

From PAH to fullerenes: Closing a nano bowl with a nano lid

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Table S1. Comparison of the reaction enthalpies and Gibbs free energies (kJmol⁻¹) computed using HO and quasiharmonic approximations at various temperatures.

T, K	ΔE	ΔG							
		500		1000		1500		2000	
		HO	quasiharm	HO	quasiharm	HO	quasiharm	HO	quasiharm
$C_{40}H_{10}+H \rightarrow C_{40}H_9+H_2$	26.0	10.3	10.3	-8.0	-8.2	-24.8	-25.1	-40.3	-40.5
$C_{60}H_{18}+H \rightarrow C_{60}H_{17}+H_2$	44.6	35.0	35.5	22.7	23.7	11.5	13.0	1.5	3.5
$C_{60}H_{16}+H \rightarrow C_{60}H_{15}+H_2$	28.1	19.1	19.5	7.0	7.8	-4.1	-2.8	-13.9	-12.3
$C_{60}H_{14}+H \rightarrow C_{60}H_{13}+H_2$	23.6	15.1	15.5	4.4	5.0	-5.3	-4.2	-13.6	-12.2
$C_{60}H_{12}+H \rightarrow C_{60}H_{11}+H_2$	24.6	15.2	15.4	2.6	3.0	-9.0	-8.4	-19.5	-18.5
$C_{60}H_{10}+H \rightarrow C_{60}H_9+H_2$	10.0	1.5	0.9	-9.5	-10.8	-19.3	-21.3	-27.9	-30.6
$C_{60}H_8+H \rightarrow C_{60}H_7+H_2$	24.0	14.7	14.8	2.1	2.3	-9.4	-9.1	-19.8	-19.4
$C_{60}H_6+H \rightarrow C_{60}H_5+H_2$	8.1	-0.4	-0.4	-11.4	-11.4	-21.3	-21.3	-29.9	-29.9
$C_{60}H_4+H \rightarrow C_{60}H_3+H_2$	23.3	13.8	13.8	1.3	1.3	-10.0	-10.0	-20.1	-20.1
$C_{60}H_2+H \rightarrow C_{60}H+H_2$	-95.1	-106.5	-106.5	-120.8	-120.8	-134.2	-134.2	-146.3	-146.3
H loss									
$C_{40}H_9+C_{20}H_{10} \rightarrow C_{60}H_{18}+H$	-48.5	-9.4	10.6	14.8	56.3	34.2	97.2	50.6	135.1
$C_{60}H_{17} \rightarrow C_{60}H_{16}+H$	-9.2	-41.3	-50.6	-78.3	-97.5	-116.0	-145.1	-153.8	-192.7
$C_{60}H_{15} \rightarrow C_{60}H_{14}+H$	105.9	69.5	66.2	27.4	20.6	-15.6	-25.9	-58.8	-72.6
$C_{60}H_{13} \rightarrow C_{60}H_{12}+H$	44.8	9.3	5.3	-30.9	-39.1	-71.8	-84.3	-112.7	-129.5
$C_{60}H_{11} \rightarrow C_{60}H_{10}+H$	98.3	59.8	58.1	15.6	12.1	-29.5	-34.9	-74.8	-82.0
$C_{60}H_9 \rightarrow C_{60}H_8+H$	45.6	8.1	5.3	-34.1	-40.0	-77.0	-86.1	-120.1	-132.2
$C_{60}H_7 \rightarrow C_{60}H_6+H$	90.4	49.7	48.8	3.1	1.1	-44.4	-47.4	-92.0	-96.1
$C_{60}H_5 \rightarrow C_{60}H_4+H$	65.7	25.5	25.5	-19.8	-19.8	-65.9	-65.9	-112.2	-112.2
$C_{60}H_3 \rightarrow C_{60}H_2+H$	-120.5	-157.3	-157.3	-196.1	-196.1	-235.1	-235.1	-274.2	-274.2
$C_{60}H \rightarrow C_{60}+H$	162.8	135.0	135.0	97.9	97.9	59.7	59.7	21.5	21.5
Overall									
$C_{40}H_{10}+C_{20}H_{10} \rightarrow C_{60}+10H_2$	552.9	167.1	166.0	-309.8	-312.2	-786.8	-790.6	-1256.4	-1261.4

Table S2. Equilibrium concentration ratios $[C_{60}H_{x-2}]/[C_{60}H_{x-1}]$ in the $C_{60}H_{x-1} \rightarrow C_{60}H_{x-2} + H$ reactions at typical flame mole fractions of H atoms x_H and constant $[H] = 5 \times 10^{15}$ molecule cm^{-3} at various temperatures.

T,K	500			1000			1500			2000		
x_H or [H]	0.0004	const [H]	0.01	0.0004	const [H]	0.01	0.0004	const[H]	0.01	0.0004	const[H]	0.01
$x = 18$	5.16E+07	6.06E+07	2.06E+06	3.09E+07	1.81E+07	1.23E+06	2.74E+07	1.07E+07	1.10E+06	2.60E+07	7.64E+06	1.04E+06
$x = 16$	1.38E-04	1.62E-04	5.51E-06	9.25E+01	5.43E+01	3.70E+00	8.72E+03	3.41E+03	3.49E+02	8.60E+04	2.52E+04	3.44E+03
$x = 14$	2.68E+02	3.14E+02	1.07E+01	1.03E+05	6.02E+04	4.10E+03	7.90E+05	3.09E+05	3.16E+04	2.20E+06	6.45E+05	8.79E+04
$x = 12$	1.62E-03	1.65E-03	6.49E-05	4.43E+02	2.25E+02	1.77E+01	3.09E+04	1.04E+04	1.23E+03	2.60E+05	6.60E+04	1.04E+04
$x = 10$	3.57E+02	4.19E+02	1.43E+01	1.51E+05	8.87E+04	6.04E+03	1.20E+06	4.71E+05	4.81E+04	3.42E+06	1.00E+06	1.37E+05
$x = 8$	1.61E-02	1.89E-02	6.44E-04	1.73E+03	1.02E+03	6.93E+01	8.82E+04	3.45E+04	3.53E+03	6.34E+05	1.86E+05	2.54E+04
$x = 6$	5.44E+00	6.39E+00	2.18E-01	2.72E+04	1.59E+04	1.09E+03	4.94E+05	1.93E+05	1.98E+04	2.13E+06	6.26E+05	8.53E+04
$x = 4$	6.79E+19	7.98E+19	2.72E+18	4.39E+13	2.58E+13	1.76E+12	3.85E+11	1.51E+11	1.54E+10	3.63E+10	1.07E+10	1.45E+09
$x = 2$	1.98E-11	2.32E-11	7.91E-13	1.92E-02	1.13E-02	7.68E-04	2.08E+01	8.14E+00	8.32E-01	6.86E+02	2.01E+02	2.74E+01

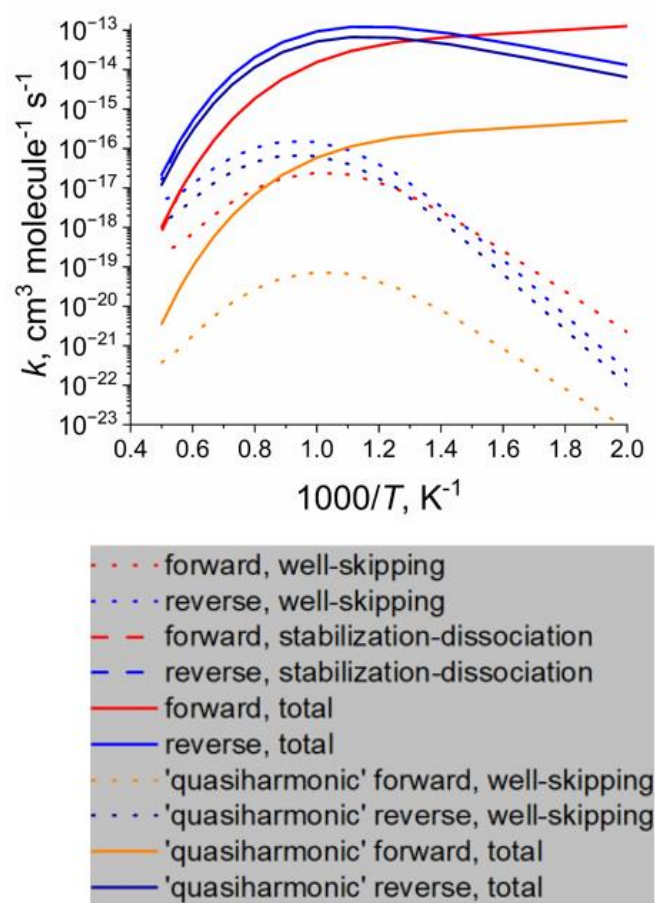


Figure S1. Rate constants for the $\text{C}_{40}\text{H}_9 + \text{C}_{20}\text{H}_{10} \rightarrow \text{C}_{60}\text{H}_{18} + \text{H}$ reaction in forward and reverse directions calculated using HO and quasi-harmonic approximations.

Input file for RRKM-ME calculations for the C₄₀H₉ + C₂₀H₁₀ reaction

```

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1700. 1800. 1900. 2000.
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1750. 1800. 2000. 2250. 2500.
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!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
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ExcessEnergyOverTemperature   100
ModelEnergyLimit[kcal/mol]    900
WellCutoff                    10
ChemicalEigenvalueMax         0.2
ChemicalEigenvalueMin         1.e-6      #only for direct diagonalization method
CalculationMethod              direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput               eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber             0
!ReductionNumber               5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
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EnergyRelaxation
Exponential
! Factor[1/cm]                 260 ! Frenklach
! Power                         0.
! Factor[1/cm]                 247 ! Jasper universal
! Power                         0.85
! Factor[1/cm]                 424 ! Jasper calc N2
! Power                         0.62
! Factor[1/cm]                 125 ! SJK guess
! Power                         0.85
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LennardJones
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!Sigmas[angstrom]              4.6 4.6 ! N2 pyrene-Frenklach
! Epsilons[1/cm]              206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
! Sigmas[angstrom]             5.06 5.06 ! N2 Jasper extrapolation to C16
! Epsilons[1/cm]              32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
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! Sigmas[angstrom]             3.6154 10.91359478
! Epsilons[1/cm]              390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
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OutputTemperatureSize          20

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Well ip1
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C 5.0991575324 -0.5632077756 -0.291042066
C 5.2232619199 0.7367182356 0.3205007962
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C 0.7446222097 2.8087222142 -2.0915828506
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Core RigidRotor

SymmetryFactor 0.5

End

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1638.3024	1641.4168	1660.1777
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ElectronicLevels[1/cm] 1		
0 2		
End		
End		
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C	0.1013749752	-2.3789688326 -1.0483752833
C	1.4357270757	-2.5213117744 -1.5924806123
C	2.1578946973	-1.4337651861 -2.06880116
C	1.6223772807	-0.0884514621 -2.0516475471
C	1.6989705747	2.349004865 -1.5858376857

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 H 1.9292613232 -3.4898461556 -1.5508153753
 H 3.1875280735 -1.594947987 -2.3806603808
 H 2.2940591725 3.2585391807 -1.540971481
 H 3.3411811547 1.2411620876 -2.3758413482
 H -3.2273764948 1.3801799334 2.3603078503
 H -3.3577042939 -1.0378490256 2.3572295228
 H -2.1302276849 -3.4038164394 1.3772140355
 H -0.3056692625 -4.2500178306 0.028987428

Core RigidRotor
 SymmetryFactor 5
 End

Frequencies[1/cm] 84

140.7775	141.8922	142.3173
281.8467	282.2812	311.8267
312.0680	409.5615	409.6129
438.8131	438.8476	452.8308
453.1059	542.0046	547.7660
547.8603	559.8178	604.9719
612.3044	612.6253	648.0155
648.3518	649.5188	673.0567
673.2082	759.3730	759.4482
772.3237	772.9044	812.4415
812.7146	833.7571	833.9871
856.2916	869.7673	869.8548
937.4422	953.6671	960.2083
960.5143	968.8406	969.2946
1051.9040	1091.5776	1091.7207
1171.7586	1171.9032	1172.0981
1172.1222	1197.1583	1197.4074
1224.1539	1224.4673	1244.7979
1269.6835	1342.9540	1343.2096
1392.0233	1392.1219	1440.9376
1441.0044	1458.8246	1459.0431
1480.5066	1486.1369	1486.2718
1497.7890	1497.8396	1527.1299
1668.7697	1668.8240	1669.9817
1670.3181	1671.8910	3174.2813
3174.9348	3175.1083	3175.7679
3175.8475	3191.5459	3191.6357
3192.7383	3192.8415	3194.2595

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

End

Fragment c40h9

RRHO

Geometry[angstrom] 49

C 2.4359897853 0.0967968941 -2.8131180127
 C 1.1344753957 -0.217512293 -3.372690928
 C 0.8742051617 -1.6259340379 -3.1413729921
 C 2.0126135232 -2.1819086837 -2.436434385
 C 2.9788099026 -1.117437125 -2.2332389045
 C 3.6789830465 -1.0480773739 -1.0352345167
 C 3.8997395471 0.214011034 -0.3733026349
 C 3.3764838585 1.3853247991 -0.9330897501
 C 2.625249652 1.3096722645 -2.161656501

C -0.4104944292 -2.0408902709 -2.8064057663
 C -0.6282157978 -3.0449509118 -1.7933892211
 C 0.4713840479 -3.5636002646 -1.094690452
 C 1.7994811507 -3.1134205679 -1.4273740077
 C 0.0974748561 0.6988884299 -3.2472555837
 C -1.2386743387 0.2691707532 -2.9175318929
 C -1.4897256104 -1.0904689456 -2.698499123
 C 3.4783603855 -2.0311068466 5.599541E-4
 C 2.5463085224 -3.0562267505 -0.1939683656
 C 1.5564379189 2.2723203959 -2.0556200066
 C 0.3007063166 1.9681427941 -2.5939238752
 C -0.8971196877 2.3764537624 -1.9319634987
 C -0.7678809534 3.2822457755 -0.8771494473
 C 0.5098050717 3.5926334395 -0.3301439424
 C 1.670447075 3.000428029 -0.8325433291
 C 3.9256613371 0.0289866102 1.0426450928
 C 3.6375722918 1.1395921755 1.838547293
 C 3.1055118393 2.3315023267 1.2690702883
 C 2.8555219251 2.4233377826 -0.101613475
 C 1.7447844839 -3.5287885324 0.8889746481
 C 2.0864704616 -3.1026719643 2.1742485917
 C 3.0359765355 -2.06035468 2.37223711
 C 3.6493438202 -1.432176179 1.2862431779
 C -1.8747060531 -2.7813768786 -1.1163585966
 C -1.9411311486 -3.3207554049 0.1455199779
 C -0.8786611737 -3.8401882725 0.8968575211
 C 0.3959212803 -3.8535873605 0.3060326201
 C -1.8986611315 1.269526474 -2.1409103482
 C -2.9598273054 0.8570814868 -1.3318642642
 C -3.2183811991 -0.5250583613 -1.108826547
 C -2.416016971 -1.5053180066 -1.6950034396
 H -1.6441059274 3.6168033232 -0.3269088548
 H 0.5338997661 4.1461875927 0.6055463799
 H 3.627718575 1.0535950556 2.9225310057
 H 2.7205328553 3.0853702554 1.9516660081
 H 1.5008185431 -3.4190134165 3.0341245853
 H 3.1199185453 -1.6407892191 3.3718721764
 H -1.0183003857 -4.0673774299 1.9515942154
 H -3.4864437247 1.573579235 -0.7059263089
 H -3.9245616398 -0.7913979117 -0.3266956748

Core RigidRotor
 SymmetryFactor 0.5
 End

Frequencies[1/cm] 141

86.0880	86.4900	171.8894
178.3809	181.4091	195.3181
199.4531	312.8920	317.0556
337.9214	339.1979	340.2639
360.9350	362.8313	378.1306
383.3990	410.1044	419.6604
423.0144	446.7463	449.5694
460.1212	464.2493	490.1299
497.0413	502.3883	509.3281
520.1341	537.4813	543.1539
543.3413	575.7455	581.1616
598.6671	599.9459	602.2960
608.8565	625.4260	626.9836
628.7935	655.2646	656.4095
685.6993	687.1249	700.0124
704.2609	713.9481	715.9235
719.1977	731.7356	737.2033
738.5706	753.9911	762.1585
764.1902	765.6564	768.5363
783.4383	784.4825	817.2124

821.6266	826.8754	832.2865
834.9507	837.4703	847.0472
850.9904	884.8526	891.1631
939.8392	947.5561	949.2766
951.4221	967.0793	990.8014
1001.2732	1006.4317	1007.9790
1038.7046	1085.4378	1092.8037
1113.5811	1118.2962	1144.3025
1150.0208	1167.8038	1183.7524
1186.6567	1200.7810	1207.2605
1231.6846	1245.0177	1249.8479
1260.8159	1263.1079	1269.2111
1295.9856	1306.8261	1323.8189
1325.6737	1334.2973	1336.2061
1347.7959	1357.6848	1369.9074
1378.1459	1394.9665	1398.6724
1418.7173	1432.4479	1435.2060
1436.4756	1439.1098	1445.5135
1446.8364	1448.5073	1450.9038
1498.5755	1506.3793	1507.1306
1534.3073	1573.2543	1576.2957
1595.8189	1598.4124	1598.6763
1604.6535	1610.4401	1617.7179
1618.5036	1635.8658	1636.9319
3177.7532	3178.8022	3179.6241
3180.9459	3182.5902	3193.8926
3195.1210	3196.2013	3199.9422
ZeroEnergy[kcal/mol] 0.0		
ElectronicLevels[1/cm] 1		
0 2		
End		
GroundEnergy[kcal/mol] 0.00		
End		
!-----h_c60h18_p2-----		
Bimolecular p2		
Fragment c60h18		
RRHO		
Geometry[angstrom] 78		
C 6.0649301284	-0.4950920623	-2.7093860106
C 4.9179985186	-0.8166410309	-3.5387057303
C 4.4284083908	-2.1226395772	-3.1408012747
C 5.2749211661	-2.6106612514	-2.0686618235
C 6.2849718977	-1.6043613272	-1.7997661586
C 6.6616940616	-1.3477754575	-0.4869172281
C 6.8643730402	0.0018723385	-0.0210088597
C 6.6528417647	1.0717753665	-0.8985850157
C 6.2353438179	0.8063255042	-2.2532776929
C 3.0582652853	-2.3535773641	-3.0912637896
C 2.4639505543	-3.0962056928	-2.0069098526
C 3.2845952796	-3.5659258215	-0.9754350854
C 4.7007234145	-3.3028569426	-1.0095287243
C 4.0086626239	0.1825211144	-3.8644595891
C 2.5885780978	-0.0665336072	-3.8397283326
C 2.1163268815	-1.326767848	-3.4538535032
C 6.0848117334	-2.0845026239	0.6105951504
C 5.1107579925	-3.0557780508	0.3513170109
C 5.3069757852	1.8492779617	-2.6148044414
C 4.201492086	1.539574376	-3.4156359692
C 2.9377464293	2.1663369771	-3.1913664831
C 2.9099275771	3.2548142309	-2.3171354383
C 4.0346465011	3.5694818322	-1.502227847
C 5.1985149169	2.799590748	-1.5542818919
C 6.5062305639	0.1050010152	1.3576477079
C 6.1670226931	1.3720066877	1.83701905

C 5.9524616945 2.4607065201 0.9443979794
 C 6.0737342381 2.2927936685 -0.4366874032
 C 4.007594142 -3.2400315702 1.2388431215
 C 4.0640284103 -2.5910742838 2.4741191547
 C 5.0550051828 -1.6027429883 2.7379456901
 C 5.9977452128 -1.2531511208 1.7687015995
 C 1.1417361808 -2.6242606086 -1.745695533
 C 0.5975063791 -2.8768962998 -0.4693580759
 C 1.46068282 -3.3419804213 0.5797884511
 C 2.8184129011 -3.5706713658 0.3730374042
 C 1.8883530793 1.1213318131 -3.4694051913
 C 0.6107009471 0.9642201555 -2.9300784893
 C 0.1240501689 -0.3181555599 -2.5461054317
 C 0.9195525752 -1.4601110153 -2.6836586834
 C -4.3840067558 -0.4549517377 1.7935528652
 C -3.0381351157 -0.6641833922 2.1831795867
 C -2.4854115643 -1.6628476952 1.3422885913
 C -3.4933442305 -2.0631475012 0.4293720006
 C -4.6646125126 -1.3198048007 0.7080988309
 C -5.6299985151 -1.0455096428 -0.2466953147
 C -6.4786364424 0.0821476955 0.0746653353
 C -6.2055371178 0.9294822542 1.142061687
 C -5.0543345278 0.7391076215 1.9991249345
 C -1.1307759352 -1.7659351959 1.0750827462
 C -0.8041377388 -2.5280008772 -0.1336848138
 C -1.8158199319 -2.8975383522 -1.0295516881
 C -3.20826178 -2.5789476293 -0.8226752079
 C -2.2758577587 0.3100385702 2.8050528264
 C -0.8494103127 0.1052031651 2.6902914946
 C -0.306156582 -0.8751749891 1.8679957081
 C -5.4517932825 -1.7593150648 -1.494190215
 C -4.3014187627 -2.4882008374 -1.7687783074
 C -4.3436686201 1.6825315678 2.8370787672
 C -3.0240269047 1.4787906431 3.2197833465
 H 1.9729807777 3.7608521424 -2.0967469723
 H 3.8904928188 4.2977768822 -0.7075994263
 H 5.8713019533 1.5077990491 2.8747043692
 H 5.5054295066 3.3640149893 1.3527825444
 H 3.245878527 -2.6852018607 3.1844353992
 H 4.9353883987 -0.998286867 3.6339973028
 H 1.0459386763 -3.3611803549 1.583989436
 H 0.033074418 1.8309629859 -2.6173707253
 H -0.7984307085 -0.3552906932 -1.9757373732
 H -7.3064759833 0.333089022 -0.5847597237
 H -6.8309747335 1.8093952552 1.2753583378
 H -1.5122377027 -3.4000520444 -1.9444790582
 H -0.1687564437 0.7944385495 3.1852886399
 H 0.77357837 -0.9040666906 1.7537675789
 H -6.1967540603 -1.6556017834 -2.279927748
 H -4.1900821001 -2.9268994846 -2.757646503
 H -4.8204761646 2.6222981712 3.1067822964
 H -2.5192232917 2.2668455124 3.7741476814

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 228

13.3152	20.1215	28.0604
67.5407	83.2017	104.2719
131.6222	138.5763	146.7026
165.8305	174.7951	183.9728
191.7076	193.3097	225.1112
265.6283	284.9932	300.3242
314.9921	317.1919	324.2852
340.3957	341.6369	353.3033

357.2321	366.7059	374.8654
381.9509	399.6902	412.9218
415.0271	421.1107	425.0555
437.7200	444.1704	451.2181
452.5491	453.9113	463.6419
470.1867	481.4734	494.7242
497.3720	508.6912	514.1480
516.3467	533.6611	542.8126
547.1370	549.5053	552.3134
561.8054	575.8010	584.3671
587.2303	597.3356	601.7450
605.0503	609.6663	611.4381
617.6477	618.4698	626.3894
629.6321	645.6080	648.3374
653.1905	655.6078	666.7544
674.0819	679.0469	687.0015
689.5654	703.8915	709.8404
713.8303	719.0608	721.0394
722.0346	730.2265	737.6740
740.3939	744.3637	761.6919
762.9664	764.8201	767.7776
769.0350	772.5555	774.7493
783.5811	785.7852	798.6964
808.8584	810.5741	816.4215
816.9202	823.5961	828.9722
834.9370	836.6533	840.2834
843.2140	851.6682	859.2780
875.5916	886.2609	890.6953
898.1001	913.1986	924.3620
940.1255	946.7126	948.2613
953.6552	958.1060	964.0503
964.6779	969.5523	972.3522
981.5519	1002.1577	1005.9899
1009.3491	1042.6196	1044.8361
1070.5663	1086.6565	1093.3512
1098.1380	1111.5588	1119.0280
1145.1307	1148.9756	1154.0777
1170.4262	1172.0481	1174.6989
1178.9940	1187.8634	1192.2136
1199.2287	1202.8650	1209.5357
1215.2208	1220.8730	1227.7964
1239.0962	1245.4191	1250.2085
1252.1246	1265.8570	1267.1134
1271.2329	1294.8530	1301.9668
1310.2363	1325.6430	1330.6245
1336.0219	1337.9767	1341.1634
1342.8933	1352.7262	1357.0857
1367.8270	1377.4348	1384.6427
1388.1819	1392.4826	1401.4512
1417.4214	1432.5109	1433.4730
1435.9965	1436.6520	1441.1754
1443.2153	1445.2387	1448.0715
1450.9370	1451.0013	1457.3360
1462.7496	1471.8895	1481.0761
1487.0604	1494.8400	1500.0494
1506.0606	1506.9811	1508.0959
1522.9676	1565.9000	1575.7279
1585.1425	1596.7261	1598.1587
1598.4419	1604.2630	1614.4711
1617.6642	1620.0338	1637.2211
1637.7911	1659.3935	1666.6548
1668.9735	1669.7390	1671.6945
3176.1278	3177.0790	3177.5622
3178.9204	3179.0311	3179.8949

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3180.8874      3185.1625      3192.7488
3193.2068      3193.5124      3194.3483
3194.6307      3195.6391      3196.2918
3196.3566      3206.8524      3218.4800
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] -11.60
End
!-----bar_ts1-----
Barrier      ts1 p1 ip1
RRHO
Geometry[angstrom] 79
C 4.9034121184 0.1520486906 -2.9249562956
C 3.6016052274 -0.1629404665 -3.4843632835
C 3.3405885377 -1.5700268805 -3.2503190062
C 4.4810148236 -2.1258662779 -2.5468868287
C 5.4467509589 -1.0614471159 -2.3441063429
C 6.1469398309 -0.991434507 -1.1457950518
C 6.3661236799 0.2710842751 -0.4843676285
C 5.8436879629 1.4420383777 -1.0459534553
C 5.0931583992 1.365152575 -2.2746802843
C 2.0561152881 -1.9805418059 -2.9073874142
C 1.8382436947 -2.9760038464 -1.8859719186
C 2.9412135755 -3.5042068513 -1.2017956177
C 4.2692275344 -3.0565528267 -1.5377488089
C 2.5647517336 0.7540453201 -3.3595848821
C 1.2282419939 0.3265219963 -3.0293532607
C 0.976703258 -1.0324005304 -2.8031879139
C 5.9470502061 -1.9745119718 -0.109677233
C 5.0153987278 -3.0001620575 -0.304683187
C 4.0253594787 2.3292654199 -2.1710354405
C 2.7696999632 2.0248590225 -2.7093429576
C 1.5717424987 2.4359202553 -2.049386116
C 1.7011293777 3.3437877996 -0.9964001759
C 2.9787908736 3.6540010965 -0.4491441501
C 4.139560389 3.0600160333 -0.9494866768
C 6.3913542339 0.0871594936 0.9316130176
C 6.1024220029 1.1987815928 1.7259700064
C 5.5715624393 2.3904267937 1.1547298578
C 5.3226345657 2.4814533854 -0.2162521085
C 4.2125458817 -3.4750387452 0.7771416022
C 4.5538610609 -3.0477606434 2.0621123155
C 5.5018117406 -2.003347297 2.2606990824
C 6.116559139 -1.3746988693 1.1758972925
C 0.5957149953 -2.7214730923 -1.2074902396
C 0.4984992568 -3.2810828524 0.0555966263
C 1.5864953912 -3.822986066 0.768934099
C 2.8653857164 -3.8082892021 0.1915411382
C 0.5681912916 1.330919766 -2.2579035885
C -0.4923363197 0.9213818682 -1.448342665
C -0.7507053899 -0.4605308214 -1.2202790245
C 0.0506300856 -1.4465328308 -1.7972639715
C -3.99647643 0.2109738871 1.1291542734
C -2.9887716833 -0.2562619337 2.0072085521
C -2.7835044093 -1.6331131637 1.7456267267
C -3.6778580288 -2.014933003 0.7077447693

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C	-4.4223341689	-0.877634219	0.3298793048
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C	-5.2886511274	0.6491790453	-1.2717782053
C	-4.8683778922	1.7190559169	-0.488378113
C	-4.0994883952	1.5307872547	0.7252600209
C	-1.5951982612	-2.2823721582	2.0088277704
C	-1.4219113101	-3.5442703125	1.2653166675
C	-2.3652623784	-3.9399725581	0.2779157653
C	-3.4494515992	-3.0900928842	-0.1373570191
C	-2.0134637296	0.5660764362	2.5461510009
C	-0.8439117709	-0.1408790056	3.0175914406
C	-0.6458797522	-1.4947468913	2.7602727181
C	-4.9358278061	-1.9167389383	-1.7456442295
C	-4.2109965234	-3.0419105845	-1.3702495403
C	-3.2209727866	2.4358442678	1.4394763379
C	-2.2319105233	1.9781533723	2.3034253246
H	0.8243009181	3.6770016177	-0.4462684918
H	3.0030841314	4.2087559691	0.4860028664
H	6.0920346875	1.114088531	2.8101383545
H	5.1866755073	3.1454139905	1.8362865801
H	3.9684836032	-3.3643862331	2.922289255
H	5.5836907142	-1.5831119542	3.2603533128
H	1.455022747	-4.0977999273	1.8146880422
H	-1.0199413633	1.6349074205	-0.820128797
H	-1.4573358331	-0.7162109589	-0.4391303688
H	-5.7849643572	0.8662989941	-2.2148800851
H	-5.0545967957	2.7271382303	-0.8518152946
H	-0.7915970418	-4.3216548502	1.6851517188
H	-2.1778612524	-4.8751943608	-0.2434465823
H	-0.0458296248	0.4103798762	3.509633858
H	0.3024453476	-1.9362351262	3.0553554842
H	-5.4071209536	-1.912251152	-2.7258034078
H	-4.1456239504	-3.8710240244	-2.070739684
H	-3.2773882189	3.5037807048	1.2400269705
H	-1.5549971545	2.7068266445	2.7440875555

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 230

9.9138	16.9828	
25.0609	47.8510	62.1044
92.0888	100.4711	127.7235
142.4846	149.6121	174.3587
181.8094	186.2082	197.0537
210.3211	272.0772	285.7638
309.7475	314.6204	318.4445
324.1160	337.4822	339.5289
343.4953	352.1322	363.5798
378.6472	385.1644	401.7790
406.9353	410.9082	414.1854
420.8371	428.8557	437.5010
440.2299	448.3737	450.6828
451.3364	459.3815	468.4651
491.3063	495.9235	501.5340
510.1155	515.3592	524.8556
540.2236	542.3885	543.8422
547.5687	548.0396	558.3177
577.2660	581.0082	585.8882
599.3724	599.8495	603.8019
605.1931	609.0789	616.0874
621.4815	626.8657	628.8413
643.3928	645.6432	649.1450
655.8468	656.6495	663.8668
679.6348	683.3037	686.4319

702.6118	704.3882	714.9087
716.2854	718.5964	731.0164
736.8440	737.2572	751.6966
755.8246	757.1222	761.2805
762.5420	765.0043	767.0769
772.4987	782.5279	784.1989
786.5594	804.3513	813.8454
814.6834	817.8095	824.7823
826.9191	830.8762	834.9745
838.5686	840.5152	846.5464
852.2224	857.6636	861.8323
869.1597	880.2011	889.9741
924.9262	937.7801	944.9354
947.1976	947.8405	953.5722
955.9688	959.2113	964.6277
969.6091	972.8128	996.8047
1001.5137	1007.1473	1011.3020
1039.4195	1048.0508	1085.1579
1088.0306	1091.2942	1094.1174
1114.3156	1118.6637	1134.4562
1145.0950	1151.1770	1168.5834
1169.3926	1170.9693	1172.6951
1186.0765	1187.9613	1189.6650
1197.1378	1200.9732	1209.1085
1217.0786	1222.4191	1230.4412
1243.1417	1248.4387	1249.9643
1260.4536	1263.9382	1266.6161
1268.7526	1297.3644	1308.5728
1324.6386	1328.3171	1334.9104
1336.3571	1336.8929	1342.8098
1348.4334	1357.6916	1369.9533
1371.9023	1378.5873	1388.9353
1393.2214	1399.2231	1423.4545
1427.3079	1432.2544	1433.2000
1434.9673	1436.4611	1439.8430
1441.1369	1445.1673	1447.2763
1447.9743	1450.7108	1455.4373
1470.7282	1475.1990	1483.7408
1487.6945	1495.7967	1501.5900
1506.4082	1507.1774	1520.6549
1535.4476	1569.6720	1575.3753
1595.3818	1598.1861	1598.9089
1604.7494	1610.4100	1617.5576
1618.0936	1636.2261	1637.0062
1645.7121	1660.9036	1668.4441
1669.6649	1671.5724	3157.7320
3175.0695	3176.6899	3177.7521
3178.2747	3179.0904	3180.6132
3181.1545	3188.4704	3189.5253
3192.3290	3192.9070	3194.2483
3195.2432	3195.5089	3197.5516
3199.2759	3201.1943	3240.8119
ZeroEnergy[kcal/mol] -4.54		
ElectronicLevels[1/cm] 1		
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RRHO		
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C 6.6180461723 -1.2529913298 -0.5355914887
C 6.770204362 0.0899610478 -0.0329774277
C 6.4804778499 1.1746141694 -0.8689863507
C 6.0337660051 0.9307610607 -2.218319175
C 2.986707279 -2.3535577092 -3.0597180234
C 2.4646280263 -3.1580219826 -1.9830864827
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C 4.7385721226 -3.2845808815 -1.0617805182
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C 3.9307973447 1.5989210033 -3.2931789029
C 2.6463049905 2.1561888576 -3.010615569
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C 3.7289339382 3.560109558 -1.3130349024
C 4.9255390083 2.8489511676 -1.4244545748
C 6.4513284099 0.1332168908 1.3585841114
C 6.0686092304 1.3673128885 1.888396831
C 5.7743645804 2.4710851363 1.0380003469
C 5.8590237648 2.3514617698 -0.3507541271
C 4.1138760415 -3.3263694467 1.2070832509
C 4.1777852161 -2.7134785919 2.4604199754
C 5.1273031334 -1.6855270451 2.7259009865
C 6.0215210094 -1.2600759222 1.7410079043
C 1.1275464671 -2.7626172514 -1.6668475394
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C 1.5550184888 -3.5458928017 0.6188532731
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C 0.3884967246 0.8335372173 -2.7189640385
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C -2.4040659531 -1.6570939939 1.3523473333
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C -4.5404528414 -1.1989859932 0.647323132
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C -5.9078565962 1.1899964594 0.8837715668
C -4.7881847485 0.9756155296 1.7753164835
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C -0.7735482975 -2.7984964695 0.0035842845
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C -3.1609551684 -2.6675708543 -0.7638244643
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C -0.6566124581 0.082918643 2.5932743775
C -0.1784732235 -0.9979255346 1.8572939704
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C -4.2297182021 -2.5583499761 -1.7384639247
C -4.019913974 1.92247864 2.5573303605
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 H 0.0684668952 0.7561749806 3.0451090534
 H 0.8968683481 -1.1169543441 1.7650178038
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 H -4.1351521911 -3.0720263038 -2.6922401686
 H -4.4282526863 2.9123087534 2.7488916744
 H -2.1708703531 2.4355427981 3.4872352446

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 826.3165

WellDepth[kcal/mol] 34.89

WellDepth[kcal/mol] 6.03

End

Frequencies[1/cm] 230

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30.1100	66.2069	82.6912
104.2316	131.1660	140.0955
148.6213	166.5023	176.1913
188.3210	191.6483	194.1438
224.2794	263.6702	283.8061
298.5285	313.9072	316.3757
323.9388	340.2744	341.5232
348.1506	356.9440	365.1955
374.0996	381.8028	395.0668
397.9450	412.8836	414.5752
420.3961	426.1940	437.5946
445.3560	448.8549	451.0291
457.5546	463.4064	468.1805
482.7634	494.9027	496.1167
504.1044	509.8878	514.9993
517.4280	532.5451	542.9200
546.4970	552.8355	555.8261
562.5068	575.0488	583.4218
587.0034	597.6236	601.6238
604.5438	609.3999	611.1326
616.2517	623.1406	626.6873
629.7779	645.5726	648.1197
653.7877	656.0824	665.6288
676.7139	678.0451	687.1814
690.2333	703.3050	709.5929
712.8107	717.0987	719.2378
721.7453	731.5110	738.9309
739.5222	743.0228	760.7867
762.0971	763.8769	767.3890
767.7177	770.6713	773.9868
783.9973	785.6775	796.6592
807.2120	812.3453	816.6769
818.8509	824.9810	830.6519
834.9313	836.1511	840.2591
842.9441	851.6470	858.2204
874.7954	884.4345	886.8741
890.9401	901.9571	923.5434
941.0104	947.9452	950.6699
954.3497	957.8498	964.0206
964.3459	969.2280	972.0101
981.2348	1002.1100	1005.6202
1009.1220	1042.0025	1043.1888

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1098.6766	1111.2186	1118.6545
1143.9665	1146.3045	1154.2332
1168.0272	1172.3711	1174.1543
1177.9547	1187.5182	1191.3925
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1214.1447	1219.8051	1227.4749
1239.5911	1242.5018	1250.6856
1252.1957	1265.3958	1267.4429
1270.5155	1291.0356	1299.9335
1306.3630	1320.6303	1324.7001
1332.8023	1338.1125	1338.7236
1342.5007	1350.9261	1357.8117
1366.4205	1376.9148	1384.4486
1386.9839	1391.8311	1401.2369
1411.8992	1432.6381	1433.2096
1435.7491	1436.5343	1440.6935
1442.9417	1445.5868	1446.6472
1449.9405	1450.6503	1454.9721
1456.0505	1470.9771	1476.1329
1486.5387	1490.2776	1499.0426
1506.2272	1507.0416	1507.8103
1522.1705	1566.3291	1575.6761
1585.2770	1597.0746	1598.2064
1598.6122	1604.4301	1614.6617
1617.7994	1620.3287	1637.2802
1637.6893	1645.4084	1660.2991
1665.7461	1667.8433	1670.4268
3176.6497	3177.8527	3178.0733
3178.9543	3179.9867	3180.0736
3182.1570	3185.7089	3191.9280
3193.7950	3194.3185	3195.0428
3195.1624	3196.3368	3196.9972
3199.3460	3209.6448	3221.1207
ZeroEnergy[kcal/mol] -5.57		
ElectronicLevels[1/cm] 1		
0 2		
End		
!-----		
End		

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H₁₇

```

!TemperatureList[K]          700. 800. 900. 1000. 1100. 1200. 1300. 1400. 1500. 1600.
1700. 1800. 1900. 2000.
TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650.
1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
!TemperatureList[K]          300 500. 1000 1500. 2000
!TemperatureList[K]          300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
!PressureList[bar]           0.1
!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature     0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature   100
ModelEnergyLimit[kcal/mol]    900
WellCutoff                    10
ChemicalEigenvalueMax         0.2
ChemicalEigenvalueMin         1.e-6      #only for direct diagonalization method
CalculationMethod              direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput               eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber             0
!ReductionNumber               5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                 260 ! Frenklach
! Power                         0.
! Factor[1/cm]                 247 ! Jasper universal
! Power                         0.85
! Factor[1/cm]                 424 ! Jasper calc N2
! Power                         0.62
! Factor[1/cm]                 125 ! SJK guess
! Power                         0.85
ExponentCutoff                 15
End
CollisionFrequency
LennardJones
!Epsilons[1/cm]                203.0 203.0 ! N2 pyrene-Frenklach
!Sigmas[angstrom]              4.6 4.6 ! N2 pyrene-Frenklach
! Epsilons[1/cm]              206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
! Sigmas[angstrom]             5.06 5.06 ! N2 Jasper extrapolation to C16
! Epsilons[1/cm]              32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
! Sigmas[angstrom]             3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
! Epsilons[1/cm]              101.5 1188.706851
! Sigmas[angstrom]             3.6154 10.90383901
! Epsilons[1/cm]              390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
! Sigmas[angstrom]             4.46 4.46 ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
! Epsilons[1/cm]              189. 216.0 ! N2 , CH2CCH ! from Jasper calc
! Sigmas[angstrom]             3.30 4.11 ! N2 , CH2CCH ! from Jasper calc
Masses[amu]                    28. 737.
End
OutputTemperatureStep[K]       100
OutputTemperatureSize          20

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OutputReferenceEnergy[kcal/mol] 0.

