4 9 10 11
            Axis                     3 5
            Symmetry                    1
            MassExpansionSize              11
            GridSize                   100
       End
     End

Tunneling      Eckart
ImaginaryFrequency[1/cm]  1408.0448
WellDepth[kcal/mol]  43.5
WellDepth[kcal/mol]  40.0
End
```

Frequencies[1/cm] 24
178.4722 300.0672 483.8526
580.0511 695.4542 726.6736
810.2172 856.5672 893.2677
992.6331 1049.7635 1137.4214
1203.8760 1248.9520 1351.6601
1415.8046 1430.0633 1706.0739
1756.3894 1852.5029 3162.7289
3203.7092 3226.7653 3259.1630
ZeroEnergy[kcal/mol] -58.0
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts19b----------
Barrier ts19b ip02 ip04
RRHO
Geometry[angstrom] 11
C -1.7998323032 -0.5340248962 0.5699786516
C -0.3330506928 -0.4617497362 0.8066887856
C 0.5711947704 -0.327844661 -0.2513036751
C 1.9226408956 -0.2263815038 -0.076053904
O -2.2156560724 0.6578377439 0.0162713436
O -2.2041667622 -1.057346143 -0.6301008188
H -2.3733139505 -0.8747869199 1.4426057285
H 0.0302899483 -0.4574833278 1.8312737807
H 0.1509096667 -0.3252233015 -1.2517217653
H 2.5966737558 -0.139918487 -0.9191473441
H 2.3659307444 -0.2353837677 0.9140342173
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 706.0344
WellDepth[kcal/mol] 18.2
WellDepth[kcal/mol] 93.2
End
Frequencies[1/cm] 26
113.6656 153.9236
203.0342 365.8496 392.1451
581.6562 711.9427 815.7287
891.0083 917.9289 946.1734
1025.6340 1033.9670 1223.4875
1231.7878 1247.8472 1287.6960
1335.0592 1393.9901 1495.2352
1553.3031 2998.8874 3139.6709
3154.2300 3176.3535 3236.4117
ZeroEnergy[kcal/mol] -27.5
ElectronicLevels[1/cm] 1
0 2
End

!----------
!-------ts_ts32f----------
Barrier ts32f ip32 ip48
RRHO
Geometry[angstrom] 11
C -1.3682474815 -0.5886717186 0.093197048
C -1.2052684923 0.7961503452 0.3150000158
C 0.0162487275 1.2527376522 -0.1743159976
C 0.999078467 0.2405392505 -0.4337048226
O -0.4073242982 -1.250600803 -0.408563359
O 1.7446870559 -0.3431387596 0.5136839517
H -2.314319254 -1.1000253631 0.2910855928
H -2.0145371147 1.4368607273 0.638226462
H 0.1594251005 2.2492674239 -0.577698588
H 1.5237667869 0.2005837713 -1.3850647146
H 1.2980795029 -0.2395525261 1.3659894116
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 511.5892
WellDepth[kcal/mol] 33.8
WellDepth[kcal/mol] 24.4
End
Frequencies[1/cm] 26
175.2991 289.8297
444.2036 483.1657 554.8561
615.7635 709.3794 796.0281
856.8938 899.2074 956.5775
1015.2181 1068.1686 1093.4720
1217.3580 1285.2260 1330.6401
1387.9779 1445.5257 1488.5279
1512.2603 3073.3222 3150.1582
3166.2712 3209.9912 3760.0451
ZeroEnergy[kcal/mol] -95.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts33b----------
Barrier ts33b ip06 ip33
RRHO
Geometry[angstrom] 11
C -1.4041241363 0.6205316069 -0.2224929014
C -0.0706383874 0.6171831697 0.0941773691
C 0.7073537381 -0.5568535235 -0.0019076945
C 0.4018719876 -1.5019606209 -0.9605457015
O -2.2033707631 -0.436025376 -0.3825010803
O -1.6661928339 -1.707605606 -0.5187977432
H -2.0156966566 1.5150131369 -0.2005269877
H 0.3230839571 1.5236460566 0.5424279988
H 1.4861649405 -0.7465688576 0.7306528256

H 0.8207904838 -2.500781442 -0.9109141591
H -0.0076693298 -1.2066705439 -1.9136529256
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 383.7232
WellDepth[kcal/mol] 19.6
WellDepth[kcal/mol] 65.1
End
Frequencies[1/cm] 26
192.2142 296.2810
337.4894 502.1548 545.3420
682.6385 776.1426 839.8975
877.4428 899.9708 910.3246
974.1588 1007.7086 1058.1253
1102.3540 1260.7601 1265.4235
1403.6597 1484.6091 1536.1795
1575.7352 3147.6084 3156.8159
3164.4323 3197.2113 3252.7611
ZeroEnergy[kcal/mol] -24.8
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts33gmin------------
Barrier ts33gmin ip33 ip60
RRHO
Geometry[angstrom] 11
C -1.2196214516 -0.2175749566 -0.3092594024
C -0.1908602351 0.6624256811 0.3428058321
C 1.0322563432 1.015165449 -0.2641403139
C 1.6472970158 -0.33229128 -0.4129554151
O -2.3583329955 -0.2599982248 0.0794475933
O 0.8623083094 -0.8470627054 0.7013258839
H -0.868029432 -0.804405134 -1.1761231486
H -0.624570798 1.2762480128 1.1325969
H 1.577694913 1.9156157509 -0.0125898006
H 1.4344254568 -0.8799035471 -1.3396553206
H 2.7251578739 -0.3580400459 -0.2211468081
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 697.0061
WellDepth[kcal/mol] 29.4
WellDepth[kcal/mol] 22.4
End

Rotor Hindered #115.6312
Group 5 7
Axis 1 2

Symmetry 1
Potential[kcal/mol] 12
0 1.238390176 3.790032422 4.75244388 2.089355931 1.92764671 4.467240771 5.734182633
7.096694206 8.752503761 7.87624937 2.250312141
End

Frequencies[1/cm] 25
216.5858
305.5240 364.1828 487.0431
615.6804 731.6826 884.8909
949.7023 981.7878 1031.6782
1056.8845 1087.4474 1143.1831
1157.9673 1293.7388 1357.8013
1383.1057 1444.4367 1513.2079
1790.0878 2957.1673 2996.9036
3044.5964 3120.3672 3195.5823
ZeroEnergy[kcal/mol] -60.5
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_35a_37a----------
Barrier ts_35a_37a ip04b ip35
Union
RRHO
Geometry[angstrom] 11
C -1.3569774608 -0.2278426676 0.0037630342
C 0.4566738178 1.2725420023 -0.0949222739
C 1.3865818139 0.2983414019 -0.0751511134
C 0.9944304692 -1.0462708486 0.3107519763
O -0.6206301002 -1.1762466492 -0.4156374409
O -0.8650633499 1.0367083837 0.1765448765
H -2.3045458192 -0.3657073566 0.5203277892
H 0.6351638399 2.3079368438 -0.3485957946
H 2.3836693458 0.5068771351 -0.4442900055
H 1.5584734022 -1.8710893618 -0.1119336436
H 0.6949410414 -1.2223068829 1.3393805957
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 701.875
WellDepth[kcal/mol] 38.6
WellDepth[kcal/mol] 10.9
End
Frequencies[1/cm] 26
227.4804 322.6296
451.7657 512.2786 608.2094
648.7367 702.8481 828.1651
882.4527 908.5091 985.1484
1009.2061 1052.6113 1092.1503
1137.7171 1239.4085 1322.2375

1386.0158 1424.4107 1491.7748
1632.6175 3113.3831 3125.4544
3173.7307 3194.8577 3219.8465
ZeroEnergy[kcal/mol] -82.6
ElectronicLevels[1/cm] 1
0 2
End
RRHO
Geometry[angstrom] 11
C 0.9799463295 0.9233019711 0.2058168492
C 0.4623388919 -1.238642035 0.1348477957
C -0.8566084285 -1.0018562567 0.2666242027
C -1.4153101286 0.2032616453 -0.3077267334
O 1.2885368264 -0.2897594265 -0.4462604325
O -0.1217559705 1.4802384719 -0.0460141576
H 1.5225211285 1.0633376824 1.1443358498
H 0.9838220362 -2.1025388282 0.5302932779
H -1.4554041634 -1.6437737044 0.903959957
H -1.3634350382 0.3164054089 -1.3835265914
H -2.3136384833 0.6167710711 0.1370339828
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 715.8637
WellDepth[kcal/mol] 47.2
WellDepth[kcal/mol] 19.5
End
Frequencies[1/cm] 26
144.6099 359.5369
413.4862 489.4717 619.3423
693.1000 734.7815 792.9823
865.2816 909.5213 953.4754
1001.2831 1014.1275 1056.8315
1142.7490 1221.4675 1298.9291
1387.1386 1394.6402 1491.0139
1618.1002 3057.2431 3135.3203
3159.2879 3189.3610 3216.4629
ZeroEnergy[kcal/mol] -74.0
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------ts_ts37b----------
Barrier ts37b ip35 ip37
RRHO
Geometry[angstrom] 11
C 0.7006949824 -0.8456440506 -0.3609786525
C 0.7308783019 0.9948214469 -0.1956843377
C -0.6205772133 1.2134024603 -0.1419205007
C -1.3475709002 -0.0152644653 0.3023363288

O 1.2491526326 -0.0572584528 0.6278052486
O -0.5950097398 -1.1778807454 -0.2264872153
H 1.3252041251 -1.5379611473 -0.9075683897
H 1.4796040397 1.609500014 -0.6766265296
H -1.0972236071 1.999212542 -0.7105690844
H -1.363835865 -0.1324288975 1.3911233895
H -2.3625617564 -0.1003257043 -0.0834812569
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 611.7501
WellDepth[kcal/mol] 18.2
WellDepth[kcal/mol] 14.6
End
Frequencies[1/cm] 26
259.0427 418.6485
521.4555 590.2691 632.2457
656.2374 767.7632 824.7745
851.5756 932.9124 969.6051
1051.0412 1110.0556 1141.3318
1159.1307 1224.7266 1289.7745
1356.5257 1387.1892 1485.7677
1493.9047 3022.1682 3116.3034
3201.1401 3216.3311 3224.0306
ZeroEnergy[kcal/mol] -75.3
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts38b----------
Barrier ts38b ip38min ip33
RRHO
Geometry[angstrom] 11
C -1.6785718092 -0.4509549337 -0.0816667187
C -0.7340113024 0.6540714606 -0.0040810367
C 0.6360390679 0.528010484 0.0034748361
C 1.4569419894 -0.7228704552 -0.1625363763
O -1.3743903735 -1.6317435764 -0.0290293289
O 2.7118951008 -0.637480796 -0.3114435507
H -2.7398257535 -0.1506325828 -0.1852781284
H -1.1476319644 1.656453924 0.0319749685
H 1.262952614 1.4081715703 0.1152007171
H 1.1304236722 -0.4480706111 1.0149819087
H 0.8913727586 -1.6296764836 -0.3996652907
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1361.4048
WellDepth[kcal/mol] 44.7
WellDepth[kcal/mol] 18.2

End
Frequencies[1/cm] 26
167.9053 182.2048
195.2320 333.7730 410.8785
505.0009 737.7746 798.8473
911.1872 957.7935 1004.0460
1021.0954 1037.2683 1155.0178
1204.9769 1322.8957 1353.2006
1426.0164 1479.6266 1524.7810
1712.6640 1921.1569 2920.1714
3065.7829 3159.8751 3176.9134
ZeroEnergy[kcal/mol] -71.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts38d----------
Barrier ts38d ip38min ip48
RRHO
Geometry[angstrom] 11
C -1.3871978762 0.08134367 0.9402697945
C -0.7622223762 -0.9305168237 0.1859863933
C 0.9111067593 0.8619816227 -0.0051005674
C 0.5130029562 -0.5482243883 -0.2939001914
O 1.9264822658 0.7936141792 0.7581761883
O -0.808458363 1.19611365 1.0616235431
H -2.3584702196 -0.0714792595 1.4225542102
H -1.1826498596 -1.9194953928 0.0627395241
H 0.7059234242 1.7695881851 -0.5669850555
H 0.9507982049 -1.0071958261 -1.1771592892
H 1.6026520843 -0.4941366165 0.6815834501
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1744.3216
WellDepth[kcal/mol] 48.1
WellDepth[kcal/mol] 51.2
End
Frequencies[1/cm] 26
96.0028 219.2284
342.1494 458.4623 572.1061
632.1431 775.4767 820.6570
870.9078 921.4261 941.2302
1042.9505 1055.7786 1103.9709
1151.2753 1256.8733 1318.4445
1385.9414 1457.5317 1498.2846
1552.8169 1752.0695 3058.7475
3140.1542 3156.8690 3212.5839
ZeroEnergy[kcal/mol] -68.3
ElectronicLevels[1/cm] 1
0 2

End
!----------
!-------ts_ts38e----------
Barrier ts38e ip38min ip40
RRHO
Geometry[angstrom] 11
C -1.6772880354 0.0933503371 0.6218922296
C -0.6362044088 -0.8395133019 0.6235407137
C 1.3611445576 0.7408525065 0.3947580559
C 0.4891881435 -0.3536247487 -0.1371903325
O 2.5141871188 0.8925311627 0.076503147
O -1.5258282747 1.0909403842 -0.1746925792
H -2.5832239542 0.0396238084 1.2214225231
H -0.7254777835 -1.8337046647 1.042477583
H 0.8587103722 1.4277014142 1.105979821
H -0.4093436526 0.6164028299 -0.6453603349
H 1.0727459171 -1.0733277275 -0.7050778267
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1882.7885
WellDepth[kcal/mol] 29.7
WellDepth[kcal/mol] 29.8
End
Frequencies[1/cm] 26
140.1463 192.0952
276.8056 476.6593 513.0586
614.6913 737.9221 834.7465
902.4322 948.1697 1002.4296
1018.6427 1087.8619 1130.4944
1269.6379 1290.0703 1329.9443
1409.8530 1416.2310 1483.3814
1734.0476 1775.0747 2900.2006
3146.1134 3151.9437 3201.6276
ZeroEnergy[kcal/mol] -86.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_38g_39amin----------
Barrier ts_38g_39amin ip38min ip39
Union
RRHO
Geometry[angstrom] 11
C -1.8466857238 0.0300913319 0.4881051197
C -0.4671582411 -0.4257154604 0.6298054357
C 1.4322255617 0.586146525 0.3566876956
C 0.5075015529 -0.1878451373 -0.5295439094
O 2.5866793564 0.6584364133 0.5875216063
O -2.2398897253 0.7118865906 -0.4428873922
H -2.5310683954 -0.2630438871 1.3078248866

H -0.2757676413 -1.2605840035 1.2976998815
H 0.3402921607 0.6597037684 1.2498038355
H 0.0214028426 0.476317685 -1.2512344939
H 0.9392442525 -1.054328826 -1.0329686655
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1765.3773
WellDepth[kcal/mol] 37.6
WellDepth[kcal/mol] 37.9
End
Frequencies[1/cm] 26
90.1139 152.5858
245.2906 279.9218 460.6245
646.3694 684.6271 728.2121
856.0514 930.0279 981.3632
1023.6764 1059.8910 1147.4564
1182.4501 1219.9631 1363.5591
1405.4284 1445.5078 1679.5154
1698.5849 1908.4084 2922.3142
3046.8777 3116.0121 3160.5903
ZeroEnergy[kcal/mol] -78.8
ElectronicLevels[1/cm] 1
0 2
End
RRHO
Geometry[angstrom] 11
C -1.8240219108 0.4919048285 -0.0047657101
C -0.4266232794 0.5163357728 -0.0922336582
C 1.9054693278 -0.4556971684 0.0985957556
C 0.4231725508 -0.7274465677 -0.0471826477
O 2.3996158064 0.6413793903 0.0991331257
O -2.6962561049 -0.3356472255 0.0987106212
H -1.2389526999 1.1439063391 0.9513825873
H 0.0509531602 1.4594396489 -0.3261651555
H 2.5340997863 -1.3658943245 0.1996864405
H 0.2775273701 -1.3096699175 -0.9701801846
H 0.1024379934 -1.4033727761 0.7550238257
Core MultiRotor
#1 2 4 3 s 11 30. 39.9568 143.4391
#2 4 3 5 s 11 30.
SymmetryFactor 0.5
InterpolationEnergyMax[kcal/mol] 100
PotentialEnergySurface[kcal/mol]
/home/dporfirev/C4H5+O2/kin/dat/ts_39a_min_double.dat
InternalRotation
Group 1 6 7 8
Axis 2 4
Symmetry 1
MassExpansionSize 11
GridSize 100

