Supporting Information

Circumstellar Origin of Chrysene ($C_{18}H_{12}$) via Self-Recombination of Resonantly-Stabilized 1-Indenyl Radicals and Implications to the Aromaticity of the Carbonaceous Asteroid Ryugu

Souvick Biswas[1], Shane J. Goettl[1], Vladislav S. Krasnoukhov[2], Nureshan Dias[3], Valeriy N. Azyazov[2], Sabrina Arias[4], Stanislaw F. Wnuk[4], Musahid Ahmed[3*], Alexander M. Mebel[4*], Ralf I. Kaiser[1*]

[1] Department of Chemistry, University of Hawai'i at Manoa, Honolulu, Hawaii 96822, United States

[2] Samara National Research University, Samara 443086, Russian Federation

[3] Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

[4] Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, United States

* Corresponding author. E-mail: mahmed@lbl.gov (https://orcid.org/0000-0003-1216-673X)
mebela@fiu.edu (https://orcid.org/0000-0002-7233-3133)
ralfk@hawaii.edu (https://orcid.org/0000-0002-7233-7206)

Contents

S1. Methods:

S1.1. Experimental: The experiments were performed at the Chemical Dynamics Beamline (9.0.2.) of the Advanced Light Source (ALS) using a high-temperature chemical reactor consisting of a resistively heated silicon carbide (SiC) tube of 20 mm heating length and 1 mm inner diameter.[21,27,30] This device was located inside the source chamber of a molecular beam setup, which was equipped with a Wiley−McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS). The indenyl radical ($C_9H_7^{\bullet}$) was prepared in situ by pyrolysis of the 1-bromoindene (C_9H_7Br) precursor synthesized in house using the procedure reported in previous work.[30] The vapor of 1-bromoindene (C_9H_7Br) (stored in a Swagelok particulate filter at room temperature of 298 ± 3 K) was seeded in helium carrier gas at total pressures of 150 ± 10 torr at the reactor inlet through a 0.2 mm nozzle. The temperature of the SiC tube was determined using a Type-C thermocouple to be 1223 ± 20 K. The products formed in the reactor passed through a 2 mm skimmer located 10 mm downstream of the reactor and entered the main chamber, which houses the Re-TOF-MS. The neutral products within the supersonic molecular beam were then photoionized in the extraction region of the mass spectrometer by utilizing quasi-continuous tunable synchrotron vacuum ultraviolet (VUV) light. VUV single photon ionization represents essentially a fragment-free ionization technique and is accepted as a soft ionization method compared to the harsher conditions of electron impact ionization with the latter leading to excessive fragmentation of the parent ion.[53] The ions formed via soft photoionization were extracted and ultimately detected by a microchannel plate detector through an ion lens. Under our experimental conditions, modeling suggested that the residence time in the reactor tube was few tens of microseconds.[36] Photoionization efficiency (PIE) curves, which report ion counts as a function of photon energy with a step interval of 0.05 eV at a well-defined mass-to-charge ratio (m/z), were produced by integrating the signal recorded at the specific m/z for the species of interest. Due to the weak signal in these experiments, extended data accumulation times of up to 15 min per step had to be accounted for, and each step was repeated three times.

S1.2. Computational: The geometry of the reactants, products, intermediates, and transition states were optimized using the B3LYP hybrid density functional method with the 6-311G** basis set. The same B3LYP/6-311G** approach was used to compute vibrational frequencies and zero-point vibrational energy corrections (ZPE) at the optimized structures. Intrinsic reaction coordinate (IRC) calculations were carried out to confirm connections between transition states (saddle

points) on the potential energy surface and corresponding local minima in the forward and reverse directions. The relative energies were further refined using a modified G3(MP2,CC) calculation scheme:[54-56]

$$E[G3(MP2, CC)] = E[CCSD(T)/6{-}311G^{**}] + E[MP2/G3Large] - E[MP2/6{-}311G^{**}]$$

$$+ E(ZPE) = E[CCSD(T)/6{-}311G^{**}] + \Delta EMP2 + E(ZPE)$$

Here, CCSD(T) is the coupled cluster method with single and double excitations and with accounting for triple excitations according to perturbation theory, MP2 is the second-order Meller–Plesset perturbation theory method, and ΔEMP2 = E[MP2/G3Large] − E[MP2/6-311G**] is the basis set correction. B3LYP and MP2 calculations were performed using the Gaussian 09 software,[57] and the MOLPRO 2015 package[58] was employed for CCSD(T) calculations. Note that a preliminary account of the PES involved in the C_9H_7 + C_9H_7 reaction was published earlier,[59] prior to the Wang *et al.*'s work.[41]

Temperature- and pressure-dependent rate constants and product branching ratios for the decomposition of the $C_{18}H_{13}$ radical **i2**, which is produced by the H loss from the initial C_9H_7-C_9H_7 complex **i1**, were computed using the RRKM-ME theory[60] utilizing the MESS software package.[61] Generally, the rigid rotor-harmonic oscillator approximation (RRHO) was employed in partition function calculations, which utilized the refined G3(MP2,CC) relative energies and B3LYP/6-311G** molecular parameters. Lennard-Jones and the collisional energy transfer parameters and the temperature dependence of the range parameter α for the deactivating wing of the energy transfer function in the "exponential down" model[62] of the collisional energy transfer in ME calculations were taken from the previous kinetic study of the C_9H_7 + C_5H_5 reaction.[22] Cartesian coordinates, vibrational frequencies, and relative energies of various species along the $C_{18}H_{13}$ PES in the form of an input file for RRKM-ME calculations using the MESS code are presented in Data S1.

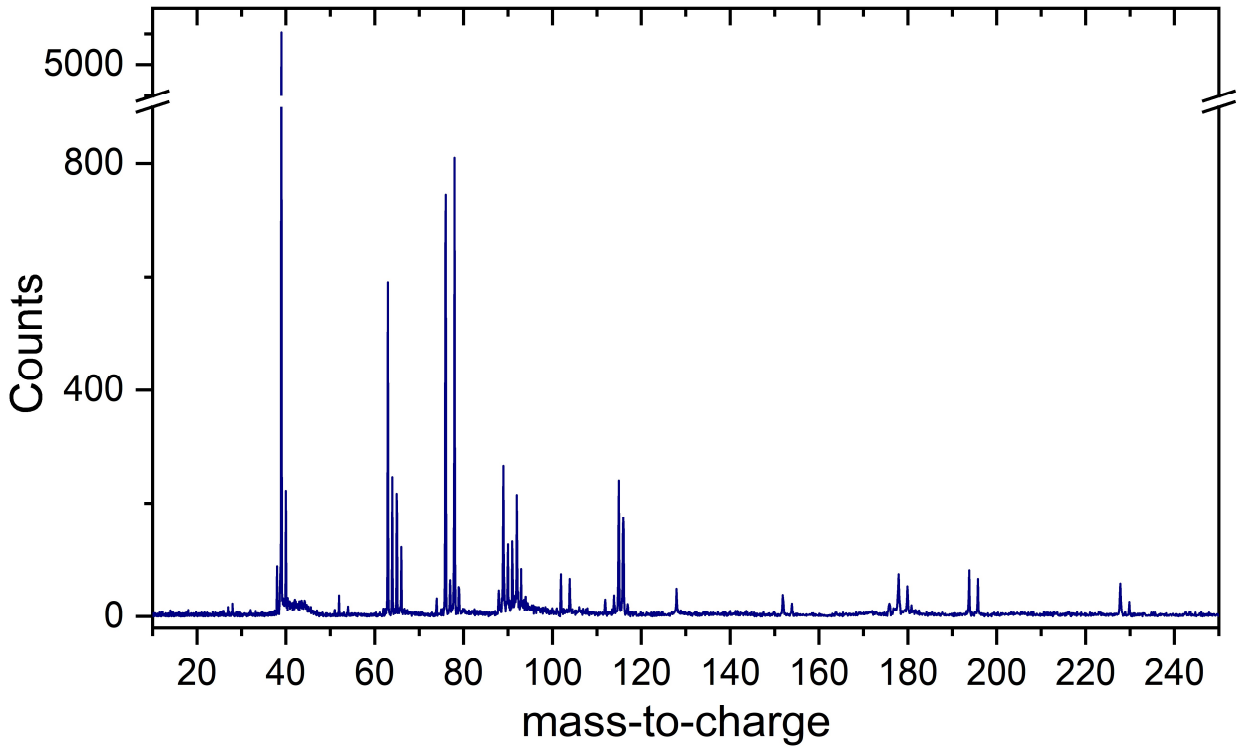


Figure S1: Complete mass spectra recorded at a photon energy of 9.50 eV where the microreactor temperature was 1223 ± 20 K for 1-bromoindene/helium molecular beam.

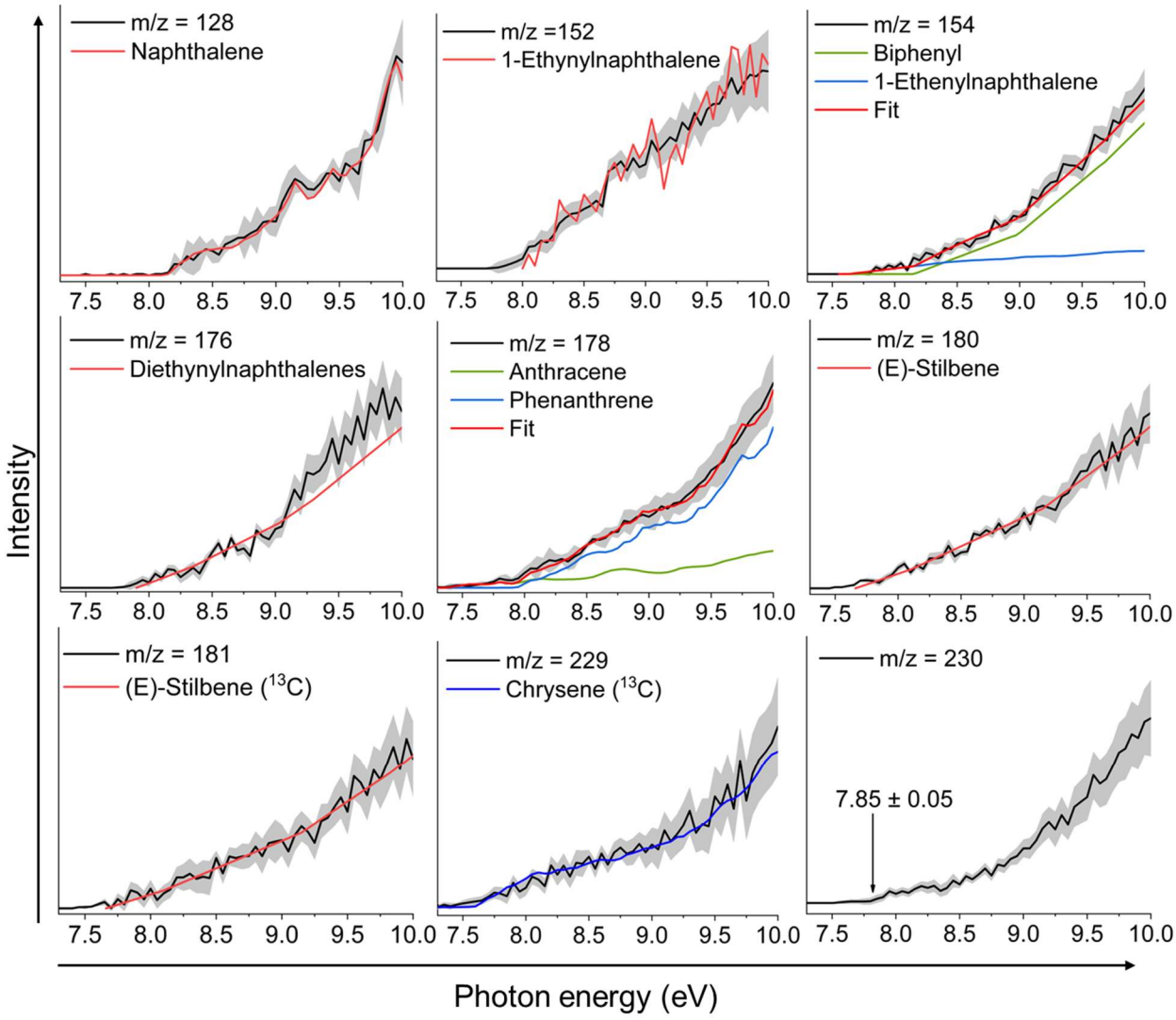


Figure S2: Photoionization efficiency curves for the additional products in the range of m/z = 128 to 230. Black: experimental PIE curves; blue/green/red: reference PIE curves. In case of multiple contributions to one PIE curve, the red line resembles the overall fit. The error bars consist of two parts: ±10% based on the accuracy of the photodiode and a 1-σ error of the PIE curve averaged over the individual scans.

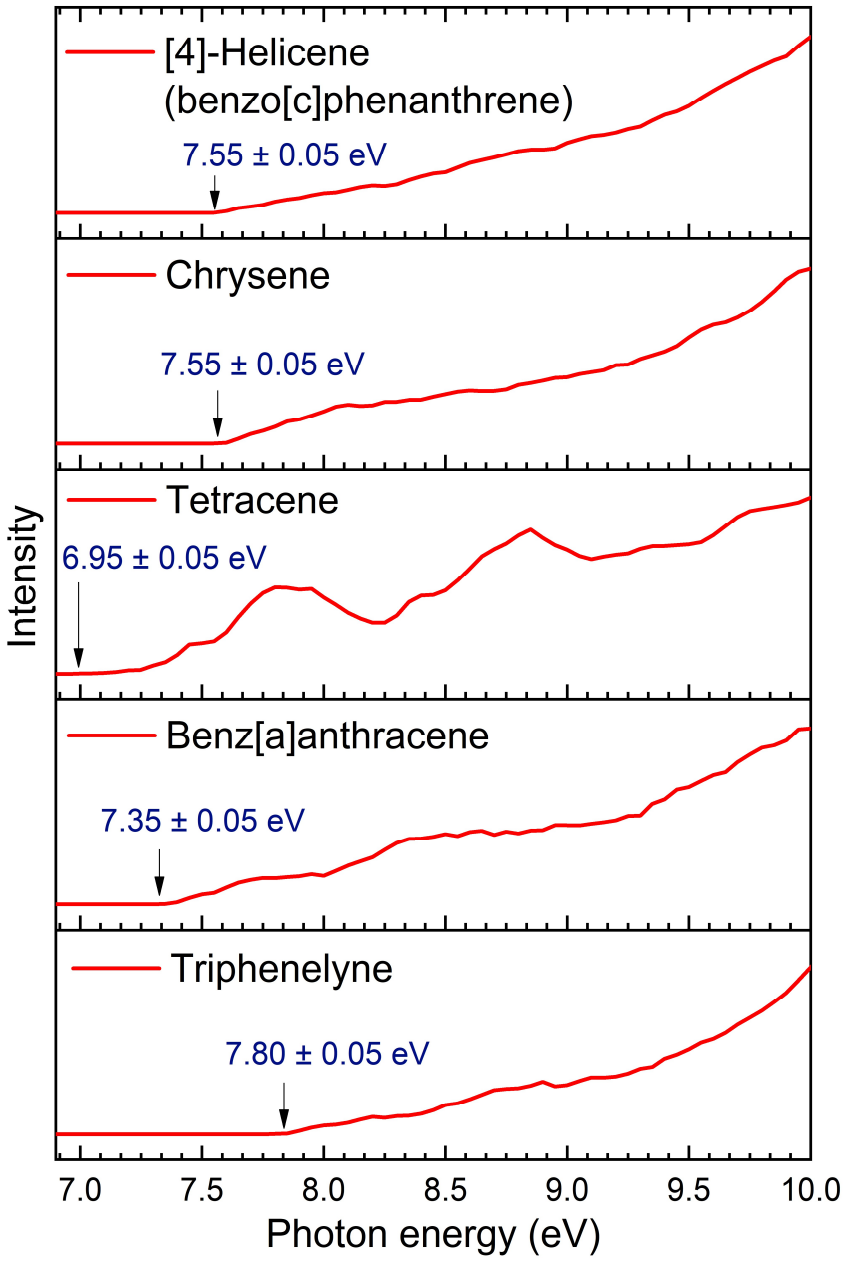


Figure S3: Reference PIE curves for plausible products at m/z = 228 ($C_{18}H_{12}$).