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Well ip1
Species
RRHO
Geometry[angstrom] 77
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C 5.2704828609 -2.6987686558 -2.065411496
C 6.3040678902 -1.7098957833 -1.8212947532
C 6.6954019612 -1.437653127 -0.5156848767
C 6.9308051961 -0.0845421732 -0.076178525
C 6.7368640134 0.9736443405 -0.9717761422
C 6.3043925541 0.6928116277 -2.3186055805
C 3.0535336159 -2.4117075614 -3.0793918723
C 2.449705703 -3.1206988556 -1.9776998383
C 3.266216961 -3.5875990743 -0.9416566463
C 4.6872077969 -3.3563788841 -0.989465774
C 4.0532128925 0.0888466314 -3.9022126131
C 2.6285444072 -0.1287932151 -3.8648170646
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C 5.1118073732 -3.0941127493 0.3637938521
C 5.396607389 1.7493077666 -2.6925849671
C 4.2785328827 1.4490159943 -3.4793359879
C 3.030143382 2.106650112 -3.2580911966
C 3.0322844127 3.2118044162 -2.4044675606
C 4.1695641636 3.5168702683 -1.6034976784
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C -0.4227224876 -0.9331293567 2.0122448416
C -5.4226062527 -1.6752551069 -1.6197414529

C	-4.2505734491	-2.3627895376	-1.9048286043
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C	-3.2467067329	1.2662846563	3.4045964981
H	2.1082396231	3.7423217151	-2.1871885002
H	4.0470651543	4.26290673	-0.8217521491
H	5.9943014879	1.496754534	2.7983783729
H	5.6583931773	3.3322134596	1.2449742514
H	3.2774992158	-2.6327092793	3.2035905836
H	5.0061409886	-0.9757802235	3.6101506815
H	1.0453605331	-3.2987298844	1.6249356164
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H	-5.0624013974	2.3797969372	3.2985485802
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Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 225

12.1529	21.2980	26.3773
66.2081	82.6526	103.8187
130.5729	136.4476	146.6976
162.3121	175.3822	182.8804
191.7224	195.0501	224.3855
262.1687	286.7058	301.9383
314.2487	316.0160	323.7003
340.2891	341.9868	355.2399
357.2179	366.7863	374.5570
382.2009	397.9979	410.7948
415.3574	420.4614	426.4708
437.5060	443.3671	450.9233
451.5895	453.5901	461.8086
469.9842	480.3631	493.0511
496.0042	507.9021	512.7677
515.9180	532.8331	542.8941
546.5236	548.4015	551.6858
563.8956	572.5759	583.9686
588.3256	596.1855	601.8013
604.6154	608.8630	610.9625
614.7990	616.7859	626.6676
629.2559	644.8200	646.9385
652.3558	656.0369	661.9027
673.3960	678.0511	686.8684
690.1544	703.1461	708.5274
713.3063	718.4765	720.5013
721.5363	729.3594	738.4761
739.7957	742.7987	755.3216
761.9541	763.8401	766.8179
767.7704	771.0980	774.5036
783.3192	785.6252	797.3909
804.8171	808.1426	816.5263
818.1329	824.4732	830.3214
834.9988	837.3618	840.4226
843.3849	852.3812	858.8342
875.4239	884.9285	890.5930
905.2351	921.4148	940.4607
947.3487	949.8894	954.5239
958.3850	962.2059	964.2356
970.0960	972.5170	980.1567

1002.0598	1005.6795	1009.2278
1042.2927	1043.3015	1064.1710
1086.3741	1089.9767	1094.6388
1108.3302	1118.9261	1145.4180
1146.3035	1154.1685	1170.2295
1171.6167	1172.6716	1177.7815
1187.7213	1191.6352	1201.3491
1202.7737	1209.4461	1220.3017
1227.5656	1235.8308	1238.9895
1249.7375	1251.2667	1256.9637
1266.1223	1270.0726	1281.7766
1295.2529	1301.7128	1313.9203
1324.2263	1325.0383	1332.5827
1337.8104	1341.4785	1349.7965
1357.3619	1364.4340	1376.9086
1379.8225	1384.8790	1389.2063
1399.2765	1405.4873	1432.7598
1433.3758	1436.0668	1436.3722
1440.3925	1442.9033	1445.4783
1447.7336	1450.2064	1450.6683
1454.0052	1458.9683	1467.8946
1476.2971	1480.1527	1485.3011
1494.8624	1506.4258	1506.8414
1508.0042	1518.7262	1565.2709
1575.6068	1584.5146	1596.7768
1598.0313	1598.3651	1604.2274
1614.1427	1617.4808	1619.5005
1620.0540	1637.2965	1637.8090
1651.6721	1665.6387	1668.1335
1671.0218	3177.4900	3177.5362
3178.2648	3178.8458	3179.5756
3181.0889	3184.3389	3184.9537
3193.5442	3194.4841	3194.5922
3195.7853	3196.1024	3197.0172
3207.2068	3208.0071	3220.7474
ZeroEnergy[kcal/mol] 0.00		
ElectronicLevels[1/cm] 1		
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End		
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Well ip2		
Species		
RRHO		
Geometry[angstrom] 77		
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C 5.0089634844	-2.820959245	-3.0700658306
C 5.6856686173	-3.1273375593	-1.8237515812
C 6.6492801709	-2.0737310438	-1.5578078544
C 8.6684373379	-1.644686378	-0.2558350665
C 7.0442411239	-0.2456100022	0.0560671708
C 6.9298655058	0.7013507351	-0.9711354473
C 6.6457742169	0.2589305365	-2.3121862823
C 3.6541593985	-3.1273324765	-3.2172539361
C 2.9226497149	-3.6979093799	-2.1118994589
C 3.5491601552	-3.9225542724	-0.8944886616
C 4.9586301306	-3.6590686095	-0.7594723259
C 4.5947488725	-0.6189580548	-4.0600182027
C 3.2117539438	-0.93386815	-4.2057477989
C 2.7429780321	-2.1995318242	-3.860668784
C 6.1383879163	-2.220556579	0.8498441555
C 5.1666739156	-3.1899582578	0.5870804977

C	5.7284398738	1.2263583834	-2.8713827236
C	4.6910892819	0.7772593351	-3.6951223733
C	3.3998846565	1.3709699609	-3.6206012797
C	3.2734168556	2.5652632901	-2.9030856754
C	4.3284256935	3.028841295	-2.0792637286
C	5.5169594307	2.2958078819	-1.954409499
C	6.5372768547	0.034626179	1.3589516676
C	6.1790873575	1.3600016535	1.6442037279
C	6.0634627704	2.3178664518	0.6077932706
C	6.3046382842	1.9637276449	-0.7260473346
C	3.9276745325	-3.1887535287	1.3064874936
C	3.8488553047	-2.3834675702	2.4505930715
C	4.8497867895	-1.4207429658	2.732119081
C	5.936889043	-1.2390833283	1.8672169371
C	1.5855251807	-3.1668342427	-2.1288090436
C	0.8544087225	-2.9581199915	-0.9320258319
C	1.533606575	-3.1902036927	0.2992078693
C	2.8732633276	-3.6117807896	0.3438637598
C	2.4093118548	0.274645789	-3.8857974493
C	1.1482792493	0.1435768908	-3.4067987474
C	0.4302331277	-1.2313844748	-3.3241523739
C	1.4524075647	-2.3183255258	-3.2457988005
C	-4.4402259386	-0.3406708572	0.0676724501
C	-3.6700210068	-1.4049109919	0.5864975557
C	-2.6673523101	-1.7245791892	-0.3615194889
C	-2.836006295	-0.8684691906	-1.469550992
C	-3.9305212642	-0.0142791866	-1.2080716013
C	-4.0932552339	1.2219262982	-1.8028401731
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C	-5.478250898	1.7889632951	0.1829766094
C	-5.138045243	0.5524717324	0.8594074784
C	-1.4781276653	-2.3496220088	-0.0465468949
C	-0.4274905693	-2.2228098793	-1.0717702911
C	-0.6166594116	-1.3668389283	-2.2034328741
C	-1.8274235346	-0.5748971006	-2.3615312924
C	-3.562526369	-1.6776097647	1.9352788306
C	-2.4521755928	-2.5519139275	2.2476362413
C	-1.4789798278	-2.8824017129	1.309831423
C	-3.1724916688	1.4576343031	-2.896300717
C	-2.1096054426	0.6025894431	-3.1704022574
C	-5.1843777009	0.1786391432	2.2590982279
C	-4.440791949	-0.8815202957	2.768497567
H	2.3094330358	3.0620926932	-2.823492354
H	4.1181179642	3.8555185492	-1.4048154807
H	5.7931300931	1.6266156596	2.6252330742
H	5.5947509071	3.2691261106	0.8485492561
H	2.9356106996	-2.351378719	3.0399724076
H	4.648601769	-0.6995750559	3.5207501103
H	1.0922691251	-2.8025233915	1.2091219334
H	0.6259848039	0.9969726872	-2.9846287756
H	-0.1358396617	-1.3388517594	-4.269444417
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H	-6.0771777559	2.5344681764	0.7012454511
H	-2.3333203624	-2.9344259821	3.2589367592
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H	-3.2667273191	2.3620183654	-3.4932871868
H	-1.4409753398	0.8805203941	-3.9797324923
H	-5.7583054078	0.7848632575	2.9563509526
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Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 225
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256.6235	298.9658	310.4036
313.2415	319.8724	323.6398
332.8547	350.0662	352.0098
371.5963	378.2694	380.2670
401.2912	404.4157	412.3304
415.6353	425.8450	435.5611
440.2278	445.9112	460.5781
463.3794	473.1778	476.2637
484.4052	490.5360	497.4788
506.9744	511.9896	517.2888
522.0044	546.7127	548.6329
551.1103	552.3113	566.5448
572.5399	587.9321	591.8756
593.0521	599.3710	605.1921
607.7778	610.3809	612.8812
625.0215	628.5601	637.5791
645.7011	651.3120	653.9438
660.0631	660.9204	670.4697
682.5565	692.1855	693.8986
700.7553	703.5688	708.3225
711.9275	714.0490	726.6357
728.4018	732.7693	737.7202
744.5278	749.1685	757.2713
761.7938	765.8439	768.1592
774.3087	779.5746	780.2932
788.4990	795.6304	804.0224
809.9795	811.0721	812.6922
816.8517	823.7579	826.3534
837.5523	841.6651	845.6406
849.5196	855.7494	880.5879
882.6452	894.8667	909.9090
911.5103	942.2706	946.8560
950.2675	957.7673	958.3149
962.5917	965.6607	971.0058
973.1565	980.4179	1002.1254
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1163.0392	1166.2506	1172.7350
1177.4602	1179.9625	1187.2563
1188.9110	1198.6398	1201.5552
1211.5476	1215.6380	1225.3727
1230.6218	1234.5303	1240.5535
1242.3136	1249.5690	1253.1423
1263.2705	1276.8651	1282.6795
1293.0890	1297.1091	1313.8951
1320.9633	1327.4371	1332.5889
1334.7127	1341.0769	1342.9190
1350.6604	1355.1637	1358.4255
1370.9519	1371.4670	1377.9900
1381.4012	1395.0251	1399.2771
1423.3398	1425.1521	1432.2028
1435.1131	1439.7554	1440.1783
1441.9586	1447.1068	1450.7355
1457.9973	1460.2076	1465.2879
1473.7531	1475.1279	1485.3463
1490.9238	1498.4376	1503.3434
1505.0526	1517.5555	1538.1798
1543.9625	1568.8906	1584.9924

1589.3279	1594.8618	1598.1481
1602.9137	1610.1622	1616.7208
1626.5025	1643.2849	1665.9686
1677.0465	1677.4208	1681.3490
1685.1021	2922.3885	3177.2445
3177.9737	3177.9873	3178.9513
3180.3248	3181.5031	3183.2763
3194.1654	3194.2018	3195.1390
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3209.0368	3225.5114	3245.0907

ZeroEnergy[kcal/mol] -31.9
ElectronicLevels[1/cm] 1
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End
End
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Bimolecular p1
Fragment c60h16
RRHO
Geometry[angstrom] 76

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C	4.5136918007	-2.8153264219	-2.8435776091
C	5.186973761	-3.0972176163	-1.5891971403
C	6.1412391926	-2.031443504	-1.3383577627
C	6.3392146081	-1.5704155237	-0.0432913567
C	6.4916794148	-0.1628255919	0.2353436581
C	6.3943413914	0.7587775264	-0.8145592856
C	6.1436077214	0.2815214093	-2.1530498097
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C	2.4266679667	-3.7025097156	-1.8790471205
C	3.0586370084	-3.9216402561	-0.6575799591
C	4.4603901722	-3.6225985084	-0.5214890117
C	4.1450252248	-0.6368551112	-3.9229217448
C	2.7436401067	-0.9394194286	-4.0550457532
C	2.2651245532	-2.1732299528	-3.6212569695
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C	4.6598823172	-3.1333982008	0.8213477533
C	5.2524134348	1.234084451	-2.7702105306
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C	2.9528117245	1.371744173	-3.6178907711
C	2.8081210113	2.5781516486	-2.929713512
C	3.8356476079	3.0568540402	-2.0706848093
C	5.0131133606	2.3279589835	-1.8859503264
C	5.9610873764	0.1439207919	1.524442168
C	5.5769637949	1.4658695708	1.7639800189
C	5.4781373601	2.4014486117	0.6981529258
C	5.7625647947	2.0233234786	-0.6166076154
C	3.4316850084	-3.1619463938	1.5469557262
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C	4.2989090748	-1.3289233548	2.9256684544
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C	0.3624613356	-2.9956839042	-0.7126721136
C	1.0390361565	-3.2491409457	0.540469278
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C	1.9637895167	0.2573733726	-3.8505636392
C	0.6802290003	0.1480392062	-3.3296011831
C	0.1639681445	-1.1165297365	-2.8534296114
C	0.9948858627	-2.2352939749	-2.9734263422
C	-4.8693724418	-0.2772929301	0.2542188076
C	-4.1425811287	-1.3863763087	0.7364579624
C	-3.1090220995	-1.6664474387	-0.1861818622

C	-3.2071918002	-0.7367175555	-1.2452982304
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C	-4.4389172585	1.382309102	-1.509888209
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C	-5.9004995492	1.8475577024	0.4487891049
C	-5.5980103079	0.5709796522	1.0663634627
C	-1.9616498326	-2.3601669527	0.1303000277
C	-0.8790555264	-2.2208964919	-0.8499792882
C	-0.9803078858	-1.2619145469	-1.9423700825
C	-2.1673594903	-0.4123025482	-2.0887272498
C	-4.1074012303	-1.7565637142	2.0660490739
C	-3.0329091724	-2.6787333249	2.3661768509
C	-2.0309198973	-2.9782340527	1.4474175167
C	-3.4904648106	1.6533161202	-2.5691371125
C	-2.4297896823	0.7982965283	-2.8549998082
C	-5.7164128139	0.1047715558	2.4342778903
C	-5.0133885086	-1.0001229305	2.9069303728
H	1.8426014664	3.0765253811	-2.8854010501
H	3.5964740355	3.8929162584	-1.4177973359
H	5.1570577515	1.7524376356	2.7252439817
H	4.9883055104	3.3499213273	0.9053585362
H	2.4118408979	-2.312568896	3.2539619286
H	4.0704510188	-0.594682517	3.694540637
H	0.5807025589	-2.871978862	1.4474871653
H	0.1663515444	1.0516126145	-3.0222156084
H	-5.5717288593	3.2307835997	-1.1410446346
H	-6.5175041174	2.5672501416	0.9821242481
H	-2.9662291401	-3.1276875371	3.3546981988
H	-1.2645985265	-3.6769433518	1.7626001181
H	-3.5685413779	2.5747492475	-3.1418882641
H	-1.7676141151	1.0858766793	-3.6634598644
H	-6.3172046744	0.670930408	3.1425235722
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Core RigidRotor
SymmetryFactor 1
End

Frequencies[1/cm] 222

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183.3821	183.4611	201.2713
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278.3055	300.8119	310.0266
321.9103	325.7069	337.7365
342.0694	349.6107	355.8198
375.3180	381.8356	389.5834
403.3829	406.0089	415.8523
418.0823	435.4083	436.5666
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551.7849	552.0004	572.3025
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599.0866	603.7868	607.6664
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627.4417	631.2164	639.7001
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774.6626	781.7347	782.3891
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812.5006	816.5754	818.0477
818.7583	828.7341	832.3426
838.2184	848.4403	853.9799
860.6608	870.5162	884.1196
890.0142	911.9187	912.6624
915.5102	943.4735	949.1176
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966.4021	967.5862	977.3788
978.9102	992.4371	1005.0513
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1221.2801	1222.0470	1230.0429
1240.8506	1248.8807	1252.9110
1255.8886	1265.9605	1271.7607
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1314.3442	1326.5316	1328.3960
1333.3418	1333.4580	1338.2461
1350.7272	1353.8996	1367.0243
1374.5461	1381.9191	1391.2716
1395.0652	1397.0840	1414.7110
1424.3455	1427.7226	1434.8836
1436.4485	1437.5951	1440.2332
1446.2675	1446.3396	1451.0024
1452.5446	1458.8129	1462.0256
1465.2944	1473.7493	1486.0832
1494.1185	1496.3055	1496.9446
1506.4746	1508.9955	1518.3405
1565.7047	1569.3758	1577.6585
1598.0973	1599.5400	1602.5495
1613.1329	1615.8312	1617.0421
1624.3866	1628.8349	1635.1101
1668.3242	1678.5044	1679.8231
1685.0226	1685.9299	3177.0273
3177.7436	3178.2148	3179.4310
3180.3741	3182.9238	3183.0396
3193.9930	3194.2081	3195.1377
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3218.1664	3234.3152	3234.4549
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] -2.2		
End		
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Barrier ts1 ip1 ip2		
RRHO		
Geometry[angstrom] 77		
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C	6.6310488561	-2.0591925824	-1.1957548009
C	6.6879319944	-1.4756516397	0.0629394302
C	6.7991963638	-0.0454472185	0.2190354685
C	6.8135558044	0.7713125394	-0.9183169588
C	6.7260493592	0.16846175	-2.224321163
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C	4.9373504792	-2.9799627089	0.8953562828
C	5.9196836771	1.0498037149	-3.0338831375
C	5.0326035099	0.5054302077	-3.9674808669
C	3.7576476067	1.1044202227	-4.2094360086
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C	5.7048104189	1.7029473208	1.4719278613
C	5.7178555677	2.5317790705	0.3160218797
C	6.1560798976	2.039683616	-0.9161001494
C	3.6466699087	-2.9663953993	1.5034537792
C	3.4255063831	-2.0425276417	2.5279515608
C	4.3546838452	-0.9962802161	2.7794412531
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C	2.6940374889	-3.523218609	0.4813542158
C	2.7993898418	-0.0263651146	-4.4777384444
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C	-1.6249845422	-2.5201070488	-0.2882275734
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 SymmetryFactor 0.5
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 Tunneling Eckart
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 WellDepth[kcal/mol] 44.41
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ZeroEnergy[kcal/mol] 2.6
 ElectronicLevels[1/cm] 1
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 End

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H₁₅

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1700. 1800. 1900. 2000.
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1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
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!TemperatureList[K]          300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
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0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature    0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature  100
ModelEnergyLimit[kcal/mol]   900
WellCutoff                   10
ChemicalEigenvalueMax        0.2
ChemicalEigenvalueMin        1.e-6      #only for direct diagonalization method
CalculationMethod             direct
!RateOutput                   one_path.out
!LogOutput                    one_path.log
EigenvalueOutput              eigenvalue.out
!EigenvectorOutput            eigenvector_test.out
!EigenvectorNumber            0
!ReductionNumber              5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                260 ! Frenklach
! Power                       0.
! Factor[1/cm]                247 ! Jasper universal
! Power                       0.85
! Factor[1/cm]                424 ! Jasper calc N2
! Power                       0.62
! Factor[1/cm]                125 ! SJK guess
! Power                       0.85
ExponentCutoff                15
End
CollisionFrequency
LennardJones
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!Sigmas[angstrom]             4.6 4.6 ! N2 pyrene-Frenklach
! Epsilons[1/cm]              206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
! Sigmas[angstrom]             5.06 5.06 ! N2 Jasper extrapolation to C16
! Epsilons[1/cm]              32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
! Sigmas[angstrom]             3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
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C 4.2208919551 0.7309284069 -3.6679358291
C 2.913865833 1.302209735 -3.7165935285
C 2.7212698968 2.5210534715 -3.0625440363
C 3.7089065445 3.0417513491 -2.1812307847
C 4.8950078374 2.3439245423 -1.9399439344
C 5.7953164954 0.256368324 1.5470267563
C 5.3672215736 1.5716762494 1.7452566801
C 5.275461598 2.4817437455 0.6564871467
C 5.6102516993 2.084705615 -0.6408216539
C 3.371851455 -3.1313473316 1.5807582568
C 3.2115101946 -2.2827457406 2.6781309943
C 4.1423792581 -1.2390469949 2.9374954681
C 5.2381059644 -1.0297979061 2.0964426704
C 1.1277985692 -3.2695979268 -1.9035037675
C 0.3578650267 -3.0940102471 -0.7493721173
C 1.0071299301 -3.3215758699 0.5237239216
C 2.3542087531 -3.6544528848 0.5981908296
C 1.956305001 0.1574879948 -3.9404952588
C 0.6623802492 0.0323840755 -3.4514955379
C 0.1885550403 -1.2232381108 -2.914662533
C 1.0327953231 -2.3341558462 -3.0017622926
C -4.767196406 -0.2167329822 0.2676040257
C -4.1209794444 -1.4036487961 0.6813395038
C -3.1069914095 -1.7022251114 -0.2592574596
C -3.1465112649 -0.7083262587 -1.2670260661
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C -5.4250521408 0.6326820418 1.1390725489
C -1.989277171 -2.4565269502 0.0357121879
C -0.8817995534 -2.3225246795 -0.9146794594
C -0.9364414781 -1.3409231173 -1.9843759474
C -2.0607227587 -0.4117456356 -2.0737435493
C -4.1015446185 -1.8402144996 1.9926698512
C -3.080109643 -2.8316366324 2.2491839504
C -2.089546629 -3.1322749236 1.3201759362
C -3.1865520492 1.8231944819 -2.3791231421

C -2.237877076 0.877282675 -2.6685483519
 C -5.5762341429 0.0988003624 2.4777122618
 C -4.951131756 -1.0760328321 2.8820898944
 H 1.7438923927 2.9975984567 -3.0609615191
 H 3.4295857588 3.8872297553 -1.5570088125
 H 4.9112729663 1.8673290878 2.6871426256
 H 4.7545693062 3.4206734854 0.828514305
 H 2.2811854839 -2.2780699417 3.2411874465
 H 3.8697359632 -0.4962269933 3.6833594131
 H 0.5114964767 -2.9550147963 1.4158364092
 H 0.0824773819 0.9247908482 -3.2325170717
 H -5.1676523575 3.4347069697 -0.864929003
 H -6.181015542 2.6954232699 1.2036496127
 H -3.0406474029 -3.3286275405 3.2159050554
 H -1.3521848033 -3.8763619035 1.5999170587
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 H -6.1324702492 0.6669807513 3.2198700778
 H -5.0465275238 -1.3783872873 3.9224701739

Core RigidRotor
 SymmetryFactor 0.5
 End

Frequencies[1/cm] 219

21.8751	31.2577	65.6569
81.1167	103.5711	114.6394
138.2716	155.5108	181.3547
183.3050	185.0909	204.7722
220.0491	249.2140	253.0530
274.5722	302.4418	315.0336
321.3142	323.2900	334.9618
341.2433	349.1427	355.0810
373.5962	381.4447	389.7491
402.9714	407.2709	417.1755
418.6197	434.9081	436.9539
444.0532	449.5750	452.8531
471.2830	478.7085	479.2202
483.8516	490.0100	505.0672
512.2776	517.9723	518.5539
521.9332	542.5101	550.2444
551.0176	551.5214	570.2856
575.3897	589.2170	592.0612
599.9281	604.3446	606.4109
607.3049	611.6638	612.2457
627.9780	631.6381	639.7440
644.8784	650.7408	656.3808
664.6142	666.1318	684.6606
686.8349	697.9375	702.8818
705.3388	707.2517	715.5574
716.4031	719.8843	730.8750
734.2723	737.8768	742.2971
754.9147	755.5531	762.6115
763.3645	768.4315	770.2316
775.5303	780.4996	781.3652
786.9127	792.3506	794.6185
811.0470	814.1882	818.6044
821.5255	828.1315	832.3872
843.2704	847.7960	857.7553
860.0401	871.4150	883.9326
889.1814	900.8595	909.6168
913.6355	943.6404	949.3095
951.6369	958.9623	962.5792
966.8756	968.0601	980.5554
989.2606	1004.5080	1011.2978
1039.7646	1049.3538	1062.5371
1076.8714	1091.5656	1103.3407

1112.2421	1119.2955	1119.6957
1147.1215	1160.1947	1167.8697
1168.9587	1180.6899	1184.9351
1187.4491	1198.4520	1201.4796
1202.8688	1210.9082	1222.1716
1227.2720	1238.1081	1246.6821
1250.2246	1253.4690	1254.4705
1271.2717	1276.3714	1293.7963
1303.5409	1304.8939	1320.6848
1324.4955	1329.1643	1330.2790
1337.0352	1348.7737	1350.8925
1359.2063	1374.1682	1378.3306
1385.3544	1392.7998	1395.6240
1400.2119	1412.4492	1423.1626
1425.9824	1434.7352	1435.2693
1437.4514	1445.3460	1446.0084
1449.0982	1450.3843	1452.8634
1456.3171	1463.7577	1471.8223
1475.6577	1483.1264	1493.3507
1496.7649	1502.2101	1509.5013
1513.4494	1564.5061	1569.2738
1576.4868	1597.9870	1598.9886
1601.9123	1612.4184	1615.4317
1617.1596	1624.1032	1627.1436
1628.5061	1634.9346	1661.2406
1670.4347	1675.0235	1677.1486
3175.6007	3177.9189	3178.8549
3178.9201	3179.7652	3180.8620
3183.9195	3186.3383	3194.9026
3194.9268	3195.9053	3196.1706
3197.1003	3214.6649	3228.7046
ZeroEnergy[kcal/mol] 0.00		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
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Well ip2		
Species		
RRHO		
Geometry[angstrom] 75		
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C 4.7289899643	-1.0953446464	-3.1306390669
C 4.5183384389	-2.4774941396	-2.764731284
C 5.0893791301	-2.6843738269	-1.4510855066
C 5.7136713195	-1.4430238373	-1.0250007639
C 5.6563007003	-1.0592776637	0.3069761331
C 5.4060061645	0.3130593085	0.6815431423
C 5.1603538938	1.2581574859	-0.3190191564
C 5.18421144	0.8497446647	-1.7013647796
C 3.3009204821	-3.0831204034	-3.0995078648
C 2.5878639245	-3.8719649263	-2.1016764859
C 3.125353636	-4.0365716924	-0.8328983997
C 4.4027106688	-3.4512032323	-0.509899838
C 3.7065891504	-0.3808342611	-3.7691212465
C 2.4603791769	-1.0019154303	-4.1388152751
C 2.31317902	-2.365612773	-3.8571290175
C 4.9857674454	-1.877609129	1.2916332378
C 4.3371948059	-3.0470188013	0.8717059078
C 4.1253046946	1.5763801844	-2.3574622285
C 3.3868516671	0.9533766723	-3.3564820186
C 1.9593181739	1.1798714333	-3.4821464606
C 1.4414238517	2.2751294438	-2.7365501517

C 2.19894782 2.904151012 -1.7321012271
 C 3.5100618442 2.486292091 -1.4349702159
 C 4.690729217 0.3617239428 1.9176466472
 C 3.9431470964 1.5166967625 2.1885020336
 C 3.6893792799 2.4719994251 1.1755000501
 C 4.180777801 2.2857499729 -0.1257853225
 C 3.0813487344 -3.4199186991 1.4406870866
 C 2.6728131883 -2.7513060127 2.6022569809
 C 3.3387155311 -1.5809193581 3.0363146732
 C 4.4169111721 -1.0560374755 2.3070013061
 C 1.1735314729 -3.6641897766 -2.2480708688
 C 0.2853380224 -3.6521822429 -1.1293844372
 C 0.8930789256 -3.8951723793 0.1620756308
 C 2.2672767211 -4.0093893353 0.3276121052
 C 1.3675354952 -0.0229356001 -4.0114228952
 C -0.0800778414 -0.5652654145 -4.1130148681
 C -0.0561774314 -1.9744269702 -3.4486247328
 C 1.0143849829 -2.8049775662 -3.3886203172
 C -3.7245915432 0.5289665076 -0.0899927786
 C -3.4961593668 -0.7673301964 0.4625618276
 C -2.9210145923 -1.5973893083 -0.5431270324
 C -2.8876751505 -0.7966985451 -1.723505257
 C -3.3194952126 0.5133249308 -1.4491021725
 C -2.7741610206 1.616705797 -2.107318716
 C -2.9662141192 2.8602464543 -1.3872362267
 C -3.4166034816 2.8914069423 -0.0728728215
 C -3.7051050127 1.6849954957 0.6752538406
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 C -2.6450372118 -2.2162763991 2.13253824
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 H 3.3820852446 1.6026177404 3.1159782181
 H 2.9492234399 3.2420686708 1.3786003303
 H 1.7307621984 -3.0052769611 3.0822576067
 H 2.8732751029 -0.9968567231 3.8266421643
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 H -2.5573729516 -2.5350509661 3.1688754727
 H -1.5577692193 -3.9106666098 1.4780914019
 H -1.3809963178 2.2023259407 -3.6977214985
 H -3.7658200475 2.3139144117 2.7786139912
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Core RigidRotor
 SymmetryFactor 0.5
 End

Frequencies[1/cm] 219

30.3233	35.9455	69.2337
95.4164	122.0978	144.8368
169.9107	182.4066	185.4714
193.1733	216.6035	228.5977
257.2541	263.6087	279.7599
300.4052	306.6069	322.3353
324.4739	333.3671	347.4523

352.4351	355.4728	375.9977
381.2373	395.2435	399.9628
400.8679	409.4217	428.0586
430.5529	438.0171	442.9836
447.2838	457.2478	469.0888
480.9971	485.8385	490.2836
493.8912	507.1093	514.3692
518.8168	519.6341	524.6722
539.5060	545.2582	554.1718
555.3126	563.0936	570.9285
579.7001	589.7981	598.7572
599.4534	604.7246	609.4623
615.0899	621.2827	625.3998
636.3487	644.8728	647.7534
652.8313	656.5525	665.1391
672.7146	680.5768	692.3014
695.0726	700.2274	709.7779
712.3935	714.1637	716.2243
723.6607	728.9418	734.5650
738.5405	748.8337	750.5862
756.6557	760.1362	762.0235
765.2000	767.7054	775.4879
778.7937	781.2722	783.9202
787.7493	795.8426	801.8717
807.8048	812.4958	818.7705
821.3284	823.8857	827.5705
844.6363	848.3278	859.4990
867.5762	880.4724	892.0367
902.9709	924.6704	934.5837
942.0113	944.8779	950.9193
956.1226	959.0812	966.9970
967.8789	978.9750	981.7952
998.2833	1009.8947	1025.2704
1041.7993	1073.4899	1081.0668
1093.5521	1095.7485	1111.7728
1114.8411	1124.7254	1134.7889
1150.0955	1160.1262	1170.3353
1175.1230	1179.8523	1181.4944
1187.9577	1190.4737	1199.3206
1207.0228	1213.9537	1222.5448
1223.9191	1228.6954	1237.4008
1245.8838	1256.4351	1258.3184
1262.5918	1266.7904	1289.7727
1297.8612	1304.0493	1316.5131
1317.2135	1320.0746	1328.0753
1331.1358	1339.8294	1344.9187
1348.1006	1357.9542	1364.7196
1368.0234	1380.5401	1384.9584
1396.5172	1406.7747	1414.0452
1419.0340	1422.8076	1430.1463
1431.9765	1437.0503	1442.4293
1443.1667	1447.5285	1452.0922
1458.8484	1460.9820	1465.7815
1472.2759	1477.9462	1487.4738
1494.8282	1504.2982	1510.7720
1517.4652	1528.8693	1549.0221
1554.7088	1569.6171	1580.4312
1587.2650	1593.0642	1601.4242
1609.1652	1615.5141	1616.9200
1630.7931	1641.5981	1653.1906
1659.5949	1684.6224	1751.2157
2984.4537	3173.2235	3176.9125
3178.6917	3181.1384	3182.2363
3186.5075	3190.5761	3192.9982

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3194.3155      3195.0043      3197.5785
3216.7616      3265.0583      3267.9240
ZeroEnergy[kcal/mol] -17.8
ElectronicLevels[1/cm] 1
0 2
End
End
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!-----h_c60h14_p1-----
Bimolecular p1
Fragment c60h14
RRHO
Geometry[angstrom] 74
C 4.5266208952 -0.4240257023 -1.9242047934
C 3.7606066682 -1.0751991189 -2.9725480016
C 3.5188972672 -2.4432691553 -2.5651522504
C 4.079890208 -2.622251241 -1.2401994034
C 4.7232898806 -1.3813274231 -0.8501645295
C 4.6528456637 -0.9504764022 0.4680609633
C 4.4417866395 0.4399862148 0.7909745147
C 4.2595412125 1.3648234447 -0.2446874096
C 4.2792236738 0.9045715745 -1.6121118242
C 2.3064438375 -3.0443030631 -2.8933466864
C 1.5765290881 -3.8210330805 -1.8984205694
C 2.0919658496 -3.9417430711 -0.6122523801
C 3.3651294111 -3.3464819033 -0.2881264295
C 2.7540789262 -0.3554682537 -3.626062184
C 1.4955015991 -0.9568970129 -3.9610904563
C 1.3267985281 -2.3122683155 -3.6598902552
C 3.9419040533 -1.7171580833 1.4632833781
C 3.2829943465 -2.8916865821 1.0775759997
C 3.266727243 1.655023164 -2.3131523957
C 2.4946560403 1.0195835225 -3.2905830303
C 1.1087128811 1.3284876455 -3.4544526624
C 0.6486168437 2.4706199557 -2.787674575
C 1.4290032081 3.1127221011 -1.7878236323
C 2.694123015 2.6334477514 -1.4478321966
C 3.7034466309 0.5562582508 2.0067169238
C 3.0013717492 1.74556281 2.22298789
C 2.8197410199 2.6859771533 1.1730549544
C 3.3379890402 2.4453734817 -0.1028189537
C 2.0140511522 -3.2288567548 1.6372593084
C 1.5889073201 -2.5014230052 2.7514358822
C 2.2666883911 -1.3180894418 3.1523878696
C 3.3723958647 -0.8468018798 2.4388518208
C 0.1664862682 -3.6169827414 -2.0760048419
C -0.7395531288 -3.5879383119 -0.9794821455
C -0.155451538 -3.7736657585 0.3340272268
C 1.2156666074 -3.8709012136 0.5302969627
C 0.4149058598 0.0499450428 -3.8581468312
C -0.8876759478 -0.4098276436 -3.6068685546
C -0.9901049139 -1.8368996772 -3.2394348295
C 0.0413944459 -2.7300287369 -3.21371657
C -4.7273578941 0.5661546943 0.1091286631
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C -3.9681795557 -1.5567951815 -0.43489039
C -3.8688800187 -0.6961022143 -1.5695280499
C -4.2665717891 0.6125212462 -1.2307702849
C -3.6519156694 1.7312205133 -1.7962006111
C -3.8366828373 2.9397690243 -1.017427521
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C -4.7014859026 1.6772054272 0.9392054619
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C	-3.7835450896	-2.3164996147	2.2161754317
C	-3.1596404623	-3.054295009	1.2178400705
C	-2.6347781482	1.4979761942	-2.8169361946
C	-2.1703312997	0.2062544935	-3.0951968375
C	-4.7619384117	1.3777666441	2.3533175217
C	-4.621152808	0.0835429789	2.8313610789
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H	0.9368277503	3.8644661559	-1.1755085258
H	2.4151150652	1.8824738219	3.1284888465
H	2.1055847843	3.4898330481	1.3349631673
H	0.6280254969	-2.7120371655	3.2148251508
H	1.7851373097	-0.6910392138	3.8989624267
H	-0.7718345401	-3.5493024971	1.1942726934
H	-3.4754872463	3.888213692	-1.4094545022
H	-4.3695554759	3.844117024	0.8378604225
H	-3.7333163136	-2.6865554009	3.2378192782
H	-2.6857464747	-3.9864701544	1.5071562053
H	-2.1512300224	2.3655804044	-3.2513748105
H	-4.8276765285	2.1928324755	3.0705159895
H	-4.5850364722	-0.0718095307	3.9072876313

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 216

33.9421	36.0562	71.3320
96.6098	128.1226	148.8755
172.7775	181.0075	185.7636
197.1112	216.1247	233.5374
258.2023	275.1922	283.4822
296.8939	311.3070	322.4796
331.7236	338.3704	349.4396
355.4415	360.3053	379.7789
386.7512	396.5153	403.5479
407.3484	416.3901	434.9325
436.2570	442.5720	451.8172
454.3718	458.8483	472.6027
485.7865	487.8745	492.7037
495.2226	504.4462	514.7016
517.4724	524.6366	527.8003
539.8165	550.7513	554.9914
556.8630	566.8294	577.4953
581.8581	597.1577	602.0821
607.3995	608.9989	612.2937
617.5344	624.8872	630.6599
641.3805	646.9293	652.1811
655.4191	664.3544	670.4401
677.4127	693.3751	699.1287
700.6154	705.8871	713.7649
717.6247	720.3626	721.2726
730.9471	737.2399	737.4742
742.2665	747.5902	752.6400
757.1761	761.4660	762.7773
767.2010	769.1422	770.2041
776.7615	783.7969	788.1490
792.8855	795.1215	802.6092
805.7606	815.9311	818.6410
823.8858	825.6199	829.5868
847.1025	852.4119	869.3097
882.2888	886.3907	898.8221
907.1460	911.2462	931.9591
943.7074	945.6793	951.0657

958.9708	963.3505	968.3803
974.9157	984.4521	993.7198
1010.6759	1023.1620	1040.8091
1066.3688	1076.7590	1083.5604
1093.0056	1103.7881	1113.1894
1130.0776	1138.5889	1147.2462
1163.5619	1168.3386	1172.2636
1180.9823	1181.5968	1191.9872
1196.0033	1202.1809	1206.5385
1215.7353	1223.1928	1229.8116
1239.0143	1246.8949	1250.6905
1255.5791	1267.0365	1273.4643
1298.1925	1300.6997	1305.8091
1317.8985	1325.7314	1327.3756
1335.5932	1345.1158	1348.0758
1355.5442	1360.8410	1366.3766
1374.5314	1377.3861	1386.6505
1398.0305	1404.4528	1408.1719
1424.9107	1428.6425	1432.7452
1435.4085	1439.1619	1443.0948
1445.4318	1446.2549	1451.1423
1451.8332	1458.8066	1460.6667
1465.6462	1474.9542	1483.1781
1487.7308	1499.1684	1507.3088
1509.9681	1516.1865	1545.5511
1561.6591	1575.0478	1592.1275
1596.7947	1600.0683	1608.0219
1609.4404	1614.0441	1620.8529
1626.8713	1635.8846	1636.6098
1652.7283	1657.1071	1682.1158
1748.8834	3174.9198	3177.7943
3178.9314	3180.4400	3182.3523
3186.9349	3191.9682	3194.6089
3194.9552	3196.8245	3211.0771
3221.9454	3253.5026	3276.6308
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] 25.3		
End		
!-----bar_ts1-----		
Barrier ts1 ip1 ip2		
RRHO		
Geometry[angstrom] 75		
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C 3.5318458457	-1.1301903237	-2.0775225245
C 3.1483242795	-2.4282969808	-1.5614334022
C 3.6143633561	-2.5184870446	-0.1938438008
C 4.3151664517	-1.2863766785	0.1278762113
C 4.180041212	-0.726841696	1.3903819254
C 4.0268189007	0.6973065875	1.5655501985
C 3.973282286	1.5256787555	0.4387152479
C 4.0777142368	0.9400232524	-0.8749779679
C 1.9027086513	-2.9647547833	-1.9043858387
C 1.0775322992	-3.5983581524	-0.8928336413
C 1.5174069632	-3.6619046904	0.4250927551
C 2.804064387	-3.1133449764	0.7729375827

