# Supporting Information for

# Unconventional Gas-Phase Preparation of the Prototype Polycyclic Aromatic Hydrocarbon Naphthalene ($C_{10}H_8$) via the Reaction of Benzyl ($C_7H_7$) and Propargyl ($C_3H_3$) Radicals Coupled with Hydrogen-Atom Assisted Isomerization

Chao He, Ralf I. Kaiser*

*Department of Chemistry, University of Hawai'i at Mānoa, Honolulu, HI 96822, USA*

Wenchao Lu, Musahid Ahmed*

*Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

Vladislav S. Krasnoukhov[a,b], Pavel S. Pivovarov[b], Marsel V. Zagidullin[a], Valeriy N. Azyazov[a]

[a] *Lebedev Physical Institute, Samara 443011, Russian Federation*

[b] *Samara National Research University, Samara 443086, Russian Federation*

Alexander N. Morozov, Alexander M. Mebel

*Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, USA*

Corresponding Author Prof. Dr. Ralf I. Kaiser: ralfk@hawaii.edu

Corresponding Author Prof. Dr. Musahid Ahmed: mahmed@lbl.gov

Corresponding Author Prof. Dr. Alexander M. Mebel: mebela@fiu.edu

**Experimental & Computational - Experimental**

The experiments were carried out 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.[1] This device is located inside the source chamber of a molecular beam setup, which is equipped with a Wiley-McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS).[2] The molecular beam apparatus is designed to study the elementary chemical reactions and ultimately leading to PAH growth in situ via the reactions of aromatic radicals. In detail, propargyl radicals ($C_3H_3$) were prepared in situ by pyrolysis of the propargyl bromide ($C_3H_3Br$; Sigma Aldrich, > 98%),[3] whereas a continuous beam of benzyl radicals ($C_7H_7$) was generated in situ through the pyrolysis of benzylbromide ($C_7H_7Br$; Sigma Aldrich, 98%).[4] The reactants were seeded in helium carrier gas at total pressures of 200 ± 10 torr at the reactor inlet. The temperature of the SiC tube was determined using a Type-C thermocouple to be 1473 ± 10 K. The precursor propargyl bromide ($C_3H_3Br$; Sigma Aldrich, > 98%) [3] was kept in a bubbler at a temperature of 199 K obtained in a dry ice-ethanol bath, whereas benzylbromide ($C_7H_7Br$; Sigma Aldrich, 98%)[4] precursor was also stored in a bubbler at room temperature of 298 ± 3 K. At this temperature, each precursor dissociates to the corresponding radical in situ followed by the reaction of benzyl ($C_7H_7$) and propargyl ($C_3H_3$) radicals. The products formed in the reactor passed through a 2 mm skimmer located 10 mm downstream the reactor and entered the main chamber, which houses the ReTOF-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 considered as a soft ionization method compared to the harsher conditions of electron impact ionization with latter normally leading to excessive fragmentation of the parent ion.[5] The ions formed via soft photoionization were extracted and ultimately detected by a microchannel plate detector through an ion lens. Under our experimental condition, the residence time in the reactor tube is few tens to hundreds of microseconds.[6, 7] 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. Control experiments were also proceeded by expanding neat helium carrier gas with each precursor separately into the resistively-heated silicon carbide tube, but no naphthalene was detected. Finally, reference PIE curve of naphthalene was

recorded via helium-seeded naphthalene ($C_{10}H_8$; Sigma Aldrich; 99%)[8] in the present work within the same experimental setup. Due of the weak signal in these experiments, extended data accumulation times of up to 15 min per step have to be accounted for and each step was repeated in triplicate. No unexpected or unusually high safety hazards were encountered during the course of this study.

## Experimental & Computational - Computational

### Calculation Methods

*Electronic structure*

Ab initio calculations were applied to investigate the potential energy surface (PES) for the benzyl + propargyl reaction. Initially, geometries of the reactants, products, all local $C_{10}H_{10}$ local minima, and transition states were optimized using the B3LYP[9-11] density functional theory (DFT) method with the 6-311G** basis set. Vibrational frequencies and zero-point vibrational energies (ZPE) were calculated using the same level of theory. Then single-point energies were refined within the G3(MP2,CC) model chemistry approach[12-14] where the overall energy is computed as

E[G3(MP2,CC)] = E[CCSD(T)/6-311G**] + E[MP2/G3Large] – E[MP2/6-311G**] + ZPE

Here, CCSD(T) is the coupled clusters method with single and double excitations with perturbative treatment of triple excitations and MP2 is the second order Møller−Plesset perturbation theory. $\Delta E_{MP2}$ = E[MP2/G3Large] – E[MP2/6-311G**] is the basis set correction to the CCSD(T)/6-311G** energy computed as a difference of the MP2 energies with the 6-311G** and G3Large basis sets.

Diradical (singlet open shell) compounds involved in the reaction mechanism were treated using the unrestricted UB3LYP/6-311G** approach for geometry optimization and vibrational frequencies calculations, whereas their total energies were refined employing the composite triplet-singlet gap method:[15, 16]

$E^S = E^T$ [G3(MP2,CC] + $\Delta E^{S-T}$(CASPT2(10,10)/cc-pVTZ) + $ZPE^S$

where $E^T$[G3(MP2,CC] is the G3(MP2,CC) of the triplet state without ZPE at the open shell singlet optimized geometry, $\Delta E^{S-T}$(CASPT2(10,10)/cc-pVTZ) is the singlet-triplet energy gap computed using the multireference second-order perturbation theory CASPT2 method[17, 18] with the active space consisting of 10 electrons distributed on 10 orbitals and with the cc-pVTZ basis set,[19] and $ZPE^S$ is the singlet state ZPE. The electronic structure calculations were carried out utilizing the Gaussian 09[20] and MOLPRO 2015[21] program packages.

*Rate constants*

The computed PES and molecular parameters were utilized in calculations of reaction rate constants and product branching ratios using the Rice-Ramsperger-Kassel-Marcus (RRKM) theory – Master Equation (ME) approach[22, 23] approach as implemented in the MESS

package.[24] For reaction steps with distinct barriers, the rigid-rotor-harmonic-oscillator (RRHO) model was used for computing the number of states of transition states and the density of states of the related local minima with Eckart's tunneling corrections.[25] Internal rotations were treated within the hindered rotor approximation for the partition function, with the rotational potentials taken from the B3LYP/6-311G(d,p) calculations by Matsugi and Miyoshi.[16] For the initial barierrless association of the benzyl and propargyl radicals, the *E,J*-resolved rate constant in the high-pressure (HP) limit was computed within variable reaction coordinate-transition state theory (VRC-TST).[26-28] The details of the VRC-TST calculations are provided in the previous work.[29] For the other barrierless dissociation reactions leading to various $C_{10}H_9$ + H and $C_6H_5$ + $C_4H_5$ products, phase space theory[30] was employed to assess *E,J*-resolved rate constants of their reverse bimolecular association reactions at the HP limit. Potential power exponents and prefactors in the phase space theory calculations were fit to match the HP rate constants to those of the closest analogous prototype reactions evaluated in the work of Klippenstein and co-workers[31] and our earlier publication[32] within state-of-the-art VRC-TST calculations.

The Lennard-Jones, ($\varepsilon$/cm$^{-1}$, $\sigma$/Å) = (390, 4.46), and the collisional energy transfer, $n$ = 0.62, $\alpha_{300}$ = 424 cm$^{-1}$, parameters for ME calculations were taken from the previous study of the $C_9H_x$/Ar systems[33] and were used within the "exponential down" model[34] of the collisional energy transfer for the temperature dependence of the range parameter $\alpha$ for the deactivating wing of the energy transfer function $\alpha(T) = \alpha_{300}(T/300\ \mathrm{K})^n$. In the limit of low pressure, the present RRKM-ME calculations took into account infrared radiative stabilization of $C_{10}H_{10}$ intermediates using the theoretical approach by Klippenstein and coworkers[35] as implemented in the MESS package. The molecular parameters including optimized Cartesian coordinates, vibrational frequencies, relative energies, and hindered rotor potentials in the form of an input file for RRKM-ME calculations using the MESS code are provided in Table S1.

*CFD and kinetics simulations of processes in the micro reactor*

Modeling of the gas flow and kinetics of the $C_7H_7$ + $C_3H_3$ system was carried out employing the COMSOL Multiphysics package[36] using the formalism and physical parameters described in detail in previous publications.[7, 37] A gas mixture of He ($p_{inlet}$ = 200 Torr), $C_3H_3Br$ ($p$ = 1 Torr), and $C_7H_7Br$ ($p$ = 1.6 Torr) was introduced at the room temperature upstream of the choke orifice. The maximum temperature is 1,473 K at the SiC microreactor surface. We implied the following simplified kinetic mechanism:

$C_3H_3Br \rightarrow C_3H_3 + Br$ (R0a)[3]

$C_6H_5CH_2Br \rightarrow C_6H_5CH_2 + Br$ (R0b)[38, 39]

$C_7H_7 + C_3H_3$ → 3-butynylbenzene (**i1**) (R1)[29]

$C_7H_7 + C_3H_3$ → 2,3-butadienylbenzene (**i2**) (R2)[29]

$C_7H_7 + C_3H_3$ → methyleneindanyl radicals (**p3** + **p4** + **p5**) + H (R3)[29]

(**i1** + **i2**) → (**p3** + **p4** + **p5**) + H (R4)[29]

$C_7H_7 + C_3H_3 \rightarrow C_6H_5CH_2CCCCH_2$ (**p6**) + H (R5)[29]

$C_7H_7 + C_3H_3 \rightarrow C_6H_5 + i\text{-}C_4H_5$ (**p7**) (R6)[29]

**p6** + H → $C_6H_5 + i\text{-}C_4H_5$ (**p7**) (R7)[29]

**p6** + H → (**p3** + **p4** + **p5**) + H (R8)[29]

$C_6H_5 + i\text{-}C_4H_5$ (**p7**) → (**p3** + **p4** + **p5**) + H (R9)[29]

(**p3** + **p4** + **p5**) → benzofulvene (**p1**) + H (R10)[33]

(**p3** + **p4** + **p5**) → naphthalene (**p0**) + H (R11)[33]

**p1** + H → **p0** + H (R12)[33]

Temperature- and pressure-dependent rate constants were taken from the literature specified in the references provided following the reaction designation.

Figure S6 illustrates temperature, pressure, and axial and cross section average gas stream velocities profiles along the reactor computed as a result of the CFD simulations and used for kinetic modeling alongside with the mechanism described here.

**Comparison of calculated rate constants for the high-temperature combustion environments with the earlier work**

Figure S7 compares the rate constants of various reactions in the proposed mechanisms computed here ($C_7H_7 + C_3H_3$) and in our previous work on the $C_{10}H_9$ PES[33] at 1 atm with those from Matsugi and Miyoshi.[16] For (R3) (Fig. S7(a)), our rate constant is higher than the values of Matsugi and Miyoshi at lower temperatures by from a factor of 8 at 500 K, a factor of 2 at 1000 K, to 40-50% around 1400-1500 K. However, the rate constants practically coincide at high temperatures above 1600 K, i.e., in the temperature regime most relevant to these mechanisms. The rate constants for (R1) and (R2) both in forward (Fig. S7(b)) and reverse (Fig. S7(c)) directions are in general quite similar. For example, at 1000 K the differences in the forward rate constants are within 40-45%, whereas those for the reverse rate constants are 22-34%. However, there are two main differences: first, the **i1**/**i2** branching ratio controlled by the entrance channel rate constants is notably higher in the present calculations and second, the forward rate constants computed by Matsugi and Miyoshi[16] rapidly drop off to very small values at temperatures above 1500 K. Our results indicate that the forward rate constants for the formation of **i1** and **i2** decrease relatively slightly with temperature and remain high (above $10^{-12}$ $cm^3$ $molecule^{-1}$ $s^{-1}$) up to 1800 K. Above this temperature, our calculations show **i1** and **i2** to become unstable and to merge with their decomposition products, mostly dissociating back to $C_7H_7 + C_3H_3$. The agreement for the rate constants for (R4) is reasonably close (Fig. S7(d)); the present values are somewhat higher, by factors of around 2.5 in the 1000-1800 K range. Comparing the rate constants for the unimolecular decomposition of the methyleneindanyl radicals **p3**, **p4**, **p5** to benzofulvalene (**p1**) and naphthalene (**p0**) computed by our group in 2016[33] and by Matsugi and Miyoshi,[16] one can see significant differences (Fig. S7(e)). Our rate constants for the formation of **p1** are generally by more than order of magnitude higher than the values of Matsugi and Miyoshi, whereas for the formation of **p0** the differences are smaller and decrease from a factor of 8.5 at 800 K to a factor of 1.4 at 2000 K. Additionally, our calculations predicted a much higher yield of benzofulvene as compared with naphthalene, whereas Matsugi and Miyoshi predicted opposite.[16] The differences in the rate constants for the bimolecular reaction of H-assisted isomerization of benzofulvene to naphthalene (R12) are less pronounced (Fig. S7(f)). Our rate constants computed in 2016 are higher at lower temperatures by from a factor of 4.7 at 500 K to 1.8 at 1000 K. At higher temperatures, Matsugi and Miyoshi's values are slightly higher but the differences are within 30%. Summarizing, while the present calculations of the kinetics of the $C_7H_7 + C_3H_3$ reaction qualitatively support the mechanism proposed by Matsugi and Miyoshi,[16] the quantitative

differences in the calculated rate constants warrant their inclusion in an updated detailed kinetic mechanism of naphthalene formation in combustion flames.

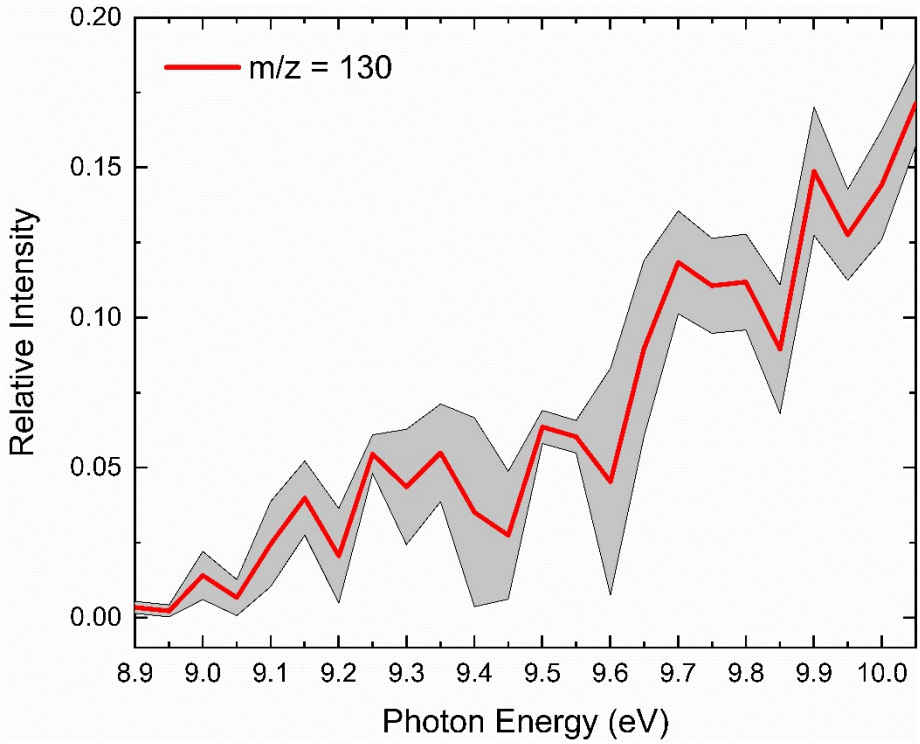


**Figure S1**. PIE curve for the species (m/z = 130) in the benzyl ($C_7H_7$•) + propargyl ($C_3H_3$•) system. The error bars consist of two parts: ±10% based on the accuracy of the photodiode and a 1 σ error of the PIE curve averaged over the individual scans.