```
      End
      InternalRotation
           Group                    5 9
           Axis                   3 4
           Symmetry                 1
           MassExpansionSize          11
           GridSize                 100
      End
    End

Tunneling      Eckart
ImaginaryFrequency[1/cm]  1516.9585
WellDepth[kcal/mol]  42.0
WellDepth[kcal/mol]  42.3
End
Frequencies[1/cm]  24
154.5264            232.3866            482.9855
604.6282            671.2202            701.2598
742.8565            897.4498           1012.3458
1048.4757           1146.9498           1196.2274
1226.9596           1301.0401           1403.1977
1410.2047           1429.5080           1804.0087
1817.3720           1895.0965           2889.2423
2993.2720           3039.6157           3202.5266
ZeroEnergy[kcal/mol]  -74.4
ElectronicLevels[1/cm] 1
0  2
End
End
!---------------------------------
!-------ts_ts39d------------
Barrier      ts39d  ip39  ip67
RRHO
Geometry[angstrom]   11
C  -1.7512988947   -0.496601183   -0.7798695572
C  -1.161100653   0.662972893   0.027308888
C  0.6101225915   -0.9997976183   -4.567946E-4
C  0.3666119705   0.4857992166   0.124288104
O  -0.18363458   -1.6215659427   -0.7388408188
O  -2.4714223989   -0.540093035   -1.7087993322
H  -1.6233155185   0.6278591103   1.0182156547
H  -1.4482373697   1.6007085105   -0.4504434562
H  1.2983408838   -1.537315083   0.6615025287
H  0.7687585701   0.8905601493   1.0542985242
H  0.8621443989   1.0063539824   -0.7050377406
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  631.0984
WellDepth[kcal/mol]  21.3
WellDepth[kcal/mol]  34.1
```

```
End
Frequencies[1/cm]  26
110.3602            187.5417
374.3959            459.0217            521.7088
618.4027            737.2961            783.0626
906.4147            928.3406            993.6981
1020.4717           1143.7023           1205.2058
1280.5067           1289.4864           1335.9481
1462.9061           1476.7528           1485.8964
1914.2838           3003.4686           3033.1130
3044.5250           3095.5639           3103.5552
ZeroEnergy[kcal/mol]  -95.4
ElectronicLevels[1/cm] 1
0  2
End
!---------------------------------
!-------ts_ts39f_min------------
Barrier      ts39f  ip39  p12_p12
RRHO
Geometry[angstrom]   11
C         1.685068   -0.142598   -0.562751
C         0.193452    1.030097    0.595225
C        -1.735933   -0.338244   -0.283366
C        -1.029653    1.001045   -0.253982
O        -1.410576   -1.297374    0.366959
O         2.602608   -0.488731    0.018699
H         0.768354    1.947967    0.640955
H         0.223326    0.390659    1.469050
H        -2.616750   -0.381120   -0.960508
H        -0.811716    1.290010   -1.291076
H        -1.777078    1.739523    0.085557
     Core                            MultiRotor
#4 2 1 6 s 11 30. 37.5621              200.7988
#2 4 3 5 s 11 30.
       SymmetryFactor  0.5
       InterpolationEnergyMax[kcal/mol]        100
       PotentialEnergySurface[kcal/mol]
/home/dporfirev/C4H5+O2/kin/dat/ts_39f_min_double.dat
       InternalRotation
            Group                    6
            Axis                   2 1
            Symmetry                 1
            MassExpansionSize           11
            GridSize                 100
       End
       InternalRotation
            Group                    5 9
            Axis                   3 4
            Symmetry                 1
            MassExpansionSize           11
            GridSize                 100
       End
```

End

Tunneling Eckart
ImaginaryFrequency[1/cm] 286.9825
WellDepth[kcal/mol] 12.1
WellDepth[kcal/mol] 5.8
End

Frequencies[1/cm] 24
88.4159 124.4840 259.3191
290.4078 531.7063 673.8257
681.8959 817.2272 859.8287
994.6359 1030.5923 1123.7028
1218.3071 1361.7457 1409.6493
1420.0158 1451.2923 1816.1232
2085.5516 2876.9474 2951.0770
3018.0844 3134.9438 3236.8649
ZeroEnergy[kcal/mol] -104.6
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts40a------------
Barrier ts40a ip33 ip40
RRHO
Geometry[angstrom] 11
C -1.6145218711 -0.4338960734 0.0421386973
C -0.7406999266 0.6819043789 -0.1501788495
C 0.6070321942 0.4914752373 -0.0478499537
C 1.2299487957 -0.8518706533 -0.0289713887
O -1.2136194772 -1.6166739396 0.1515682687
O 2.2838206488 -1.0555337007 0.68331784
H -2.6843373423 -0.2464324733 0.1945123229
H -1.1777116259 1.6727236124 -0.1666783339
H 1.2653452509 1.3371771586 0.1382388125
H 0.1580006792 -1.5023487034 0.3258610661
H 1.1499536741 -1.3905328436 -1.0013404816
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1576.3144
WellDepth[kcal/mol] 13.2
WellDepth[kcal/mol] 39.8
End
Frequencies[1/cm] 26
177.1578 259.8748
416.6645 428.3775 508.6021
513.7295 741.1178 811.3366
917.9571 989.3739 997.7102
1020.0404 1050.3337 1177.2633
1200.1553 1294.8170 1337.0212

1372.1983 1424.6345 1504.9372
1571.9444 1668.4658 2829.1286
3046.8936 3144.7494 3193.1530
ZeroEnergy[kcal/mol] -76.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts40c----------
Barrier ts40c ip45min ip32
RRHO
Geometry[angstrom] 11
C 1.6809125826 -0.2069093301 -0.061382841
C 0.9019980718 1.0499815033 -0.1837209667
C -0.406758137 1.1839144014 0.095064104
C -1.3275740412 0.1253052352 0.5451618073
O 1.2179130086 -1.3020610641 0.1576152865
O -1.9094906545 -0.724578126 -0.358697586
H 2.7770072915 -0.0737117567 -0.1872083131
H 1.4708592553 1.9241018052 -0.4933185451
H -0.8254873448 2.1877978561 -0.0207399926
H -1.2835997694 -0.2826003106 1.5459916515
H -1.6646512629 -0.4570312137 -1.2512856047
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 521.0029
WellDepth[kcal/mol] 23.8
WellDepth[kcal/mol] 32.8
End

Rotor Hindered #50.7475
Group 11
Axis 4 6
Symmetry 1
Potential[kcal/mol] 12
0 1.215862582 1.47621631 0.825677119 0.41089328 1.296183809 2.872738903 5.280995208
4.678899756 2.083771095 1.071347123 1.014432003
End

Frequencies[1/cm] 25
135.3671
200.8165 249.6002 296.1232
466.6823 520.9737 755.2614
841.7886 903.7500 989.4559
1001.4471 1035.7275 1177.7373
1239.4922 1288.3179 1383.0177
1425.2039 1441.0561 1636.7124
1784.4240 2880.9051 3048.9976
3138.4267 3196.7179 3817.7049
ZeroEnergy[kcal/mol] -96.1

ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts40e------------
Barrier ts40e ip40 ip48
RRHO
Geometry[angstrom] 11
C 1.3758300523 -0.847880564 0.2952130197
C 1.0547041813 0.518912382 0.1460015361
C -0.3210917908 0.714116085 0.0518433978
C -1.0938537817 -0.4525579047 -0.2634450873
O 0.445533747 -1.7105424244 0.2342094329
O -1.21357354 -0.9641628991 -1.4955633068
H 2.3931266658 -1.1838185482 0.5141376303
H 1.7778046809 1.3099147475 0.2920559403
H -0.8227168175 1.599126921 0.427820637
H -1.9639449764 -0.7244504288 0.3290143191
H -0.468109421 -0.6576783662 -2.0312465189
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 512.0684
WellDepth[kcal/mol] 21.4
WellDepth[kcal/mol] 24.4
End
Frequencies[1/cm] 26
175.2045 290.0344
444.3352 483.1603 554.7433
615.7564 709.3197 796.0712
856.8809 899.0650 956.6544
1015.3427 1068.1685 1093.4402
1217.3786 1285.1875 1330.5986
1388.0040 1445.6185 1488.6183
1512.3043 3073.4262 3150.1547
3166.4884 3210.0501 3760.0936
ZeroEnergy[kcal/mol] -95.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts40g------------
Barrier ts40g ip40 ip55
RRHO
Geometry[angstrom] 11
C 1.564762056 -0.3251631114 0.1058658958
C 0.5897771373 0.7792048811 0.0068279852
C -0.7424497841 0.6360350412 -0.076956267
C -1.4295042117 -0.6705198052 -0.0223574033
O 2.2168088286 -0.7320566094 -1.0329588269
O -2.6293480492 -0.7904947547 -0.1262927295

H 2.2011537301 -0.4146062586 0.9788726807
H 0.992930042 1.7972407631 -0.0214831439
H -1.3927926468 1.5000439585 -0.1764208238
H -0.7683933356 -1.5473896002 0.1280451528
H 1.6520152334 -0.5571645043 -1.7949545201
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 239.2938
WellDepth[kcal/mol] 16.6
WellDepth[kcal/mol] 17.1
End

Rotor Hindered #369.4497
Group 11
Axis 1 5
Symmetry 1
Potential[kcal/mol] 12
0 0.944903941 1.742405879 3.790973686 6.391687182 3.629076212 1.331951856
0.909324147 2.74428769 5.214981199 4.583330045 1.374559757
End

Frequencies[1/cm] 25
138.0051 173.5316
247.1177 391.0213
492.0556 583.0198 709.3864
800.2041 949.2169 1018.3994
1033.3624 1092.9441 1171.3315
1218.9585 1274.1083 1362.6112
1406.9629 1435.6415 1662.3805
1774.9482 2914.7050 3033.7863
3167.5424 3172.8318 3805.9470
ZeroEnergy[kcal/mol] -99.9
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts40i----------
Barrier ts40i ip40 ip32
RRHO
Geometry[angstrom] 11
C 1.6356685905 -0.0507167133 -0.1089328785
C 0.8900979523 1.1027998889 0.0754660528
C -0.4912089099 1.2285821627 0.0994642583
C -1.4467106956 0.1570545426 -0.300796833
O 1.1578314874 -1.3137218725 -0.1928639891
O -2.0275151911 -0.5771437686 0.4669316501
H 2.7120324648 -0.0194146831 -0.21461933
H 1.4783560227 1.9997118444 0.2429878285
H -0.9392268755 2.1799333356 0.3677504953
H 0.2584924084 -1.3657551005 0.1576595529

H -1.6195412539 0.0562783638 -1.3964198072
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 298.0398
WellDepth[kcal/mol] 6.9
WellDepth[kcal/mol] 19.3
End
Frequencies[1/cm] 26
126.9589 164.0571
305.3243 383.5883 430.3557
541.8981 643.6453 735.4835
755.0267 901.4395 912.2043
1003.5719 1050.2898 1159.3937
1236.2263 1356.2945 1382.7137
1414.1040 1458.2849 1528.4311
1761.8479 2851.4924 3152.8892
3167.7506 3209.5757 3766.8455
ZeroEnergy[kcal/mol] -109.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts41a----------
Barrier ts41a ip40 ip49min
RRHO
Geometry[angstrom] 11
C 1.4229646657 -0.2842019801 0.1941963896
C 0.689828987 0.9361563895 -0.1583060457
C -0.6494003332 0.7470121217 -0.2587042736
C -1.0322981727 -0.5498793182 0.2828887768
O 1.7070501765 -1.1313538512 -0.8774275104
O -1.970488016 -1.2758481457 0.179338961
H 2.2516186583 -0.1918085093 0.9031839054
H 1.177969218 1.8993329617 -0.2655106781
H -1.3890172223 1.4778309725 -0.5617813319
H 0.2270803562 -0.8489660027 0.7544325276
H 2.1532716824 -1.9139826381 -0.5352837206
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1565.778
WellDepth[kcal/mol] 37.1
WellDepth[kcal/mol] 27.1
End
Frequencies[1/cm] 26
121.0255 237.1688
339.3038 369.0773 395.2700
582.4471 602.0793 701.8316
783.1287 889.8419 938.5889

957.2051 1035.1990 1089.1624
1163.0204 1247.1105 1275.6754
1333.7108 1440.7167 1553.8108
1657.9317 1871.9205 3040.2231
3160.3983 3200.6426 3806.9336
ZeroEnergy[kcal/mol] -79.4
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts45a----------
Barrier ts45a ip45min ip33
RRHO
Geometry[angstrom] 11
C -1.7116343649 -0.451677242 0.0162365177
C -0.7249973217 0.6334174353 0.0025423387
C 0.6280678892 0.4800551879 0.0224315273
C 1.3531784167 -0.764188338 0.0770919896
O -1.4585413458 -1.6387460933 0.1084831412
O 2.7307487794 -0.7609469845 -0.0023314574
H -2.7645745317 -0.1130376347 -0.067403127
H -1.1306747907 1.6396247683 -0.0387015742
H 1.2558909859 1.3677973877 0.0075758647
H 2.0504054194 -0.8676281565 1.0914773148
H 0.830502864 -1.6988173302 -0.1182805355
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1968.8514
WellDepth[kcal/mol] 54.0
WellDepth[kcal/mol] 24.0
End
Frequencies[1/cm] 26
144.9288 165.2560
191.4706 329.6843 384.9865
495.2682 595.3623 768.5352
816.2749 947.7110 983.7520
1012.2956 1022.7949 1086.2913
1170.6892 1229.2751 1319.8993
1425.1532 1452.1102 1577.1355
1739.6712 2364.4821 2904.0987
3131.4315 3146.1081 3167.5020
ZeroEnergy[kcal/mol] -65.9
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts45b----------
Barrier ts45b ip45min ip48
RRHO
Geometry[angstrom] 11

C 0.9685377159 -0.7313280998 1.1924210733
C 0.8495089044 0.3275134797 0.2832471569
C -0.4216108086 0.3704843049 -0.2872360732
C -1.2200964728 -0.7971322228 -0.0579127502
O -0.027464049 -1.5276009776 1.3349616625
O -2.5237024109 -0.697533811 0.233764957
H 1.8474107566 -0.8854397694 1.820880436
H 1.6122121072 1.0817467005 0.1487107485
H -0.865870833 1.2558109559 -0.7282168332
H -1.0257482151 -1.7423264595 -0.5513963445
H -2.6846556949 0.1658288991 0.639173967
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 402.7715
WellDepth[kcal/mol] 19.2
WellDepth[kcal/mol] 18.8
End
Frequencies[1/cm] 26
195.9311 346.5236
461.8936 543.7967 578.4345
610.7554 665.1396 798.5753
856.7724 894.7919 1011.3985
1047.5148 1081.7025 1119.9233
1234.6753 1268.6029 1307.1560
1381.3130 1456.7755 1487.6895
1509.3376 3096.8078 3168.4590
3172.6183 3216.5971 3758.3059
ZeroEnergy[kcal/mol] -100.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts48a----------
Barrier ts48a ip48 ip52
RRHO
Geometry[angstrom] 11
C 1.1899589311 0.9965430392 0.3786814669
C 1.0411852941 -0.4751075108 0.8127352333
C -0.1695916155 -0.8300792491 0.373879825
C -0.7421684735 0.4325387545 -0.2031132633
O 1.4429068979 1.0659064304 -0.9833982465
O -0.1718674511 1.4836785587 0.5190663166
H 1.8906111102 1.6242679249 0.9330819302
H 1.8225951186 -1.083364369 1.2432000046
H -0.6260563486 -1.8073806262 0.3161618816
H 0.1036282627 0.5756148275 -1.1819975094
H -1.7874377259 0.5632812199 -0.4616316391
Core RigidRotor
SymmetryFactor 0.5
End

Tunneling Eckart
ImaginaryFrequency[1/cm] 1852.6486
WellDepth[kcal/mol] 60.5
WellDepth[kcal/mol] 35.4
End
Frequencies[1/cm] 26
379.8606 436.3980
576.8159 646.7740 677.2835
747.0128 805.2031 866.8994
903.4009 923.5363 944.4162
994.1962 1021.7621 1031.1449
1133.1254 1219.4099 1236.1157
1262.6360 1305.0095 1328.6275
1569.8616 1803.8041 3089.8338
3177.3137 3220.6064 3245.2154
ZeroEnergy[kcal/mol] -59.0
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts48c----------
Barrier ts48c ip60 ip52
RRHO
Geometry[angstrom] 11
C 0.7526513792 -0.6627547241 -0.0893948024
C 0.7997193289 0.7989392268 -0.4862516775
C -0.3500122468 0.9587516798 0.4875785511
C -1.3417563352 -0.1272586054 0.2199076266
O 1.8860178943 1.4978860991 -0.4790985924
O -0.4369340112 -1.2542587577 -0.0852213664
H 1.6122516975 -1.3021881739 0.0998056786
H 0.3752175577 0.7914264157 -1.5431786141
H -0.382587034 1.671719743 1.2986882532
H -1.9388878971 -0.4524073992 1.0709816341
H -1.9963253333 0.044086496 -0.6427866909
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 590.8723
WellDepth[kcal/mol] 54.1
WellDepth[kcal/mol] 65.6
End
Frequencies[1/cm] 26
241.9208 293.1411
352.1117 415.8951 577.0766
642.9509 703.4360 812.4094
854.8472 891.7866 960.5686
992.3893 1016.0418 1065.9470
1164.2016 1178.4518 1235.0176
1273.5850 1346.2832 1404.8497
1493.8938 2506.1601 3026.1445

3116.0483 3156.4275 3229.9742
ZeroEnergy[kcal/mol] -28.8
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts52a----------
Barrier ts52a ip52 ip37
RRHO
Geometry[angstrom] 11
C 1.1797491073 1.1206697638 0.4959607179
C 1.1338110887 -0.3600907643 0.5997129391
C -0.1732427059 -0.7354472098 0.2739117734
C -0.9572996952 0.5036037818 -0.0457293176
O 1.7727872849 0.6220061281 -0.6397945788
O -0.1266405466 1.6055319703 0.3610994498
H 1.767801586 1.7775038457 1.1336126001
H 1.9214460745 -0.9793987343 0.996500088
H -0.5508350015 -1.7421942175 0.1673763035
H -1.1814440933 0.5703601988 -1.119202585
H -1.903470099 0.5751102373 0.5015676096
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 462.5934
WellDepth[kcal/mol] 6.8
WellDepth[kcal/mol] 2.3
End
Frequencies[1/cm] 26
220.8024 361.0625
527.1090 589.3830 777.5734
794.6401 834.3416 908.0953
940.1833 967.2651 1003.4118
1073.6668 1085.5493 1104.2184
1188.2924 1211.1679 1303.7430
1342.9455 1351.3604 1413.3931
1487.3969 2990.6897 3037.3081
3127.7743 3222.2448 3253.6981
ZeroEnergy[kcal/mol] -87.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts52b----------
Barrier ts52b ip52 ip54
RRHO
Geometry[angstrom] 11
C -0.9859345642 0.0074704462 0.2362973435
C -0.1059665482 1.2124619458 0.0562439585
C 1.1858593674 0.9362100224 -0.0608643463
C 1.4955738458 -0.5399975402 -0.0544901717

O -2.0892627057 -0.1837539571 -0.2469682987
O 0.3025578382 -1.2548899018 -8.543142E-4
H -0.810779986 -0.4675931629 1.25913758
H -0.5591390047 2.1945694962 0.0481571458
H 1.9704192153 1.6732203855 -0.183862415
H 2.019363137 -0.8057712078 -0.9906822366
H 2.174314405 -0.8107765262 0.7700697547
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 542.0699
WellDepth[kcal/mol] 19.6
WellDepth[kcal/mol] 31.3
End
Frequencies[1/cm] 26
170.4611 328.5029
424.8280 530.7439 576.5953
720.9153 769.7340 818.6739
909.9377 931.1232 967.7245
995.9763 1051.8101 1131.7939
1141.6318 1180.2574 1311.1138
1342.2720 1446.5365 1610.1181
1668.4948 2514.8463 2922.5603
2964.8853 3188.6071 3219.7764
ZeroEnergy[kcal/mol] -74.8
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts52d----------
Barrier ts52d ip52 ip33
RRHO
Geometry[angstrom] 11
C 1.1974815152 -0.356344926 -0.315014332
C 0.1349960593 0.714685075 -0.3151459871
C -1.0461733713 0.3528797575 0.1680598338
C -1.108857767 -1.1021873224 0.5492148739
O 1.9024451636 -0.5337627754 0.7129993862
O 0.0407656335 -1.7333740513 0.0508566429
H 1.5765081565 -0.6900195325 -1.2935777997
H 0.3921157479 1.718457674 -0.6328192081
H -1.8895396505 1.0162118536 0.3203064628
H -1.2242484098 -1.2502909328 1.6316350904
H -1.9508960774 -1.6175408196 0.056622037
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 547.4628
WellDepth[kcal/mol] 22.8
WellDepth[kcal/mol] 18.3