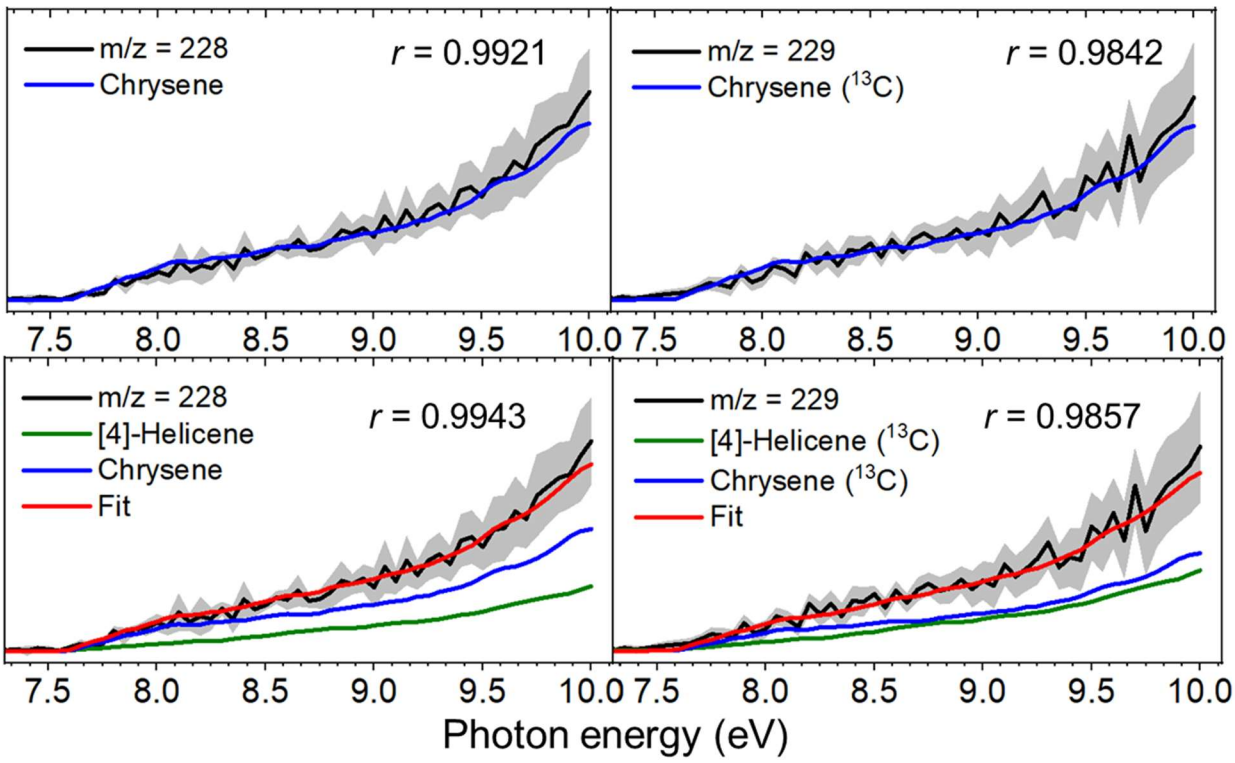
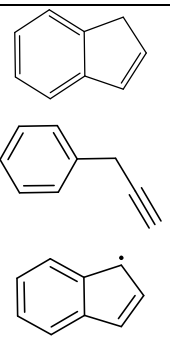
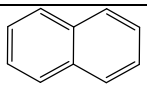
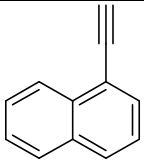
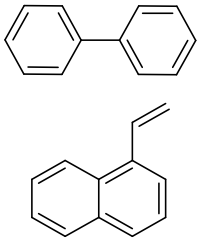
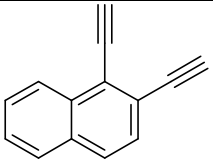
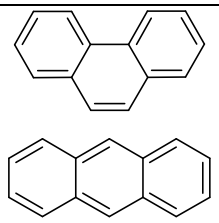
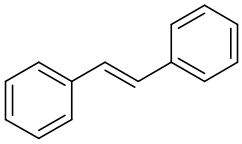
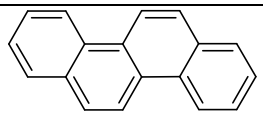
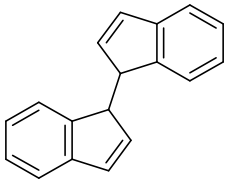


Figure S4: Most probable fits for the PIE curve recorded at m/z = 228 ($C_{18}H_{12}$) with corresponding Pearson correlation coefficients (*r*). Contribution from [4]-helicene may be considered; however, fitting with chrysene only achieves $r > 0.99$ suggesting an excellent fit already.

Table S1: Assignment of the mass-growth products from 1-indenyl self-recombination reaction.

Mass	Molecular formula	Name	Structure
116	C_9H_8	Indene 3-Phenyl-1-propyne Indenyl radical (^{13}C)	
128	$C_{10}H_8$	Naphthalene	
152	$C_{12}H_8$	1-Ethynylnaphthalene	
154	$C_{12}H_{10}$	Biphenyl 1-Ethenylnaphthalene	
176	$C_{14}H_8$	Diethynylnaphthalenes	
178	$C_{14}H_{10}$	Phenanthrene Anthracene	
180	$C_{14}H_{12}$	(E)-Stilbene	

228	$C_{18}H_{12}$	Chrysene	
230	$C_{18}H_{14}$	1H,1'H-1,1'-biindene (adduct)	

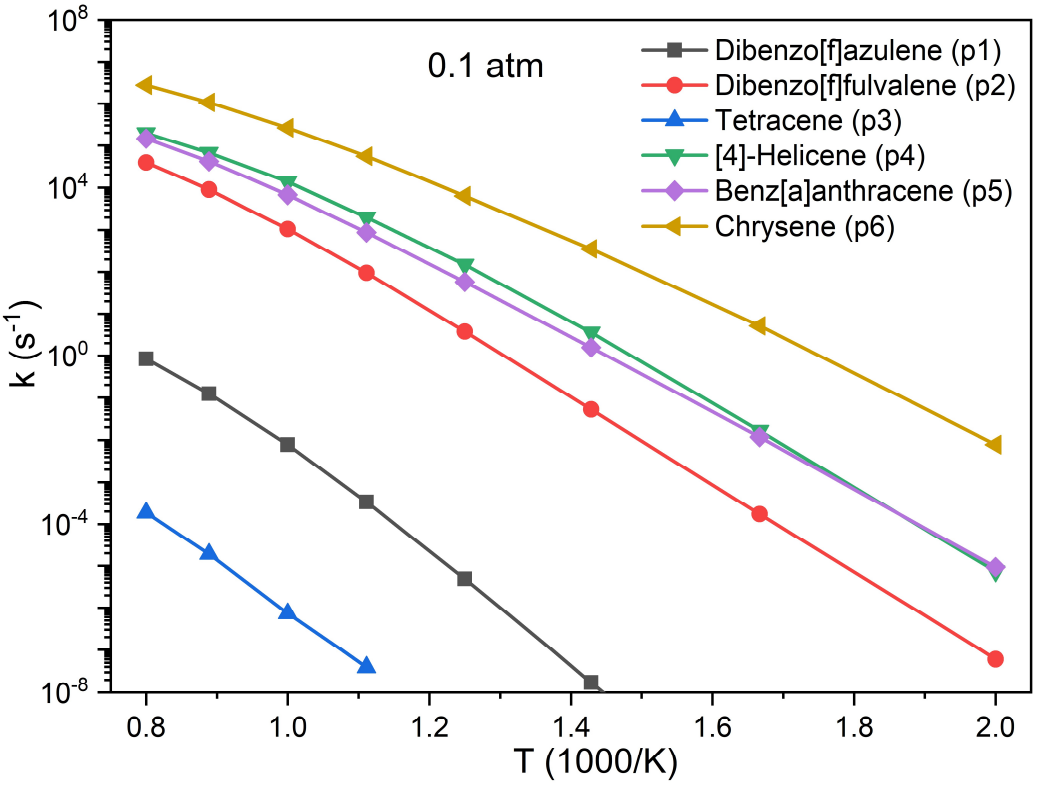


Figure S5: Calculated rate constants for the formation of $C_{18}H_{12}$ isomers at 0.1 atm pressure.

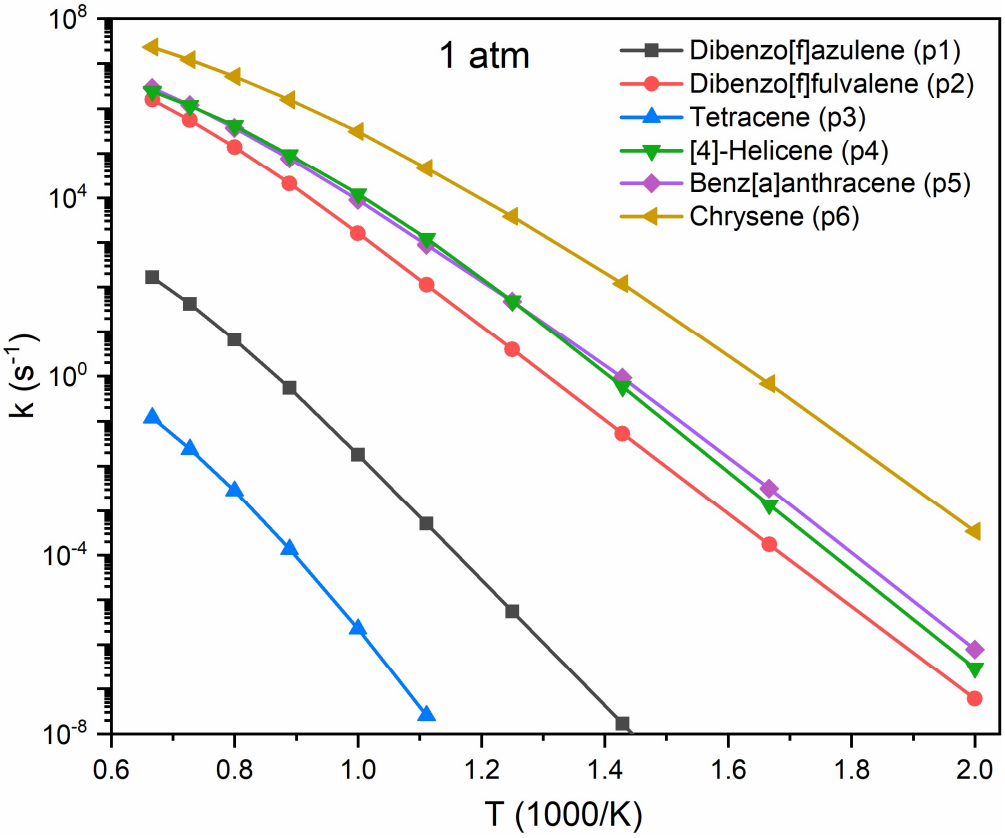


Figure S6: Calculated rate constants for the formation of $C_{18}H_{12}$ isomers at 1 atm pressure.

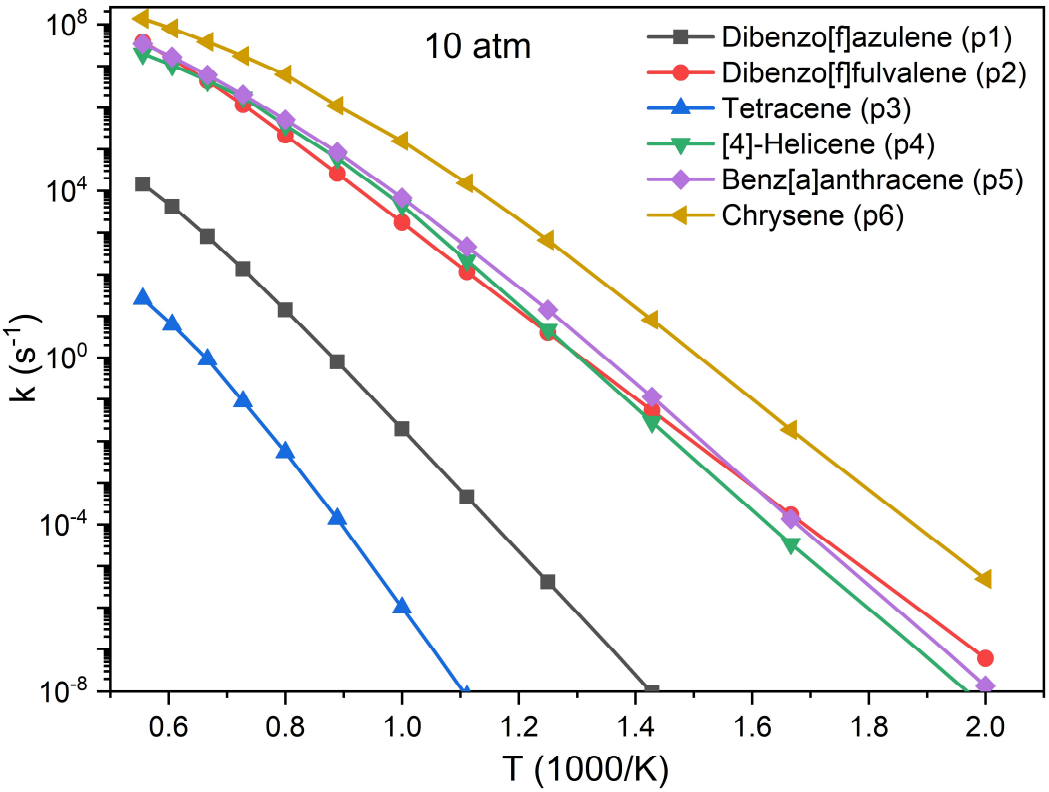


Figure S7: Calculated rate constants for the formation of $C_{18}H_{12}$ isomers at 10 atm pressure.

Data S1. Input file for RRKM-ME calculations of the unimolecular decomposition and dissociation on the $C_{18}H_{13}$ PES using the MESS package.

```
TemperatureList[K]              500. 600. 700. 800. 900. 1000. 1125. 1250. 1375. 1500. 1650. 1800. 2000. 2250.
2500.
PressureList[atm]               0.01 0.1 1. 10. 100.
EnergyStepOverTemperature       0.2     #Ratio of discretization energy step to T
ExcessEnergyOverTemperature     60
ModelEnergyLimit[kcal/mol]      600
WellCutoff                      10
ChemicalEigenvalueMax           0.2
ChemicalEigenvalueMin           1.e-6   #only for direct diagonalization method
CalculationMethod               direct
EigenvalueOutput                        eigenvalue.out
Model
EnergyRelaxation
Exponential
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]      390. 390.    ! N2
Sigmas[angstrom]    4.46 4.46    ! N2
Masses[amu]         28. 229.
End
OutputTemperatureStep[K]  100
OutputTemperatureSize  24
OutputReferenceEnergy[kcal/mol]  0.

!-------well_i1------------
Well    i1
Species
RRHO
Geometry[angstrom]   31
C    4.760984   -0.095444    0.347612
C    4.020995   -1.091527    0.979828
C    2.620831   -1.114701    0.884224
C    1.981126   -0.126546    0.147567
C    2.740674    0.893426   -0.500234
C    4.124018    0.908310   -0.399325
C    0.574608    0.131713   -0.136197
C    0.507792    1.285314   -0.942654
C    1.794956    1.764063   -1.175751
C   -0.565395   -0.738430    0.312782
```

C -0.846159 -1.882211 -0.659271
C -2.135138 -1.885962 -1.033938
C -2.845806 -0.780308 -0.385999
C -1.925631 -0.072119 0.411268
C -4.580935 0.733895 0.286730
C -3.666608 1.436310 1.073706
C -2.328323 1.034703 1.142000
C -4.179607 -0.381195 -0.450057
H 5.841744 -0.094376 0.433012
H 4.530925 -1.857796 1.552513
H 2.057931 -1.897054 1.382955
H 4.710124 1.680014 -0.887373
H -0.406246 1.726543 -1.312719
H 2.054194 2.637860 -1.758414
H -0.304377 -1.170234 1.290570
H -0.075829 -2.569458 -0.981457
H -2.595775 -2.594191 -1.711510
H -5.614435 1.059866 0.247660
H -3.997199 2.301120 1.637906
H -1.621614 1.586153 1.752855
H -4.893740 -0.924199 -1.059752
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
17.9217 56.1214 64.0295
144.1633 156.5009 202.8618
220.1822 230.6421 331.5360
394.5046 414.1621 417.4183
441.1716 466.8458 546.0861
557.8704 559.3060 572.0141
595.0381 641.0493 641.9078
710.3761 726.6872 734.3573
747.6831 755.6488 760.7509
782.8670 788.2668 838.1221
860.9716 867.5408 872.4795
879.8905 893.6981 895.5573
941.0549 948.7851 959.4537
977.2385 979.3283 989.8322
1024.7196 1039.9945 1042.7474
1049.8256 1088.1358 1094.3616
1132.1956 1171.8634 1179.6638
1182.8807 1189.0901 1191.5109
1205.2999 1228.4270 1262.5167
1299.9641 1304.5667 1322.6314
1343.0596 1371.4597 1384.1766
1422.4094 1451.2174 1487.2346
1488.9053 1490.9249 1492.8950