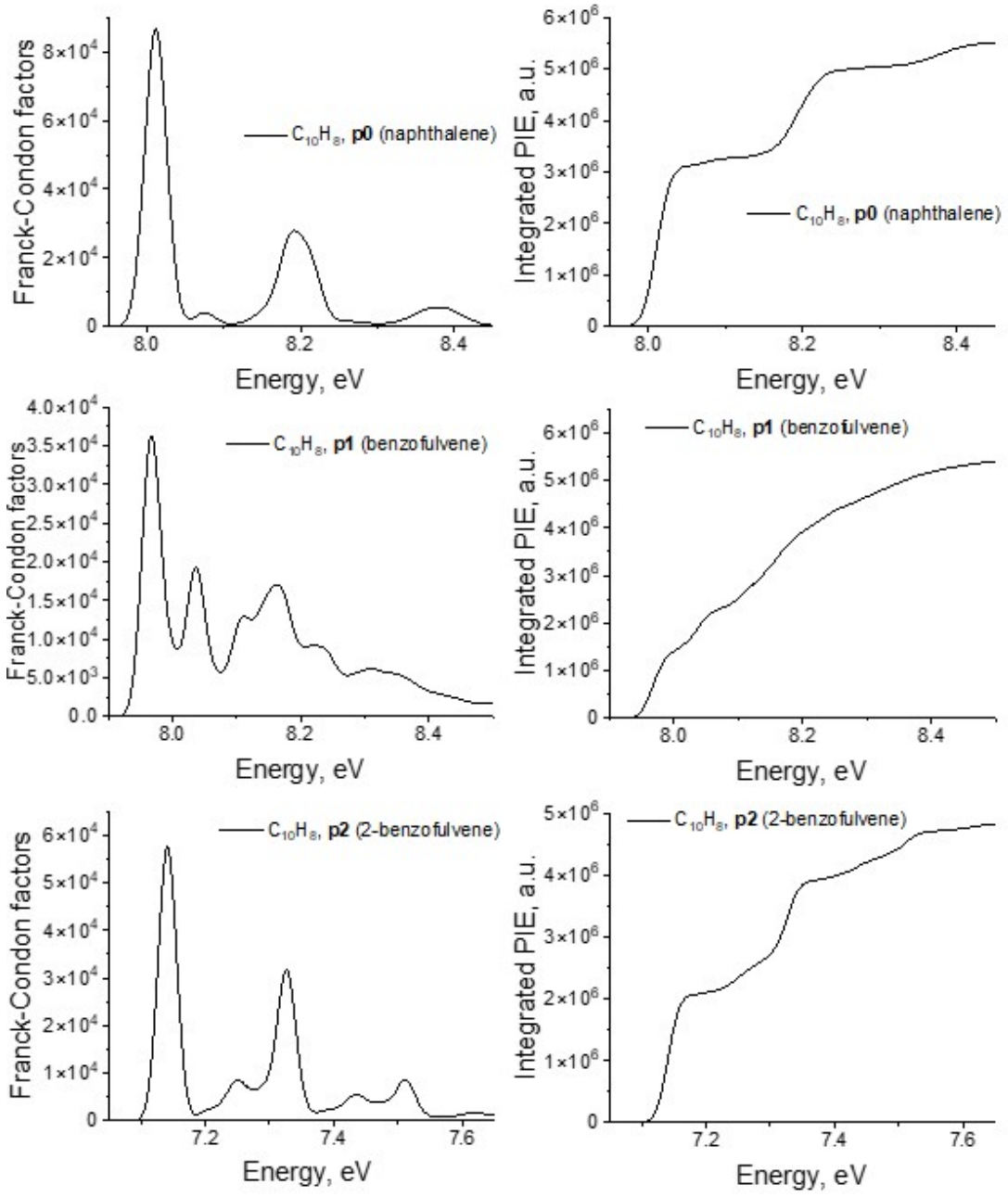


**Figure S2**. Computed ionization Franck-Condon factors and integrated PIE curves for three isomers of $C_{10}H_8$.

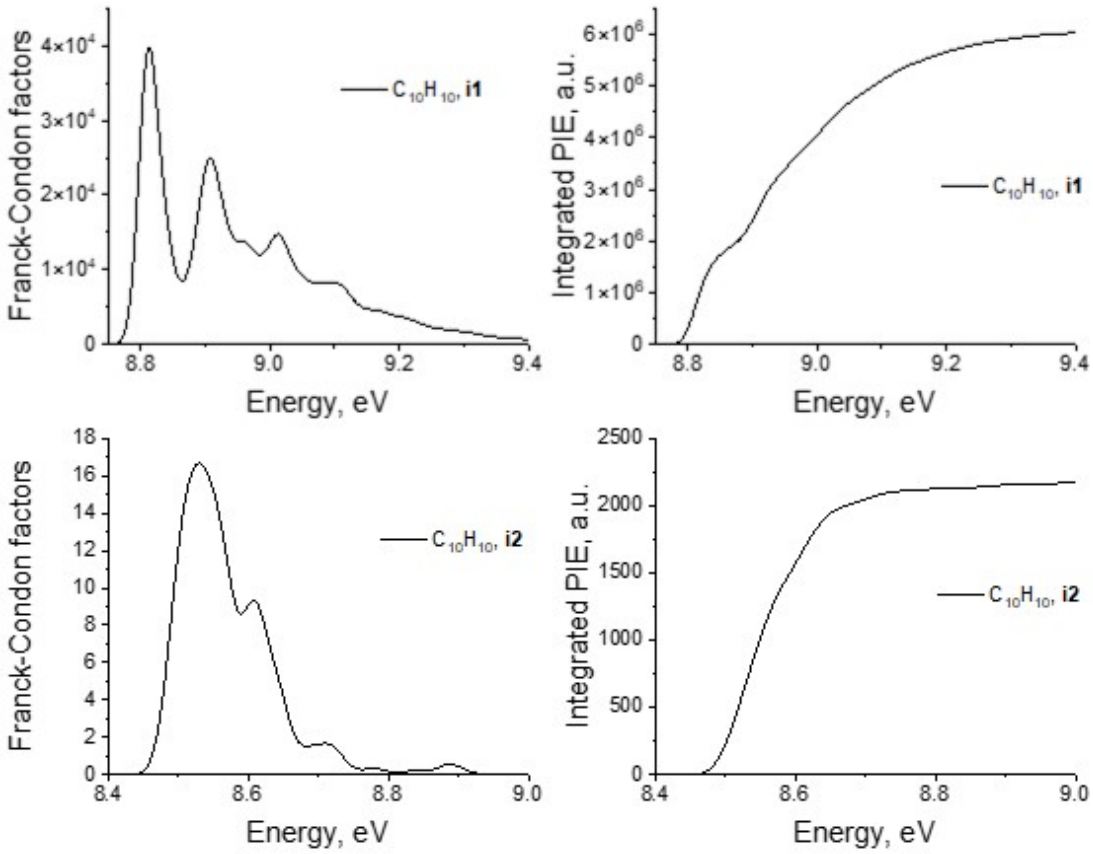


**Figure S3**. Computed ionization Franck-Condon factors and integrated PIE curves for two isomers of $C_{10}H_{10}$.

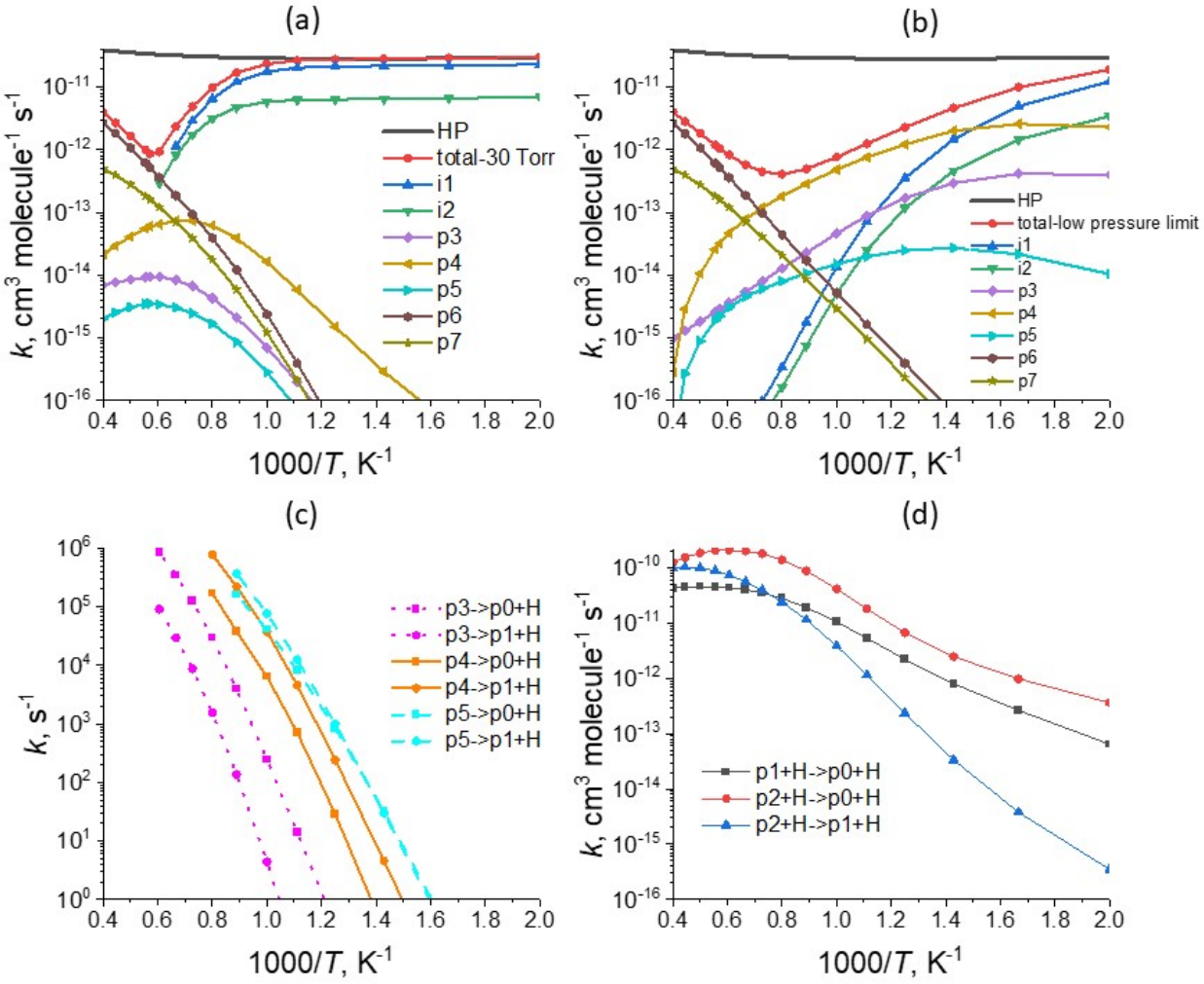


**Figure S4**. Calculated total and individual product channel rate constants for the benzyl – propargyl radical-radical reaction at 30 Torr (a) and in the limit of low pressure (b). Rate constants for thermal unimolecular decomposition of methylene-indanyl radicals (c) and hydrogen atom assisted isomerization of benzofulvenes to naphthalene (d) at 30 Torr.

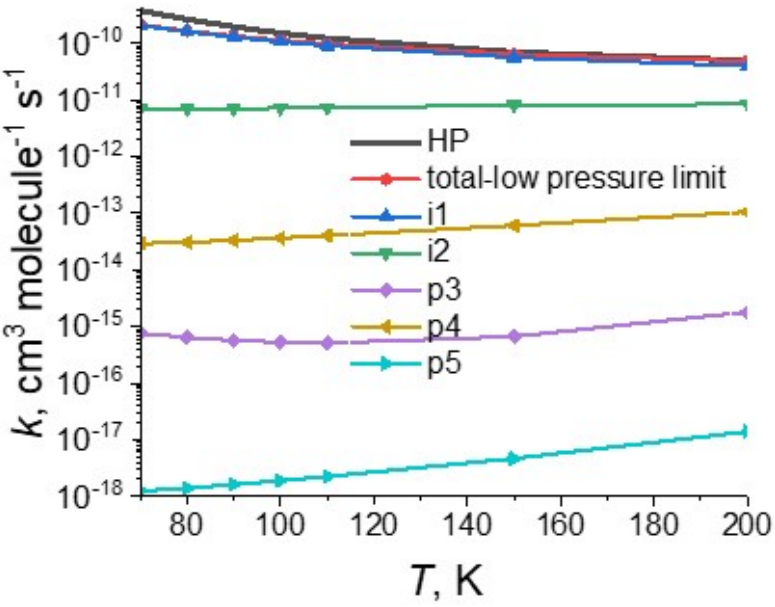


**Figure S5**. Calculated total and individual product channel rate constants for the $C_7H_7$ + $C_3H_3$ reaction at low temperatures in the limit of low pressure.

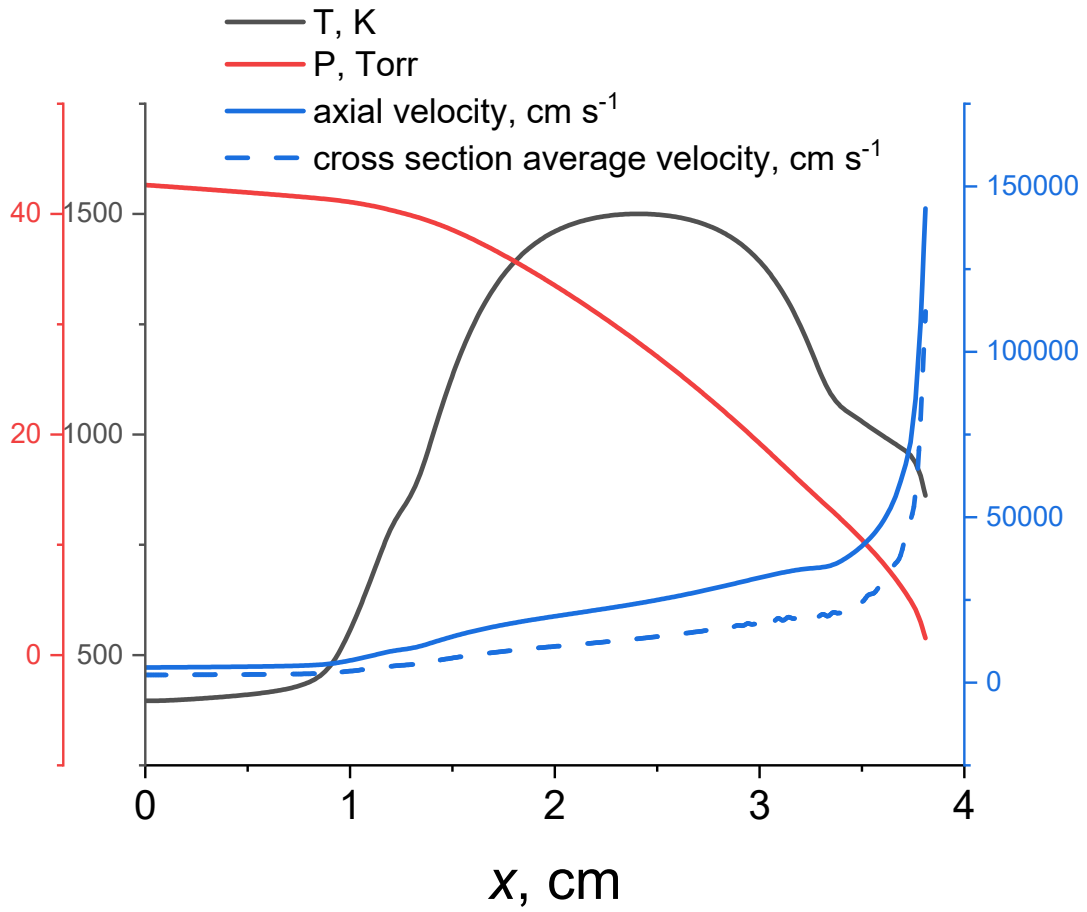


**Figure S6**. CFD simulation of distributions of temperature T, pressure P, axial velocity, and cross section average velocity for the gas stream along the axis of the microreactor under the experimental conditions. $x$ = 0 corresponds to the inlet of SiC tube.

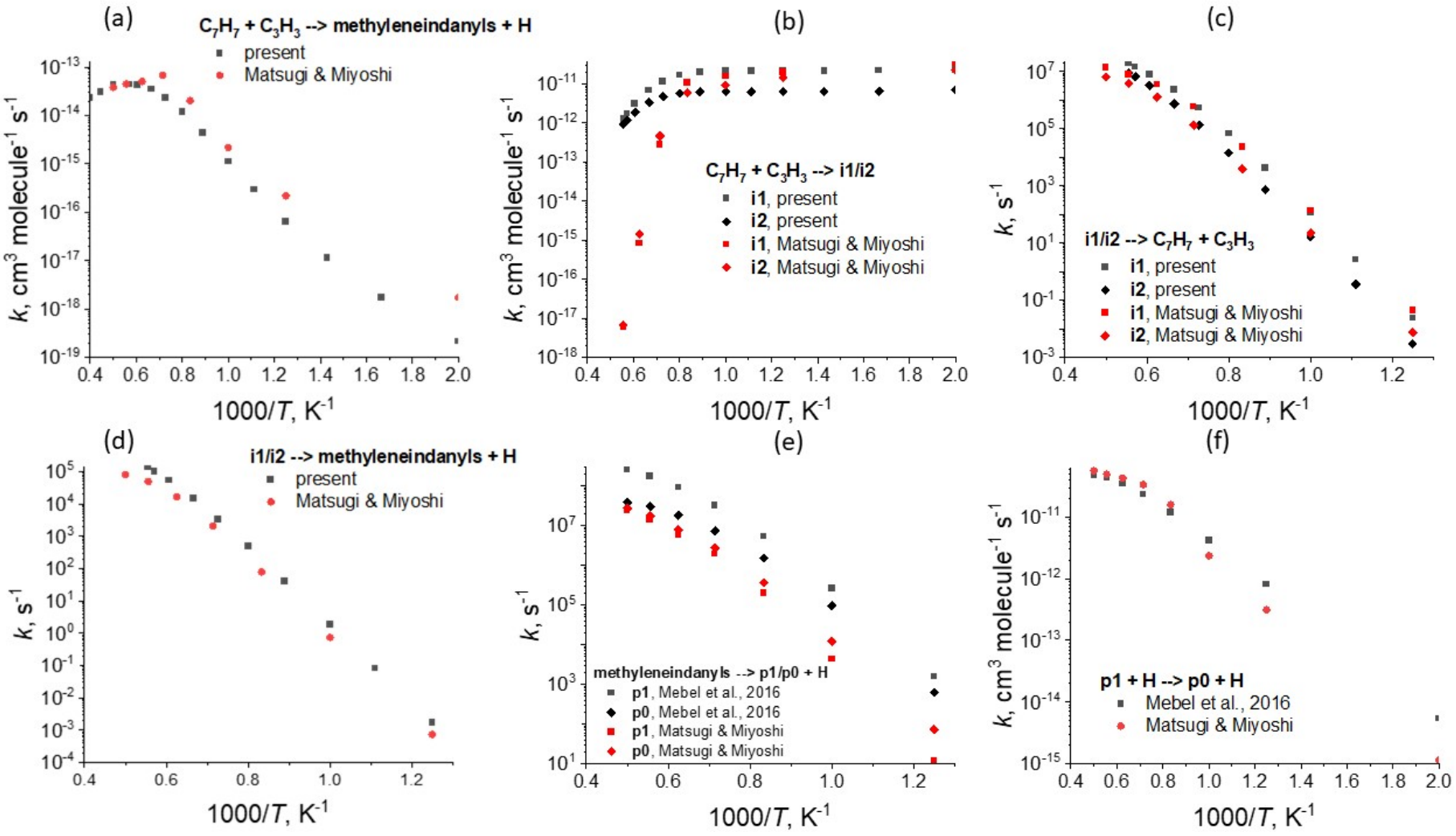


**Figure S7**. Comparison of rate constants for the key reactions involved in the $C_7H_7 + C_3H_3 \rightarrow$ naphthalene + 2H mechanism calculated here and in the previous literature at 1 atm.