```
End
Frequencies[1/cm]  26
164.4815            296.6351
344.6140            500.9711            634.3255
728.5745            802.9447            894.7497
937.9691            950.3117            965.8913
1024.6081           1045.9561           1138.5857
1169.1380           1309.7424           1345.1626
1359.5656           1447.4492           1458.6852
1690.0006           2952.7547           2973.7140
3004.1688           3177.0093           3199.4466
ZeroEnergy[kcal/mol]  -71.6
ElectronicLevels[1/cm] 1
0  2
End
!---------------------------------
!-------ts_ts54a------------
Barrier     ts54a  ip54  ip49min
RRHO
Geometry[angstrom]   11
C  -1.3686965822   -0.6378798132   -0.1739213688
C  -0.6537112656   0.6154521552   -0.2029419637
C  0.6821698528   0.7779231401   -0.1663687303
C  1.6890374716   -0.3343295399   -0.2092104417
O  -2.2081725131   -1.1853839617   -0.7987284714
O  1.1190047989   -1.6316699384   -0.182019173
H  -1.3098703821   1.4810562702   -0.1319647135
H  1.0835059384   1.7855431097   -0.1146236383
H  2.2694525457   -0.2745944084   -1.1368316103
H  2.4078168698   -0.1986021406   0.61381769
H  0.6908792659   -1.760061873   0.671234421
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  194.3716
WellDepth[kcal/mol]  2.0
WellDepth[kcal/mol]  2.4
End
Frequencies[1/cm]  26
113.9244            172.6339
258.9680            356.1170            381.8667
442.5300            694.8972            762.1574
800.4174            897.5734            919.1625
983.9522            1080.1112           1180.6101
1209.0841           1370.8746           1374.6541
1409.7784           1487.4999           1618.2217
1949.1578           2968.0225           3034.4583
3126.4202           3163.4084           3816.4086
ZeroEnergy[kcal/mol]  -104.1
ElectronicLevels[1/cm] 1
0  2
```

End
!----------
!-------ts_ts54b----------
Barrier ts54b ip54 ip58
RRHO
Geometry[angstrom] 11
C -1.0164500379 -0.5479486993 -0.1413327135
C -0.5729444168 0.7781462769 -0.4118287546
C 0.7956330408 1.0081272703 -0.0092772319
C 1.4735869936 -0.3395466652 -0.0127474387
O -1.9171081825 -1.283350357 -0.0050186924
O 0.5166921339 -1.2138770576 -0.633810318
H -1.3118327861 1.5602315623 -0.5284821361
H 1.2906900923 1.9655917454 -0.0547460586
H 2.4045434667 -0.3633040979 -0.5879728149
H 1.6862151028 -0.7133060405 1.0010084591
H -0.0585814067 -0.2002269375 -1.3353513003
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1791.6777
WellDepth[kcal/mol] 49.9
WellDepth[kcal/mol] 71.9
End
Frequencies[1/cm] 26
193.3008 245.5455
344.8153 381.8056 478.3800
611.6984 650.4153 765.0166
857.4087 930.2800 970.3272
992.9931 1030.7442 1075.8856
1174.0159 1241.8563 1298.2471
1324.2474 1370.7509 1489.8552
1711.2862 2008.8164 2952.5990
3041.7063 3202.8925 3239.3865
ZeroEnergy[kcal/mol] -56.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts55a----------
Barrier ts55a ip55 ip45min
RRHO
Geometry[angstrom] 11
C 1.2949310284 -0.5401868362 0.0679519079
C 0.5133859183 0.5693445383 -0.1935297744
C -0.8727750681 0.6122630109 -0.1690792183
C -1.7308539526 -0.5435674325 0.2253305179
O 2.6499411784 -0.5503389539 0.0590422158
O -2.1682690072 -1.3671675442 -0.5402787109
H 0.8890153322 -1.5177461832 0.2932428206
H 1.0354456852 1.4913241077 -0.4495233514

H -1.3889944099 1.5340454026 -0.4151619191
H -1.9714934244 -0.611325189 1.3119960755
H 2.9796227199 0.3310530794 -0.1544015636
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 275.595
WellDepth[kcal/mol] 8.4
WellDepth[kcal/mol] 11.3
End

Rotor Hindered #418.0116
Group 11
Axis 1 5
Symmetry 1
Potential[kcal/mol] 12
0 1.243598505 4.104414726 5.764805101 4.051829423 1.504767997 0.396021302 1.16603832
3.614831744 5.439002122 3.98951772 1.23801367
End

Frequencies[1/cm] 25
133.8010 158.5461
277.6159 353.2245
472.1910 602.8382 649.2197
773.2265 907.2025 920.0271
997.7845 1106.8019 1169.7076
1270.8515 1290.9208 1387.8487
1412.4471 1448.1542 1552.7521
1783.2905 2834.1956 3107.0771
3168.8512 3207.0457 3799.3898
ZeroEnergy[kcal/mol] -108.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts55c----------
Barrier ts55c ip55 ip49min
RRHO
Geometry[angstrom] 11
C 1.0776255392 -0.5548271494 0.2711874102
C 0.4728978611 0.7700966239 0.3053103332
C -0.8714315452 0.7513435819 0.0610387214
C -1.3050419681 -0.5337692793 -0.4228175481
O 2.3408522247 -0.7149449816 -0.2457303903
O -2.3245208945 -1.1478703946 -0.5037188066
H 0.9721338864 -1.1962876846 1.1429939571
H 1.0668365684 1.6676326989 0.4445116355
H -1.5564538992 1.5854076115 0.1417055733
H -0.0233675739 -1.0824181287 -0.4561726898
H 2.4510538011 -0.1112838979 -0.9893951958
Core RigidRotor

SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1387.523
WellDepth[kcal/mol] 31.3
WellDepth[kcal/mol] 20.8
End
Frequencies[1/cm] 26
208.9588 224.5532
269.2105 439.2647 482.5660
538.1731 636.6368 724.3972
771.0502 856.0963 941.9138
1008.1946 1079.8376 1104.3352
1190.1785 1225.9554 1292.7978
1341.7121 1447.8764 1527.2598
1645.3394 1863.9614 3133.1989
3163.9491 3206.7775 3807.0325
ZeroEnergy[kcal/mol] -85.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts55d----------
Barrier ts55d ip55 ip38min
RRHO
Geometry[angstrom] 11
C 1.3440872562 -0.6461783123 -0.2385948722
C 0.5496194066 0.5612749255 -0.1622563082
C -0.8661407146 0.6379006964 -0.1321385818
C -1.6980089756 -0.481980418 0.199375613
O 2.3228400973 -0.5784587828 0.5569705738
O -2.9228301018 -0.4695821167 0.2012009804
H 1.2109684031 -1.527656459 -0.8681744592
H 1.0848207476 1.3931352024 -0.6269863317
H -1.362494156 1.5847456114 -0.3137727842
H -1.1471682558 -1.4150941169 0.4676430616
H 1.6509952931 0.5304787701 0.8823501085
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 2160.4616
WellDepth[kcal/mol] 56.7
WellDepth[kcal/mol] 56.1
End
Frequencies[1/cm] 26
109.2672 158.4907
234.8547 321.3234 419.3555
532.9446 690.8981 736.8326
815.6919 926.1642 975.7332
991.9804 1081.6501 1131.5763
1202.0132 1257.1824 1353.4940

1412.4660 1461.6497 1504.2298
1643.4174 1727.4846 2816.8087
3090.0287 3122.8790 3182.4049
ZeroEnergy[kcal/mol] -60.3
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts57a----------
Barrier ts57a ip57 ip49min
RRHO
Geometry[angstrom] 11
C -1.717902721 -0.3689409892 -0.351289203
C -0.8237732407 0.5490214297 -0.0236378747
C 0.565339363 0.2599069295 0.3362322965
C 1.1499652343 -1.1297784566 0.2408309874
O -2.5130161799 -1.164048271 -0.6345288667
O 2.0614422396 -0.7109268558 -0.7825566567
H -1.171955152 1.5747866385 -0.0805706383
H 1.4133478433 0.4421388118 -0.6539114052
H 0.9830795169 0.8794601996 1.1276283952
H 1.6570950207 -1.484033992 1.1430365178
H 0.4488760757 -1.8978734445 -0.1100905525
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1859.2536
WellDepth[kcal/mol] 23.9
WellDepth[kcal/mol] 41.4
End
Frequencies[1/cm] 26
88.4740 139.3145
214.8729 387.6611 511.8813
581.0422 628.9964 706.5848
822.8883 884.9868 986.2933
1044.6338 1102.5203 1158.5084
1172.0680 1181.9875 1305.1025
1358.0793 1414.7475 1527.9255
1924.1586 2206.9201 2995.6405
3052.6687 3120.6185 3171.2046
ZeroEnergy[kcal/mol] -65.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts57d----------
Barrier ts57d ip57 ip39
RRHO
Geometry[angstrom] 11
C -1.7478176821 -0.0674708789 0.1228381517
C -0.4857300924 -0.0055980149 0.5858778938

C 0.5496146731 0.9180313961 -0.0577258888
C 1.5846578878 -0.1483323415 -0.493754147
O -2.7662866268 -0.2727319397 -0.393168746
O 2.7000047992 -0.254321392 0.0271788036
H -0.366008897 -0.2345364055 1.6399253452
H 0.1448250042 1.4805668869 -0.9020303491
H 0.5422982203 -1.1230974919 0.0590120994
H 1.3832529576 -0.5632706857 -1.5068536982
H 0.9822157561 1.609113867 0.6658485354
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1366.6918
WellDepth[kcal/mol] 26.5
WellDepth[kcal/mol] 54.2
End
Frequencies[1/cm] 26
64.4781 139.9035
187.0250 406.7115 448.4485
464.2613 596.8087 675.2491
835.8825 850.3548 890.8247
1037.9060 1060.9316 1118.7088
1141.3773 1159.1245 1252.7067
1328.9914 1343.3766 1468.7973
1619.0561 2174.4998 2835.9840
3060.2236 3125.7620 3168.3919
ZeroEnergy[kcal/mol] -62.5
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts58a------------
Barrier ts58a ip52 p7_p7
RRHO
Geometry[angstrom] 11
C 0.9367954471 -0.2772336976 0.023275093
C 0.0028499975 0.8921713583 -0.1069329175
C -1.2474001616 0.4423059028 -0.1383542609
C -1.2377622619 -1.05286496 -0.0056740481
O 2.1360779376 -0.330524933 -0.2021818567
O 0.1424036457 -1.4211081478 0.0158003303
H 0.369488609 1.9058951 -0.1611103626
H 1.0923384107 -0.0412110284 1.6009444498
H -2.1544192129 1.0233142425 -0.2385322193
H -1.7204163261 -1.3908804662 0.9200101561
H -1.7245480852 -1.5564903706 -0.8474823641
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1065.8888

WellDepth[kcal/mol] 18.2
WellDepth[kcal/mol] 21.5
End
Frequencies[1/cm] 26
188.7213 339.2006
431.0701 482.8087 562.7460
654.1451 714.1160 782.4079
823.3744 867.2796 944.1630
961.9153 1024.7439 1049.2241
1092.1563 1125.5301 1202.3144
1332.2405 1364.6787 1492.7874
1647.7981 1676.8915 3012.4970
3049.6108 3209.9824 3248.5410
ZeroEnergy[kcal/mol] -76.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts58c----------
Barrier ts58c ip58 ip67
RRHO
Geometry[angstrom] 11
C 0.8586724791 -0.0069843677 -0.0180178555
C -0.0483155813 1.2266240744 0.0128985857
C -1.4351224222 0.6528480505 0.0384332226
C -1.2758442963 -0.8277719317 -0.0239912833
O 2.04983428 -0.0565379287 -0.0021251381
O 0.0800614311 -1.147214477 -0.0501461832
H 0.1498597936 1.8246006572 -0.8861375492
H -2.3208269127 1.1398237182 -0.3445614498
H -1.668432667 -0.1834101902 1.0434060989
H -1.9307329625 -1.5183158257 -0.5402032011
H 0.2296178582 1.8517932207 0.8671127529
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 2041.1593
WellDepth[kcal/mol] 43.7
WellDepth[kcal/mol] 45.1
End
Frequencies[1/cm] 26
133.6070 278.0280
489.8151 550.2906 612.6410
682.0606 732.7853 800.0499
835.6291 943.2708 984.3835
1027.4155 1104.1147 1128.2495
1162.0780 1260.1080 1297.7231
1306.1624 1331.9400 1463.9878
1878.1209 2125.8706 3003.6635
3045.9222 3172.3660 3204.1590
ZeroEnergy[kcal/mol] -84.4

ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts58e------------
Barrier ts58e ip58 p10_p10
RRHO
Geometry[angstrom] 11
C -0.866242 -0.007383 -0.000746
C 0.017145 1.238085 0.039068
C 1.393784 0.668966 -0.097988
C 1.280503 -0.671874 -0.114961
O -2.050572 -0.111264 0.041359
O -0.030812 -1.115457 -0.106069
H -0.153913 1.769028 0.982403
H 2.318307 1.223490 -0.123773
H 2.012228 -1.436928 -0.318901
H 1.795894 -1.028780 1.791928
H -0.272585 1.920202 -0.766217
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 634.2337
WellDepth[kcal/mol] 36.9
WellDepth[kcal/mol] 4.3
End
Frequencies[1/cm] 26
161.3394 261.7500
354.1887 491.0110 492.3164
579.5016 676.3007 713.6178
807.3728 837.1498 941.0874
955.9260 987.9163 1053.0869
1093.3933 1158.0550 1166.2420
1282.1186 1364.2111 1434.1780
1584.4873 1897.7538 3035.9110
3068.3040 3241.2864 3261.422
ZeroEnergy[kcal/mol] -91.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts58f------------
Barrier ts58f ip58 p7_p7
RRHO
Geometry[angstrom] 11
C 0.8426970 -0.0273630 0.0366410
C -0.0450370 1.1733870 0.0940260
C -1.3218210 0.7538440 0.1360540
C -1.3472450 -0.7331690 -0.0331660
O 2.0337700 -0.1040880 0.0819360
O 0.0258800 -1.1305350 -0.0752880

H 0.2979950 1.6465930 -1.8171170
H -2.2132790 1.3575310 0.2371580
H -1.8415960 -1.2457800 0.7989160
H -1.8353850 -1.0421140 -0.9649760
H 0.3435080 2.1605550 0.2915100
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 627.5312
WellDepth[kcal/mol] 34.7
WellDepth[kcal/mol] 4.3
End
Frequencies[1/cm] 26
199.3880 263.6247
309.5653 401.4506 496.4531
692.7395 706.4338 786.2382
807.3976 870.6223 946.6543
972.9396 1017.2369 1052.6428
1106.7758 1134.0704 1201.4668
1343.7426 1365.3456 1489.4662
1593.4058 1869.2307 3022.2119
3054.1576 3215.2840 3246.6064
ZeroEnergy[kcal/mol] -93.4
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts60b----------
Barrier ts60b ip60 ip19min
RRHO
Geometry[angstrom] 11
C 1.276873865 -0.0963749409 0.3899078043
C 0.0918183224 -0.0467948127 -0.5672753602
C -0.9741753663 0.9531289349 -0.2619888641
C -1.7880632035 0.2028507187 0.6054142778
O 2.3971069874 0.2160257501 0.0854827155
O -0.8308989455 -1.1365487683 -0.3225659982
H 1.023314692 -0.4584894223 1.4105493576
H 0.4713065371 -0.0029936699 -1.5937954631
H -1.3701507512 1.6319199723 -1.0064158673
H -1.4121684326 -0.1969299711 1.5381039314
H -2.8727467048 0.2987652092 0.5687364663
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 762.0844
WellDepth[kcal/mol] 24.0
WellDepth[kcal/mol] 28.1
End

Rotor Hindered #81.9860
Group 5 7
Axis 1 2
Symmetry 1
Potential[kcal/mol] 12
0 0.532065381 1.044866218 0.919740806 1.278990046 1.877069437 0.715800189
0.448920361 2.042543715 3.889555443 2.599772231 0.629392119
End

Frequencies[1/cm] 25

172.0533
292.5233 362.2064 462.7024
609.3108 723.6716 867.3524
888.0857 956.8082 984.9125
1053.0052 1062.4446 1105.8653
1194.3061 1256.4977 1290.6366
1363.9383 1401.2581 1531.5809
1815.0966 2875.3149 3039.2551
3106.5819 3191.0046 3208.3500
ZeroEnergy[kcal/mol] -58.9
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts67b----------
Barrier ts67b ip67 ip69
RRHO
Geometry[angstrom] 11
C -0.9702356846 -0.0560664257 0.190024381
C -0.2706082791 1.128620755 -0.3492078752
C 1.1249573791 -0.9484122807 -0.147327098
C 1.6166849467 0.224786509 0.3602110553
O -0.1852988405 -1.2351284434 0.1167224878
O -2.0594248073 -0.1142705247 0.6733690354
H -0.579932615 2.0800248226 0.0667904157
H -0.0322669323 1.1275329779 -1.4063035456
H 1.5753737392 -1.5385531529 -0.9358640444
H 1.3217998364 0.5697111279 1.3435322362
H 2.5602512574 0.612688635 -0.0073850483
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 613.5548
WellDepth[kcal/mol] 36.5
WellDepth[kcal/mol] 14.6
End
Frequencies[1/cm] 26
126.7880 330.2703
468.5665 519.8355 571.1429
608.2070 669.5743 711.9590

770.1324 805.6540 887.5870
943.0700 961.9718 1018.6947
1073.8695 1181.7791 1265.0961
1419.2925 1436.0603 1553.6889
1858.5418 3137.5922 3138.8706
3189.0779 3222.0458 3234.1714
ZeroEnergy[kcal/mol] -93.0
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts67d----------
Barrier ts67d ip67 p10_p10
RRHO
Geometry[angstrom] 11
C -0.870543 0.034785 0.001304
C 0.119775 1.187850 -0.129557
C 1.201739 -0.832888 -0.082741
C 1.448175 0.484024 -0.113835
O -0.134299 -1.153912 0.012858
O -2.056676 0.037946 0.081213
H -0.033778 1.897838 0.686055
H -0.076416 1.720885 -1.065761
H 1.869529 -1.680012 -0.093236
H 1.962515 0.806634 1.946729
H 2.411073 0.939750 -0.277375
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 374.0243
WellDepth[kcal/mol] 36.7
WellDepth[kcal/mol] 2.7
End
Frequencies[1/cm] 26
153.4448 254.6515
319.2273 454.9593 492.8432
566.8331 676.6542 772.7148
803.4369 833.3748 911.8135
957.2528 984.4709 1049.9043
1091.8817 1166.4403 1175.8816
1281.6763 1366.9341 1439.7248
1618.6553 1900.9938 3048.3028
3090.3646 3242.6254 3262.4923
ZeroEnergy[kcal/mol] -92.8
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts68b----------
Barrier ts68b ip04b ip52
RRHO

Geometry[angstrom] 11
C 1.3778290559 -0.579689346 0.1911744581
C 0.4885953856 0.5597961714 -0.2233507948
C -0.869453399 0.4028165807 -0.0440906299
C -1.3993854036 -0.8776742715 -0.0101100681
O 0.7073382605 -1.7182975934 0.5356866936
O 1.6489684451 -0.1358349765 1.4668306734
H 2.2468083457 -0.7555099677 -0.4670341755
H 0.9575760153 1.5213233001 -0.4035153484
H -1.4820948639 1.2476352518 0.2576229079
H -1.046243055 -1.6715113011 -0.6446966019
H -2.3373847866 -1.0621388478 0.5084618856
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 512.2789
WellDepth[kcal/mol] 107.0
WellDepth[kcal/mol] 80.2
End
Frequencies[1/cm] 26
157.8059 191.7591
437.9143 479.0601 525.9846
627.0929 749.8716 837.2157
877.8332 944.2627 995.6079
1023.6842 1040.9096 1107.2528
1172.7926 1243.8927 1251.0628
1308.5209 1405.6438 1509.4994
1555.5084 2920.8058 3136.3686
3150.9321 3189.1982 3279.9095
ZeroEnergy[kcal/mol] -14.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts68d----------
Barrier ts68d ip68 ip52
RRHO
Geometry[angstrom] 11
C -1.3884859748 0.326026736 0.2704187053
C -0.057628363 0.8883725038 -0.1089138868
C 0.9866962886 0.0492973861 -0.1224726473
C 0.8507646325 -1.3928502013 0.0230415214
O -1.4281584242 -1.055494578 0.1895261928
O -2.3663678225 0.0612562773 -0.6753666553
H -1.7852885436 0.7535275247 1.2014413512
H 0.0586987188 1.9619616462 -0.207223515
H 1.9977395222 0.4551589172 -0.1810017423
H 0.4321386843 -1.9974924037 -0.7672827125
H 1.4587902817 -1.9088948084 0.7615493885
Core RigidRotor
SymmetryFactor 0.5

End
Tunneling Eckart
ImaginaryFrequency[1/cm] 766.0917
WellDepth[kcal/mol] 25.3
WellDepth[kcal/mol] 75.8
End
Frequencies[1/cm] 26
68.5739 131.2541
267.8373 394.1679 456.4976
530.4462 662.9929 748.0281
830.5673 928.0610 934.5401
967.0140 1015.7588 1054.7641
1180.5731 1217.1366 1280.6225
1374.0096 1422.5838 1466.8623
1648.8481 2997.9965 3092.0190
3127.3939 3181.9606 3247.6849
ZeroEnergy[kcal/mol] -18.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts68g----------
Barrier ts68g ip02 ip68
RRHO
Geometry[angstrom] 11
C 0.7944155325 -0.0443854781 0.3705945265
C -0.3292197372 0.2789532705 -0.4991483044
C -1.6926300652 0.4986680413 0.0067449871
C -2.6430352394 -0.43186976 0.0741437443
O 2.0340409788 0.5733094593 0.1001972281
O 1.8023144062 -0.8754318558 -0.1551945735
H 0.5835560645 -0.1971425903 1.4278783205
H -0.0931195078 0.4260197419 -1.5488652792
H -1.9282202566 1.5098329014 0.3478086826
H -3.6295400428 -0.1986436043 0.4585757999
H -2.4686311332 -1.4508051259 -0.2547521319
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 222.1424
WellDepth[kcal/mol] 14.6
WellDepth[kcal/mol] 12.8
End
Frequencies[1/cm] 26
66.4309 226.4754
339.1170 351.8467 458.8906
596.9699 651.8380 772.7822
816.8495 966.1212 978.0926
1006.7946 1085.1878 1141.8286
1160.0628 1223.1372 1288.1267
1316.5773 1430.7658 1458.7218

1682.7869 3067.4822 3120.9024
3134.0628 3162.6844 3220.0792
ZeroEnergy[kcal/mol] -31.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts68i----------
Barrier ts68i ip68 ip04b
RRHO
Geometry[angstrom] 11
C -1.9701220655 0.3019634825 0.3895435205
C -0.4832250338 0.4142929564 0.3781000521
C 0.4467328699 -0.5698622482 0.0093797283
C 0.1714874146 -1.8747586476 -0.3036847878
O -2.4178598502 0.1522535945 -0.9055984393
O -2.5602975835 -0.9219567052 0.5823034515
H -2.4414225918 1.1201056079 0.9528783202
H -0.0954790949 1.4048336138 0.6010763619
H 1.4850582041 -0.2492267473 -0.0256789647
H -0.8395482729 -2.2554770113 -0.2720244791
H 0.9700310039 -2.5455718956 -0.5971037635
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 711.1968
WellDepth[kcal/mol] 22.3
WellDepth[kcal/mol] 99.6
End
Frequencies[1/cm] 26
65.5033 216.1211
237.2192 368.3422 412.1842
525.9531 744.7020 796.9089
854.7354 938.2449 948.0260
1009.9564 1059.0788 1138.9605
1230.5768 1259.6993 1293.7272
1389.8905 1443.3461 1473.9510
1545.2742 2984.4100 3134.4018
3154.1681 3160.3310 3264.2382
ZeroEnergy[kcal/mol] -21.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_91a_91c----------
Barrier ts_91a_91c ip90min ip91
Union
RRHO
Geometry[angstrom] 11
C -1.796475 0.336106 0.208385
C -0.427459 0.648377 0.248637

C 0.636493 -0.271452 -0.225284
C 1.881516 -0.448887 0.552437
O -2.477950 -0.603701 -0.121635
O 1.865531 0.340194 -0.633968
H -1.450655 1.348358 -0.527391
H -0.135811 1.561733 0.754435
H 0.297300 -1.091640 -0.852121
H 2.013789 0.101202 1.480909
H 2.410276 -1.396462 0.483940
Core RigidRotor
SymmetryFactor 0.5
End

Tunneling Eckart
ImaginaryFrequency[1/cm] 1527.8180
WellDepth[kcal/mol] 42.8
WellDepth[kcal/mol] 42.1
End

Rotor Hindered #69.3541
Group 1 5 7 8
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 0.878513426 2.555658307 2.814631515 1.933294296 1.498555652 2.304779973
3.299068918 3.588915598 3.721382873 2.700738524 0.838541065
End

Frequencies[1/cm] 25
160.9217
290.1038 361.2778 570.6113
622.7643 714.9159 838.6771
856.3497 923.4112 1068.2422
1100.5493 1141.9007 1163.5251
1176.3488 1193.5347 1270.0305
1327.7601 1443.8579 1521.8399
1797.5552 1887.3391 3081.2152
3136.9840 3172.2428 3187.0030
ZeroEnergy[kcal/mol] -51.2
ElectronicLevels[1/cm] 1
0 2
End

RRHO
Geometry[angstrom] 11
C -1.800063 0.389185 0.011867
C -0.430287 0.691683 -0.016027
C 0.639815 -0.338206 -0.118444
C 1.887978 -0.230776 0.659926
O -2.494818 -0.596144 -0.025335
O 1.864383 0.103097 -0.725351
H -0.146798 1.732489 -0.125594

H -1.342282 0.998320 1.075609
H 0.301044 -1.324057 -0.425796
H 2.020298 0.606136 1.341738
H 2.426561 -1.139827 0.915593
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1530.3200
WellDepth[kcal/mol] 43.3
WellDepth[kcal/mol] 42.6
End

Rotor Hindered #60.0288
Group 1 5 7 8
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 0.536771703 1.60378901 2.419174971 2.43153691 1.252320889 0.813252429 2.066891088 3.666977791 4.183480935 2.544927893 0.692080327
End

Frequencies[1/cm] 25
160.5794
298.4870 357.0639 577.3931
609.9035 708.5276 826.7108
857.4640 933.8338 1075.9102
1099.2396 1143.0551 1154.0573
1174.8646 1200.4326 1271.8607
1318.3172 1439.8733 1522.6855
1800.7742 1863.7972 3080.6911
3133.9572 3171.7884 3184.5850
ZeroEnergy[kcal/mol] -50.7
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------ts_ts91b----------
Barrier ts91b ip91 p4_p4_db
RRHO
Geometry[angstrom] 11
C -1.907122 0.156731 0.100462
C -0.809746 0.929512 0.156444
C 1.138707 0.157603 -0.622545
C 1.705611 -0.954642 0.121566
O -2.703881 -0.676964 -0.074507
O 2.142840 0.424563 0.303002
H -0.835623 1.813529 -0.470625
H -0.364160 1.058712 1.137198
H 1.311673 0.392046 -1.672492
H 1.154524 -1.374455 0.960244

H 2.457213 -1.605843 -0.317840
Core RigidRotor
SymmetryFactor 0.5
End

Tunneling Eckart
ImaginaryFrequency[1/cm] 467.5804
WellDepth[kcal/mol] 43.1
WellDepth[kcal/mol] 9.2
End

Rotor Hindered #22.8011
Group 1 5 7 8
Axis 2 3
Symmetry 1
Potential[kcal/mol] 12
0 0.096950232 0.184738823 0.295180511 0.569527704 0.856927096 0.889432093
0.676329836 0.334713615 0.258157445 0.235943606 0.106802132
End

Frequencies[1/cm] 25
90.2148
155.0370 192.0137 407.0756
411.4343 554.4126 776.5734
811.7463 848.6820 929.9175
1043.9767 1052.5316 1070.7890
1096.9052 1127.4944 1160.4108
1324.6188 1391.0233 1522.3593
2154.2926 3075.1668 3090.7896
3130.7142 3162.5597 3213.5554
ZeroEnergy[kcal/mol] -50.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_tsp1a----------
Barrier tsp1a ip04 p1_p1
RRHO
Geometry[angstrom] 11
C 2.2502083716 -0.2381907372 0.1728769157
C -0.4152400355 -0.0668551171 -0.1292121481
C -1.8128226069 -0.364275053 0.0852099292
C -2.7592266387 0.5860962861 0.011888908
O 2.3056428949 0.9392547079 0.059268454
O 0.4702609792 -0.9380664411 -0.1212926738
H 2.742406962 -1.030368862 -0.4219637219
H -0.127105139 0.9837681392 -0.2908084189
H -2.0605531029 -1.4013478551 0.2880825497
H -3.8086086436 0.3590452501 0.1528100985
H -2.5033080412 1.6201866823 -0.1959598924
Core RigidRotor
SymmetryFactor 0.5

End
Tunneling Eckart
ImaginaryFrequency[1/cm] 519.8052
WellDepth[kcal/mol] 38.6
WellDepth[kcal/mol] 11.6
End
Frequencies[1/cm] 26
102.7317 119.7476
145.7372 267.4020 300.3078
454.0738 544.7464 613.4250
773.8355 944.4181 959.2641
990.4409 1024.5863 1060.7772
1190.9450 1299.0236 1368.6747
1446.4881 1568.2250 1638.1854
1814.9516 2877.2941 2998.0125
3138.6495 3169.8737 3231.2280
ZeroEnergy[kcal/mol] -82.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_tsp1bmin----------
Barrier tsp1bmin ip19min p1_p1
RRHO
Geometry[angstrom] 11
C 1.3684410571 -0.3014480206 -0.4005024766
C -0.1995871795 0.6875896601 0.3923923569
C -1.2874869899 0.0015385276 -0.3645835762
C -1.9488764179 -1.0559596475 0.1086855293
O 2.0457891773 -1.0231492847 0.2223135291
O 0.1751490543 1.8474611072 0.1067913858
H 1.5347712013 0.1396445303 -1.4020120192
H -0.0326712618 0.2777093097 1.4083126461
H -1.5323124642 0.4449125656 -1.3263374105
H -2.752744883 -1.5250026 -0.4460540718
H -1.7086132937 -1.4827501477 1.0782291072
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 313.2769
WellDepth[kcal/mol] 3.2
WellDepth[kcal/mol] 9.9
End

Rotor Hindered #45.9630
Group 5 7
Axis 1 2
Symmetry 1
Potential[kcal/mol] 12
0 0.431663847 0.904366821 0.687562258 0.57843834 1.118222089 2.834272565 2.019074857
2.080508046 2.397902396 2.451240711 0.577999083

End

Frequencies[1/cm] 25

128.0711
191.9263 269.3084 285.9630
373.4083 552.2762 647.5296
704.5117 905.2032 967.2028
1008.8476 1038.1274 1125.5011
1146.3404 1290.6180 1352.3400
1427.9312 1510.5584 1672.9867
1922.9261 2896.3819 2903.5592
3129.0813 3152.4811 3218.6567
ZeroEnergy[kcal/mol] -83.8
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_tsp1d----------
Barrier tsp1d ip04b p1_p1
RRHO
Geometry[angstrom] 11
C 2.7906143112 -0.6866803478 0.3023629474
C 0.3464284799 0.390444977 -0.1461330057
C -1.0933112175 0.5616958703 -0.0337773121
C -1.9477088919 -0.4689017818 0.0661736736
O 3.2292224769 0.410094947 0.3640393194
O 0.9043306591 -0.7171308788 -0.2049009392
H 3.0588494617 -1.5194997951 -0.3753919425
H 0.9731011023 1.294524101 -0.1583241046
H -1.4546513015 1.5854874684 -0.0353102463
H -3.0160427754 -0.3142288907 0.1530764919
H -1.5815133047 -1.4890156696 0.0684021182
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 514.4805
WellDepth[kcal/mol] 42.2
WellDepth[kcal/mol] 14.7
End
Frequencies[1/cm] 26
63.1866 116.0643
187.7676 229.2106 283.0186
447.7021 574.4178 672.3418
755.1220 971.1529 976.6194
993.1793 1018.0777 1057.3273
1082.9114 1311.0049 1394.0000
1440.4249 1531.4848 1663.0497
1823.5143 2869.8468 3009.8306
3146.8041 3164.1595 3241.1628
ZeroEnergy[kcal/mol] -79.0

ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_tsp1g----------
Barrier tsp1g ip38min p1_p1
RRHO
Geometry[angstrom] 11
C -1.7783134617 -0.1547056558 -0.4701320181
C -0.7573251889 0.9038216434 -0.4311013853
C 1.7178760806 -0.5522426786 0.2029211509
C -0.001693247 1.1108864402 0.6713003525
O 2.7283410573 -0.2848214351 -0.3310781212
O -1.9305833918 -0.9925585975 0.3980067592
H -2.4259085763 -0.1561658837 -1.3711390876
H -0.6205334105 1.5011132899 -1.3274091845
H 1.074918168 -1.4464781987 0.0189065053
H -0.2215418352 0.5680689851 1.5825247983
H 0.7181078055 1.9174780909 0.7286162305
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 210.0774
WellDepth[kcal/mol] 27.4
WellDepth[kcal/mol] 4.7
End

Rotor Hindered #81.5612
Group 5 9
Axis 3 4
Symmetry 1
Potential[kcal/mol] 12
0 0.449987127 1.042795437 1.254517172 1.25828223 1.28444938 1.620731769 2.410327086
2.408444557 2.01273701 1.7372603 0.747301171
End

Frequencies[1/cm] 25
49.5966
129.5699 196.5410 273.7947
319.4251 497.4490 627.9202
703.0421 943.8953 979.1240
994.5259 1026.3484 1074.7012
1090.6551 1294.1972 1417.7785
1430.5380 1582.1089 1746.1552
1910.5281 2765.1978 2900.0924
3150.3185 3164.3037 3246.0913
ZeroEnergy[kcal/mol] -89.0
ElectronicLevels[1/cm] 1
0 2
End
!----------

!-------ts_tsp4b------------
Barrier tsp4b ip21min p4_p4
RRHO
Geometry[angstrom] 11
C 1.7605875601 -0.0564773712 0.119045655
C 0.9920426421 1.0770597395 0.0749271216
C -1.4857804274 0.1106854733 0.3263588473
C -2.2371794242 -0.9204175074 -0.0992626459
O -0.7542100455 0.8625315065 -0.4848008515
O 2.057514125 -1.1801980269 0.0574278201
H 0.8411799867 1.5419870081 1.0449216164
H 1.2617447142 1.7610138507 -0.7217762228
H -1.5032318624 0.3951280919 1.3858998194
H -2.9138939844 -1.4264921756 0.5776173333
H -2.2223452841 -1.218215589 -1.1407264931
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 609.9772
WellDepth[kcal/mol] 25.7
WellDepth[kcal/mol] 22.6
End

Rotor Hindered #48.4451
Group 1 6 7 8
Axis 2 5
Symmetry 1
Potential[kcal/mol] 12
0 0.446661326 1.476969322 1.962410741 2.053525133 2.190824232 1.714418951
0.869728292 0.511294814 0.552522194 0.583332915 0.26173425
End

Frequencies[1/cm] 25
64.4693
163.6336 239.7802 399.7056
421.5092 517.1796 695.6032
738.0130 861.2007 915.6658
980.3475 1013.9059 1042.8147
1086.7399 1209.7517 1318.0727
1389.7564 1425.7638 1607.3000
2119.1450 3021.5800 3131.6576
3146.3925 3215.9024 3241.4683
ZeroEnergy[kcal/mol] -72.3
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_tsp4c------------
Barrier tsp4c ip16 p4_p4
RRHO
Geometry[angstrom] 11

C 1.907665633 -0.2023816303 -0.0118961597
C 1.255006218 0.9488965366 0.0858044499
C -1.3042088861 -0.2427173395 -0.1093351885
C -2.6789462728 -0.3034064602 0.1279029222
O -0.7145976263 0.8541554977 -0.3192487727
O 2.0730698337 -1.3898098081 -0.0310185213
H 2.73996924 0.639641541 0.384771696
H 1.3944639345 1.8453139573 -0.4934798992
H -0.7253365694 -1.1737162956 -0.1347239332
H -3.1850077243 -1.2555891761 0.225749693
H -3.2533027803 0.6135761772 0.1753097135
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 910.6503
WellDepth[kcal/mol] 67.8
WellDepth[kcal/mol] 61.2
End
Frequencies[1/cm] 26
54.9143 68.4315
126.7177 192.7302 259.8661
464.0902 522.4447 537.5512
579.2121 689.2091 827.2762
852.3319 991.0409 1014.5175
1131.8987 1183.6481 1270.8491
1344.9241 1451.3069 1489.8134
1960.3682 2084.3698 3050.1335
3149.0443 3260.6833 3300.4511
ZeroEnergy[kcal/mol] -33.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_tsp4dmin----------
Barrier tsp4dmin ip39 p4_p4
RRHO
Geometry[angstrom] 11
C -1.9552736012 0.2394119226 -0.1803121948
C -0.6761326074 0.5130371182 -0.5359403985
C 1.9973693464 -0.270469129 -0.261691322
C 0.765386576 -0.9256859084 0.1088508142
O 2.5125974144 0.6386285583 0.3796454549
O -2.923493833 -0.2514745799 0.2315793072
H -0.2173610939 1.341958252 -0.0046360749
H -0.5071240363 0.5088464605 -1.6081144578
H 2.4452171683 -0.6002798991 -1.2240624488
H 0.4602867238 -1.8080177021 -0.4437800441
H 0.4921229427 -0.8926660931 1.1574013645
Core RigidRotor
SymmetryFactor 0.5
End

Tunneling Eckart
ImaginaryFrequency[1/cm] 506.1586
WellDepth[kcal/mol] 31.2
WellDepth[kcal/mol] 9.4
End

Rotor Hindered #47.1414
Group 1 6 7 8
Axis 2 4
Symmetry 1
Potential[kcal/mol] 12
0 0.662712878 1.449107896 1.297501579 1.491276541 2.280809107 2.415598167
1.631838689 0.808169601 0.851154008 1.084650326 0.507027749
End

Frequencies[1/cm] 25
86.2870
136.6677 246.3498 411.8086
431.7665 510.1826 584.4321
805.6865 876.7488 926.2626
981.8339 996.0050 1064.4563
1071.7241 1161.9669 1397.1735
1401.6999 1467.2276 1663.6229
2155.5374 2870.5169 3123.1820
3124.9359 3204.3143 3224.1567
ZeroEnergy[kcal/mol] -85.5
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_tsp4e----------
Barrier tsp4e ip69 p4_p4
RRHO
Geometry[angstrom] 11
C -1.1627863028 -0.0132181823 0.0329768339
C -1.0525605428 1.2580100843 -0.4247135044
C 1.5440529694 -0.2947779073 -0.3267994419
C 1.7113328982 0.4524498876 0.836125447
O 0.4497199785 -0.7774891529 -0.7452877614
O -1.7236610593 -0.8573375748 0.613658871
H -1.9005446764 1.9083872308 -0.2515374234
H -0.2200392939 1.5924415039 -1.0128288256
H 2.4313187935 -0.4938532775 -0.9427152116
H 0.9135188866 0.5546660489 1.5584121515
H 2.675923349 0.887771339 1.063358865
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 473.5172
WellDepth[kcal/mol] 24.3
WellDepth[kcal/mol] 14.6

End
Frequencies[1/cm] 26
71.9767 140.2688
188.5065 371.9726 433.0641
447.8228 567.4239 591.5869
635.2063 645.4679 803.6454
962.0184 980.4289 1014.3223
1106.9387 1233.5856 1344.4878
1434.3619 1473.6795 1506.6838
2050.3342 3024.9433 3160.7732
3176.6058 3265.7659 3323.5009
ZeroEnergy[kcal/mol] -80.3
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts86a----------
Barrier ts86a ip06 ip86
RRHO
Geometry[angstrom] 11
C -1.68964362 0.0560807485 -0.2318026432
C -0.5694828035 0.6412568012 0.1880882153
C 0.5587111308 -0.2778821465 0.5020191909
C 1.5758754463 -0.5086102546 -0.4128151542
O -1.7094904794 -1.2989035084 -0.3446504481
O -0.5921762934 -1.8040252585 0.3422761852
H -2.6008201888 0.5209354577 -0.5841620067
H -0.4607675849 1.7159719475 0.2303448088
H 0.7647111781 -0.4907154794 1.5466238233
H 1.4698129907 -0.2039762576 -1.4470202835
H 2.434863224 -1.11179005 -0.1456906879
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 568.6183
WellDepth[kcal/mol] 19.1
WellDepth[kcal/mol] 15.2
End
Frequencies[1/cm] 26
165.2810 239.3355
353.9210 485.3393 545.2119
619.0592 695.4893 826.6407
837.1104 862.6373 916.2818
926.5604 1029.1048 1052.0582
1100.7590 1174.2360 1260.5946
1342.3327 1422.4486 1505.0771
1665.5886 3140.2200 3142.9678
3207.3661 3229.0029 3242.2691
ZeroEnergy[kcal/mol] -25.3
ElectronicLevels[1/cm] 1
0 2

End
!----------
!-------ts_ts86c----------
Barrier ts86c ip86 ip90min
RRHO
Geometry[angstrom] 11
C -1.3921666224 0.5463925637 -0.1550593465
C -0.2688343521 1.2159689077 0.1218088666
C 0.8042723151 0.2240083713 0.4855764193
C 2.0038790599 0.0534097924 -0.3589358928
O -1.3892730681 -0.7854178205 -0.1536878029
O 0.3184100017 -1.037587412 0.0367653724
H -2.3645291966 0.9801071446 -0.3804633427
H -0.1698637403 2.28777153 0.1900363308
H 1.0226478446 0.2123046855 1.5625917272
H 1.9306737931 0.2654173227 -1.417069222
H 2.8601149651 -0.4943320855 0.0133168906
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 730.0084
WellDepth[kcal/mol] 12.1
WellDepth[kcal/mol] 65.6
End
Frequencies[1/cm] 26
180.6171 307.6909
355.7590 427.9700 524.2471
635.1834 688.0549 729.8319
798.6588 873.2884 889.1048
948.0582 1058.6457 1083.0926
1156.2151 1179.0717 1264.2309
1324.9394 1368.7571 1456.7138
1633.3182 2980.0744 3142.6381
3151.9534 3245.7010 3272.5615
ZeroEnergy[kcal/mol] -28.4
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_86e_86p----------
Barrier ts_86e_86p ip86 ip38min
Union
RRHO
Geometry[angstrom] 11
C -1.2408838883 0.3111036141 -0.8369056883
C -0.3154323178 0.5774715512 0.1134872787
C 0.3808593379 -0.7468583423 0.4342611613
C 1.6291410492 -0.4068980822 -0.2906434985
O -1.3264505648 -0.9199026363 -1.2802301578
O -0.409203448 -1.7555329035 -0.1076600991
H -1.9934482432 0.9996140897 -1.210430644

H -0.1221875003 1.5203104003 0.5969088511
H 0.4836988861 -0.9383586481 1.5082100543
H 1.7065336319 -0.6473481327 -1.3427197837
H 2.3390180573 0.2799820899 0.1524635259
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1090.6034
WellDepth[kcal/mol] 14.4
WellDepth[kcal/mol] 90.3
End
Frequencies[1/cm] 26
143.2492 273.0924
386.4455 451.4683 480.1530
607.1811 677.5475 701.9620
818.7748 840.4552 884.2029
920.1950 1046.0097 1091.8436
1101.4103 1140.5942 1164.2872
1304.3156 1318.9020 1438.0595
1471.6910 3027.1893 3149.9149
3167.6735 3266.2835 3268.5611
ZeroEnergy[kcal/mol] -26.1
ElectronicLevels[1/cm] 1
0 2
End
RRHO
Geometry[angstrom] 11
C 1.401367 0.611397 0.146445
C 0.209308 1.107611 -0.278366
C -0.807501 -0.009639 -0.354374
C -2.043322 0.132708 0.462989
O 1.594696 -0.650637 0.264539
O -0.153573 -1.209091 -0.249064
H 2.197089 1.261002 0.521484
H -0.035178 2.150027 -0.415754
H -1.152883 0.058739 -1.425962
H -2.625177 -0.753679 0.682169
H -2.471952 1.109278 0.654094
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 666.4428
WellDepth[kcal/mol] 16.0
WellDepth[kcal/mol] 91.9
End
Frequencies[1/cm] 26
102.4152 154.3099
290.0783 374.8276 481.0522
538.8272 625.4998 680.7671
735.4520 848.0487 867.1281

890.1695 976.3600 1074.7152
1117.7303 1135.9160 1172.2918
1209.8150 1342.9718 1394.5067
1436.5772 2695.0821 3083.4219
3137.4355 3238.8430 3254.7228
ZeroEnergy[kcal/mol] -24.5
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------ts_ts90a----------
Barrier ts90a ip90min ip33
RRHO
Geometry[angstrom] 11
C -1.5020017199 -0.2337555812 0.0459359334
C -0.3636471525 0.6915951481 -0.0274233986
C 0.9542781284 0.3636085825 -0.2569019525
C 1.5074510985 -1.0256385088 -0.3527097973
O -1.4754099094 -1.4209129858 -0.2105035265
O 1.6319671442 -0.8161793343 1.010343485
H -2.4518513832 0.2487987655 0.3545016752
H -0.6064477327 1.7408754454 0.1150744653
H 1.6893572999 1.1574663247 -0.278558495
H 0.7997007096 -1.7990641916 -0.6463370784
H 2.4560695171 -1.0674636646 -0.9004283106
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 442.6846
WellDepth[kcal/mol] 15.8
WellDepth[kcal/mol] 11.7
End
Frequencies[1/cm] 26
103.8634 152.9092
247.4930 366.0913 400.3943
721.5036 802.1033 843.9433
935.7964 987.0015 1015.3040
1050.7706 1148.8965 1169.9175
1240.1186 1276.8887 1407.7124
1440.3306 1486.0052 1519.1371
1730.6859 2904.4732 3008.4661
3126.9191 3154.9672 3203.2274
ZeroEnergy[kcal/mol] -78.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts90c----------
Barrier ts90c ip90min ip94
RRHO

Geometry[angstrom] 11
C -1.3728329169 -0.1843506587 -0.0246186292
C -0.4218446192 0.7803004558 0.099406703
C 0.9763979103 0.4299110224 -0.0744804608
C 1.3116602038 -0.9842752766 -0.2775028645
O -1.1531029749 -1.4599089555 -0.2305660202
O 1.634356302 -0.5264464957 0.9626476988
H -2.4349495827 0.0706655399 0.0091208921
H -0.7135880787 1.8067884166 0.2661736463
H 1.6923838464 1.1949623513 -0.3499224827
H 0.1969643467 -1.5314276258 -0.3119422258
H 2.0712035632 -1.4575257736 -0.9018932569
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1242.6071
WellDepth[kcal/mol] 33.3
WellDepth[kcal/mol] 13.9
End
Frequencies[1/cm] 26
183.3687 238.5177
374.6088 516.8605 571.7598
610.4771 715.0997 858.5493
874.6919 903.7264 978.6921
1040.3218 1077.1177 1122.2034
1155.9576 1226.6865 1261.0996
1278.3955 1364.8774 1444.4466
1503.4603 1640.8182 3082.8068
3084.1350 3173.6689 3220.0349
ZeroEnergy[kcal/mol] -60.7
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts94a------------
Barrier ts94a ip94 ip40
RRHO
Geometry[angstrom] 11
C -1.2265521231 -0.1001519475 0.2138036747
C -0.1534054223 0.7184522308 0.0082000316
C 1.1455276624 0.2345179285 -0.2994890543
C 1.5444083772 -1.1687206089 -0.2140951125
O -1.2234568599 -1.4216959314 0.1733620583
O 2.0840040069 -0.7890396924 0.9179629688
H -2.2046737676 0.3051087021 0.4553796778
H -0.3078542865 1.784057018 0.1202299229
H 1.9225694268 0.957939253 -0.5254999978
H 2.0330157361 -1.8231666577 -0.940176192
H -0.27964775 -1.7183982945 0.0459760225
Core RigidRotor
SymmetryFactor 0.5