1599.9822 1616.0947 1623.8797
1635.3896 1648.8387 2983.7517
3157.7951 3159.3656 3163.5099
3166.9291 3174.6770 3176.1592
3187.1953 3188.3738 3190.4376
3206.2899 3220.0611 3229.0073
ZeroEnergy[kcal/mol] 23.6
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i1-1----------
Well i1-1
Species
RRHO
Geometry[angstrom] 31
C -4.661100 0.007281 -0.389323
C -4.048497 -1.246622 -0.433468
C -2.670260 -1.374462 -0.234657
C -1.919275 -0.231909 0.008082
C -2.538368 1.039341 0.053462
C -3.911285 1.159752 -0.145535
C -0.468635 -0.037685 0.253178
C -0.304190 1.423930 0.435243
C -1.501328 2.035517 0.320872
C 0.563359 -0.979050 -0.404307
C 0.322182 -1.131386 1.074035
C 1.560042 -0.715136 1.746616
C 2.511093 -0.312612 0.781681
C 1.955810 -0.472631 -0.527315
C 4.552661 0.494060 -0.217189
C 4.003168 0.318995 -1.495809
C 2.696019 -0.159372 -1.653262
C 3.822277 0.191464 0.922806
H -5.731118 0.085759 -0.546416
H -4.646985 -2.130255 -0.624366
H -2.207607 -2.355755 -0.272224
H -4.392849 2.131332 -0.113470
H 0.643946 1.902780 0.630007
H -1.680397 3.099161 0.410089
H 0.160664 -1.670282 -1.135207
H -0.311943 -1.904070 1.490923
H 1.693292 -0.690270 2.819426
H 5.565468 0.869551 -0.121506
H 4.596192 0.559428 -2.370660
H 2.274618 -0.280656 -2.645384
H 4.254678 0.326423 1.908131

Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
57.8675 65.9235 84.6353
148.8900 177.7289 240.7037
253.4386 273.0018 338.4758
406.1789 427.9593 444.7512
455.1260 499.6779 536.8064
551.0791 574.9017 587.9005
607.6154 631.5378 645.0190
672.3369 697.6986 742.8014
749.4713 757.6295 763.3148
769.4172 788.1435 809.0756
847.9576 861.4350 871.8104
873.6033 880.9352 892.0655
937.2614 942.0923 946.5004
949.6353 981.5497 981.6108
1003.2801 1029.7240 1034.4868
1043.7144 1072.1562 1096.0503
1120.6841 1137.6767 1167.9241
1178.6726 1192.2964 1197.9021
1207.1840 1236.1859 1241.8393
1270.9681 1310.7102 1320.5054
1333.2078 1346.5595 1351.9138
1391.8701 1402.8338 1460.8713
1480.0658 1491.2620 1500.6557
1585.3641 1587.6642 1611.8019
1626.1445 1644.8838 3153.4833
3160.7419 3161.5001 3162.2376
3167.4022 3171.8593 3173.1630
3177.4812 3186.2854 3188.9256
3199.4269 3212.7877 3234.0822
ZeroEnergy[kcal/mol] 37.4
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i1-2----------
Well i1-2
Species
RRHO
Geometry[angstrom] 31
C -4.829549 -0.385077 0.107602
C -4.462339 0.988205 0.360891
C -3.175905 1.415219 0.232094
C -2.171966 0.482237 -0.185023

C -2.524419 -0.942932 -0.332851
C -3.906339 -1.325403 -0.230622
C -0.824703 0.615094 -0.420433
C -0.230582 -0.763731 -0.556693
C -1.381517 -1.688865 -0.495237
C 0.680631 -0.258480 0.714938
C 0.284284 1.228804 0.420934
C 1.513500 1.800478 -0.228032
C 2.585657 0.891826 -0.142043
C 2.154969 -0.333825 0.459500
C 4.816926 -0.020317 -0.307142
C 4.384808 -1.209748 0.297070
C 3.043560 -1.369164 0.676447
C 3.938498 1.028666 -0.534143
H -5.874001 -0.662836 0.200383
H -5.241075 1.686515 0.646798
H -2.914258 2.454429 0.400355
H -4.198043 -2.355334 -0.406066
H 0.447972 -0.959537 -1.388706
H -1.343424 -2.744061 -0.733492
H 0.312976 -0.675681 1.649144
H -0.071426 1.830365 1.263149
H 1.563043 2.790758 -0.661957
H 5.856925 0.079616 -0.598048
H 5.092369 -2.012558 0.469054
H 2.713072 -2.296706 1.132320
H 4.282797 1.947099 -0.996468
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
48.4659 78.6840 97.8849
140.2239 172.2614 224.2958
276.9687 285.8229 337.6865
402.1697 444.9261 447.3524
460.5935 509.6952 541.4304
549.4119 561.6220 571.8677
600.8802 645.6717 661.0900
704.7810 730.6103 738.4425
755.8790 761.6406 767.5967
780.9835 796.0958 811.6441
847.2777 857.1740 865.9823
868.3142 873.8800 892.5730
939.8263 961.6907 972.2422
979.6386 989.5592 994.9180
1008.5505 1032.0659 1037.3634
1069.1397 1110.5800 1132.7220
1142.2091 1159.8972 1168.1251

1177.5054 1181.8920 1184.9097
1208.0116 1214.4061 1234.1356
1249.8434 1285.0298 1293.6967
1297.9904 1338.3333 1366.7069
1385.8350 1401.5021 1439.9632
1455.9012 1495.8039 1510.8579
1560.6789 1578.8077 1586.7562
1602.5355 1666.8174 3037.1002
3087.7571 3130.6090 3156.7721
3159.7667 3163.7398 3165.4617
3175.6965 3177.6326 3185.6556
3188.7533 3197.7272 3200.5132
ZeroEnergy[kcal/mol] 70.0
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i2-1----------
Well i2-1
Species
RRHO
Geometry[angstrom] 31
C -4.227107 -1.330944 0.033450
C -3.118480 -2.059758 0.467288
C -1.848670 -1.473593 0.501616
C -1.715113 -0.155832 0.096405
C -2.829718 0.582138 -0.342752
C -4.093975 -0.002925 -0.375763
C -0.455711 0.722925 0.037943
C -1.053527 2.034062 -0.495874
C -2.375715 1.928651 -0.700411
C 0.560044 0.175241 -0.928531
C 0.128079 0.936056 1.416927
C 1.413710 0.692407 1.715080
C 2.362819 0.189901 0.739027
C 1.895797 -0.067352 -0.597035
C 4.589854 -0.546490 0.107108
C 4.144862 -0.804327 -1.200311
C 2.829625 -0.572424 -1.547793
C 3.698079 -0.055588 1.058734
H -5.203256 -1.802877 0.014557
H -3.243255 -3.090084 0.781084
H -0.987875 -2.040247 0.839557
H -4.958856 0.559056 -0.711682
H -0.433798 2.903656 -0.667886
H -3.024047 2.712492 -1.072704
H 0.211889 -0.024790 -1.936350

```
H     -0.556035    1.309368    2.171332
H      1.774719    0.869383    2.724078
H      5.623729   -0.729986    0.375273
H      4.839186   -1.187676   -1.939836
H      2.486830   -0.772039   -2.557633
H      4.041660    0.140863    2.069563
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  87
36.9129              62.9955              81.5317
166.9718             184.5181             226.5870
263.7073             283.9962             328.9561
358.6806             402.5307             437.6552
456.2673             485.9547             506.4793
538.5624             551.9303             579.6724
591.9436             600.2143             618.6886
670.5258             715.5744             722.5079
747.3538             752.2082             758.4017
768.5808             778.5516             803.1649
803.6849             855.3615             866.8313
868.8700             888.9958             910.8258
942.1524             951.7324             966.9873
975.2868             980.2315             990.5706
990.9994            1032.3502            1042.3696
1043.1234            1089.4231            1129.4478
1135.9948            1144.1463            1165.8912
1175.6353            1182.1433            1201.8700
1226.3698            1246.4384            1254.2330
1293.4956            1295.6550            1334.7663
1341.3558            1382.2638            1405.5358
1421.8767            1456.1487            1482.2719
1489.9225            1499.7553            1559.9660
1597.2837            1602.6375            1633.1765
1643.5457            1662.4302            3147.2914
3155.9922            3159.7184            3160.2059
3167.2245            3168.0458            3174.4659
3175.2503            3177.1018            3187.4979
3188.5143            3188.5949            3218.7461
ZeroEnergy[kcal/mol] 25.7
ElectronicLevels[1/cm]       1
0  2
End
End
!----------------------------------
!-------well_i2x1------------
Well       i2x1
Species
```

RRHO
Geometry[angstrom] 31
C 0.953026 -1.028620 1.121102
C 1.868983 -2.030027 1.277979
C 3.075360 -2.070836 0.521518
C 3.411295 -1.020422 -0.329900
C 2.533579 0.045824 -0.490348
C -0.009503 0.368613 -0.890681
C 0.627533 1.442299 -0.013030
C -2.089708 0.519384 0.493828
C -0.229907 2.039209 1.024773
C -2.049122 -0.962496 -1.428640
C -3.402044 0.100856 0.754106
C -4.029157 -0.838215 -0.055928
C -3.352680 -1.364692 -1.157134
C -1.393036 -0.041870 -0.604610
C 1.182062 -0.010936 0.106188
C 2.763965 1.366735 -1.004664
C 1.728747 2.188512 -0.688660
C -1.465090 1.577297 1.281878
H 0.033405 -1.021499 1.692644
H 1.679251 -2.814481 2.002690
H 3.764500 -2.894817 0.663502
H 4.384559 -0.996815 -0.810003
H 0.298105 0.336854 -1.930637
H 0.178920 2.868005 1.593154
H -1.521131 -1.377245 -2.280950
H -3.933406 0.530651 1.597237
H -5.043523 -1.152316 0.162138
H -3.838646 -2.091295 -1.798423
H 3.656576 1.662143 -1.541488
H 1.652436 3.241114 -0.929889
H -2.056878 2.026012 2.073359
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
65.1358 85.4653 110.6804
174.1994 191.4041 216.8904
257.5954 335.7026 357.7061
392.4690 412.5392 424.9164
455.0453 496.2380 506.5739
520.0274 538.6147 558.8468
588.5722 621.9498 632.8575
663.1519 685.4029 701.5006
730.0892 741.2144 749.6161
764.2423 777.5311 803.9712
812.7144 819.9989 841.1816

886.4182 893.4212 912.6384
916.6822 937.3558 952.2601
966.3375 978.1401 984.7079
990.6865 1009.1874 1013.6810
1059.4799 1082.4323 1111.6757
1128.6226 1153.7088 1177.7257
1182.7737 1187.1344 1203.6641
1227.0953 1238.2347 1266.9025
1282.3080 1293.8309 1327.9676
1333.7361 1358.1972 1378.2152
1408.0650 1438.4566 1444.4352
1484.7291 1510.2795 1527.7996
1546.7813 1593.9362 1598.0967
1637.8561 1669.4456 3142.4791
3154.0605 3156.7067 3157.8025
3162.9656 3163.8703 3174.5526
3175.4071 3186.3080 3188.5374
3188.8922 3195.6626 3208.2994
ZeroEnergy[kcal/mol] 43.9
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i2x2----------
Well i2x2
Species
RRHO
Geometry[angstrom] 31
C -3.879492 -1.373062 -0.066885
C -3.625509 -0.089629 -0.523200
C -2.373498 0.522951 -0.319689
C -1.342778 -0.207476 0.321679
C -1.637742 -1.477592 0.820831
C -2.886852 -2.064861 0.628081
C -2.165544 1.903520 -0.679925
C 0.120268 1.879892 0.143552
C 1.264212 -0.348438 0.089358
C 3.697803 -0.364700 -0.037088
C 3.677039 -1.683636 -0.471902
C 2.455320 -2.321068 -0.670756
C 1.379039 2.501011 0.330443
C 2.517182 1.753918 0.484927
C -0.981292 2.548128 -0.404671
C 1.260141 -1.654160 -0.386835
C 2.504740 0.328751 0.223179
C 0.019740 0.424965 0.564405
H -4.850973 -1.826344 -0.228614

H -4.404662 0.472495 -1.027704
H -0.882224 -2.017537 1.380334
H -3.084537 -3.054506 1.023823
H -2.982703 2.440373 -1.148527
H 4.642985 0.156292 0.077248
H 4.606050 -2.204546 -0.674484
H 2.424489 -3.339095 -1.042374
H 1.442707 3.583899 0.278780
H 3.476476 2.240146 0.625784
H -0.871588 3.599179 -0.655273
H 0.322088 -2.168208 -0.546613
H 0.145246 0.446766 1.664600
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
66.0835 80.7121 117.3765
167.1978 198.0848 238.9122
257.0858 321.0726 362.6839
408.3295 419.4260 427.8240
448.3684 497.0811 512.4555
524.9502 539.0217 560.5900
567.8995 624.8168 663.6817
694.4054 701.6768 733.1133
749.5803 752.1156 767.8711
797.3246 802.1358 810.0241
827.9043 854.5189 887.0029
894.2117 932.0572 935.6840
947.4967 953.3805 959.6153
967.8962 987.2407 993.8017
1061.3687 1066.4352 1104.9876
1128.5433 1144.0441 1149.8897
1173.8344 1183.0005 1186.8886
1211.5516 1221.3755 1229.2493
1238.0179 1240.3608 1290.9588
1295.0757 1320.7627 1326.8910
1336.3062 1360.6499 1401.3211
1443.3144 1456.4879 1479.4191
1503.3007 1517.4673 1527.8964
1560.4402 1603.8495 1612.6804
1630.2375 1634.0072 2875.7716
3148.7409 3152.2184 3157.1596
3157.8940 3165.8914 3169.3152
3173.6253 3175.9008 3177.7215
3184.9722 3189.0682 3204.9889
ZeroEnergy[kcal/mol] 11.9
ElectronicLevels[1/cm] 1
0 2

End
End
!----------
!-------well_i2-2----------
Well i2-2
Species
RRHO
Geometry[angstrom] 31
C 4.771981 -0.313530 -0.410294
C 4.329883 0.971869 -0.806233
C 3.008562 1.357241 -0.628469
C 2.108454 0.462745 -0.037501
C 2.552453 -0.850617 0.369948
C 3.909817 -1.220654 0.166259
C 0.716888 0.601885 0.293012
C 0.242008 -0.710284 0.888537
C 1.485449 -1.557666 0.917361
C -0.830234 -1.210874 -0.037634
C -0.087874 1.720906 0.252618
C -1.474182 1.748776 0.466976
C -2.407637 0.715782 0.291006
C -2.065717 -0.622721 -0.188434
C -4.771815 0.235463 -0.144313
C -4.415732 -0.991597 -0.783713
C -3.115035 -1.386272 -0.825844
C -3.801980 1.052645 0.357077
H 5.809999 -0.584375 -0.569362
H 5.035631 1.658367 -1.259509
H 2.679563 2.340245 -0.947189
H 4.256424 -2.203966 0.464110
H -0.174552 -0.549837 1.895439
H 1.517210 -2.569976 1.297655
H -0.624195 -2.120922 -0.592906
H 0.389882 2.676914 0.053971
H -1.906698 2.731446 0.636005
H -5.813475 0.531638 -0.095171
H -5.189135 -1.611113 -1.223457
H -2.843185 -2.333657 -1.279349
H -4.069210 2.016653 0.777616
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
48.1673 73.7185 112.9277
167.7332 185.7833 211.4566
257.2282 283.1000 311.2621
359.4469 421.3160 433.5489
451.0962 473.8977 514.6371

527.9894 544.3595 553.5661
570.6855 604.0396 608.2965
658.2648 683.1417 712.8788
732.2411 748.9401 750.8765
758.2486 769.5544 785.3437
824.6528 842.1034 856.8075
863.7793 879.4014 917.7203
921.1626 946.8431 965.2703
977.9147 981.5652 984.2826
1022.4453 1024.9034 1039.0689
1090.1035 1108.3168 1138.6955
1142.1475 1165.5349 1182.0934
1193.6959 1204.2031 1222.0549
1238.6734 1246.9535 1268.2293
1309.7035 1318.6399 1331.4491
1366.4418 1377.0842 1410.3036
1419.9895 1429.8507 1460.7074
1480.1739 1510.9243 1543.2336
1564.7591 1583.8083 1595.8781
1605.3419 1656.7064 2949.6064
3130.5129 3147.1980 3151.9661
3156.8811 3161.4891 3162.0087
3168.8348 3175.6169 3179.2047
3188.1492 3189.4359 3207.1736
ZeroEnergy[kcal/mol] 43.3
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i4-2----------
Well i4-2
Species
RRHO
Geometry[angstrom] 31
C -4.552617 -0.879702 -0.146681
C -3.689032 -1.913699 0.215802
C -2.327664 -1.667837 0.353169
C -1.795615 -0.388996 0.137555
C -2.678802 0.664037 -0.213335
C -4.045084 0.396523 -0.359508
C -0.355582 -0.100126 0.220088
C -0.892783 2.331903 -0.103283
C -2.143176 2.005498 -0.442017
C 0.602701 -1.029129 -0.010667
C 0.027608 1.327268 0.565098
C 1.481051 1.624982 0.362693
C 2.435493 0.636361 0.137883