C	2.6390683667	-0.4112992701	-2.8731861019
C	1.3479481124	-0.9487562186	-3.1937925053
C	1.0135064328	-2.2320505199	-2.7697049572
C	3.3649301801	-1.3567006899	2.4018746205
C	2.6701265934	-2.5318034163	2.0861231804
C	3.1792120692	1.6821015904	-1.7271472268
C	2.4610742205	1.0078553201	-2.7165209329
C	1.1078112267	1.3765456412	-3.0261617983
C	0.6394178008	2.5829201288	-2.4813826821
C	1.3724742486	3.2668009963	-1.4782468941
C	2.5875392849	2.7612172792	-0.9986503469
C	3.2126024937	0.9659915722	2.7072539697
C	2.5616077501	2.203377085	2.7544955713
C	2.5075577645	3.0446569697	1.6113788574
C	3.1045142387	2.6598998576	0.4055720022
C	1.3570194487	-2.7569834712	2.5984840335
C	0.9071391774	-1.9056968636	3.6129346116
C	1.6161201893	-0.7194646672	3.9372396736
C	2.7828855567	-0.3685259456	3.2484050572
C	-0.3004690888	-3.2983692431	-1.1558737501
C	-1.2564458807	-3.1916093674	-0.1253696485
C	-0.76468711	-3.3243293429	1.2340152371
C	0.5877957604	-3.4583520797	1.5106255841
C	0.3761437904	0.1197109273	-3.320433179
C	-1.0168395724	-0.2181621689	-3.2039470951
C	-1.3046129144	-1.4832277859	-2.4721005219
C	-0.3361713512	-2.459524633	-2.3258685428
C	-5.3974671766	0.7385135594	0.9999261826
C	-5.2347491853	-0.6382698436	1.3173122732
C	-4.4842558038	-1.24826768	0.2739147988
C	-4.2531112894	-0.2448335727	-0.708221548
C	-4.7682587272	0.9852873405	-0.2467481702
C	-4.2004809506	2.2108389049	-0.5820450801
C	-4.542395808	3.2847507914	0.3271279105
C	-5.1921310291	3.0516432152	1.5322711005
C	-5.5519911242	1.7186792244	1.9679763084
C	-3.6065499723	-2.3040342658	0.5066175414
C	-2.4809934158	-2.4429162181	-0.4305488498
C	-2.3925227011	-1.5218335199	-1.5418308496
C	-3.1643208577	-0.3081897592	-1.5407846121
C	-5.2396479017	-1.1035738695	2.6234326641
C	-4.607758541	-2.3917017116	2.7877690022
C	-3.830588181	-2.9562863258	1.7851872496
C	-3.1357931681	2.1574223813	-1.5809486462
C	-2.648403736	0.9341861588	-1.9884330195
C	-5.7838330912	1.2148341298	3.3036322361
C	-5.6387579307	-0.1305053419	3.6147222694
H	-0.3762541324	2.9113509991	-2.6789326876
H	0.8752153811	4.0841685417	-0.9615407331
H	1.9220736079	2.4575079156	3.5963706708
H	1.8307446337	3.89506207	1.6442193454
H	-0.0860956355	-2.0306247421	4.0375107329
H	1.1263306007	-0.003312205	4.5927309767
H	-1.4211179538	-3.0124559244	2.0369988229
H	-1.7479888713	0.2214613262	-3.8731111418
H	-4.2061837459	4.2959510321	0.10867245
H	-5.3451709656	3.8911454532	2.2069596985
H	-4.6702333974	-2.9067387551	3.7438340183
H	-3.3433683658	-3.9034108981	1.9948020091
H	-2.6621263827	3.0850770073	-1.8967472633
H	-5.9881278502	1.9146105679	4.1109359315
H	-5.7365941465	-0.4366530817	4.6538250672

Core RigidRotor
SymmetryFactor 0.5

End
Tunneling Eckart
ImaginaryFrequency[1/cm] 581.6592
WellDepth[kcal/mol] 16.46
WellDepth[kcal/mol] 40.95

End
Frequencies[1/cm] 218

24.4390	37.3103	
69.5480	85.4637	117.5384
151.5826	165.8415	176.5443
177.7918	188.8331	195.2159
220.8908	246.4231	264.3342
281.1520	297.6257	308.5832
320.8664	326.1899	331.6850
338.7291	348.3579	356.7106
376.1418	382.5174	387.7615
391.0659	399.4502	413.8239
425.0949	429.1359	435.6533
441.3347	447.2080	457.0691
467.3722	473.8032	482.9388
487.3392	487.9942	501.5374
507.7258	513.8430	517.6880
520.6191	527.8939	540.3450
551.7118	553.0778	556.0108
571.6323	576.3107	591.4831
597.2136	598.8521	605.7495
607.5845	610.6207	617.3242
622.1241	629.2098	640.0468
645.6334	648.9273	653.0901
656.7743	665.6848	669.8679
685.0545	694.1391	695.9512
701.5174	706.0285	711.7941
715.0722	716.6522	718.9463
734.3779	736.1350	739.0784
746.0071	752.0872	755.9461
761.2942	765.6369	767.1110
771.9878	773.7311	779.7964
782.6905	784.5211	793.2794
796.8000	807.1321	810.1160
816.1609	820.9605	823.7957
829.0359	844.3068	847.8455
859.5256	861.0505	868.5184
885.7896	893.8365	909.3466
914.1005	939.0046	945.9580
949.8270	957.6862	958.8579
966.8886	968.2483	982.9560
987.2799	1002.2310	1010.6070
1039.3752	1042.0421	1065.3867
1079.7023	1088.9705	1098.7074
1113.3438	1115.9117	1123.3513
1132.2215	1150.2997	1165.8272
1168.7971	1173.7527	1182.9230
1184.2383	1193.5195	1198.3970
1203.3240	1212.1220	1220.7303
1225.3846	1234.5607	1239.2501
1252.4087	1252.8391	1258.6146
1270.7832	1283.5964	1299.2637
1302.0855	1304.4380	1314.6181
1322.1543	1328.5504	1335.0809
1338.8896	1340.5828	1344.8984
1354.2439	1359.6228	1363.5727
1369.5649	1376.1806	1390.0763
1393.8436	1402.0687	1411.6959
1421.3577	1426.7757	1430.6964

1432.6657	1437.3600	1441.5177
1442.0797	1444.8440	1447.9410
1450.1369	1460.1777	1467.3671
1474.6476	1477.9601	1479.6069
1494.5871	1502.5727	1506.8171
1513.9540	1542.4538	1561.4100
1572.2378	1576.9425	1588.0289
1594.4303	1597.6251	1604.6504
1612.1238	1617.0296	1621.8486
1625.1955	1632.1581	1647.1759
1655.0918	1661.6220	1665.7467
3171.8105	3175.5540	3177.1673
3179.1728	3180.6681	3182.1393
3186.3768	3192.5961	3194.5113
3195.2375	3196.8678	3198.6787
3208.3259	3213.1067	3234.5864

ZeroEnergy[kcal/mol] 23.2
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-----
Barrier ts2 ip2 p1
RRHO
Geometry[angstrom] 75
C 4.5269095407 -0.4203420701 -1.3970601849
C 3.7627554185 -1.0713054445 -2.4467978648
C 3.5233749506 -2.4405710177 -2.0417648751
C 4.0847367725 -2.620604566 -0.7172925009
C 4.7261784123 -1.3790526297 -0.3247021859
C 4.6554063947 -0.9501616244 0.9940506679
C 4.4414254192 0.4394326346 1.3194404453
C 4.2552159319 1.3652014759 0.2852964854
C 4.2757068478 0.9070001967 -1.0826918351
C 2.3115579417 -3.0432007259 -2.371053004
C 1.58230191 -3.8202154741 -1.3761435751
C 2.0981036027 -3.9422386049 -0.0905443475
C 3.3707399966 -3.3463967072 0.2340786495
C 2.7555070771 -0.3529461077 -3.1001732846
C 1.4984007771 -0.9567597285 -3.4375607011
C 1.3315773655 -2.3126776253 -3.1380409641
C 3.9465399588 -1.7199272222 1.9885747933
C 3.2885236097 -2.8942245655 1.6004322464
C 3.2597028762 1.6549416128 -1.7813543849
C 2.4906181247 1.019673331 -2.7601790506
C 1.10178828 1.3222002684 -2.9222753576
C 0.6367726124 2.4610479137 -2.250930682
C 1.4151774807 3.1036070115 -1.2507416032
C 2.6832232318 2.6291463132 -0.913008452
C 3.7035202139 0.5513425323 2.5360080072
C 2.9982337472 1.7383650689 2.7551096716
C 2.8123894801 2.6795390295 1.7070594228
C 3.3297628759 2.4424180048 0.4299187022
C 2.0199960585 -3.2337811827 2.1597541796
C 1.5949469914 -2.5099513846 3.2764496863
C 2.271824578 -1.3273108505 3.6799227657
C 3.3763828039 -0.8526370582 2.9662927935
C 0.1720160414 -3.6167387262 -1.5536297752
C -0.7338796295 -3.5890749469 -0.4568759658
C -0.1492376511 -3.7769121779 0.8564093685
C 1.2217686379 -3.8736373315 1.0521049362
C 0.4171784408 0.0468495205 -3.3331770857
C -0.8978459915 -0.4184425997 -3.1170663849
C -0.9901374022 -1.8453517183 -2.723634756

C	0.0449361956	-2.7329227657	-2.6927362177
C	-4.7213746003	0.5680972678	0.6259459593
C	-4.5475687556	-0.7615796405	1.1177674997
C	-3.9599257361	-1.5556003899	0.088775833
C	-3.8643117533	-0.6990842157	-1.0489983351
C	-4.2640300931	0.6099899805	-0.7152379509
C	-3.6538816928	1.7276451089	-1.2876029978
C	-3.8392212228	2.9388633166	-0.513159552
C	-4.3432197599	2.9165527394	0.7814712865
C	-4.6961683428	1.682425093	1.4513213209
C	-3.0661814006	-2.6021361338	0.3656759705
C	-2.0242828785	-2.8865854279	-0.6566658327
C	-2.0616843802	-2.0585704756	-1.8157304223
C	-2.8572095564	-0.8900075933	-1.931591835
C	-4.3811867394	-1.0283788323	2.4686031789
C	-3.7707165788	-2.3058992118	2.7417872095
C	-3.1484190726	-3.0471387068	1.7450438187
C	-2.6413362994	1.491472133	-2.3128516908
C	-2.1760752366	0.1998797724	-2.5847243518
C	-4.7526404358	1.3884086367	2.866750743
C	-4.6087242661	0.0962336539	3.3496466387
H	-0.3893289558	2.7847544277	-2.3485312532
H	0.9208168672	3.8524397937	-0.6366554937
H	2.4129321089	1.8723264545	3.6616454607
H	2.0964711141	3.4813035073	1.8714211606
H	0.6347098939	-2.7229544436	3.7400452321
H	1.7905690021	-0.7032084454	4.42915858
H	-0.7653562132	-3.5545448871	1.7172428432
H	-1.6072218857	-0.5634739653	-5.2679652159
H	-3.4820712241	3.8868380353	-0.9100212203
H	-4.3693557567	3.8497094513	1.3397970259
H	-3.7192607411	-2.6727804312	3.7645294372
H	-2.6752544778	-3.9788712506	2.0367723501
H	-2.1645947188	2.3571680117	-2.7587555821
H	-4.8180649652	2.206126688	3.5809691606
H	-4.5699341703	-0.0547640787	4.4260882418

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 373.0864

WellDepth[kcal/mol] 45.5

WellDepth[kcal/mol] 2.4

End

Frequencies[1/cm] 218

34.2743	34.6939	
71.0962	96.2310	127.3931
148.2642	173.0519	177.2631
183.0030	186.9030	196.0366
212.1873	221.2971	233.5098
258.9156	274.4353	283.2393
296.2975	311.1252	322.7369
331.8595	338.1657	349.9304
355.2440	360.2473	379.9108
386.5381	396.5719	403.3957
406.6030	415.8773	434.2758
435.9650	441.8393	451.5903
454.5456	458.0935	472.2623
485.0794	487.4831	492.7071
494.5576	504.7872	515.2277
515.9234	524.3409	527.3248
539.3103	550.4088	554.2004
554.7789	566.1944	577.1973
580.6738	597.8220	602.2083

606.6259	609.2909	611.5546
617.5220	624.4569	630.9424
641.1594	647.0757	651.7594
654.7941	664.7747	670.1175
677.1417	691.4050	697.7151
700.2589	705.7402	712.2268
717.9710	719.6577	720.6477
730.8971	734.3945	737.7377
743.4364	745.0452	752.0695
755.5646	760.7027	762.5298
766.6723	768.7232	769.8947
776.1587	783.8183	788.0139
792.9553	794.6009	802.8782
806.2279	815.8243	818.2229
824.3799	825.6771	829.4072
847.0107	851.9121	868.7945
882.0474	885.8506	896.5054
906.7250	911.7786	933.4722
944.3208	946.1953	951.3739
959.1161	963.3807	967.5571
974.7046	984.8963	992.8734
1010.5591	1023.2433	1040.6344
1065.8948	1076.6321	1083.1268
1092.4246	1102.8032	1114.4620
1129.8750	1138.6378	1146.5952
1164.5927	1167.5598	1171.9413
1178.8378	1181.0562	1191.8585
1194.2908	1202.3547	1206.0454
1215.2381	1223.3603	1229.7909
1239.0119	1246.1733	1250.5714
1255.4180	1267.5854	1272.8709
1297.7835	1300.8378	1306.0211
1317.9337	1325.4444	1327.4763
1336.0057	1344.9922	1347.8201
1354.4617	1360.6333	1366.3290
1374.1642	1377.0913	1384.6055
1397.9058	1403.0598	1405.7354
1424.3440	1426.4924	1431.9213
1434.3255	1438.7249	1442.9198
1444.6552	1445.1826	1448.7381
1451.2880	1457.1152	1459.0890
1463.8198	1474.8600	1482.8195
1487.4026	1498.6522	1507.7359
1509.8972	1515.9924	1543.2974
1559.6129	1574.7903	1590.1895
1596.2138	1599.5382	1606.5311
1609.4678	1613.2433	1620.3314
1626.4677	1635.9611	1636.6289
1653.0427	1657.5412	1680.4643
1749.3610	3174.7065	3177.3600
3178.8844	3180.5986	3181.8265
3188.3909	3192.0673	3194.7400
3194.9118	3196.9388	3211.5462
3220.7660	3253.2051	3276.7479
ZeroEnergy[kcal/mol] 27.7		
ElectronicLevels[1/cm] 1		
0 2		
End		
!-----		
End		

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H₁₃

```

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1700. 1800. 1900. 2000.
TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650.
1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
!TemperatureList[K]          300 500. 1000 1500. 2000
!TemperatureList[K]          300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
!PressureList[bar]           0.1
!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature    0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature   100
ModelEnergyLimit[kcal/mol]    900
WellCutoff                    10
ChemicalEigenvalueMax         0.2
ChemicalEigenvalueMin         1.e-6      #only for direct diagonalization method
CalculationMethod             direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput              eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber             0
!ReductionNumber              5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                 260 ! Frenklach
! Power                        0.
Factor[1/cm]                   247 ! Jasper universal
Power                          0.85
! Factor[1/cm]                 424 ! Jasper calc N2
! Power                        0.62
! Factor[1/cm]                 125 ! SJK guess
! Power                        0.85
ExponentCutoff                 15
End
CollisionFrequency

```

```

LennardJones
!Epsilons[1/cm]      203.0 203.0 ! N2 pyrene-Frenklach
!Sigmas[angstrom]    4.6 4.6 ! N2 pyrene-Frenklach
!   Epsilons[1/cm]    206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
!   Sigmas[angstrom]  5.06 5.06 ! N2 Jasper extrapolation to C16
!   Epsilons[1/cm]    32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
!   Sigmas[angstrom]  3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
!   Epsilons[1/cm]    101.5 1184.960648
!   Sigmas[angstrom]  3.6154 10.88427413
!   Epsilons[1/cm]    390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Sigmas[angstrom]  4.46 4.46 ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Epsilons[1/cm]    189. 216.0 ! N2 , CH2CCH ! from Jasper calc
!   Sigmas[angstrom]  3.30 4.11 ! N2 , CH2CCH ! from Jasper calc
Masses[amu]          28. 733.
End
OutputTemperatureStep[K] 100
OutputTemperatureSize 20
OutputReferenceEnergy[kcal/mol] 0.
!-----
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Well      ip1
Species
RRHO
Geometry[angstrom] 73
C 4.4810502025 -0.3861298289 -1.8786911395
C 3.7596331808 -1.0681115669 -2.939606274
C 3.5200880509 -2.4315481589 -2.5141616008
C 4.0462360611 -2.5798224062 -1.1712198929
C 4.6580351201 -1.3221769779 -0.7830137708
C 4.5401160655 -0.8711440082 0.5247248211
C 4.2933365411 0.5198930544 0.8175746784
C 4.1269434375 1.424197218 -0.2384956444
C 4.2027476657 0.9439646043 -1.5968578932
C 2.3239247781 -3.0548945655 -2.8639004657
C 1.5803154889 -3.828571512 -1.8777502069
C 2.065864612 -3.9251501917 -0.5773385965
C 3.3192208169 -3.3027414351 -0.228209591
C 2.7701704152 -0.3743425582 -3.643323039
C 1.528891697 -1.0014383686 -4.0010889363
C 1.3549250497 -2.3495882404 -3.6689550446
C 3.8167557416 -1.6356464403 1.5121867792
C 3.192645739 -2.8296471419 1.1281476163
C 3.2050182852 1.6682769068 -2.3451134659
C 2.4827238228 1.0055601782 -3.3412124609
C 1.0988960481 1.2886845092 -3.5491277868

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C	0.5788476733	2.4235595364	-2.9167984973
C	1.3138466856	3.0943185892	-1.9002759353
C	2.5791256032	2.6461434386	-1.5148357371
C	3.5169070837	0.6413604483	2.0086634936
C	2.7843697248	1.8192732902	2.1813005436
C	2.6170035438	2.738374445	1.1099060118
C	3.1800216477	2.4884613742	-0.1449980751
C	1.9171892189	-3.1842341008	1.6603907715
C	1.4470789388	-2.4478859883	2.7503701043
C	2.088555746	-1.2437058594	3.1487666588
C	3.2024772261	-0.760782522	2.4562300231
C	0.1716060005	-3.6448441791	-2.092971536
C	-0.7592375216	-3.6163758238	-1.0178262681
C	-0.2049829647	-3.783768703	0.3111812758
C	1.1610465513	-3.8567420172	0.5422450548
C	0.4434621621	-0.0050921508	-3.9346892027
C	-0.8473772454	-0.4612843878	-3.6567699737
C	-0.9777094674	-1.8810989206	-3.289483741
C	0.0604682919	-2.7706516687	-3.2430828139
C	-4.5379441888	0.6080968499	0.1884595805
C	-4.4542412895	-0.7510692605	0.6198480282
C	-3.927111316	-1.5344386656	-0.4503984056
C	-3.7959473738	-0.6462992752	-1.5603820851
C	-4.0940397863	0.6750857249	-1.1573169461
C	-3.4002393387	1.7830975071	-1.6726479478
C	-3.4759053213	2.9622619245	-0.8351253566
C	-3.9785848183	2.9124982581	0.4575932713
C	-4.4240763061	1.6778614081	1.0653704964
C	-3.0865658984	-2.6342546614	-0.2188462849
C	-2.0485437055	-2.9168937819	-1.2416689043
C	-2.0700468921	-2.0820976627	-2.3969012614
C	-2.8309075508	-0.8828992221	-2.4821058355
C	-4.2967467658	-1.0872490411	1.9562934603
C	-3.7681514555	-2.4116692379	2.1706384125
C	-3.1917694086	-3.1389797128	1.1383933026
C	-2.4609343248	1.4592630964	-2.7117744526
C	-2.0795556635	0.1956505196	-3.1088672519
C	-4.4971816608	1.326500448	2.4661195301
C	-4.4433714219	0.0074607078	2.8894318539
H	-0.4610680603	2.7041820061	-3.0602329258
H	0.7868928421	3.8399686485	-1.3097882493
H	2.1676995838	1.9603667528	3.0657279886
H	1.8828299026	3.530386668	1.2369397126
H	0.4783713244	-2.6711185651	3.1910069113
H	1.5738839537	-0.6150644015	3.8715243838
H	-0.8442979512	-3.5597768889	1.1543641055

H -3.0452360548 3.8941788891 -1.1913638222
H -3.9306253701 3.8149776316 1.0627542931
H -3.7403081858 -2.8278681386 3.1751453441
H -2.7692443463 -4.1088080308 1.3809997895
H -4.501232167 2.1147603111 3.2154092888
H -4.4110207031 -0.1956026763 3.9574667331

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 213

31.2984	36.7223	73.4151
91.5561	126.2343	149.4644
178.9184	181.9600	192.2349
197.8043	214.4133	234.0551
259.9090	276.2372	290.2072
296.5961	312.1421	326.3226
332.4754	338.9937	352.8041
357.9044	364.4748	380.8228
387.9009	398.3265	401.7652
406.8535	418.5251	432.9923
436.0600	441.8510	452.8491
455.9530	460.1135	474.7510
484.4209	487.0173	492.4637
493.5114	505.1267	514.7277
516.0219	524.8116	528.7924
538.8185	550.3755	554.2799
555.0104	568.0112	576.5460
580.5632	596.0643	601.4490
607.1207	609.1691	610.7683
617.1875	625.5767	631.3295
640.6740	643.7227	652.9915
654.5718	666.5943	670.7451
677.4590	693.4478	696.7065
701.5345	705.1083	713.7331
716.8331	719.2612	721.4271
727.3180	735.7818	740.2839
740.7581	747.8245	753.1216
755.6409	759.7735	762.4716
765.9865	769.1244	769.5794
771.3237	780.1309	786.5746
790.3257	795.7071	801.6911
814.2965	816.9119	819.1353
823.4121	827.6473	832.5646
847.8250	850.9309	869.9741
882.7244	890.4882	900.2055
908.1106	941.2264	947.1175

948.6705	952.9554	959.0601
963.8472	967.8604	975.0723
987.9140	995.3718	1011.2144
1026.0777	1038.9874	1064.7230
1072.5226	1084.5728	1092.1294
1103.7106	1115.9152	1129.6238
1139.8180	1149.3787	1162.9283
1167.5533	1171.9760	1179.9892
1191.4218	1195.5458	1202.6311
1206.0700	1213.4542	1223.4025
1228.8061	1237.8308	1247.1235
1248.6207	1252.6490	1264.1917
1267.1330	1275.4868	1298.1707
1304.0359	1307.5024	1311.7709
1323.3807	1329.1811	1335.5555
1343.8851	1348.0448	1352.5639
1363.1825	1373.9125	1376.0281
1377.1358	1384.0987	1399.3064
1401.1678	1411.0091	1429.2900
1432.6823	1435.2582	1438.5978
1442.0238	1445.6069	1446.2674
1449.1422	1450.6307	1456.5415
1458.4022	1470.3894	1474.5491
1480.4743	1482.5808	1496.6561
1498.9583	1509.7724	1511.7144
1546.9843	1563.6821	1574.5538
1592.2184	1594.8916	1596.5798
1600.6076	1606.5484	1608.1814
1613.9448	1620.2964	1626.0111
1634.9671	1652.4457	1653.3197
1671.3547	1730.5366	3177.9243
3178.6935	3179.0536	3180.5855
3182.2562	3183.2284	3192.9895
3195.1026	3195.9824	3196.8392
3202.5153	3208.6688	3252.3414
ZeroEnergy[kcal/mol] 0.00		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----well_ip2-----		
Well ip2		
Species		
RRHO		
Geometry[angstrom] 73		

C 4.8667168289 -0.4320893137 -2.0675280403
 C 4.171762444 -1.1302701471 -3.125119168
 C 3.8969242972 -2.4795593807 -2.6645486004
 C 4.4302839491 -2.6097571202 -1.3219449915
 C 5.0472097664 -1.3450264904 -0.9572629084
 C 4.9572018548 -0.8861993472 0.3505264167
 C 4.6784456016 0.5046504737 0.6363321398
 C 4.4206768106 1.3737844293 -0.4309974108
 C 4.5205555229 0.8979457039 -1.794167217
 C 2.6795130329 -3.0891404552 -2.9868976541
 C 1.9166272087 -3.7848654098 -1.9597647028
 C 2.4319664243 -3.8952294649 -0.6755526235
 C 3.7136277615 -3.3123250843 -0.358729031
 C 3.2250043746 -0.4501014239 -3.9029838874
 C 2.0093564148 -1.1079310198 -4.2890411252
 C 1.7372858709 -2.4040822387 -3.8358049517
 C 4.2778023063 -1.6489598169 1.3674087689
 C 3.6349246973 -2.8430090142 1.005272927
 C 3.5222930009 1.5742597272 -2.553834698
 C 2.8827132289 0.9394638027 -3.6134456569
 C 1.4883899183 1.1644091382 -3.8711258186
 C 0.6732713301 2.259033131 -3.1533462756
 C 1.4800021894 2.7840927433 -1.9424149682
 C 2.7704588986 2.476650153 -1.6699638066
 C 3.9507962813 0.6223949394 1.8542329521
 C 3.175581124 1.7765126565 2.0382647265
 C 2.9075007087 2.6475692297 0.9561546778
 C 3.4212865389 2.3796248282 -0.3182290294
 C 2.3725497987 -3.1769678288 1.5723411595
 C 1.9479554459 -2.4508403723 2.6934422684
 C 2.6073801736 -1.2587346776 3.0733792127
 C 3.6903441437 -0.772343869 2.3285691795
 C 0.5111248521 -3.5145798881 -2.1477630309
 C -0.373437786 -3.3581354244 -1.0354166283
 C 0.2021173114 -3.5985787598 0.2697219762
 C 1.5623850926 -3.7901895114 0.4670023063
 C 0.9589934889 -0.0942648794 -4.2850872677
 C -0.3226484735 -0.4509276773 -3.9084581328
 C -0.5959965388 -1.7880753447 -3.4272723101
 C 0.4095243416 -2.7283507333 -3.3510099352
 C -2.8099464983 1.5663439661 0.3995445777
 C -3.0697898365 0.2440503756 0.8753499138
 C -2.9254741629 -0.6622442359 -0.2153152016
 C -2.7127465512 0.1460578822 -1.3658506382
 C -2.5077747173 1.4953222124 -0.9919019927
 C -1.5490607451 2.3292645297 -1.5980430536

C -1.3109982909 3.5323922193 -0.8082875988
 C -1.6885423519 3.6521399189 0.5206469635
 C -2.3345410937 2.5691762563 1.2288584514
 C -2.3820263727 -1.9443917102 -0.0560840657
 C -1.5666218251 -2.4792356926 -1.1897373272
 C -1.5982711912 -1.7240914049 -2.3992719703
 C -2.0693463376 -0.3611714095 -2.4356844703
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 C -1.1573566235 0.4802837821 -3.1688353107
 C -2.3490878631 2.2602891481 2.639796969
 C -2.6008571961 0.9768386501 3.1023145221
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 H 2.603975095 1.9148240148 2.9528768699
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 H 0.996413581 -2.6765424155 3.168619816
 H 2.1285050584 -0.6315097515 3.8214582653
 H -0.3842707328 -3.3331792475 1.1362538994
 H -0.7882717333 4.372479821 -1.2563138143
 H -1.4185922963 4.5612300418 1.0535580933
 H -2.6861807606 -1.9527834776 3.3961076653
 H -2.3108236121 -3.4484617759 1.5507046208
 H -2.0674632733 3.0269881931 3.3580369109
 H -2.5088704411 0.7795920543 4.1679399423

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 213

10.4016	48.1927	92.4930
108.9544	136.1339	173.2629
181.0391	203.2362	212.7386
217.3737	245.2882	254.1172
264.1585	278.9146	287.2961
304.2440	317.4158	335.2383
340.5916	347.9557	355.4753
359.5701	373.2477	384.2123
394.6513	399.7892	402.0999
409.5804	423.0157	435.2569
444.3555	453.1157	458.5310
468.1885	474.5534	480.4252
483.1743	493.3267	496.2027
505.2802	508.2995	517.4853
522.6231	533.0125	535.1171

545.6463	547.4086	558.5849
560.6479	575.1180	580.8110
590.8486	599.0548	601.5815
606.7097	614.8131	620.9209
628.2800	633.0953	635.1274
649.1160	653.4702	660.6208
667.0864	669.6239	672.0287
683.2856	690.5645	695.4599
699.6455	704.5741	709.7206
711.8180	723.2314	727.9294
731.5201	733.6927	736.6196
742.7405	745.8281	751.1782
754.6915	757.5930	761.1866
764.3981	769.9779	773.7542
775.5777	785.2505	787.4695
797.8486	802.0275	806.3069
810.8285	819.3194	822.2642
828.8851	837.6441	845.4421
857.5432	869.5167	880.2330
889.4421	898.4187	904.9951
930.3604	940.0546	946.2243
950.9174	956.7990	970.1186
972.7890	982.4287	986.6622
990.6451	1011.1162	1031.3312
1038.1777	1045.9656	1067.7443
1085.2190	1090.4963	1107.7996
1114.9064	1132.2441	1136.4448
1140.6065	1161.2823	1167.8476
1170.3381	1178.5233	1188.3358
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1208.9009	1215.3701	1218.9735
1227.6853	1234.7560	1239.1533
1246.2490	1258.9467	1259.4809
1267.0304	1278.4453	1283.3116
1294.3434	1305.1722	1312.4701
1313.2358	1323.2625	1327.4685
1342.3305	1344.7131	1348.4181
1351.9067	1355.0058	1361.9802
1363.6168	1369.6619	1382.1242
1387.2480	1396.8610	1400.3830
1409.7884	1422.8121	1429.1543
1430.1560	1441.2711	1443.9800
1444.6544	1450.2883	1450.8940
1457.6858	1461.4230	1470.1793
1473.9322	1484.1114	1491.1267
1503.1848	1511.0310	1514.8361

1541.1488	1558.0666	1561.6280
1573.7432	1590.7754	1595.7851
1600.7851	1601.4433	1606.8317
1610.8254	1614.7684	1623.7631
1634.7576	1653.6860	1656.4101
1663.5353	1756.6709	2931.6992
3176.8761	3178.3070	3179.5069
3181.1967	3190.2616	3194.9339
3195.6221	3196.3379	3202.9318
3212.7617	3268.8274	3277.0258

ZeroEnergy[kcal/mol] -17.1
 ElectronicLevels[1/cm] 1
 0 2
 End
 End
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 !-----h_c60h12_p1-----
 Bimolecular p1
 Fragment c60h12
 RRHO
 Geometry[angstrom] 72
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 C 3.1726325316 -1.460899444 -3.0716913384
 C 2.8911019887 -2.8062344742 -2.6037550299
 C 3.4277321582 -2.9329314282 -1.2622726234
 C 4.0641896239 -1.6773032582 -0.9050072355
 C 3.9841220764 -1.2074277861 0.397582911
 C 3.73916673 0.188903778 0.6751820408
 C 3.5097743517 1.0631228005 -0.3969258128
 C 3.5827462562 0.5712066132 -1.7523300903
 C 1.6721867298 -3.4152912279 -2.9227807683
 C 0.9086765813 -4.1084959167 -1.8929901758
 C 1.4218113374 -4.2022560882 -0.6057315393
 C 2.705040129 -3.6226402649 -0.293501627
 C 2.2243876385 -0.7767609301 -3.8406022161
 C 1.0036592929 -1.4365243348 -4.2280061101
 C 0.7318939554 -2.7349828683 -3.7763124103
 C 3.2905069863 -1.9548384497 1.4208645381
 C 2.6302374603 -3.1396023851 1.0649764219
 C 2.5652196693 1.2614385203 -2.5062434643
 C 1.8960914968 0.6097292006 -3.5342162513
 C 0.4798065886 0.8131668483 -3.7080393154
 C -0.2621008717 1.6772787868 -2.8480474197
 C 0.512730189 2.4115821232 -1.8652547639
 C 1.8586477515 2.1703428745 -1.641700108
 C 3.0112143379 0.3268671986 1.8925100601

C 2.2581254436 1.4929769864 2.0673116333
 C 2.0101541687 2.3658574252 0.9776033125
 C 2.5230317763 2.0862588211 -0.2924825423
 C 1.3630548301 -3.4562268294 1.6353924342
 C 0.9469624959 -2.71379009 2.7444490297
 C 1.6262075553 -1.526203406 3.1174908776
 C 2.7198815381 -1.065108669 2.376707913
 C -0.4960015245 -3.8493858322 -2.0862341842
 C -1.3850951918 -3.6887355468 -0.9815682264
 C -0.8094971326 -3.9067419576 0.3324349854
 C 0.549841947 -4.0837719866 0.5337234915
 C -0.048775484 -0.4360746423 -4.2084110304
 C -1.328135266 -0.7857274403 -3.8509542951
 C -1.6112544913 -2.1385254973 -3.3803789794
 C -0.598464846 -3.0624770515 -3.2948676297
 C -3.8081172668 1.2164232459 0.4596520469
 C -4.0853474058 -0.1082811937 0.9204632944
 C -3.9362390094 -1.0071110003 -0.1748166024
 C -3.7049877963 -0.194979612 -1.3177855526
 C -3.4841026953 1.1531159447 -0.926249729
 C -2.5121007716 1.9799153729 -1.5059539647
 C -2.2653906265 3.1691399489 -0.7070955001
 C -2.6634036107 3.2857939238 0.6182630929
 C -3.3338020971 2.2074098209 1.3052973046
 C -3.4067965077 -2.2954484267 -0.0187254598
 C -2.5857207982 -2.8243615489 -1.1480825552
 C -2.6188863565 -2.0715629609 -2.3620462619
 C -3.080022585 -0.7011651278 -2.3968659219
 C -3.8970377062 -0.4841640977 2.2415748267
 C -3.7503915315 -1.9086550886 2.4252128856
 C -3.5061546504 -2.759663665 1.3552894841
 C -1.7038227459 1.3894495797 -2.613836813
 C -2.156747636 0.1365436635 -3.1300943607
 C -3.3750710548 1.8866915893 2.713529759
 C -3.643946709 0.6017531541 3.1605004876
 H -0.0255031015 2.9446546868 -1.0958930669
 H 1.6815633325 1.6448543229 2.9766497661
 H 1.256707017 3.1382280596 1.1113956692
 H -0.0106313586 -2.9170016921 3.2175874998
 H 1.1520561838 -0.8847969167 3.8565224702
 H -1.4025519879 -3.6358508758 1.1930533323
 H -1.7203770244 4.001257084 -1.1423372533
 H -2.3864470215 4.1856175208 1.1630686379
 H -3.7496952887 -2.3279691512 3.4288933777
 H -3.3557414545 -3.8121605904 1.5755235302
 H -3.0995508164 2.645173422 3.4427435187

H -3.5705503204 0.3944306227 4.2256690548

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 210

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188.9965	202.7387	220.4564
247.0281	264.1510	269.6592
280.4320	284.1062	312.7302
319.7144	333.6763	339.0885
352.0313	358.8885	360.3899
364.3336	386.5838	388.0589
401.4129	405.3124	414.0601
426.9998	438.7660	438.8566
446.5660	457.4523	461.0937
470.8828	485.8492	488.6841
495.9811	499.1744	510.8194
511.0070	524.0433	528.1699
530.3334	535.9727	546.3289
553.4396	556.0153	563.1220
567.3139	577.4477	584.6003
603.6263	606.9333	607.4991
609.6799	619.5798	633.2768
634.2672	636.2324	643.4225
649.9290	667.8454	670.1314
674.2405	676.9498	681.6372
695.6542	702.0372	707.5640
711.4322	711.8717	720.6905
721.5758	730.6889	731.2187
739.8014	740.8975	746.1716
751.9163	753.2186	754.6106
759.0652	760.8301	763.2971
767.1435	771.7448	774.0658
782.1367	784.0762	790.4815
799.2310	802.6312	811.4433
818.8813	822.7716	828.4773
829.7558	834.4268	851.2386
872.9632	881.9609	884.5305
900.5737	904.7012	906.6705
943.6490	948.0051	954.4287
961.1899	964.8247	975.0686
987.2466	989.5153	990.3764
1016.2790	1033.5449	1039.5692
1053.5765	1076.4914	1084.9732
1101.1223	1112.6844	1125.5824

1128.1512	1143.6466	1145.2036
1166.5733	1172.5213	1176.2219
1182.7614	1190.9273	1192.4556
1195.3869	1207.8222	1217.4602
1219.9790	1238.5255	1244.3856
1246.3114	1249.7397	1251.9168
1266.2505	1281.0883	1283.1549
1297.5151	1299.8896	1300.9098
1315.0658	1317.1802	1327.1177
1330.2973	1343.5769	1346.3369
1351.2245	1358.5656	1358.5968
1360.6471	1369.1432	1373.8169
1378.9390	1388.1300	1395.4441
1404.8552	1428.6830	1430.3607
1432.9167	1441.2881	1444.9885
1448.9722	1449.5164	1451.5089
1455.3857	1455.9497	1464.3368
1470.6155	1473.3565	1485.4696
1493.1199	1496.2616	1509.7914
1517.1277	1544.1205	1558.7696
1571.0625	1584.8381	1598.3417
1600.8208	1604.6796	1606.5257
1613.7468	1615.6960	1622.4182
1623.0565	1634.7216	1652.8824
1655.1937	1662.0115	1760.9984
3178.2928	3180.0780	3181.2759
3181.3290	3181.8119	3195.5109
3196.1949	3197.8228	3204.2548
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ZeroEnergy[kcal/mol] 0.0		
ElectronicLevels[1/cm] 1		
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Atom		
Mass[amu] 1		
ElectronicLevels[1/cm] 1		
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GroundEnergy[kcal/mol] 10.7		
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Barrier ts1 ip1 ip2		
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Geometry[angstrom] 73		
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C 4.4055781596 -2.6535928364 -1.2656824457
C 5.060368748 -1.4015604994 -0.9245625854
C 4.9559612061 -0.893960935 0.3643503683
C 4.7304323123 0.5133933206 0.6004376094
C 4.5676954911 1.3717351658 -0.4925407104
C 4.6602825567 0.8377505179 -1.8288993626
C 2.6510645659 -3.1123279168 -2.9367406608
C 1.8711581822 -3.7895614032 -1.9097878398
C 2.3727435 -3.8836094683 -0.6158285466
C 3.6582224724 -3.3110571673 -0.2949317314
C 3.2703827769 -0.5174146082 -3.8815542302
C 2.015443135 -1.1118223532 -4.2426277258
C 1.7254060082 -2.4026781686 -3.7860168446
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C 3.5656972537 -2.794004583 1.0506915312
C 3.6977649255 1.5471336944 -2.6204492314
C 3.015854278 0.8877617819 -3.6393398007
C 1.660168104 1.2169215034 -3.9328911315
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C 3.2308649481 1.8843782827 1.9037628688
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C 2.2893406374 -3.0910512718 1.6092866107
C 1.8535677906 -2.3109476064 2.6858618682
C 2.5257484388 -1.1113110791 3.0314910343
C 3.6370044661 -0.6778543556 2.3003979439
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C -0.4251969598 -3.3578249996 -1.0175670902
C 0.1344271862 -3.5719766185 0.300688814
C 1.4916852789 -3.746159308 0.5142298433
C 1.0024796128 -0.0478654504 -4.261817741
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 C -2.7161301344 0.7825188382 3.1738227754
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 H 2.3250041622 3.5463273911 0.8803509069
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 H 2.0376412004 -0.4455485688 3.7391902291
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 H -1.3222597937 4.3514695926 1.3131773122
 H -2.8511805414 -2.1492086416 3.360920502
 H -2.4389324507 -3.5751081475 1.4608550043
 H -2.1264281393 2.8047750773 3.5114719147
 H -2.6388484502 0.541364809 4.2316026517

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 447.0957

WellDepth[kcal/mol] 10.1

WellDepth[kcal/mol] 27.2

End

Frequencies[1/cm] 212

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169.7288	182.9822	190.2987
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265.9211	277.6885	291.5895
302.9759	321.1152	326.4433
336.9912	338.1378	355.6352
360.0042	363.8450	379.9271
383.3680	390.7669	398.9709
404.4306	417.5163	432.7912
434.7391	439.1682	453.7375

457.6343	464.6050	471.7422
479.1631	487.8155	493.3306
494.1405	503.4218	514.0910
516.8356	518.0745	531.9691
534.0587	544.5020	549.7235
557.9965	562.9416	570.0270
580.2147	585.2573	598.9118
604.3618	606.9506	610.5746
618.5262	628.7787	629.5228
637.6167	640.5520	651.3225
655.4101	666.9376	669.4520
672.9742	682.4674	695.0975
700.8096	703.0045	709.7871
712.4821	717.7288	721.1437
726.0919	730.6477	734.5351
741.5546	743.8455	746.6374
751.5185	754.3267	759.1649
761.3697	765.2709	769.1136
770.1193	779.0708	783.0436
787.1924	791.5990	796.1219
801.4847	814.5072	817.7798
821.9808	827.5142	830.7639
840.5110	850.4933	867.3290
874.2061	882.5781	893.1936
899.4628	914.6298	941.4235
950.1024	956.0310	958.4660
966.4693	967.1482	974.8949
989.5812	1004.0882	1013.5106
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1070.3509	1081.3378	1097.0874
1101.4439	1106.5235	1129.3669
1141.3338	1141.7173	1160.1513
1168.3551	1175.1585	1178.1470
1189.6859	1194.2218	1197.8500
1209.8759	1215.7062	1219.8616
1226.9597	1236.4236	1243.9815
1247.1655	1253.9839	1264.1437
1265.3102	1278.3688	1297.6802
1301.7788	1307.0386	1307.7147
1318.8753	1323.6803	1331.1296
1342.2001	1344.2579	1349.7302
1357.7387	1364.1630	1371.8842
1374.5432	1378.3571	1381.4479
1391.9276	1399.9541	1403.4366
1422.8952	1431.3657	1432.6603
1436.6033	1442.0723	1444.9644

1445.6577	1450.8366	1452.8216
1456.8952	1467.7339	1469.2981
1474.0055	1484.3374	1486.7061
1494.2032	1507.9136	1509.9187
1537.0877	1551.8031	1564.7632
1573.5046	1586.3937	1591.2976
1597.4368	1601.0966	1606.0045
1611.0220	1616.4361	1619.3220
1630.7704	1643.9441	1652.3430
1653.7136	1734.4156	3177.0777
3180.0881	3180.2424	3181.1851
3182.4301	3193.1140	3194.3606
3196.3230	3198.3708	3203.3970
3204.1329	3214.6724	3270.1077

ZeroEnergy[kcal/mol] 10.1
 ElectronicLevels[1/cm] 1
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 Barrier ts2 ip2 p1
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 C 3.4304093781 -2.9311551812 -1.2652832964
 C 4.0627031507 -1.674074769 -0.9056444855
 C 3.9804398552 -1.2070436486 0.3980665456
 C 3.7282557132 0.1876555842 0.6782541595
 C 3.4928048878 1.0619455245 -0.3919496356
 C 3.571128033 0.5741605028 -1.7486531422
 C 1.6752021545 -3.4123253533 -2.9266538902
 C 0.9124333689 -4.1067011585 -1.8974393553
 C 1.4263974712 -4.2045207045 -0.6111647507
 C 2.7092642979 -3.6245185252 -0.2977940634
 C 2.2233294427 -0.7732752684 -3.8417156451
 C 1.0046578778 -1.4334769641 -4.2309131976
 C 0.7342107293 -2.7321079147 -3.77954342
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 C 2.6341128538 -3.1453887925 1.062098368
 C 2.5545591227 1.2607254012 -2.5025472969
 C 1.8918225882 0.6131017632 -3.5371159295
 C 0.4788931269 0.8193297289 -3.7254261994
 C -0.2743371409 1.7216329677 -2.8970438622
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 C 1.9882118928 2.3554391046 0.9856606369
 C 2.5019014165 2.0800959177 -0.2850149852
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 H 1.1503854211 -0.9015799444 3.8603860057
 H -1.3958233809 -3.6406177221 1.1910999587
 H -1.7379495899 4.0131702989 -1.1687356702
 H -2.3933791278 4.2015207244 1.1406332676

H -3.7280923858 -2.3130510379 3.4330175798
 H -3.3421986435 -3.8022169317 1.582778756
 H -3.0854405284 2.6625066151 3.4292541139
 H -3.5474945064 0.4132076593 4.2211309683
 Core RigidRotor
 SymmetryFactor 0.5
 End
 Tunneling Eckart
 ImaginaryFrequency[1/cm] 623.9871
 WellDepth[kcal/mol] 32.0
 WellDepth[kcal/mol] 4.2
 End
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 263.5285 278.6575 282.4381
 287.2082 306.7519 315.1430
 319.4060 334.0506 338.7809
 350.3896 358.1557 361.2410
 365.5755 386.8398 388.3919
 402.3051 405.5014 412.1541
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 495.8200 497.8347 510.0693
 511.2918 522.8899 527.3706
 529.8190 535.8204 545.9956
 553.4695 555.3880 562.4681
 567.3795 577.4077 582.9943
 602.5675 606.6498 607.3173
 608.9388 619.3720 633.0862
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 673.9629 676.9989 682.0506
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 739.9246 740.4618 745.9269
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 756.9058 759.7679 763.7438
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 782.1678 783.3409 790.1725
 799.2727 803.1041 810.2253
 815.9303 822.4410 825.0631

830.0439	833.6833	851.0262
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987.0103	989.5519	990.3079
1014.8273	1032.9973	1038.8310
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1179.0574	1187.9275	1191.3668
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1328.3858	1343.9886	1346.2126
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1453.2910	1456.1463	1463.6364
1470.2396	1473.9361	1485.9041
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1571.3976	1583.8332	1597.8289
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1613.7960	1615.0862	1619.0923
1622.2517	1634.3288	1653.1698
1654.6087	1659.8921	1761.0269
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ZeroEnergy[kcal/mol] 14.9		
ElectronicLevels[1/cm] 1		
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End		

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H₁₁

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1700. 1800. 1900. 2000.
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1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
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1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
!PressureList[bar]           0.1
!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature    0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature   100
ModelEnergyLimit[kcal/mol]    900
WellCutoff                    10
ChemicalEigenvalueMax         0.2
ChemicalEigenvalueMin         1.e-6      #only for direct diagonalization method
CalculationMethod              direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput               eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber             0
!ReductionNumber               5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                 260 ! Frenklach
! Power                        0.
Factor[1/cm]                   247 ! Jasper universal
Power                          0.85
! Factor[1/cm]                 424 ! Jasper calc N2
! Power                        0.62
! Factor[1/cm]                 125 ! SJK guess
! Power                        0.85
ExponentCutoff                 15
End
CollisionFrequency