**Table S1.** Optimized Cartesian coordinates (Å) and vibrational frequencies ($cm^{-1}$) for all intermediates, transition states, reactants and products involved in the reaction of benzyl + propargyl system. The data are given in the format of an input file for the MESS package.

```
# -------declarations-----------
TemperatureList[K]          300. 500. 600. 700. 800. 900. 1000. 1125.
1250. 1375. 1500. 1650. 1750. 1800. 2000. 2250. 2500.
!PressureList[atm]           0.03947368 1. 10. 100.
!TemperatureList[K]          70. 80. 90. 110. 150. 200.
PressureList[atm]           1E-18
EnergyStepOverTemperature   0.2            # *Ratio of discretization
energy step to T*
ExcessEnergyOverTemperature 70
ModelEnergyLimit[kcal/mol]      900
WellCutoff                  10
ChemicalEigenvalueMax       0.2
ChemicalEigenvalueMin       1.e-6          # *Only for direct
diagonalization method*
CalculationMethod           low-eigenvalue
EigenvalueOutput                        eigenvalue.out
Reactant                    w0             # *Ground energy of bimolecular
species will be used as a reference*
Model
EnergyRelaxation
Exponential
Factor[1/cm]                424            # C9Hx/Ar
Power                               0.62
ExponentCutoff                  15
End
CollisionFrequency
LennardJones
Epsilons[1/cm]              390.  390.     # C9Hx/Ar
Sigmas[angstrom]            4.46  4.46     # C9Hx/Ar
Masses[amu]                 28.   130.
End
OutputTemperatureStep[K]          100
OutputTemperatureSize             20
OutputReferenceEnergy[kcal/mol]   0.

# -------w0-----------
Bimolecular        w0
Fragment        C7H7
 RRHO
   Geometry[angstrom]   14
C  0.994159   -8.0E-6   0.0
C  0.25121   -1.216512   -1.24E-4
C  0.251213   1.216472   -1.13E-4
C  -1.13158   1.209837   -5.0E-5
C  -1.836277   1.7E-5   9.8E-5
C  -1.131545   -1.209843   -1.0E-6
C  2.398095   3.7E-5   1.62E-4
H  0.790904   -2.157628   -4.7E-5
H  0.790845   2.157619   4.3E-5
```

```
H  -1.673995   2.149038   -6.0E-5
H  -2.919988   -8.0E-6   4.03E-4
H  -1.674008   -2.14901   -7.1E-5
H  2.957234   -0.927196   -7.4E-5
H  2.957365   0.927187   -2.3E-5
  Core  RigidRotor
     SymmetryFactor 2
  End
  Frequencies[1/cm]  36
    198.6753               359.1271               390.3132
    478.5981               502.1989               534.2124
    628.2287               684.5079               707.1720
    773.7403               829.1817               830.9751
    898.3874               969.6051               971.5974
    989.5358               994.6024              1035.9429
   1116.3450              1174.6158              1184.4537
   1288.0078              1327.3102              1351.9221
   1473.6465              1489.6398              1502.0160
   1576.6083              1598.3058              3144.6847
   3157.8381              3160.3300              3172.6310
   3177.3169              3190.8265              3241.3375
  ZeroEnergy[kcal/mol]     0.0
  ElectronicLevels[1/cm]        1
         0  2
 End
Fragment        C3H3
 RRHO
   Geometry[angstrom]   6
C  0.11578   -5.0E-6   -2.1E-5
C  1.337865   -1.0E-6   -1.6E-5
C  -1.251358   -3.0E-6   7.0E-6
H  2.400059   1.0E-6   1.24E-4
H  -1.806931   -0.929803   2.8E-5
H  -1.806851   0.929853   2.8E-5
  Core  RigidRotor
     SymmetryFactor 2
  End
  Frequencies[1/cm]  12
    352.0219               403.2308               468.4763
    637.8092               681.8420              1031.3626
   1089.2851              1455.3919              2011.1052
   3139.2898              3229.7773              3467.8791
  ZeroEnergy[kcal/mol]     0.0
  ElectronicLevels[1/cm]        1
         0  2
 End
 GroundEnergy[kcal/mol] 0.0
 End

# -------well_i1-----------
Well          i1
Species
RRHO
Geometry[angstrom]   20
```

```
C  -3.3501175844   -8.234513E-4   -0.2986146486
C  -4.5216160598   -0.0027110189   -0.0305067963
C  -1.919844054   0.0014063952   -0.5911744936
H  -5.5590910538   -0.0046244442   0.197233102
H  -1.6716321569   0.8803447716   -1.1959846376
H  -1.670514658   -0.8717912343   -1.2037879996
C  0.4349060375   -0.0013711318   0.368675861
C  1.1329585126   -1.2013932625   0.1958004963
C  1.1315686959   1.2010588539   0.2071546774
C  2.4856686903   1.205966098   -0.1193881599
C  3.1679840505   0.0033389906   -0.2904978589
C  2.4870744263   -1.2016324453   -0.1307666547
C  -1.0426501366   -0.003707608   0.6877377294
H  0.6118300598   -2.1449966299   0.3257006572
H  0.6093319917   2.1427787192   0.3459599167
H  3.0088952915   2.1487741937   -0.2351976268
H  4.2226438466   0.0051405145   -0.5415936495
H  3.0113891996   -2.1426993991   -0.2554735463
H  -1.2984483765   -0.8844368727   1.282756942
H  -1.2995347221   0.8714129613   1.2905126901
Core  RigidRotor
SymmetryFactor  1.0
End
      Rotor     Hindered     ! 49.4130
        Group                  1 2 3 4 5 6 19 20
        Axis                   7 13
        Symmetry                2
        Potential[kcal/mol]     6
0       0.444603288     1.333809864     1.778413152     1.333809864
        0.444603288
End
      Rotor     Hindered     ! 64.8388
        Group                  1 2 4 5 6
        Axis                   13 3
        Symmetry                3
        Potential[kcal/mol]     4
0       2.275911365     4.551822731     2.275911365
End
Frequencies[1/cm]  52
               84.3924
174.6256              283.0948              323.6283
369.4841              415.7948              444.1272
526.8242              604.1707              636.7163
664.9629              675.4977              716.4144
766.1921              771.1124              828.4034
856.8263              918.5414              972.0387
978.3918             1001.0780             1011.2962
1011.9187             1018.3790             1050.7761
1105.7851             1180.5010             1187.1680
1202.8703             1226.1491             1295.8233
1306.3683             1341.0116             1361.7603
1371.0719             1476.5024             1485.1911
1501.2293             1528.0168             1625.7711
1647.2672             2220.8995             3023.6220
```

```
3045.6034               3051.1105               3087.7784
3152.3728               3153.5456               3166.7654
3176.0166               3188.2186               3477.2834
       InfraredIntensities[km/mol]     52
 0.1032
 0.0505                  0.7277                  2.1139
 4.6577                  0.0064                  2.5404
21.9237                  3.3069                  0.0161
45.3080                 45.0199                 42.3290
24.3137                  0.0340                  1.0227
 0.0149                  0.8477                  0.4300
 0.0004                  0.0175                  0.2151
 1.3663                  0.1588                  3.5911
 5.0308                  0.5112                  0.3503
 0.0868                  0.1538                  2.6039
 0.1862                  0.0308                  0.3997
 0.7115                  1.9020                  6.3163
 5.5115                 13.1052                  1.1654
 5.8467                  7.3116                  7.9259
28.2934                  2.3244                 19.8888
 9.8170                  5.5157                  5.6377
34.9249                 19.2759                 74.1208
ZeroEnergy[kcal/mol] -67.6
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i2-----------
Well          i2
Species
RRHO
Geometry[angstrom]   20
C  -3.047023   0.049489   -0.27926
C  -1.937542   -0.599904   -0.500261
C  -4.1557   0.696819   -0.051496
H  -1.701852   -0.903003   -1.519038
H  -5.077537   0.175254   0.189056
H  -4.199658   1.78106   -0.097984
C  0.458634   -0.397412   0.288845
C  1.540681   -1.236479   0.013074
C  0.673011   0.985642   0.301567
C  1.935611   1.513459   0.050899
C  3.00875   0.665387   -0.22219
C  2.807476   -0.711566   -0.241147
C  -0.922393   -0.965918   0.566253
H  1.392285   -2.311762   2.7E-4
H  -0.159419   1.650859   0.506386
H  2.083979   2.587657   0.068522
H  3.992751   1.076318   -0.418056
H  3.635152   -1.379773   -0.452278
H  -0.850296   -2.057266   0.628316
H  -1.284449   -0.616445   1.5371
Core  RigidRotor
```

```
SymmetryFactor  1.0
End
      Rotor     Hindered     ! 22.5037
        Group                  1 2 3 4 5 6 19 20
        Axis                   7 13
        Symmetry                2
        Potential[kcal/mol]     6
0       0.345961401     1.037884203     1.383845604     1.037884203
        0.345961401
End
      Rotor     Hindered     ! 46.3346
        Group                  1 3 4 5 6
        Axis                   13 2
        Symmetry                3
        Potential[kcal/mol]     4
0       1.083631165     2.16726233      1.083631165
End
Frequencies[1/cm]  52
132.8520
184.4864               281.1099               324.5297
351.0429               415.3650               471.6782
512.9008               577.0990               630.6151
637.5674               715.7902               763.1666
827.8106               857.3193               873.4890
881.5446               918.2383               925.0700
978.9029              1001.0600              1017.1470
1020.9619              1024.3931              1051.2861
1102.9800              1143.5972              1181.1807
1199.2698              1202.9112              1215.8614
1302.7468              1341.3858              1361.7342
1372.7132              1477.6911              1479.4207
1487.7545              1527.8807              1626.8474
1646.3343              2051.8564              3025.1937
3069.2156              3111.7445              3120.0717
3153.3842              3158.7558              3168.4186
3176.6204              3182.4974              3187.9531
       InfraredIntensities[km/mol]     52
 0.6487
 0.1515                 0.8615                 3.5183
 5.6236                 0.0816                 0.1986
 8.4596                17.3601                 5.2396
 0.6944                42.1651                23.8240
 2.4402                 0.0637                50.1620
 6.0631                16.3201                 4.8437
 0.0712                 0.0548                 0.6747
 0.4957                 1.4133                 4.5872
 6.3295                 0.3543                 0.0760
 0.1158                 0.1950                 1.3166
10.4890                 2.7318                 1.5718
 0.9302                 0.9776                 7.1177
11.3148                13.1982                 0.6416
 6.5705                56.3929                26.2968
 9.2615                 7.5735                 6.4437
 7.7575                 1.4531                 9.3059
```

```
36.7543                 3.7577                19.8165
ZeroEnergy[kcal/mol] -68.6
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_w22-----------
Well          w22
Species
RRHO
Geometry[angstrom]   20
C  -2.079962   1.057475   -4.9E-5
C  -2.520787   -1.451612   -1.6E-5
C  -0.756782   1.782323   -9.8E-5
C  -0.202762   -0.458094   1.7E-4
C  0.281752   0.927624   3.9E-5
C  0.654294   -1.504231   9.8E-5
C  2.091661   -1.265146   -1.03E-4
C  2.614715   -0.029294   -1.81E-4
C  1.765609   1.220088   1.6E-4
C  -1.677114   -0.41616   6.3E-5
H  -2.687771   1.308129   0.878216
H  -2.687792   1.307933   -0.878659
H  -3.595352   -1.306452   7.0E-6
H  -2.167621   -2.476755   -1.65E-4
H  -0.681727   2.863571   -2.74E-4
H  0.293738   -2.526944   4.5E-5
H  2.751845   -2.126385   -2.23E-4
H  3.691102   0.107863   -3.85E-4
H  2.029861   1.835182   0.871137
H  2.029964   1.83601   -0.870199
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
46.5753               120.9058              216.1267
268.0704               293.7885              450.0959
454.8653               496.2201              505.0368
533.1447               627.2721              674.5776
712.7406               719.6716              737.0780
810.8648               859.1754              884.4850
900.1530               902.1384              933.2695
962.6708               976.9919              989.4821
995.9390              1024.0136             1074.2368
1165.4407              1168.0221             1194.8895
1219.8187              1267.6299             1285.6074
1303.6047              1349.5856             1396.3772
1425.7570              1446.0680             1459.4497
1468.2870              1615.7207             1659.0857
1695.0292              1704.1795             2989.9029
2999.2008              3005.4144             3023.9525
3134.3648              3151.0312             3167.8662
3178.6718              3182.2570             3213.6623
```

```
       InfraredIntensities[km/mol]     54
 0.0128                  0.0145                  5.5274
 0.0071                  7.1242                  0.2115
 4.0585                  0.2443                  0.8255
 0.4977                  6.6869                 18.0993
30.1556                  0.6789                 16.0654
13.4193                  4.2498                  3.9005
 2.1719                 41.9523                  8.1723
 0.8647                  0.3312                  0.0379
11.4143                  3.6132                  2.7623
 0.9604                  0.4367                  0.3646
 1.3798                  0.2979                  0.0106
13.1883                  2.7261                  1.3727
 1.5676                  4.8731                  8.3930
 3.1432                  1.8948                  0.8926
 3.9156                  7.6125                 28.0504
15.2225                 35.0376                 19.0728
 8.2626                  4.3494                 31.3791
26.0234                 14.0272                  8.9249
ZeroEnergy[kcal/mol] -71.0
ElectronicLevels[1/cm]        1
0  1
End
End
# -------well_w24-----------
Well          w24
Species
RRHO
Geometry[angstrom]   20
C  -2.420961   -0.621707   -0.359208
C  -1.259954   -1.381486   0.298293
C  -2.348434   0.853698   -0.053656
C  0.095574   0.723486   0.091728
C  0.071355   -0.687401   0.101722
C  1.324115   1.387208   -0.001444
C  2.515392   0.6732   -0.09754
C  2.488407   -0.718832   -0.099627
C  1.26877   -1.389757   0.002704
C  -1.172624   1.458099   0.156571
H  -2.39423   -0.761048   -1.450392
H  -3.375184   -1.037902   -0.023825
H  -1.21241   -2.409242   -0.071908
H  -1.454833   -1.444624   1.378225
H  -3.268345   1.429712   -0.055921
H  1.340485   2.472569   -0.0065
H  3.459523   1.200961   -0.173016
H  3.411313   -1.28249   -0.178368
H  1.250757   -2.475366   0.009742
H  -1.126917   2.528388   0.334706
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
134.3217              152.3858              266.0589
```

```
355.2704                391.9905                424.0729
488.4376                504.0600                560.1072
594.8905                695.5925                708.3478
757.1178                758.9420                800.1522
820.7355                887.1970                893.2006
945.8593                953.2429                984.6597
991.3788               1026.1758               1044.8484
1060.3227               1135.0782               1175.8964
1182.6674               1190.9390               1212.3908
1228.8494               1248.3249               1307.1678
1331.0276               1359.6830               1374.4775
1423.7603               1472.2832               1482.5464
1484.8632               1517.3298               1609.5923
1644.0459               1687.3982               2975.5415
2991.7641               3057.5631               3064.3891
3145.7779               3151.9351               3157.0507
3168.3252               3171.2303               3186.1876
       InfraredIntensities[km/mol]     54
 1.0265                  0.0547                  3.4475
 0.6074                  1.0179                  3.4356
 1.5484                  2.7311                  6.1274
 2.6273                  4.3906                 11.4058
 1.9630                 29.7851                 38.2339
 2.6990                  2.5653                  4.4440
 0.1079                  2.2799                  0.2629
 0.5076                  4.1304                  3.6315
 4.5808                  3.5092                  0.1991
 0.0142                  1.0129                  1.2495
 1.7553                  2.9756                  5.1964
 1.0140                  4.0424                  0.5725
 0.2791                  3.6532                  2.4139
 9.8751                 12.4269                  0.1628
 0.2384                  0.0145                 23.5211
41.7965                 38.7554                 29.6625
 3.1156                 12.1715                  0.7300
26.5746                 36.9323                 26.2420
ZeroEnergy[kcal/mol] -103.3
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i9-----------
Well          i9
Species
RRHO
Geometry[angstrom]   20
C  2.108404   -0.056884   9.0E-6
C  3.445295   -0.153539   1.3E-5
C  1.295363   1.235977   4.4E-5
C  -0.128132   -0.697794   9.5E-5
C  -0.140392   0.757861   8.0E-5
C  -1.420695   -1.475309   -1.7E-5
C  -2.645756   -0.592257   -1.0E-5
```

```
C  -2.571666   0.746629   -2.3E-5
C  -1.294774   1.455635   -7.6E-5
C  1.15164   -1.153433   -4.3E-5
H  3.939567   -1.118465   -8.2E-5
H  4.080686   0.724721   -9.0E-6
H  1.518054   1.846649   -0.880511
H  1.518143   1.846666   0.880438
H  -1.45617   -2.146411   0.869676
H  -1.455947   -2.146086   -0.869979
H  -3.61043   -1.088682   2.53E-4
H  -3.483152   1.335402   1.61E-4
H  -1.296387   2.540454   -2.31E-4
H  1.449908   -2.195564   -1.43E-4
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
55.8888               138.9239               192.6447
270.9121               324.3354               449.8627
461.0189               464.2146               481.1436
573.0083               629.7947               638.8806
685.7873               732.4412               771.0813
852.6412               864.9907               867.1821
878.4874               891.5858               934.9660
957.4067               966.0572               970.6816
989.5531              1020.8008              1122.5835
1173.9656              1182.9496              1206.7662
1214.8134              1235.0451              1281.6561
1315.6441              1342.1992              1403.5466
1426.3754              1445.7851              1454.3076
1457.4051              1610.5836              1629.7900
1683.7705              1702.8269              2986.1429
2994.1825              3036.1971              3065.5314
3134.5929              3151.6494              3165.7787
3177.8018              3182.2317              3215.8540
       InfraredIntensities[km/mol]     54
  0.4383                 0.5992                 2.0747
  0.9152                 9.7093                 0.7202
  3.5855                 6.7491                 0.7116
  6.0165                14.2796                 5.9065
 16.1677                21.3966                 2.6377
 16.2725                26.7501                 2.2984
  5.6072                17.6113                 6.1483
  2.4960                 2.2724                 0.5401
  0.0412                 2.5725                 1.6163
  0.1974                 0.1860                 0.5181
  1.4909                 3.4248                 0.2596
  3.0186                 0.1616                 0.7347
  1.6433                 5.8165                 5.6697
  4.8785                10.2780                 6.4327
 46.1834                 8.1649                23.0731
 13.0146                11.4414                 8.9215
  7.4389                 5.3262                29.3706
 33.8547                10.2235                13.3873
```

```
ZeroEnergy[kcal/mol] -73.7
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i6-----------
Well          i6
Species
RRHO
Geometry[angstrom]   20
C  2.52693   -0.244268   0.353888
C  3.809268   -0.210357   0.118809
C  1.242651   -0.271317   0.574924
H  4.370198   0.718336   0.169108
H  0.871025   -0.438948   1.583189
C  -0.74662   1.071589   -0.1701
C  0.177371   -0.10128   -0.512893
C  -2.025769   0.754253   0.455333
C  -2.514712   -0.501715   0.468319
C  -1.786637   -1.600217   -0.157206
C  -0.555468   -1.41867   -0.652356
C  -0.377603   2.338508   -0.41321
H  0.701419   0.120322   -1.446001
H  -2.60003   1.57466   0.873942
H  -3.482265   -0.706135   0.913466
H  -2.267643   -2.570365   -0.223156
H  -0.007737   -2.235062   -1.110569
H  -1.007389   3.172573   -0.12363
H  0.561431   2.575796   -0.900407
H  4.364528   -1.110345   -0.128988
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
46.5480                51.4143               153.6238
189.7754               233.7186               341.1813
362.6553               373.5360               462.9809
503.3661               535.7555               591.4969
618.9996               659.6175               690.5976
765.4268               787.8245               827.7945
872.6084               903.2418               906.0296
940.1463               963.7219               979.5270
986.5173               996.5903              1007.5970
1020.1177              1043.0609              1136.7505
1178.5419              1202.2975              1237.6492
1308.8932              1314.2471              1356.8486
1389.5278              1425.5888              1465.3888
1472.2367              1610.5213              1657.5410
1700.0473              2046.0849              3054.7022
3111.6860              3133.2381              3134.0544
3153.0237              3158.9967              3174.6260
3182.7248              3183.8174              3216.9444
       InfraredIntensities[km/mol]     54
```

```
  0.0361                0.0599                0.5867
  0.0729                0.4045                4.7500
  4.0636                0.3524                8.4649
  0.8109                2.8287                0.2261
 17.1410               37.2708                9.7405
 26.2664                3.4255                2.5458
 53.0790               10.6884               43.4221
  0.8977                2.3198               10.2057
  1.4840                0.7661                3.5309
  0.7042                5.4375                0.2650
  1.2250                1.7072                1.0978
  0.1375                0.0947                1.6408
  0.5272                3.4501                1.1095
  2.1272                4.1770               12.3423
  1.6157               69.0502                6.7589
  6.4118                3.0323                5.3240
  0.5263                6.4274               32.5092
  2.9680               24.9201               11.6801
ZeroEnergy[kcal/mol] -39.3
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i10-----------
Well          i10
Species
RRHO
Geometry[angstrom]   20
C  -2.058318   0.061359   -0.084948
C  -3.396595   0.127932   -0.116362
C  -1.21844   -1.21368   -0.062422
C  0.141264   0.753927   0.157945
C  0.1596   -0.736966   0.461273
C  1.393674   1.464836   0.09266
C  2.537729   0.760653   -0.081102
C  2.525086   -0.691709   -0.234094
C  1.409315   -1.412096   -0.030486
C  -1.124078   1.179053   -0.066212
H  -3.913205   1.081202   -0.123868
H  -4.011045   -0.764867   -0.134546
H  -1.109477   -1.59312   -1.084789
H  0.157889   -0.84341   1.561574
H  -1.664551   -2.00422   0.544025
H  1.400811   2.549899   0.095687
H  3.485051   1.279173   -0.181383
H  3.44722   -1.181447   -0.528862
H  1.413729   -2.492202   -0.141675
H  -1.42186   2.209136   -0.22368
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
92.7250               153.3651               237.3429
```

```
261.4535                409.2373                431.8991
470.8921                498.0565                532.4777
558.2705                649.7341                678.0905
696.9892                724.5111                782.0442
826.6468                861.2508                875.0519
885.5248                900.6004                968.4332
969.2824                976.8895                987.1363
994.1165               1055.6270               1082.0652
1167.5968               1171.5408               1193.2636
1196.7317               1248.3407               1264.9580
1295.2880               1319.4631               1355.8051
1396.5911               1437.5575               1453.2183
1480.0848               1580.2510               1621.4147
1678.0293               1688.6785               2909.8297
3025.6428               3089.4085               3134.3169
3149.3591               3158.5496               3170.4539
3182.5661               3185.5616               3215.7622
       InfraredIntensities[km/mol]     54
  0.0883                  0.6413                  0.0529
  0.8295                 10.0948                  9.0826
  3.6921                  4.2893                  4.8304
  0.0888                  1.3068                  2.5325
 11.0205                 47.9274                  8.8195
  0.8965                  4.8935                 18.1650
  4.5642                 43.4763                  3.1527
  1.2960                  0.6494                  5.7729
  0.4580                  2.5099                  1.4230
  3.7570                  1.6612                  1.2737
  0.3932                  3.9058                  1.2352
  2.2626                  1.2316                  0.2356
  3.3784                  0.1775                  0.7497
  4.7616                  0.8175                  5.3705
 15.2850                 16.8818                 26.7531
 19.8127                 27.4436                  8.8603
  3.1019                  0.1787                 35.4602
 27.2080                 12.5243                 13.1641
ZeroEnergy[kcal/mol] -71.3
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_w23-----------
Well          w23
Species
RRHO
Geometry[angstrom]   20
C  -2.3687400585   -0.61380209   -0.4516031983
C  -1.2785493959   -1.3695784231   0.3418232587
C  -2.459254229   0.8552885698   -0.3019235658
C  0.0772161433   0.7102768731   0.1579735497
C  0.0582795582   -0.6923128946   0.178475922
C  1.2870942331   1.3821826364   -0.0208742791
C  2.4777439446   0.6730094061   -0.1590079933
```

```
C  2.4608371421   -0.7201356971   -0.1340220204
C  1.2536727973   -1.3961916012   0.0269914431
C  -1.2358338416   1.4556611939   0.2892545592
H  -2.1484155661   -0.6753616597   -1.5378526194
H  -3.3533449218   -1.0834603225   -0.3544747391
H  -1.2249383463   -2.4168555329   0.0318605316
H  -1.5698697034   -1.3746585925   1.4011005748
H  1.296280809   2.4674993271   -0.0501078975
H  3.4134582966   1.2048383633   -0.2905495941
H  3.3833471537   -1.2783445971   -0.2480117773
H  1.2373731007   -2.4817263827   0.0327902321
H  -1.1330051501   2.5159842609   0.0398260986
H  -1.5639269658   1.4596431626   1.3540735144
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
113.6848               157.6226               242.9583
271.4041               350.9104               395.2862
426.4289               480.2397               504.7108
550.6847               584.5404               700.5016
730.8148               762.5167               767.4174
785.0538               856.2896               875.2272
896.9178               920.6896               952.6248
975.4694               993.1004              1053.9162
1065.2235              1093.2155              1132.2955
1182.7614              1189.6044              1195.9634
1227.1860              1239.7330              1267.0316
1280.9144              1331.1639              1346.0046
1366.9591              1399.5194              1404.5253
1482.6276              1490.5418              1520.0679
1622.8942              1646.8585              2871.6174
2917.3623              2995.8007              3042.3637
3051.4572              3061.2061              3152.0765
3156.2290              3171.1045              3186.1108
       InfraredIntensities[km/mol]     54
  1.9988                 2.6416                14.4718
  2.7251                 0.4796                 1.1152
 11.2040                 1.0478                 3.4814
  3.3674                 9.6372                 8.1307
  2.4902                22.6142                28.3498
  0.6368                 4.6079                 0.9754
  3.9425                 1.1585                 0.4519
  3.6336                 0.0407                 2.8567
  6.3976                 1.5181                 2.6233
  0.3093                22.0564                 4.1213
  1.9348                 3.8164                10.7112
  2.4079                 2.5269                 4.5264
 12.4923                16.1805                 9.6750
  2.1832                 9.7432                17.5540
  1.1376                 0.1606                23.8680
  8.6151                30.3058                25.2373
 17.7789                27.1802                12.1776
  1.3076                26.1126                25.6363
```

```
ZeroEnergy[kcal/mol] -33.0
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_w20-----------
Well          w20
Species
RRHO
Geometry[angstrom]   20
C  -2.052728   -1.016134   -0.170312
C  -2.440027   1.499726   -0.049159
C  -0.781839   -1.805918   -0.123751
C  -0.175828   0.450472   0.18562
C  0.332041   -0.960774   0.424442
C  0.72595   1.499915   0.065841
C  2.088747   1.241294   -0.059792
C  2.568851   -0.105106   -0.197932
C  1.746858   -1.170695   -0.04666
C  -1.606199   0.438658   -0.003126
H  -2.61189   -1.157452   -1.104439
H  -2.74649   -1.306929   0.636545
H  -3.502961   1.374618   -0.219843
H  -2.082134   2.51383   0.085508
H  -0.728321   -2.881217   -0.237606
H  0.366741   -1.111932   1.5314
H  0.366188   2.519778   -0.029611
H  2.785505   2.063567   -0.172163
H  3.609817   -0.257647   -0.464224
H  2.108586   -2.185251   -0.176596
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
81.6176               129.0806              169.7395
257.1586               328.6762              366.8343
413.4590               475.0763              515.6454
521.0016               533.7305              624.6081
655.2579               690.9331              697.5984
743.0649               789.2243              847.5915
856.4188               890.6209              912.5264
924.4695               970.7805              990.4712
999.4145              1032.8225             1070.4499
1095.3376              1126.0478             1144.1512
1169.5876              1221.1483             1233.4493
1255.7975              1291.7388             1318.4863
1333.0889              1387.2267             1423.8564
1435.2824              1456.0359             1509.7479
1594.6062              1621.9479             2756.7907
2935.3186              3001.6681             3137.8716
3152.0850              3156.6846             3172.3267
3187.1985              3193.9606             3220.3814
       InfraredIntensities[km/mol]     54
```

```
  0.9090                 0.6963                 3.7502
  1.4342                 5.7719                19.0604
 16.8893                 7.8293                 1.8985
  4.4785                 9.3572                18.7089
  7.8216                17.2716                36.5252
 17.7515                 8.9539                32.5801
 52.8893                26.0899                25.6197
 11.9493                57.3767                13.5458
  4.6547                22.1906                 2.7748
 48.2371                 1.0381                 7.3327
  1.4090                47.2920                56.0820
 44.8164                43.3767                 8.0941
 40.1514                 3.4777                 7.6816
  2.7542                 4.5305                 3.0251
 28.1819                 9.0430               334.7066
 84.4106                40.9939                 4.0241
 12.8260                 6.5244                23.3027
 12.5788                 1.0369                 6.6567
ZeroEnergy[kcal/mol] -22.4
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i8-----------
Well          i8
Species
RRHO
Geometry[angstrom]   20
C  2.077235   2.1E-5   0.011406
C  3.384055   -1.0E-5   -0.229119
C  1.200378   -1.241145   0.148271
C  -0.209137   0.699208   0.055771
C  -0.209132   -0.699214   0.05577
C  -1.40795   1.403311   -0.012801
C  -2.609228   0.697909   -0.08298
C  -2.609224   -0.697918   -0.082999
C  -1.407943   -1.403317   -0.01285
C  1.20037   1.24116   0.148214
H  3.943915   -0.923731   -0.331519
H  1.421824   -1.984226   -0.624112
H  1.366796   -1.733747   1.115398
H  3.943973   0.923666   -0.331541
H  -1.41217   2.488603   -0.015014
H  -3.548647   1.236504   -0.140603
H  -3.548639   -1.236517   -0.140642
H  -1.412164   -2.48861   -0.015081
H  1.421775   1.984155   -0.624264
H  1.366789   1.733875   1.11528
Core  RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  54
38.2233               170.4295               227.5328
```

```
281.5259                409.0739                433.4300
450.0702                485.6241                500.2251
598.5678                661.2524                678.8636
730.8320                753.3635                800.8436
834.6870                861.1110                875.3751
909.8366                937.9976                946.0099
952.5360                990.2528                993.2997
1047.3918               1113.5906               1164.0181
1179.3722               1186.7459               1187.4711
1225.3406               1227.0521               1271.8541
1273.1396               1329.6750               1351.8686
1446.5794               1463.9662               1471.0527
1493.1421               1514.4559               1626.2261
1650.4914               1727.1743               3000.2258
3001.7856               3049.0309               3049.5829
3126.5703               3154.7250               3159.8946
3171.7141               3185.3780               3204.3688
       InfraredIntensities[km/mol]     54
  0.2062                  0.0242                  5.7750
  0.0085                 11.0589                  0.4495
  1.2004                  1.1445                  0.0046
  0.4924                  2.1510                  0.0000
  0.0004                 60.6270                  0.4581
  1.0779                  0.3839                  0.0089
 33.5490                  1.2371                  0.3903