C 2.013575 -0.731621 -0.022999
C 4.750061 -0.076401 -0.171813
C 4.329147 -1.412153 -0.313325
C 2.976060 -1.723065 -0.244845
C 3.828913 0.925745 0.042221
H -5.614571 -1.067869 -0.256109
H -4.077745 -2.909082 0.398833
H -1.669508 -2.474070 0.655665
H -4.711759 1.205443 -0.640484
H -0.514436 3.337845 -0.252616
H -2.805208 2.744815 -0.882194
H 0.313462 -2.047167 -0.252215
H -0.173304 1.442260 1.656094
H 1.797330 2.658471 0.467085
H 5.805838 0.163686 -0.231624
H 5.058829 -2.195530 -0.481558
H 2.650801 -2.751205 -0.368724
H 4.154744 1.954873 0.151633
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
55.9969 61.0195 124.3296
148.9956 199.0787 217.7275
277.4596 291.2711 346.1570
373.6946 412.7954 426.3885
452.7213 491.0737 518.0916
523.8266 547.0630 555.9501
579.9331 619.2733 639.1999
677.0963 695.8357 700.9403
742.4696 754.5312 759.4777
768.9383 785.4716 794.9880
835.9130 858.9092 871.6135
889.2783 906.9345 915.7472
947.7336 955.4174 964.7426
976.3464 981.5081 990.5648
1041.0227 1046.0081 1064.0817
1087.7083 1135.1735 1143.6470
1163.1247 1178.2498 1184.5999
1199.2177 1225.7167 1227.7386
1235.7087 1265.9015 1283.1966
1291.7385 1323.9393 1333.1545
1347.4277 1379.6955 1415.5410
1420.5324 1450.4263 1483.1363
1498.1168 1512.1715 1558.1625
1596.5801 1605.3029 1627.0300
1648.7891 1688.2097 2783.1405
3149.1278 3152.7827 3154.9458

```
3157.4604            3158.8443            3161.4616
3167.8668            3172.1627            3174.7783
3179.7542            3188.8597            3190.2891
ZeroEnergy[kcal/mol] 20.0
ElectronicLevels[1/cm]       1
0  2
End
End
!-----------------------------------
!-------well_i44-2------------
Well       i44-2
Species
RRHO
Geometry[angstrom]   31
C     4.573770   -0.187465   -0.621309
C     3.973100    0.977639   -1.117481
C     2.628573    1.261864   -0.838014
C     1.905455    0.383702   -0.052416
C     2.511407   -0.801595    0.471542
C     3.859723   -1.083006    0.162939
C     0.476259    0.442193    0.375125
C     0.272040   -0.821559    1.223293
C     1.572225   -1.506794    1.257823
C    -0.411893   -0.705943   -0.155425
C    -0.206416    1.705898    0.698969
C    -1.544532    1.821414    0.683817
C    -2.422323    0.748213    0.229127
C    -1.865787   -0.461445   -0.250900
C    -4.639106   -0.044457   -0.378593
C    -4.083158   -1.218126   -0.888977
C    -2.707293   -1.416053   -0.830417
C    -3.811733    0.930057    0.164853
H     5.613687   -0.389372   -0.853802
H     4.552177    1.662247   -1.726539
H     2.165193    2.157799   -1.237553
H     4.333178   -1.980513    0.545808
H    -0.386070   -0.805781    2.083977
H     1.762231   -2.422944    1.800874
H     0.015475   -1.338635   -0.926330
H     0.417759    2.550801    0.971099
H    -2.009819    2.760429    0.966024
H    -5.711075    0.112869   -0.416466
H    -4.720603   -1.978695   -1.325632
H    -2.276493   -2.332259   -1.221292
H    -4.237503    1.856837    0.536098
Core  RigidRotor
SymmetryFactor  0.5
End
```

Frequencies[1/cm] 87
59.7271 88.6230 100.7093
166.2093 193.2150 252.2542
275.6307 294.9744 368.1309
386.0963 416.7671 438.2673
461.1033 510.5575 534.4676
538.4802 554.2670 564.1288
600.6660 621.4185 639.8398
682.2182 693.9410 722.6649
742.4461 747.8934 760.5430
772.8985 791.2363 808.1259
830.2502 868.8766 873.6706
880.5443 886.4441 926.4266
942.5791 951.3503 974.4652
977.7388 983.0391 990.0048
994.1494 1033.9961 1058.3486
1063.7249 1080.0249 1120.2704
1137.7219 1161.4992 1171.8007
1182.9626 1208.6940 1221.4517
1233.7279 1239.1561 1255.8450
1275.3573 1299.6426 1332.2805
1335.1339 1337.5384 1369.8404
1388.8761 1438.0324 1458.8680
1485.1775 1499.5819 1513.5615
1586.3218 1597.9966 1607.6738
1640.1488 1672.9133 3142.7957
3152.8208 3155.9595 3159.0563
3160.3133 3163.9057 3165.7099
3172.9796 3173.9607 3176.1580
3187.6349 3187.9720 3206.0610
ZeroEnergy[kcal/mol] 31.5
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i4-22----------
Well i4-22
Species
RRHO
Geometry[angstrom] 31
C -4.678419 -0.114420 -0.026830
C -4.206128 1.177140 0.222741
C -2.842326 1.424286 0.274668
C -1.903122 0.389982 0.091049
C -2.392330 -0.924579 -0.156646
C -3.771784 -1.150019 -0.218438
C -0.467795 0.613572 0.107366

C -0.129805 -1.849807 -0.172831
C -1.437862 -1.997192 -0.408514
C 0.418286 -0.573128 0.437742
C 0.107266 1.853642 -0.153081
C 1.476684 2.039187 -0.242092
C 2.396869 0.944862 -0.101939
C 1.908032 -0.350219 0.196797
C 4.671855 0.079651 -0.128644
C 4.189351 -1.191635 0.186644
C 2.819609 -1.394096 0.347688
C 3.784004 1.133723 -0.267946
H -5.744074 -0.307843 -0.069693
H -4.905906 1.989356 0.384652
H -2.495651 2.427363 0.492333
H -4.130407 -2.153847 -0.422395
H 0.560409 -2.659547 -0.375115
H -1.820727 -2.932788 -0.804349
H 0.320746 -0.713761 1.536092
H -0.540061 2.700942 -0.350348
H 1.874117 3.020787 -0.474329
H 5.735815 0.243291 -0.257604
H 4.875485 -2.021624 0.310532
H 2.465584 -2.385062 0.609847
H 4.150363 2.127025 -0.506028
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
40.0006 70.9184 126.6807
158.6523 197.3237 211.1007
264.8176 282.3687 371.3101
382.5165 413.3728 444.5977
464.4068 493.1077 511.0123
534.9399 542.7547 558.0051
569.7968 578.0713 653.1116
687.1093 690.2763 724.5142
743.6216 750.5332 768.5678
787.3014 799.4738 822.3517
849.3178 868.2686 870.6320
884.1851 894.2356 943.3355
951.4547 956.0999 975.8719
985.9476 986.5395 1003.0341
1041.4626 1061.5873 1064.6123
1129.2060 1141.5289 1151.9529
1178.8034 1182.6630 1186.6295
1205.2629 1226.0242 1233.6928
1238.8740 1253.3341 1263.2233
1305.6486 1320.1116 1331.2478

1338.8154 1349.3219 1416.6788
1434.7635 1459.8936 1480.8530
1493.3140 1523.9256 1529.3504
1584.6302 1603.9240 1629.2780
1630.5406 1681.6249 2825.1791
3152.7917 3157.8874 3158.4954
3161.6852 3164.0709 3168.0846
3175.2966 3179.4229 3183.5837
3187.8459 3190.7218 3191.7687
ZeroEnergy[kcal/mol] 13.1
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i444----------
Well i444
Species
RRHO
Geometry[angstrom] 31
C 4.512335 -0.934640 -0.078686
C 3.601137 -1.869335 -0.559400
C 2.246109 -1.549287 -0.599919
C 1.770538 -0.307948 -0.165427
C 2.693961 0.636935 0.342727
C 4.055802 0.300025 0.366585
C 0.308021 -0.034445 -0.274762
C 1.092105 2.423581 1.084491
C 2.302585 1.947252 0.894483
C -0.603242 -0.750230 0.472485
C -0.174185 0.919952 -1.216529
C -1.518579 1.129351 -1.382989
C -2.472446 0.411982 -0.614053
C -2.000942 -0.547690 0.335277
C -4.762130 -0.106736 0.007245
C -4.296481 -1.054732 0.947827
C -2.948662 -1.269453 1.106863
C -3.869990 0.608349 -0.755184
H 5.571142 -1.165177 -0.045777
H 3.939021 -2.838573 -0.908177
H 1.534731 -2.267597 -0.991767
H 4.763763 1.023857 0.757031
H 0.659609 3.334075 1.470222
H 3.149700 2.573088 1.200681
H -0.250708 -1.480292 1.193739
H 0.541334 1.472091 -1.814446
H -1.870748 1.850904 -2.113078
H -5.828165 0.053104 -0.109348

H -5.009881 -1.612526 1.544102
H -2.590123 -1.996513 1.828211
H -4.225288 1.335983 -1.477605
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
25.1847 54.6371 65.6968
99.0978 145.3920 184.4803
187.4799 219.4316 248.3886
288.0980 350.6605 395.6645
418.2078 453.4513 470.0758
486.7483 523.1846 534.0416
563.5603 582.0183 583.4694
640.5750 649.3158 674.3373
690.7834 756.2244 760.9200
769.6876 775.2477 783.7305
786.2350 831.4110 848.1895
858.4654 872.3459 895.3422
904.9302 914.6918 958.3290
961.2132 963.0772 978.1023
992.8388 994.7280 1037.2402
1045.2890 1073.8338 1133.9879
1153.9817 1171.6953 1180.0753
1185.7694 1212.1755 1216.0659
1244.3254 1260.5566 1285.6354
1294.3612 1309.2897 1329.2645
1374.0113 1394.2320 1402.5760
1461.9837 1470.9638 1497.0683
1519.9411 1538.6163 1599.6677
1606.8269 1636.8661 1641.3304
1654.0357 1667.5861 3010.9572
3156.3394 3157.4817 3159.5072
3161.6462 3165.6013 3166.9585
3174.4444 3177.6108 3186.4710
3187.3332 3189.6188 3244.6484
ZeroEnergy[kcal/mol] 47.5
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i5-2----------
Well i5-2
Species
RRHO
Geometry[angstrom] 31
C 4.843883 -0.704030 -0.379906

C 4.849463 0.720981 -0.306054
C 3.682602 1.407953 -0.090470
C 2.443567 0.729731 0.078384
C 2.437342 -0.729877 0.041177
C 3.682341 -1.402264 -0.222405
C 1.226834 1.421172 0.178494
C -0.000016 -0.714986 0.648729
C 1.264068 -1.415437 0.247026
C -1.264016 -1.415449 0.246795
C -0.000005 0.769149 0.309679
C -1.226856 1.421172 0.178638
C -2.443591 0.729728 0.078523
C -2.437336 -0.729901 0.041048
C -4.849482 0.720939 -0.305925
C -4.843866 -0.704021 -0.380040
C -3.682279 -1.402258 -0.222650
C -3.682633 1.407920 -0.090194
H 5.774635 -1.230280 -0.559968
H 5.782683 1.257837 -0.431503
H 3.685877 2.492603 -0.054690
H 3.679337 -2.486086 -0.272385
H -0.000153 -0.735871 1.770751
H 1.253603 -2.500108 0.208521
H -1.253522 -2.500112 0.208068
H 1.233560 2.502428 0.072221
H -1.233597 2.502436 0.072449
H -5.782686 1.257845 -0.431287
H -5.774567 -1.230319 -0.560219
H -3.679303 -2.486072 -0.272828
H -3.685988 2.492565 -0.054220
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 87
50.1797 65.1430 141.3208
144.6522 200.7245 253.9998
258.2640 293.1431 313.9394
353.7309 428.5667 448.9042
456.3852 478.3525 491.9236
511.6860 538.1637 544.6138
602.8714 623.7317 623.7990
671.2525 704.7753 709.8585
727.3689 746.1209 750.2799
755.8374 756.1206 783.3843
815.8991 836.5941 848.4297
866.3804 866.6694 900.4510
907.0139 934.0889 939.1757
960.1703 961.0867 983.5816

983.6307 1018.8541 1034.4664
1077.6828 1091.7707 1151.1505
1153.1123 1175.5545 1185.0253
1192.0749 1204.8060 1220.6398
1238.1914 1265.1706 1286.6680
1298.8456 1300.0838 1344.8334
1372.1618 1393.5021 1398.0261
1414.1409 1438.9305 1462.3000
1476.1677 1498.7869 1544.9439
1545.1453 1580.4223 1587.4693
1633.7048 1636.7145 2683.4654
3146.2801 3149.9459 3156.2793
3157.3194 3158.0674 3160.2324
3162.1385 3163.4131 3175.8824
3175.9699 3188.6308 3188.8827
ZeroEnergy[kcal/mol] 36.3
ElectronicLevels[1/cm] 1
0 2
End
End
!----------
!-------well_i555-2----------
Well i555-2
Species
RRHO
Geometry[angstrom] 31
C 4.702085 -0.615724 -0.215114
C 4.555921 0.634837 -0.812855
C 3.320675 1.265858 -0.770908
C 2.191322 0.693802 -0.158556
C 2.324336 -0.614853 0.403396
C 3.604228 -1.211110 0.384421
C 0.992033 1.560794 -0.157398
C -0.075972 -1.438938 0.774462
C 1.275939 -1.383642 1.065826
C -0.707524 -0.990112 -0.380338
C -0.145592 1.495788 0.493154
C -1.358284 1.445796 0.988674
C -2.434663 0.631223 0.375604
C -2.117397 -0.544156 -0.355123
C -4.784538 0.303547 -0.140088
C -4.469389 -0.825268 -0.892774
C -3.143835 -1.242135 -0.996472
C -3.773053 1.023886 0.487881
H 5.660870 -1.121485 -0.218780
H 5.397364 1.120675 -1.293234
H 3.219230 2.253372 -1.208696
H 3.713406 -2.188903 0.841915

```
H      1.081022    2.408512   -0.838221
H     -0.721512   -1.827730    1.560982
H      1.616770   -1.970222    1.915351
H     -0.121647   -0.824836   -1.279489
H     -1.598532    1.992747    1.898459
H     -5.815193    0.627408   -0.048297
H     -5.253000   -1.386738   -1.388841
H     -2.899541   -2.135714   -1.560303
H     -4.016971    1.915361    1.056404
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  87
37.6057              79.7305              92.2821
131.0162             158.5746             218.0376
230.5854             263.2219             293.1122
331.2279             343.3294             365.5884
405.0798             415.0892             445.1077
460.0250             500.4850             514.9892
554.8317             562.5579             602.5043
643.0646             658.4119             683.1303
714.0124             719.6771             736.8690
751.0044             754.3689             768.1741
793.7680             800.9563             830.9523
863.9443             880.1651             883.6661
887.1063             906.2143             909.8418
958.8369             960.0555             987.3269
992.6746            1052.8346            1062.6949
1099.6531            1115.4169            1123.9238
1148.9673            1183.3805            1187.6071
1200.1172            1203.7003            1216.4938
1232.8250            1260.8573            1264.3254
1279.1024            1299.0813            1324.0671
1338.5314            1343.5077            1429.9779
1458.1916            1476.2534            1488.3134
1497.1593            1507.8974            1513.1368
1588.0253            1598.8439            1625.9948
1634.8325            2003.0409            3086.8636
3108.9249            3118.3896            3136.5310
3148.2207            3157.2066            3157.9673
3161.5458            3165.4854            3175.7386
3176.1747            3188.3774            3190.1245
ZeroEnergy[kcal/mol] 64.5
ElectronicLevels[1/cm]       1
0  2
End
End
!----------------------------------
```

!-------h_c18h12_p1------------
Bimolecular p1
Fragment c18h12
RRHO
Geometry[angstrom] 30
C -4.760265 -0.418079 0.163858
C -3.926136 -1.517266 0.351682
C -2.533555 -1.382751 0.290027
C -1.979596 -0.136857 0.015974
C -2.837251 0.984080 -0.136811
C -4.217355 0.848833 -0.072623
C -0.582251 0.360686 -0.074280
C -0.698213 1.811506 -0.249469
C -2.002096 2.168880 -0.316803
C 0.582256 -0.360645 -0.074491
C 0.698151 -1.811431 -0.250199
C 2.001919 -2.168915 -0.316396
C 2.837261 -0.984257 -0.136112
C 1.979586 0.136557 0.017289
C 4.760313 0.418179 0.163583
C 3.926292 1.517436 0.351344
C 2.533538 1.382684 0.290488
C 4.217385 -0.848797 -0.072868
H -5.835963 -0.542728 0.216528
H -4.356859 -2.490818 0.556052
H -1.915590 -2.249272 0.480935
H -4.864414 1.711179 -0.191984
H 0.136138 2.475961 -0.400778
H -2.380066 3.167760 -0.490678
H -0.136219 -2.475760 -0.402446
H 2.379855 -3.167778 -0.490437
H 5.836044 0.542819 0.215719
H 4.357087 2.491140 0.554826
H 1.915531 2.249449 0.479687
H 4.864553 -1.711006 -0.192585
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 84
45.4272 59.1553 88.4029
152.8262 194.4518 200.5744
241.2541 278.3335 351.2234
353.7573 411.8463 420.2243
426.7658 493.8782 553.2043
562.4395 575.6042 592.8130
605.3607 631.0651 660.1054
695.3550 733.6108 748.0692
750.1576 761.4986 769.7384