```

```

LennardJones
!Epsilons[1/cm]      203.0 203.0 ! N2 pyrene-Frenklach
!Sigmas[angstrom]    4.6 4.6 ! N2 pyrene-Frenklach
!   Epsilons[1/cm]    206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
!   Sigmas[angstrom]  5.06 5.06 ! N2 Jasper extrapolation to C16
!   Epsilons[1/cm]    32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
!   Sigmas[angstrom]  3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
!   Epsilons[1/cm]    101.5 1183.084328
!   Sigmas[angstrom]  3.6154 10.87446486
!   Epsilons[1/cm]    390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Sigmas[angstrom]  4.46 4.46 ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Epsilons[1/cm]    189. 216.0 ! N2 , CH2CCH ! from Jasper calc
!   Sigmas[angstrom]  3.30 4.11 ! N2 , CH2CCH ! from Jasper calc
Masses[amu]          28. 731.
End
OutputTemperatureStep[K] 100
OutputTemperatureSize 20
OutputReferenceEnergy[kcal/mol] 0.
!-----
!-----well_ip1-----
Well      ip1
Species
RRHO
Geometry[angstrom] 71
C 3.8724248613 -0.7558254255 -2.0057710962
C 3.1713853897 -1.4692909237 -3.0562610939
C 2.8824162859 -2.8072378833 -2.5720938518
C 3.4056033558 -2.9152468333 -1.2235031969
C 4.0404510009 -1.6553074418 -0.878276739
C 3.9438459279 -1.1646161753 0.4155683858
C 3.7010228691 0.2365553947 0.6694169405
C 3.4929937825 1.0981145694 -0.4169988648
C 3.5754870554 0.5821322708 -1.7625707613
C 1.6658496204 -3.419448765 -2.8945606625
C 0.8936992659 -4.1017690896 -1.8647313217
C 1.3935189648 -4.1769700642 -0.570795589
C 2.6719844577 -3.5902989561 -0.2528528889
C 2.231194899 -0.7941687817 -3.8427071817
C 1.0096870107 -1.4562013115 -4.2261434026
C 0.7319510647 -2.7486495675 -3.7630782051
C 3.2357174492 -1.8947685616 1.4409751786
C 2.5803214737 -3.0853776002 1.0964660192
C 2.5677516093 1.2641050358 -2.5347260607
C 1.907776816 0.5980805184 -3.5594187571
C 0.4932868201 0.8003465988 -3.7404065221

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C -0.2404660979 1.6801033318 -2.8949574312
 C 0.528015427 2.464865397 -1.9493248598
 C 1.8657424261 2.2039497912 -1.6968430227
 C 2.9576115347 0.3951931943 1.8748900819
 C 2.2121062145 1.5696961151 2.0237941866
 C 1.988113097 2.4324389943 0.9203053371
 C 2.5170668631 2.1351213501 -0.339253835
 C 1.3073998698 -3.3954090039 1.65749386
 C 0.8762504118 -2.6328031629 2.7469635342
 C 1.5502372364 -1.4379791824 3.1082694433
 C 2.6536801557 -0.9890384286 2.3747564555
 C -0.5098689456 -3.8507308574 -2.0758759865
 C -1.4124054235 -3.6895884799 -0.9830934867
 C -0.8491974594 -3.8857135811 0.3401852293
 C 0.5092465124 -4.0464074045 0.5576464134
 C -0.0406273761 -0.4539258434 -4.2200344587
 C -1.3227838852 -0.7960904378 -3.8632110171
 C -1.6148767667 -2.1449842838 -3.38829699
 C -0.6034566662 -3.0715386054 -3.2904910419
 C -3.7397742875 1.1919542947 0.4997123422
 C -4.0711636269 -0.1315642448 0.9302750805
 C -3.9497227151 -1.0105555117 -0.1854359172
 C -3.6961191564 -0.184865079 -1.3161345716
 C -3.4384654875 1.1510813176 -0.8952432374
 C -2.4223725476 1.9425102325 -1.4751816239
 C -2.0926051589 3.0056606278 -0.5875263167
 C -2.4263314755 3.1696255219 0.7276960802
 C -3.1987489604 2.1245778541 1.3776173739
 C -3.4484927885 -2.3128342158 -0.0483485572
 C -2.6146020005 -2.8322245586 -1.1689269706
 C -2.6296882834 -2.0710973134 -2.3766335981
 C -3.0727554716 -0.6936668105 -2.3992457222
 C -3.9008052679 -0.5486308164 2.2424929591
 C -3.8045947646 -1.9800565557 2.39682106
 C -3.5734447504 -2.8109519005 1.3099054289
 C -1.6641479135 1.3716977537 -2.6198673107
 C -2.1413617027 0.1315630126 -3.1360446143
 C -3.2594239137 1.7748974374 2.7769744441
 C -3.5988767072 0.4969112275 3.190983145
 H -0.0261838073 3.0702276448 -1.2380925399
 H 1.6230723762 1.7380184353 2.9221293812
 H 1.2370240212 3.2102855115 1.0329191913
 H -0.0881018664 -2.8271902926 3.2101086098
 H 1.065477453 -0.7846563213 3.8297325159
 H -1.4541609055 -3.6087043652 1.1906934445
 H -2.0534787265 4.0186315669 1.2977361168

H -3.8243391819 -2.4202189526 3.3913000338
H -3.4463810649 -3.8722791076 1.5018593408
H -2.9397248519 2.4992788039 3.5223578682
H -3.538015574 0.257189893 4.2501638235

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 207

42.7567	49.8776	96.2212
108.9480	170.8325	177.1650
186.9538	197.3732	222.8274
248.6628	264.0683	274.2334
278.4039	286.5225	313.6870
320.5513	333.3984	335.8720
351.7158	357.2865	360.8336
366.3108	387.3948	388.5705
399.6554	404.7864	413.2913
430.4546	438.6737	440.6724
447.1642	455.0377	460.9439
470.4449	479.8821	488.5705
493.5781	499.9185	506.7387
510.7125	524.1497	527.9612
530.6552	536.7942	544.6175
553.0286	555.3670	559.2180
568.1296	577.6199	582.9530
600.6304	604.5778	607.1264
609.9691	614.9902	626.4534
632.8080	635.7987	638.9916
646.9073	668.2778	669.1711
674.9938	677.2666	683.2744
694.8708	701.8367	704.6884
711.7780	712.0181	720.0021
721.3339	730.1251	732.9164
739.2000	740.5521	746.3645
750.6858	752.7715	753.9890
757.8828	759.3472	763.2896
767.4356	770.9097	772.5610
779.0298	783.5812	784.2144
789.9918	800.2327	809.5583
816.5787	822.9974	826.0829
830.3643	835.2767	853.4286
871.3877	879.1206	883.2550
901.8556	903.4275	905.7810
942.0863	944.9305	951.8554
959.9274	963.3608	974.1871
987.9999	990.8472	1014.9489

1030.7061	1039.9693	1049.7832
1076.9866	1082.5410	1099.8742
1111.3709	1126.6605	1128.0360
1144.3488	1146.8326	1166.9598
1173.2016	1178.0085	1185.6730
1188.9389	1192.3658	1198.6409
1206.7963	1221.2149	1225.4866
1238.5397	1241.8136	1246.4177
1251.5676	1265.7469	1268.1345
1281.5070	1296.2359	1298.6216
1301.2786	1310.9309	1317.1367
1326.0532	1327.3519	1327.7242
1345.8517	1350.1403	1354.7406
1358.7471	1359.8759	1369.6433
1372.7504	1374.6146	1385.2810
1390.8143	1396.3868	1400.3350
1425.1926	1428.5786	1432.4353
1438.9913	1444.5476	1445.6881
1448.9642	1451.3305	1455.4999
1459.4288	1464.5345	1465.7374
1477.5697	1492.1033	1496.1499
1504.9589	1517.4167	1534.5159
1555.1163	1568.4176	1576.4933
1584.6490	1597.8502	1600.3270
1603.0596	1613.7884	1615.7284
1620.5039	1622.3580	1634.4990
1642.7187	1650.7380	1657.6580
1744.5612	3171.4731	3174.2358
3179.0233	3179.8972	3181.8702
3181.9973	3196.0509	3196.3004
3198.0397	3203.1775	3268.7722
ZeroEnergy[kcal/mol] 0.00		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----well_ip2-----		
Well ip2		
Species		
RRHO		
Geometry[angstrom] 71		
C	5.0021171837	-0.9290065902 -2.3387841453
C	4.4121646643	-1.6440051041 -3.4438414784
C	4.1792995627	-3.0124895922 -3.0225682773
C	4.6681898647	-3.147337961 -1.6626426973

C 5.2097721535 -1.8632170597 -1.2488852755
 C 5.0484703265 -1.4396131679 0.0612693685
 C 4.6819136248 -0.0755965827 0.361119569
 C 4.3985906055 0.7917098555 -0.6899537618
 C 4.565896478 0.3661174655 -2.0422584192
 C 2.9998208712 -3.6631104301 -3.4032984498
 C 2.227128712 -4.4013024448 -2.418193212
 C 2.7015275664 -4.5236023366 -1.118915659
 C 3.9478847239 -3.8997534951 -0.7412470939
 C 3.47542535 -0.9858657746 -4.2512227102
 C 2.3056112166 -1.7000536394 -4.7219943081
 C 2.0648298548 -3.0073837265 -4.2862796362
 C 4.3699001367 -2.2540138256 1.0395651601
 C 3.7959664915 -3.4628318742 0.627665672
 C 3.5250394929 1.0119824726 -2.8027686649
 C 3.0642809988 0.3684695989 -3.9482091655
 C 1.6663279646 0.5204672998 -4.3180332652
 C 0.8389081367 1.3515079344 -3.5839774251
 C 1.2942567532 2.2945233094 -2.4103459638
 C 2.7014564032 1.8376119653 -1.9072306313
 C 3.9322703409 -0.0192598693 1.5784194444
 C 3.1762118985 1.1540032236 1.7956259046
 C 2.8923036332 2.0289955132 0.7382810545
 C 3.3029254304 1.7351015998 -0.5982074199
 C 2.5242220291 -3.8617411784 1.1385198559
 C 2.0267365218 -3.17972381 2.2579004404
 C 2.6199464469 -1.973603681 2.6935573263
 C 3.7095879285 -1.4216427237 1.9999516142
 C 0.8212508802 -4.174492461 -2.6541928678
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 C 1.7870180148 -4.477380178 -0.0128127587
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 C 0.7260750458 -3.3857524602 -3.8555672786
 C -2.040299414 0.8656143144 -0.0853360518
 C -2.4458568275 -0.4185613489 0.40136667
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 C 0.0253241677 2.2015124538 -1.4655815756
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 C -2.0796525477 -2.6337364942 -0.6126297203

C -1.3073524764 -3.1889892006 -1.7576700965
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 C -0.993960779 -0.2934545617 -3.8906233548
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 C -1.5477728782 0.1471415167 2.5501868584
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 H 2.2747433987 2.8897923348 0.9528423012
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 H 2.087714171 -1.3856578769 3.4371232773
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 H 0.5525568223 2.9853576297 0.4706604176
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 H -2.1206618467 -4.1937704075 0.9365808916
 H -0.5052350014 1.9988001171 2.7133620531
 H -1.3690925901 -0.0939763849 3.5956899916

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 207

42.9536	65.9991	111.5383
148.1579	189.0475	193.3163
203.8382	229.9035	254.6573
263.6513	272.2407	285.3894
300.8741	312.8891	313.6117
328.3048	344.4087	350.5933
356.4101	364.3393	372.7384
391.4880	392.4366	399.3014
405.8972	416.2892	419.3466
440.3973	442.0841	454.3209
458.7204	463.2055	467.1831
473.6566	487.6295	492.8066
501.0209	510.8558	516.4238
526.2567	529.2026	536.6060
541.6216	549.5185	555.5498
557.8461	559.8173	568.6305
575.5105	579.9780	591.6784
601.3461	603.0683	610.7124
613.3417	628.0850	633.4137
636.8451	643.6607	649.3182
663.5410	668.4153	675.1624

682.5028	688.4625	696.5321
701.5631	707.1147	711.4711
714.6720	720.1067	722.5779
726.8214	735.3950	740.9659
743.8746	745.4564	750.7041
750.9824	753.6108	756.6003
757.8293	761.9304	763.6919
764.8866	769.6958	774.5283
784.4484	786.8339	790.9532
793.1217	798.9577	806.4200
812.1306	822.8652	828.7671
835.4201	841.5636	854.3810
877.2823	885.1561	887.8926
905.7994	929.7817	940.2469
942.8743	952.3876	957.7172
962.8465	979.2937	984.6344
992.1233	998.2186	1027.1860
1030.9808	1047.4677	1064.0651
1081.0614	1088.5157	1101.2506
1117.7322	1119.9109	1140.9544
1148.3131	1155.0495	1169.4769
1171.7787	1174.6234	1184.9618
1186.9609	1193.0962	1203.1569
1211.6635	1220.4954	1230.4766
1236.0352	1238.3399	1243.1787
1247.5441	1258.9806	1267.2909
1271.4539	1280.9280	1292.9827
1296.5027	1309.3802	1311.9918
1316.3663	1321.6283	1326.0487
1337.0256	1343.4322	1347.5051
1355.0304	1360.6636	1361.4127
1364.8684	1371.5942	1377.9321
1385.0751	1392.6587	1410.2951
1416.1747	1421.0723	1422.5052
1428.2733	1436.5376	1441.0877
1442.4715	1447.1192	1450.8672
1455.1375	1461.6564	1477.2180
1485.7688	1486.9833	1499.6016
1500.0660	1508.2817	1533.8328
1538.9355	1544.7598	1559.9432
1572.9370	1583.4362	1588.1419
1592.4844	1602.2825	1607.5241
1614.4510	1623.4022	1628.5162
1632.3094	1639.0638	1648.8011
1676.7016	2984.5958	3174.7538
3179.7917	3182.9184	3185.8245

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3192.4566      3199.3081      3202.3636
3245.3168      3285.6692      3295.0441
ZeroEnergy[kcal/mol] -15.6
ElectronicLevels[1/cm]      1
0 2
End
End
!-----
!-----h_c60h10_p1-----
Bimolecular p1
Fragment      c60h10
RRHO
Geometry[angstrom] 70
C 3.6525657697 -0.1491306855 -1.7443709133
C 3.0625358698 -0.8749221609 -2.8466070276
C 2.829345613 -2.2422245905 -2.4127271608
C 3.3163253823 -2.3645782545 -1.0531155195
C 3.8598215448 -1.079689105 -0.6474488204
C 3.7134856037 -0.6509141779 0.6609096102
C 3.364881581 0.7170994288 0.9597765703
C 3.0632603866 1.5811942828 -0.0979759048
C 3.2175786422 1.1459924946 -1.456294192
C 1.6492577596 -2.8923677789 -2.7894149095
C 0.8748751942 -3.6233208158 -1.7991025678
C 1.3475726043 -3.7311107354 -0.4973639415
C 2.5944786672 -3.1087537809 -0.1241502846
C 2.1349633794 -0.2288084084 -3.6628206468
C 0.9653812276 -0.9420626157 -4.1344749118
C 0.7182482887 -2.2443563657 -3.6824357697
C 3.0430891865 -1.4596905762 1.6512680738
C 2.4515611565 -2.6638092102 1.242260104
C 2.1943249976 1.7956678807 -2.2308157503
C 1.7248765249 1.1355173898 -3.3645164712
C 0.3463424519 1.282983724 -3.7179392387
C -0.468998608 2.0873775904 -2.9236246884
C -0.0152268326 2.7623839195 -1.6818499062
C 1.3446966421 2.6155140254 -1.3356847321
C 2.6387836038 0.7912654824 2.1807232525
C 1.9030040693 1.9603891188 2.3993420187
C 1.6163671147 2.8429793939 1.3258705511
C 2.0166293916 2.5413904535 0.0133321821
C 1.1799745779 -3.0479217366 1.7595912279
C 0.697274486 -2.3594833364 2.8764494696
C 1.3127345763 -1.1570257939 3.3091301439
C 2.4074831921 -0.6253936578 2.6186765003
C -0.5294336456 -3.3982354739 -2.0402452697

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C -1.4568955057 -3.2688765786 -0.9671778166
 C -0.9212520774 -3.512575306 0.3594336289
 C 0.4318850728 -3.6712770316 0.6095354316
 C -0.131363344 0.0038275471 -4.2236447775
 C -1.4283747538 -0.4082000798 -3.9398807603
 C -1.6714964101 -1.7390717021 -3.3953506268
 C -0.6207230531 -2.61605579 -3.2511637533
 C -3.3891049168 1.6218730946 0.5277270602
 C -3.818356196 0.3409537147 1.0005053003
 C -3.9003601529 -0.5353757115 -0.135696431
 C -3.7321965538 0.2637465781 -1.3063207857
 C -3.3480198152 1.592317122 -0.8864958688
 C -2.3221869452 2.2415369939 -1.5527813758
 C -1.2632913053 2.9059827937 -0.8264525775
 C -1.4587375588 3.1071340882 0.5446202242
 C -2.4939546821 2.3994094142 1.2692399891
 C -3.4512017525 -1.8627718528 -0.0273802203
 C -2.6608276638 -2.4081145344 -1.1618088108
 C -2.7011183874 -1.6639877621 -2.380748996
 C -3.1999497953 -0.301873633 -2.4339724071
 C -3.5214549261 -0.1047967152 2.2801718555
 C -3.5821371205 -1.5379347971 2.437970534
 C -3.5326489322 -2.3692857637 1.3339556105
 C -1.8507637612 1.7202302954 -2.7984119861
 C -2.3286490421 0.4908747232 -3.281383804
 C -2.4188075748 2.0614183187 2.6758091846
 C -2.9309921709 0.872494841 3.1636588652
 H 1.3890790358 2.1325431818 3.3420100773
 H 0.9902734887 3.6979878802 1.538587542
 H -0.2671860956 -2.6156984901 3.3078215082
 H 0.7860108726 -0.5593513249 4.0490952003
 H -1.544667712 -3.2795552672 1.2074995469
 H -0.7246667975 3.6288918444 1.1363805895
 H -3.5691087257 -1.9810356132 3.4312681126
 H -3.511810301 -3.4422284522 1.5012488287
 H -1.8503781814 2.7008560372 3.3475546253
 H -2.7667666585 0.6190520128 4.2085572051
 Core RigidRotor
 SymmetryFactor 0.5
 End
 Frequencies[1/cm] 204
 47.4086 67.4706 116.0441
 150.7522 194.7357 201.2559
 210.7020 231.0158 254.0900
 265.0740 276.5015 290.3561
 303.3816 318.9830 321.2316

332.8620	345.3897	356.3562
360.2894	366.7361	382.4997
393.7279	397.5766	405.3913
408.6155	415.8682	433.8303
442.5009	449.9609	458.7340
462.5899	468.8466	474.6726
486.0516	491.8445	497.6878
501.2470	517.5728	520.7494
525.7417	530.9163	538.6979
544.6330	553.6502	556.7405
563.5898	564.0163	571.0576
578.9885	585.4917	594.3355
605.5843	607.6022	616.0626
620.1718	632.0901	634.8069
638.9363	647.7771	652.5553
669.2023	679.8024	680.9021
690.5318	703.0063	708.0197
708.7524	711.7162	717.2349
718.8756	720.4066	724.8513
731.1030	738.2426	741.7402
746.3381	748.4374	750.1064
754.8950	756.6892	758.6042
762.1274	764.7389	766.1620
769.4213	773.9195	776.8388
785.0492	786.0665	788.8431
796.5182	803.3648	808.4962
822.8422	825.5447	830.9717
833.5436	842.3442	869.6405
879.8363	882.1967	896.3093
908.8485	939.6954	945.5390
957.4093	959.7494	964.4815
971.3735	985.1877	991.6865
996.9325	1017.9962	1036.2113
1041.5660	1069.6183	1078.7148
1088.5500	1099.2859	1111.3881
1122.0808	1138.0595	1142.9056
1159.1069	1165.6244	1175.3143
1180.8442	1185.0339	1187.8242
1198.2238	1207.5485	1212.5598
1225.9728	1234.2433	1242.4268
1245.3173	1254.4994	1266.4414
1272.2710	1275.1496	1283.3716
1300.7530	1304.3827	1310.5597
1316.2967	1317.7504	1327.6578
1341.6329	1349.7048	1352.7421
1355.0096	1358.2147	1364.7624

1368.5184	1371.2935	1373.7575
1379.9328	1392.0603	1401.7106
1410.8786	1419.9159	1426.7061
1434.9261	1437.0949	1442.6142
1443.7694	1446.7986	1450.6914
1453.2418	1455.8703	1466.2262
1478.8646	1484.4934	1492.7595
1498.4854	1504.1431	1515.3497
1544.1256	1549.1053	1564.8879
1579.9702	1585.8344	1592.8648
1597.5146	1601.5916	1612.5157
1615.9168	1620.0735	1623.0329
1625.0068	1634.8597	1641.1445
1647.3936	1674.8740	3175.9312
3180.8358	3182.3075	3186.3654
3193.5157	3198.6025	3201.2493
3248.8668	3288.6837	3307.6361
ZeroEnergy[kcal/mol]		0.0
ElectronicLevels[1/cm]		1
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End		
Fragment		H
Atom		
Mass[amu]		1
ElectronicLevels[1/cm]		1
0 2		
End		
GroundEnergy[kcal/mol]		23.5
End		
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C	3.7678238681	-0.659148303 -1.9045400971
C	3.1221173828	-1.4031343958 -2.9657166588
C	2.8468542354	-2.7395208341 -2.4748552375
C	3.3333634005	-2.8188570564 -1.1097697179
C	3.9261185858	-1.5387574425 -0.7613909182
C	3.7710294737	-1.0306627178 0.5201770269
C	3.4849757139	0.3673744562 0.7450518525
C	3.2927316952	1.208089863 -0.3547986279
C	3.4169022627	0.6703927235 -1.6811132016
C	1.6513943986	-3.3792428939 -2.8250944804
C	0.8668822758	-4.0674028831 -1.8124395105
C	1.3328061828	-4.1211534354 -0.5035877475
C	2.5861150548	-3.4975994995 -0.1532597766

C 2.1946488725 -0.7562233103 -3.7922749542
 C 0.9929525861 -1.4473094163 -4.1992687649
 C 0.7257574338 -2.7370114838 -3.7272697496
 C 3.0448346677 -1.7603072954 1.5313210277
 C 2.4364861855 -2.974604562 1.1849440717
 C 2.4009310632 1.3086078794 -2.4722799878
 C 1.8392690096 0.6291274226 -3.544385156
 C 0.4278340777 0.8062668992 -3.8038909799
 C -0.3327106869 1.7009581939 -3.0340862093
 C 0.3426315702 2.6410879221 -2.0873648309
 C 1.6743018223 2.278509098 -1.6746089716
 C 2.7025946227 0.527855233 1.9280166239
 C 1.9652644297 1.7142042173 2.0492673265
 C 1.7719977903 2.5673493044 0.9357274355
 C 2.298650915 2.2416395415 -0.325544083
 C 1.1534346804 -3.3109966403 1.70775213
 C 0.6613247012 -2.5389934377 2.7656849106
 C 1.2868423545 -1.3194764537 3.1285054252
 C 2.4069059807 -0.8524237229 2.4297508394
 C -0.5366189056 -3.8480831046 -2.0667750902
 C -1.4730624689 -3.7040157751 -1.0011999196
 C -0.94244591 -3.883843144 0.3361050044
 C 0.4134820404 -4.0035480863 0.5949940045
 C -0.0786560797 -0.4699754557 -4.254736543
 C -1.3729694689 -0.8373989701 -3.938333502
 C -1.6498757315 -2.1757020011 -3.4261968981
 C -0.618081388 -3.0787021689 -3.2865808425
 C -3.4482523105 1.1261791977 0.5474350901
 C -3.9139971114 -0.1642777725 0.9613014413
 C -3.9364384901 -1.0094344849 -0.1940334019
 C -3.6852658883 -0.1783116847 -1.3255203269
 C -3.2968301371 1.1251395945 -0.8653452811
 C -2.2372915031 1.8081859177 -1.4789108981
 C -1.4351327611 2.5846278791 -0.609544202
 C -1.6549431876 2.7287043491 0.7407174179
 C -2.6491206552 1.8976537095 1.392814265
 C -3.509727974 -2.3435214493 -0.1018065465
 C -2.6815077195 -2.8616954498 -1.220415624
 C -2.6824344243 -2.0952935663 -2.4243795952
 C -3.1217537334 -0.712764441 -2.4431127749
 C -3.7072928876 -0.6483631142 2.2455093622
 C -3.765279939 -2.0847930844 2.3582263689
 C -3.6473393454 -2.8879322716 1.236517727
 C -1.6976529495 1.3117038384 -2.7357286463
 C -2.210015892 0.0855701087 -3.2359978627
 C -2.6622605995 1.5133043091 2.7865564173

C -3.1871743207 0.302361293 3.1989821722
 H -0.0064478944 3.6638286708 -1.991911582
 H 1.3718338227 1.9061169026 2.9400054606
 H 1.0662844525 3.3836912329 1.0370660987
 H -0.3147212543 -2.7509595618 3.1951316628
 H 0.7565587977 -0.6672713706 3.8181307321
 H -1.5754031059 -3.6217792514 1.1696255137
 H -1.001535855 3.3361094154 1.3608278134
 H -3.7939582698 -2.5541919617 3.3390931945
 H -3.6031062748 -3.9642159029 1.3776822756
 H -2.1592785354 2.1441725783 3.5162036547
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 Core RigidRotor
 SymmetryFactor 0.5
 End
 Tunneling Eckart
 ImaginaryFrequency[1/cm] 602.897
 WellDepth[kcal/mol] 17.3
 WellDepth[kcal/mol] 32.9
 End
 Frequencies[1/cm] 206

47.7851	62.0675	
109.4810	134.0154	186.0938
188.9551	198.4494	219.1079
251.1461	264.1242	272.3451
282.3696	294.2576	303.4666
314.7393	331.2884	339.0472
350.5751	353.5696	362.0076
374.4760	387.0580	392.9046
396.7224	404.0495	407.8660
425.1747	437.2485	442.7548
451.2501	453.8119	462.2775
474.4281	475.5301	483.1470
489.5456	494.4985	503.3276
512.5180	515.6309	525.2270
533.5160	540.5061	544.6925
545.1558	554.5647	558.2195
563.0211	571.1234	582.3164
586.2947	596.9240	604.2936
606.9041	613.7289	620.3836
632.0828	634.9330	637.9818
647.1987	653.7251	669.6340
671.2815	672.9928	678.9324
687.4690	700.9044	702.7787
708.6352	712.5344	714.7581
720.0662	725.2684	730.5956

736.3943	740.3111	741.6279
744.9948	750.0828	750.9335
756.5083	759.9039	760.2233
761.8076	765.9195	766.8952
770.0629	780.6249	786.5149
788.9052	793.8664	797.5534
806.9654	814.9903	822.3418
824.6974	828.6014	838.0473
863.9782	872.0109	881.3850
890.9146	903.4454	907.2532
939.8448	943.3667	952.5019
956.0388	961.3702	975.0082
986.1020	992.5005	1008.6028
1035.9817	1037.7510	1050.7313
1072.1327	1076.4502	1091.9106
1112.1045	1121.5488	1127.2220
1130.8365	1150.2019	1163.1920
1170.5216	1174.6537	1183.2013
1187.3828	1191.6662	1201.4530
1206.2129	1224.6257	1225.2675
1239.2205	1242.4869	1245.1906
1254.1704	1267.2596	1273.1440
1276.2608	1285.3584	1299.7813
1302.1552	1310.4937	1315.9269
1318.9539	1330.0929	1332.3945
1338.2133	1345.6516	1350.3513
1353.3469	1357.3719	1362.5321
1367.0982	1369.0489	1375.9425
1384.6449	1394.2127	1398.8083
1409.8348	1420.9626	1427.8599
1431.7552	1433.0527	1438.4404
1441.8309	1448.9155	1449.3509
1453.3274	1461.0759	1463.6746
1479.5019	1489.4959	1495.5995
1502.2591	1513.3780	1517.4296
1545.9944	1564.1243	1566.2587
1576.4822	1579.8256	1593.4536
1596.7072	1600.2170	1606.5604
1612.3415	1616.6929	1630.3733
1632.4487	1640.5506	1647.3452
1696.8632	3175.3301	3179.8299
3182.0415	3185.3793	3192.1524
3193.3751	3194.2186	3198.4358
3199.8729	3230.5226	3276.3188

ZeroEnergy[kcal/mol] 17.3

ElectronicLevels[1/cm] 1

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0 2
End
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!-----bar_ts2-----
Barrier    ts2 ip2 p1
RRHO
Geometry[angstrom] 71
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C 3.064577943 -1.0484296316 -2.8448862849
C 2.8312974915 -2.4157337034 -2.4119409877
C 3.3174944611 -2.5388794718 -1.051893678
C 3.860401756 -1.2540849678 -0.6451975857
C 3.7121594888 -0.8257374554 0.6631043047
C 3.3615734967 0.5418077443 0.9614968357
C 3.0617255095 1.4060949293 -0.0958978384
C 3.2188249063 0.9716279043 -1.4536824669
C 1.6509429685 -3.0652561275 -2.7893630571
C 0.8761175585 -3.796394885 -1.7997750622
C 1.3485083892 -3.9060017024 -0.4981873926
C 2.5952698767 -3.2839844926 -0.1238897335
C 2.1373969149 -0.4015907814 -3.6614251179
C 0.9678120811 -1.114294593 -4.1333772894
C 0.7202695322 -2.4168118956 -3.6824912976
C 3.040676533 -1.6350846622 1.6521800648
C 2.4511201882 -2.8398234631 1.24260314
C 2.1956026011 1.6215305781 -2.2284650217
C 1.7274429518 0.9625222624 -3.3633247419
C 0.3485023887 1.1114707714 -3.7191238847
C -0.4674846199 1.919805209 -2.9311568572
C -0.0130309041 2.6183674034 -1.6957380665
C 1.3476125165 2.4411715053 -1.3348767437
C 2.6327505394 0.6147156937 2.181330841
C 1.8960004581 1.7838616063 2.3993467054
C 1.6104453787 2.6663211818 1.3264304412
C 2.0127724068 2.3658037616 0.0130580056
C 1.1796998989 -3.2255933323 1.7593226493
C 0.6951874352 -2.5378757622 2.8759794159
C 1.3082569932 -1.334496982 3.3088265379
C 2.4027942455 -0.8014366848 2.618839841
C -0.5281763446 -3.5705372359 -2.0410940264
C -1.4557147359 -3.4414221379 -0.9678625201
C -0.9205354494 -3.6881537702 0.3582162624
C 0.4325399173 -3.8480804739 0.6084014982
C -0.1285706954 -0.1681298016 -4.2229977885
C -1.4259507893 -0.5800602771 -3.940721022
C -1.6695520836 -1.9108774559 -3.3956306283

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C -0.6190897341 -2.7882025502 -3.2515487029
 C -3.3835076281 1.4552422373 0.5251175212
 C -3.8115278268 0.1745575242 0.9999036821
 C -3.89436324 -0.7034920888 -0.1350110459
 C -3.7269799401 0.0943063325 -1.3065227141
 C -3.343676859 1.4236051522 -0.8888031667
 C -2.3175942746 2.0716835898 -1.5562101009
 C -1.2635169726 2.742107987 -0.8321894598
 C -1.4574907322 2.9463613793 0.5374967585
 C -2.488909553 2.2351436044 1.2646666511
 C -3.4461791314 -2.031052505 -0.0256976368
 C -2.6581652064 -2.5784685839 -1.1612019138
 C -2.6983549897 -1.8347350699 -2.3803397127
 C -3.1959832004 -0.4722548389 -2.4341267249
 C -3.5132099133 -0.2692762775 2.279760915
 C -3.5742900107 -1.7022380123 2.439342347
 C -3.5268447923 -2.5353319392 1.3364420373
 C -1.8463609436 1.5496909267 -2.8014036166
 C -2.3251957158 0.3192814099 -3.2828947508
 C -2.4116491468 1.8985006327 2.6714419295
 C -2.9221888301 0.7096038609 3.1612373536
 H 0.0163143556 4.7691975712 -2.435932094
 H 1.3821056045 1.9562150126 3.3419528379
 H 0.9857317715 3.5221569856 1.5392653705
 H -0.2694187741 -2.7952949691 3.3062765292
 H 0.7803652466 -0.737732237 4.0486479974
 H -1.5439252708 -3.4564189859 1.2065933599
 H -0.7271101494 3.4767353119 1.1261546132
 H -3.5607815374 -2.1441599893 3.433165328
 H -3.5075097812 -3.6079861704 1.5055680727
 H -1.8437866278 2.5395347413 3.3421398952
 H -2.7567714546 0.4579263546 4.20636085
 Core RigidRotor
 SymmetryFactor 0.5
 End
 Tunneling Eckart
 ImaginaryFrequency[1/cm] 353.5849
 WellDepth[kcal/mol] 41.4
 WellDepth[kcal/mol] 2.4
 End
 Frequencies[1/cm] 206
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 115.4032 150.1068 171.1216
 193.8882 199.6668 205.3206
 211.5953 230.6605 254.0482
 265.0334 276.3360 289.6859

303.4229	318.4790	321.2983
332.6162	345.5562	356.0372
359.7688	366.6506	382.2367
393.5611	397.6084	404.7535
408.3953	415.9674	433.0768
441.7615	449.9241	458.1200
462.8282	468.7696	474.4464
485.2905	491.3767	497.7427
501.1893	515.9915	519.5633
525.4877	530.6252	538.1054
544.1322	553.1931	556.4200
562.9036	564.0257	570.7399
578.8657	584.6336	593.7109
604.9762	607.2894	615.7866
620.1589	632.0750	634.1162
638.9335	647.5350	652.3710
668.9982	679.4356	680.8211
690.2705	702.2914	705.9482
708.6721	711.3046	716.4877
718.0574	720.1051	724.1331
730.6933	738.2149	742.5017
745.9583	748.6511	750.0958
754.9413	756.4621	758.5588
762.1049	764.0360	766.1892
769.1267	772.7025	776.5551
784.9807	785.5083	788.8123
796.4694	803.0026	807.2505
821.4168	825.4703	830.4650
833.2063	841.9918	868.8838
879.0692	882.2537	896.3005
908.9837	939.1236	944.2488
956.8317	959.2367	964.2363
971.2160	984.7860	990.9030
996.6068	1017.9594	1036.0598
1041.2352	1069.0870	1078.2431
1087.6518	1098.6358	1111.6371
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1158.5895	1165.6727	1175.1604
1179.1550	1184.2224	1187.6084
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1244.8375	1254.8893	1266.5239
1272.5199	1274.5879	1283.3877
1300.5460	1304.7282	1310.7296
1315.5121	1317.8107	1328.2761
1341.2214	1348.9798	1351.7894

1354.4691	1358.1446	1363.1727
1367.8209	1369.3975	1373.1526
1379.6922	1390.5415	1399.3718
1409.2921	1416.8134	1425.5739
1434.3866	1437.0009	1442.2999
1443.3130	1446.1793	1449.4199
1452.7093	1455.4703	1465.0570
1479.0579	1484.7303	1493.0904
1498.4023	1503.5635	1515.3628
1542.1988	1547.0904	1564.2663
1579.4743	1583.6400	1592.5952
1596.5885	1600.4318	1611.7419
1615.6853	1619.6998	1623.0521
1625.4668	1634.8665	1641.1899
1647.4620	1675.1518	3176.0541
3180.9346	3182.6370	3187.1175
3193.6702	3198.7139	3201.3583
3250.4272	3288.4876	3307.4354

ZeroEnergy[kcal/mol] 25.8

ElectronicLevels[1/cm] 1

0 2

End

!-----

End

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H₉

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1700. 1800. 1900. 2000.
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1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
!TemperatureList[K]          300 500. 1000 1500. 2000
!TemperatureList[K]          300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
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!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature    0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature   100
ModelEnergyLimit[kcal/mol]    900
WellCutoff                    10
ChemicalEigenvalueMax         0.2
ChemicalEigenvalueMin         1.e-6      #only for direct diagonalization method
CalculationMethod              direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput               eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber             0
!ReductionNumber               5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                 260 ! Frenklach
! Power                        0.
Factor[1/cm]                   247 ! Jasper universal
Power                          0.85
! Factor[1/cm]                 424 ! Jasper calc N2
! Power                        0.62
! Factor[1/cm]                 125 ! SJK guess
! Power                        0.85
ExponentCutoff                 15
End
CollisionFrequency