```
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  410.1904
WellDepth[kcal/mol]  5.1
WellDepth[kcal/mol]  47.0
End
Frequencies[1/cm]  26
151.0648            228.4831
287.9360            450.9882            536.8929
719.2659            799.0905            842.9120
858.5082            928.8935            942.7056
1003.4393           1085.2570           1175.7494
1267.5945           1283.0067           1315.5775
1396.2069           1440.4919           1494.1930
1629.1501           3050.9080           3102.6828
3149.2206           3177.5060           3196.7279
ZeroEnergy[kcal/mol]  -69.5
ElectronicLevels[1/cm] 1
0  2
End
!---------------------------------
!---------------------------------
Barrier B6      ip48    p2_p2
   Variational
            RRHO                                ! R=1.4
        Geometry[angstrom]              11
C       -1.3311200    -0.6988760    -0.1546890
C       -1.4068350    0.6862070     -0.1701110
C       -0.1680690    1.1838610     0.1918310
C       0.7553950     0.0260140     0.4312360
O       -0.0995370    -1.1452210    0.1906800
O       1.8956380     -0.0212630    -0.3734980
H       -2.0675500    -1.4540840    -0.3803000
H       -2.2878820    1.2539440     -0.4305830
H       0.1365220     2.2131640     0.3003790
H       1.1270250     -0.0733900    1.4552000
H       1.6268540     0.2090050     -1.2717440
        Core    RigidRotor
          SymmetryFactor                0.5
        End
      Frequencies[1/cm]                 26
                                        345.9804            442.9845
 521.8116           544.7392           625.7272
 659.6480           756.0000           815.4749
 873.8939           882.9127           979.0763
1026.6694           1079.4509          1123.5799
1176.0912           1261.8427          1297.4696
1350.1105           1398.7736          1442.8200
1496.0932           3050.8632          3223.6028
3241.8434           3255.5159          3783.9487
      ZeroEnergy[kcal/mol]              -119.5
      ElectronicLevels[1/cm]            1
```