  0.0157                  0.0001                  3.7483
  4.0792                  0.9523                  0.0587
  0.0239                  1.0682                  0.2238
  4.0879                  9.1560                  0.0158
  0.5382                  0.7526                  7.6634
  1.8768                  5.9906                  2.7057
  6.1780                 23.5620                  0.8932
  0.3455                 22.8280                 26.7147
 19.2841                 13.8659                 19.1924
 12.9485                  6.4508                  2.0742
 31.5013                 27.1864                 14.0989
ZeroEnergy[kcal/mol] -97.1
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i5-----------
Well          i5
Species
RRHO
Geometry[angstrom]   20
C  -2.0466222427   1.0510214001   -0.0699711668
C  -2.3891137917   -1.4666669064   0.0587022551
C  -0.7285956597   1.7818522468   0.0114782526
C  -0.1726156232   -0.4188985339   -0.6587887281
C  0.306116745   0.9727079408   -0.2650015979
C  0.7537949626   -1.5034567711   -0.1770360732
C  2.0405255357   -1.2159255074   0.0747580181
```

```
C  2.5587570875   0.1489041234   -0.015781207
C  1.7323072024   1.2076656704   -0.1653026037
C  -1.6300509428   -0.4104157255   -0.2076083144
H  -2.6900644144   1.2233370687   0.7994195255
H  -2.6254970254   1.3703890328   -0.9504863107
H  -3.4154056661   -1.3547020621   0.3923580059
H  -2.0212111731   -2.481443402   -0.0442518958
H  -0.6487911313   2.8318526384   0.2678573656
H  -0.1684277937   -0.4699195553   -1.7653962904
H  0.3845036012   -2.520894477   -0.1066483366
H  2.7280257455   -2.0030937585   0.3662925708
H  3.6250004495   0.3027184084   0.1101444664
H  2.1103684042   2.2240967667   -0.1286076565
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
70.3886               162.3685              230.5931
271.4513               374.1747               428.9178
469.9192               500.7944               516.9266
564.0009               660.6785               674.5818
701.1741               705.8310               782.0884
835.7677               841.3674               874.1700
907.5020               911.7123               962.1069
968.9362               978.0979               990.5310
991.8948              1009.4848              1064.2941
1161.7978              1169.6558              1181.2976
1197.8829              1227.3308              1258.6450
1286.1484              1303.6134              1345.1699
1397.2736              1442.2045              1448.0035
1468.1227              1593.7506              1655.0536
1695.8771              1731.5827              2884.2312
2969.1301              3038.0038              3130.9367
3152.9163              3160.1868              3174.2666
3182.7440              3183.8395              3207.4107
       InfraredIntensities[km/mol]     54
  0.1572                 1.6377                 0.0594
  0.1025                11.1148                 4.2529
  3.4040                 4.3546                 0.7172
  4.2856                 2.4089                 5.6594
 14.5715                14.9402                 0.9862
 36.6706                 7.2334                 9.6749
  2.9570                42.1846                 2.5484
  1.2075                 2.0728                 0.5649
  9.9006                 0.9250                 5.5500
  0.9402                 1.9145                 3.9856
  2.6573                 1.4397                 0.6908
  8.6402                 4.9985                 0.1945
  0.6096                 1.1471                 2.5663
  2.6625                 2.6760                 1.4176
  0.6628                28.1267                26.4796
 34.9948                27.8331                 9.0653
  2.4388                 3.5750                30.6058
 23.2298                18.6784                13.0827
```

```
ZeroEnergy[kcal/mol] -66.3
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i3-----------
Well          i3
Species
RRHO
Geometry[angstrom]   20
C  1.9803257619   0.9127691822   -0.2452549923
C  2.3810646137   -1.5344278809   -0.209942221
C  0.8678373205   1.8867621492   0.0465920935
C  0.1729187736   -0.4129137702   0.5406427222
C  -0.3229205913   0.969610041   0.1875014298
C  -0.7874658475   -1.5016527228   0.1673098128
C  -2.087302377   -1.2068023832   -0.1264251899
C  -2.5495245591   0.1314090858   -0.2150129883
C  -1.6266941289   1.2050915141   -0.1239508301
C  1.6074157241   -0.4113686064   -0.0200333725
H  2.9661245602   1.2166843165   -0.5762904705
H  3.3937681582   -1.4543368827   -0.5874651037
H  2.0072228509   -2.5286775743   -5.981067E-4
H  0.732083692   2.6383995603   -0.7396199343
H  1.0713905513   2.4497166353   0.9742405321
H  0.2995882345   -0.4611922192   1.6453277544
H  -0.4527807062   -2.5319527845   0.2176565784
H  -2.7853088904   -2.0140179723   -0.3247271633
H  -3.588377977   0.3290900509   -0.4488658246
H  -1.9543021635   2.2099992611   -0.3751157262
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
83.8714               166.2822              217.4983
266.8277               365.4301               407.0569
476.2055               518.0470               524.6548
526.3262               538.5269               642.2846
675.2699               685.4584               698.0955
755.5646               776.1634               800.1601
840.4870               901.1469               936.3566
937.4656               962.1549               995.5230
1002.3108              1015.5841              1046.7538
1113.3617              1136.3743              1150.8973
1181.5952              1216.7093              1244.4498
1253.3003              1290.0158              1336.0546
1359.1299              1387.7217              1415.7717
1430.1441              1463.7304              1511.6715
1540.1897              1611.5189              2807.2682
2931.0064              3025.2386              3141.6197
3146.8319              3153.1880              3173.1065
3187.4285              3190.6888              3231.3798
       InfraredIntensities[km/mol]     54
```

```
  1.1219                1.6712                1.9359
 10.1008               14.2842               11.5637
  1.5746               18.3090                2.4894
  3.9565                2.8123               22.9722
 37.4746               39.8259               18.5308
 58.2777               14.7596               16.1943
  1.5481               16.1846                8.8706
 31.7558                1.7644                1.0345
 25.2139               11.2739               15.8058
  4.7207                0.1343                4.7507
  4.5611                4.5678               82.1165
 15.2521                1.3322               41.2862
  7.5858               18.7043                4.5114
  3.3564               20.2759                7.0327
 23.6118               14.6129               13.5143
  1.4301                7.1051                4.1529
 25.7686               16.9390               13.9485
  6.2724               10.2896               10.7058
ZeroEnergy[kcal/mol] -31.0
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i7-----------
Well          i7
Species
RRHO
Geometry[angstrom]   20
C  -2.010532   0.07724   -0.088176
C  -3.330046   0.107856   -0.488072
C  -1.261272   -1.202453   0.299601
C  0.205174   0.745252   0.571936
C  0.173481   -0.748403   0.311847
C  1.440646   1.4143   0.033945
C  2.534795   0.674726   -0.303357
C  2.51225   -0.745597   -0.285681
C  1.294071   -1.431862   -0.050514
C  -1.151485   1.164747   0.046928
H  -3.925635   -0.795007   -0.546078
H  -3.808981   1.040585   -0.761886
H  -1.441737   -2.026913   -0.395395
H  -1.596002   -1.538188   1.292799
H  0.205112   0.915814   1.673631
H  1.467276   2.498411   -0.002022
H  3.44295   1.177376   -0.620965
H  3.401771   -1.300997   -0.556581
H  1.24348   -2.50116   -0.23591
H  -1.430727   2.195239   -0.138328
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
77.5041               138.5667               236.8987
```

```
273.4956                386.5490                389.7727
457.8030                490.5074                502.0959
536.4830                546.5638                638.4691
642.0760                675.3846                732.6753
756.9492                772.3647                796.8774
862.4060                868.5326                906.0760
953.4678                963.2453                986.9121
998.4673               1029.3507               1061.9326
1116.4407               1151.2665               1156.5748
1187.2106               1214.8463               1226.5059
1246.3410               1295.3391               1339.5134
1359.1121               1379.9611               1421.0371
1428.1152               1468.5431               1508.8960
1540.3607               1609.1679               2786.0598
2973.0849               3062.9324               3138.6243
3146.4075               3151.1426               3169.8360
3185.7064               3189.9930               3229.4317
       InfraredIntensities[km/mol]     54
   0.8515                  1.2999                  5.5631
   2.0873                  9.0888                  7.7853
  11.5497                  8.1426                  4.6967
   6.0061                  3.7201                  3.0032
  14.0244                 31.9996                 37.7865
  21.5800                 76.0855                 15.8704
   0.2490                  3.7147                 12.2893
   2.2923                  3.3811                  1.7112
  19.1976                 18.5836                  4.9540
   2.2332                  1.0310                  4.2035
   0.0287                 29.2792                 37.4091
   0.9729                 96.9265                  6.1023
   0.3378                 27.2692                  3.5185
   1.2053                 10.5379                 31.9747
  22.3247                 12.1470                227.9162
  35.5576                 25.4668                  3.3247
  20.8713                 15.6509                 20.0376
   4.9755                  6.8697                 10.4040
ZeroEnergy[kcal/mol] -30.7
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_w25-----------
Well          w25
Species
RRHO
Geometry[angstrom]   20
C  -2.464069   -0.664834   5.91E-4
C  -1.216848   -1.499611   -4.32E-4
C  -2.464067   0.664835   5.1E-4
C  0.070927   0.699999   -2.1E-4
C  0.070944   -0.70001   -2.65E-4
C  1.295135   1.381036   1.15E-4
C  2.50363   0.697512   3.06E-4
```

```
C  2.503643   -0.697497   1.98E-4
C  1.295159   -1.381038   -6.4E-5
C  -1.216849   1.499606   -6.09E-4
H  -3.408527   -1.202053   0.001367
H  -1.228463   -2.169681   -0.871584
H  -1.227778   -2.170903   0.86971
H  -3.408495   1.202061   0.001221
H  1.292663   2.467172   2.12E-4
H  3.439235   1.245597   5.59E-4
H  3.439261   -1.245561   3.43E-4
H  1.292688   -2.467174   -9.4E-5
H  -1.228355   2.169418   -0.871938
H  -1.227874   2.171141   0.869358
Core  RigidRotor
SymmetryFactor  2.0
End
Frequencies[1/cm]  54
38.2667               149.1980               241.3446
351.6678               381.7985               441.5118
466.9265               503.5549               507.5730
609.2684               668.6691               721.8389
740.0891               760.5464               780.9305
873.7130               904.7560               934.1054
941.0470               978.1349               979.9589
990.4013              1006.3230              1014.0494
1064.0593              1135.2850              1183.5944
1198.8108              1202.7264              1207.3957
1227.7220              1231.3621              1278.2148
1332.0106              1376.6468              1376.7457
1420.0435              1469.2695              1471.8821
1487.2840              1528.6907              1622.8216
1649.3914              1738.0794              2986.0673
2987.0611              2996.3609              2996.7262
3134.1587              3147.2393              3150.7880
3157.0938              3169.2088              3184.8932
       InfraredIntensities[km/mol]     54
  0.5066                 0.0000                 7.1390
  0.2307                 0.0000                 7.7405
  0.2456                 0.0323                 0.0000
  0.3534                15.0993                 0.0000
  0.3762                79.0080                 2.2857
  0.0000                 0.1913                 0.0349
  3.0918                 0.0000                 0.7582
  0.0000                 7.2190                 0.0003
  3.1763                 2.1199                 0.0194
  0.0502                 1.5786                 0.2299
  1.9240                 0.0000                 0.9805
  0.9148                 2.6165                 0.1620
  0.0002                 0.0063                 3.8182
  9.9861                21.5571                 4.2343
  0.1673                 5.2079                 1.7200
 66.9270                42.4884                 0.1019
  9.4795                15.9371                 0.8893
 50.0695                25.0371                25.8142
```

```
ZeroEnergy[kcal/mol] -100.4
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_i4-----------
Well          i4
Species
RRHO
Geometry[angstrom]   20
C  2.094505   0.902502   0.210774
C  2.339631   -1.611077   -0.139929
C  0.888909   1.822206   -0.113127
C  0.111489   -0.446114   0.014425
C  -0.303029   0.892955   -0.037305
C  -0.834646   -1.473706   0.055021
C  -2.188031   -1.151009   0.046029
C  -2.598559   0.184704   -0.003306
C  -1.657156   1.212507   -0.046635
C  1.583581   -0.521148   0.015743
H  2.971703   1.11525   -0.403089
H  2.390428   1.03503   1.256462
H  3.422288   -1.553868   -0.140414
H  1.903078   -2.594334   -0.274764
H  0.975549   2.240977   -1.122395
H  0.806935   2.667548   0.575085
H  -0.521801   -2.510935   0.105254
H  -2.930908   -1.939962   0.084224
H  -3.656737   0.42172   -0.004528
H  -1.980707   2.247659   -0.085979
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
84.5517               138.0100              215.5948
268.9215               400.4903              450.7019
460.2469               530.9611              544.9570
569.4396               652.0730              685.7564
742.5396               749.0016              789.3646
813.4150               852.9816              882.5430
894.8314               912.7588              950.9433
986.3311               990.4940             1032.5968
1046.9080              1106.4037             1134.1256
1168.4340              1180.2475             1197.3653
1221.9733              1260.4815             1292.4873
1310.7043              1329.7506             1359.8114
1446.2456              1474.0931             1493.4939
1494.3859              1505.2521             1620.7539
1644.2381              1701.7357             3019.8443
3032.6652              3066.1654             3088.4128
3134.5734              3156.4575             3164.0896
3174.4277              3186.5118             3213.5124
       InfraredIntensities[km/mol]     54
```

```
  0.0972                0.3676                4.7142
  0.4717                4.2653                1.7424
  0.5383                3.6283                0.3980
  0.3803                1.2187                2.0644
 30.1209                0.3729               28.1148
  1.6968                0.9503                2.2432
 37.9599                0.9827                1.5296
  0.3740                0.0181                1.2948
  2.8527                0.9887                1.9001
  0.3017                0.8418                2.5742
  0.7667                0.5646                0.2606
  1.1320                3.0395                9.1104
  2.2953                1.5140                1.9205
 13.7411                9.4782                0.2918
  2.0900               26.8555               30.3221
 17.3445               29.7949               28.0695
  7.2402                5.0216                3.9950
 27.4724               24.7597               12.6729
ZeroEnergy[kcal/mol] -100.0
ElectronicLevels[1/cm]        1
0  1
End
End

# -------well_w3-----------
Well          w3
Species
RRHO
Geometry[angstrom]   20
C  -2.6019683559   -0.1532656955   -0.3270015205
C  -3.7145455084   0.20750227   -0.0499907422
C  -1.2482409267   -0.6027081478   -0.6349439487
C  1.1277075521   -0.9384385575   0.1550001688
C  -0.2049885211   -0.2711655859   0.4896647312
C  2.1687865721   -0.1022731595   -0.4312607973
C  2.0872145404   1.2429533369   -0.4105917454
C  0.9496722499   1.9180715681   0.2022786013
C  -0.1035025221   1.225215154   0.6552516705
C  1.3217203181   -2.2501976882   0.3694282956
H  -4.700997269   0.5250447011   0.1832598736
H  -1.2503748132   -1.6871603822   -0.7864426
H  -0.9104641116   -0.1511027893   -1.5733724106
H  -0.5986766332   -0.7092364297   1.412252316
H  3.0435781363   -0.5970551669   -0.8409079663
H  2.890225845   1.8447295966   -0.8219118348
H  0.9737879039   2.9989822919   0.2901849231
H  -0.9541628728   1.7296114404   1.0993842547
H  2.2454499961   -2.7374731493   0.0774212985
H  0.5708124201   -2.8694836071   0.8480924322
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  54
53.9539               83.7332              130.1773
```

```
190.4266                243.9398                345.9402
370.4429                379.3909                458.8692
519.5014                525.7106                590.3349
661.8363                664.1978                678.6862
686.3707                763.1501                784.1051
830.9795                842.7839                903.0856
951.5896                959.8824                984.0838
986.8318                990.5968               1001.4340
1010.7075               1057.6751               1180.3921
1202.4129               1204.7961               1278.1555
1313.1513               1324.3771               1353.6116
1393.9381               1431.2382               1466.1830
1472.4952               1612.3052               1654.4307
1702.3559               2218.4481               3026.6022
3035.4719               3066.7348               3131.8138
3154.6157               3162.1019               3178.2066
3186.7793               3214.2251               3477.1523
       InfraredIntensities[km/mol]     54
 0.0298                  0.1704                  0.0968
 0.2751                  0.9536                  4.5995
 3.4841                  1.2647                  8.5470
 3.1607                  8.5554                  3.7845
43.7226                  1.7192                 45.4162
37.9190                 25.0145                  6.6869
 1.5702                  0.5868                 45.6004
 0.6634                  5.3282                  4.0391
 0.6767                  2.6986                  0.4464
 0.7627                  3.5987                  1.4376
 0.7589                  1.6795                  2.5488
 0.1089                  1.6970                  6.4452
 0.3246                  4.8530                  0.9922
 4.0991                  1.5845                 17.9587
 1.9616                  5.8350                  5.8304
 9.8474                 10.5240                  5.2791
 0.2209                 12.4491                 27.8447
16.0610                 13.2813                 72.5279
ZeroEnergy[kcal/mol] -38.6
ElectronicLevels[1/cm]        1
0  1
End
End

# -------h2_C10H8_p2-----------
Bimolecular       p2
Fragment        C10H8
RRHO
Geometry[angstrom]   18
C  2.04873   0.0   -1.3E-5
C  3.394047   0.0   -4.38E-4
C  1.180156   1.183531   2.0E-4
C  -0.112197   -0.744362   3.49E-4
C  -0.112197   0.744362   3.5E-4
C  -1.37002   -1.441006   2.47E-4
C  -2.523655   -0.725475   -4.31E-4
```

```
C  -2.523655   0.725475   -4.29E-4
C  -1.37002   1.441006   2.49E-4
C  1.180155   -1.183531   2.03E-4
H  3.959894   0.925154   -7.52E-4
H  3.959894   -0.925154   -7.51E-4
H  1.531017   2.205649   -1.3E-5
H  -1.385276   -2.525547   7.21E-4
H  -3.47967   -1.237462   -8.24E-4
H  -3.47967   1.237462   -8.22E-4
H  -1.385276   2.525547   7.24E-4
H  1.531017   -2.205649   -2.0E-6
Core  RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  48
115.7296               207.6102               265.4528
265.6551               448.0460               459.6923
502.4908               504.0584               568.3363
649.9687               650.6876               667.8077
720.5520               741.8401               789.2342
796.1351               826.3613               854.4655
908.8369               939.8182               965.2235
965.7608               974.2106               981.1868
995.0955              1140.5767              1177.9413
1186.6224              1193.9145              1222.8690
1303.0345              1372.5389              1394.8970
1428.2405              1460.9062              1539.6324
1569.6399              1600.6385              1674.6711
1685.6053              3137.4138              3158.1274
3165.0719              3177.2632              3186.7122
3218.0126              3220.1894              3224.5731
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  1
End
Fragment        h2
RRHO
Geometry[angstrom]   2
H  -0.8584806313   0.3111295618   0.2448078961
H  -1.2000193687   -0.0244155618   0.8145141039
Core  RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  1
4419.1625
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  1
End
GroundEnergy[kcal/mol] -58.3
End

# -------C4H5_C6H5_p7-----------
Bimolecular        p7
```

```
Fragment        C6H5
RRHO
Geometry[angstrom]   11
C  -2.36E-4   -1.396028   0.0
C  -1.223654   -0.770723   0.0
C  1.223556   -0.770924   0.0
C  1.211926   0.631211   0.0
C  0.0   1.32196   0.0
C  -1.211542   0.63183   0.0
H  -2.158085   -1.320755   0.0
H  2.157456   -1.321858   0.0
H  2.15027   1.176086   0.0
H  1.54E-4   2.406051   0.0
H  -2.150086   1.176517   0.0
Core  RigidRotor
SymmetryFactor 2.0
End
Frequencies[1/cm]  27
400.9605               426.4786               601.9001
620.2031               673.2085               721.3618
812.6504               892.3554               964.2589
988.6384               993.0286              1016.5317
1049.8674              1072.4077              1174.9732
1176.0810              1301.4469              1324.0613
1462.6872              1470.6151              1574.2771
1630.2259              3155.1702              3161.1286
3173.2989              3175.9637              3187.0914
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment        C4H5
RRHO
Geometry[angstrom]   9
C  -0.6234965585   0.1527517685   2.7603E-5
C  0.6801437921   0.4993917905   5.79736E-5
C  -1.8799899928   -0.1757125362   2.5904E-6
C  1.7569416245   -0.384449124   8.86847E-5
H  0.8956869769   1.5673845046   -2.78292E-5
H  -2.4369606583   -0.3232125182   -0.9248650987
H  -2.437326275   -0.3219874073   0.9248424877
H  2.7729245902   -0.0133107433   -2.50785E-5
H  1.602794501   -1.4557377347   1.026671E-4
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  21
206.5200               213.7048               495.6014
524.8347               572.8674               741.9907
883.8231               907.2270               937.3437
980.9474              1090.2238              1194.1738
1376.9555              1449.1388              1492.6535
1909.3729              3068.2826              3111.2790
3126.6627              3152.0133              3252.2770
```

```
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
GroundEnergy[kcal/mol] 21.8
End

# -------h1_C10H9_p6-----------
Bimolecular       p6
Fragment        C10H9
RRHO
Geometry[angstrom]   19
C  -0.493964   -0.519347   0.008765
C  -0.511986   0.874296   0.021247
C  -1.722898   1.566998   0.012658
C  -2.929171   0.874044   -0.008454
C  -2.919446   -0.520482   -0.021278
C  -1.71104   -1.209216   -0.01286
C  0.801752   -1.326241   0.02211
H  0.424873   1.418446   0.037047
H  -1.719494   2.651395   0.022281
H  -3.869753   1.413111   -0.015391
H  -3.853479   -1.071158   -0.038427
H  -1.711922   -2.295225   -0.023337
H  0.801085   -1.977456   0.907327
H  0.798072   -2.011346   -0.836901
C  4.281187   0.74072   -0.020972
C  3.098885   0.053806   -0.006697
C  2.040542   -0.562681   0.005626
H  4.297914   1.823341   -0.056257
H  5.229531   0.217508   0.002796
Core  RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]  51
9.1304                44.7336               77.0808
161.6371               190.8068              247.0117
329.1675               405.5700              414.8738
423.3338               469.8105              604.4733
635.7290               665.7824              712.3065
736.7966               792.5749              842.8092
857.4815               888.8354              953.5825
979.3719              1003.9808             1018.7892
1029.4271              1051.7566             1103.7933
1181.6528              1195.8868             1204.4613
1224.2443              1245.1994             1305.8805
1347.9915              1367.4384             1454.0503
1463.4503              1485.0018             1528.6827
1628.8635              1647.8417             2141.3399
2987.3049              3003.0673             3136.1939
3149.8986              3163.0430             3173.1808
3184.3303              3191.3253             3223.9021
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
```

```
0  2
End
Fragment        H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]        1
0  2
End
GroundEnergy[kcal/mol] 17.4
End

# -------h2_C10H8_p14-----------
Bimolecular       p14
Fragment        C10H8
RRHO
Geometry[angstrom]   18
C  2.429234   -0.70735   -1.68E-4
C  1.243601   -1.400109   -4.05E-4
C  2.429377   0.707268   -4.4E-5
C  1.7E-5   0.715677   2.16E-4
C  1.13E-4   -0.715622   1.09E-4
C  -1.243612   1.400374   -1.4E-4
C  -2.42949   0.707357   -2.74E-4
C  -2.429367   -0.707548   5.0E-5
C  -1.243392   -1.400369   3.48E-4
C  1.243532   1.400406   2.58E-4
H  3.371925   -1.2429   2.5E-4
H  1.242244   -2.485239   4.17E-4
H  3.372302   1.242531   -6.26E-4
H  -1.241983   2.485504   -3.82E-4
H  -3.372432   1.242526   -1.83E-4
H  -3.372192   -1.242943   -3.74E-4
H  -1.241746   -2.485511   2.45E-4
H  1.241804   2.485519   9.52E-4
Core  RigidRotor
SymmetryFactor 4
End
Frequencies[1/cm]  48
173.5114              186.4476              365.7018
395.8040              479.5856              488.2794
518.9567              519.8899              634.9169
636.1406              729.1294              773.2233
786.8882              798.4266              808.7787
849.4535              896.8248              950.9625
956.9628              974.2650              992.5317
999.8545             1035.6337             1046.3463
1151.0779             1169.1036             1171.8931
1185.2232             1232.2231             1269.9329
1286.9322             1391.2947             1398.5366
1417.9531             1490.5015             1491.6581
1548.5843             1613.9916             1641.4252
1671.1274             3156.3050             3158.0395
3160.4742             3163.9084             3174.3013
3175.6869             3187.0828             3188.2630
```

```
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  1
End
Fragment        h2
RRHO
Geometry[angstrom]   2
H  -0.8584806313   0.3111295618   0.2448078961
H  -1.2000193687   -0.0244155618   0.8145141039
Core  RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  1
4419.1625
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  1
End
GroundEnergy[kcal/mol] -99.6
End

# -------h1_C10H9_p5-----------
Bimolecular       p5
Fragment        C10H9
RRHO
Geometry[angstrom]   19
C  -2.07207   -1.017546   -1.53E-4
C  -2.421267   1.510136   3.79E-4
C  -0.793101   -1.804877   -2.55E-4
C  -0.148346   0.425276   7.0E-6
C  0.305909   -0.935449   1.24E-4
C  0.768874   1.471236   -2.82E-4
C  2.133593   1.184472   -2.16E-4
C  2.587519   -0.148931   1.76E-4
C  1.697234   -1.206402   3.34E-4
C  -1.61382   0.441457   -1.94E-4
H  -2.694311   -1.23903   -0.877325
H  -2.694297   -1.239008   0.877062
H  -3.500268   1.405095   5.11E-4
H  -2.029846   2.520998   8.99E-4
H  -0.742682   -2.885306   -5.0E-4
H  0.43181   2.502261   -6.01E-4
H  2.85458   1.99379   -5.28E-4
H  3.654348   -0.344416   3.28E-4
H  2.053521   -2.230617   6.4E-4
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  51
98.2212               180.2672               245.9736
267.0355               399.1984               465.6482
469.0492               534.4811               551.5839
552.4676               608.8821               676.1590
684.0336               745.4599               757.2383
```

```
782.3519               860.6388               873.7475
883.1060               899.4699               928.7646
943.6584               979.8313              1000.2384
1032.0211              1098.7469              1130.2355
1145.6364              1164.0718              1197.9530
1242.5857              1275.5889              1312.1139
1332.8773              1386.6327              1444.8391
1451.1361              1454.9932              1503.8168
1578.6663              1602.8567              1673.2544
2997.7826              3013.8864              3136.9465
3160.0775              3166.8756              3177.6129
3188.7980              3208.1615              3217.0914
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment        H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]        1
0  2
End
GroundEnergy[kcal/mol] -13.4
End

# -------h1_C10H9_p1-----------
Bimolecular       p1
Fragment        C10H9
RRHO
Geometry[angstrom]   19
C  3.3091053427   0.1559001896   8.769993E-4
C  2.008583083   0.456713622   5.790582E-4
C  4.5762798473   -0.1307865254   0.0010999328
C  -0.4426086263   -0.215153564   1.629964E-4
C  -1.3614853893   -1.294517448   1.214113E-4
C  -0.9831513315   1.0951671832   -3.4602E-6
C  -2.353119321   1.3035298858   -1.906506E-4
C  -3.2389188088   0.2224757546   -2.197107E-4
C  -2.7301939618   -1.07839081   -6.25599E-5
C  0.9612085394   -0.4963093064   3.647458E-4
H  1.7566800707   1.5152055607   8.692711E-4
H  5.1353971627   -0.2582819243   0.9266275582
H  5.1359856377   -0.2575023962   -0.9241655195
H  -0.9752581771   -2.3085045488   2.476841E-4
H  -0.3213490444   1.9529159791   -1.22689E-5
H  -2.73919585   2.3170464097   -3.218649E-4
H  -4.3092687735   0.3923473827   -3.627278E-4
H  -3.4077969088   -1.9251254029   -8.33507E-5
H  1.2506415088   -1.5422970415   3.704561E-4
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  51
69.9162                95.7715               103.2779
```

```
225.3716                230.0652                296.3907
376.9358                410.8492                494.6885
509.1049                546.0593                627.1571
634.8159                691.5309                752.1513
805.2898                834.7245                859.1475
883.0681                901.6485                913.5769
971.2854                990.8055                992.0402
1000.7014               1040.9790               1059.4701
1100.3437               1173.3305               1184.3408
1192.1682               1242.0810               1300.0854
1338.1120               1354.7018               1430.3297
1467.1012               1499.0070               1511.7601
1592.2365               1614.9887               1948.2263
3079.3923               3124.7029               3141.1257
3157.1723               3161.0634               3164.4881
3174.6608               3183.0460               3191.8202
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment        H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]        1
0  2
End
GroundEnergy[kcal/mol] 11.8
End

# -------h1_C10H9_p3-----------
Bimolecular       p3
Fragment        C10H9
RRHO
Geometry[angstrom]   19
C  -2.066573   -0.06128   2.4E-5
C  -3.43224   -0.100359   1.81E-4
C  -1.228264   1.216647   -2.26E-4
C  0.176804   -0.71253   -5.1E-5
C  0.19347   0.707497   6.1E-5
C  1.386176   -1.428444   -3.9E-5
C  2.584087   -0.722842   1.7E-5
C  2.593242   0.67647   7.2E-5
C  1.39181   1.397701   1.09E-4
C  -1.179944   -1.163091   -7.9E-5
H  -4.026278   0.805659   1.73E-4
H  -3.96502   -1.043959   2.53E-4
H  -1.442789   1.832245   -0.88049
H  -1.443051   1.83277   0.879577
H  1.384342   -2.512957   -4.5E-5
H  3.525051   -1.261947   -3.0E-6
H  3.538797   1.206684   7.4E-5
H  1.409123   2.482827   1.05E-4
H  -1.491577   -2.199938   -6.1E-5
Core  RigidRotor
```

```
SymmetryFactor 1.0
End
Frequencies[1/cm]  51
107.2854                197.4040                269.8732
274.4375                423.9136                449.5162
463.4823                488.2501                542.9561
594.9856                600.1944                667.6426
722.3320                750.7749                790.9983
805.9823                815.0955                867.3432
873.6848                888.7209                929.6171
962.6779                981.9853                982.8102
1037.0743               1117.6931               1165.8559
1169.5088               1188.8115               1196.1402
1223.4811               1276.6787               1325.6325
1344.4708               1383.5600               1409.7392
1452.0208               1477.4612               1502.2124
1538.7312               1605.0493               1624.2556
3029.6281               3057.8460               3138.8472
3157.5643               3163.9492               3175.8573
3187.5787               3197.1411               3227.1005
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment        H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]        1
0  2
End
GroundEnergy[kcal/mol] -20.4
End

# -------h1_C10H9_p4-----------
Bimolecular       p4
Fragment        C10H9
RRHO
Geometry[angstrom]   19
C  -2.041609   0.931976   -3.4E-5
C  -2.463875   -1.520944   -1.92E-4
C  -0.86193   1.860737   1.64E-4
C  -0.156142   -0.417162   2.33E-4
C  0.311959   0.906579   1.3E-5
C  0.742958   -1.481823   2.18E-4
C  2.110335   -1.209607   -1.8E-5
C  2.573976   0.107751   -1.77E-4
C  1.674347   1.17562   -1.38E-4
C  -1.64119   -0.409053   -1.04E-4
H  -3.070891   1.266475   -3.53E-4
H  -3.541533   -1.414286   -0.00109
H  -2.062618   -2.526183   8.5E-4
H  -0.855762   2.522694   0.87758
H  -0.855691   2.523649   -0.876471
H  0.391915   -2.507982   3.98E-4
```