```

```

LennardJones
!Epsilons[1/cm]      203.0 203.0 ! N2 pyrene-Frenklach
!Sigmas[angstrom]    4.6 4.6 ! N2 pyrene-Frenklach
!   Epsilons[1/cm]    206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
!   Sigmas[angstrom]  5.06 5.06 ! N2 Jasper extrapolation to C16
!   Epsilons[1/cm]    32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
!   Sigmas[angstrom]  3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
!   Epsilons[1/cm]    101.5 1181.20585
!   Sigmas[angstrom]  3.6154 10.86463759
!   Epsilons[1/cm]    390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Sigmas[angstrom]  4.46 4.46 ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Epsilons[1/cm]    189. 216.0 ! N2 , CH2CCH ! from Jasper calc
!   Sigmas[angstrom]  3.30 4.11 ! N2 , CH2CCH ! from Jasper calc
Masses[amu]          28. 729.
End
OutputTemperatureStep[K] 100
OutputTemperatureSize 20
OutputReferenceEnergy[kcal/mol] 0.
!-----
!-----well_ip1-----
Well      ip1
Species
RRHO
Geometry[angstrom] 69
C 3.6450712392 -0.0876390713 -1.7224603457
C 3.0626087107 -0.8182712016 -2.8285014053
C 2.8262641985 -2.1832472817 -2.3914609205
C 3.302659496 -2.3018152611 -1.0275685725
C 3.8346847129 -1.0124906846 -0.618462284
C 3.6627634345 -0.5788012641 0.6864104157
C 3.297077384 0.7881511384 0.9731883998
C 3.0317617657 1.6538015208 -0.0929336038
C 3.219159461 1.213731603 -1.4499695686
C 1.6510913402 -2.8383765529 -2.7766612085
C 0.8748954412 -3.575041388 -1.7927527258
C 1.3427135708 -3.6874762076 -0.489857614
C 2.5804267707 -3.0537507971 -0.1059412007
C 2.1438828861 -0.1782109171 -3.6605367997
C 0.9729158785 -0.8921345376 -4.1296351615
C 0.722473519 -2.1911509983 -3.6726699687
C 2.9851750187 -1.3929816285 1.6680286702
C 2.4204383471 -2.6105296935 1.2597004023
C 2.2140960686 1.8604588211 -2.2538087158
C 1.7406706972 1.1922253028 -3.3829729323
C 0.3607889232 1.3408453676 -3.7423820243

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C -0.4577362806 2.1578383966 -2.9623490137
 C 0.0104057806 2.8333209872 -1.7363483357
 C 1.3578613554 2.6836052202 -1.3808539043
 C 2.5243204134 0.8528824921 2.1688875316
 C 1.7133575419 1.9775260642 2.3453421313
 C 1.4405313502 2.8531164362 1.2606249575
 C 1.9653096619 2.5965529361 -0.0136387047
 C 1.1535139166 -3.0168939405 1.7693669634
 C 0.6473280526 -2.3331543774 2.878994784
 C 1.2309395561 -1.1140702699 3.3056017645
 C 2.3187588206 -0.5645696521 2.6182114128
 C -0.5295897607 -3.3502257088 -2.0375383286
 C -1.4599312455 -3.2285809565 -0.9666169524
 C -0.931258835 -3.494098409 0.3582392394
 C 0.421260805 -3.6452634136 0.6126918524
 C -0.1221108481 0.0557534994 -4.2249600838
 C -1.4198533672 -0.3494502241 -3.9309062781
 C -1.6662792689 -1.6786402014 -3.3840431242
 C -0.6180354577 -2.5604151505 -3.2431006399
 C -3.283053078 1.6770644148 0.5640230209
 C -3.7259841471 0.4012870301 1.0387457051
 C -3.848948052 -0.4649973171 -0.1026090975
 C -3.6882858056 0.3379568192 -1.2715561271
 C -3.2899385875 1.6639924234 -0.8554500022
 C -2.2976832154 2.3249235701 -1.5613800786
 C -1.2021401877 2.9769621929 -0.8554577735
 C -1.371564584 3.1025827628 0.5045242462
 C -2.3408505589 2.4203828738 1.3021165504
 C -3.4256760056 -1.8010449022 -0.0083651337
 C -2.6532965851 -2.3519548251 -1.1521433824
 C -2.690989602 -1.5988172371 -2.3646561498
 C -3.1792997176 -0.231212797 -2.4099744696
 C -3.4142768162 -0.0627245296 2.3085923505
 C -3.5180760822 -1.4941088562 2.4594482642
 C -3.5083075042 -2.3174622566 1.3492924021
 C -1.8407977924 1.7954868444 -2.8127643333
 C -2.3162508971 0.5549038578 -3.2711450461
 C -2.2321415884 2.0610775672 2.6999210736
 C -2.7735203178 0.8854359615 3.186992832
 H 1.1229078845 2.0990160336 3.2500285252
 H 0.6923040403 3.6257618582 1.4059639025
 H -0.3147179838 -2.6078569898 3.3042525529
 H 0.6845622512 -0.5215105589 4.0352490291
 H -1.5588340122 -3.2775647472 1.2069565916
 H -3.5069242676 -1.9434658113 3.4498650243
 H -3.5194490824 -3.3919432143 1.5070506627

H -1.6303419543 2.67954729 3.3599697101
H -2.5958778051 0.6172935456 4.2259440428

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 201

55.8618	67.3592	116.0305
146.6242	193.5693	200.7928
210.3724	233.1432	254.3701
265.3773	277.4166	288.5490
304.9442	318.4040	321.7549
331.2094	351.8292	359.3755
363.7061	370.2278	381.8797
394.0710	399.9313	406.6231
409.3454	414.5686	433.5125
444.4468	448.8124	459.6418
464.0114	470.1554	474.7484
485.1339	493.3542	495.0980
502.9463	513.3031	520.3394
527.0960	529.1755	539.3378
545.4946	551.2370	556.1072
562.1972	564.6973	570.4923
577.9817	584.8321	591.7603
605.1967	609.0084	615.8355
618.0858	630.9536	633.7297
638.5478	650.7259	653.1431
666.3106	680.1707	681.3498
690.2926	700.6034	706.9138
708.4360	712.3697	718.2011
719.8892	722.6542	723.7834
733.2941	738.7684	742.6461
745.4398	748.2156	748.7741
750.8940	756.3061	757.8439
759.9030	763.0017	766.5407
768.1007	771.0471	777.2005
783.9309	785.9799	789.1349
797.1037	804.2068	805.0317
818.3406	821.3306	831.1686
835.3316	843.1485	878.9613
882.8173	899.4175	905.8753
931.6612	941.4653	943.9275
958.4886	960.7526	970.3884
985.5813	991.3596	994.8407
1021.5660	1036.2184	1041.7763
1071.6272	1079.6104	1089.3172
1100.2183	1114.5715	1121.8521

1138.6293	1143.2351	1159.1046
1167.5161	1173.7621	1183.6611
1188.5687	1198.1581	1206.8954
1213.7884	1224.5993	1234.0374
1237.7974	1242.9396	1253.4348
1256.2325	1268.9009	1271.4280
1276.5178	1291.4803	1298.6406
1304.0644	1305.9802	1314.1470
1318.8233	1328.6943	1341.0781
1350.2944	1352.4035	1356.4907
1360.9834	1363.3760	1368.0007
1373.9446	1375.2253	1383.0780
1385.3028	1398.2316	1423.6700
1428.0736	1433.5793	1436.9094
1440.0919	1442.9777	1446.7664
1451.6512	1452.7500	1454.6392
1466.4127	1473.3078	1480.5105
1489.3123	1494.7014	1498.3181
1513.4069	1540.5007	1551.1814
1563.9018	1574.3832	1584.4841
1587.6149	1596.5597	1596.8632
1601.6870	1612.6828	1613.2005
1618.1108	1620.1722	1632.0282
1638.8102	1645.3341	1667.0551
3181.1876	3181.5666	3182.9231
3186.3746	3197.7712	3201.3219
3202.0426	3204.4135	3291.7680
ZeroEnergy[kcal/mol] 0.0		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----well_ip2-----		
Well ip2		
Species		
RRHO		
Geometry[angstrom] 69		
C 5.1053416666 -0.1919739325 -1.2427411172		
C 4.563237776 -0.9454193113 -2.3607045111		
C 4.3325498112 -2.3086451421 -1.9126578723		
C 4.7682652277 -2.4013518054 -0.5325513524		
C 5.248810049 -1.092910634 -0.1238588358		
C 4.9493997886 -0.6340595447 1.163011099		
C 4.4978651822 0.6995551571 1.3810859506		
C 4.3462507288 1.581495936 0.3164132392		

C 4.6866737514 1.1277305876 -1.0249637569
 C 3.1812329544 -2.9908256398 -2.3211226971
 C 2.4068090674 -3.7581072655 -1.3588235699
 C 2.8602625871 -3.8781146685 -0.0495322519
 C 4.0542793089 -3.1865053326 0.3661973037
 C 3.6617846074 -0.3363302573 -3.2377036679
 C 2.4941803868 -1.065209349 -3.6974471621
 C 2.2512929122 -2.3575246469 -3.227238717
 C 4.2576631105 -1.4729251006 2.1205019198
 C 3.8214518217 -2.749098139 1.727875925
 C 3.7579872319 1.7503022244 -1.9279052488
 C 3.2669699814 1.0457138843 -3.0288376848
 C 1.8727665047 1.1809863078 -3.4041062488
 C 1.0376082924 2.0236439242 -2.6567383091
 C 1.5343759292 2.7039817812 -1.4787182214
 C 2.8668061531 2.5806550313 -1.1178300837
 C 3.5473469029 0.7181311555 2.4939989262
 C 2.5650977436 1.6511067741 2.5373166484
 C 2.2558690872 2.6762479767 1.4288559166
 C 3.2328707184 2.4815749326 0.2593174488
 C 2.5846917584 -3.251747624 2.2127417923
 C 2.000055658 -2.6067761759 3.3133368051
 C 2.4456579373 -1.3301194575 3.7133723054
 C 3.4787028695 -0.6903405977 3.0142029459
 C 1.0024255816 -3.5500626162 -1.6153486721
 C 0.0575836551 -3.4708451392 -0.5499591618
 C 0.564735214 -3.7953958937 0.7639238137
 C 1.9194711729 -3.9043728333 1.0374392345
 C 1.3922445983 -0.1235796268 -3.8153601642
 C 0.0961933194 -0.5282614576 -3.4844592722
 C -0.1382153191 -1.8541913835 -2.9305963293
 C 0.9124150948 -2.73881386 -2.804382269
 C -1.434219106 1.4217744923 1.0867365485
 C -1.9709301956 0.1750120334 1.5667597472
 C -2.2026839817 -0.6595418254 0.418042373
 C -2.0668295862 0.1527673017 -0.7426422117
 C -1.5901465227 1.4485478178 -0.3204244361
 C -0.6774032318 2.1374816542 -1.0833996127
 C 0.4931593965 2.6962528224 -0.4403912914
 C 0.7340962196 2.5725118489 0.9400490124
 C -0.3515628852 2.0213028124 1.7660010956
 C -1.8524310922 -2.0180198877 0.4715260054
 C -1.121043389 -2.5665806747 -0.7044061458
 C -1.1550762995 -1.784754638 -1.8975752424
 C -1.6241833387 -0.4091499006 -1.9141210759
 C -1.6850967822 -0.3337506684 2.8204711403

C -1.8823586615 -1.7554243881 2.9474253654
 C -1.9384385587 -2.5562691069 1.820231263
 C -0.3256989596 1.6354360521 -2.3953253672
 C -0.7949229602 0.3787010426 -2.8086317282
 C -0.3640367498 1.6990338486 3.1913294015
 C -1.014505886 0.5931313733 3.701774132
 H 1.8325907169 1.5679019866 3.3230852981
 H 2.3839395693 3.6919977007 1.8477240578
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 H -0.0824887069 -3.6419394686 1.6105433724
 H -1.8902611523 -2.2251950902 3.9283277224
 H -2.015980266 -3.6306982474 1.9589691773
 H 0.1652425194 2.3422923443 3.8878615222
 H -0.9404880569 0.3834901331 4.7664536951

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 201

75.2726	90.8621	161.1192
187.2854	205.1040	243.6392
257.5888	263.9794	269.3091
278.6783	285.2116	299.9636
309.8650	320.9526	333.7401
357.4001	357.4373	359.4886
376.4996	383.5142	391.1572
400.4925	409.4116	414.6511
418.9671	421.4726	431.3851
447.6739	464.9695	467.7558
472.3067	481.0935	483.3989
492.1687	493.9164	507.2912
511.4299	515.3871	524.0407
529.2370	537.1476	542.6068
550.3159	554.8108	565.6249
566.4408	571.9391	577.1893
580.6924	593.1502	604.1201
610.6789	615.3238	619.2494
627.1883	639.1624	640.5199
656.3420	665.6626	671.9109
675.9965	688.7109	690.0549
696.8160	697.7623	703.1844
710.6072	714.4474	717.2506
720.3163	724.4959	732.4361
736.1105	739.5857	743.7511
745.0514	745.7839	747.2214
750.5864	755.6006	757.9202

760.7546	765.6979	770.6838
779.2738	780.4101	785.4037
787.5582	791.3568	794.7553
796.3165	804.8369	808.2745
824.6620	829.5682	839.1581
850.8164	869.8744	880.9565
886.3625	898.1867	920.9964
935.4814	946.9404	963.1964
972.7049	983.8736	986.6225
988.3594	990.4224	1027.5543
1034.3794	1043.1346	1054.6061
1074.6124	1090.0014	1093.0928
1108.7852	1126.7800	1137.8449
1140.5917	1149.6751	1164.3345
1178.5190	1181.7645	1189.9750
1199.2789	1202.3263	1206.2586
1213.9181	1227.5123	1228.4013
1234.5948	1239.8148	1247.1845
1253.0712	1260.7062	1267.4761
1270.8830	1279.5010	1286.5333
1300.2328	1302.9963	1311.4548
1322.3395	1328.9723	1336.6600
1337.8737	1345.9516	1347.7598
1352.5811	1355.0918	1362.2063
1364.6109	1366.3497	1375.0363
1377.3799	1384.4749	1393.0183
1404.4138	1417.6649	1426.0827
1432.5143	1439.6524	1441.9589
1446.3256	1449.9249	1454.2138
1458.7314	1466.4593	1477.3111
1486.3776	1492.5454	1494.3527
1499.3495	1537.0848	1547.2038
1554.0616	1561.5775	1576.3886
1587.3815	1594.6345	1596.3569
1600.4762	1600.7702	1607.4797
1615.7964	1625.0145	1629.7637
1649.1899	1652.8345	1666.6075
2937.1829	3179.6087	3181.2924
3186.0147	3200.3723	3200.9344
3201.8396	3297.5891	3303.0150
ZeroEnergy[kcal/mol] -14.2		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		

!-----h_c60h8_p1-----

Bimolecular p1

Fragment c60h8

RRHO

Geometry[angstrom] 68

C	3.5814460698	0.4212524315	-1.7075100877
C	3.0373882532	-0.3302434089	-2.8260760796
C	2.8120162156	-1.6960049178	-2.3834215038
C	3.2569205369	-1.7996582089	-1.0088772922
C	3.7337161544	-0.4876373431	-0.5900507154
C	3.4734199997	-0.0473174109	0.7008750368
C	3.0093995034	1.3008519918	0.9375150217
C	2.8202401129	2.1674184611	-0.1316023622
C	3.1551049964	1.7349996811	-1.4783473163
C	1.6601093443	-2.3789977519	-2.7916857995
C	0.8889430285	-3.1470498153	-1.8281818049
C	1.3470977616	-3.2739632515	-0.5228589027
C	2.5503255218	-2.5876580028	-0.1100944164
C	2.1341614325	0.2779785761	-3.7030501123
C	0.969445126	-0.4538009008	-4.1667158715
C	0.7289806835	-1.7466728565	-3.6958419403
C	2.7963467065	-0.8932806021	1.6587496475
C	2.3362191768	-2.1593051853	1.2545472003
C	2.220918591	2.3587300528	-2.3852050561
C	1.7369601392	1.6581370665	-3.4925133899
C	0.3409122288	1.7909452208	-3.8727306379
C	-0.5016680458	2.6329317587	-3.1453661286
C	-0.0069817214	3.3062250027	-1.9483957932
C	1.3139720328	3.1649136912	-1.5828004093
C	2.0818204121	1.3002940085	2.0336316742
C	0.9938558182	2.1577406643	2.0021080682
C	0.6492259747	2.9433148904	0.8355763903
C	1.638430774	2.9966653057	-0.1858911303
C	1.0954928935	-2.6537125899	1.7433118282
C	0.5230819147	-2.0126636813	2.8486572001
C	0.9851076565	-0.7412019755	3.2545198531
C	2.0205215321	-0.1085052758	2.5559335663
C	-0.5179785415	-2.9375244913	-2.0803152577
C	-1.4562112701	-2.8503046131	-1.0139535951
C	-0.9420293532	-3.1689994051	0.3014022732
C	0.4122619186	-3.2942346311	0.5667573094
C	-0.1344716221	0.482797154	-4.2903345424
C	-1.4293959173	0.0800127638	-3.9603045321
C	-1.6622267798	-1.2486557372	-3.4025251678
C	-0.6095456529	-2.1281581751	-3.2725785375
C	-2.9735567503	2.0458191318	0.6023663156

C -3.5146135867 0.8025215071 1.0841095695
 C -3.7308439497 -0.0386769278 -0.062969614
 C -3.5923807231 0.7670286853 -1.2280189711
 C -3.1202046009 2.0668088477 -0.8131125637
 C -2.2200484596 2.7639929644 -1.5789926862
 C -1.041530713 3.3250625845 -0.9341349963
 C -0.7814745304 3.161461146 0.4587978938
 C -1.904746252 2.6451386205 1.2887508573
 C -3.3729936003 -1.3954003128 -0.0010061723
 C -2.6381096959 -1.9480280899 -1.1724208385
 C -2.6770533688 -1.175825334 -2.3709079176
 C -3.1517066921 0.2003446387 -2.3974085372
 C -3.2355364974 0.299053801 2.3432194451
 C -3.4240776418 -1.1241710758 2.4731890294
 C -3.4634678994 -1.9293040919 1.3486993466
 C -1.8658891915 2.2532724337 -2.8895248715
 C -2.3260946422 0.9868309249 -3.2937795135
 C -1.9151980716 2.3312304379 2.7089122095
 C -2.5699151352 1.226525094 3.2236572143
 H 0.2332802659 1.9946974653 2.7470740199
 H -0.4109096066 -2.3715562965 3.2733375895
 H 0.3825614504 -0.1879883388 3.9703374378
 H -1.5836533336 -3.0050814278 1.1508172505
 H -3.4352574052 -1.5903543251 3.4557412484
 H -3.5304209518 -3.0040459036 1.4905814263
 H -1.3615895997 2.9645810002 3.3959946963
 H -2.4892554231 1.0143113515 4.2872894456

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 198

79.7816	100.5141	165.5555
201.3762	211.1526	250.2115
264.6655	267.3477	277.5297
283.3047	291.2467	298.0229
318.4177	329.6539	342.5225
361.2981	365.0449	368.4663
380.9888	385.6625	403.8892
407.5628	415.5775	418.0100
424.0256	425.9091	437.3820
452.9996	471.6523	473.2992
475.7015	484.5969	490.2278
501.0167	503.2412	510.3352
518.2701	521.6461	531.1820
534.8956	542.7981	550.4836
556.4287	561.5764	569.0201

573.6884	576.4098	584.5894
587.9727	597.5328	613.4995
614.6781	618.5241	623.9507
629.7916	642.2221	648.7577
662.2145	673.4343	678.3934
682.9907	692.3937	700.6172
701.2346	705.1744	714.4586
718.6868	721.0813	721.5727
730.8636	733.5304	737.3871
738.6848	742.8069	745.0523
745.0661	747.5421	751.1273
757.1007	757.3508	760.5498
764.9762	768.0021	768.8216
778.7928	779.6644	786.9969
788.4411	793.5351	796.7201
807.4084	811.3032	818.6917
831.9017	832.4837	842.5350
865.3880	882.8797	886.1339
899.2334	901.5106	946.9013
957.2653	959.5391	968.0083
978.9484	987.5979	991.1297
995.3028	1010.4326	1039.3747
1041.3993	1076.0798	1090.3073
1096.6159	1100.9444	1115.2641
1127.4908	1133.6020	1144.9542
1165.0822	1167.0195	1183.4316
1185.9917	1191.4181	1194.8757
1203.9107	1217.4621	1227.9490
1231.1761	1239.8074	1245.0602
1257.4137	1264.0021	1270.4198
1273.3314	1273.4887	1283.3484
1295.9058	1301.2787	1305.8753
1314.4985	1322.4504	1330.7881
1337.3471	1347.1186	1347.2512
1350.8156	1353.0500	1357.0473
1361.4558	1364.8004	1368.2763
1372.7354	1375.2774	1385.9014
1389.1122	1426.5704	1426.8214
1434.5556	1438.6800	1441.9566
1449.2410	1451.0564	1453.9940
1456.3289	1471.7607	1472.0068
1478.8673	1490.4204	1493.7278
1495.6629	1508.6417	1538.8539
1549.7864	1559.3303	1566.9406
1580.5970	1590.8105	1597.1547
1599.6647	1608.7142	1612.0987

1620.5955	1624.6108	1626.9170
1636.4849	1637.0495	1651.6270
1671.4556	3180.7926	3182.2477
3185.0950	3200.9116	3200.9145
3201.5235	3298.5309	3298.6530

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] 10.9
 End
 !-----bar_ts1-----
 Barrier ts1 ip1 ip2
 RRHO
 Geometry[angstrom] 69
 C 3.6176607087 -0.0553925392 -1.6883482236
 C 3.0574235091 -0.8035269939 -2.7948723576
 C 2.8122310591 -2.1626824278 -2.3412114859
 C 3.2547952677 -2.2578657881 -0.9632344564
 C 3.760080692 -0.9569770237 -0.5613906007
 C 3.5132334736 -0.4959524243 0.7262631871
 C 3.1108910088 0.8626391238 0.9589729247
 C 2.942843296 1.7268033072 -0.1210515694
 C 3.2114843403 1.2625917844 -1.4637214561
 C 1.6484285753 -2.8281481217 -2.7409373598
 C 0.8649304893 -3.5752796551 -1.7706118802
 C 1.3126144435 -3.6814365136 -0.4584517408
 C 2.523766158 -3.0113976451 -0.0512893063
 C 2.1540754073 -0.1774395388 -3.6575187092
 C 0.9811652432 -0.8955373561 -4.1191607264
 C 0.726902176 -2.1878047331 -3.6505782334
 C 2.8082586948 -1.300007902 1.6959916657
 C 2.3102193122 -2.5516754107 1.3039018127
 C 2.2599311148 1.9064407753 -2.3286902779
 C 1.7669436409 1.2048212507 -3.4299806882
 C 0.3782383394 1.3508047347 -3.794208026
 C -0.4394266762 2.186423493 -3.0297866939
 C 0.0579402593 2.8763792593 -1.8351819588
 C 1.4037942107 2.7667598953 -1.4984049552
 C 2.2451954175 0.9416850401 2.1044345208

C 1.4321029743 2.0574987693 2.2265987913
 C 1.202494595 2.9684855487 1.1151897414
 C 1.8941404495 2.6912357597 -0.121220039
 C 1.0490755284 -2.9978981413 1.7898134095
 C 0.4834083864 -2.3070106626 2.8674894694
 C 0.9934781342 -1.048280928 3.2681181503
 C 2.0738889137 -0.4694498383 2.5930150289
 C -0.5379333262 -3.3625002223 -2.0367922698
 C -1.4867231196 -3.2661485351 -0.9795330684
 C -0.9813179659 -3.5544647791 0.346620384
 C 0.3699766142 -3.6668058709 0.6256247407
 C -0.1121112404 0.0543845809 -4.2325721385
 C -1.4107119689 -0.3427773699 -3.9176671714
 C -1.6617084324 -1.6708042194 -3.3714091112
 C -0.6166302187 -2.5593024766 -3.2338161013
 C -3.0334885896 1.6113486781 0.6428322952
 C -3.5526807611 0.3584519097 1.1068224056
 C -3.7709736897 -0.4706053799 -0.0496603158
 C -3.6084116752 0.3473678721 -1.2055774902
 C -3.1402091612 1.644184899 -0.7731291037
 C -2.1964441955 2.3191704817 -1.5184369506
 C -1.0523353186 2.9233151404 -0.853664326
 C -0.9808281186 2.8801741695 0.5287264516
 C -1.9865887936 2.2450402308 1.3460604993
 C -3.4200652081 -1.8282956032 0.0045450241
 C -2.6698384131 -2.3735606661 -1.1571155154
 C -2.6885514563 -1.5933776224 -2.3518174206
 C -3.1501026634 -0.2144073397 -2.3714667664
 C -3.2473063308 -0.1577136789 2.3562636019
 C -3.4559170008 -1.5800792031 2.4793455666
 C -3.5185644041 -2.3742122247 1.3498789865
 C -1.811718996 1.8122513662 -2.8099686883
 C -2.2970393575 0.5680438482 -3.2464569112
 C -1.8959533063 1.8577701941 2.7403333994
 C -2.5253440869 0.7298853506 3.2335950044
 H 0.8161318963 2.1885451567 3.1091541541
 H 0.8671493314 3.9764277345 1.3367075134
 H -0.4749424371 -2.615428261 3.2769871685
 H 0.3993755934 -0.4613817408 3.9632017377
 H -1.6294525793 -3.3722099247 1.1866982097
 H -3.4650248851 -2.0527167015 3.4589309956
 H -3.5995336112 -3.4496328709 1.4805053133
 H -1.2725319267 2.4392336461 3.4118759185
 H -2.3709003401 0.4535653332 4.2742290214

Core RigidRotor

SymmetryFactor 0.5

End
 Tunneling Eckart
 ImaginaryFrequency[1/cm] 447.2786
 WellDepth[kcal/mol] 4.4
 WellDepth[kcal/mol] 18.6
 End
 Frequencies[1/cm] 200

69.0870	91.8096	
139.2973	182.4898	201.4167
227.9265	250.1416	254.6172
270.6458	279.7430	283.1199
308.5048	313.1677	318.2599
336.3270	357.0961	362.7622
365.9981	376.3624	378.6472
388.0537	400.0309	406.2552
409.7093	415.5234	425.6037
440.2907	450.7668	462.2624
468.0684	468.4251	471.5100
484.3349	492.1626	494.5450
501.8520	506.8903	514.2945
524.4841	526.7694	531.9942
543.9597	548.1076	551.7692
558.3367	563.8696	570.1879
575.0538	582.5299	592.2040
601.8911	609.5704	613.9659
618.5294	623.2781	638.4506
639.8306	643.3336	654.4686
658.8077	678.0067	678.3070
690.0725	699.2233	701.7002
703.5068	711.8210	715.6674
716.3094	719.5599	722.4288
731.2424	735.9134	737.6646
742.2195	744.3896	746.2298
748.3093	748.5563	756.6400
758.8226	759.6201	765.4746
768.6217	771.6796	777.8060
784.4133	786.5184	788.9953
790.2430	798.9702	803.5075
815.8080	825.1125	829.4868
833.0357	849.2829	858.5617
882.0053	890.2907	900.8528
917.6514	945.1274	949.5819
960.6190	967.7157	969.5757
989.7011	990.0567	998.9769
1026.1913	1032.0371	1042.0720
1067.2332	1086.3325	1088.3692

1094.5075	1103.1331	1120.5869
1135.5926	1141.2600	1155.8787
1163.8466	1175.5291	1180.7838
1188.9884	1196.3760	1205.9491
1218.9692	1219.6232	1229.8815
1233.8543	1241.1176	1248.1886
1258.5941	1267.2727	1269.9837
1274.9279	1289.5444	1295.4014
1302.0088	1307.2792	1312.2514
1317.1134	1325.9766	1337.2525
1347.0975	1347.8119	1353.8084
1355.9674	1361.6939	1364.9995
1369.3328	1375.5375	1379.2884
1381.1772	1389.0325	1396.0714
1416.2435	1425.7724	1429.1505
1437.9322	1440.6645	1445.8247
1448.7549	1453.4350	1454.7810
1461.8184	1472.3990	1477.5491
1487.6315	1491.4384	1494.4631
1506.8977	1533.7794	1542.1629
1553.6227	1561.7177	1569.8007
1582.6951	1586.9121	1597.3048
1598.1152	1608.8103	1609.9725
1615.1576	1620.5228	1625.1932
1633.3553	1648.1036	1662.8568
3179.8502	3181.6236	3188.7378
3192.0030	3199.3874	3204.9246
3209.8066	3228.3315	3301.2889

ZeroEnergy[kcal/mol] 4.4
 ElectronicLevels[1/cm] 1
 0 2
 End
 !-----
 !-----bar_ts2-----
 Barrier ts2 ip2 p1
 RRHO
 Geometry[angstrom] 69
 C 3.580642512 -0.0702830102 -1.7089029628
 C 3.0378982625 -0.8230981924 -2.8269878843
 C 2.8127273951 -2.1885761183 -2.3831087591
 C 3.2563236618 -2.2900111478 -1.0077986375
 C 3.7318267177 -0.9776360768 -0.5907130387
 C 3.4668307726 -0.5346116868 0.6992413973
 C 3.0036323025 0.8118206012 0.9323038355
 C 2.8196144378 1.6805744254 -0.1361158602
 C 3.1551914153 1.2442520302 -1.4819523987

C 1.6611501519 -2.8721497393 -2.7911211357
 C 0.8900611461 -3.6400430992 -1.82740276
 C 1.3476826496 -3.765874814 -0.5216752715
 C 2.5491359405 -3.0774488837 -0.1086176191
 C 2.1347497134 -0.2157104494 -3.7044692179
 C 0.9700893928 -0.9479418282 -4.1675391643
 C 0.7298392225 -2.2405100439 -3.6958394755
 C 2.7879995659 -1.3794983913 1.6572989876
 C 2.3323087856 -2.6475838283 1.255274257
 C 2.2218411422 1.8668039143 -2.388938696
 C 1.7374540595 1.1645353136 -3.4949239688
 C 0.341672846 1.2968355504 -3.875101082
 C -0.5002876532 2.1395427702 -3.1469085213
 C -0.0052329637 2.8143851353 -1.9523885313
 C 1.3167387225 2.6766527673 -1.5867658072
 C 2.0717846871 0.8130498426 2.028586485
 C 0.9972095111 1.6787485478 2.0047229388
 C 0.6629964957 2.5094514896 0.851399445
 C 1.6461167931 2.5184795725 -0.1919183282
 C 1.0926223848 -3.144141508 1.7438284529
 C 0.5175976398 -2.5025002158 2.8476994024
 C 0.9753884655 -1.2288553779 3.2512294938
 C 2.0099552035 -0.5952850679 2.552342587
 C -0.5167829068 -3.4313244105 -2.0799998049
 C -1.4554674389 -3.3447300697 -1.0135893677
 C -0.9420817445 -3.6647724943 0.301440698
 C 0.4122290327 -3.7876010526 0.5675417578
 C -0.1339731353 -0.0113571048 -4.2911491848
 C -1.4286831904 -0.4143969558 -3.9599333716
 C -1.6613186796 -1.742481249 -3.4015963733
 C -0.608564635 -2.6221205249 -3.2720346858
 C -2.9691185257 1.554094032 0.6014966922
 C -3.5083275862 0.3109076484 1.0850978731
 C -3.7271269732 -0.5313475426 -0.0608083874
 C -3.5907809915 0.273637528 -1.226607719
 C -3.1184093798 1.5738170458 -0.812758226
 C -2.2177788202 2.2692861981 -1.5794359776
 C -1.0400883918 2.8309222674 -0.935639351
 C -0.7828058948 2.6748801707 0.4546967026
 C -1.8993080032 2.1557466921 1.286061288
 C -3.3696568607 -1.8880516795 0.0015752351
 C -2.636723655 -2.4416968697 -1.1708993874
 C -2.6758602617 -1.6693842879 -2.3694057807
 C -3.1504299816 -0.2933813801 -2.3959421488
 C -3.2271376813 -0.1906140779 2.3442884997
 C -3.4155546802 -1.6137058141 2.4759191194

C -3.4578402122 -2.420128078 1.3523327413
 C -1.8641539387 1.75869277 -2.8896441216
 C -2.3250498536 0.4926922258 -3.2932497743
 C -1.909811789 1.8445836094 2.7076449738
 C -2.5625616859 0.7395274993 3.2234426311
 H 0.2376992879 1.5295380218 2.753194893
 H 0.9099216357 4.3221308106 1.7254670255
 H -0.4153924803 -2.8634667883 3.2727004726
 H 0.3713266176 -0.6758588287 3.9658602178
 H -1.5844788594 -3.5028985377 1.1505528227
 H -3.4256510925 -2.0789286553 3.4589310025
 H -3.5261656088 -3.494558075 1.4958661715
 H -1.3610837852 2.4832038293 3.3937092663
 H -2.4835552302 0.5301246466 4.2877454154

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 612.9129

WellDepth[kcal/mol] 33.2

WellDepth[kcal/mol] 8.2

End

Frequencies[1/cm] 200

79.4482	99.2729	
165.1234	199.8749	210.0147
244.1352	260.1545	266.6652
272.0946	278.8460	283.1437
290.2073	298.8325	303.7231
317.8206	329.5845	341.6158
362.9582	365.3183	368.3428
380.8849	386.1083	403.7232
406.8876	415.4271	418.6182
424.5155	426.9045	436.4660
452.9941	470.7625	474.3940
475.4325	484.1100	490.0106
499.9292	502.7787	510.3975
518.4240	521.5388	530.8641
534.6004	542.0779	549.7841
556.1359	561.6257	569.3241
573.6182	576.5672	583.6557
587.4400	597.3568	613.0736
614.3892	618.1634	622.8829
629.1328	642.1872	647.8291
662.1712	673.5055	678.1022
682.5662	692.2224	700.1654
700.9930	704.5255	714.1631

718.9422	720.6438	721.2427
730.0911	733.0053	737.3682
738.9000	742.8783	745.1566
745.2632	747.3219	751.1550
755.8430	756.5341	760.7175
764.7038	768.2124	768.4923
778.9160	779.4958	787.2139
788.3683	793.5568	796.8945
807.3324	809.5236	817.4938
831.6682	832.0010	843.2177
864.4467	882.4451	885.8438
897.5477	900.9276	945.1283
956.4568	957.6853	966.8490
978.3527	988.2268	991.5795
994.9096	1009.1396	1039.1991
1041.5849	1074.2138	1090.5484
1092.2144	1100.4658	1115.0901
1125.5287	1133.6299	1144.4788
1161.3858	1166.4741	1181.0946
1185.1516	1189.8618	1194.5923
1204.1350	1216.9585	1228.2312
1229.4663	1239.7903	1244.6943
1257.0025	1263.3901	1266.4750
1272.9679	1273.7174	1282.4748
1295.1785	1299.9393	1305.0423
1314.2321	1322.2670	1330.8729
1337.3110	1344.8660	1347.3388
1351.3118	1353.5155	1356.2797
1361.3143	1364.8466	1367.6433
1373.0976	1375.7473	1385.8726
1389.3593	1426.6693	1427.0602
1434.9623	1435.9934	1441.4411
1449.0194	1450.8992	1453.8219
1454.1863	1471.0335	1471.7448
1479.7437	1488.9866	1493.3959
1494.8567	1507.6663	1537.2279
1547.9185	1560.2385	1565.5761
1579.9549	1588.8803	1596.8342
1598.6260	1608.3777	1610.9115
1619.1211	1623.1439	1626.3670
1634.3042	1636.1986	1651.8029
1671.4946	3180.9135	3182.2627
3185.8491	3201.0965	3201.6594
3202.1048	3299.6592	3303.5924

ZeroEnergy[kcal/mol] 19.1

ElectronicLevels[1/cm] 1

0 2

End

!-----

End

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H₇