769.9093 805.4907 822.0973
868.0596 868.6065 887.1374
887.2519 894.6349 943.3841
944.2992 949.8148 950.6569
986.7868 987.1209 1043.3612
1045.4704 1074.2655 1080.4283
1089.2089 1111.3693 1127.9025
1139.5115 1179.6049 1185.1864
1203.0171 1212.9518 1216.8156
1233.1103 1310.0332 1320.4640
1347.0895 1352.2033 1396.5214
1399.7367 1476.3897 1478.5492
1487.9694 1491.2418 1566.2448
1571.7791 1624.3546 1624.4167
1629.3145 1641.3408 1646.5486
3162.5902 3162.6119 3172.9056
3172.9635 3186.2295 3186.3778
3204.7202 3205.0360 3208.5009
3209.0723 3260.0024 3260.7755
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] 66.6
End
!-------h_c18h12_p2----------
Bimolecular p2
Fragment c18h12
RRHO
Geometry[angstrom] 30
C -4.901882 -0.285972 -0.000011
C -4.518437 1.084708 0.000058
C -3.191207 1.445208 0.000079
C -2.202244 0.435923 0.000024
C -2.590438 -0.954837 -0.000042
C -3.966811 -1.293275 -0.000055
C -0.784203 0.499672 -0.000025
C -0.305757 -0.908745 0.000022
C -1.430313 -1.752406 -0.000067
C 1.011345 -1.342628 0.000055
C -0.001050 1.644533 -0.000037
C 1.381636 1.770050 -0.000034

C 2.406671 0.796088 -0.000013
C 2.236789 -0.641953 0.000037
C 4.843373 0.473690 -0.000025
C 4.677310 -0.931954 0.000027
C 3.414444 -1.456516 0.000055
C 3.747369 1.293606 -0.000043
H -5.958154 -0.533074 -0.000032
H -5.288209 1.847907 0.000084
H -2.911376 2.493409 0.000112
H -4.273637 -2.333594 -0.000099
H -1.397763 -2.833032 -0.000097
H 1.122633 -2.425162 0.000063
H -0.545413 2.585610 -0.000019
H 1.746074 2.792963 -0.000045
H 5.839755 0.901114 -0.000052
H 5.542756 -1.583939 0.000043
H 3.280343 -2.532806 0.000092
H 3.883416 2.369457 -0.000081
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 84
52.6007 80.5213 143.0387
158.5372 177.8918 261.4921
282.8420 301.6654 317.9238
365.1920 415.7546 447.9013
465.2500 494.7646 528.9861
535.0116 560.7412 561.5530
564.7382 627.2277 694.4885
703.5865 704.8470 734.0932
740.7712 749.1526 760.8999
777.3943 793.6332 808.7846
835.9548 862.2161 870.3928
879.9034 913.6989 947.4194
953.9896 965.0913 973.3199
979.5656 987.7099 996.7266
1018.6632 1030.1536 1078.9387
1132.1287 1151.3898 1177.3982
1184.9720 1190.2216 1192.1176
1241.6654 1251.9566 1307.7432
1322.6466 1338.0964 1353.5821
1376.8978 1395.3108 1421.0250
1433.8473 1443.8524 1465.4251
1505.7511 1527.9810 1536.2320
1567.3755 1579.0608 1612.9534
1623.5931 1650.2912 1656.1528
3129.2527 3134.0528 3153.5387
3156.7983 3162.9446 3163.2647

3168.3547 3175.0361 3180.3299
3186.5695 3192.8163 3212.0402
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] 67.8
End
!-------h_c18h12_p3----------
Bimolecular p3
Fragment c18h12
RRHO
Geometry[angstrom] 30
C -4.547935 -0.915538 -0.000095
C -3.620160 -1.966520 0.000413
C -2.263172 -1.699572 0.000493
C -1.772031 -0.378582 0.000069
C -2.717875 0.683272 -0.000220
C -4.096512 0.389122 -0.000345
C -0.342253 -0.061206 0.000010
C -0.942691 2.351678 0.000027
C -2.260954 2.049012 -0.000266
C 0.651471 -1.034502 -0.000252
C 0.062470 1.321580 0.000153
C 1.415595 1.646824 0.000258
C 2.416976 0.664463 0.000157
C 2.020501 -0.715196 -0.000164
C 4.750979 -0.011285 0.000097
C 4.359675 -1.376957 -0.000249
C 3.033084 -1.717591 -0.000380
C 3.806334 0.980206 0.000287
H -5.611195 -1.126751 -0.000203
H -3.965570 -2.994197 0.000756
H -1.572491 -2.532926 0.001020
H -4.803895 1.211987 -0.000611
H -0.614472 3.385801 0.000118
H -3.006443 2.837321 -0.000465
H 0.385942 -2.084634 -0.000645
H 1.704433 2.693541 0.000368
H 5.805362 0.241225 0.000203
H 5.120053 -2.149767 -0.000393
H 2.733583 -2.760600 -0.000640

```
H      4.103678    2.023753    0.000543
Core  RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm]  84
66.9359              70.4615              145.3989
165.1291             187.1977             270.9691
290.3474             307.4216             359.3443
399.2283             430.3906             454.7784
476.7993             498.2541             522.8615
540.8467             549.8397             578.1102
587.7403             636.7265             663.7052
700.0569             734.8556             751.8932
760.2086             771.8697             773.8370
794.6553             804.8080             820.9278
856.7081             879.7390             888.3856
889.8611             906.4235             920.0195
954.5328             968.1689             981.9821
992.5062             995.6079             999.8145
1034.3586            1063.9312            1122.9354
1155.9820            1168.2846            1178.9667
1187.5109            1197.5994            1222.5424
1241.0049            1261.9117            1288.9852
1302.4448            1322.6231            1346.0367
1369.2100            1385.9878            1416.9221
1442.1248            1451.9735            1473.6760
1487.1115            1514.0017            1535.5321
1587.7471            1599.3257            1630.9778
1650.1367            1661.5518            1669.2133
3153.8101            3156.6377            3157.5264
3159.9557            3161.5702            3169.4537
3174.8545            3176.1238            3178.8922
3186.3936            3187.8119            3200.5992
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] 29.9
End
!-------h_c18h12_p4------------
Bimolecular   p4
Fragment       c18h12
```

RRHO
Geometry[angstrom] 30
C 4.665950 0.073472 0.000021
C 4.150325 -1.236007 -0.000018
C 2.789191 -1.452813 -0.000015
C 1.868269 -0.376508 0.000029
C 2.399501 0.945955 0.000003
C 3.800308 1.142563 0.000003
C 0.428694 -0.562933 0.000060
C 0.153275 1.868883 -0.000100
C 1.501443 2.052716 -0.000070
C -0.428695 0.562943 0.000007
C -0.153270 -1.868874 0.000095
C -1.501437 -2.052712 0.000005
C -2.399498 -0.945953 -0.000052
C -1.868270 0.376512 0.000026
C -4.665952 -0.073482 -0.000064
C -4.150333 1.235998 0.000088
C -2.789200 1.452811 0.000126
C -3.800304 -1.142568 -0.000121
H 5.737895 0.234965 0.000028
H 4.828357 -2.082092 -0.000039
H 2.431117 -2.473424 -0.000070
H 4.181417 2.158486 -0.000010
H -0.488158 2.739494 -0.000264
H 1.914594 3.055968 -0.000137
H 0.488170 -2.739482 0.000219
H -1.914584 -3.055965 -0.000001
H -5.737896 -0.234981 -0.000117
H -4.828369 2.082081 0.000184
H -2.431137 2.473425 0.000288
H -4.181407 -2.158493 -0.000208
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 84
46.1283 75.2688 130.6027
176.0054 186.9355 234.7640
291.4715 294.0029 383.7555
390.4639 438.2189 483.8795
485.7424 487.6932 520.3217
544.8320 563.5756 577.1619
579.6594 586.3348 685.4111
691.4515 695.5015 742.0697
751.9529 774.2199 782.4628
791.1036 827.1302 836.4548
864.4067 872.7708 879.1126
890.8590 893.4401 946.8485

954.7618 962.0198 974.2936
992.4684 994.0199 1038.0132
1057.3658 1061.9667 1102.0852
1161.1700 1173.4134 1177.6181
1187.2595 1205.4883 1213.8057
1249.6373 1256.9923 1275.7979
1284.4832 1323.0692 1354.1570
1381.7806 1387.0562 1394.7041
1456.0745 1462.5847 1463.4986
1484.9417 1521.0484 1556.3184
1559.4883 1606.2594 1638.1852
1648.3002 1658.3245 1660.2822
3159.6366 3159.8576 3164.0807
3165.1207 3169.8798 3170.5262
3185.1417 3185.5892 3194.5899
3194.8594 3211.7961 3212.1028
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] 27.4
End
!-------h_c18h12_p5----------
Bimolecular p5
Fragment c18h12
RRHO
Geometry[angstrom] 30
C 4.880892 0.714616 -0.000176
C 4.880898 -0.714602 -0.000194
C 3.706381 -1.407175 -0.000114
C 2.446445 -0.724865 0.000032
C 2.446454 0.724865 0.000066
C 3.706370 1.407189 -0.000041
C 1.233687 -1.404476 0.000075
C 0.000041 0.725005 0.000180
C 1.233667 1.404444 0.000223
C -1.233740 1.404500 0.000200
C 0.000037 -0.725045 0.000089
C -1.233750 -1.404485 0.000087
C -2.446395 -0.724907 0.000106
C -2.446369 0.724924 0.000077
C -4.880887 -0.714641 -0.000126