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H  2.821547   -2.028163   -1.41E-4
H  3.6408   0.301681   -4.16E-4
H  2.039263   2.197671   -1.42E-4
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  51
138.8133              190.1179              244.6336
258.4211              412.9391              457.9508
468.9236              524.0911              537.0384
561.9048              611.8354              677.8857
702.1255              732.3106              755.2261
761.0925              786.0837              841.5495
872.5232              924.7836              944.5991
954.3103              988.7664             1015.9128
1046.3478             1099.5006             1139.1661
1151.8925             1179.2813             1207.7274
1234.2941             1248.9391             1323.6220
1343.8281             1384.6453             1412.2618
1450.1750             1493.8211             1497.3618
1519.2547             1623.5201             1649.8843
2990.4294             3004.1788             3148.0491
3157.0438             3164.5635             3175.2272
3186.9590             3201.5905             3239.1650
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment        H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]        1
0  2
End
GroundEnergy[kcal/mol] -16.7
End

# -------h2_C10H8_p1-----------
Bimolecular       p1
Fragment        C10H8
RRHO
Geometry[angstrom]   18
C  -2.012832   1.038215   6.5E-5
C  -2.493059   -1.428195   -1.84E-4
C  -0.893864   1.794936   1.69E-4
C  -0.166178   -0.418846   1.03E-4
C  0.285894   0.921392   -7.0E-6
C  0.740318   -1.467852   3.15E-4
C  2.109134   -1.176762   1.0E-5
C  2.555122   0.145027   -2.11E-4
C  1.646304   1.207611   -1.02E-4
C  -1.647744   -0.388225   -9.2E-5
H  -3.033549   1.395482   -1.97E-4
H  -3.566955   -1.280101   -2.29E-4
```

```
H  -2.138954   -2.452694   -3.22E-4
H  -0.853705   2.876428   2.85E-4
H  0.404314   -2.499472   4.59E-4
H  2.829971   -1.986471   9.0E-6
H  3.619915   0.350077   -2.54E-4
H  2.000386   2.23294   -1.43E-4
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  48
132.0431               197.9707               257.4459
316.3119               413.2315               458.8737
539.0289               553.3154               570.7645
659.2631               665.7351               723.1518
759.3601               767.4854               792.1323
813.7669               867.7070               886.5176
933.3723               943.6486               945.4828
953.1108               986.4274              1041.3921
1090.5629              1105.5042              1142.9534
1180.2076              1209.6071              1243.5938
1323.6045              1341.7764              1392.5178
1447.8902              1482.4715              1491.8766
1580.3985              1630.3704              1647.5099
1696.5765              3140.2089              3158.9081
3165.0174              3175.4383              3187.9274
3198.2739              3220.6299              3223.7287
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  1
End
Fragment        h2
RRHO
Geometry[angstrom]   2
H  -0.8584806313   0.3111295618   0.2448078961
H  -1.2000193687   -0.0244155618   0.8145141039
Core  RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm]  1
4419.1625
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  1
End
GroundEnergy[kcal/mol] -78.3
End

# -------h1_C10H9_p2-----------
Bimolecular       p2
Fragment        C10H9
RRHO
Geometry[angstrom]   19
C  -3.1671790544   0.1006662167   -0.2799117155
C  -1.9835202931   -0.5545286124   -0.5046150495
```