```

!TemperatureList[K]          700. 800. 900. 1000. 1100. 1200. 1300. 1400. 1500. 1600.
1700. 1800. 1900. 2000.
TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650.
1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
!TemperatureList[K]          300 500. 1000 1500. 2000
!TemperatureList[K]          300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
!PressureList[bar]           0.1
!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature    0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature   100
ModelEnergyLimit[kcal/mol]    900
WellCutoff                    10
ChemicalEigenvalueMax         0.2
ChemicalEigenvalueMin         1.e-6      #only for direct diagonalization method
CalculationMethod             direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput              eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber            0
!ReductionNumber              5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                260 ! Frenklach
! Power                        0.
Factor[1/cm]                  247 ! Jasper universal
Power                          0.85
! Factor[1/cm]                424 ! Jasper calc N2
! Power                        0.62
! Factor[1/cm]                125 ! SJK guess
! Power                        0.85
ExponentCutoff                15
End
CollisionFrequency

```

```

LennardJones
!Epsilons[1/cm]      203.0 203.0 ! N2 pyrene-Frenklach
!Sigmas[angstrom]    4.6 4.6 ! N2 pyrene-Frenklach
!   Epsilons[1/cm]    206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
!   Sigmas[angstrom]  5.06 5.06 ! N2 Jasper extrapolation to C16
!   Epsilons[1/cm]    32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
!   Sigmas[angstrom]  3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
!   Epsilons[1/cm]    101.5 1179.325206
!   Sigmas[angstrom]  3.6154 10.85479223
!   Epsilons[1/cm]    390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Sigmas[angstrom]  4.46 4.46 ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Epsilons[1/cm]    189. 216.0 ! N2 , CH2CCH ! from Jasper calc
!   Sigmas[angstrom]  3.30 4.11 ! N2 , CH2CCH ! from Jasper calc
Masses[amu]          28. 727.
End
OutputTemperatureStep[K] 100
OutputTemperatureSize 20
OutputReferenceEnergy[kcal/mol] 0.
!-----
!-----well_ip1-----
Well      ip1
Species
RRHO
Geometry[angstrom] 67
C 3.5774504004 0.4046810366 -1.7003449598
C 3.0314630293 -0.3508762953 -2.8156078917
C 2.8006991944 -1.7131335199 -2.3661742553
C 3.2404326431 -1.8096678762 -0.9891048679
C 3.720988237 -0.4976073744 -0.5764707945
C 3.4560513303 -0.0484311153 0.7108889614
C 3.0010387327 1.303014787 0.9395093327
C 2.8300984427 2.1663345562 -0.1354658623
C 3.1600582134 1.7223775122 -1.4801466892
C 1.6482486295 -2.3953546755 -2.7746241319
C 0.8719297959 -3.1576441923 -1.8107688082
C 1.3228614747 -3.2737032889 -0.5016355367
C 2.5249583578 -2.5867166753 -0.0880724327
C 2.1313560187 0.2556657864 -3.697210295
C 0.9653755419 -0.4748578862 -4.1592486498
C 0.7212240045 -1.7654666871 -3.6844954311
C 2.7715322002 -0.8826711722 1.6721159853
C 2.3055943784 -2.1474697103 1.2722880371
C 2.2261777089 2.3430371612 -2.390724846
C 1.7378878306 1.637901458 -3.4931270754
C 0.3411450493 1.7716595404 -3.8715814015

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C -0.4998672853 2.6162114611 -3.1451142704
 C -2.36144E-5 3.2961963846 -1.9549649453
 C 1.3226665299 3.1566042791 -1.5926918755
 C 2.0793884936 1.3219229396 2.0437531955
 C 1.0178082731 2.2146899576 2.0204232313
 C 0.674671855 2.9618698905 0.8300372747
 C 1.6553238181 3.0024688487 -0.1965476486
 C 1.0601223835 -2.6329001231 1.7581169839
 C 0.4874862569 -1.9802419555 2.856352131
 C 0.9590896231 -0.7110001299 3.2618637081
 C 2.0027591431 -0.0872078531 2.5677367391
 C -0.5337075306 -2.9523227421 -2.0726487759
 C -1.4787388859 -2.8652908978 -1.0131369118
 C -0.9701424485 -3.1699684517 0.3084895538
 C 0.382890236 -3.2849687372 0.5833753101
 C -0.136668964 0.4637263159 -4.2860123519
 C -1.4333593504 0.0643626452 -3.9590249415
 C -1.6712317247 -1.2643048289 -3.4039667147
 C -0.6198546637 -2.145136499 -3.2674537216
 C -2.9623716003 2.013109039 0.6167575141
 C -3.5050884619 0.7656827182 1.0917965393
 C -3.7429710218 -0.059714093 -0.0642172867
 C -3.5967243439 0.7532930037 -1.2234338024
 C -3.1155301372 2.0490393826 -0.8004885933
 C -2.2116994289 2.742284015 -1.5693174086
 C -1.029619901 3.3098054526 -0.9358754957
 C -0.7528124896 3.1416246865 0.4489915961
 C -1.8525038017 2.5908474903 1.281099475
 C -3.4059727209 -1.4225875912 -0.0184183412
 C -2.6632071231 -1.9687038495 -1.1841570361
 C -2.6916590602 -1.1907169877 -2.3780917882
 C -3.1582195832 0.1881655765 -2.3961457728
 C -3.2061239649 0.2257633521 2.335562907
 C -3.4391912193 -1.1917764583 2.4542243859
 C -3.5071045274 -1.978327373 1.3203069624
 C -1.8633816071 2.2359008261 -2.8828508045
 C -2.3279753286 0.9725557242 -3.290101075
 C -1.8207534236 2.1582658512 2.6330499118
 C -2.4464102348 1.0954018245 3.2121799382
 H 0.261735916 2.1328235093 2.7946546876
 H -0.451793469 -2.3289491743 3.2778226139
 H 0.3578926095 -0.1510525281 3.9728811601
 H -1.6172091314 -3.0016489519 1.1527444372
 H -3.4515883904 -1.6673675034 3.4320488745
 H -3.5948616235 -3.0541764866 1.4429527356
 H -2.2960252902 0.8452676723 4.2604113082

Core RigidRotor
SymmetryFactor 0.5
End

Frequencies[1/cm] 195

80.0745	96.8702	159.3939
190.4355	210.6780	253.7009
260.5368	270.7580	274.3240
283.2402	291.4066	301.3435
322.1035	328.1628	338.9070
362.8187	365.7062	369.5312
380.4736	385.3234	400.5151
406.7627	413.3454	415.8153
424.1172	426.5580	437.7193
452.7403	463.4677	474.6099
476.1733	485.8435	489.6838
497.0444	502.1981	509.8453
517.3566	522.1792	531.7328
533.4937	541.5178	550.3382
554.6016	559.8831	567.4602
570.9482	576.4815	582.8818
585.7854	594.8791	611.0291
613.9403	618.3192	622.5411
623.4936	633.2839	646.0373
661.6333	672.5435	680.6543
681.6947	694.0987	697.2021
702.8334	704.8908	714.2485
718.4743	720.7775	721.1518
729.4345	733.1477	736.0532
738.6939	742.3569	743.6829
744.5984	748.8870	750.9398
756.1486	757.3542	760.3507
764.7539	766.7004	767.9376
774.8629	778.3487	779.1580
786.5940	787.1793	798.3547
805.0801	808.4910	816.1627
825.8438	831.9416	846.1227
865.7044	880.7085	891.7296
899.2295	915.2819	945.1672
950.5872	959.0426	965.9102
979.7371	989.6764	992.3946
1008.8012	1038.2463	1039.8150
1072.9654	1090.6101	1098.6863
1100.0729	1113.4070	1128.0694
1133.6715	1145.5173	1165.6105
1169.7910	1180.8737	1190.4728
1190.8819	1194.1327	1201.7533

1221.5860	1225.7269	1231.2070
1238.4908	1251.0658	1259.2297
1263.4639	1271.0743	1272.8502
1283.7220	1294.8522	1297.6143
1305.9942	1310.8348	1321.7501
1327.3549	1334.6116	1339.0956
1342.8730	1346.1453	1349.3050
1356.7797	1360.0704	1361.6772
1366.0717	1370.8438	1374.3447
1381.4665	1388.5045	1392.0385
1421.8688	1427.1231	1429.2560
1433.2142	1444.3505	1448.0991
1451.3756	1451.9015	1468.0333
1470.9401	1471.3067	1485.3048
1489.9122	1494.5346	1507.8872
1521.0798	1544.4352	1555.9026
1566.4203	1570.8906	1581.9230
1592.6208	1596.4915	1608.2314
1611.7671	1618.5786	1622.9501
1623.8522	1634.3613	1634.9013
1642.2674	1662.7842	3170.8056
3177.9430	3182.7322	3186.5703
3200.5213	3203.8513	3298.8879
ZeroEnergy[kcal/mol] 0.00		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----well_ip2-----		
Well ip2		
Species		
RRHO		
Geometry[angstrom] 67		
C	3.5036460867	0.4080146228 -1.5736301929
C	3.0121910721	-0.3407169802 -2.7173065579
C	2.781398007	-1.7108265254 -2.289786793
C	3.1749823784	-1.8134054823 -0.8974162255
C	3.5868397314	-0.489463848 -0.4513542794
C	3.2017115505	-0.0523735483 0.816594557
C	2.6543989284	1.2680248081 1.0305948734
C	2.6669134297	2.1582217457 -0.0377830355
C	3.0723573835	1.7243276982 -1.3568546845
C	1.6462458124	-2.3977598014 -2.7356543647
C	0.8571359621	-3.1855141387 -1.8029208944
C	1.287179227	-3.3402739902 -0.4925619284

C 2.4576550386 -2.6289444508 -0.0358479671
 C 2.1377858946 0.2665172948 -3.6224158681
 C 0.9833935704 -0.4630702175 -4.1120193474
 C 0.7309785981 -1.7566714871 -3.6529712942
 C 2.512047717 -0.9199511227 1.7170174678
 C 2.1690852422 -2.2140956081 1.3191137285
 C 2.1950002879 2.3624740205 -2.3193034049
 C 1.7406691848 1.6519523022 -3.4345239306
 C 0.3558084538 1.7881373976 -3.863227928
 C -0.502016841 2.6685441089 -3.2022381971
 C -0.0189490013 3.4204751469 -2.0505832721
 C 1.2886650145 3.2384844138 -1.5966823733
 C 1.6161710688 1.2054938665 2.0636230757
 C 0.5475481625 2.3484113804 2.1178594871
 C 0.5500114155 3.1309970037 0.7574207335
 C 1.5647755006 3.1020886558 -0.1817070113
 C 0.949800898 -2.7987276003 1.7762627806
 C 0.378005828 -2.2383392161 2.9433133222
 C 0.7295588628 -0.9479066298 3.3464370512
 C 1.6123373772 -0.1525225453 2.5503177989
 C -0.5464882661 -2.9633359371 -2.0771756076
 C -1.5021454374 -2.8982526761 -1.0258624312
 C -1.0282661347 -3.3031396626 0.2765846378
 C 0.3263949792 -3.415144799 0.5754835407
 C -0.1154287947 0.4758701851 -4.2610035233
 C -1.4176192725 0.0803825743 -3.9414954977
 C -1.6606643104 -1.2406056473 -3.3843274849
 C -0.6141109481 -2.1318743684 -3.2523209954
 C -2.8608631571 2.0793787438 0.6133540413
 C -3.3042124382 0.8255718489 1.1167341487
 C -3.6539029335 -0.0034017747 -0.0174534112
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 C -3.0964752745 2.1288117362 -0.8119973969
 C -2.2453131362 2.8357999487 -1.6462177341
 C -1.0777757678 3.499664363 -1.0862361515
 C -0.7782945386 3.3316290427 0.2795279269
 C -1.6742180393 2.6011168445 1.1315007052
 C -3.3348921984 -1.3705768314 0.0181572423
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 C -3.0914193297 -1.1176080076 2.4720814481
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 C -1.8738010509 2.2802785883 -2.9333904143
 C -2.317981321 0.9971758749 -3.2898135671

C -0.9815974732 1.9633288206 2.2085299411
 C -1.6378337966 0.945647531 2.8884009048
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 H -3.5529311301 -2.9627040308 1.5313834146
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Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 195

97.2668	135.4723	184.5160
237.3581	245.6219	263.7316
272.8484	281.9851	285.6106
302.9785	314.2972	316.3729
331.8982	332.3059	353.9690
361.0829	371.9934	380.6967
392.2994	400.8964	404.0229
406.1494	420.1469	424.7267
433.5516	439.7337	449.5094
455.7790	469.7876	473.2117
488.5663	494.1160	500.9998
503.1903	507.3455	519.1915
520.1199	531.5084	537.9901
544.2739	547.8094	549.8523
557.8586	561.9198	568.1213
572.0608	575.9582	579.4718
587.1541	609.6898	611.2023
622.9925	629.6237	632.9551
635.8672	653.5353	662.6995
670.9168	675.3026	682.1039
689.6005	695.7156	701.1847
703.7344	713.1224	713.8352
717.1020	721.3753	723.1863
729.1735	732.5883	738.6738
739.1080	743.0958	744.6283
747.7372	749.3343	751.5149
755.9468	758.8295	760.6253
761.6025	763.7705	771.5286
774.0141	782.2481	784.7692
787.8389	796.3185	799.7996
806.2043	813.1108	818.3711
830.4702	849.4959	864.9233
880.6593	892.7897	895.5491

925.6387	943.3861	949.0842
959.5197	975.0196	982.1721
990.8688	996.6333	1008.2465
1019.4323	1046.4860	1061.8579
1068.5733	1086.8156	1103.4901
1106.8974	1119.5657	1122.3600
1139.7263	1154.1168	1162.6526
1168.7934	1181.2674	1192.2786
1196.2861	1203.3802	1205.2440
1208.5697	1224.7698	1230.1028
1233.7995	1241.5118	1256.3814
1263.8705	1265.2783	1271.1203
1273.2730	1279.6566	1291.1395
1298.0341	1306.1600	1318.9279
1323.1880	1325.5881	1330.1290
1339.1625	1341.0756	1346.6419
1351.8716	1356.2013	1359.2224
1363.4219	1368.6178	1370.4753
1380.4231	1385.8301	1403.4160
1407.7904	1416.0016	1425.6686
1430.6513	1435.0808	1443.1992
1453.1750	1455.8873	1462.3311
1470.3576	1471.7812	1476.4147
1482.4137	1499.0515	1500.7759
1528.1698	1531.5583	1537.7019
1546.4539	1561.9464	1569.0582
1578.1862	1587.2771	1593.8984
1604.2392	1605.6663	1611.5025
1613.7085	1617.0304	1629.0789
1629.9468	1643.1550	2988.5386
3181.1905	3189.3798	3198.8648
3228.4234	3298.6443	3322.6509
ZeroEnergy[kcal/mol] -18.9		
ElectronicLevels[1/cm] 1		
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End		
End		
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Bimolecular p1		
Fragment c60h6		
RRHO		
Geometry[angstrom] 66		
C	3.6032450435	-0.1857747035 -1.6834027151
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C	2.7661046612	-2.2687852335 -2.3689665298

C 3.202802745 -2.3980157938 -0.9907157999
 C 3.7559879761 -1.1243136921 -0.5765639189
 C 3.574985519 -0.6834406829 0.7242039895
 C 3.300855852 0.7062931288 1.0091166956
 C 3.0802693451 1.5860596401 -0.0610339106
 C 3.2166795022 1.1256795266 -1.4137799145
 C 1.6163967034 -2.9304850331 -2.8046187196
 C 0.8457610291 -3.7305715962 -1.8693929359
 C 1.2380230418 -3.8078243282 -0.5324039286
 C 2.4390858094 -3.1438976416 -0.0822181889
 C 2.0897281758 -0.2368146592 -3.603381595
 C 0.9157881379 -0.9384561798 -4.0856935286
 C 0.6834686146 -2.2621999911 -3.6965171251
 C 2.7945308959 -1.4503900583 1.6665662666
 C 2.1898407086 -2.6314921169 1.2543798845
 C 2.2068330933 1.7988522614 -2.1923066593
 C 1.6955597618 1.1316174654 -3.3015047407
 C 0.304027353 1.2799936761 -3.6151850633
 C -0.4900324843 2.0723269234 -2.7873184944
 C 0.0175527923 2.7755352681 -1.5887233101
 C 1.3952524818 2.6556699212 -1.2989679376
 C 2.5344268802 0.84018281 2.1967840627
 C 1.931000063 2.0840956249 2.4189745579
 C 1.7393820826 2.9803064174 1.3411720985
 C 2.0955825662 2.6073752493 0.0319251562
 C 0.8096744906 -2.8892129304 1.601900274
 C 0.0530378907 -1.9537234754 2.3564700023
 C 0.8099740982 -0.8677997134 2.9472077722
 C 2.1016525349 -0.5566181145 2.5520294772
 C -0.5602365261 -3.5799253359 -2.1999897117
 C -1.5109822783 -3.511017345 -1.1799355463
 C -1.0872251394 -3.5137722552 0.213287404
 C 0.246602696 -3.6669974425 0.5230932509
 C -0.1852756805 0.0087882481 -4.1296111939
 C -1.4798948065 -0.4129234525 -3.8420291632
 C -1.7267005224 -1.7897419444 -3.4301938815
 C -0.661956673 -2.6871089916 -3.3409706521
 C -2.922231601 1.3235726807 0.9083724657
 C -3.009027268 -0.0604177544 1.324826872
 C -3.412694434 -0.8266125939 0.187123202
 C -3.5312625176 0.0554285818 -0.9583226252
 C -3.1285575567 1.3667294113 -0.5006980634
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 C -1.1701300284 2.8694074948 -0.6513137827
 C -1.2480710906 3.0818457956 0.7269388222
 C -2.0668961894 2.2227666273 1.5426450757

C -2.9192410705 -2.1069417417 0.0420050853
 C -2.633357115 -2.6139256376 -1.2874134648
 C -2.7503003593 -1.7690941378 -2.4027436068
 C -3.1738549456 -0.3935756789 -2.2203111621
 C -2.1270927773 -0.5262324235 2.3125879403
 C -1.4031312609 -1.7946358947 2.0410537775
 C -1.9088734652 -2.5895770111 0.9741917512
 C -1.8541040644 1.6580849371 -2.5699876884
 C -2.3478248586 0.4490092517 -3.0732787399
 C -1.7352385301 1.8462844926 2.9040627888
 C -1.7630707946 0.5192991253 3.2636742854
 H 1.4403245782 2.3124126694 3.3614969183
 H 1.216422393 3.9067092871 1.538079741
 H 0.2745929495 -0.0981089344 3.4733123022
 H -0.5369763042 3.7107614793 1.2341073584
 H -1.3578486317 2.5838669556 3.6082323984
 H -1.4539503604 0.2440657736 4.2677787319

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 192

102.1461	136.7746	194.2151
241.1727	248.7499	265.1039
278.4460	285.5548	293.7422
307.0664	318.0568	322.6346
333.6632	341.0923	360.0408
368.7150	377.2375	383.4361
398.8122	404.8228	409.0917
415.7469	422.4243	432.2135
441.4341	449.1003	455.6667
465.5570	472.2831	478.7783
498.2589	503.7174	507.5166
509.5807	516.9216	522.7833
525.8736	529.4925	538.8885
548.0125	552.9965	556.6437
559.8615	565.7739	571.5186
572.1128	578.6310	585.4851
595.5588	613.2919	615.6179
624.2761	629.4961	639.5686
646.7591	654.5977	672.0036
680.1397	687.5230	695.6162
702.9900	706.9972	712.0214
716.2411	716.6354	719.3394
721.4562	722.1994	729.2673
736.5467	741.1421	742.0943
742.6622	744.5843	746.7823

748.0494	750.9103	753.0578
756.7526	760.7404	763.3270
768.8921	770.5122	770.9583
777.5829	779.5203	786.9289
792.3628	795.7176	799.0969
805.6979	811.1872	830.2690
833.0479	850.7651	868.5089
880.4002	884.2417	897.1351
946.2470	956.3121	967.1236
974.2097	980.0391	984.4305
993.0442	997.0514	1012.9050
1038.7469	1058.9823	1082.9058
1087.7429	1096.0815	1106.6249
1110.2605	1131.5114	1135.8802
1147.3752	1168.6347	1177.1835
1179.6908	1190.1996	1199.2189
1206.0039	1207.4066	1219.5432
1227.8319	1233.4478	1249.5362
1259.2484	1264.9231	1267.3359
1270.0898	1280.7228	1287.5194
1301.0656	1304.0337	1317.4110
1321.6297	1322.5399	1334.8131
1336.0287	1342.0240	1346.6302
1353.0805	1357.0178	1363.1254
1364.4224	1365.8380	1368.5880
1376.8156	1382.1609	1393.5769
1402.2646	1414.3103	1425.8436
1429.7134	1441.4770	1442.0880
1446.9136	1450.9009	1462.8681
1465.1099	1470.4396	1470.7980
1476.8433	1485.7949	1496.9557
1507.3525	1537.2315	1540.3289
1552.5801	1563.9406	1575.0608
1579.5091	1589.8923	1592.0104
1604.6122	1608.7142	1614.4772
1616.2695	1619.2275	1624.6396
1627.0013	1633.6227	1644.8314
3182.0615	3191.0510	3200.3339
3236.9081	3317.3384	3321.6303
ZeroEnergy[kcal/mol]		0.0
ElectronicLevels[1/cm]		1
0 1		
End		
Fragment	H	
Atom		
Mass[amu]	1	

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ElectronicLevels[1/cm]      1
0 2
End
GroundEnergy[kcal/mol] 21.6
End
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RRHO
Geometry[angstrom] 67
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C 3.0558227748 -0.4053444511 -2.7590746324
C 2.8128050058 -1.7664435071 -2.3113183717
C 3.2343197223 -1.8630986097 -0.9272694449
C 3.7026894802 -0.5492636299 -0.5093433971
C 3.3901362214 -0.0958767087 0.7676366733
C 2.9044803197 1.2423317917 0.981047868
C 2.8353826017 2.1218389574 -0.0890202877
C 3.1834457565 1.6705518197 -1.42313754
C 1.6601991268 -2.4409373257 -2.7305612838
C 0.8717646699 -3.2025854734 -1.7764958973
C 1.3082796635 -3.3230332477 -0.4626004119
C 2.5041918229 -2.6359315559 -0.0349835746
C 2.1687230859 0.206899856 -3.6501271533
C 1.0004932133 -0.5146686949 -4.1190525397
C 0.7439171113 -1.8039870326 -3.6481723278
C 2.7035870995 -0.9242882138 1.7192079314
C 2.2610348344 -2.1926370949 1.320096648
C 2.2683475046 2.2993210019 -2.3501858976
C 1.7842011941 1.5941811477 -3.454261659
C 0.3905377881 1.738230363 -3.846645482
C -0.4498266738 2.6024626238 -3.1424268579
C 0.0546690638 3.3113522582 -1.9713324808
C 1.3718814709 3.1443657239 -1.5789485976
C 1.9760103653 1.2733408499 2.093716534
C 0.9952287767 2.3295500504 2.1317177364
C 0.7214926842 3.0219106958 0.8359532843
C 1.6922813185 3.007387437 -0.1771850092
C 1.0165999782 -2.6945565049 1.7971449737
C 0.4578607801 -2.0632998344 2.9184037409
C 0.916048696 -0.7924091022 3.3312675834
C 1.9189830765 -0.1214836777 2.6090869955
C -0.5308645875 -2.9902336376 -2.0530050809
C -1.4857991515 -2.9095103585 -1.0033750711
C -0.9941100353 -3.2345588185 0.3199066568
C 0.3571886617 -3.3431494316 0.613148407
C -0.0939433052 0.4323804523 -4.2534081322

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 C -1.6459546852 -1.2827753649 -3.3814633339
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 C -0.6668165619 3.1581168877 0.4083244416
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 C -3.3905307591 -1.4492802454 -0.0106118751
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 C -2.6713861493 -1.2027107709 -2.3602570187
 C -3.1188260244 0.1829737153 -2.3637327833
 C -2.9382514554 0.1303904772 2.3215521267
 C -3.280588 -1.2689521285 2.453525538
 C -3.4800045598 -2.0270419384 1.3226433557
 C -1.8160921888 2.223265151 -2.8673405469
 C -2.2854191541 0.9588009404 -3.262367528
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 C -1.9047993444 0.8170852383 3.0590899662
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 H -0.4556186299 -2.4427217641 3.3688044723
 H 0.3610376096 -0.2757205928 4.1043220179
 H -1.6528245677 -3.0891748628 1.1581275475
 H -3.2632601632 -1.7520891527 3.4277989839
 H -3.6449911639 -3.0958560397 1.4290488966
 H -1.5640818393 0.3981568579 4.0007931061
 Core RigidRotor
 SymmetryFactor 0.5
 End
 Tunneling Eckart
 ImaginaryFrequency[1/cm] 629.8407
 WellDepth[kcal/mol] 16.2
 WellDepth[kcal/mol] 35.0
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 Frequencies[1/cm] 194
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 175.9028 218.4104 232.0988
 258.6748 269.4521 282.6672
 286.7731 291.0432 309.9232
 327.3163 330.7379 341.9782
 351.0123 361.4769 368.6799
 378.9800 386.5633 395.9924

403.7548	410.2542	418.2747
425.4208	431.2359	437.3069
451.9109	457.1002	468.4749
477.6677	480.5751	488.8620
497.0151	502.5627	507.0392
513.1943	521.3190	524.4997
532.9693	538.3374	544.7448
549.9182	554.1482	561.2482
567.8168	569.0440	576.2355
578.2434	586.3652	604.8806
612.2351	616.5229	623.0898
628.1047	634.5590	635.8095
658.4180	670.0438	673.2999
675.4675	686.3345	691.6486
699.0277	705.7168	710.7808
713.2259	717.3790	720.5129
722.5995	728.6039	732.2431
736.6873	741.0483	743.0068
744.5942	746.1837	748.2467
750.2646	753.6910	757.7104
760.3652	761.5227	764.9865
769.9356	773.3503	776.1909
780.6258	786.4051	788.2581
797.5396	801.4335	808.7019
821.2417	825.2631	835.0301
866.2993	870.0305	879.9468
895.6883	897.0052	939.5607
947.7634	954.3014	964.6880
979.2947	988.3011	991.6924
1008.9504	1031.8006	1041.9793
1072.0416	1082.7503	1086.1884
1099.5031	1115.4416	1125.1382
1130.4328	1136.4024	1155.5404
1170.0404	1177.8878	1186.0709
1188.1022	1196.9864	1205.4408
1215.9082	1221.7261	1229.4928
1240.3411	1254.6496	1258.1794
1265.3859	1267.5244	1274.8309
1280.7799	1287.9971	1298.5898
1304.3273	1313.9773	1317.3702
1324.5690	1329.7415	1333.5763
1337.5059	1342.9010	1347.9882
1349.6436	1355.9241	1357.9849
1364.1933	1367.8760	1372.9932
1376.2196	1384.9976	1391.7440
1406.4578	1417.9620	1425.1571

1427.6157	1434.5789	1440.3909
1442.5548	1452.4104	1461.4081
1468.9810	1469.6811	1481.4735
1486.7528	1491.6479	1504.3262
1505.6661	1535.1083	1548.6938
1552.2777	1564.8339	1575.4442
1577.7158	1590.6563	1594.9837
1603.7059	1612.8679	1614.4917
1618.3293	1623.0048	1630.6143
1633.6637	1648.4633	3179.3724
3191.2917	3194.7231	3197.0665
3198.9194	3238.9212	3308.2299

ZeroEnergy[kcal/mol] 16.2
 ElectronicLevels[1/cm] 1
 0 2
 End
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 !-----bar_ts2-----
 Barrier ts2 ip2 p1
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 Geometry[angstrom] 67
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 C 3.0244322211 -0.3486757322 -2.7792947149
 C 2.785990402 -1.7092808691 -2.3307068805
 C 3.2139172051 -1.8050095463 -0.9497102704
 C 3.6906599927 -0.4924437768 -0.5326121692
 C 3.4083620075 -0.0393936327 0.7512285408
 C 2.9619243649 1.31426649 0.9794239239
 C 2.8267530871 2.1788521396 -0.102524605
 C 3.1592227496 1.7268632681 -1.4453123801
 C 1.6344454149 -2.3889474837 -2.7471627216
 C 0.8518501877 -3.152456843 -1.7898898023
 C 1.2946949723 -3.2721190685 -0.478274386
 C 2.4921573234 -2.582889884 -0.0557200796
 C 2.131020409 0.2607996274 -3.6653385286
 C 0.9639527738 -0.4649446496 -4.1324114806
 C 0.7135003768 -1.7552644671 -3.6610504174
 C 2.7125961301 -0.874230363 1.7009045233
 C 2.2594007122 -2.1425760942 1.3011822306
 C 2.2357525149 2.3533278554 -2.3659298107
 C 1.7443167941 1.6457928445 -3.4660934216
 C 0.3488212045 1.7849594243 -3.8501011923
 C -0.4911918596 2.637313298 -3.1317345302
 C 0.0149078567 3.329965022 -1.9523112137
 C 1.3391495485 3.1867948925 -1.5828946851
 C 2.0096420945 1.3262204333 2.0801807841

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 C 0.6854256416 3.0025311799 0.8280867889
 C 1.6749002317 3.0415623965 -0.184290183
 C 1.0153591474 -2.6372301811 1.7811381932
 C 0.4458760372 -1.9979970803 2.8888863041
 C 0.9090006069 -0.7258003173 3.2972186564
 C 1.9352376965 -0.0845883199 2.5933530475
 C -0.5523490871 -2.9443109633 -2.0593629779
 C -1.5030236733 -2.8623858369 -1.0055711524
 C -1.0032560881 -3.1803416787 0.3167584028
 C 0.3484882513 -3.2916771454 0.6007907283
 C -0.134035465 0.478102867 -4.2619706475
 C -1.4324835425 0.0846810796 -3.9357137548
 C -1.6774541725 -1.2437488652 -3.3860626339
 C -0.63093319 -2.1309802477 -3.2507686128
 C -2.9072688487 2.0042595854 0.6568476214
 C -3.4460754609 0.7611696621 1.1264176924
 C -3.738352382 -0.0456578975 -0.0363187859
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 C -0.7254686907 3.156540828 0.4338844154
 C -1.7516018237 2.5225951082 1.2747933639
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 C -3.1572227525 0.2147531937 -2.3693595716
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 C -3.3759363971 -1.222253904 2.4574774196
 C -3.5191047931 -1.9887635102 1.3221661215
 C -1.8568523168 2.2571188143 -2.861327
 C -2.3247828718 0.9949836139 -3.2645264002
 C -1.4499640404 1.9806871033 2.5565178446
 C -2.1167892866 0.9172328896 3.126456245
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 H -0.4827600498 -2.3614482586 3.3210225138
 H 0.3283482179 -0.1830652843 4.0351902572
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 H -3.6516804069 -3.0618673935 1.4294163879
 H -1.7971328409 0.5124041603 4.0831991505
 Core RigidRotor
 SymmetryFactor 0.5
 End
 Tunneling Eckart

ImaginaryFrequency[1/cm] 1765.8932

WellDepth[kcal/mol] 44.6

WellDepth[kcal/mol] 4.1

End

Frequencies[1/cm] 194

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347.1955	363.9785	371.5904
379.1339	383.6799	392.7770
400.9916	406.9799	416.0443
424.6983	428.0673	436.5164
445.0426	456.2449	469.5338
477.4284	478.8533	490.2261
496.6312	498.8906	504.4773
513.7293	520.9491	525.3462
532.9812	540.0396	544.5188
551.9148	556.6297	561.3482
568.9789	569.3672	576.4501
582.4248	587.2575	604.6607
613.8572	619.1193	625.6588
628.9662	635.0032	635.1539
654.5757	665.5794	674.7397
679.0877	689.4345	692.6035
700.2540	705.2561	712.5841
713.2783	719.5119	721.1619
721.9576	731.8058	733.8281
737.7249	740.9223	741.6964
743.0067	745.2970	748.6336
750.9283	751.2667	756.4463
761.3196	764.5750	766.0638
768.1557	774.6592	778.9875
784.4681	787.7884	789.4738
800.6652	807.3248	812.1397
822.2421	825.1707	835.7509
867.7375	876.9185	885.4455
899.6166	902.9348	942.3127
951.8276	963.6767	970.1516
979.8488	990.1969	994.1014
1010.5086	1035.1020	1040.2751
1080.0611	1091.3310	1096.0012
1106.5156	1114.7327	1127.1059
1131.7237	1143.8323	1160.7727
1173.7177	1181.4673	1183.9811

1189.9996	1194.9458	1204.1416
1216.3950	1224.5059	1229.2947
1233.7421	1248.0737	1258.1964
1264.0793	1268.9644	1269.8785
1277.1000	1284.3872	1302.1515
1304.9670	1310.6476	1317.7366
1323.2130	1331.6836	1337.0640
1341.4361	1346.2338	1349.1071
1353.6650	1360.7900	1364.0292
1366.0587	1368.6666	1371.5738
1380.1939	1389.0955	1400.5569
1405.6769	1422.7491	1427.3037
1428.8318	1443.5038	1446.8043
1450.5354	1453.7371	1465.3841
1469.6748	1471.1798	1477.7940
1489.2172	1491.8282	1505.7275
1513.9686	1541.6713	1555.0113
1560.4130	1563.8426	1578.9829
1591.7371	1593.5370	1604.0967
1606.5899	1609.3611	1615.1867
1619.7458	1623.0525	1628.4685
1633.6411	1641.0402	1654.2925
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3198.1448	3222.9433	3302.2856
ZeroEnergy[kcal/mol] 25.7		
ElectronicLevels[1/cm] 1		
0 2		
End		
!-----		
End		

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H₅

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!TemperatureList[K]          700. 800. 900. 1000. 1100. 1200. 1300. 1400. 1500. 1600.
1700. 1800. 1900. 2000.
TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650.
1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
!TemperatureList[K]          300 500. 1000 1500. 2000
!TemperatureList[K]          300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
!PressureList[bar]           0.1
!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature     0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature    100
ModelEnergyLimit[kcal/mol]     900
WellCutoff                     10
ChemicalEigenvalueMax          0.2
ChemicalEigenvalueMin          1.e-6      #only for direct diagonalization method
CalculationMethod              direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput               eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber             0
!ReductionNumber               5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                 260 ! Frenklach
! Power                         0.
Factor[1/cm]                   247 ! Jasper universal
Power                          0.85
! Factor[1/cm]                 424 ! Jasper calc N2
! Power                         0.62
! Factor[1/cm]                 125 ! SJK guess
! Power                         0.85
ExponentCutoff                 15
End
CollisionFrequency

```