C -4.880885 0.714662 -0.000297
C -3.706424 1.407191 -0.000159
C -3.706433 -1.407210 0.000062
H 5.826503 1.244952 -0.000293
H 5.826516 -1.244921 -0.000267
H 3.705807 -2.492201 -0.000115
H 3.705805 2.492212 -0.000031
H 1.234060 -2.490223 0.000143
H 1.233986 2.490195 0.000393
H -1.233914 2.490245 0.000279
H -1.234012 -2.490234 0.000150
H -5.826566 -1.244859 -0.000167
H -5.826543 1.244911 -0.000589
H -3.705781 2.492220 -0.000282
H -3.705795 -2.492225 0.000240
Core RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm] 84
56.6754 89.8280 150.2796
163.3044 191.7626 271.7219
305.0869 317.8223 318.2240
383.2114 448.2815 474.3326
478.2823 483.7332 505.6268
518.9255 562.7178 567.2275
618.6251 634.7197 645.0898
734.0283 745.3469 757.3559
757.9571 762.8837 769.3994
778.2237 788.4012 844.1979
854.6493 864.7453 867.8661
891.9901 910.6415 916.1856
917.0128 945.2627 972.0201
973.5122 995.7022 995.9011
1020.5239 1022.5643 1146.8846
1150.1331 1151.9071 1186.1890
1189.2765 1204.1602 1223.3793
1224.2005 1291.0527 1298.7092
1315.6163 1318.1242 1359.8133
1367.6265 1411.7573 1418.0364
1424.2221 1432.4559 1479.5584
1482.0734 1501.4468 1557.2775
1578.0639 1583.4247 1608.8643
1648.4208 1663.2450 1677.3562
3154.6971 3156.4726 3157.0431
3158.7305 3159.8414 3159.8864
3163.4341 3164.5224 3176.4047
3176.4898 3188.3037 3188.5765
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] 38.5
End
!-------h_c18h12_p6------------
Bimolecular   p6
Fragment       c18h12
RRHO
Geometry[angstrom]   30
C    -3.851725   -1.511287    0.107391
C    -3.737252   -0.173356   -0.190682
C    -2.479890    0.474617   -0.186466
C    -1.287837   -0.279756    0.055618
C    -1.458327   -1.636069    0.437682
C    -2.699975   -2.235782    0.460748
C    -2.402395    1.890059   -0.345936
C    -0.000002    0.394828   -0.000005
C    -0.000001    1.810241   -0.000013
C     1.287838   -0.279758   -0.055616
C     3.737251   -0.173351    0.190681
C     3.851727   -1.511285   -0.107377
C     2.699978   -2.235788   -0.460718
C     1.216389    2.534127    0.192321
C     2.402393    1.890064    0.345915
C    -1.216387    2.534124   -0.192352
C     1.458328   -1.636076   -0.437657
C     2.479887    0.474617    0.186461
H    -4.822672   -1.993279    0.110064
H    -4.621020    0.418283   -0.405797
H    -0.606054   -2.206519    0.773895
H    -2.787348   -3.270204    0.773786
H    -3.315840    2.444304   -0.533266
H     4.621018    0.418293    0.405791
H     4.822675   -1.993275   -0.110050
H     2.787351   -3.270214   -0.773739
H     1.166548    3.616909    0.236449
H     3.315839    2.444308    0.533245
H    -1.166553    3.616906   -0.236487
H     0.606057   -2.206537   -0.773856
Core  RigidRotor
SymmetryFactor 0.5
```

End
Frequencies[1/cm] 84
80.1408 83.8735 127.2521
175.4162 208.1464 258.9000
279.5023 323.3223 378.6621
418.8692 439.1281 440.4861
478.8613 519.6027 524.8538
526.6596 553.1042 588.0812
590.4664 632.3899 686.2894
690.1362 706.5660 756.1619
761.7071 769.4765 769.7033
811.1523 817.6590 827.1191
852.9954 865.7488 883.2107
889.1695 962.4867 965.5444
970.0924 978.7673 981.4062
993.5770 1006.5416 1015.0466
1055.8492 1072.1334 1130.0767
1153.7814 1168.4149 1178.9308
1182.1556 1190.3494 1217.8548
1235.8489 1239.1117 1254.4605
1279.2070 1325.6614 1352.1585
1368.0729 1385.3538 1397.4086
1449.5735 1449.7102 1456.2038
1484.2511 1532.3035 1534.2626
1557.9103 1596.9072 1638.1900
1647.4974 1648.6671 1667.3145
3157.4732 3158.7597 3160.1067
3161.3175 3169.9058 3170.4409
3177.1667 3179.3826 3186.5058
3187.1424 3213.4364 3231.2947
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] 32.5
End
!-------bar_ts1-1----------
Barrier ts1-1 i1 i1-1
RRHO
Geometry[angstrom] 31
C 4.682401 0.008579 -0.267582
C 4.053646 1.244932 -0.434522

C 2.663124 1.355372 -0.348452
C 1.913029 0.212188 -0.090187
C 2.551028 -1.046240 0.073866
C 3.936062 -1.145330 -0.014105
C 0.468674 -0.006562 0.052093
C 0.296950 -1.438589 0.291725
C 1.512194 -2.043352 0.309102
C -0.573224 1.000757 -0.384981
C -0.375815 1.192088 1.086762
C -1.549035 0.761541 1.763102
C -2.514858 0.330101 0.803780
C -1.971548 0.485481 -0.503661
C -4.545684 -0.516174 -0.173481
C -4.005747 -0.350333 -1.456037
C -2.708448 0.145131 -1.625263
C -3.812877 -0.188859 0.960169
H 5.762461 -0.055768 -0.338903
H 4.650305 2.127673 -0.634990
H 2.188630 2.322542 -0.482203
H 4.431854 -2.102730 0.107157
H -0.659677 -1.919083 0.433415
H 1.693129 -3.097936 0.469202
H -0.224359 1.742374 -1.098474
H 0.391469 1.817130 1.516917
H -1.671451 0.737923 2.837040
H -5.552299 -0.905285 -0.067258
H -4.599511 -0.610435 -2.324767
H -2.291910 0.259832 -2.620244
H -4.237866 -0.320626 1.949149
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 446.1661
WellDepth[kcal/mol] 16.1
WellDepth[kcal/mol] 2.3
End
Frequencies[1/cm] 86
56.4965 64.3659
84.5077 161.3429 174.0327
230.8209 255.1956 270.0782
378.9575 415.2455 429.5093
451.9154 462.8421 529.0143
544.5411 559.4920 573.9233
592.2544 607.2550 636.6706
679.9026 712.1814 733.1290
748.4566 753.9206 757.0614
772.5635 792.3690 801.0122

851.4831 866.2231 871.7816
877.7859 878.4862 893.1395
928.8244 938.8516 948.3775
950.7589 978.4158 986.0415
1022.3965 1036.5458 1041.4568
1078.3446 1082.0242 1095.0458
1122.3233 1135.6619 1172.7317
1177.4931 1188.6813 1197.2945
1221.4754 1233.4070 1245.3528
1272.3946 1320.7795 1325.4526
1345.5861 1351.2018 1358.6642
1393.9871 1403.7076 1470.3681
1475.1633 1490.7765 1502.5413
1552.6632 1598.4935 1617.9935
1625.2985 1635.7692 3128.5544
3152.6569 3160.5701 3160.7474
3167.4825 3172.3820 3177.4971
3185.9639 3188.7555 3203.4461
3211.9172 3230.8666 3233.7040
ZeroEnergy[kcal/mol] 39.7
ElectronicLevels[1/cm] 1
0 2
End
!-----------------------------------
!-------bar_ts1-2------------
Barrier ts1-2 i1 i1-2
RRHO
Geometry[angstrom] 31
C -4.876652 -0.258856 0.073197
C -4.495878 1.110582 -0.191001
C -3.201888 1.453248 -0.436308
C -2.195094 0.433573 -0.424606
C -2.569636 -0.951425 -0.052342
C -3.962438 -1.263415 0.132077
C -0.851919 0.454121 -0.686994
C -0.253748 -0.872761 -0.297111
C -1.439558 -1.712316 0.074274
C 0.754255 -0.343401 0.809262
C 0.471878 1.157158 0.862691
C 1.596562 1.860837 0.490273
C 2.659709 0.939830 0.152193
C 2.196282 -0.380629 0.357331
C 4.797600 0.073337 -0.520215
C 4.334921 -1.230380 -0.319592
C 3.025540 -1.463544 0.116231
C 3.967360 1.167545 -0.290751
H -5.928273 -0.477938 0.224672
H -5.272702 1.866764 -0.210305

H -2.923844 2.476737 -0.662246
H -4.268390 -2.286202 0.325106
H 0.320798 -1.364461 -1.088848
H -1.406346 -2.781767 0.242655
H 0.596474 -0.853572 1.761315
H -0.355854 1.578735 1.413900
H 1.677614 2.939176 0.448558
H 5.814798 0.232364 -0.860371
H 4.998069 -2.068531 -0.501275
H 2.675055 -2.479599 0.266983
H 4.328823 2.177275 -0.451801
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 407.5235
WellDepth[kcal/mol] 72.3
WellDepth[kcal/mol] 25.9
End
Frequencies[1/cm] 86
36.8856 52.6615
100.7885 120.7441 154.9528
226.2113 260.3835 293.7364
330.3725 403.6189 435.3442
447.5954 456.9705 518.2748
543.1421 547.9558 555.6918
569.2555 610.6039 650.1188
703.6749 726.4401 741.1632
752.5994 756.1500 760.0578
786.0880 798.0451 814.3746
849.2789 856.6468 866.8134
874.9621 889.0358 910.6467
929.4147 948.1504 956.7739
975.3983 985.2525 988.6708
996.9384 1008.4212 1024.0999
1040.7205 1082.8048 1119.3757
1127.4022 1149.2344 1164.1548
1174.8369 1183.5765 1189.9062
1203.9642 1230.1862 1234.9303
1245.9886 1251.9507 1307.3852
1334.0975 1340.9287 1377.3026
1388.1340 1411.0697 1443.3940
1484.5375 1495.2017 1510.3620
1551.2665 1582.6353 1613.7081
1632.8953 1662.9015 3045.3246
3077.9287 3156.6058 3158.0291
3165.3627 3166.0409 3176.4915
3176.7371 3186.9418 3188.6184

3190.3972 3200.8154 3223.9883
ZeroEnergy[kcal/mol] 95.9
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_ts2-1------------
Barrier ts2-1 i1-1 i2-1
RRHO
Geometry[angstrom] 31
C -4.645222 0.075746 0.401656
C -3.995870 1.308396 0.461586
C -2.612629 1.395488 0.261448
C -1.901397 0.234745 0.003647
C -2.555496 -1.011533 -0.059604
C -3.930432 -1.095851 0.139880
C -0.431647 0.017477 -0.243661
C -0.336464 -1.475051 -0.451900
C -1.549740 -2.040016 -0.346549
H -5.716972 0.026961 0.559126
H -4.566445 2.207605 0.664629
H -2.116663 2.359728 0.308180
H -4.440762 -2.051920 0.093627
H 0.596001 -1.979639 -0.659082
H -1.770739 -3.094490 -0.455835
C 0.524279 0.736051 0.642333
C 0.200196 0.953049 -1.283076
C 1.512435 0.793124 -1.716617
C 2.455989 0.290276 -0.747343
C 1.939036 0.365846 0.576992
C 4.598489 -0.386192 0.140749
C 4.098584 -0.278867 1.439673
C 2.771045 0.103049 1.660045
C 3.785126 -0.094045 -0.952757
H 0.143407 1.443792 1.369164
H -0.475192 1.654282 -1.760098
H 1.842058 1.215513 -2.659038
H 5.629752 -0.680479 -0.017838
H 4.742662 -0.490331 2.285630
H 2.389019 0.180499 2.672381
H 4.186180 -0.141668 -1.959859
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 644.679
WellDepth[kcal/mol] 16.3
WellDepth[kcal/mol] 28.0

End
Frequencies[1/cm] 86
61.7618 67.9724
86.0361 158.1527 184.0116
247.9702 255.9266 270.2268
367.3040 394.9175 428.5411
449.0250 469.5666 519.6169
525.0685 554.0168 567.0312
584.7728 597.0394 638.1133
663.3005 672.9747 692.2019
700.7099 749.8080 759.5837
761.5798 763.9347 792.9319
804.9946 823.2316 858.2533
871.2666 874.9028 886.5904
897.8795 943.2503 947.2397
962.4559 977.1739 981.3364
986.8993 1017.1698 1044.0476
1044.2952 1092.6513 1117.2662
1132.2279 1137.5341 1179.6938
1179.9793 1192.0839 1199.6525
1220.2344 1232.1739 1246.6176
1283.3184 1309.4155 1315.2405
1342.3732 1347.2837 1385.2994
1393.8751 1437.7215 1485.5035
1488.8381 1490.9085 1500.5500
1601.0560 1603.2511 1618.6194
1636.8753 1648.8044 3156.8692
3159.1115 3163.3937 3164.1283
3165.1822 3174.5898 3175.5327
3176.9550 3181.6122 3187.1396
3188.8773 3192.8294 3232.1073
ZeroEnergy[kcal/mol] 53.7
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_ts2-2----------
Barrier ts2-2 i1-2 i2-2
RRHO
Geometry[angstrom] 31
C -4.683622 -0.204351 0.755268
C -4.220172 1.148708 0.870817
C -2.963256 1.509563 0.460688
C -2.104431 0.521024 -0.088042
C -2.566784 -0.859826 -0.198697
C -3.893086 -1.188212 0.235236
C -0.804678 0.612103 -0.591952
C -0.361106 -0.797527 -1.022580

C -1.567549 -1.643993 -0.722546
C 0.917468 -1.293788 -0.332208
C 0.214361 1.574385 -0.446206
C 1.384391 1.308753 -1.141589
C 2.501371 0.712022 -0.379984
C 2.162884 -0.654935 -0.041416
C 4.649720 0.500560 0.708368
C 4.365911 -0.832216 1.021387
C 3.157570 -1.399488 0.655558
C 3.711197 1.261601 0.001488
H -5.688159 -0.438357 1.090302
H -4.889871 1.894328 1.284364
H -2.629102 2.538458 0.536320
H -4.251861 -2.208295 0.153613
H -0.202690 -0.809555 -2.118901
H -1.627962 -2.703643 -0.933407
H 0.857809 -2.327402 -0.005620
H 0.220112 2.222755 0.428843
H 1.241153 0.815877 -2.103635
H 5.596086 0.940494 1.000620
H 5.096065 -1.427937 1.558005
H 2.948446 -2.433167 0.911862
H 3.928842 2.290146 -0.263896
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 265.3244
WellDepth[kcal/mol] 18.6
WellDepth[kcal/mol] 45.3
End
Frequencies[1/cm] 86
53.7223 75.5955
113.5930 162.1051 204.8417
238.5768 246.2397 303.2917
313.3206 364.2070 393.6944
428.6046 461.2442 485.4882
513.1816 532.3721 536.4053
543.1498 570.5253 606.7146
620.8911 649.7256 692.4823
695.8363 724.2081 748.5553
760.1870 763.8776 774.1211
796.0604 808.4420 850.9651
856.7216 866.8034 882.2684
893.0535 946.0896 956.7607
965.3736 978.2913 991.8065
1002.0602 1028.3092 1038.3396
1061.6135 1100.1859 1122.9792

1150.1631 1155.9699 1165.0083
1171.5793 1177.2854 1201.9491
1218.2237 1237.4701 1245.2680
1284.5826 1292.7694 1309.6590
1323.8483 1354.1073 1387.5337
1392.7569 1425.9269 1439.7549
1449.1075 1488.7428 1498.1102
1548.4305 1562.3503 1564.4884
1607.6382 1638.7785 2890.8116
3078.2836 3109.2745 3149.3399
3156.2601 3160.9933 3167.5780
3168.7343 3175.7479 3179.7124
3188.6479 3190.0450 3203.6003
ZeroEnergy[kcal/mol] 88.6
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_ts444----------
Barrier ts444 i2-1 i444
RRHO
Geometry[angstrom] 31
C -4.534400 -0.863066 0.019450
C -3.631950 -1.770900 0.567961
C -2.272082 -1.457084 0.627588
C -1.810289 -0.237210 0.140579
C -2.724098 0.676695 -0.419262
C -4.082379 0.358834 -0.474524
C -0.356327 0.138170 0.202769
C -0.825754 2.060357 -0.820888
C -2.132825 1.921904 -0.924353
C 0.560279 -0.479074 -0.664400
C 0.163766 0.714053 1.423090
C 1.504430 0.783303 1.654904
C 2.448556 0.257919 0.720740
C 1.955445 -0.392485 -0.456514
C 4.726613 -0.211118 0.021926
C 4.243988 -0.858942 -1.136149
C 2.891440 -0.949725 -1.368521
C 3.843367 0.332185 0.930471
H -5.589884 -1.107203 -0.026134
H -3.982301 -2.722731 0.950827
H -1.569207 -2.162376 1.057291
H -4.782285 1.065842 -0.907659
H -0.092130 2.812414 -1.069696
H -2.785185 2.679131 -1.364354
H 0.188331 -1.001165 -1.539376
H -0.542494 1.109794 2.143769

```
H      1.875217    1.235086    2.569457
H      5.794692   -0.145349    0.195517
H      4.946073   -1.284979   -1.844148
H      2.519951   -1.446371   -2.258856
H      4.212544    0.825010    1.824156
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  435.2595
WellDepth[kcal/mol]  26.2
WellDepth[kcal/mol]  4.4
End
Frequencies[1/cm]  86
46.8165              59.1118
72.2231             158.8060             179.7374
200.8162             234.0789             244.8698
311.9009             360.2926             397.3128
413.8842             463.8164             469.7393
485.4120             519.1679             532.6976
562.3387             581.5183             614.9584
624.3236             637.8012             658.8099
697.1355             748.0288             765.9659
769.8658             773.5694             778.6799
788.2693             819.4032             851.2895
857.3321             874.1669             888.1546
897.1939             903.5570             949.7676
956.3421             958.3375             978.8507
990.5921             990.8267            1019.4136
1043.4137            1058.0075            1127.3006
1150.0968            1171.3585            1172.8247
1181.6055            1192.6471            1212.5144
1237.8375            1259.5879            1280.3623
1289.7098            1307.0603            1334.6939
1348.8638            1380.1012            1405.1032
1454.5404            1474.8597            1483.4256
1509.1825            1522.8670            1576.9828
1598.8098            1623.8367            1636.2006
1642.3716            1644.7896            3071.3500
3156.1900            3158.4291            3158.4738
3161.9647            3166.4659            3170.1293
3174.8064            3176.2452            3183.7140
3187.5111            3188.0643            3242.1223
ZeroEnergy[kcal/mol]  51.9
ElectronicLevels[1/cm] 1
0  2
End
!----------------------------------
```

```
!-------bar_ts44-2------------
Barrier      ts44-2  i2-1  i44-2
RRHO
Geometry[angstrom]   31
C     4.526069   -0.151182   -0.717900
C     3.858853    0.950399   -1.265931
C     2.523231    1.206966   -0.936822
C     1.881005    0.362038   -0.047714
C     2.552142   -0.753675    0.521127
C     3.885526   -1.012020    0.167516
C     0.458281    0.377567    0.440558
C     0.420490   -0.779816    1.421381
C     1.653788   -1.437665    1.410534
C    -0.422428   -0.630748   -0.260400
C    -0.216099    1.659064    0.793097
C    -1.549338    1.791643    0.726841
C    -2.424948    0.736331    0.228770
C    -1.844054   -0.451664   -0.306738
C    -4.634188   -0.073645   -0.377914
C    -4.064699   -1.223902   -0.934444
C    -2.690612   -1.407269   -0.904407
C    -3.813099    0.897151    0.188115
H     5.560240   -0.334682   -0.988392
H     4.380492    1.607177   -1.952628
H     2.002595    2.053334   -1.372341
H     4.412299   -1.862722    0.586053
H    -0.381994   -0.911960    2.130284
H     1.889527   -2.330276    1.974133
H     0.050557   -1.367894   -0.894146
H     0.410840    2.473801    1.137883
H    -2.015114    2.725696    1.025958
H    -5.708630    0.066864   -0.397099
H    -4.699041   -1.977562   -1.387599
H    -2.252042   -2.302646   -1.332367
H    -4.249276    1.803451    0.596248
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  543.029
WellDepth[kcal/mol]  11.6
WellDepth[kcal/mol]  5.8
End
Frequencies[1/cm]  86
55.9640              84.8831
101.5882             174.1638             190.7005
252.1390             275.0777             291.2071
372.4150             402.3720             416.6490
```

442.2678 496.0006 504.5565
526.6497 546.3922 556.0149
577.4405 605.1264 629.3563
678.4287 712.6730 721.1223
748.2247 754.3167 760.5118
765.8920 782.8324 796.7115
807.8384 853.5955 868.7523
876.9234 880.2147 888.0331
912.7556 946.5203 948.0550
968.7259 981.0511 983.5275
991.8298 1012.1601 1039.0841
1053.3643 1084.1892 1119.6802
1135.7196 1155.7034 1174.9819
1176.4039 1195.7434 1218.8578
1227.1006 1246.4317 1271.9359
1276.8149 1295.2214 1335.3659
1337.6398 1350.5192 1374.5355
1399.6476 1435.3631 1473.7645
1477.3596 1499.2469 1503.3375
1579.2941 1603.3456 1621.0244
1629.7517 1672.3342 3152.8770
3157.1084 3158.7230 3161.6438
3165.7826 3175.0892 3175.7754
3179.4714 3187.4721 3189.3793
3202.9309 3204.4847 3236.4759
ZeroEnergy[kcal/mol] 37.3
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_ts4-2----------
Barrier ts4-2 i444 i4-2
RRHO
Geometry[angstrom] 31
C -4.538592 -0.858582 -0.035256
C -3.696782 -1.817982 0.520683
C -2.333588 -1.556463 0.636108
C -1.788699 -0.341334 0.211054
C -2.643275 0.636188 -0.355836
C -4.009445 0.350689 -0.473478
C -0.331430 -0.088656 0.311772
C -0.926647 2.413359 -0.657479
C -2.127212 1.913817 -0.881380
C 0.589523 -0.957622 -0.215587
C 0.123806 1.141553 0.905341
C 1.487560 1.403359 0.996257
C 2.442329 0.530526 0.424560
C 1.987357 -0.682326 -0.186770

```
C      4.736708   -0.085789   -0.091322
C      4.285577   -1.277299   -0.701121
C      2.939493   -1.566586   -0.745325
C      3.836353    0.796131    0.459157
H     -5.600984   -1.051884   -0.131683
H     -4.096952   -2.764734    0.865339
H     -1.676591   -2.297212    1.078282
H     -4.661797    1.092463   -0.922956
H     -0.434859    3.320760   -0.979674
H     -2.826989    2.469254   -1.514091
H      0.251299   -1.867981   -0.699977
H     -0.558751    1.691487    1.541632
H      1.831308    2.293555    1.512590
H      5.798503    0.131543   -0.059807
H      5.003915   -1.964693   -1.133293
H      2.591709   -2.482443   -1.212075
H      4.181969    1.711980    0.927449
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  348.3515
WellDepth[kcal/mol]  0.1
WellDepth[kcal/mol]  31.1
End
Frequencies[1/cm]  86
57.4812             69.7549
100.3327            145.5635            194.1658
211.6876            237.9288            265.8189
308.4002            354.8250            395.6453
422.4219            454.4511            477.9968
481.2912            521.8101            531.4549
560.3992            581.8053            610.9829
636.7726            653.0634            683.4701
696.3166            752.3402            768.2537
771.0472            775.2038            782.2165
787.3591            827.2257            855.3477
871.7268            879.3943            896.6291
907.8614            917.1406            947.3185
960.0880            961.8737            967.9870
990.9251            991.8590           1029.7754
1043.8523           1068.6437           1131.1233
1147.7394           1164.5309           1173.8372
1184.3879           1213.9922           1217.2968
1238.4467           1256.9121           1282.1108
1289.1162           1317.9141           1325.5480
1369.4746           1383.4651           1400.4544
1452.1361           1473.5897           1495.0693
```