```
C  -4.2190678362   0.6856530687   -0.0687796814
C  0.3969809482   -0.3712343464   0.2994639265
C  1.4553186975   -1.2396758347   0.023587299
C  0.6441255509   1.0066042814   0.3005976051
C  1.9180921841   1.5008683912   0.0389286804
C  2.9679922724   0.624160295   -0.2338999218
C  2.7329709057   -0.7476701633   -0.2415500631
C  -1.000380889   -0.9005367772   0.5830062348
H  -1.7304370731   -0.8374682179   -1.5220849422
H  -5.1351561818   1.1927435429   0.1090787472
H  1.2801788566   -2.3109448315   0.020045459
H  -0.1699124908   1.6937106699   0.5073263275
H  2.0931706781   2.5710721499   0.0480592243
H  3.9607962443   1.0090164294   -0.4379494134
H  3.543005236   -1.4374143855   -0.4516699987
H  -0.9470194534   -1.9919206243   0.6893680712
H  -1.3647113018   -0.5105262519   1.5372172105
Core  RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]  51
23.8709                26.8950               132.6340
184.6464               281.7661               328.4623
388.2717               415.1293               442.0402
468.6234               538.6912               573.3201
635.4077               641.6737               646.8799
715.8930               763.0808               821.1367
857.4995               873.8992               924.3309
979.4148              1001.8752              1017.1015
1024.3840              1051.0543              1102.2523
1143.4917              1181.2521              1191.7030
1203.3047              1212.5665              1296.0131
1338.3737              1360.2531              1401.6608
1473.0578              1485.5001              1527.3192
1626.3566              1645.0422              2013.3657
2999.6799              3067.4793              3150.9417
3154.2802              3159.3677              3168.9576
3177.2446              3188.6502              3468.5476
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment        H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]        1
0  2
End
GroundEnergy[kcal/mol] 19.6
End

# -------h1_C10H9_p12-----------
Bimolecular       p12
Fragment        C10H9
```

```
RRHO
Geometry[angstrom]   19
C  2.446641   -0.513347   -6.2E-5
C  1.226407   -1.381968   8.5E-5
C  2.365945   0.8532   -6.2E-5
C  -0.104388   0.792469   7.0E-6
C  -0.088258   -0.626739   -6.0E-6
C  -1.350583   1.456385   1.8E-5
C  -2.540146   0.7477   -8.0E-6
C  -2.517484   -0.649799   -4.6E-5
C  -1.296438   -1.320513   -4.9E-5
C  1.130728   1.521757   2.8E-5
H  3.413405   -1.004856   -1.44E-4
H  1.257745   -2.059255   0.868609
H  1.257769   -2.059587   -0.868164
H  3.27952   1.439327   -1.44E-4
H  -1.363349   2.541544   2.7E-5
H  -3.486921   1.276263   5.0E-6
H  -3.444921   -1.211049   -7.3E-5
H  -1.282882   -2.40662   -7.9E-5
H  1.097203   2.60508   5.3E-5
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  51
86.0667               172.1344              251.0656
357.5737               429.6094              471.5310
485.5430               506.4692              541.6557
612.7051               660.3964              713.9658
747.7418               751.4459              791.8633
794.5749               871.2099              920.8227
931.9666               954.5132              959.5321
966.5833               984.7572             1056.8223
1092.6382              1139.3179             1175.6202
1179.3283              1201.8461             1202.5165
1234.0543              1277.4316             1309.2880
1356.0487              1393.8304             1439.2594
1445.6397              1473.6849             1515.7469
1559.5059              1599.1827             1629.7487
2952.2734              2952.4859             3148.8035
3152.5568              3158.0580             3171.2889
3172.5326              3182.9429             3187.1206
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]        1
0  2
End
Fragment        H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]        1
0  2
End
GroundEnergy[kcal/mol] -24.0
End
```

```
# -------h1_C10H9_p13-----------
Bimolecular       p13
Fragment        C10H9
RRHO
Geometry[angstrom]   19
C  2.498545   -0.697531   -5.2E-5
C  1.17813   -1.396929   -7.1E-5
C  2.385467   0.799183   9.0E-6
C  -0.064016   0.722015   1.1E-5
C  -0.043264   -0.718056   8.0E-6
C  -1.287696   1.3915   -2.6E-5
C  -2.493813   0.693714   -6.7E-5
C  -2.486404   -0.711099   6.0E-6
C  -1.292869   -1.40351   8.1E-5
C  1.202832   1.433007   6.8E-5
H  3.101925   -1.022986   0.866013
H  3.1019   -1.022913   -0.866158
H  1.177837   -2.482266   2.6E-5
H  3.309313   1.368937   5.2E-5
H  -1.292165   2.477103   6.0E-6
H  -3.43404   1.232557   -1.93E-4
H  -3.425132   -1.254209   5.7E-5
H  -1.290007   -2.488594   2.05E-4
H  1.168895   2.5186   1.84E-4
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  51
123.3347              173.0144              257.7164
357.9903              393.8082              459.7952
498.4553              504.2186              542.9712
615.2203              687.2613              700.4505
750.4204              759.2844              784.9193
788.2145              863.5324              900.9898
926.8348              927.8706              942.5778
974.6647              995.4948             1036.7673
1053.1506             1139.3661             1163.2684
1177.7355             1183.5210             1202.7389
1249.9945             1294.9554             1340.6531
1358.5897             1413.0465             1436.2870
1446.8400             1459.4012             1504.7200
1562.2803             1603.7669             1676.1235
2913.0958             2926.1623             3145.4274
3154.6715             3157.5034             3160.5475
3167.8210             3173.6738             3188.6360
ZeroEnergy[kcal/mol]     0.0
ElectronicLevels[1/cm]       1
0  2
End
Fragment        H
Atom
Mass[amu] 1
ElectronicLevels[1/cm]       1
```

```
0  2
End
GroundEnergy[kcal/mol] -18.9
End

!-------ch2_ts1------------
Barrier      ts1  i1  w0
RRHO
 Stoichiometry C10H10
 Core     Rotd
 File ch2_flux.out
 SymmetryFactor 4.0
End
Frequencies[1/cm]  48
    198.6753               359.1271               390.3132
    478.5981               502.1989               534.2124
    628.2287               684.5079               707.1720
    773.7403               829.1817               830.9751
    898.3874               969.6051               971.5974
    989.5358               994.6024              1035.9429
   1116.3450              1174.6158              1184.4537
   1288.0078              1327.3102              1351.9221
   1473.6465              1489.6398              1502.0160
   1576.6083              1598.3058              3144.6847
   3157.8381              3160.3300              3172.6310
   3177.3169              3190.8265              3241.3375
    352.0219               403.2308               468.4763
    637.8092               681.8420              1031.3626
   1089.2851              1455.3919              2011.1052
   3139.2898              3229.7773              3467.8791
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm] 1
0  1
End

!-------ch_ts2------------
Barrier      ts2  i2  w0
RRHO
 Stoichiometry C10H10
 Core     Rotd
 File ch_flux.out
 SymmetryFactor 4.0
End
Frequencies[1/cm]  48
    198.6753               359.1271               390.3132
    478.5981               502.1989               534.2124
    628.2287               684.5079               707.1720
    773.7403               829.1817               830.9751
    898.3874               969.6051               971.5974
    989.5358               994.6024              1035.9429
   1116.3450              1174.6158              1184.4537
   1288.0078              1327.3102              1351.9221
   1473.6465              1489.6398              1502.0160
   1576.6083              1598.3058              3144.6847
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   3157.8381              3160.3300              3172.6310
   3177.3169              3190.8265              3241.3375
    352.0219               403.2308               468.4763
    637.8092               681.8420              1031.3626
   1089.2851              1455.3919              2011.1052
   3139.2898              3229.7773              3467.8791
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i1_w23-----------
Barrier      i1_w23  i1  w23
RRHO
Geometry[angstrom]   20
C  2.373008    0.879236   -0.429116
C  1.332175    1.546897    0.098935
C  2.389870   -0.606221   -0.411533
C  -0.037413   -0.702596    0.226097
C  -0.120896    0.703910    0.267306
C  -1.197290   -1.419540   -0.055672
C  -2.415647   -0.766496   -0.239914
C  -2.487300    0.627019   -0.153496
C  -1.343511    1.370900    0.099649
C  1.312877   -1.309572    0.467464
H  1.150754    2.614450    0.126439
H  3.385014   -0.966078   -0.128390
H  2.282966   -0.907659   -1.464873
H  0.735003    1.123754    1.141733
H  -1.146273   -2.501932   -0.117520
H  -3.310515   -1.341780   -0.446418
H  -3.437046    1.131752   -0.289596
H  -1.384230    2.453466    0.146381
H  1.597055   -1.157988    1.517498
H  1.292036   -2.389202    0.296435
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1179.2925
WellDepth[kcal/mol]  71.2
WellDepth[kcal/mol]  31.2
End
Frequencies[1/cm]  53
137.2491               170.8078
254.9056               324.5039               359.0623
393.4871               440.4985               471.8839
537.1297               573.2680               642.6833
673.2437               731.7973               751.9970
762.3748               788.0379               854.0469
872.3772               913.9154               946.9279
958.4453               981.2927               988.2754
1002.3867              1049.8243              1112.9976
1137.1144              1166.0719              1181.9031
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1193.7110              1218.5829              1296.8754
1307.6662              1334.5688              1346.5616
1372.9084              1425.8587              1460.3075
1490.5043              1492.8394              1548.9644
1612.4734              1628.6980              2065.9554
2987.0282              2998.3555              3047.3518
3065.1108              3159.7290              3167.1100
3176.4559              3178.9679              3191.2896
ZeroEnergy[kcal/mol]  3.6
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_w23_w24-----------
Barrier      w23_w24  w23  w24
RRHO
Geometry[angstrom]   20
C  2.408833   -0.595718   0.393182
C  1.274056   -1.375261   -0.299141
C  2.467454   0.898808   0.175316
C  -0.091867   0.705297   -0.10398
C  -0.064578   -0.698861   -0.124983
C  -1.306958   1.382837   0.01437
C  -2.5006   0.674273   0.118373
C  -2.476836   -0.718933   0.100186
C  -1.265436   -1.398708   -0.022121
C  1.204197   1.439954   -0.153493
H  2.295975   -0.665156   1.488475
H  3.375013   -1.057952   0.174061
H  1.232251   -2.406781   0.062157
H  1.49987   -1.437997   -1.373995
H  -1.313912   2.468422   0.030952
H  -3.442091   1.203218   0.212686
H  -3.402337   -1.277959   0.182428
H  -1.253577   -2.484003   -0.034919
H  1.121723   2.526527   -0.232082
H  1.997497   1.249561   -1.096016
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  925.1332
WellDepth[kcal/mol]  3.3
WellDepth[kcal/mol]  73.6
End
Frequencies[1/cm]  53
127.3492               153.5151
259.8385               347.1074               397.1399
418.0431               492.2033               494.5328
554.5146               596.9195               694.4052
725.7072               756.1405               767.8220
797.5138               834.6238               880.0133
894.9270               941.0365               958.5331
975.8161               998.2581              1033.7132
```

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1057.3338               1132.0205               1150.8709
1183.6593               1200.9468               1215.3945
1231.9798               1249.9161               1298.4234
1311.6913               1339.3913               1365.0337
1378.6092               1421.2865               1456.0563
1479.9109               1491.8708               1520.3412
1622.5951               1646.1554               2152.8146
2969.1922               2984.3366               3056.7059
3058.5230               3076.8291               3154.6525
3158.9518               3173.2811               3187.8744
ZeroEnergy[kcal/mol]  -29.7
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i2_w3-----------
Barrier      i2_w3  i2  w3
RRHO
Geometry[angstrom]   20
C  4.6823298447   0.4913228987   -1.4697204058
C  4.1334397684   -0.5231033734   -1.0084221187
C  5.7971520837   1.3400053827   -1.3751180572
H  3.35821919   -1.2579471378   -1.0601098211
H  5.5849518342   2.4029525928   -1.268181934
H  6.5506152331   1.1715604687   -2.1440682322
C  6.5503622818   -0.4938232749   0.392033017
C  7.6654361533   -1.284006036   -0.0209796676
C  6.6428128168   0.9577088186   0.2095484236
C  7.9902066209   1.5128898371   0.0740147659
C  9.0400905683   0.7095430581   -0.234615057
C  8.8672007978   -0.7091655699   -0.3270830584
C  5.3177538519   -1.0473918991   0.7164133412
H  7.5582212992   -2.3642241548   -0.0312051871
H  5.9843549733   1.5255800618   0.8640654725
H  8.1201476685   2.5868281211   0.158043417
H  10.0258467054   1.1337914347   -0.3922668262
H  9.7140430009   -1.3299434714   -0.5971718927
H  5.216604418   -2.1275418488   0.7545186194
H  4.6255878897   -0.4941939084   1.3382772014
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  508.7033
WellDepth[kcal/mol]  49.7
WellDepth[kcal/mol]  19.7
End
Frequencies[1/cm]  53
125.0145               135.6843
217.1986               248.8807               336.8143
372.9202               380.5750               417.6528
517.7224               552.8933               559.2741
618.4297               653.6477               717.1906
746.5086               781.0324               803.6303
```

```
818.6262                850.9217                889.7057
960.3927                972.5623                981.8805
989.8630                996.6765               1015.4058
1076.6525               1079.2551               1116.2159
1137.7251               1176.6110               1185.2871
1199.1667               1312.4769               1335.8387
1400.2915               1445.1866               1473.4098
1488.8684               1546.7607               1552.3733
1659.1635               1980.3109               3080.8261
3104.1536               3130.4779               3138.2133
3153.2777               3158.3046               3172.7606
3184.9864               3215.8206               3371.2250
ZeroEnergy[kcal/mol]  -18.9
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i7_i10-----------
Barrier      i7_i10  i7  i10
RRHO
Geometry[angstrom]   20
C  2.0965084925   -0.0719130515   -0.0275480535
C  3.4505446459   -0.0697894634   5.0667E-4
C  1.2433891396   1.2136162667   -0.0505751479
C  -0.1448987971   -0.7586632008   0.056010778
C  -0.1896379032   0.7398675265   0.0341982916
C  -1.4360648034   -1.4460408938   -0.0332443886
C  -2.5929831596   -0.7134642349   -0.0381645651
C  -2.6056916549   0.7057753867   -0.0088542562
C  -1.4042494884   1.4130212356   0.0135107999
C  1.2080194069   -1.1945713039   -0.0387627729
H  4.01785778   0.8531258372   -0.0019399995
H  4.0119052826   -0.9963367819   0.0062442501
H  1.3785992931   1.7425843308   -1.0014836372
H  1.5174906182   1.9134287827   0.7436507381
H  -0.1839875905   -0.2758767874   1.1502448292
H  -1.4571951874   -2.5272112655   -0.0942934759
H  -3.5411826642   -1.2392280732   -0.084735158
H  -3.549483518   1.2352180856   -0.0095849968
H  -1.4082172849   2.4981907792   -0.0051138736
H  1.5186473926   -2.2287031746   -0.0086060316
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1588.3882
WellDepth[kcal/mol]  15.9
WellDepth[kcal/mol]  56.5
End
Frequencies[1/cm]  53
80.3992               184.8897
227.5611                271.7236                413.5060
439.3884                449.8478                485.4517
527.9041                573.2593                595.8127
```

```
645.1256                653.1578                698.1315
723.1349                753.8022                774.4570
805.0936                849.7937                871.6710
909.3937                942.8578                958.3844
976.0112                986.1440               1008.7137
1100.4995               1156.1854               1168.7862
1174.3911               1190.0098               1226.0522
1234.6821               1301.2964               1333.7676
1375.2907               1433.2783               1447.3517
1461.2840               1483.8033               1521.4297
1610.3166               1635.6845               2314.1656
3018.1785               3060.8926               3138.4134
3161.0858               3164.1533               3190.3207
3200.8286               3218.7354               3220.6945
ZeroEnergy[kcal/mol]  -14.8
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i3_i5-----------
Barrier      i3_i5  i3  i5
RRHO
Geometry[angstrom]   20
C  2.0120035928   1.0156788127   -0.0569861042
C  2.4753047821   -1.4499539932   -0.1169467836
C  0.7530575098   1.8247407572   -0.0718456876
C  0.1850582896   -0.4141444938   0.4362148848
C  -0.3558996378   0.9744286233   0.1381136539
C  -0.7272895924   -1.5105510029   -0.017206394
C  -2.0455273745   -1.2407392966   -0.1727440877
C  -2.5786743311   0.0930591834   -0.0567342688
C  -1.7342681731   1.1828536297   0.0324213182
C  1.668376904   -0.3790236956   0.0436748443
H  2.9901102439   1.4298508598   -0.2539103677
H  3.5366076725   -1.3332724529   -0.3032658835
H  2.0989883339   -2.4612224864   -0.0295930491
H  1.2057068696   1.496931912   -1.1520411425
H  0.7420508216   2.9075585581   -0.0289389189
H  0.2236103   -0.4512638442   1.5494388967
H  -0.3375882919   -2.5147285114   -0.1373969783
H  -2.7298605477   -2.0434658291   -0.4292939761
H  -3.6479028283   0.2413150098   -0.1485800992
H  -2.1303215428   2.1908662601   -0.0489568568
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1792.4784
WellDepth[kcal/mol]  23.3
WellDepth[kcal/mol]  58.6
End
Frequencies[1/cm]  53
111.5361                162.0191
228.2948                300.9398                394.6095
```

```
442.2736                489.4717                513.1253
535.3883                582.5290                598.0469
659.8414                688.2957                690.9391
713.2699                772.2366                808.9144
827.3879                839.8022                906.5193
932.4217                938.7232                971.8500
990.1313               1001.4327               1017.0863
1070.2250               1151.4412               1168.7279
1187.1942               1219.1542               1220.1212
1245.3868               1256.5116               1309.3157
1328.3696               1387.9449               1433.9406
1441.6532               1460.7121               1544.9348
1626.8884               1634.6823               2242.9475
2796.5194               3141.8080               3149.2334
3153.8739               3179.9993               3185.3219
3188.1136               3225.6863               3227.6456
ZeroEnergy[kcal/mol]  -7.7
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i6_i7-----------
Barrier      i6_i7  i6  i7
RRHO
Geometry[angstrom]   20
C  1.868927   -0.342185   -0.248188
C  2.932981   -0.090175   -1.027129
C  1.245657   1.114434   0.920715
C  -0.282992   -0.766992   0.84983
C  -0.07295   0.726487   0.655683
C  -1.534651   -1.297793   0.210901
C  -2.36371   -0.507447   -0.506322
C  -2.112036   0.898027   -0.655561
C  -0.989805   1.472673   -0.119403
C  0.928742   -1.25985   0.053193
H  3.822017   0.392217   -0.63603
H  2.899954   -0.276748   -2.095787
H  1.583869   2.087314   0.575877
H  1.748287   0.758431   1.815004
H  -0.215776   -1.082001   1.902103
H  -1.753107   -2.353167   0.339857
H  -3.247224   -0.931883   -0.971616
H  -2.811071   1.500894   -1.22366
H  -0.787247   2.526408   -0.283563
H  1.039318   -2.304538   -0.224493
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  583.3271
WellDepth[kcal/mol]  27.6
WellDepth[kcal/mol]  19.0
End
Frequencies[1/cm]  53
```

```
94.3466                137.7701
237.6095                291.1230                364.9862
408.8432                435.9588                502.8979
524.0169                541.4423                577.1188
614.2365                700.7850                726.1568
769.4223                786.9629                799.0379
834.4412                875.3526                934.9473
959.6372                970.4551                976.2691
986.6140                993.6284               1005.2871
1044.1167               1056.0615               1129.6447
1178.5487               1193.9877               1238.0768
1288.5776               1316.0662               1340.1069
1378.2072               1427.1327               1462.9013
1489.2663               1522.2398               1546.9431
1661.3718               1774.5044               2942.7331
3110.6681               3121.9639               3151.0073
3153.4537               3157.1794               3171.1146
3185.8602               3186.4605               3200.7049
ZeroEnergy[kcal/mol]  -11.7
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_w20_w22-----------
Barrier      w20_w22  w20  w22
RRHO
Geometry[angstrom]   20
C  -2.0525653512   -1.0373161413   -0.0640176904
C  -2.4325078547   1.491944071   -0.0346278343
C  -0.7763041055   -1.8352694071   -0.1393455337
C  -0.1418593148   0.4575221373   -0.0445465438
C  0.3258558493   -0.9551347563   -0.0801004263
C  0.7494744487   1.4921473727   -0.0318891306
C  2.1528505674   1.2581921469   -0.0640064223
C  2.6360261443   -0.0378438642   -0.1164688292
C  1.7925821851   -1.1560144807   -0.1564807136
C  -1.6083585442   0.4342754271   -0.04461186
H  -2.7050158014   -1.2319127427   -0.926942932
H  -2.6575303466   -1.2752313503   0.8230701128
H  -3.5096559342   1.3706262666   -0.0371552638
H  -2.056750616   2.5086665388   -0.0265443336
H  -0.7182316354   -2.9129547585   -0.1149753748
H  0.6974320386   -1.2068490282   1.0069447507
H  0.3859040283   2.514784558   -0.007265484
H  2.8386429399   2.0951788519   -0.044136073
H  3.7065235724   -0.2109218553   -0.1504351251
H  2.1814847401   -2.1655313899   -0.1878846251
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1125.0332
WellDepth[kcal/mol]  20.8
WellDepth[kcal/mol]  60.5
```

```
End
Frequencies[1/cm]  53
73.0135               177.2544
206.3133               270.5134               373.7702
439.5559               459.9276               508.9129
527.6481               537.1804               556.2491
613.4049               647.7137               664.0125
720.4768               739.8996               773.9155
843.5179               871.2899               886.9922
892.9610               927.5313               946.7816
951.4736               998.6473              1029.8725
1064.3109              1102.8607              1153.2447
1176.1259              1182.4919              1235.9393
1272.4882              1274.0426              1329.4205
1408.4574              1441.2011              1448.2897
1469.5745              1477.6048              1526.8185
1643.2731              1678.9366              2499.1123
2968.9552              2980.5315              3136.7221
3158.9612              3165.0149              3195.2916
3201.1286              3216.3388              3226.8358
ZeroEnergy[kcal/mol]  -10.5
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_w23_w25-----------
Barrier      w23_w25  w23  w25
RRHO
Geometry[angstrom]   20
C  -2.401142   -0.602975   -0.295095
C  -1.25309   -1.420395   0.282953
C  -2.496679   0.79558   -0.261394
C  0.069479   0.703155   0.140648
C  0.066867   -0.698483   0.148611
C  1.28286   1.379677   -0.015135
C  2.480408   0.682257   -0.136976
C  2.474682   -0.711858   -0.122631
C  1.269959   -1.394701   0.011387
C  -1.241297   1.457083   0.261833
H  -2.252814   0.01497   -1.374336
H  -3.294457   -1.169159   -0.567549
H  -1.204503   -2.413399   -0.172616
H  -1.49423   -1.581617   1.343778
H  1.284822   2.465134   -0.038561
H  3.413829   1.222562   -0.249281
H  3.402467   -1.263292   -0.225404
H  1.260003   -2.480408   0.006905
H  -1.136064   2.469875   -0.13634
H  -1.491338   1.599288   1.328194
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  922.2347
```

```
WellDepth[kcal/mol]  3.7
WellDepth[kcal/mol]  71.1
End
Frequencies[1/cm]  53
95.8879               164.5573
248.6667               353.9870              413.5765
418.9303               477.8822              506.3633
516.6069               596.6689              701.4464
715.7276               756.8482              763.6109
788.3502               859.8709              884.3476
896.9856               940.7071              968.9206
977.7665               979.0503              993.4033
1061.3290              1130.1890             1162.5927
1181.9249              1185.1070             1201.9573
1220.0584              1258.0479             1271.7396
1290.9610              1345.9499             1357.3548
1390.6711              1445.8229             1454.3617
1469.3404              1487.6951             1522.5872
1622.9005              1646.4328             2183.3365
2955.6292              2991.5468             3057.2445
3058.7762              3081.9998             3151.7135
3155.7420              3171.2291             3186.3653
ZeroEnergy[kcal/mol]  -29.3
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_w25_p14-----------
Barrier      w25_p14  w25  p14
RRHO
Geometry[angstrom]   20
C  2.4073701599   -0.673665537   -1.4592135747
C  1.3043122616   -1.3037344354   -0.7945163658
C  2.4044737601   0.6921791334   -1.449065348
C  -0.0154399235   0.7058610687   -0.9824629033
C  -0.0124505002   -0.704549438   -0.9929428263
C  -1.2295434998   1.402128658   -1.0706320265
C  -2.4163887844   0.69891262   -1.2015464168
C  -2.4134139677   -0.7045260248   -1.2119738263
C  -1.2235945025   -1.4045716331   -1.0914866935
C  1.2987771123   1.3076075257   -0.7750983854
H  3.2662539022   -1.2516152924   -1.7779892565
H  1.3441991177   -2.3754374402   -0.6212252039
H  3.2608903342   1.2784399979   -1.7591838982
H  -1.2325941115   2.4869193533   -1.0503426768
H  -3.3545651901   1.2347491404   -1.2927127535
H  -3.3493132958   -1.2429212978   -1.3111206815
H  -1.2220452791   -2.4895472547   -1.0873196454
H  1.3341150533   2.3767776141   -0.5859031804
H  1.5064365657   -0.4916135965   0.4895555783
H  1.5044447876   0.4773708383   0.4967090845
Core  RigidRotor
SymmetryFactor  0.5
End
```

```
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1545.863
WellDepth[kcal/mol]  47.7
WellDepth[kcal/mol]  46.9
End
Frequencies[1/cm]  53
168.9356               202.5067
357.0925               407.2669               492.9838
507.6580               555.7239               605.5632
619.5114               728.7852               740.7510
764.7244               767.2201               805.1513
813.7256               853.8262               875.2268
927.4809               944.9425               966.2650
971.6120               990.5888              1011.4418
1015.5100              1048.0913              1075.8092
1095.1427              1147.8040              1157.1694
1180.2491              1237.7929              1247.1273
1274.6765              1300.6086              1328.7059
1335.4433              1367.8242              1381.2288
1454.8640              1494.2062              1527.6157
1572.0091              1606.4512              1654.4870
1747.3497              3150.0053              3152.2206
3157.6140              3163.2754              3174.4735
3178.7416              3187.1521              3196.4352
ZeroEnergy[kcal/mol]  -52.7
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i8_p2-----------
Barrier      i8_p2  i8  p2
RRHO
Geometry[angstrom]   20
C  2.0520558509   -7.65445E-5   0.0307271419
C  3.2851770758   -3.149454E-4   -0.4732359707
C  1.1839531468   -1.1539615276   0.3717898319
C  -0.1472247314   0.7167569648   0.1109857535
C  -0.1465009588   -0.7187600268   0.114023803
C  -1.3647325876   1.4217996743   -0.0191121822
C  -2.5302011145   0.7074165673   -0.1753173993
C  -2.5294846187   -0.7130333077   -0.1723106605
C  -1.3632978007   -1.4255745095   -0.0130844207
C  1.1827901672   1.1543919391   0.3669249961
H  3.8045687797   -0.92575542   -0.694386188
H  3.8033981519   0.9248824465   -0.6981167324
H  1.511591144   -2.1852314585   0.328055503
H  -1.3747072276   2.506284829   -0.0121117521
H  -3.4709630434   1.2311419427   -0.3042015408
H  -3.4697176054   -1.2382483611   -0.2989746806
H  -1.3721794975   -2.5100297498   -0.0014919031
H  1.5093904665   2.1857948877   0.3187819643
H  1.2512782562   -0.4692935423   1.8403670976
H  1.2507761466   0.4761571417   1.8383453394
Core  RigidRotor
```

```
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1507.3526
WellDepth[kcal/mol]  70.3
WellDepth[kcal/mol]  31.5
End
Frequencies[1/cm]  53
126.6985               208.0502
278.4900               297.7785               435.0219
449.1394               515.7333               552.5366
585.7557               604.9312               676.3100
724.2889               734.4534               762.2084
774.5508               803.0504               845.6010
885.4314               893.2090               905.2202
936.3878               944.8729               964.1686
965.8842               979.5794               994.5184
1024.5890              1136.1090              1178.2549
1182.5403              1204.8285              1218.7257
1272.5827              1276.6641              1301.3990
1346.3116              1370.7838              1388.7181
1451.7014              1484.7835              1530.2048
1576.7568              1658.0716              1732.9966
1899.4966              3139.0348              3159.1614
3166.7175              3177.2774              3187.0898
3195.3387              3197.3304              3223.2389
ZeroEnergy[kcal/mol]  -26.8
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i3_i4-----------
Barrier      i3_i4  i3  i4
RRHO
Geometry[angstrom]   20
C  1.9898161128   0.9090229987   0.3648056701
C  2.4105611378   -1.5043780819   -0.3896619515
C  0.8661640762   1.8350326005   -0.0328008776
C  0.1654191827   -0.3981625255   0.1948688556
C  -0.3264941721   0.9318027631   -0.1009836171
C  -0.7610553084   -1.4817109409   0.2128456166
C  -2.1133607736   -1.2030489113   0.1052664956
C  -2.572990305   0.104432138   -0.1147343557
C  -1.6742072129   1.1777039799   -0.2292130314
C  1.6664466776   -0.4416804725   -0.0571428889
H  3.0091354886   1.277691146   0.4195810409
H  3.4926904932   -1.4483656251   -0.3956026338
H  1.9589685542   -2.4565988181   -0.6366583496
H  1.0695942812   2.2340357401   -1.041725455
H  0.7160324341   2.6997740487   0.6205227158
H  0.6547810824   0.063644618   1.3299507339
H  -0.4070990435   -2.4991674583   0.3285817478
H  -2.8338047842   -2.0117958875   0.1624021283
H  -3.6376075334   0.2867539837   -0.2042194894
```

```
H  -2.0422753877   2.1830687044   -0.4052353547
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1699.8015
WellDepth[kcal/mol]  18.0
WellDepth[kcal/mol]  87.0
End
Frequencies[1/cm]  53
136.1165               188.8946
257.5322               260.2142               419.4512
444.1206               473.2326               523.6969
549.9799               594.1407               635.7751
694.0850               700.1116               741.9199
747.9155               778.7664               803.9528
834.5960               852.7723               906.2562
928.8431               946.1903               988.4598
1003.7880              1029.8994              1058.1479
1085.5614              1122.4212              1141.4947
1168.6098              1192.5235              1202.6621
1234.5710              1302.7875              1316.0181
1372.1233              1416.9484              1431.0808
1451.7452              1486.5123              1502.4021
1567.9527              1637.1643              1694.5656
2958.1505              3060.8970              3142.8869
3161.4050              3164.1511              3167.7544
3184.8388              3192.2383              3225.3620
ZeroEnergy[kcal/mol]  -13.0
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i5_p1-----------
Barrier      i5_p1  i5  p1
RRHO
Geometry[angstrom]   20
C  1.9923109502   1.0231178162   -0.21583972
C  2.4409597116   -1.3796479386   0.559940125
C  0.854684306   1.7778548868   0.1823263045
C  0.2109270074   -0.3979555234   -0.2545171764
C  -0.2528251529   0.931396506   0.1388634638
C  -0.7334738381   -1.4772244006   -0.2677293659
C  -2.0620668194   -1.1983924209   -0.1127041575
C  -2.5215931381   0.1308670275   0.1433748763
C  -1.6445363769   1.1747548638   0.2790118233
C  1.6655557768   -0.4085101197   0.0956012483
H  3.0048764209   1.4091989194   -0.1932976876
H  3.4903080284   -1.2086206264   0.7706047749
H  2.0506709929   -2.3710156527   0.7579170416
H  0.8222127236   2.8552466188   0.2774401359
H  -0.3943239129   -2.4928313101   -0.4401223499
H  -2.7917844666   -1.9987083822   -0.1708391369
H  -3.5866475285   0.302095281   0.2532742977
```