```
                0       2
    End
            RRHO                                ! R=1.5
        Geometry[angstrom]              11
C       -1.3307120      -0.7065640      -0.1759970
C       -1.4190750      0.6762040       -0.1946210
C       -0.1950570      1.1800560       0.2107300
C       0.7205260       0.0305040       0.4552910
O       -0.1043150      -1.1337040      0.2202960
O       1.9534370       -0.0147800      -0.3915570
H       -2.0458610      -1.4753450      -0.4210260
H       -2.2956120      1.2386700       -0.4793260
H       0.1021580       2.2105050       0.3248730
H       1.1350530       -0.0562520      1.4610960
H       1.6571990       0.1890870       -1.2879520
        Core    RigidRotor
          SymmetryFactor                0.5
        End
      Frequencies[1/cm]                 26
                                        326.3743        410.8586
 480.0946           529.7665        629.2132
 662.1169           758.0139        829.4746
 846.2351           881.8514        902.8414
 998.3660          1046.8092        1117.1381
1161.4859           1219.2179       1288.5330
1352.7774           1396.8865       1397.5101
1494.9553           3079.0023       3228.3455
3247.3577           3261.7791       3787.4953
      ZeroEnergy[kcal/mol]              -117.4
      ElectronicLevels[1/cm]            1
                0       2
    End
            RRHO                                ! R=1.6
        Geometry[angstrom]              11
C       -1.3313680      -0.7113930      -0.1982440
C       -1.4284080      0.6691890       -0.2203520
C       -0.2193450      1.1756790       0.2302610
C       0.6866900       0.0342430       0.4802730
O       -0.1161620      -1.1236200      0.2495170
O       2.0121520       -0.0115650      -0.4083260
H       -2.0276800      -1.4897910      -0.4649260
H       -2.2975770      1.2287950       -0.5310080
H       0.0717000       2.2067680       0.3520710
H       1.1446340       -0.0462120      1.4647070
H       1.6955890       0.1756190       -1.3019980
        Core    RigidRotor
          SymmetryFactor                0.5
        End
      Frequencies[1/cm]                 26
                                        300.5102        319.5680
 376.3113           528.8276        617.7002
 673.3622           689.7981        808.5512
```