```

LennardJones
!Epsilons[1/cm]      203.0 203.0 ! N2 pyrene-Frenklach
!Sigmas[angstrom]    4.6 4.6 ! N2 pyrene-Frenklach
!   Epsilons[1/cm]    206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
!   Sigmas[angstrom]  5.06 5.06 ! N2 Jasper extrapolation to C16
!   Epsilons[1/cm]    32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
!   Sigmas[angstrom]  3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
!   Epsilons[1/cm]    101.5 1177.442388
!   Sigmas[angstrom]  3.6154 10.84492872
!   Epsilons[1/cm]    390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Sigmas[angstrom]  4.46 4.46 ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Epsilons[1/cm]    189. 216.0 ! N2 , CH2CCH ! from Jasper calc
!   Sigmas[angstrom]  3.30 4.11 ! N2 , CH2CCH ! from Jasper calc
Masses[amu]          28. 725.
End
OutputTemperatureStep[K] 100
OutputTemperatureSize 20
OutputReferenceEnergy[kcal/mol] 0.
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C 3.6362795659 -1.1641882966 -0.6396857177
C 3.4478014152 -0.7194624393 0.6595306591
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C 0.569492788 -2.3079974921 -3.7607399524
C 2.672895265 -1.4933234574 1.601325582
C 2.0764342203 -2.6809159205 1.1924423187
C 2.1154901284 1.7570461739 -2.2869713587
C 1.5972695488 1.0858324108 -3.39254248
C 0.2048521344 1.23802241 -3.7085277924

```

C -0.5900524877 2.0407976704 -2.8891396958
 C -0.0672795815 2.7338874968 -1.7017415687
 C 1.2997369829 2.6114501476 -1.407774849
 C 2.3725185175 0.7956706282 2.1168230668
 C 1.688082865 2.0008884746 2.3079499748
 C 1.4754922819 2.8836395519 1.2201175628
 C 1.945997531 2.5494811143 -0.0601424074
 C 0.6991106064 -2.9477959457 1.5439216237
 C -0.0568209815 -2.0229812061 2.3111511525
 C 0.6979301429 -0.9414105303 2.908293148
 C 1.975752638 -0.6083053705 2.4892627984
 C -0.6768591559 -3.6193573824 -2.2609684655
 C -1.6261307729 -3.547654663 -1.2394934852
 C -1.201557265 -3.5595122646 0.153496287
 C 0.1329253716 -3.7172900394 0.4610854979
 C -0.2911797376 -0.0364125481 -4.2056781109
 C -1.5863436625 -0.4494804823 -3.9059100815
 C -1.8374915838 -1.8231367894 -3.4879041041
 C -0.7771472916 -2.7264048782 -3.4015007991
 C -2.9660485339 1.2931113453 0.8551211213
 C -3.0831721236 -0.0901121049 1.274471538
 C -3.4989233114 -0.8479409046 0.1356928064
 C -3.610233003 0.0380446184 -1.0075936845
 C -3.1929535752 1.3467180818 -0.5534897151
 C -2.3291381826 2.1055420568 -1.3453997701
 C -1.2219952602 2.8305918812 -0.742106792
 C -1.2741992019 2.9594453586 0.6251098357
 C -2.0635060488 2.1591227882 1.4926118326
 C -3.0214654678 -2.1347418262 -0.0123794566
 C -2.7422201124 -2.6420965503 -1.343321772
 C -2.8563600386 -1.7950112072 -2.4563768525
 C -3.2697265489 -0.4154992033 -2.2730741755
 C -2.2171172122 -0.5770786964 2.2652055202
 C -1.5109627176 -1.8536095451 1.9937518159
 C -2.0189682418 -2.6347735051 0.9187471189
 C -1.9562966686 1.6378109239 -2.6526254313
 C -2.4486479249 0.4197368163 -3.1366416633
 C -1.753677446 1.7785254318 2.8579173315
 C -1.8386565483 0.4574804096 3.222823369
 H 1.1359031666 2.1870887488 3.2243296509
 H 0.8214469822 3.7359691445 1.3700784529
 H 0.1647861732 -0.1854525297 3.4545836754
 H -1.3698035989 2.5118406499 3.5612622541
 H -1.5626864649 0.1746711755 4.2345130953

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 189

110.0458	132.0231	199.6040
226.4020	253.7555	268.1942
283.2011	285.0866	292.3951
307.7432	320.8903	324.0392
330.7028	340.1963	361.4718
373.7341	379.4708	382.1848
400.0950	405.7163	408.4514
415.1607	421.5854	434.1307
441.3179	442.9709	457.2803
468.2774	474.4516	481.2446
497.8536	504.1750	507.5610
509.9712	516.4359	522.1340
523.7604	528.0961	536.1117
547.2965	554.1302	557.0416
560.4915	567.7406	569.6434
570.6208	578.8274	582.2742
595.2654	608.6983	613.9988
619.7562	627.1084	637.7900
649.6094	659.6365	670.0903
679.0757	687.8418	694.5745
701.7163	705.7174	712.1204
716.1647	717.3309	720.0427
721.8578	723.4078	728.8347
736.6894	740.6990	741.4137
743.5196	744.5453	745.6201
748.2973	750.2877	751.8017
754.4989	756.9877	762.6566
764.3550	769.5581	770.5620
776.8288	778.8219	787.2549
792.1435	792.6175	798.2750
804.4872	812.6915	826.8011
831.6540	855.5851	870.0252
882.4215	894.1017	929.8633
945.8755	959.3873	971.6586
976.3311	981.3202	990.3247
998.8774	1012.8980	1038.3756
1066.6801	1084.0307	1087.3164
1098.5537	1105.9064	1110.1289
1129.5340	1136.1980	1145.9184
1171.4535	1179.9754	1186.4277
1198.2115	1199.0108	1206.9731
1219.7041	1227.6226	1232.1255
1247.8638	1251.9601	1262.6084
1265.4431	1268.1127	1276.4976

1281.2502	1294.0894	1300.4493
1306.5460	1313.8356	1320.8107
1325.8225	1330.1321	1338.9171
1341.2985	1346.0488	1352.2857
1359.2828	1362.0114	1365.3861
1369.0905	1369.4589	1373.1026
1380.7185	1390.6759	1419.5691
1425.5562	1425.8629	1440.4095
1444.0110	1448.1362	1450.2063
1457.2495	1462.6640	1464.5864
1469.8113	1472.4635	1486.2021
1494.6237	1502.9692	1534.6252
1541.0214	1551.4510	1562.0696
1571.0447	1575.2432	1582.3140
1591.6763	1594.0762	1603.9044
1607.3500	1613.7415	1615.6759
1617.0541	1624.7722	1630.1861
1641.3845	3188.4186	3197.5905
3207.1500	3212.1616	3328.9605
ZeroEnergy[kcal/mol] 0.0		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----well_ip2-----		
Well ip2		
Species		
RRHO		
Geometry[angstrom] 65		
C	3.4817810361	-0.1980185927 -1.7738447561
C	2.9098188316	-0.9335515349 -2.8830685228
C	2.6728830235	-2.3024532234 -2.44135327
C	3.0991515756	-2.4071251481 -1.0585551175
C	3.6139032166	-1.1124194446 -0.6568533
C	3.3500218824	-0.6466560867 0.632975175
C	2.9678974954	0.7082679493 0.8639862914
C	2.8256033898	1.5993124302 -0.1975703804
C	3.1027753154	1.1302567256 -1.5470274117
C	1.5346723864	-2.9858580867 -2.8733166149
C	0.7758591733	-3.7970829468 -1.9376853741
C	1.1765086809	-3.8754287863 -0.6029820771
C	2.3584933687	-3.1792166104 -0.153827732
C	1.9953275404	-0.307497807 -3.7336464949
C	0.8164963755	-1.0241764357 -4.1875099104
C	0.5917159107	-2.3365847614 -3.7683965119

C 2.6094077227 -1.4525268638 1.5809353982
 C 2.0925998529 -2.6853983766 1.1899312328
 C 2.1504191139 1.7708772583 -2.416662466
 C 1.6121906163 1.0740786836 -3.497200126
 C 0.2032575751 1.2135563688 -3.8147136163
 C -0.6036562787 2.0323055577 -3.0109224909
 C -0.0533418389 2.7184445778 -1.8638402104
 C 1.3029785252 2.6161680994 -1.5753178007
 C 2.0883291808 0.8019846209 2.0250916076
 C 1.2387775957 1.8570890951 2.1477802172
 C 0.8492369142 2.79481362 0.9931297246
 C 1.745126408 2.5369054914 -0.2182080856
 C 0.7396931489 -3.0276702917 1.5569815051
 C -0.0369762928 -2.1679304697 2.3780505105
 C 0.6757080478 -1.0840788803 3.0047724938
 C 1.8787530442 -0.6219225891 2.4876689431
 C -0.6322707944 -3.657115543 -2.2579751751
 C -1.5799344727 -3.6059867113 -1.230430869
 C -1.1553962947 -3.6424655909 0.1590453118
 C 0.1870235389 -3.7820526891 0.4607073167
 C -0.2891735284 -0.0787632357 -4.248004426
 C -1.5791921586 -0.4943610877 -3.9054018421
 C -1.8124763103 -1.8628332847 -3.4691570563
 C -0.7478469182 -2.7632984603 -3.3950281871
 C -2.715186136 1.2065186438 0.8869281711
 C -2.9643703898 -0.1679295907 1.3250147706
 C -3.4138321882 -0.9045160686 0.185826502
 C -3.5154700126 -0.0099554677 -0.9483091012
 C -3.0277706742 1.2769431548 -0.4969185265
 C -2.2144341911 2.0471792691 -1.316028163
 C -1.0337376689 2.6733683114 -0.7661474983
 C -0.6947726261 2.5811312811 0.5955980816
 C -1.6570107794 1.932552602 1.4717574233
 C -2.971636554 -2.2069396515 0.0222267369
 C -2.696959392 -2.696754292 -1.3179282782
 C -2.8176014595 -1.8408257792 -2.4213066688
 C -3.2208311316 -0.4602857342 -2.2259192272
 C -2.1647739457 -0.7193290075 2.3319192035
 C -1.4909770925 -2.0015349233 2.0536593298
 C -1.9850971533 -2.7452322758 0.9459110063
 C -1.9436159836 1.6071417131 -2.6719356285
 C -2.4327828659 0.3765267457 -3.1203936858
 C -1.5293577703 1.5822782468 2.8883519669
 C -1.7824635637 0.3052345615 3.3031278425
 H 0.6272858971 1.9263074642 3.0325691677
 H 0.9518691764 3.8444819728 1.3206530298

H 0.131315422 -0.4103441747 3.6394476475
H -1.2372244153 2.3342348383 3.6161575209
H -1.6722551013 0.048370221 4.3535544745

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 189

167.2223	172.8730	244.8215
258.1844	268.7207	283.6493
291.4917	311.0763	316.9899
324.2697	326.8840	349.1203
350.3599	361.6789	372.9240
377.9304	382.3012	399.3600
403.4716	411.5353	417.2681
426.7726	429.3865	435.8093
441.9074	449.0273	469.9568
475.9973	498.0189	500.0022
503.5039	508.3988	515.4482
516.3521	521.5948	523.7943
529.3783	539.5680	541.6647
548.9555	555.7424	563.6313
564.5121	569.8790	571.0589
573.8403	579.2470	582.1381
604.2875	606.0601	617.4341
635.2476	639.8750	657.5810
666.7289	676.6601	680.3449
684.4258	689.5816	696.6051
706.5185	710.9192	714.6244
716.9091	718.7322	722.2783
728.9028	731.1966	731.9369
737.0714	739.8748	742.7915
744.7760	745.3718	745.8530
746.8373	749.5069	750.2692
753.3443	757.4062	760.1309
764.9390	766.6554	776.4480
780.1137	787.7180	792.2729
797.9699	798.3693	805.4616
821.0515	827.6153	839.0399
857.4792	861.3749	874.4347
888.1598	913.7676	946.3707
954.6563	968.0875	973.3477
979.8970	986.8589	1001.7518
1022.6531	1030.8585	1056.3221
1073.3173	1083.1622	1093.0338
1102.6156	1107.8047	1117.7785
1127.4489	1147.0515	1169.1782

1179.2064	1186.7176	1193.7642
1194.5545	1198.9375	1210.1206
1214.1985	1226.6562	1239.3040
1241.4609	1251.6883	1258.4799
1264.4545	1269.2093	1272.8475
1274.7809	1277.3626	1300.9852
1304.3593	1310.8107	1315.0473
1324.6390	1329.2785	1333.7910
1338.3673	1343.7752	1346.6146
1348.5533	1349.0332	1361.1731
1362.8887	1367.0448	1370.4293
1372.8843	1378.4043	1389.1168
1395.9783	1411.4291	1428.8939
1433.7017	1440.9962	1449.0743
1450.0485	1452.1970	1461.0177
1462.0054	1475.4072	1483.9555
1484.6845	1496.1586	1521.2551
1541.5738	1545.3844	1549.1749
1561.6446	1568.3234	1577.4137
1586.2325	1595.2993	1600.4040
1602.1796	1606.7625	1609.3766
1610.7024	1617.3060	1628.2029
1633.3540	2959.5105	3179.7469
3197.6476	3289.6627	3328.6308
ZeroEnergy[kcal/mol] -17.0		
ElectronicLevels[1/cm] 1		
0 2		
End		
End		
!-----		
!-----h_c60h4_p1-----		
Bimolecular p1		
Fragment c60h4		
RRHO		
Geometry[angstrom] 64		
C	3.4734580268	0.2210420165 -1.8239270435
C	2.8890874756	-0.5116539811 -2.9298540513
C	2.6565501226	-1.882172352 -2.492505883
C	3.0971708987	-1.9966572832 -1.1162513626
C	3.6184882081	-0.7016200627 -0.7095273009
C	3.4002990456	-0.2515726175 0.5845625346
C	3.0350530915	1.1249240745 0.8388456198
C	2.8429861266	2.002307331 -0.2278829195
C	3.0950876187	1.5464078256 -1.5843278884
C	1.5154751385	-2.5656546456 -2.9208561155
C	0.7623152561	-3.3768812375 -1.9807909299

C 1.1711938669 -3.4581903985 -0.6501345723
 C 2.3631911335 -2.7669886908 -0.2079470651
 C 1.9702410413 0.1146132239 -3.7761697071
 C 0.7907159248 -0.6022944823 -4.2282639941
 C 0.567888401 -1.9155269584 -3.8091845895
 C 2.6648293314 -1.0568869759 1.5350633409
 C 2.1170961414 -2.2761770536 1.1374107944
 C 2.1288408148 2.1860899604 -2.451302308
 C 1.5889912699 1.495107546 -3.5355280452
 C 0.1768580363 1.6341564484 -3.8464502203
 C -0.6318386961 2.4534181847 -3.0562203375
 C -0.0749304201 3.1309255791 -1.8953245673
 C 1.2708309253 3.005028556 -1.6113839884
 C 2.1848277916 1.2072228492 1.9865469491
 C 1.2052807648 2.1889024903 2.0381142423
 C 0.7772449387 2.8896157276 0.8523667639
 C 1.6875631535 2.8703551281 -0.2354868586
 C 0.7594000367 -2.6011991776 1.5105290313
 C -0.0059428761 -1.7285756924 2.3259928996
 C 0.7246680471 -0.6493389537 2.9445477165
 C 1.9435487293 -0.2171438504 2.4412936641
 C -0.649391919 -3.235357503 -2.2924356206
 C -1.5870776863 -3.176518433 -1.2596140712
 C -1.1505382281 -3.209049735 0.1278409411
 C 0.1915992229 -3.3562555793 0.4186534517
 C -0.3160128725 0.3405018554 -4.2854946366
 C -1.6039805668 -0.0702106409 -3.9388273114
 C -1.8368306359 -1.4424621244 -3.5008890954
 C -0.7709436565 -2.3405368047 -3.4298701343
 C -2.7184490437 1.6506817126 0.8545467778
 C -2.9520322493 0.2745775781 1.293680059
 C -3.4050095707 -0.4655099792 0.1588923388
 C -3.5183435236 0.4235900517 -0.978376637
 C -3.0349630943 1.7152026488 -0.5370057643
 C -2.2402547529 2.4932608243 -1.3619729481
 C -1.0484976687 3.1240990002 -0.8155459889
 C -0.6875466972 3.0173475907 0.5555831319
 C -1.6892723454 2.393730185 1.4465595653
 C -2.9632000289 -1.7678903159 -0.0021106228
 C -2.7035956259 -2.265366166 -1.3421009086
 C -2.8338420356 -1.4159702594 -2.4488021968
 C -3.2372301668 -0.0320801319 -2.2569635017
 C -2.1417048075 -0.2715835105 2.2971486314
 C -1.4633758907 -1.5547768075 2.0148161807
 C -1.9692708027 -2.3023934402 0.9161745419
 C -1.9728592747 2.0414078834 -2.7165055896

C -2.457401699 0.8026246176 -3.1568129141
 C -1.5506097479 2.0418587743 2.8555764745
 C -1.7694469042 0.7528910383 3.2669165804
 H 0.540396241 2.1684693619 2.8823590146
 H 0.1807477663 0.0428127073 3.5612060564
 H -1.2341527158 2.7887509005 3.5788800071
 H -1.6240043847 0.4919141728 4.3118753803

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 186

177.0031	186.9698	257.9733
261.4895	270.7017	294.8804
295.1057	318.1200	320.2396
325.6028	330.9997	350.3133
351.6651	368.3858	381.9775
383.3974	392.1963	401.3533
413.4604	415.9568	426.7302
431.7536	436.8536	443.2487
450.3458	450.7065	475.0108
481.3405	506.0424	507.2869
514.5846	515.1446	520.8865
522.9998	525.8792	531.2470
536.3014	544.2886	547.5755
555.5670	560.9762	567.1857
567.7773	572.3380	575.5044
577.4660	580.1195	591.2965
611.3473	619.3551	620.0110
640.8764	644.1413	672.0826
677.3667	683.1303	687.7079
689.6575	695.3020	703.1568
710.1177	717.8637	719.2951
721.2249	721.2923	732.8473
733.6967	736.5018	739.3066
741.5580	744.1375	746.1091
746.5959	746.9005	749.6526
750.1241	751.9101	754.0456
757.5095	759.7678	762.5736
771.0053	772.5678	775.7444
780.8917	783.7215	790.7698
794.9862	799.3230	816.3714
823.4250	831.5803	838.0246
868.5735	885.4712	888.8607
909.8993	941.0306	949.7343
977.6319	978.6209	982.5692
987.1531	994.6841	1003.4502

1039.8060	1076.4330	1079.4406
1095.8587	1102.9728	1105.5904
1109.2711	1114.8946	1137.5806
1147.7558	1177.3775	1182.5733
1187.5836	1195.7885	1196.8108
1204.5342	1214.3993	1225.8039
1245.6770	1248.4843	1259.2663
1262.7502	1263.2799	1270.7791
1273.4698	1282.7690	1287.0260
1298.6812	1303.9435	1314.4054
1316.3218	1327.3391	1332.8108
1332.9622	1340.6219	1341.5843
1349.5910	1350.3029	1354.8093
1360.6432	1361.9549	1369.6227
1370.5512	1375.0677	1379.1187
1384.0617	1420.8259	1422.4405
1438.5113	1444.3572	1449.7901
1452.1748	1453.6547	1463.9431
1465.2021	1471.2049	1478.4673
1490.9191	1492.4417	1492.7363
1529.1191	1541.3560	1542.6910
1557.7705	1564.5168	1570.3641
1585.3001	1592.7446	1601.9436
1609.6868	1612.6487	1613.2427
1614.4809	1618.2294	1623.5748
1625.5276	1639.1013	3180.1260
3197.2091	3317.0018	3319.0946
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] 15.7		
End		
!-----bar_ts1-----		
Barrier ts1 ip1 ip2		
RRHO		
Geometry[angstrom] 65		
C 3.438543679 -0.207949853 -1.8317901727		
C 2.8624887806 -0.9369701619 -2.9383514461		
C 2.6268628195 -2.30782312 -2.5024994605		

C 3.0576785185 -2.4206782131 -1.1212588258
 C 3.5778602871 -1.1301553361 -0.7138682541
 C 3.349082528 -0.6758520438 0.5786082652
 C 3.000624627 0.6978222441 0.833683706
 C 2.831922248 1.5772133882 -0.2397364013
 C 3.0538795167 1.1115623788 -1.5904250829
 C 1.4864900614 -2.9871807499 -2.9355027662
 C 0.7264877009 -3.7967706043 -1.9993531088
 C 1.1243488401 -3.8754168922 -0.6643193212
 C 2.3115634668 -3.1853175394 -0.2144582974
 C 1.9421663842 -0.2998313787 -3.7731652521
 C 0.7673887602 -1.0158005182 -4.2370376295
 C 0.544385575 -2.3334188538 -3.8286782022
 C 2.5975212749 -1.468542083 1.5222802999
 C 2.0522211262 -2.6859949866 1.125740388
 C 2.0805468922 1.76861966 -2.4254182121
 C 1.5531142271 1.0768384361 -3.5145521948
 C 0.1500348997 1.2138333823 -3.8264636386
 C -0.650279237 2.0188398438 -3.0123779547
 C -0.1108139078 2.7154987679 -1.8455677865
 C 1.2534767709 2.6279697547 -1.5671138339
 C 2.1671651469 0.8088841981 1.9959530424
 C 1.4256028071 1.9717587338 2.1580198803
 C 1.1721324616 2.8720434943 1.0482665475
 C 1.803537988 2.5615377602 -0.2106094609
 C 0.689015265 -3.004092467 1.4871068828
 C -0.0838769515 -2.1195517737 2.2818306448
 C 0.63938427 -1.0232138258 2.8869065062
 C 1.8730961456 -0.6106985456 2.4127159349
 C -0.682209407 -3.6581726313 -2.3232670998
 C -1.6302540564 -3.603437831 -1.2984494509
 C -1.2052377947 -3.6294958069 0.0931545112
 C 0.1342565887 -3.7699347309 0.396466887
 C -0.339257156 -0.0736704956 -4.2902362082
 C -1.6283861511 -0.4945655444 -3.9655096206
 C -1.8635819071 -1.8678863306 -3.5389256154
 C -0.7959746399 -2.7638444103 -3.4609582304
 C -2.876490212 1.210450784 0.8222241364
 C -3.0640618283 -0.1693851725 1.2466407803
 C -3.4933651463 -0.9147861808 0.1047061617
 C -3.6005746971 -0.0211256755 -1.0314977348
 C -3.1490990012 1.2770510847 -0.5754852112
 C -2.3175489185 2.0446754864 -1.3851655792
 C -1.1728774001 2.7271915536 -0.8095389015
 C -1.0155656162 2.7270711967 0.5648649348
 C -1.8886262619 2.0031803593 1.4363204109

C -3.0312346604 -2.2084297465 -0.0543682919
 C -2.7521426612 -2.7019622074 -1.3915656245
 C -2.8733437077 -1.8482590668 -2.4976687266
 C -3.2870477071 -0.4692592276 -2.3056837298
 C -2.2350294943 -0.6908236524 2.2481666862
 C -1.5395319285 -1.9658827406 1.9672428849
 C -2.0353815011 -2.7268498359 0.8724058336
 C -2.0007342723 1.5969968651 -2.7198728499
 C -2.488555197 0.3707904214 -3.1860788128
 C -1.6651462881 1.633159421 2.8249990502
 C -1.8507113657 0.3335112581 3.216139601
 H 0.8616895926 2.1381158813 3.0682329755
 H 0.8618614559 3.8891952499 1.2652632473
 H 0.0948027654 -0.3146514942 3.4805171896
 H -1.3061133165 2.3674201509 3.5403295301
 H -1.6544410806 0.0542009727 4.2478020711

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 443.8797

WellDepth[kcal/mol] 7.2

WellDepth[kcal/mol] 24.2

End

Frequencies[1/cm] 188

141.7860	170.3786	
223.5036	261.7590	272.7373
280.0339	290.2051	298.0814
313.0483	321.7484	327.1356
335.0139	343.4371	364.5195
373.9232	378.0642	389.0131
394.4219	406.6274	408.4086
417.4218	423.0211	431.1904
437.6901	441.3064	449.0403
470.5883	474.9648	484.4945
500.3583	500.6275	506.3968
512.4421	515.3800	523.1073
524.0667	527.9133	535.8510
547.9508	554.0680	556.6366
559.5500	562.8382	568.3159
569.6266	574.7425	578.2150
586.3424	601.2723	610.5396
617.9493	623.8936	638.7743
645.2357	658.7199	667.8090
677.8871	686.6473	689.5382
700.1237	704.2312	711.0708

715.9816	717.9178	718.7083
720.5653	725.2233	729.5596
735.4953	738.8730	739.8640
741.8949	745.0526	745.8956
747.6629	749.5253	750.4735
753.8604	754.9146	757.4896
764.0843	765.0354	770.6861
775.7957	777.0013	781.4244
787.5860	792.8508	798.3087
808.0592	816.5987	825.6756
836.4454	852.2819	860.8610
875.9290	888.8984	913.6211
947.7244	959.7807	974.6402
975.8551	984.5412	987.4274
1001.4158	1022.8698	1033.4172
1070.2179	1083.1143	1085.5163
1091.8149	1104.5869	1107.2648
1125.1200	1127.8558	1143.5209
1168.9182	1178.1421	1186.6022
1194.9908	1195.7167	1205.2863
1212.6143	1225.1003	1238.3118
1246.5151	1250.4325	1262.3619
1265.5048	1268.5709	1273.9249
1277.2197	1291.2487	1302.4696
1308.0049	1310.9003	1318.1027
1326.2261	1328.7463	1335.5425
1340.0063	1342.3190	1350.1327
1354.5947	1361.2185	1363.0768
1367.7650	1369.3305	1373.7077
1380.4692	1385.4171	1392.6940
1409.0983	1419.6594	1436.2317
1442.0361	1447.1186	1450.8888
1454.8038	1457.4692	1462.6345
1466.8309	1472.1817	1485.9365
1492.6621	1494.8042	1522.9778
1537.0701	1543.5224	1548.9267
1558.8425	1566.9083	1574.7627
1581.4567	1595.0862	1599.8709
1605.4439	1611.5648	1613.0267
1614.4370	1618.7801	1622.7151
1636.2658	3183.1126	3190.5407
3203.0033	3230.7576	3342.2927

ZeroEnergy[kcal/mol] 7.2
ElectronicLevels[1/cm] 1
0 2
End

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!-----bar_ts2-----
Barrier    ts2 ip2 p1
RRHO
Geometry[angstrom] 65
C 3.4795057238 -0.1855113184 -1.7621280495
C 2.905796644 -0.9205005454 -2.8718636124
C 2.6759976748 -2.2920571792 -2.43594612
C 3.1080401602 -2.4044556544 -1.05666514
C 3.6205575767 -1.1074031543 -0.6469676859
C 3.3895191202 -0.657495209 0.6456697174
C 3.0151915392 0.7151685019 0.8953493678
C 2.8315102339 1.5945919054 -0.1709146891
C 3.094915353 1.1386240087 -1.5255495035
C 1.5403487529 -2.9798787384 -2.8711399998
C 0.784744905 -3.7945414357 -1.9360179019
C 1.1856618377 -3.8748109743 -0.6027864328
C 2.3713528059 -3.1781094501 -0.1529873665
C 1.9897613617 -0.2975911586 -3.723538824
C 0.8156205031 -1.019097603 -4.1825798358
C 0.5954708714 -2.3332392505 -3.7650301434
C 2.6518675759 -1.4662294578 1.5918323405
C 2.1141873053 -2.6888301157 1.1910276076
C 2.1323980876 1.774674065 -2.3977427131
C 1.6014968077 1.0812137326 -3.4847091507
C 0.1908337023 1.2146362729 -3.8038981057
C -0.6254185691 2.0306679672 -3.0173852066
C -0.0777849498 2.7095741826 -1.8538703491
C 1.2675720106 2.5923143541 -1.5621954926
C 2.1551374643 0.7944526716 2.0393026874
C 1.1864287729 1.7806716563 2.093977874
C 0.7697601238 2.5154212962 0.911915517
C 1.6799661225 2.4647829817 -0.1859849353
C 0.7559956579 -3.0210517335 1.5558911261
C -0.0184723611 -2.1532765755 2.3679311617
C 0.7022962989 -1.0703590457 2.9912270499
C 1.9209370572 -0.6307813087 2.4941805575
C -0.625520706 -3.6587655474 -2.2562273012
C -1.5701979322 -3.6049531304 -1.2291486947
C -1.1423336009 -3.6367190111 0.1610328465
C 0.1987358414 -3.7779408958 0.4600616077
C -0.2943763106 -0.0806107936 -4.2460523816
C -1.5827937265 -0.4969104392 -3.9068359388
C -1.8127275845 -1.869957534 -3.4708027987
C -0.743748628 -2.7639941143 -3.3939437386
C -2.7309859286 1.2156581427 0.8804077273

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C -2.963854349 -0.1611698555 1.3179861601
 C -3.4078716634 -0.9024112577 0.1803092705
 C -3.5174613395 -0.012900864 -0.9570462439
 C -3.0408902638 1.2800628042 -0.5115013676
 C -2.2426393995 2.0600565024 -1.3311692531
 C -1.057318432 2.6944367263 -0.7779759551
 C -0.7058445978 2.5904461766 0.5931905983
 C -1.7038388919 1.9601686228 1.4771763745
 C -2.960286982 -2.2031114838 0.020906224
 C -2.6899866037 -2.6983271799 -1.3179227749
 C -2.8163268434 -1.8482545547 -2.4246045061
 C -3.2263304157 -0.4663324961 -2.2340872587
 C -2.1579251319 -0.7049165149 2.3259741125
 C -1.4742033814 -1.9854303358 2.047420294
 C -1.9698253028 -2.7341510619 0.9447494054
 C -1.966419228 1.6117261805 -2.6848656785
 C -2.4440766703 0.3720061551 -3.1289365473
 C -1.57336985 1.6093140934 2.8880463385
 C -1.7937883575 0.3208789101 3.2983579254
 H 0.5220832445 1.7715150351 2.9387353711
 H 1.0062298204 4.4679037928 1.6266975715
 H 0.1518091091 -0.3818593964 3.6059153769
 H -1.2680424755 2.3592193435 3.6129672074
 H -1.6585715893 0.0607612929 4.3449232779

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 522.4572

WellDepth[kcal/mol] 36.7

WellDepth[kcal/mol] 4.0

End

Frequencies[1/cm] 188

176.2806	185.1690	
240.1478	255.3035	261.3735
267.2716	271.1139	294.8453
296.4594	317.4974	323.4541
326.1005	330.4164	350.8751
352.0783	368.4369	381.8472
383.6394	392.3956	401.8549
414.0886	414.6289	426.1678
431.5864	436.4623	442.9432
449.7929	450.9146	474.6494
480.9981	505.7942	506.8552
514.5274	514.7350	520.7881
522.9774	525.8726	530.1835

536.0348	543.4369	546.8193
555.4694	560.5075	567.3788
567.8946	572.2002	575.6767
577.3238	579.1594	591.5932
610.3628	617.2111	619.4726
641.0705	643.2522	671.1802
676.7164	682.6427	687.4453
689.4318	694.1252	702.9821
710.2278	717.1307	718.9019
721.0687	721.2396	732.5969
733.9634	736.0205	739.6232
741.7212	743.5877	745.7987
746.8623	747.1208	749.2416
750.1978	751.8995	754.0140
757.5148	758.4203	761.7444
770.2385	772.4526	775.2661
780.6043	783.1512	790.3119
795.0471	799.3503	815.7249
824.2145	831.6466	837.9920
868.3111	884.6975	888.4462
905.6631	939.3028	949.4339
977.0132	978.2451	981.8667
986.7336	993.0557	1004.6202
1040.0876	1075.8946	1078.8559
1093.0103	1102.7187	1104.7953
1106.9133	1114.5357	1136.5090
1145.9540	1174.6944	1182.4148
1186.6824	1194.6330	1197.1484
1203.5340	1211.6327	1225.4778
1245.3724	1248.1257	1258.8559
1260.5786	1262.8775	1271.7429
1273.0424	1281.6209	1286.2866
1298.4807	1303.5805	1314.2295
1315.4161	1327.4120	1332.4637
1332.7891	1340.1504	1341.6180
1349.0630	1349.8789	1354.3086
1360.1750	1362.2877	1369.1059
1370.4831	1374.5131	1378.8971
1384.3992	1419.1678	1422.8393
1436.6523	1442.8953	1449.5604
1451.8271	1452.6488	1463.9040
1464.0847	1472.3967	1476.4599
1490.0044	1491.3080	1493.1889
1526.5654	1540.8203	1541.9773
1556.7379	1564.3634	1570.0284
1581.8918	1591.6092	1601.2374

1609.2301	1611.8385	1612.2199
1613.5483	1617.1997	1622.1487
1624.3855	1638.2776	3180.5700
3197.8369	3318.5875	3320.4853

ZeroEnergy[kcal/mol] 19.7
 ElectronicLevels[1/cm] 1
 0 2
 End
 !-----
 End

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H₃

```

!TemperatureList[K]          700. 800. 900. 1000. 1100. 1200. 1300. 1400. 1500. 1600.
1700. 1800. 1900. 2000.
TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650.
1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
!TemperatureList[K]          300 500. 1000 1500. 2000
!TemperatureList[K]          300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
!PressureList[bar]           0.1
!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature    0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature   100
ModelEnergyLimit[kcal/mol]    900
WellCutoff                    10
ChemicalEigenvalueMax         0.2
ChemicalEigenvalueMin         1.e-6      #only for direct diagonalization method
CalculationMethod             direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput              eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber             0
!ReductionNumber              5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                 260 ! Frenklach
! Power                        0.
Factor[1/cm]                   247 ! Jasper universal
Power                          0.85
! Factor[1/cm]                 424 ! Jasper calc N2
! Power                        0.62
! Factor[1/cm]                 125 ! SJK guess
! Power                        0.85
ExponentCutoff                 15
End
CollisionFrequency

```

```

LennardJones
!Epsilons[1/cm]      203.0 203.0 ! N2 pyrene-Frenklach
!Sigmas[angstrom]    4.6 4.6 ! N2 pyrene-Frenklach
!   Epsilons[1/cm]    206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
!   Sigmas[angstrom]  5.06 5.06 ! N2 Jasper extrapolation to C16
!   Epsilons[1/cm]    32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
!   Sigmas[angstrom]  3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
!   Epsilons[1/cm]    101.5 1175.557388
!   Sigmas[angstrom]  3.6154 10.83504696
!   Epsilons[1/cm]    390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Sigmas[angstrom]  4.46 4.46 ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Epsilons[1/cm]    189. 216.0 ! N2 , CH2CCH ! from Jasper calc
!   Sigmas[angstrom]  3.30 4.11 ! N2 , CH2CCH ! from Jasper calc
Masses[amu]          28. 723.
End
OutputTemperatureStep[K] 100
OutputTemperatureSize 20
OutputReferenceEnergy[kcal/mol] 0.
!-----
!-----well_ip1-----
Well      ip1
Species
RRHO
Geometry[angstrom] 63
C 3.4599583157 0.2409827335 -1.8281217061
C 2.8826691636 -0.4953594357 -2.9352432238
C 2.6469546614 -1.8637199696 -2.494483462
C 3.0764405173 -1.9727836811 -1.1139341346
C 3.5918615172 -0.6776636674 -0.7069698299
C 3.3634715407 -0.2217186253 0.5850635513
C 3.0050683845 1.1587007411 0.8189056388
C 2.832020709 2.0366356757 -0.2511278043
C 3.0871948951 1.5700409186 -1.602191161
C 1.5099858502 -2.5487614341 -2.9293452215
C 0.7522246995 -3.3599722656 -1.9932718588
C 1.1523595361 -3.4412575562 -0.6591781069
C 2.3369490343 -2.7395852335 -0.2076776004
C 1.9704189472 0.1282160514 -3.7909554095
C 0.7930085179 -0.5895555659 -4.2469381365
C 0.5682947326 -1.9017383203 -3.826116775
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C 2.0802247233 -2.2459956401 1.1351416155
C 2.1257054109 2.2069727409 -2.4776969823
C 1.588544728 1.5100568514 -3.5586841893
C 0.1771287316 1.6481098071 -3.8742146599

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C -0.6343485493 2.4694006956 -3.0883410458
 C -0.0806616195 3.1555269014 -1.9315177149
 C 1.2657633335 3.0329511163 -1.6463153558
 C 2.1448912885 1.2605638151 1.9528403239
 C 1.1973454955 2.2674589589 2.011279896
 C 0.7693739057 2.9487069955 0.815774489
 C 1.6809613103 2.9115651021 -0.2697329891
 C 0.7253520218 -2.5955743692 1.4979087374
 C -0.0676942951 -1.7098523123 2.2780054275
 C 0.645301868 -0.6111557696 2.8301782453
 C 1.8647687505 -0.1462457398 2.4147578823
 C -0.6574853002 -3.2227603335 -2.3175692909
 C -1.6051229406 -3.1711180061 -1.2941892649
 C -1.1790732792 -3.2137096314 0.0958466501
 C 0.1636470513 -3.3558784197 0.4022339987
 C -0.3135392594 0.3530331363 -4.3110059996
 C -1.6028538696 -0.0570732314 -3.9684098648
 C -1.8377974973 -1.4289850008 -3.5318496964
 C -0.7724072395 -2.3272642138 -3.4553890437
 C -2.7127759174 1.6589693855 0.8244268245
 C -2.9577740876 0.2864034971 1.2615606411
 C -3.4207862071 -0.4546122488 0.125497254
 C -3.5226089831 0.4375692654 -1.0100456261
 C -3.0350444348 1.7281428521 -0.5670055625
 C -2.2436322361 2.5073829325 -1.3947371112
 C -1.0561663594 3.1493218608 -0.8517909808
 C -0.695217974 3.0532174874 0.5190918205
 C -1.6793355509 2.4006572631 1.413645682
 C -2.9943347455 -1.7636889955 -0.0434771476
 C -2.7222669239 -2.2570905636 -1.3821436045
 C -2.8410591523 -1.4024760864 -2.4852373661
 C -3.2406269688 -0.0179277703 -2.2900975435
 C -2.1340186393 -0.2707984761 2.2448287233
 C -1.5075829685 -1.5639960327 1.9617931154
 C -2.0130247097 -2.3159929457 0.8755316308
 C -1.9750677958 2.0549083843 -2.7480214772
 C -2.4580420101 0.8155609483 -3.1880597504
 C -1.4806893727 2.0188718297 2.8057147956
 C -1.6395516041 0.7098716461 3.1948756462
 H 0.5578427827 2.2656799658 2.8707360398
 H -1.136164036 2.7508415614 3.5300714219
 H -1.40471157 0.4174561902 4.2136590508
 Core RigidRotor
 SymmetryFactor 0.5
 End
 Frequencies[1/cm] 183

152.9818	183.5022	245.5542
263.3446	269.6285	285.3211
299.9658	314.4397	322.3839
326.3016	336.5503	342.3555
355.1566	368.2568	383.5066
387.0650	392.4970	399.6445
414.1061	416.8029	422.1497
431.0735	436.0413	441.1733
449.3186	454.1889	476.8118
481.9138	505.8333	507.6674
512.5405	514.1334	518.9255
523.7351	525.5081	531.4345
534.8254	541.1167	549.6339
556.6674	558.9546	566.1577
568.9379	570.8563	573.2787
576.0977	578.7759	590.8630
613.8061	614.7674	619.3328
640.5233	644.4068	669.3259
671.6007	682.2780	687.3041
687.9999	694.4476	703.6524
706.9342	715.8641	719.5131
720.9363	721.2392	731.3593
733.8353	735.1636	737.5051
740.4174	745.1239	746.0439
746.4431	747.2936	748.3353
749.9648	751.7081	752.2901
755.1441	759.0502	760.5039
769.1723	771.5115	776.9808
778.8574	784.6574	790.9218
794.0858	797.0908	810.0560
815.7789	828.9782	832.2527
867.4186	881.4073	888.2174
944.6593	950.8785	971.0966
981.2156	982.0576	985.7953
990.6562	998.4516	1034.3476
1079.0228	1082.8627	1096.2325
1103.3712	1109.7659	1112.6611
1116.6709	1138.7844	1146.1069
1178.8714	1185.5440	1194.0584
1197.2445	1202.3504	1207.5186
1221.6820	1226.0563	1244.9467
1248.4889	1258.1219	1262.3338
1264.6161	1272.8304	1279.8869
1284.4734	1289.9302	1301.2744
1305.8608	1311.3424	1318.8047
1329.7331	1332.5194	1335.7108

1340.0353	1348.7618	1349.1694
1353.5298	1356.0070	1362.1340
1364.5681	1371.7979	1375.2924
1378.1824	1381.8871	1392.4881
1420.5938	1431.4858	1438.9116
1450.7070	1451.6680	1455.0666
1461.4070	1462.4700	1467.1941
1473.0413	1485.0658	1488.3581
1491.2327	1509.4163	1534.4104
1541.9358	1554.6069	1560.4664
1568.9160	1573.8717	1588.5297
1596.8566	1607.9155	1611.1965
1612.3564	1613.1452	1615.5111
1618.1171	1621.5092	1634.7034
3190.5354	3211.0232	3360.7891

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_ip2-----

Well ip2

Species

RRHO

Geometry[angstrom] 63

C	3.3940285274	0.3470075766	-1.3975635804
C	2.8116382301	-0.3848923713	-2.5077963146
C	2.5780361366	-1.7511790847	-2.074334793
C	3.0138559963	-1.8661837757	-0.6950801607
C	3.5147117397	-0.5665931099	-0.273660454
C	3.2704909411	-0.1125622037	1.0228236319
C	2.9056305272	1.2737981529	1.2539123678
C	2.80198821	2.1547666743	0.1709621903
C	3.0457585556	1.6809768581	-1.1792388223
C	1.4375090816	-2.4360010181	-2.5060874879
C	0.6920926245	-3.2631758795	-1.5794688444
C	1.110235473	-3.3729852865	-0.2478677741
C	2.3007674875	-2.6627267198	0.2009397424
C	1.9012331702	0.2449504137	-3.3610723003
C	0.7165905	-0.4662127944	-3.8095014271
C	0.4888373648	-1.7787015472	-3.3905787898
C	2.532167402	-0.93979884	1.9601897288
C	2.0619619079	-2.1963860144	1.5547010244
C	2.0947811922	2.3359694242	-2.0647097552
C	1.5340936797	1.6306046131	-3.1336477695

C 0.1219493004 1.77665321 -3.4415975041
 C -0.6780328231 2.617304083 -2.6633237268
 C -0.0946217696 3.3433711487 -1.5479896274
 C 1.2630915615 3.2062837813 -1.25670684
 C 1.9420488476 1.316216162 2.332115156
 C 0.8975795905 2.2143288741 2.2950141711
 C 0.7595765068 3.0830110796 1.1596207032
 C 1.7031859274 3.0873421529 0.1244265988
 C 0.7339223644 -2.6051926536 1.9330213618
 C -0.0545236353 -1.7351030259 2.6870526679
 C 0.4459066028 -0.4797522184 3.1539214953
 C 1.7101843884 -0.0770254361 2.7775877069
 C -0.7218320714 -3.1120521563 -1.883141496
 C -1.6581835478 -3.0740767953 -0.8503489279
 C -1.2228533031 -3.1835650236 0.5345656525
 C 0.1418824734 -3.3403934035 0.823358231
 C -0.3837200328 0.4809754221 -3.8601291513
 C -1.668965757 0.0782775861 -3.4892359059
 C -1.9064244639 -1.2909895946 -3.0569200968
 C -0.8470264682 -2.1980997437 -3.007595067
 C -2.5258589798 1.753889132 1.3720358058
 C -3.0063602854 0.4178805443 1.9659725312
 C -3.3853597434 -0.3481279934 0.6797116303
 C -3.4536167191 0.5586748788 -0.4297898203
 C -2.9341500941 1.8463810312 -0.0066524748
 C -2.2438918463 2.6545021937 -0.9152783961
 C -1.0692330507 3.3584562731 -0.4717490756
 C -0.6515120609 3.2125677768 0.8537749217
 C -1.4006378766 2.4175789277 1.7929031938
 C -3.0109685 -1.6612388849 0.4479104321
 C -2.7590968298 -2.1294564594 -0.8988746547
 C -2.8843802036 -1.2575155576 -1.9843809567
 C -3.2439100948 0.120492529 -1.7466026258
 C -1.8662536596 -0.2636576271 2.6901449551
 C -1.4708480034 -1.5646185423 2.3754892707
 C -2.0589149436 -2.3296244353 1.3355293506
 C -2.0112856459 2.1940440111 -2.2729836509
 C -2.4967476718 0.9497323662 -2.6774329475
 C -0.4786705284 1.9615226296 2.9290842569
 C -0.7274278932 0.4750099877 3.4049724527
 H -3.8820212461 0.5583309578 2.6234618123
 H -0.60535517 2.6132823218 3.804195856
 H -0.9395693921 0.5185794227 4.4840003192
 Core RigidRotor
 SymmetryFactor 0.5
 End