```
1514.1956          1529.2276          1589.8488
1597.2449          1620.9566          1637.2851
1644.5869          1648.9168          3036.5951
3156.6585          3157.0724          3160.0902
3161.9437          3164.5376          3166.5483
3174.6633          3177.1422          3178.1426
3187.5589          3189.1572          3218.2962
ZeroEnergy[kcal/mol]  51.1
ElectronicLevels[1/cm] 1
0  2
End
!---------------------------------
!-------bar_ts4-22------------
Barrier     ts4-22  i44-2  i4-22
RRHO
Geometry[angstrom]   31
C     4.594791   -0.182098   -0.541945
C     4.037889    1.017716   -0.990640
C     2.685730    1.301918   -0.759967
C     1.900061    0.383639   -0.079812
C     2.466783   -0.832451    0.397657
C     3.819624   -1.107112    0.152445
C     0.452816    0.502710    0.217171
C     0.195593   -1.107493    1.106297
C     1.524748   -1.558753    1.202818
C    -0.385933   -0.650088   -0.228419
C    -0.182361    1.698980    0.689491
C    -1.534322    1.827258    0.725328
C    -2.413098    0.780477    0.233762
C    -1.862948   -0.419416   -0.277443
C    -4.638205   -0.021103   -0.333122
C    -4.088671   -1.190827   -0.857888
C    -2.708417   -1.379724   -0.830995
C    -3.806702    0.954213    0.201561
H     5.642575   -0.390450   -0.727794
H     4.653820    1.734060   -1.522189
H     2.256777    2.231157   -1.119517
H     4.261811   -2.028303    0.516891
H    -0.504858   -1.204107    1.927983
H     1.834283   -2.241802    1.984851
H    -0.003109   -1.211587   -1.081091
H     0.455134    2.507445    1.032130
H    -1.986679    2.737499    1.103209
H    -5.711571    0.130836   -0.348352
H    -4.731536   -1.953166   -1.282928
H    -2.280466   -2.291108   -1.236209
H    -4.230454    1.872441    0.595214
Core  RigidRotor
```

SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 646.5307
WellDepth[kcal/mol] 8.7
WellDepth[kcal/mol] 27.1
End
Frequencies[1/cm] 86
62.8508 84.8445
102.3928 167.5062 195.7366
248.3585 264.2873 304.5431
379.1181 394.3051 422.1986
449.7440 482.3751 506.4445
530.1991 540.7290 551.8089
574.4708 609.9598 628.1706
656.6958 682.3080 697.3470
746.1090 750.9029 758.5218
767.7615 779.5245 804.1428
836.5019 846.7293 869.6111
885.9084 889.3306 910.4045
944.1772 953.6260 960.0187
977.3055 978.4244 990.3107
1008.5364 1044.4293 1059.4590
1109.1486 1129.6137 1139.3781
1159.9492 1165.9217 1176.9458
1183.2570 1221.5466 1225.5524
1234.4778 1243.9964 1275.6875
1295.0598 1310.0940 1331.6020
1337.0340 1340.7420 1377.8944
1415.9927 1451.2021 1476.2794
1481.6918 1502.5545 1515.5475
1570.6146 1598.7179 1615.8812
1621.6060 1639.0985 3073.7738
3156.7012 3158.4748 3159.5712
3161.6429 3165.1892 3166.2556
3174.5174 3175.1856 3179.0529
3185.2618 3188.0212 3188.9089
ZeroEnergy[kcal/mol] 40.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_ts555-4----------
Barrier ts555-4 i4-22 i555-2
RRHO
Geometry[angstrom] 31
C 4.445253 -0.751262 -0.331806
C 3.990617 -0.187488 -1.524060

C 2.751908 0.442082 -1.583741
C 1.940817 0.525823 -0.430922
C 2.382361 -0.117087 0.774231
C 3.635138 -0.714380 0.809382
C 0.704622 1.178547 -0.386986
C 0.119065 -0.352294 1.749751
C 1.436155 -0.111966 1.906976
C -0.503119 -0.928020 0.553606
C -0.244741 2.069057 -0.144474
C -1.642424 1.855169 0.164786
C -2.375346 0.677289 0.170009
C -1.758223 -0.641614 0.046569
C -4.529203 -0.314852 -0.405687
C -3.866080 -1.519756 -0.806600
C -2.525453 -1.667089 -0.608757
C -3.811357 0.743160 0.064979
H 5.419118 -1.224607 -0.289214
H 4.614206 -0.222365 -2.410518
H 2.412560 0.904750 -2.502720
H 3.976435 -1.176479 1.730287
H -0.549155 -0.151984 2.584630
H 1.811200 0.165360 2.888120
H -0.013047 -1.819905 0.166168
H 0.033221 3.126683 -0.215603
H -2.220578 2.770632 0.258864
H -5.604328 -0.235888 -0.520911
H -4.445844 -2.329066 -1.235661
H -2.031878 -2.603800 -0.846791
H -4.301847 1.684749 0.289818
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 293.4439
WellDepth[kcal/mol] 79.4
WellDepth[kcal/mol] 28.0
End
Frequencies[1/cm] 86
57.2773 84.2440
93.4445 143.9284 159.5416
208.6329 242.0881 258.7439
276.8813 356.6107 383.8546
399.7658 436.1238 445.6059
463.2979 486.2158 501.0232
522.5513 546.7427 561.1338
603.6247 657.6772 675.5567
693.3128 722.8904 734.4027
744.6341 750.4385 759.1023

776.3319 789.8030 816.6784
842.7171 859.9169 876.1076
896.2679 920.1932 942.9396
952.2019 963.4747 978.7683
979.4131 1006.1764 1037.1426
1054.4366 1057.7906 1112.5149
1147.6317 1151.9867 1169.0612
1182.6956 1185.2385 1198.5178
1221.6285 1240.3872 1269.7819
1303.9492 1320.4193 1332.7751
1382.5852 1406.5340 1415.4990
1431.6833 1458.7512 1469.3827
1474.7824 1539.8039 1556.7700
1568.7143 1600.0842 1624.8248
1641.5757 1742.8915 3016.5151
3118.0552 3126.5722 3141.3836
3151.8063 3156.2760 3158.7482
3160.7829 3167.1477 3174.9824
3184.1249 3187.6890 3192.2068
ZeroEnergy[kcal/mol] 92.5
ElectronicLevels[1/cm] 1
0 2
End
!-----------------------------------
!-------bar_ts5-2------------
Barrier ts5-2 i555-2 i5-2
RRHO
Geometry[angstrom] 31
C 4.774193 -0.563622 -0.256189
C 4.582916 0.723534 -0.851659
C 3.354797 1.322806 -0.811246
C 2.240869 0.685513 -0.190988
C 2.420866 -0.640914 0.396230
C 3.743071 -1.215469 0.348705
C 1.001196 1.309838 -0.067753
C -0.006881 -0.740000 1.020976
C 1.372584 -1.272174 1.019705
C -0.828436 -0.980795 -0.237736
C -0.111580 0.681063 0.511538
C -1.389715 1.363412 0.766573
C -2.523111 0.640707 0.412890
C -2.189887 -0.575069 -0.302654
C -4.858154 0.329898 -0.147195
C -4.512917 -0.792327 -0.940674
C -3.201346 -1.229773 -1.028806
C -3.885810 1.039401 0.518137
H 5.757463 -1.019897 -0.289662
H 5.420303 1.220907 -1.326722

H 3.207422 2.303618 -1.251727
H 3.894909 -2.191507 0.797287
H 0.883690 2.328683 -0.425290
H -0.564289 -0.940260 1.940810
H 1.558242 -2.193794 1.562636
H -0.355977 -1.527311 -1.044793
H -1.413739 2.369571 1.168325
H -5.895157 0.639854 -0.086229
H -5.291671 -1.324339 -1.475568
H -2.956892 -2.106411 -1.619397
H -4.140234 1.924712 1.091210
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 799.1231
WellDepth[kcal/mol] 2.9
WellDepth[kcal/mol] 31.1
End
Frequencies[1/cm] 86
52.7473 90.5636
99.4967 172.0584 211.3342
249.8586 284.0157 324.4054
339.3342 346.9403 419.0984
438.5072 457.0021 468.2700
514.6435 527.6494 554.7076
556.3931 594.7395 621.4904
640.3782 673.3902 711.4111
721.6451 736.7557 742.1896
748.6935 754.6141 764.6088
777.9655 814.2125 836.1637
851.0093 857.0474 888.8504
907.6480 920.4901 940.6184
962.6737 970.0936 987.8123
1009.3571 1015.6662 1030.9117
1061.1135 1119.8717 1129.5426
1139.1625 1163.9771 1171.7473
1192.8596 1199.0627 1211.9822
1226.8595 1249.0236 1261.7145
1287.6213 1298.9318 1319.4818
1349.2930 1354.9487 1397.7617
1402.9205 1423.9111 1448.4654
1450.7962 1486.9319 1510.5677
1550.4895 1555.1145 1599.8650
1602.4139 1649.1364 3024.3010
3153.5955 3156.0909 3157.4887
3157.9517 3162.1567 3162.8692
3174.6842 3175.9919 3179.3620

3182.5095 3187.4371 3189.3271
ZeroEnergy[kcal/mol] 67.4
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_tsp1----------
Barrier tsp1 i1 p1
RRHO
Geometry[angstrom] 31
C -4.767939 0.395315 0.105071
C -3.944741 1.490981 0.351052
C -2.549936 1.363353 0.322806
C -1.986095 0.128243 0.024053
C -2.832836 -0.991992 -0.187335
C -4.214093 -0.862826 -0.157227
C -0.588624 -0.358371 -0.041272
C -0.682588 -1.798539 -0.262468
C -1.983662 -2.164928 -0.378564
C 0.576109 0.377804 0.031418
C 0.695836 1.821802 -0.234733
C 1.995939 2.152227 -0.404413
C 2.829068 0.970037 -0.200960
C 1.974796 -0.127246 0.073547
C 4.749814 -0.440990 0.071795
C 3.916620 -1.515220 0.377979
C 2.525412 -1.363393 0.391970
C 4.209793 0.816804 -0.211496
H -5.845184 0.514519 0.132108
H -4.385639 2.455688 0.574519
H -1.938282 2.224352 0.556067
H -4.855225 -1.722271 -0.321002
H 0.164266 -2.449392 -0.405790
H -2.347513 -3.160544 -0.595449
H 0.501585 0.761595 2.126704
H -0.141587 2.485664 -0.371837
H 2.372526 3.133300 -0.662074
H 5.825236 -0.578583 0.068647
H 4.349128 -2.479669 0.618392
H 1.904261 -2.201948 0.677353
H 4.859196 1.658917 -0.424981
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 570.2029
WellDepth[kcal/mol] 45.8
WellDepth[kcal/mol] 2.8

End
Frequencies[1/cm] 86
46.4912 66.7883
89.5139 155.3746 179.5752
199.0406 221.3015 242.1015
271.2453 307.0974 355.4197
371.5676 413.3821 423.2029
427.6911 493.2460 552.5532
563.4653 574.8791 590.3310
605.3718 624.6805 659.7456
690.5523 733.7118 746.6647
750.1859 760.3968 770.0521
770.9066 803.2833 817.4476
868.4376 869.0141 886.8935
888.6128 894.7180 940.5099
944.1258 949.9006 954.2017
987.2470 989.1192 1042.5466
1044.3767 1069.7126 1080.0093
1089.3155 1110.0031 1126.8568
1137.8591 1179.8725 1184.5136
1201.9225 1211.9940 1213.6580
1234.3203 1308.6097 1319.4562
1347.2338 1350.6033 1393.8637
1398.8289 1473.9063 1479.2452
1487.2198 1491.7661 1551.0391
1569.9203 1586.7965 1624.1668
1626.5849 1639.9449 1641.5436
3163.0766 3163.2123 3173.3941
3173.5648 3186.2574 3186.7307
3201.6678 3204.4349 3207.6866
3207.9009 3256.7007 3259.3943
ZeroEnergy[kcal/mol] 69.4
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_tsp2----------
Barrier tsp2 i2-2 p2
RRHO
Geometry[angstrom] 31
C 4.892857 -0.275791 -0.139334
C 4.503183 1.094999 -0.156986
C 3.179052 1.454329 -0.085751
C 2.192996 0.443679 0.004667
C 2.587790 -0.946527 0.027443
C 3.965241 -1.283007 -0.048116
C 0.781214 0.512841 0.084015
C 0.299322 -0.897698 0.189073

C 1.442588 -1.746345 0.121751
C -1.015521 -1.339642 0.004509
C -0.006662 1.657432 0.065834
C -1.386648 1.775179 0.086911
C -2.410944 0.796723 0.040496
C -2.236094 -0.638839 -0.040103
C -4.845255 0.475136 -0.066187
C -4.674428 -0.925287 -0.170720
C -3.411312 -1.449789 -0.159620
C -3.750289 1.292498 0.032706
H 5.948212 -0.519329 -0.197204
H 5.269090 1.858844 -0.227233
H 2.896659 2.501496 -0.099728
H 4.274248 -2.322405 -0.032042
H 0.440216 -0.835504 2.044935
H 1.410067 -2.826142 0.149566
H -1.116878 -2.420075 -0.064554
H 0.534950 2.599122 0.030961
H -1.756323 2.796045 0.105301
H -5.841963 0.901436 -0.069472
H -5.537320 -1.575378 -0.254183
H -3.274910 -2.523325 -0.231052
H -3.888594 2.365869 0.101168
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 871.3355
WellDepth[kcal/mol] 36.8
WellDepth[kcal/mol] 12.3
End
Frequencies[1/cm] 86
52.8932 79.3154
142.3425 158.3128 176.0870
255.9851 262.5914 286.5529
306.4420 328.9445 357.8678
406.1496 435.4848 449.7458
470.7287 491.6810 532.6404
533.9269 556.0737 564.0571
569.3303 624.7523 679.3663
695.8686 704.1403 730.1183
737.3374 748.0550 760.0725
773.8604 788.4129 808.0493
833.8737 861.2367 869.5685
876.8754 912.5518 926.5286
956.4977 964.1429 970.2413
976.3634 989.4605 994.1933
1017.8058 1034.0959 1083.2738

1131.8817 1151.3987 1174.9575
1180.9729 1188.0285 1190.4411
1238.1278 1246.7216 1288.3339
1322.9150 1337.6646 1346.1944
1374.3560 1394.6472 1415.9874
1424.1138 1440.2428 1457.6344
1499.6055 1525.0966 1531.4206
1564.0580 1573.7923 1594.0497
1613.3068 1647.5133 1652.3355
3135.7999 3136.0129 3154.7252
3158.8270 3163.5327 3165.5944
3168.5900 3177.0306 3180.7258
3187.6503 3193.3142 3218.7040
ZeroEnergy[kcal/mol] 80.1
ElectronicLevels[1/cm] 1
0 2
End
!-----------------------------------
!-------bar_tsp3------------
Barrier tsp3 i4-2 p3
RRHO
Geometry[angstrom] 31
C -4.546816 -0.925398 -0.070189
C -3.627331 -1.973347 0.061887
C -2.269880 -1.707696 0.113096
C -1.774780 -0.391792 0.035940
C -2.713192 0.668998 -0.084196
C -4.088804 0.377037 -0.140851
C -0.343930 -0.081638 0.061526
C -0.948255 2.348889 -0.020217
C -2.251399 2.036924 -0.151431
C 0.645373 -1.044441 -0.000384
C 0.060857 1.315215 0.178635
C 1.429438 1.638737 0.057807
C 2.421625 0.653490 0.014948
C 2.021604 -0.726304 -0.001761
C 4.752789 -0.030845 -0.080981
C 4.357180 -1.392938 -0.090320
C 3.026349 -1.728473 -0.054773
C 3.811672 0.964465 -0.032910
H -5.609739 -1.134011 -0.111238
H -3.977522 -2.997103 0.129575
H -1.582977 -2.536250 0.229644
H -4.791929 1.197877 -0.236703
H -0.615045 3.380494 -0.046234
H -2.990587 2.817574 -0.297098
H 0.378846 -2.091898 -0.075379
H -0.060027 1.386758 1.912991

```
H      1.717199    2.685051    0.049693
H      5.807374    0.218930   -0.110877
H      5.113060   -2.169043   -0.128105
H      2.723474   -2.770403   -0.067316
H      4.112877    2.006733   -0.023897
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1010.7371
WellDepth[kcal/mol]  19.8
WellDepth[kcal/mol]  9.9
End
Frequencies[1/cm]  86
66.5315              69.6324
141.3827             160.6781             187.5601
265.3004             288.5969             304.7894
354.7692             388.0117             419.8318
437.2251             464.3274             479.3956
503.6249             512.9408             532.4571
552.5413             565.4174             581.8949
586.5568             634.2756             661.6350
703.4612             731.5436             750.0442
763.4480             767.5356             770.9841
798.7156             801.4460             815.7565
857.4177             879.7148             886.3884
891.4476             905.6707             920.0789
956.2719             965.6202             982.6988
992.1772             993.0964             994.9425
1036.1876            1064.9004            1119.7263
1152.7959            1166.3851            1173.5789
1186.7790            1195.4955            1220.5522
1239.1214            1260.8872            1275.5624
1299.3870            1315.9494            1338.7521
1359.0580            1383.4112            1405.2388
1436.6264            1445.4759            1469.4722
1487.7167            1505.8462            1526.5113
1581.2967            1591.6778            1619.0889
1646.1695            1652.8011            1669.1785
3157.5186            3158.3622            3160.5794
3161.7205            3163.5810            3170.2899
3175.7902            3177.5878            3179.9341
3186.7355            3188.7983            3199.1070
ZeroEnergy[kcal/mol]  39.8
ElectronicLevels[1/cm] 1
0  2
End
!----------------------------------
```