```
 856.4271            882.3943            915.2078
1000.3102           1053.3708           1117.6609
1157.7114           1170.1475           1285.1156
1334.5115           1360.0271           1398.5742
1494.4756           3109.1807           3232.4502
3251.0320           3266.0012           3786.4063
      ZeroEnergy[kcal/mol]                  -112.5
      ElectronicLevels[1/cm]                1
                  0       2
    End
          RRHO                                  ! R=1.7
        Geometry[angstrom]                      11
C       -1.3340620      -0.7137230      -0.2193610
C       -1.4362950      0.6645840       -0.2458330
C       -0.2408300      1.1704770       0.2479340
C       0.6523660       0.0372580       0.5049620
O       -0.1334520      -1.1143930      0.2747920
O       2.0732050       -0.0111230      -0.4206270
H       -2.0136110      -1.4988490      -0.5080700
H       -2.2959590      1.2234320       -0.5822470
H       0.0455020       2.2017390       0.3782220
H       1.1538240       -0.0421640      1.4649180
H       1.7451400       0.1683900       -1.3123600
        Core    RigidRotor
          SymmetryFactor                0.5
        End
      Frequencies[1/cm]                 26
                                        214.1467            277.8787
 338.1820            532.8176            592.2361
 684.5593            696.9466            819.0317
 864.6031            883.7660            921.7969
1005.2209           1059.5108           1103.2177
1131.1451           1156.3028           1260.6568
1287.5729           1361.9421           1402.7877
1495.0197           3142.4033           3236.1817
3253.3858           3268.6490           3783.1369
      ZeroEnergy[kcal/mol]                  -106.8
      ElectronicLevels[1/cm]                1
                  0       2
    End
          RRHO                                  ! R=1.8
        Geometry[angstrom]                      11
C       -1.3404760      -0.7133300      -0.2377780
C       -1.4439990      0.6623590       -0.2694090
C       -0.2586360      1.1643320       0.2622930
C       0.6168370       0.0393990       0.5278630
O       -0.1553840      -1.1060370      0.2933890
O       2.1378950       -0.0135430      -0.4264430
H       -2.0061850      -1.5025720      -0.5466470
H       -2.2925900      1.2228850       -0.6293900
H       0.0249210       2.1952370       0.4012420
H       1.1634930       -0.0442380      1.4590230
```