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H  -1.9998698032   2.1719542767   0.5163621704
H  1.5469114363   0.6881270321   -1.5441691821
H  0.7124766824   0.0091251462   -1.6090744855
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1876.6877
WellDepth[kcal/mol]  43.9
WellDepth[kcal/mol]  55.9
End
Frequencies[1/cm]  53
136.4309               191.2773
269.4146               307.6596               429.5781
458.3752               533.9717               559.0083
572.9974               656.6151               692.4314
715.7168               728.8440               743.0274
773.1723               814.9248               831.6514
869.6368               879.1372               919.3997
952.3262               969.9446               983.9542
996.8226              1013.3716              1017.0670
1062.1712              1091.8710              1153.1779
1182.3610              1217.2458              1252.8579
1299.7787              1311.6520              1333.1500
1384.8413              1400.2681              1424.7406
1446.4202              1493.3461              1521.1935
1566.0019              1581.0402              1658.2116
1756.7559              3140.5959              3158.2465
3165.1280              3176.7284              3182.4346
3186.5694              3206.1404              3222.6201
ZeroEnergy[kcal/mol]  -22.4
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i9_i10-----------
Barrier      i9_i10  i9  i10
RRHO
Geometry[angstrom]   20
C  1.8333968496   -0.0902590338   -1.261372179
C  3.1614585706   -0.0887032673   -1.4326892981
C  1.0016039783   1.1180851187   -0.7981035427
C  -0.3500630949   -0.8189555166   -1.2050209939
C  -0.4310861817   0.6135356526   -0.8811388606
C  -1.6482501118   -1.3938001864   -0.8221448001
C  -2.815945781   -0.7068378545   -1.205542349
C  -2.7709867627   0.6560057668   -1.4920754161
C  -1.5821600515   1.3374978048   -1.2390372961
C  0.9183325898   -1.2247728775   -1.411329552
H  3.7568749968   0.8016337828   -1.2657237428
H  3.6896817773   -0.9824320459   -1.7448108574
H  1.1599378633   1.9981510602   -1.426903592
H  1.2741718233   1.3987200332   0.2238161345
H  -1.7173033567   -2.4423269936   -0.5489692031
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H  -3.7689660934   -1.2228522596   -1.1629078269
H  -3.6733000219   1.1954303281   -1.7520028613
H  -1.557148893   2.4225973815   -1.2415410449
H  1.2489961962   -2.2436827721   -1.5643373208
H  -1.1534532965   -0.2616261214   0.2033716021
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1640.6346
WellDepth[kcal/mol]  52.6
WellDepth[kcal/mol]  50.2
End
Frequencies[1/cm]  53
79.5004               204.0205
248.2707               289.8024               412.4655
462.5689               479.0107               486.7600
567.2741               615.2633               651.6982
687.8160               694.0468               743.5801
788.9376               837.3069               847.9720
854.3703               867.2231               897.0056
940.3783               960.8244               966.6631
989.2103              1048.6071              1074.3837
1134.5173              1161.4680              1167.1568
1182.9920              1193.3605              1228.0007
1237.7537              1276.5876              1297.2021
1356.2886              1411.8875              1449.8098
1463.9497              1466.8508              1538.3585
1578.4042              1678.2190              1688.0515
3040.4519              3074.6255              3134.4098
3154.5398              3162.4115              3174.1207
3194.4682              3201.0964              3214.4450
ZeroEnergy[kcal/mol]  -21.1
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i4_w23-----------
Barrier      i4_w23  i4  w23
RRHO
Geometry[angstrom]   20
C  2.301118   -0.443932   -0.554338
C  1.326607   1.409412   0.7101
C  1.379795   -1.404178   0.235208
C  0.040791   0.641948   0.02625
C  0.006879   -0.761075   0.180099
C  -1.155768   1.358038   -0.167988
C  -2.363861   0.68223   -0.191899
C  -2.395609   -0.708542   -0.03058
C  -1.213142   -1.426661   0.144263
C  1.661987   0.953439   -0.587984
H  3.299058   -0.372121   -0.104193
H  2.433137   -0.812997   -1.574604
H  1.670495   0.954916   1.651876
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H  1.006802   2.441493   0.835633
H  1.688183   -1.542976   1.278369
H  1.364929   -2.398573   -0.215642
H  -1.121441   2.434512   -0.288147
H  -3.28697   1.230806   -0.339633
H  -3.344869   -1.23161   -0.056585
H  -1.24211   -2.507533   0.23414
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  365.5828
WellDepth[kcal/mol]  77.3
WellDepth[kcal/mol]  10.3
End
Frequencies[1/cm]  53
145.5414               173.0127
239.6836               355.3315               399.2642
424.6661               448.7571               511.1874
514.3621               624.4332               683.0434
707.2799               752.4436               790.4696
816.6204               844.6557               876.2402
956.8830               958.0300               971.6635
989.9893              1021.6360              1026.3877
1052.2874              1103.9409              1119.2786
1139.4355              1165.6863              1181.0111
1183.2712              1206.7986              1271.6453
1307.5158              1321.3615              1340.6557
1358.3628              1466.3337              1477.5972
1493.9374              1497.3939              1525.9883
1601.7897              1623.0233              2957.5182
3010.7627              3018.6120              3055.0476
3082.7461              3118.5375              3161.6584
3171.8053              3183.0380              3193.0406
ZeroEnergy[kcal/mol]  -22.7
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i7_i9-----------
Barrier      i7_i9  i7  i9
RRHO
Geometry[angstrom]   20
C  2.1014035152   -0.0619396479   -0.0205972635
C  3.4561656923   -0.0736780471   -0.0761326119
C  1.2583266852   1.2222116203   0.0432573487
C  -0.1385002703   -0.7397010769   0.0812644556
C  -0.1740914404   0.7426131427   0.050580416
C  -1.4462410023   -1.4315021035   -0.0264451565
C  -2.6249636578   -0.662935888   -0.0565469408
C  -2.5984562002   0.7158015286   -0.0528746214
C  -1.3447081048   1.4195127671   -0.0077906668
C  1.2114150539   -1.1781772456   -0.0239331515
H  4.0306732112   0.8444333538   -0.1009029386
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H  4.0089100648   -1.0049828372   -0.1103520626
H  1.4552634768   1.8788374943   -0.8101164934
H  1.4860730577   1.8010728326   0.9453881325
H  -0.5537650986   -1.0462497284   1.160638648
H  -1.4669515078   -2.513637483   -0.0215706987
H  -3.5739599398   -1.1861018895   -0.0961342156
H  -3.5238411739   1.2769260255   -0.0820172784
H  -1.3472326355   2.5046201058   -0.0414666007
H  1.522870274   -2.2132429236   -0.0463783004
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1691.2997
WellDepth[kcal/mol]  13.8
WellDepth[kcal/mol]  56.8
End
Frequencies[1/cm]  53
78.6453               171.3003
253.2249               273.6893               383.6724
447.8756               462.0980               481.0763
534.7646               569.4173               609.6522
645.1443               669.9747               688.0396
738.0020               765.2792               777.9194
794.2756               859.2551               869.5774
886.8814               937.4721               946.5301
976.9050               980.0500              1013.9471
1064.4419              1153.6289              1168.7304
1171.6615              1193.7044              1221.5645
1253.3345              1303.5270              1335.4696
1400.8249              1421.5203              1450.0594
1455.9696              1469.1899              1513.7402
1597.3647              1670.1891              2301.4525
3023.6646              3052.8460              3137.6409
3158.1327              3170.0336              3194.4834
3202.1712              3208.0359              3220.3499
ZeroEnergy[kcal/mol]  -16.9
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i4_w20-----------
Barrier      i4_w20  i4  w20
RRHO
Geometry[angstrom]   20
C  2.2244951143   0.8718528839   -0.0092431128
C  2.4638300071   -1.666014717   -0.0845380899
C  1.0072389339   1.7561182461   -0.0059622683
C  0.2323825698   -0.5070258551   -0.1415261246
C  -0.1891636959   0.9038270565   -0.2348618023
C  -0.7157522823   -1.5134444032   -0.0938305497
C  -2.0799592954   -1.2052557664   -0.0599723712
C  -2.5014251769   0.1434994246   -0.0223634397
C  -1.6098036711   1.1873998518   -0.056732156
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C  1.6891521348   -0.5680833443   -0.0800305774
H  2.9161808265   1.0839899334   -0.8350600194
H  2.8054548338   1.0259506039   0.911218381
H  3.544094372   -1.5980271917   -0.0277959116
H  2.0396838361   -2.6616213761   -0.1402359839
H  1.0154261416   2.8293898877   -0.13461756
H  0.0854526382   1.2342475545   -1.3227979445
H  -0.3995012263   -2.5504751659   -0.0437122754
H  -2.8150347268   -1.9994883981   -0.0207632596
H  -3.5613928789   0.360401787   0.0614203716
H  -1.9498624544   2.2158679883   -0.0159333062
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1293.9854
WellDepth[kcal/mol]  81.0
WellDepth[kcal/mol]  12.3
End
Frequencies[1/cm]  53
77.0357               169.7505
198.4306               268.3740               391.6165
428.9971               465.0280               489.9530
526.3438               541.3658               549.4244
648.5114               665.2358               715.4311
722.0925               767.5693               822.6439
848.9312               854.5297               885.1945
917.8323               932.5505               961.2007
995.4734              1010.8722              1024.6805
1092.8390              1124.3507              1144.5033
1160.3491              1179.2587              1202.4735
1271.3142              1285.3632              1320.7575
1341.3368              1434.9068              1439.1272
1451.0204              1456.2976              1535.0209
1603.7579              1654.2343              2376.7977
2980.6921              2996.0536              3138.2167
3156.7567              3161.5528              3178.3227
3192.8985              3217.3810              3218.5968
ZeroEnergy[kcal/mol]  -19.0
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i7_i8-----------
Barrier      i7_i8  i7  i8
RRHO
Geometry[angstrom]   20
C  2.1002173886   -0.0798831116   -0.017729194
C  3.4528123775   -0.0856252407   0.0291598513
C  1.2526227754   1.2100834583   -0.0331226347
C  -0.1496444112   -0.7511981078   0.0202321206
C  -0.1828974889   0.7445521264   0.0371827741
C  -1.4457049869   -1.4252517245   -0.0727713453
C  -2.5986585755   -0.6825345356   -0.0450206231
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C  -2.5985344747   0.7316268176   0.0211753229
C  -1.3895490918   1.4271121162   0.0532772575
C  1.2041654645   -1.1970130528   -0.0661184641
H  4.0244942207   0.8341645495   0.0554708936
H  4.0096458661   -1.0148181371   0.0187916516
H  1.3956534453   1.7422283396   -0.9814968179
H  1.5251650955   1.905240551   0.7654249101
H  -0.151137793   -0.3591810466   1.1343186714
H  -1.4776799796   -2.5048644013   -0.1539161055
H  -3.5510493293   -1.200586801   -0.0916139267
H  -3.5370453066   1.2698628556   0.0461423458
H  -1.3842691531   2.5124364614   0.0672702235
H  1.505957443   -2.2338642896   -0.0436392622
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1011.2627
WellDepth[kcal/mol]  10.7
WellDepth[kcal/mol]  77.1
End
Frequencies[1/cm]  53
79.9532               183.1375
227.8567               273.7655               415.9940
446.7999               449.9657               485.8310
528.8668               573.3370               596.3897
645.7924               649.3382               697.4775
717.6487               759.0099               774.3044
799.2421               849.2912               858.7703
886.2340               927.4504               953.8455
976.2279               984.1076              1016.7743
1101.9615              1160.3108              1170.4330
1178.4907              1190.5616              1227.3989
1236.6980              1301.3185              1336.4174
1379.6005              1444.0351              1449.2836
1463.8662              1496.1612              1527.1036
1625.9724              1640.7979              2446.2753
3015.0837              3063.2051              3138.8559
3160.7771              3164.0294              3190.0792
3200.7860              3220.2348              3220.8835
ZeroEnergy[kcal/mol]  -24.6
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i1_i6-----------
Barrier      i1_i6  i1  i6
RRHO
Geometry[angstrom]   20
C  -2.0058978926   0.9567390739   -0.6189084436
C  -2.6492233493   -0.243390365   -0.5604381318
C  -0.948055038   1.5820858302   -0.2905850382
H  -3.5711771079   -0.3282346626   0.0096809098
H  -2.6090846959   -0.8891083934   -1.4346431918
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H  -0.5473245975   2.5585589356   -0.4986325684
C  -0.097908991   -0.7704561335   0.4830713174
C  0.850295844   -1.4529729583   -0.3345052176
C  0.1465902362   0.6412453914   0.7963159932
C  1.5052719699   1.129649362   0.5594454095
C  2.3937746887   0.4118889432   -0.1740941093
C  2.0540480975   -0.8908040071   -0.6559045151
C  -1.3551390844   -1.3081175744   0.7611933954
H  0.6131886245   -2.4596993284   -0.6649463196
H  -0.2836655015   0.975732013   1.7390970417
H  1.7706238137   2.1115342861   0.938080849
H  3.3805321351   0.8125420597   -0.3800071655
H  2.7730603514   -1.4430420548   -1.2502642871
H  -1.5583138969   -2.339347534   0.4897425
H  -1.9004036061   -0.9481638837   1.6254325719
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  502.3399
WellDepth[kcal/mol]  48.7
WellDepth[kcal/mol]  20.4
End
Frequencies[1/cm]  53
115.6086               128.2783
230.6732               258.6363               351.8216
374.3303               379.6391               425.6094
515.7030               559.8472               580.7785
617.5418               654.6977               735.8420
747.7548               805.9954               824.4494
846.4488               877.7287               887.5564
968.4136               979.4426               991.2412
992.5095              1013.3384              1029.6466
1045.8119              1053.3619              1081.1227
1109.4168              1183.4340              1185.3372
1200.0966              1306.8474              1336.1052
1398.2275              1445.9054              1475.5777
1490.6483              1543.0684              1547.3779
1661.2821              1912.2214              3096.0949
3101.1656              3126.4149              3151.2114
3155.6720              3167.1831              3171.6200
3185.2738              3208.0646              3277.6618
ZeroEnergy[kcal/mol]  -18.9
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i2_i3-----------
Barrier      i2_i3  i2  i3
RRHO
Geometry[angstrom]   20
C  -1.57767   0.59707   -0.15017
C  -2.07766   -0.66817   -0.17626
C  -1.90449   1.81414   -0.65705
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```
C  0.15694   -0.9846   0.30974
C  1.28234   -1.2993   -0.42239
C  -0.03654   0.36276   0.83537
C  1.07378   1.28114   0.6802
C  2.18455   0.93076   -0.04688
C  2.30606   -0.35939   -0.602
C  -1.1382   -1.75143   0.31598
H  -3.11317   -0.87455   -0.42861
H  -1.59941   2.73445   -0.17238
H  -2.38839   1.90223   -1.62401
H  1.36523   -2.28029   -0.87973
H  -0.53422   0.43867   1.80559
H  1.01319   2.26066   1.14217
H  2.9943   1.64188   -0.17183
H  3.19132   -0.62435   -1.16793
H  -1.11389   -2.62831   -0.33957
H  -1.4296   -2.10817   1.31699
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  828.1626
WellDepth[kcal/mol]  44.9
WellDepth[kcal/mol]  7.3
End
Frequencies[1/cm]  53
80.4977               173.1844
215.6256               288.3516               354.9985
380.0581               455.3939               473.3927
503.6933               538.5324               609.4655
651.0804               711.1076               726.2549
737.4753               764.7876               806.2152
838.9896               884.7104               928.3970
932.3782               973.0346               976.6287
1002.8257              1021.6618              1036.0292
1086.8665              1138.7937              1161.1273
1166.7117              1186.4344              1211.2716
1261.3247              1313.3391              1329.3550
1350.6638              1446.8944              1467.0105
1485.4012              1493.9031              1545.6658
1605.3286              1625.8687              2945.5592
3038.8081              3044.6669              3124.9455
3154.2733              3158.1886              3158.7025
3173.2057              3188.1471              3206.6624
ZeroEnergy[kcal/mol]  -23.7
ElectronicLevels[1/cm] 1
0  1
End