```
!-------bar_tsp4------------
Barrier      tsp4  i4-22  p4
RRHO
Geometry[angstrom]   31
C    -4.670107   -0.073047   -0.082295
C    -4.160870    1.235714   -0.018387
C    -2.800140    1.456288    0.027290
C    -1.876033    0.383337    0.015602
C    -2.402228   -0.940215   -0.043721
C    -3.798502   -1.140157   -0.094996
C    -0.440466    0.576668    0.048922
C    -0.160094   -1.875049    0.029013
C    -1.499308   -2.050030   -0.064730
C     0.425534   -0.559414    0.170069
C     0.143969    1.873650    0.012728
C     1.494917    2.056679    0.001004
C     2.397873    0.951065   -0.007892
C     1.876790   -0.370517    0.049197
C     4.662733    0.082056   -0.120171
C     4.152580   -1.225843   -0.063112
C     2.791251   -1.443657    0.022356
C     3.794579    1.150774   -0.091136
H    -5.740692   -0.238742   -0.118969
H    -4.841786    2.079255   -0.001736
H    -2.445283    2.476520    0.083598
H    -4.176179   -2.156244   -0.141761
H     0.485431   -2.742021    0.025321
H    -1.912149   -3.049279   -0.155559
H     0.453743   -0.582285    1.955933
H    -0.495237    2.745266   -0.025510
H     1.906161    3.059933   -0.034273
H     5.732319    0.245961   -0.184818
H     4.830727   -2.071441   -0.083641
H     2.435697   -2.463705    0.076628
H     4.172380    2.166972   -0.133652
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  960.8916
WellDepth[kcal/mol]  22.8
WellDepth[kcal/mol]  8.5
End
Frequencies[1/cm]  86
42.2594              75.4396
129.2866             170.8424             188.8069
228.4455             287.1884             294.7561
378.7309             388.0284             423.6506
```

439.3036 454.5768 487.5729
495.9294 507.0167 533.6321
544.5364 570.8608 576.7594
583.6402 592.8040 685.4795
693.1664 699.5453 743.9965
752.6934 774.5434 778.9553
792.7004 825.9584 849.8641
863.8315 876.6133 881.3065
889.8783 895.3971 949.5361
957.1459 965.4980 976.3339
991.6174 993.5726 1036.2668
1059.0536 1062.9123 1099.4905
1159.2049 1172.4607 1177.4421
1186.6791 1201.3112 1214.3131
1247.1430 1251.6612 1275.0751
1279.4607 1318.8934 1345.1506
1371.6747 1377.6715 1381.9841
1454.5648 1459.6365 1463.9768
1482.8084 1513.6085 1551.2058
1558.1320 1594.7693 1630.9231
1645.9518 1652.1803 1654.8818
3160.3579 3160.7034 3164.5707
3166.2728 3170.8231 3171.6646
3185.9520 3186.3673 3194.6008
3197.6029 3210.7923 3215.1718
ZeroEnergy[kcal/mol] 35.9
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_tsp5----------
Barrier tsp5 i5-2 p5
RRHO
Geometry[angstrom] 31
C -0.704926 -0.153686 4.878729
C 0.723169 -0.116401 4.877242
C 1.412557 -0.032915 3.701892
C 0.729319 0.023303 2.446608
C -0.722821 0.000534 2.447567
C -1.401025 -0.100403 3.707343
C 1.412153 0.055716 1.232434
C -0.721324 0.236972 0.000000
C -1.406136 0.068554 1.245095
C -1.406136 0.068554 -1.245095
C 0.742117 0.102216 0.000000
C 1.412153 0.055716 -1.232434
C 0.729319 0.023303 -2.446608
C -0.722821 0.000534 -2.447567

C 0.723169 -0.116401 -4.877242
C -0.704926 -0.153686 -4.878729
C -1.401025 -0.100403 -3.707343
C 1.412557 -0.032915 -3.701892
H -1.232741 -0.221802 5.823288
H 1.256375 -0.158230 5.820179
H 2.497340 -0.011124 3.700346
H -2.485682 -0.123584 3.708459
H 2.497312 0.019415 1.235977
H -2.491037 0.050545 1.240763
H -2.491037 0.050545 -1.240763
H 2.497312 0.019415 -1.235977
H 1.256375 -0.158230 -5.820179
H -1.232741 -0.221802 -5.823288
H -2.485682 -0.123584 -3.708459
H 2.497340 -0.011124 -3.700346
H -0.715384 1.918011 0.000000
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1050.3894
WellDepth[kcal/mol] 27.8
WellDepth[kcal/mol] 25.6
End
Frequencies[1/cm] 86
55.6284 84.5871
147.6453 158.3179 193.2330
268.3758 298.9520 302.0170
316.3562 370.6267 433.0967
469.6500 471.6627 479.7598
483.6353 522.4640 525.5696
559.0154 575.9023 581.9982
618.6618 632.4667 641.0462
732.3096 742.1823 752.4714
755.3161 761.1307 764.8159
781.7808 787.3809 833.7162
850.4616 855.3407 864.2053
885.4991 908.7910 911.4626
919.0881 944.5130 970.2879
971.5946 993.7660 993.8936
1019.4436 1022.3142 1124.3519
1146.1691 1149.7481 1184.1508
1187.9017 1200.7568 1212.8475
1221.5076 1288.4441 1289.0637
1304.1740 1309.5101 1344.1659
1357.2465 1391.5210 1416.9922
1417.5820 1424.6796 1470.8558

1477.5955 1498.9614 1535.2576
1561.7791 1570.7883 1600.3691
1628.1472 1656.2162 1666.5665
3155.3312 3157.9720 3159.3069
3160.1761 3162.6229 3163.7106
3165.1081 3167.7932 3177.2184
3177.3128 3189.0868 3189.3451
ZeroEnergy[kcal/mol] 64.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_ts22-44----------
Barrier ts22-44 i2-2 i44-2
RRHO
Geometry[angstrom] 31
C 4.659309 -0.293083 -0.528311
C 4.142278 0.910350 -1.048756
C 2.815599 1.274734 -0.821723
C 2.006150 0.441030 -0.054873
C 2.525225 -0.790720 0.482808
C 3.872924 -1.145471 0.224670
C 0.625270 0.587852 0.371803
C 0.249654 -0.661475 1.112666
C 1.519941 -1.448851 1.200946
C -0.617440 -1.005423 -0.057990
C -0.168248 1.751741 0.412291
C -1.531590 1.769928 0.595382
C -2.419826 0.685823 0.330670
C -1.945998 -0.561497 -0.210138
C -4.700583 0.049665 -0.267566
C -4.213422 -1.099422 -0.932842
C -2.870191 -1.379912 -0.923467
C -3.822586 0.922007 0.327641
H 5.692914 -0.553384 -0.728393
H 4.784181 1.554409 -1.638601
H 2.421434 2.194062 -1.240841
H 4.278420 -2.071313 0.617348
H -0.304326 -0.514890 2.042872
H 1.607669 -2.405216 1.698141
H -0.227430 -1.740032 -0.755061
H 0.344854 2.701672 0.291246
H -2.001566 2.734120 0.764884
H -5.764238 0.259283 -0.261429
H -4.903954 -1.765237 -1.437913
H -2.497729 -2.278816 -1.403751
H -4.189025 1.841690 0.772217
Core RigidRotor

SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 247.7815
WellDepth[kcal/mol] 0.2
WellDepth[kcal/mol] 11.6
End
Frequencies[1/cm] 86
59.8021 98.5686
105.6708 185.6790 196.4787
258.2125 269.8945 311.7400
368.8433 417.9598 433.2615
445.2196 472.8789 506.1106
534.1533 547.8398 555.4026
569.5444 595.7238 607.3826
650.9270 685.8494 716.4673
741.4727 754.1539 760.7511
765.4736 772.8369 788.5466
820.4232 841.1631 863.3425
866.8761 877.3645 919.8203
940.1274 943.1428 960.3189
979.1800 985.2074 995.0338
1025.1239 1031.5479 1040.3719
1084.1955 1125.0254 1135.3550
1153.5800 1167.7185 1182.4904
1186.5401 1205.6931 1215.0209
1235.2846 1252.3279 1275.9293
1294.8520 1309.9022 1328.6005
1354.3907 1376.9739 1387.3661
1418.7110 1440.4585 1455.2642
1474.0933 1502.7277 1537.5379
1541.4748 1573.8590 1599.7408
1608.2560 1644.3156 3055.1509
3140.4435 3155.1022 3157.6054
3159.2523 3161.0386 3162.7471
3168.6309 3174.6741 3178.3322
3187.9745 3189.0910 3211.0854
ZeroEnergy[kcal/mol] 43.1
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_ts2x1----------
Barrier ts2x1 i2-1 i2x1
RRHO
Geometry[angstrom] 31
C 0.990979 -1.020354 1.133033
C 1.890673 -2.051307 1.243443

C 3.089178 -2.081703 0.485034
C 3.431342 -1.011692 -0.337906
C 2.562647 0.070139 -0.453217
C -0.058983 0.400404 -0.913059
C 0.627175 1.410390 -0.009715
C -2.104267 0.517681 0.494414
C -0.230149 2.017759 1.036568
C -2.075419 -0.953934 -1.442539
C -3.407738 0.087536 0.767971
C -4.038290 -0.852387 -0.040595
C -3.370079 -1.366440 -1.154574
C -1.412973 -0.027812 -0.621275
C 1.249275 0.024008 0.180666
C 2.762416 1.389143 -0.996475
C 1.701030 2.184078 -0.710065
C -1.471550 1.571014 1.282601
H 0.076503 -1.015469 1.713030
H 1.687182 -2.859911 1.937088
H 3.765390 -2.921706 0.590983
H 4.392993 -0.993104 -0.840810
H 0.306297 0.301462 -1.927149
H 0.191252 2.833225 1.614316
H -1.555556 -1.359348 -2.304155
H -3.932064 0.507333 1.620597
H -5.046898 -1.176707 0.188131
H -3.859148 -2.093229 -1.793447
H 3.644181 1.694098 -1.545885
H 1.579182 3.221497 -0.993154
H -2.060911 2.022716 2.074601
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 404.1764
WellDepth[kcal/mol] 18.7
WellDepth[kcal/mol] 0.5
End
Frequencies[1/cm] 86
62.8634 87.3027
112.1178 183.2990 191.6010
223.3094 296.3701 335.5144
365.1489 392.8727 416.7830
446.8394 465.9562 504.6691
522.3294 542.0572 549.8536
573.5837 621.1092 626.3622
653.1042 695.1458 702.4871
726.0379 744.6061 754.0219
762.8780 770.7175 801.0939

822.4682 838.9446 851.9572
879.1476 898.0077 900.5926
923.6330 937.0605 945.3044
951.5846 969.0005 983.4385
991.1578 1013.9207 1019.4968
1057.2822 1084.3446 1114.3119
1131.0166 1154.0398 1174.0096
1180.3735 1182.3057 1206.4154
1224.2238 1239.6796 1276.1011
1284.1073 1294.7810 1333.6800
1338.2880 1358.8158 1378.3343
1417.6187 1436.4826 1462.4045
1481.3902 1503.0558 1532.4036
1562.1130 1588.2819 1598.2697
1629.9453 1673.3332 3153.3272
3157.7466 3157.9299 3162.8059
3165.4007 3175.2754 3176.7028
3180.7761 3185.8947 3189.3386
3190.3450 3194.3545 3211.1576
ZeroEnergy[kcal/mol] 44.4
ElectronicLevels[1/cm] 1
0 2
End
!-----------------------------------
!-------bar_ts2x2------------
Barrier ts2x2 i2x1 i2x2
RRHO
Geometry[angstrom] 31
C 1.912712 -2.092572 1.200473
C 3.175106 -2.008167 0.566427
C 3.467762 -0.931571 -0.271080
C 2.510401 0.044131 -0.521775
C -0.020090 0.423317 -0.889271
C 0.570613 1.495332 -0.023303
C -1.410384 -0.009207 -0.597343
C -2.092806 0.512280 0.528097
C -1.455879 1.529983 1.352776
C -0.227763 2.015745 1.071878
C -2.065204 -0.911215 -1.437345
C -3.400873 0.077055 0.790694
C -4.031097 -0.839944 -0.041505
C -3.364593 -1.331111 -1.164072
C 1.145831 -0.128928 -0.018163
C 0.916835 -1.184993 0.934635
C 2.736569 1.393318 -0.984963
C 1.722434 2.214096 -0.622591
H 1.720498 -2.903834 1.894074
H 3.932532 -2.754435 0.774942

H 4.470123 -0.808597 -0.669254
H 0.233732 0.462892 -1.946605
H -2.019207 1.925063 2.191517
H 0.203330 2.806360 1.677041
H -1.543934 -1.297045 -2.307327
H -3.923702 0.474748 1.654544
H -5.041422 -1.166069 0.178133
H -3.853112 -2.041922 -1.820751
H -0.061847 -1.299107 1.383327
H 3.646389 1.709793 -1.479168
H 1.699169 3.286873 -0.771879
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 400.5856
WellDepth[kcal/mol] 1.6
WellDepth[kcal/mol] 33.6
End
Frequencies[1/cm] 86
66.5392 82.1640
135.3746 171.6182 200.2787
227.0917 286.8077 343.2936
382.2095 400.6142 423.1211
426.0744 461.9441 508.0207
527.1044 534.1856 566.9121
591.6962 602.9782 635.9518
650.3561 697.2517 710.2974
727.1315 739.9345 744.2302
770.7436 780.8516 788.7751
816.9646 826.7411 841.2082
888.3432 898.6078 914.7056
919.8005 935.1631 954.1774
962.1533 974.9590 990.7538
1019.4075 1031.6610 1058.5382
1066.3077 1092.1626 1124.7118
1135.3983 1159.5753 1177.7522
1183.4598 1195.8388 1205.5644
1230.6680 1236.6903 1270.8675
1285.3759 1292.4893 1324.8543
1331.8617 1366.2583 1382.7526
1423.4080 1445.8947 1452.2994
1485.7387 1513.5087 1530.6132
1569.1391 1585.1348 1596.6898
1638.0993 1641.4598 3102.0254
3156.2518 3157.2177 3158.7418
3163.3002 3165.5131 3175.2210
3177.2902 3181.3959 3186.0533

3189.1902 3195.6706 3203.4202
ZeroEnergy[kcal/mol] 45.5
ElectronicLevels[1/cm] 1
0 2
End
!----------
!-------bar_tsp6----------
Barrier tsp6 i2x2 p6
RRHO
Geometry[angstrom] 31
C -3.867040 -1.487635 0.032187
C -3.727131 -0.154297 -0.280270
C -2.467232 0.484603 -0.217331
C -1.303649 -0.273987 0.108688
C -1.498735 -1.618174 0.502892
C -2.743567 -2.213954 0.460400
C -2.366962 1.897090 -0.408768
C 0.022491 1.819929 0.015222
C 1.288782 -0.299517 -0.016805
C 3.742481 -0.205838 0.107024
C 3.832363 -1.543825 -0.207873
C 2.660842 -2.258601 -0.501076
C 1.248726 2.526252 0.179711
C 2.427676 1.865847 0.334281
C -1.178873 2.538478 -0.239780
C 1.422823 -1.650527 -0.406383
C 2.491689 0.447450 0.172382
C 0.002394 0.394393 0.143261
H -4.840186 -1.963070 -0.012183
H -4.593540 0.438631 -0.554078
H -0.667666 -2.181627 0.900718
H -2.855061 -3.243628 0.780946
H -3.266547 2.453275 -0.649133
H 4.640117 0.378352 0.280777
H 4.798865 -2.031331 -0.264375
H 2.723326 -3.293429 -0.818443
H 1.218939 3.610565 0.189132
H 3.350986 2.412045 0.494667
H -1.119371 3.617963 -0.329722
H 0.547936 -2.218992 -0.682372
H 0.139737 0.415142 1.997510
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 858.9536
WellDepth[kcal/mol] 27.3
WellDepth[kcal/mol] 6.7

End
Frequencies[1/cm] 86
79.3921 84.1422
126.1356 175.1759 206.6002
256.6636 271.0597 320.5386
375.5543 416.6193 426.8262
435.1685 440.8223 451.7153
498.2262 524.2988 527.1495
534.9853 553.1789 584.3860
596.5636 634.4869 686.1249
694.5612 706.8281 754.7746
761.3817 768.0541 771.5587
814.6520 818.3431 828.4069
855.1743 865.2445 885.7433
890.7905 961.9196 964.7822
969.9196 978.1462 980.4374
993.2725 1005.3830 1012.5520
1057.0476 1072.4667 1125.5608
1152.5736 1168.4652 1176.4345
1181.4587 1188.5927 1220.6801
1232.4947 1237.7717 1251.9102
1280.6674 1322.1682 1342.0898
1361.7788 1371.0867 1386.6579
1448.9402 1449.6339 1454.2060
1482.9540 1525.8285 1533.3787
1556.5433 1590.7192 1624.7981
1642.5686 1645.8599 1656.7141
3158.4073 3159.8031 3160.9721
3162.3366 3171.0450 3171.6913
3178.0156 3180.0234 3187.0180
3187.6941 3211.6262 3228.9346
ZeroEnergy[kcal/mol] 39.2
ElectronicLevels[1/cm] 1
0 2
End
!----------
End