```
H       1.8079160      0.1687700     -1.3176060
        Core    RigidRotor
          SymmetryFactor                  0.5
        End
      Frequencies[1/cm]                   26
                                          206.7658          255.9151
 297.6530          541.5804          576.9828
 702.6299          725.1359          831.7428
 871.5654          885.3930          915.2421
1012.3201         1050.6697         1070.8177
1126.9954         1155.4958         1182.4373
1284.4760         1365.0915         1411.0945
1497.5308         3178.5704         3239.5039
3254.7203         3270.2782         3778.0256
      ZeroEnergy[kcal/mol]                -101.2
      ElectronicLevels[1/cm]              1
                0       2
    End
            RRHO                                ! R=1.9
        Geometry[angstrom]                11
C       -1.3520990     -0.7102800     -0.2526110
C       -1.4530020      0.6622700     -0.2893090
C       -0.2723910      1.1575390      0.2725980
C        0.5800610      0.0406280      0.5474620
O       -0.1807420     -1.0988740      0.3038490
O        2.2070940     -0.0187060     -0.4249810
H       -2.0081660     -1.5012990     -0.5771830
H       -2.2900080      1.2269930     -0.6684860
H        0.0104950      2.1875740      0.4198580
H        1.1771330     -0.0523590      1.4424150
H        1.8843150      0.1787890     -1.3163880
        Core    RigidRotor
          SymmetryFactor                  0.5
        End
      Frequencies[1/cm]                   26
                                          193.1614          228.5920
 260.0409          555.0749          572.7534
 725.2902          757.2552          840.9430
 878.3098          886.6308          888.3880
 997.6262         1025.2772         1078.6771
1095.0429         1129.5616         1164.9910
1283.2289         1370.0290         1423.2221
1503.4322         3216.7255         3242.2451
3255.3818         3271.4415         3770.7870
      ZeroEnergy[kcal/mol]                -96.9
      ElectronicLevels[1/cm]              1
                0       2
    End
            RRHO                                ! R=2.0
        Geometry[angstrom]                11
C       -1.3692330     -0.7057740     -0.2637250
C       -1.4651700      0.6633790     -0.3038600
```

```
C       -0.2837110      1.1512970       0.2782180
C       0.5428490       0.0410480       0.5626480
O       -0.2070110      -1.0935270      0.3063040
O       2.2813170       -0.0254560      -0.4166340
H       -2.0204260      -1.4969930      -0.5973960
H       -2.2922240      1.2336980       -0.6956060
H       0.0000130       2.1802000       0.4325320
H       1.1980750       -0.0645280      1.4104930
H       1.9716980       0.1997860       -1.3070720
        Core    RigidRotor
          SymmetryFactor                0.5
        End
      Frequencies[1/cm]                 26
                                        170.9659        190.7033
 231.1518        570.7134        579.0153
 744.4335        784.1381        807.4333
 870.5161        884.0751        888.9891
 937.2209       1028.5035       1051.4429
1087.0227       1136.9796       1171.7631
1282.0327       1378.8653       1436.3312
1513.4633       3242.5806       3252.0617
3259.8924       3272.9965       3762.4700
      ZeroEnergy[kcal/mol]              -94.4
      ElectronicLevels[1/cm]            1
                0       2
    End
          RRHO                                  ! R=2.1
        Geometry[angstrom]              11
C       -1.3902770      -0.7017300      -0.2714750
C       -1.4814590      0.6643360       -0.3128890
C       -0.2954450      1.1470280       0.2789090
C       0.5067970       0.0412900       0.5735480
O       -0.2314550      -1.0901880      0.3030010
O       2.3602750       -0.0316180      -0.4033250
H       -2.0402960      -1.4927440      -0.6075790
H       -2.3021270      1.2396010       -0.7103570
H       -0.0098910      2.1749910       0.4366630
H       1.2229190       -0.0765310      1.3654310
H       2.0611420       0.2235880       -1.2901240
        Core    RigidRotor
          SymmetryFactor                0.5
        End
      Frequencies[1/cm]                 26
                                        133.9458        169.9075
 201.3465        584.0370        588.6226
 719.4414        758.5982        804.8692
 860.1148        885.3889        889.8741
 896.2007       1023.3381       1047.6277
1090.8930       1146.4994       1179.0052
1280.9858       1390.3320       1447.8110
1526.0574       3243.8397       3254.6928
3273.1031       3289.4620       3755.4729
```

```
      ZeroEnergy[kcal/mol]                -93.3
      ElectronicLevels[1/cm]              1
                0       2
    End
          RRHO                                  ! R=2.2
      Geometry[angstrom]                11
C     -1.4130230    -0.6991030    -0.2766170
C     -1.5009500    0.6644670     -0.3180010
C     -0.3089570    1.1449630     0.2758440
C     0.4728500     0.0418610     0.5812810
O     -0.2532630    -1.0883620    0.2970580
O     2.4424190     -0.0360990    -0.3877260
H     -2.0638700    -1.4902130    -0.6104000
H     -2.3187870    1.2429740     -0.7163870
H     -0.0213910    2.1723890     0.4335820
H     1.2480890     -0.0854770    1.3115300
H     2.1431870     0.2428860     -1.2680200
      Core    RigidRotor
        SymmetryFactor              0.5
      End
     Frequencies[1/cm]                26
                                      96.0919          165.5101
 176.5262          574.5058          593.3983
 657.4273          762.2968          795.3645
 841.9752          885.3878          890.7918
 894.7684         1020.1737         1050.1319
1092.1845         1153.7913         1184.2990
1280.6105         1400.2104         1458.2775
1538.5779         3244.2174         3255.0692
3274.7442         3309.2456         3750.4467
      ZeroEnergy[kcal/mol]                -92.9
      ElectronicLevels[1/cm]              1
                0       2
    End
          RRHO                                  ! R=2.3
      Geometry[angstrom]                11
C     -1.4356900    -0.6982200    -0.2797940
C     -1.5222850    0.6634160     -0.3213620
C     -0.3245890    1.1447360     0.2700810
C     0.4411840     0.0435090     0.5871750
O     -0.2726660    -1.0872220    0.2910810
O     2.5262840     -0.0380690    -0.3715950
H     -2.0879070    -1.4901570    -0.6083990
H     -2.3398840    1.2430790     -0.7184980
H     -0.0354750    2.1721260     0.4249620
H     1.2689770     -0.0895590    1.2555670
H     2.2136320     0.2461870     -1.2461150
      Core    RigidRotor
        SymmetryFactor              0.5
      End
     Frequencies[1/cm]                26
                                      66.0543          136.0771
```

```
 196.4610          517.1271          599.6193
 647.6125          761.4810          770.8250
 844.0786          886.0498          891.2149
 894.6679         1018.9352         1051.9988
1092.5932         1158.2662          1187.0624
1280.8673         1406.0652          1467.9200
1549.2643         3244.4133          3255.3098
3275.9712         3317.5263          3746.6886
      ZeroEnergy[kcal/mol]                -92.7
      ElectronicLevels[1/cm]              1
                0        2
    End
                  RRHO                                          ! R=2.4
         Geometry[angstrom]               11
C        -1.4569070    -0.6991660    -0.2819050
C        -1.5441530    0.6609390     -0.3253490
C        -0.3425940    1.1459330     0.2627330
C        0.4114730     0.0469750     0.5926460
O        -0.2903210    -1.0859920    0.2873460
O        2.6104980     -0.0367480    -0.3560910
H        -2.1096710    -1.4929590    -0.6044540
H        -2.3627700    1.2395700     -0.7219260
H        -0.0530740    2.1738700     0.4126870
H        1.2812510     -0.0880550    1.2060410
H        2.2759270     0.2214100     -1.2311310
         Core    RigidRotor
          SymmetryFactor                  0.5
         End
      Frequencies[1/cm]                   26
                                          47.4690          117.4600
 207.0830          464.3091          603.7559
 647.8007          748.1001          764.8046
 847.9984          886.4544          891.0583
 894.1122         1018.2026         1053.0423
1092.5432         1160.8353          1188.3111
1281.5084         1408.6770          1475.8535
1557.5750         3244.5065          3255.4527
3276.8437         3313.5947          3743.2263
      ZeroEnergy[kcal/mol]                -92.6
      ElectronicLevels[1/cm]              1
                0        2
    End
   End
!----------------------------------
!----------------------------------
Barrier B01     R1  ip01        #  C4H5 + O2 -> C4H5O2
   RRHO
    Stoichiometry                    C4H5O2
    Core      PhaseSpaceTheory
     FragmentGeometry[angstrom]      9
C  -2.2252263104  -0.1329069303   0.7036896199
C  -1.0987044023   0.3811812311   0.2578795059
```

```
C   0.2312750848   -0.2118844585    0.4372002199
C   1.3571224669    0.3362955855   -0.0285820036
H  -2.5539304092   -1.0012804533    1.2562522939
H  -1.1290731454    1.3234676776   -0.2923591235
H   0.2738445866   -1.1502800974    0.9836036907
H   2.3211869874   -0.1334313989    0.1248312137
H   1.3475521417    1.2723418442   -0.5778084169
      FragmentGeometry[angstrom]      2
O  0.000000    0.000000    0.602812
O  0.000000    0.000000   -0.602812
      SymmetryFactor                2.
      PotentialPrefactor[au]        7.0e+39
      PotentialPowerExponent        66.0
    End
    Frequencies[1/cm]               22
  165.1774            294.0886            487.6438
  583.3995            723.5481            833.2967
  902.5485            935.2666            937.1869
 1028.2566           1155.6660           1259.7751
 1319.2532           1440.8385           1625.9938
 1673.7751           3084.7801           3133.1800
 3147.5881           3221.3039           3232.9558
 1641.2330
    ElectronicLevels[1/cm]          1
          0      2
    ZeroEnergy[kcal/mol]              0.0
  End
!----------------------------
Barrier B02     R2  ip06        #  C4H5 + O2 -> C4H5O2
  RRHO
    Stoichiometry                   C4H5O2
    Core     PhaseSpaceTheory
      FragmentGeometry[angstrom]     9
C    1.897962   -0.191368   -0.000092
C    0.690235    0.331319   -0.000056
C   -0.561595   -0.422979   -0.000046
C   -1.772013    0.142834    0.000061
H    2.920223    0.155064    0.000845
H    0.591864    1.423777   -0.000241
H   -0.468457   -1.505173   -0.000037
H   -2.676027   -0.453821    0.000172
H   -1.895133    1.221313    0.000059
      FragmentGeometry[angstrom]     2
O  0.000000    0.000000    0.602812
O  0.000000    0.000000   -0.602812
      SymmetryFactor                2.
      PotentialPrefactor[au]        7.0e+39
      PotentialPowerExponent        66.0
    End
    Frequencies[1/cm]               22
 178.7766             302.0739             513.8394
 564.2009             727.6085             788.0309
```

```
 862.4874             937.7053             948.7805
1031.0575            1174.8101            1252.2327
1317.1405            1443.7681            1631.3128
1684.0409            3017.0178            3133.2943
3153.7895            3221.6895            3245.6675
  1641.2330
    ElectronicLevels[1/cm]          1
          0       2
    ZeroEnergy[kcal/mol]              0.0
  End
!--------------------
End
```

Input file for MESS calculations for the C_4H_5O secondary reaction