Frequencies[1/cm] 183

247.8620	251.1193	263.7898
265.7808	266.1925	327.5924
334.8255	337.9892	344.8558
347.4196	357.9225	360.9071
392.7245	396.3776	398.4422
400.5762	404.1355	411.1722
423.7927	428.0268	433.4034
444.1321	454.3462	469.0162
479.6621	484.9012	495.7820
508.0948	513.2247	527.8230
529.8028	532.7369	534.4313
539.0007	546.8720	549.8729
554.4214	559.0125	562.0571
564.1526	566.6432	569.1580
571.0238	575.0538	577.2812
583.4721	584.0688	587.3162
654.2849	656.7712	666.1783
673.7727	677.1390	687.8147
702.1058	708.3337	709.2123
711.8645	718.9173	719.8859
720.4486	725.3655	729.1648
731.5921	733.8353	736.1935
738.3999	739.9221	742.9974
745.4037	748.4238	749.4441
750.7915	751.7873	752.6239
753.1445	755.0665	756.4478
760.4460	762.5664	764.8917
772.8958	779.0988	783.8091
793.6071	800.7079	801.9809
805.0474	822.5210	829.0236
835.5006	873.3186	921.2422
936.5390	946.4362	949.4303
966.0838	970.2791	983.2962
991.1298	1037.8721	1045.4268
1062.5624	1077.4483	1081.4057
1104.5380	1111.9087	1118.3958
1124.1792	1130.2733	1152.8477
1159.1097	1167.3213	1184.5932
1187.8674	1205.3233	1206.3149
1210.9015	1215.9039	1219.4316
1231.5677	1233.7419	1246.4323
1252.3939	1254.9021	1257.0364
1260.9161	1266.3830	1269.7620
1279.1274	1288.0967	1294.6827
1297.8365	1306.7110	1318.4930

1321.3731	1329.4747	1330.6674
1335.4766	1339.9600	1342.3269
1343.9379	1355.5644	1357.4453
1363.3095	1371.3459	1375.8469
1377.9359	1384.2219	1387.8807
1391.4588	1412.8106	1421.9012
1438.8972	1446.3785	1452.3553
1454.5745	1455.2127	1458.4126
1462.1848	1465.2651	1466.4733
1483.1074	1491.1405	1524.3937
1537.4449	1546.8375	1550.7046
1562.0743	1568.5444	1595.5201
1599.6122	1602.9449	1604.1078
1606.8079	1608.6963	1610.1738
1612.0530	1627.0562	1630.1415
2968.4348	3002.1898	3034.7025

ZeroEnergy[kcal/mol] -65.6
 ElectronicLevels[1/cm] 1
 0 2
 End
 End
 !-----
 !-----h_c60h2_p1-----
 Bimolecular p1
 Fragment c60h2
 RRHO
 Geometry[angstrom] 62
 C 3.3604978312 0.344442226 -1.7193110509
 C 2.7768910296 -0.384853617 -2.8281728251
 C 2.5416133024 -1.7543562609 -2.3936934953
 C 2.9799666989 -1.8705522319 -1.0166394279
 C 3.4797862133 -0.5712308723 -0.5956209887
 C 3.2321301191 -0.1177060539 0.6999074971
 C 2.8704447798 1.269031697 0.9326091555
 C 2.7711518934 2.1525195978 -0.1485700136
 C 3.0139001798 1.6791561412 -1.4989405997
 C 1.4023899933 -2.4374709529 -2.8247078857
 C 0.6573423873 -3.2662737657 -1.8935124833
 C 1.0811074816 -3.3811223918 -0.5681360184
 C 2.2671247419 -2.6687951966 -0.119533499
 C 1.8632090045 0.2452198759 -3.6757712193
 C 0.6752966526 -0.4650346164 -4.1183581015
 C 0.4497434761 -1.7781215217 -3.7018135007
 C 2.4902096154 -0.9443928378 1.6348908324
 C 2.0234267343 -2.2012438355 1.2327681595
 C 2.0632580748 2.3361459718 -2.3820285672

C 1.4988965361 1.6324608352 -3.4477211728
 C 0.0838754049 1.7801791761 -3.7483299087
 C -0.7103030346 2.6256236896 -2.9712347134
 C -0.1219603127 3.354458084 -1.8609676322
 C 1.234717768 3.2129349881 -1.5727931147
 C 1.9061165919 1.313547883 2.0093313195
 C 0.8721920991 2.222975159 1.9777660332
 C 0.7384777055 3.0989462895 0.8454669982
 C 1.6777505516 3.0919769136 -0.1927993965
 C 0.6972116823 -2.6167277392 1.6183621121
 C -0.0949598502 -1.7537099117 2.3851308573
 C 0.4071845957 -0.4844707009 2.8371505803
 C 1.6665149555 -0.081051054 2.451778636
 C -0.7576453436 -3.1186321629 -2.1942198749
 C -1.6924175293 -3.0917150771 -1.1575133136
 C -1.2493565665 -3.2082420061 0.2209934327
 C 0.1073481006 -3.3496690648 0.5092542759
 C -0.4242227834 0.4840148084 -4.1618331992
 C -1.7064960894 0.0831004819 -3.7806772103
 C -1.9417891165 -1.2863920981 -3.3462682196
 C -0.8850565279 -2.1986453183 -3.3107483027
 C -2.5386731133 1.7774349244 1.0648559015
 C -2.778679421 0.3828450145 1.5073593204
 C -3.3567362135 -0.3340669798 0.3925906308
 C -3.4803436638 0.5829865029 -0.7262616784
 C -2.976387114 1.8792438751 -0.3096367146
 C -2.2781614889 2.679591351 -1.2213650821
 C -1.097251724 3.3816646591 -0.782328271
 C -0.6741085738 3.2465467801 0.5454203514
 C -1.4224414594 2.4628617253 1.4906546933
 C -3.0260963143 -1.6742902981 0.159906734
 C -2.792237728 -2.1407507586 -1.1944723843
 C -2.9107735811 -1.2557432409 -2.2681735595
 C -3.2699558969 0.1333274531 -2.0297380869
 C -1.8874166795 -0.2449624103 2.3489580648
 C -1.5076822386 -1.6061304243 2.0849089245
 C -2.0778269778 -2.3270383749 1.0285626996
 C -2.0453302064 2.2072239952 -2.5738848514
 C -2.5301756488 0.9592751788 -2.9708959741
 C -0.5004716875 1.9768378077 2.6158024347
 C -0.7577358902 0.4805671521 3.0901381576
 H -0.6208255701 2.6164410456 3.4999376298
 H -0.9823968555 0.5210024909 4.1639999052
 Core RigidRotor
 SymmetryFactor 2
 End

Frequencies[1/cm] 180

251.4743	253.8873	266.4349
267.3269	267.9670	331.2685
339.1723	341.3581	345.7277
352.9446	359.2430	362.8984
397.1562	400.5005	401.8201
402.0923	408.1277	425.5210
428.1468	430.8768	433.7248
447.8967	461.8298	478.4537
486.3181	488.7754	497.9262
511.5634	525.8368	531.2645
531.2968	535.0687	539.2170
541.4425	549.9752	554.6044
556.9044	560.9574	566.0234
566.4264	567.0642	573.2012
573.9368	574.8835	575.2728
582.8173	586.5328	588.8063
660.6764	663.8251	670.4099
678.0852	681.0790	708.5316
709.4253	709.9758	715.8952
719.6712	719.7317	720.5231
722.8916	725.1293	729.8197
735.3471	736.5468	737.3551
738.7226	741.6188	743.4607
745.7851	747.5066	749.3189
752.0565	752.3484	753.5213
753.9094	754.0578	756.9613
765.1758	766.0056	766.9689
776.3387	780.5944	785.9214
789.5347	796.4120	802.8475
803.2442	827.6628	830.1225
834.6348	874.3705	935.1614
948.1231	953.7188	954.0292
977.0236	983.9199	984.8144
989.0570	1050.3481	1056.6034
1077.1363	1077.8230	1101.9643
1104.2544	1112.9205	1124.1634
1129.2154	1150.7277	1161.0173
1168.7119	1178.9711	1201.8825
1210.5238	1218.4026	1218.5169
1228.6180	1233.1586	1245.7742
1249.0602	1249.1861	1256.0577
1259.6394	1260.0652	1264.1458
1273.2317	1284.4021	1294.0079
1297.8209	1305.6029	1313.8714
1315.3421	1323.1544	1333.0741

1335.1979	1337.8550	1339.7380
1345.3789	1346.9605	1354.0534
1367.6649	1370.2959	1372.4802
1373.4039	1378.9930	1380.9958
1387.4178	1389.6387	1436.1879
1450.4635	1453.7002	1454.9237
1455.5052	1457.1445	1457.5217
1458.2208	1463.3189	1467.1624
1476.9433	1494.8516	1527.8781
1539.2911	1539.7992	1550.6435
1559.6137	1570.4125	1602.0571
1602.9183	1603.0968	1605.0281
1607.8850	1608.5535	1613.5975
1614.0641	1615.7960	1628.5486
1632.2721	3029.9921	3050.3383

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] -28.8
End
!-----bar_ts1-----
Barrier ts1 ip1 ip2
RRHO
Geometry[angstrom] 63
C 3.406613175 0.4018691206 -1.4518868988
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C 2.606063253 -1.7076663593 -2.1231224128
C 3.0233899391 -1.8098841871 -0.7377082678
C 3.5182577957 -0.5104036964 -0.3276487373
C 3.2340397525 -0.0478004405 0.952499892
C 2.8754320396 1.3202066514 1.181898555
C 2.758892832 2.2005955352 0.116102403
C 3.0282815589 1.7303379928 -1.230826121
C 1.4740809145 -2.3975515541 -2.5624257143
C 0.7143520529 -3.2129013451 -1.6302969384
C 1.106560988 -3.2889230665 -0.2929948668
C 2.2825817409 -2.5781891193 0.1660409521
C 1.9295748406 0.280985268 -3.4227615379
C 0.754484246 -0.4401700646 -3.8828682623

C 0.5322523619 -1.7524190422 -3.461916869
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 C 2.0032416644 -2.0820127035 1.5029886398
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 C 1.5436345207 1.6634100682 -3.1971511184
 C 0.1322757825 1.7977123602 -3.5184955008
 C -0.6843401466 2.6238392416 -2.7438485531
 C -0.1355036544 3.329383003 -1.5962882317
 C 1.2116350393 3.2041314165 -1.3006716481
 C 2.0038212448 1.4227933913 2.3324409398
 C 1.1639875748 2.540523541 2.4007182468
 C 0.7213769555 3.1699401729 1.1587804279
 C 1.6181110378 3.0980734511 0.0761071663
 C 0.6545087456 -2.4705218824 1.8716320331
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 C 0.5169926249 -0.4933342449 3.3998782937
 C 1.7056867447 0.0433545245 2.7812716333
 C -0.6958053229 -3.0822998969 -1.9623116002
 C -1.6517206614 -3.0459154801 -0.9459229177
 C -1.2365519255 -3.1157999084 0.4455701252
 C 0.1105182629 -3.2229534709 0.7622446864
 C -0.353549419 0.4993300644 -3.9509897275
 C -1.6423184458 0.0867736341 -3.6073076067
 C -1.874933806 -1.2828278779 -3.1709611674
 C -0.8073950223 -2.1815036382 -3.0949941528
 C -2.7130466865 1.7982933961 1.1869075316
 C -2.9687215635 0.4276108419 1.6254889119
 C -3.4538380856 -0.3166069767 0.4979525437
 C -3.5526563948 0.5805612144 -0.6398749124
 C -3.0604456757 1.8731280744 -0.2023665244
 C -2.2892539412 2.6619975966 -1.0419900681
 C -1.1084049498 3.3331260706 -0.5190242282
 C -0.7355279862 3.2508283489 0.8506049192
 C -1.6727978803 2.5550951274 1.7459360268
 C -3.033780712 -1.6333922551 0.3136956674
 C -2.7639041226 -2.1198176048 -1.0269128046
 C -2.8782638515 -1.2588182855 -2.1247360702
 C -3.2739111549 0.1257926154 -1.9215689568
 C -2.0630270157 -0.1577992142 2.5316970472
 C -1.5281181051 -1.4864895705 2.2987596509
 C -2.0655363089 -2.2264237422 1.2247761148
 C -2.0224235021 2.2023256847 -2.3956462118
 C -2.498590914 0.9596034617 -2.8255760937
 C -1.2876647073 2.0999463505 3.085963751
 C -1.3216900789 0.7548348931 3.2956989435
 H 0.7064777186 2.7935365605 3.3344731268

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H 0.278711786 -0.2864548137 4.4380198022
H -0.981832322 2.8044189673 3.8509027654
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 582.271
WellDepth[kcal/mol] 17.0
WellDepth[kcal/mol] 82.7
End
Frequencies[1/cm] 182
186.6593      197.1486
263.7250      268.0859      274.0652
300.4747      315.1490      319.8003
331.9719      335.1751      349.6106
365.4282      366.5678      372.9116
383.9211      390.8901      400.2760
408.7831      414.1906      426.4761
427.9361      438.0123      440.5102
458.1789      464.5496      465.5300
491.6693      493.0323      498.0491
508.5682      514.0429      518.8861
525.6962      528.3032      532.5411
533.6171      535.0282      539.4121
551.4078      558.7387      560.7673
564.0261      569.1876      573.6740
574.5298      576.3533      581.3857
588.2348      599.1219      619.2778
634.0794      640.0516      661.3210
670.3372      675.6479      680.4383
692.3598      699.8225      707.1890
708.6189      715.7955      719.4976
720.2988      721.0447      722.1054
732.6623      736.1018      736.3376
738.4436      741.1203      742.1889
743.4429      745.0264      748.2066
749.9422      751.8783      752.7003
754.1084      754.6943      758.6175
760.8367      764.9447      767.7756
775.1911      781.6074      784.6768
787.6529      791.7348      801.5282
812.1570      823.2807      830.9917
841.2576      861.0498      877.8601
922.2505      941.6693      942.8690
973.8395      975.0304      980.0377
986.4468      994.9695      1040.0345

```

1070.0820	1081.1443	1090.6220
1095.4103	1102.4417	1109.4910
1113.7268	1135.8872	1144.1950
1152.8255	1176.5488	1181.8560
1194.0912	1203.6883	1205.6482
1214.3534	1235.6871	1242.9632
1247.8935	1258.0764	1259.0024
1263.9262	1272.5861	1276.2446
1288.8826	1291.8397	1299.4013
1303.8234	1307.9768	1318.7733
1322.0677	1329.6585	1332.2585
1336.5428	1340.0726	1344.7811
1345.3073	1353.8068	1360.4917
1362.6108	1367.2861	1371.3202
1377.2372	1380.1552	1383.8674
1386.9184	1408.8594	1426.8845
1428.7573	1442.7490	1450.9116
1454.2409	1459.9397	1461.7941
1469.6543	1478.0249	1482.7640
1490.8903	1504.0603	1524.0804
1533.0275	1552.9812	1557.6474
1559.9841	1560.9508	1577.2917
1592.4592	1603.7770	1605.3898
1610.0854	1611.8793	1613.3502
1615.9294	1616.7854	1627.9616
3192.0047	3194.9805	3367.9084

ZeroEnergy[kcal/mol] 17.0

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts2-----

Barrier ts2 ip2 p1

RRHO

Geometry[angstrom] 63

C	3.37609	0.35817	-1.35776
C	2.80851	-0.37918	-2.47121
C	2.57382	-1.74884	-2.03557
C	3.00365	-1.86434	-0.65316
C	3.48684	-0.55366	-0.22805
C	3.23032	-0.0983	1.06537
C	2.86101	1.2893	1.28986
C	2.76704	2.17429	0.2114
C	3.02174	1.69251	-1.15062
C	1.4424	-2.43545	-2.48239
C	0.68365	-3.26536	-1.55921

C 1.08608 -3.37867 -0.22856
 C 2.28214 -2.6612 0.24207
 C 1.90643 0.24215 -3.33985
 C 0.72905 -0.47599 -3.79777
 C 0.50156 -1.78065 -3.37496
 C 2.48022 -0.92592 1.99823
 C 2.03237 -2.20117 1.5939
 C 2.0799 2.33994 -2.05006
 C 1.53742 1.63196 -3.13027
 C 0.12755 1.77707 -3.45494
 C -0.67843 2.62993 -2.69861
 C -0.10748 3.36812 -1.58399
 C 1.23554 3.21612 -1.25632
 C 1.87976 1.33088 2.35298
 C 0.84542 2.24891 2.31321
 C 0.72025 3.12242 1.18031
 C 1.67092 3.11188 0.15796
 C 0.69562 -2.6271 1.97365
 C -0.10717 -1.79287 2.74972
 C 0.38542 -0.48682 3.18125
 C 1.65053 -0.06001 2.80052
 C -0.727 -3.12122 -1.88561
 C -1.6817 -3.09348 -0.86858
 C -1.26647 -3.21179 0.51991
 C 0.09451 -3.35575 0.83388
 C -0.37425 0.46585 -3.86747
 C -1.66149 0.0607 -3.5055
 C -1.89577 -1.30701 -3.06296
 C -0.83815 -2.20253 -3.00599
 C -2.57669 1.80761 1.32527
 C -2.84186 0.42928 1.77995
 C -3.40281 -0.30819 0.6716
 C -3.50335 0.59039 -0.46801
 C -2.98831 1.89988 -0.05887
 C -2.26389 2.68614 -0.95987
 C -1.09831 3.41183 -0.52085
 C -0.69178 3.27021 0.85843
 C -1.46432 2.49883 1.76952
 C -3.06501 -1.65398 0.46515
 C -2.7822 -2.14189 -0.93032
 C -2.88637 -1.27539 -2.00299
 C -3.26768 0.11752 -1.75824
 C -1.86197 -0.31488 2.66424
 C -1.5132 -1.64741 2.44225
 C -2.10958 -2.33232 1.31319
 C -2.02078 2.21703 -2.32218

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C -2.5045  0.94027 -2.71866
C -0.5446  1.96217  2.91042
C -0.70948  0.44026  3.18255
H -3.23297  0.70761  3.24902
H -0.70025  2.52083  3.8496
H -0.50183  0.28993  4.3602
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling   Eckart
ImaginaryFrequency[1/cm] 260.2477
WellDepth[kcal/mol] 38.7
WellDepth[kcal/mol] 1.8
End
Frequencies[1/cm] 182
151.8118      170.8871
251.7692      254.8232      266.7110
267.8104      268.1728      333.1418
339.2609      342.2049      346.9989
354.0035      358.9713      363.6431
397.3149      401.5657      402.4813
403.0701      408.6760      426.6572
429.2792      431.7313      435.1722
449.2986      461.4390      479.4786
486.6251      488.3256      499.1281
512.0105      526.0154      532.0273
533.6697      536.8359      539.4361
542.1105      550.9653      554.7948
556.0133      561.9078      566.1979
567.5123      568.3662      573.6552
574.3668      575.6671      576.6265
583.1475      586.6936      589.2700
661.4827      664.0432      670.9755
678.5021      681.9013      705.3158
709.5995      710.6369      718.4385
720.4865      721.6070      722.8348
723.2633      723.9645      730.6107
736.2946      737.5226      738.4661
739.9090      741.9916      744.3247
747.3047      748.0739      750.6721
752.0310      752.9011      754.8847
755.7282      756.2654      758.3223
764.3102      767.5333      767.7191
776.8314      780.6549      786.6872
789.8263      797.2827      803.7076
804.2728      827.7046      830.4068

```

834.9301	872.5503	934.7718
948.2441	954.1607	954.5791
977.1617	983.8731	985.2257
990.1885	1050.7372	1057.3506
1076.8699	1078.1925	1101.9375
1105.3988	1112.8350	1124.2650
1129.9270	1151.5120	1161.7038
1168.2536	1179.9141	1201.9671
1211.4338	1218.4346	1219.1244
1227.1900	1233.2636	1246.3622
1249.1703	1250.0447	1256.1194
1260.1894	1260.8328	1265.0051
1273.9752	1285.5432	1294.7237
1298.0949	1305.8369	1315.0083
1316.6005	1323.8172	1333.9284
1335.7112	1338.7732	1341.1462
1346.1138	1347.1932	1354.5724
1368.1466	1371.4966	1373.6781
1374.4551	1379.5988	1381.1751
1388.0391	1391.0824	1436.3509
1450.3473	1453.7933	1455.2984
1455.7741	1457.4843	1457.7398
1459.0266	1463.5846	1467.3839
1477.1866	1495.3690	1526.3068
1539.1104	1540.4311	1551.2689
1560.1792	1569.7949	1597.2576
1603.2621	1603.4011	1605.2975
1608.3740	1609.4243	1613.4329
1614.3191	1615.1973	1626.3955
1631.2197	3029.2036	3049.4483

ZeroEnergy[kcal/mol] -26.9

ElectronicLevels[1/cm] 1

0 2

End

!-----

End

Input file for RRKM-ME calculations for unimolecular decomposition of C₆₀H

```

!TemperatureList[K]          700. 800. 900. 1000. 1100. 1200. 1300. 1400. 1500. 1600.
1700. 1800. 1900. 2000.
TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650.
1750. 1800. 2000. 2250. 2500.
!TemperatureList[K]          500. 625. 750. 875. 1000 1150. 1300. 1500. 1750. 2000
!TemperatureList[K]          300 500. 1000 1500. 2000
!TemperatureList[K]          300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
!PressureList[bar]           0.1
!PressureList[atm]           0.01 0.03 0.03947368 0.1 0.3 1. 3. 10. 30. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 12.5 15. 17.5 20. 22.5 25. 27.5 30. 32.5 35. 37.5 40. 42.5
45. 47.5 50. 55. 60. 65. 70. 75. 80. 85. 90. 100.
!PressureList[atm]           0.013157894 0.03947368 0.065789473 0.105263157
0.526315789 1. 10. 100.
PressureList[atm]            0.03947368 1. 10. 100.
EnergyStepOverTemperature    0.2      #Ratio of discretization energy step to T
ExcessEnergyOverTemperature   100
ModelEnergyLimit[kcal/mol]    900
WellCutoff                    10
ChemicalEigenvalueMax         0.2
ChemicalEigenvalueMin         1.e-6      #only for direct diagonalization method
CalculationMethod              direct
!RateOutput                    one_path.out
!LogOutput                     one_path.log
EigenvalueOutput               eigenvalue.out
!EigenvectorOutput             eigenvector_test.out
!EigenvectorNumber             0
!ReductionNumber               5
Reactant p0 #ground energy of bimolecular species will be used as a reference.
Model
EnergyRelaxation
Exponential
! Factor[1/cm]                 260 ! Frenklach
! Power                        0.
Factor[1/cm]                   247 ! Jasper universal
Power                          0.85
! Factor[1/cm]                 424 ! Jasper calc N2
! Power                        0.62
! Factor[1/cm]                 125 ! SJK guess
! Power                        0.85
ExponentCutoff                 15
End
CollisionFrequency

```

```

LennardJones
!Epsilons[1/cm]      203.0 203.0 ! N2 pyrene-Frenklach
!Sigmas[angstrom]    4.6 4.6 ! N2 pyrene-Frenklach
!   Epsilons[1/cm]    206. 206. ! N2 Jasper extrapolation to C16
doi:10.1016/j.proci.2014.05.105
!   Sigmas[angstrom]  5.06 5.06 ! N2 Jasper extrapolation to C16
!   Epsilons[1/cm]    32.3 216.0 ! Ar , CH2CCH ! from new Jasper calc
!   Sigmas[angstrom]  3.91 4.11 ! Ar , CH2CCH ! from new Jasper calc
!   Epsilons[1/cm]    101.5 1173.670196
!   Sigmas[angstrom]  3.6154 10.82514686
!   Epsilons[1/cm]    390. 390. ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Sigmas[angstrom]  4.46 4.46 ! N2 , A3/A3a/A6 ! from new Jasper calc 11/22/2015
!   Epsilons[1/cm]    189. 216.0 ! N2 , CH2CCH ! from Jasper calc
!   Sigmas[angstrom]  3.30 4.11 ! N2 , CH2CCH ! from Jasper calc
Masses[amu]          28. 721.
End
OutputTemperatureStep[K] 100
OutputTemperatureSize 20
OutputReferenceEnergy[kcal/mol] 0.
!-----well_ip1-----
Well    ip1
Species
RRHO
Geometry[angstrom] 61
C 3.3857087764 0.4360492992 -1.4333384642
C 2.8185711891 -0.3007218862 -2.5459136719
C 2.5850842799 -1.6688569472 -2.10789928
C 3.0107662143 -1.7781092067 -0.7254796345
C 3.4996129683 -0.4757683825 -0.3048875172
C 3.2419882317 -0.0189972672 0.9870831214
C 2.8672449231 1.3663181585 1.2070399311
C 2.7693103901 2.2462753439 0.1244280301
C 3.0293581469 1.7693185878 -1.2225720582
C 1.4543185235 -2.3585238404 -2.5490559765
C 0.7023717793 -3.1874998725 -1.621035947
C 1.1109762568 -3.2956437737 -0.2919935003
C 2.2872606082 -2.5731475062 0.1688299623
C 1.9112684355 0.3214247322 -3.407301776
C 0.7335073008 -0.3959965436 -3.8622955667
C 0.5089855929 -1.7090448183 -3.4391887922
C 2.4929963122 -0.8454685986 1.9212898131
C 2.0292416853 -2.1056004641 1.5146758817
C 2.0839572291 2.4167818321 -2.1171079712
C 1.5369052512 1.7072054528 -3.1877665829
C 0.1251993821 1.8460807887 -3.5060444996
C -0.6830173743 2.6889050999 -2.7408398612

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C -0.1139649792 3.4219979362 -1.623275873
 C 1.2406475394 3.2888473645 -1.317933246
 C 1.8881630662 1.4061059134 2.2714537075
 C 0.8494136642 2.3178560747 2.2312002323
 C 0.7173019424 3.1863556823 1.0963012975
 C 1.669419052 3.1786318622 0.0665685318
 C 0.6923734397 -2.5337802571 1.8891325985
 C -0.1182021136 -1.6950504186 2.6505895681
 C 0.3651500322 -0.3831981299 3.0691136451
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 C -1.2314313419 -3.1388394734 0.4686613933
 C 0.1240732554 -3.2721916824 0.7742696891
 C -0.3702374106 0.5458736954 -3.9216368078
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 C -0.8274296042 -2.1341034186 -3.0634194633
 C -2.5629412816 1.8440228697 1.2680860917
 C -2.8101727113 0.461160235 1.7129368709
 C -3.3675979647 -0.2689851925 0.6001157401
 C -3.4803837954 0.6423190204 -0.5284775613
 C -2.9852148153 1.9421027139 -0.1123458246
 C -2.2748360779 2.74240766 -1.0127629688
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 C -0.6957649572 3.3250851726 0.7776142377
 C -1.4564495143 2.5445521321 1.7114095405
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 C -3.2443341326 0.1876437846 -1.8252775937
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 C -2.0210209471 2.2661419049 -2.3611483811
 C -2.4943776755 1.0144218508 -2.7589005768
 C -0.5376649204 2.0253599828 2.8328362285
 C -0.7331072578 0.5350209768 3.0498002761
 H -0.6940010045 2.5861598373 3.7704719834

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 177

254.3098	258.7649	264.0589
265.8971	266.5101	334.2858
343.9708	344.0025	347.2183

355.7496	356.3076	356.4157
397.9299	402.7953	403.1571
404.9100	408.3889	426.1092
429.4415	432.9980	436.1133
440.9407	474.2680	478.7255
486.2424	489.1524	492.6114
520.8830	521.6665	532.3797
534.0418	534.2057	537.0873
537.9341	550.8744	554.6953
562.5253	564.8594	566.5966
568.0639	570.4116	571.6766
575.0779	576.1798	580.4151
582.8087	585.8797	588.2605
666.1843	671.1290	674.5611
675.1294	679.5922	690.9818
709.9227	711.9096	712.9443
716.0684	718.8301	720.2708
720.9841	729.9267	734.1880
735.9022	737.5165	738.9029
739.9607	742.6021	745.9015
746.3748	749.8928	750.9348
751.4227	752.1411	752.7233
753.5042	754.4996	757.1741
760.9019	765.5143	771.8702
777.4839	779.0928	783.9996
786.5736	800.2780	803.2386
805.0461	825.7386	832.8631
838.0921	844.2036	943.1375
957.7312	966.0120	970.8491
976.7495	979.7978	981.9596
987.7809	1064.0891	1066.1027
1095.3634	1097.3303	1105.0358
1111.4738	1112.3678	1125.6173
1127.9912	1163.4081	1169.6785
1194.8173	1199.5973	1203.1031
1210.5622	1213.4433	1220.7774
1227.3438	1235.0466	1239.5574
1246.2186	1249.2978	1264.4732
1267.6164	1270.8751	1273.9472
1282.4832	1297.3027	1300.3270
1306.9283	1319.2716	1325.5301
1326.2427	1334.7975	1336.1047
1338.5259	1340.1241	1340.4953
1354.6509	1359.3560	1369.6805
1372.6733	1373.7639	1373.8330
1381.4900	1384.4535	1395.2805

1413.3135	1438.9946	1443.9111
1449.3754	1452.6976	1453.9638
1457.5687	1459.2820	1461.8812
1462.1516	1467.1776	1493.6793
1506.3600	1521.1104	1535.4452
1543.7885	1551.8042	1561.3150
1565.0215	1577.2573	1598.4318
1600.6101	1603.8987	1605.8650
1607.0546	1609.9745	1610.7747
1611.5981	1613.5182	2975.0406

ZeroEnergy[kcal/mol] 0.0
 ElectronicLevels[1/cm] 1
 0 2
 End
 End
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 !-----h_c60_p1-----
 Bimolecular p1
 Fragment c60
 RRHO
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 C -1.3922397864 -2.7075157357 -1.8269052299
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 C -1.5202431744 -3.1519602311 0.5968491701
 C -0.1088415059 -3.4984529404 0.5906507383
 C 0.6177588547 -3.4438453712 -0.5994507635
 C -0.0368533704 -3.0396912682 -1.8324323659
 C -3.086585334 -1.6540374922 -0.5822553403
 C -1.8035212847 -2.4453231446 1.8348879431
 C 0.4800604481 -3.0066115017 1.8249417267
 C 1.9636139083 -2.895186082 -0.6048145693
 C 0.9043589848 -2.2419926094 -2.6002776055
 C -1.8628593229 -1.5624875803 -2.5887119766
 C 2.5291783492 -2.4224483638 0.5803994387
 C 1.7720710935 -2.4789840411 1.8197274366
 C 3.2951480649 -1.1872139708 0.5782660597
 C 2.0701936967 -1.278975387 2.5834286647
 C -3.3587555787 -0.9756925234 0.606514778
 C -0.5673805215 -2.3554068806 2.5937926683
 C 3.0118511628 -0.4807058698 1.8166334173
 C -0.2809328907 -1.2031606218 3.3270547365
 C -2.7040855708 -1.3793038278 1.8396017914
 C 2.1407518929 -2.1521182172 -1.8412938461
 C 0.4528188968 -1.1420251576 -3.3311133597
 C -3.4654378062 0.4737426546 0.6082198023
 C -0.958745902 -0.7955248097 -3.3252943198

C -2.910028905 -0.9112970693 -1.8189728924
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 C -1.0650727686 0.6540221346 -3.3228597859
 C -3.0122674682 0.480648824 -1.8173559701
 C 1.0646496089 -0.6540722604 3.3221247165
 C 2.8760793144 -0.9660230409 -1.8432684191
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 C -0.480487112 3.0065519627 -1.8256636751
 C 0.1084148442 3.4983882294 -0.5913706859
 C 0.5669502198 2.3553492407 -2.5945138287
 C 3.4650117598 -0.4737956229 -0.6089410438
 C -0.9047874154 2.2419358652 2.5995564074
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 C 2.7036677433 1.379254681 -1.8403264118
 C -2.1411720254 2.1520589688 1.8405693722
 C 0.958318341 0.7954719248 3.3245558624
 C 1.8624420892 1.5624306027 2.5879915908
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 C -0.618188525 3.4437877977 0.598728569
 C 1.803098221 2.44527102 -1.8356099998
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 C 0.036426173 3.0396360553 1.8317118083
 C 3.3583295681 0.9756362691 -0.6072326989
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 C 1.3918211692 2.7074633121 1.8261832003
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 C 2.1483698243 2.7641105923 0.5865132462

Core RigidRotor

SymmetryFactor 120.

End

Frequencies[1/cm] 174

265.4143	265.6906	265.8130
265.8848	266.1182	342.1359
343.0653	343.4204	356.6703
357.2151	357.9017	358.6442
408.0087	408.2375	408.3693
408.5266	408.6659	435.9237
436.2935	437.0985	437.8905

438.4564	488.7926	488.9266
489.2941	490.0314	496.7130
535.6623	537.3896	537.8394
539.6303	540.7292	540.9394
541.6573	541.7842	566.2761
566.3774	566.7440	571.0262
571.6871	572.5948	576.1780
576.2770	576.5870	576.6512
588.1136	588.1933	588.3492
679.0270	679.1462	679.2502
679.3799	679.6203	717.2046
718.3692	718.6509	719.6826
720.5628	721.6928	722.1819
723.7972	735.6957	736.9908
738.2679	741.0298	741.9777
742.3719	742.9289	743.3837
751.0397	752.0294	752.4479
753.1346	754.1784	754.8807
755.6078	757.2194	765.8938
766.3669	766.5129	767.1492
787.2996	787.4001	787.4969
787.7217	787.7638	804.7595
805.0681	805.1419	840.3080
840.4440	840.5081	966.0140
977.3895	977.4953	977.6391
982.3191	982.4152	982.8128
982.9666	1093.9907	1094.2013
1094.5637	1094.7538	1126.3828
1126.4321	1126.6471	1127.0916
1127.2884	1200.6091	1201.0197
1201.2509	1213.8704	1214.2442
1214.3170	1244.3308	1244.5221
1245.1512	1245.4109	1245.5807
1275.9340	1276.3324	1276.6285
1276.8976	1277.0597	1302.2153
1302.2478	1302.6100	1333.5979
1334.0442	1334.2998	1334.4475
1334.4832	1334.6965	1334.9987
1335.3859	1370.2616	1370.3485
1370.6372	1370.9676	1371.1531
1371.5116	1371.8944	1372.2933
1453.6919	1454.3296	1454.4386
1454.6475	1454.7600	1459.6338
1459.7874	1460.2794	1463.4905
1463.6652	1463.9522	1464.0616
1502.9763	1537.2156	1537.4250

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1537.6266      1537.8819      1566.0223
1566.2531      1566.2554      1607.1685
1607.4263      1607.6290      1607.9394
1608.0866      1616.4096      1616.7259
1616.9089      1617.1154      1617.3669
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] 38.9
End
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Barrier      ts1 ip1 p1
RRHO
Geometry[angstrom] 61
C 3.3865286143 0.4356508839 -1.4268824141
C 2.8209686947 -0.3028073053 -2.5434344129
C 2.5887566201 -1.6694507608 -2.1066395724
C 3.0110000801 -1.7757254178 -0.7201441479
C 3.503909506 -0.47459477 -0.2998608748
C 3.2522937676 -0.0181782482 0.9946044659
C 2.8732045404 1.3673542212 1.2157493258
C 2.7615417633 2.2415175452 0.1338656628
C 3.0231195018 1.7660915286 -1.2144826546
C 1.4591009967 -2.3603785157 -2.5470335561
C 0.7047832818 -3.1866118971 -1.619226306
C 1.1100954441 -3.2885712907 -0.2878016027
C 2.2865729554 -2.568757553 0.1709289537
C 1.9141832808 0.3184935667 -3.4032173133
C 0.737667013 -0.4010708421 -3.8617365191
C 0.5147329254 -1.7132608716 -3.4422410606
C 2.4978954173 -0.8438847185 1.922601676
C 2.0249017145 -2.0934285175 1.5189301865
C 2.0785619252 2.4130072645 -2.1096568299
C 1.5354299967 1.7039841202 -3.181878296
C 0.1247014705 1.8407743234 -3.5036063992
C -0.6868105459 2.6812017418 -2.7403947534
C -0.1213095426 3.4190752988 -1.6231760239
C 1.2332185473 3.2877321512 -1.314244135
C 1.8846113574 1.3984528548 2.2803227631

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C 0.8243025131 2.3021912694 2.2220199111
 C 0.7058286723 3.2093360638 1.0949852071
 C 1.655512684 3.1814495937 0.0720645372
 C 0.6868561934 -2.5195960727 1.8936639153
 C -0.1246604532 -1.6793762028 2.6566667108
 C 0.3676099932 -0.3775301246 3.0763100953
 C 1.652818598 0.0311168684 2.7170854413
 C -0.706012724 -3.049787667 -1.940997968
 C -1.6552425887 -3.0203875009 -0.9185228
 C -1.2330878281 -3.1268248921 0.4680743259
 C 0.1214379997 -3.258172957 0.7770114475
 C -0.3682532862 0.5398239347 -3.9237620171
 C -1.6531347494 0.1310646665 -3.5639028339
 C -1.8852495083 -1.2355925201 -3.127092649
 C -0.8233070748 -2.1390278995 -3.0675988531
 C -2.587321362 1.8321026929 1.2603385766
 C -2.8199383186 0.4648554277 1.6969218168
 C -3.3857000339 -0.273325646 0.580683808
 C -3.5030687339 0.6369387845 -0.5461505474
 C -3.0097349456 1.9378812503 -0.1260142877
 C -2.2862408005 2.731011306 -1.0174295907
 C -1.1099373974 3.4496507524 -0.5586780774
 C -0.7046879058 3.3461253261 0.7732764296
 C -1.4595704852 2.5236728 1.701120011
 C -3.0222684058 -1.6039809223 0.3677696121
 C -2.7611946008 -2.0792603888 -0.980368812
 C -2.8738509799 -1.2050110045 -2.0623452305
 C -3.2525964448 0.1806351312 -1.8408770044
 C -1.9125701012 -0.1564220953 2.5562748342
 C -1.5347943116 -1.5426435389 2.3350607171
 C -2.0779944101 -2.2514627937 1.2630458663
 C -2.0249596918 2.2556317117 -2.3658507075
 C -2.4981155211 1.0063146417 -2.769037942
 C -0.5175170533 1.886252293 2.6140085194
 C -0.7374080232 0.5617257966 3.0148506034
 H -0.8376322407 3.1011801237 4.5380027728

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 309.1427

WellDepth[kcal/mol] 41.1

WellDepth[kcal/mol] 2.2

End

Frequencies[1/cm] 176

167.8789 185.8022

265.3556	265.5769	265.6384
266.2362	266.2854	342.8091
343.6742	343.9777	357.0072
357.5389	357.7300	358.4965
408.2715	408.3146	408.4706
408.6037	409.0143	436.4695
437.4438	437.5684	438.0616
438.4743	488.4029	489.1315
489.7003	490.0557	496.4158
536.3214	538.3080	538.6813
540.4636	540.7971	541.0837
541.1240	541.4095	566.5362
566.6530	566.7854	571.8286
572.1996	573.2090	576.1976
576.5579	576.6584	576.9560
587.1956	588.6175	588.6725
679.0295	679.1890	679.2818
679.6005	679.6432	715.4324
719.0948	719.3070	719.6313
719.6845	722.3748	722.9863
723.4100	736.7978	737.8202
738.2023	741.3187	742.6369
743.0037	743.2250	743.3641
751.6864	752.6096	752.6633
753.1462	754.5614	755.7225
755.9619	756.6939	766.2886
766.4433	766.5917	766.8093
786.1747	787.5950	787.7123
788.1332	788.1594	805.0497
805.1199	805.1779	840.4473
840.5623	840.6726	966.1505
976.9126	977.9373	978.4521
981.6761	982.3313	982.9881
983.4079	1094.0157	1094.5213
1095.1156	1095.1910	1125.4871
1126.8844	1126.9606	1127.2425
1127.3375	1200.6029	1201.2409
1201.5785	1213.6281	1214.2881
1214.5863	1244.0127	1244.2844
1245.1788	1245.4220	1245.5175
1275.4170	1276.3586	1276.6317
1277.0912	1277.4382	1302.0757
1302.3945	1302.8759	1333.0204
1334.1644	1334.2043	1334.4937
1335.0411	1335.0947	1335.2058
1336.0233	1368.7944	1370.0948

1371.1356	1371.1986	1371.3287
1372.1238	1372.3473	1372.6298
1452.3415	1453.7568	1454.6348
1454.6771	1454.9793	1459.3144
1460.4678	1460.6680	1463.5651
1463.6018	1464.0742	1464.1556
1502.7684	1535.6344	1537.2911
1537.3683	1538.6689	1564.2896
1566.5724	1566.6612	1603.9185
1607.7013	1607.7190	1607.8519
1608.0458	1614.9388	1616.7989
1617.0654	1617.0852	1617.1675

ZeroEnergy[kcal/mol] 41.1
 ElectronicLevels[1/cm] 1
 0 2
 End
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