```
TemperatureList[K]                500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650.
1800. 2000. 2250. 2500.
PressureList[atm]                 0.01 0.1 1. 10. 100.
EnergyStepOverTemperature         0.2         #Ratio of discretization energy step to T
ExcessEnergyOverTemperature       100
ModelEnergyLimit[kcal/mol]          600
WellCutoff                        10
ChemicalEigenvalueMax             0.2
ChemicalEigenvalueMin             1.e-6       #only for direct diagonalization method
CalculationMethod                 direct
EigenvalueOutput                                eigenvalue.out
Reactant       #ground energy of bimolecular species will be used as a reference.
Model
 EnergyRelaxation
  Exponential
   Factor[1/cm]               333    ! Jasper-Hansen H + fulvene paper
   Power                           0.7
   ExponentCutoff                  15
  End
 CollisionFrequency
  LennardJones
    Epsilons[1/cm]          68.0  285.2
    Sigmas[angstrom]        3.610  5.18
Masses[amu]           28.  69.
End
OutputTemperatureStep[K]  100
OutputTemperatureSize  20
OutputReferenceEnergy[kcal/mol]  0.
!-------------------------------------------------------------------------------------------------------
!-------w_ip78------------
Well       ip78
Species
RRHO
Geometry[angstrom]   10
C  -1.7076025385   0.6980471378   0.0478915551
C  -0.2851740289   0.5771162743   -0.208766572
C  0.443667883   -0.5621350266   0.1620802819
C  1.7829482561   -0.722739371   -0.0577921128
O  -2.3825551767   -0.161058719   0.598313032
H  -2.1746257054   1.6439363307   -0.2917108791
H  0.2153642787   1.4043019912   -0.7045820222
H  -0.1185742673   -1.35099704   0.6536366567
H  2.3013632403   -1.6230112193   0.2478164764
H  2.3711010587   0.0470556418   -0.546109416
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  24
179.6211             211.7697             271.7239
```

399.1604 592.0505 751.6503
770.9809 897.6207 922.5424
1003.7469 1038.2769 1057.2528
1213.2861 1285.0173 1350.4177
1418.7240 1472.5911 1536.9545
1671.6960 2912.8662 3137.3301
3154.4099 3163.6807 3233.2056
ZeroEnergy[kcal/mol] -18.1
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------w_ip79------------
Well ip79
Species
RRHO
Geometry[angstrom] 10
C -1.5556391295 0.5163970087 0.0513066698
C -0.2011211499 0.5613021976 -0.2266880471
C 0.3701319899 -0.6271127417 0.1975313257
C -0.7252279493 -1.4653077511 0.7819271681
O -1.9219788479 -0.6544438759 0.646133378
H -2.3479394067 1.2276179179 -0.1168265419
H 0.3055363815 1.391911529 -0.6956336262
H 1.4047677146 -0.9261893477 0.1347236801
H -0.595435245 -1.6995843278 1.8482380229
H -0.8988243578 -2.4142376089 0.2545279706
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 24
244.2787 513.0039 548.5441
623.6909 766.9385 853.3214
878.1018 923.1865 948.8339
983.6853 1042.0566 1116.2094
1164.7147 1166.3005 1299.8764
1346.8685 1398.7520 1489.8847
1499.9474 2968.0138 2977.9970
3224.0940 3241.0062 3262.7024
ZeroEnergy[kcal/mol] -15.8
ElectronicLevels[1/cm] 1
0 2
End
End
!---------------------------------
!-------w_ip80------------
Well ip80
Species
RRHO
Geometry[angstrom] 10
C -1.7660212088 0.4511616452 0.1485942598

C -0.5262921614 -0.283032754 0.2719444163
C 0.6890131261 0.2127286116 -0.2095021744
C 1.889101464 -0.4433250247 -0.1166510588
O -2.8434448382 0.048407224 0.5585886505
H -1.6843072549 1.4374026888 -0.3573619275
H -0.576246353 -1.2511883098 0.7617961249
H 0.6714522504 1.1892652971 -0.6904757802
H 1.960035403 -1.4180474939 0.3531390157
H 2.8016835728 -0.0116228843 -0.5076835263
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 24
147.5053 212.0753 274.1008
468.6102 543.1241 571.5935
819.8044 883.4067 971.2678
991.1643 1021.4055 1149.9104
1226.0426 1284.4263 1289.4898
1417.1920 1488.6333 1528.8451
1672.2147 2879.0023 3128.6752
3142.0369 3165.6147 3237.7196
ZeroEnergy[kcal/mol] -18.9
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------w_ip98----------
Well ip98
Species
RRHO
Geometry[angstrom] 10
C 1.452244 0.357033 -0.239301
C 0.063271 0.877371 0.156211
C -0.950650 -0.206239 0.385668
C -2.106779 -0.295794 -0.263762
O 1.892808 -0.727095 -0.092365
H -0.260973 1.594181 -0.601403
H -0.677607 -0.961455 1.117379
H -2.803834 -1.102576 -0.068608
H -2.400952 0.434905 -1.011246
H 0.252387 1.457476 1.069906
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 24
73.5228 143.0618 213.9739
399.1789 532.3586 697.8908
800.3540 844.3084 940.6925
953.2816 1023.9948 1111.2814
1206.8189 1277.8184 1326.0800
1431.3870 1459.4517 1700.4387

```
1921.8659            3012.8828            3087.6283
3128.0255            3152.6116            3213.8503
ZeroEnergy[kcal/mol] -10.2
ElectronicLevels[1/cm]       1
0  2
End
End
!---------------------------------
!---------------------------------
Bimolecular      p2_p2    # p2 + H (+O)
    Fragment       C4OH4
      RRHO
Geometry[angstrom]   9
C  -1.0361533866   0.1017501981   0.2098777106
C  -0.0550591156   -0.8114228046   0.4266843431
C  1.1162973563   -0.2992447869   -0.224221818
C  0.7503261011   0.8828997843   -0.782823445
O  -0.5623059121   1.1446828759   -0.5278817088
H  -2.0726957043   0.1613980545   0.4946802511
H  -0.1476811598   -1.7331597425   0.9784516615
H  2.0933777947   -0.7532489221   -0.2668729699
H  1.2721110263   1.6239333434   -1.3639430247
      Core   RigidRotor
      SymmetryFactor       1.0
      End
Frequencies[1/cm]  21
615.3161             623.2143             734.2602
758.0551             850.3972             883.9850
888.4085             894.9160            1013.6374
1057.8806            1087.0920            1164.1391
1198.7056            1285.0196            1412.2878
1510.2032            1593.2377            3240.5060
3251.3305            3276.3002            3282.8111
      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]       14.5
End
!-----------------------------------------
!-------c2h3o_c2h2o_p4_b_p4_e------------
Bimolecular   p4_p4_be
Fragment       c2h2o
RRHO
Geometry[angstrom]   5
C   -0.102492    0.000007   -0.000105
```

C 1.206856 -0.000020 0.000230
O -1.263828 0.000010 0.000017
H 1.742357 0.937839 -0.000446
H 1.742081 -0.937842 -0.000446
Core RigidRotor
SymmetryFactor 2.0
End
Frequencies[1/cm] 9
 447.1826 562.8840 596.0245
 990.8705 1171.6660 1408.2887
2233.4287 3179.5260 3272.0370
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment c2h3
RRHO
Geometry[angstrom] 5
C -0.706468 -0.142824 0.000032
C 0.586567 0.029451 0.000000
H -1.602053 0.461258 -0.000132
H 1.038322 1.025575 0.000023
H 1.283137 -0.806595 -0.000080
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 9
 711.2371 818.9859 921.6992
1045.8512 1391.1503 1650.4801
3038.1065 3133.7690 3234.1270
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 29.30
End
!---------------------------------
!-------ts_ts78a------------
Barrier ts78a ip78 ip80
RRHO
Geometry[angstrom] 10
C 1.8958701609 0.1984613212 -0.0107692907
C 0.427998715 0.438047929 -0.1518784955
C -0.528767999 -0.5192232828 0.1456104446
C -1.8924338484 -0.3405786903 0.0166351272
O 2.597643763 -0.2236436348 -0.8955239645
H 2.3333473307 0.4447157957 0.9836877777
H 0.1289332438 1.4195589413 -0.5129446187
H -0.1775606951 -1.4859633293 0.5014142727
H -2.5883767472 -1.1319700092 0.2620856193
H -2.3042939236 0.5969469592 -0.339681872
Core RigidRotor

SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 278.0177
WellDepth[kcal/mol] 8.9
WellDepth[kcal/mol] 9.7
End
Frequencies[1/cm] 23
147.7530 234.9344
412.6781 525.7351 549.1072
722.7297 810.8417 885.3723
973.5453 994.7555 1086.4118
1197.8442 1270.3288 1313.5167
1408.6114 1479.3956 1515.1032
1787.8158 2847.2195 3127.1478
3139.3578 3142.9690 3239.6618
ZeroEnergy[kcal/mol] -9.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------ts_ts78f----------
Barrier ts78f ip78 ip98
RRHO
Geometry[angstrom] 10
C 1.410107 0.404209 -0.051268
C 0.021332 0.658160 -0.075692
C -0.998666 -0.386759 0.002049
C -2.311671 -0.136511 0.011515
O 2.124378 -0.565684 -0.013268
H 0.922334 1.077453 0.973214
H -0.276354 1.681319 -0.277969
H -0.629023 -1.405495 0.066440
H -3.038402 -0.937660 0.072927
H -2.700189 0.875259 -0.048094
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1569.3349
WellDepth[kcal/mol] 58.2
WellDepth[kcal/mol] 40.3
End
Frequencies[1/cm] 23
128.2202 176.5093
380.7628 450.3205 644.9215
669.5058 767.9323 911.9677
955.4584 1028.9848 1113.3253
1180.5120 1205.1125 1314.0216
1361.4544 1464.5239 1667.3292
1792.9587 1834.1022 3134.2748
3162.7199 3177.0112 3223.1808

ZeroEnergy[kcal/mol] 30.1
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts79a------------
Barrier   ts79a ip79 p2_p2
RRHO
Geometry[angstrom]   10
C -1.0696992502   1.016665602   -0.5824652973
C 0.2681856749   1.0904654746   -0.8234166849
C 0.8125168714   -0.166984677   -0.4290832288
C -0.2372247602   -0.9026850386   0.0581298895
O -1.3987865093   -0.19798982   -0.0689371911
H -1.8852594281   1.7076240366   -0.7123360371
H 0.799711004   1.935871673   -1.2297941795
H 1.8437437593   -0.4789142736   -0.4682564683
H 0.1050310009   -0.6377519778   2.0788714466
H -0.3434453627   -1.9372419992   0.333641751
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling   Eckart
ImaginaryFrequency[1/cm] 440.7681
WellDepth[kcal/mol] 33.4
WellDepth[kcal/mol] 33.4
End
Frequencies[1/cm] 23
270.4052   298.2610
607.3408   628.2540   752.1551
782.9002   865.1012   885.1915
890.0814   894.0708   1017.3266
1055.8687   1090.2292   1159.8889
1195.2364   1284.9685   1407.3720
1485.2371   1565.4902   3244.2057
3255.2869   3277.4060   3284.6935
ZeroEnergy[kcal/mol] 17.6
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts79b------------
Barrier   ts79b ip78 ip79
RRHO
Geometry[angstrom]   10
C -0.9106800342   -1.1259416736   0.0349327011
C -1.0188854948   0.2603803785   0.1834965431
C 0.218520588   0.867034109   -0.0517668319
C 1.3039848619   -0.0440235869   -0.0020010855
O 0.2466455547   -1.6453787137   -0.178741719
H -1.7697798498   -1.7970132827   0.012129385
H -1.9674131367   0.7731231106   0.2628846527

H 0.3120588354 1.8579613817 -0.483309846
H 1.6010494191 -0.4858424964 0.9441673318
H 2.1224772563 0.0401357734 -0.7149351314
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 597.7237
WellDepth[kcal/mol] 24.7
WellDepth[kcal/mol] 22.4
End
Frequencies[1/cm] 23
303.0967 515.3091
611.4186 660.6806 802.9347
829.0354 869.0386 929.1171
1011.0723 1038.0176 1077.7512
1096.6015 1178.7328 1262.3336
1380.2086 1427.6904 1480.8210
1501.7794 3096.0864 3112.0905
3155.9179 3170.1368 3215.1533
ZeroEnergy[kcal/mol] 6.6
ElectronicLevels[1/cm] 1
0 2
End
!----------

!-------ts_ts80c----------
Barrier ts80c ip80 ip98
RRHO
Geometry[angstrom] 10
C -1.315783 -0.263339 -0.010283
C -0.044796 0.340113 0.117913
C 1.198093 -0.410283 -0.009140
C 2.402329 0.164021 -0.078028
O -2.458926 0.093049 -0.139893
H 0.008965 1.431935 0.183288
H 1.101169 -1.490586 -0.078815
H 2.526720 1.240246 -0.023020
H 3.299092 -0.428918 -0.205846
H -0.703597 -0.480140 1.120760
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1570.2010
WellDepth[kcal/mol] 50.7
WellDepth[kcal/mol] 42.0
End
Frequencies[1/cm] 23
150.7114 213.6600
351.3051 462.0331 499.1395
657.9969 876.9358 933.9218

944.4139 1018.2453 1088.9850
1150.8256 1193.2390 1280.0451
1328.0714 1464.2024 1683.6514
1799.6354 1869.0141 3046.2058
3140.2863 3149.0972 3230.1252
ZeroEnergy[kcal/mol] 31.8
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
!-------ts_ts98a------------
Barrier ts98a ip98 p4_p4_be
RRHO
Geometry[angstrom] 10
C 1.573643 0.201042 0.000023
C 0.370734 0.783530 -0.000079
C -1.450123 -0.584719 -0.000181
C -2.622647 0.007867 0.000113
O 2.515453 -0.483211 0.000084
H 0.067667 1.258235 -0.924582
H -1.200499 -1.639749 -0.000192
H -3.562063 -0.549947 0.000313
H -2.725851 1.092633 0.000164
H 0.067477 1.258197 0.924378
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 404.4421
WellDepth[kcal/mol] 47.7
WellDepth[kcal/mol] 39.50
End
Frequencies[1/cm] 23
14.5013 97.6455
191.3111 216.1137 403.4496
424.7400 521.5074 753.1047
818.4628 902.4103 946.0370
1033.9489 1083.6447 1109.2119
1394.5418 1403.4532 1635.8855
2176.2610 3046.8527 3116.0492
3153.6522 3180.6345 3240.2815
ZeroEnergy[kcal/mol] 37.5
ElectronicLevels[1/cm] 1
0 2
End
!---------------------------------
End