# -------bar_i1_p2-----------
Barrier      i1_p2  i1   p2    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
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        FragmentGeometry[angstrom]    19
C  -3.1671790544   0.1006662167   -0.2799117155
C  -1.9835202931   -0.5545286124   -0.5046150495
C  -4.2190678362   0.6856530687   -0.0687796814
C  0.3969809482   -0.3712343464   0.2994639265
C  1.4553186975   -1.2396758347   0.023587299
C  0.6441255509   1.0066042814   0.3005976051
C  1.9180921841   1.5008683912   0.0389286804
C  2.9679922724   0.624160295   -0.2338999218
C  2.7329709057   -0.7476701633   -0.2415500631
C  -1.000380889   -0.9005367772   0.5830062348
H  -1.7304370731   -0.8374682179   -1.5220849422
H  -5.1351561818   1.1927435429   0.1090787472
H  1.2801788566   -2.3109448315   0.020045459
H  -0.1699124908   1.6937106699   0.5073263275
H  2.0931706781   2.5710721499   0.0480592243
H  3.9607962443   1.0090164294   -0.4379494134
H  3.543005236   -1.4374143855   -0.4516699987
H  -0.9470194534   -1.9919206243   0.6893680712
H  -1.3647113018   -0.5105262519   1.5372172105
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  0.5            !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          1.42E-1     !do not change
        PotentialPowerExponent          7.00         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
23.8709                26.8950              132.6340
184.6464               281.7661              328.4623
388.2717               415.1293              442.0402
468.6234               538.6912              573.3201
635.4077               641.6737              646.8799
715.8930               763.0808              821.1367
857.4995               873.8992              924.3309
979.4148              1001.8752             1017.1015
1024.3840              1051.0543             1102.2523
1143.4917              1181.2521             1191.7030
1203.3047              1212.5665             1296.0131
1338.3737              1360.2531             1401.6608
1473.0578              1485.5001             1527.3192
1626.3566              1645.0422             2013.3657
2999.6799              3067.4793             3150.9417
3154.2802              3159.3677             3168.9576
3177.2446              3188.6502             3468.5476
      ElectronicLevels[1/cm]                  1
                0       2
      ZeroEnergy[kcal/mol]                    19.6      !equal to the
energy of separated products
   End

# -------bar_i2_p1-----------
Barrier      i2_p1  i2   p1    #
```

```
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  3.3091053427   0.1559001896   8.769993E-4
C  2.008583083   0.456713622   5.790582E-4
C  4.5762798473   -0.1307865254   0.0010999328
C  -0.4426086263   -0.215153564   1.629964E-4
C  -1.3614853893   -1.294517448   1.214113E-4
C  -0.9831513315   1.0951671832   -3.4602E-6
C  -2.353119321   1.3035298858   -1.906506E-4
C  -3.2389188088   0.2224757546   -2.197107E-4
C  -2.7301939618   -1.07839081   -6.25599E-5
C  0.9612085394   -0.4963093064   3.647458E-4
H  1.7566800707   1.5152055607   8.692711E-4
H  5.1353971627   -0.2582819243   0.9266275582
H  5.1359856377   -0.2575023962   -0.9241655195
H  -0.9752581771   -2.3085045488   2.476841E-4
H  -0.3213490444   1.9529159791   -1.22689E-5
H  -2.73919585   2.3170464097   -3.218649E-4
H  -4.3092687735   0.3923473827   -3.627278E-4
H  -3.4077969088   -1.9251254029   -8.33507E-5
H  1.2506415088   -1.5422970415   3.704561E-4
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          1.5E-1     !do not change
        PotentialPowerExponent          5.2         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
69.9162                95.7715              103.2779
225.3716               230.0652              296.3907
376.9358               410.8492              494.6885
509.1049               546.0593              627.1571
634.8159               691.5309              752.1513
805.2898               834.7245              859.1475
883.0681               901.6485              913.5769
971.2854               990.8055              992.0402
1000.7014              1040.9790             1059.4701
1100.3437              1173.3305             1184.3408
1192.1682              1242.0810             1300.0854
1338.1120              1354.7018             1430.3297
1467.1012              1499.0070             1511.7601
1592.2365              1614.9887             1948.2263
3079.3923              3124.7029             3141.1257
3157.1723              3161.0634             3164.4881
3174.6608              3183.0460             3191.8202
      ElectronicLevels[1/cm]                  1
                0       2
      ZeroEnergy[kcal/mol]                    11.8     !equal to the
energy of separated products
   End
```

```
# -------bar_i2_p2-----------
Barrier      i2_p2  i2   p2    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -3.1671790544   0.1006662167   -0.2799117155
C  -1.9835202931   -0.5545286124   -0.5046150495
C  -4.2190678362   0.6856530687   -0.0687796814
C  0.3969809482   -0.3712343464   0.2994639265
C  1.4553186975   -1.2396758347   0.023587299
C  0.6441255509   1.0066042814   0.3005976051
C  1.9180921841   1.5008683912   0.0389286804
C  2.9679922724   0.624160295   -0.2338999218
C  2.7329709057   -0.7476701633   -0.2415500631
C  -1.000380889   -0.9005367772   0.5830062348
H  -1.7304370731   -0.8374682179   -1.5220849422
H  -5.1351561818   1.1927435429   0.1090787472
H  1.2801788566   -2.3109448315   0.020045459
H  -0.1699124908   1.6937106699   0.5073263275
H  2.0931706781   2.5710721499   0.0480592243
H  3.9607962443   1.0090164294   -0.4379494134
H  3.543005236   -1.4374143855   -0.4516699987
H  -0.9470194534   -1.9919206243   0.6893680712
H  -1.3647113018   -0.5105262519   1.5372172105
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  0.5          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          1.67E-1     !do not change
        PotentialPowerExponent          5.70         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
23.8709               26.8950              132.6340
184.6464              281.7661              328.4623
388.2717              415.1293              442.0402
468.6234              538.6912              573.3201
635.4077              641.6737              646.8799
715.8930              763.0808              821.1367
857.4995              873.8992              924.3309
979.4148             1001.8752             1017.1015
1024.3840             1051.0543             1102.2523
1143.4917             1181.2521             1191.7030
1203.3047             1212.5665             1296.0131
1338.3737             1360.2531             1401.6608
1473.0578             1485.5001             1527.3192
1626.3566             1645.0422             2013.3657
2999.6799             3067.4793             3150.9417
3154.2802             3159.3677             3168.9576
3177.2446             3188.6502             3468.5476
      ElectronicLevels[1/cm]                  1
                0       2
```

```
      ZeroEnergy[kcal/mol]                    19.6      !equal to the
energy of separated products
   End

# -------bar_i2_p6-----------
Barrier      i2_p6  i2   p6    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -0.493964   -0.519347   0.008765
C  -0.511986   0.874296   0.021247
C  -1.722898   1.566998   0.012658
C  -2.929171   0.874044   -0.008454
C  -2.919446   -0.520482   -0.021278
C  -1.71104   -1.209216   -0.01286
C  0.801752   -1.326241   0.02211
H  0.424873   1.418446   0.037047
H  -1.719494   2.651395   0.022281
H  -3.869753   1.413111   -0.015391
H  -3.853479   -1.071158   -0.038427
H  -1.711922   -2.295225   -0.023337
H  0.801085   -1.977456   0.907327
H  0.798072   -2.011346   -0.836901
C  4.281187   0.74072   -0.020972
C  3.098885   0.053806   -0.006697
C  2.040542   -0.562681   0.005626
H  4.297914   1.823341   -0.056257
H  5.229531   0.217508   0.002796
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  0.5          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          1.67E-1     !do not change
        PotentialPowerExponent          5.70         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
9.1304               44.7336              77.0808
161.6371              190.8068             247.0117
329.1675              405.5700             414.8738
423.3338              469.8105             604.4733
635.7290              665.7824             712.3065
736.7966              792.5749             842.8092
857.4815              888.8354             953.5825
979.3719             1003.9808            1018.7892
1029.4271             1051.7566            1103.7933
1181.6528             1195.8868            1204.4613
1224.2443             1245.1994            1305.8805
1347.9915             1367.4384            1454.0503
1463.4503             1485.0018            1528.6827
1628.8635             1647.8417            2141.3399
2987.3049             3003.0673            3136.1939
3149.8986             3163.0430            3173.1808
```

```
3184.3303              3191.3253              3223.9021
      ElectronicLevels[1/cm]                   1
                0       2
      ZeroEnergy[kcal/mol]                     17.4     !equal to the
energy of separated products
   End

# -------bar_i2_p7-----------
Barrier      i2_p7  i2   p7    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    11
C  -2.36E-4   -1.396028   0.0
C  -1.223654   -0.770723   0.0
C  1.223556   -0.770924   0.0
C  1.211926   0.631211   0.0
C  0.0   1.32196   0.0
C  -1.211542   0.63183   0.0
H  -2.158085   -1.320755   0.0
H  2.157456   -1.321858   0.0
H  2.15027   1.176086   0.0
H  1.54E-4   2.406051   0.0
H  -2.150086   1.176517   0.0
        FragmentGeometry[angstrom]    9
C  -0.6234965585   0.1527517685   2.7603E-5
C  0.6801437921   0.4993917905   5.79736E-5
C  -1.8799899928   -0.1757125362   2.5904E-6
C  1.7569416245   -0.384449124   8.86847E-5
H  0.8956869769   1.5673845046   -2.78292E-5
H  -2.4369606583   -0.3232125182   -0.9248650987
H  -2.437326275   -0.3219874073   0.9248424877
H  2.7729245902   -0.0133107433   -2.50785E-5
H  1.602794501   -1.4557377347   1.026671E-4
        SymmetryFactor                 2.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]         0.267E-1     !do not change
        PotentialPowerExponent         2.12         !do not change
     End
          Frequencies[1/cm]  48                                    !
product frequencies
400.9605               426.4786               601.9001
620.2031               673.2085               721.3618
812.6504               892.3554               964.2589
988.6384               993.0286              1016.5317
1049.8674              1072.4077              1174.9732
1176.0810              1301.4469              1324.0613
1462.6872              1470.6151              1574.2771
1630.2259              3155.1702              3161.1286
3173.2989              3175.9637              3187.0914
206.5200               213.7048               495.6014
524.8347               572.8674               741.9907
883.8231               907.2270               937.3437
980.9474              1090.2238              1194.1738
```

```
1376.9555              1449.1388              1492.6535
1909.3729              3068.2826              3111.2790
3126.6627              3152.0133              3252.2770
      ElectronicLevels[1/cm]                   1
                0       2
      ZeroEnergy[kcal/mol]                     21.8     !equal to the
energy of separated products
   End

# -------bar_i8_p3-----------
Barrier      i8_p3  i8   p3    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -2.066573   -0.06128   2.4E-5
C  -3.43224   -0.100359   1.81E-4
C  -1.228264   1.216647   -2.26E-4
C  0.176804   -0.71253   -5.1E-5
C  0.19347   0.707497   6.1E-5
C  1.386176   -1.428444   -3.9E-5
C  2.584087   -0.722842   1.7E-5
C  2.593242   0.67647   7.2E-5
C  1.39181   1.397701   1.09E-4
C  -1.179944   -1.163091   -7.9E-5
H  -4.026278   0.805659   1.73E-4
H  -3.96502   -1.043959   2.53E-4
H  -1.442789   1.832245   -0.88049
H  -1.443051   1.83277   0.879577
H  1.384342   -2.512957   -4.5E-5
H  3.525051   -1.261947   -3.0E-6
H  3.538797   1.206684   7.4E-5
H  1.409123   2.482827   1.05E-4
H  -1.491577   -2.199938   -6.1E-5
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          4.00E-1     !do not change
        PotentialPowerExponent          6.70         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
107.2854               197.4040               269.8732
274.4375               423.9136               449.5162
463.4823               488.2501               542.9561
594.9856               600.1944               667.6426
722.3320               750.7749               790.9983
805.9823               815.0955               867.3432
873.6848               888.7209               929.6171
962.6779               981.9853               982.8102
1037.0743              1117.6931              1165.8559
1169.5088              1188.8115              1196.1402
1223.4811              1276.6787              1325.6325
```

```
1344.4708              1383.5600              1409.7392
1452.0208              1477.4612              1502.2124
1538.7312              1605.0493              1624.2556
3029.6281              3057.8460              3138.8472
3157.5643              3163.9492              3175.8573
3187.5787              3197.1411              3227.1005
      ElectronicLevels[1/cm]                   1
                0       2
      ZeroEnergy[kcal/mol]                     -20.4     !equal to the
energy of separated products
   End

# -------bar_i9_p3-----------
Barrier      i9_p3  i9   p3    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -2.066573   -0.06128   2.4E-5
C  -3.43224   -0.100359   1.81E-4
C  -1.228264   1.216647   -2.26E-4
C  0.176804   -0.71253   -5.1E-5
C  0.19347   0.707497   6.1E-5
C  1.386176   -1.428444   -3.9E-5
C  2.584087   -0.722842   1.7E-5
C  2.593242   0.67647   7.2E-5
C  1.39181   1.397701   1.09E-4
C  -1.179944   -1.163091   -7.9E-5
H  -4.026278   0.805659   1.73E-4
H  -3.96502   -1.043959   2.53E-4
H  -1.442789   1.832245   -0.88049
H  -1.443051   1.83277   0.879577
H  1.384342   -2.512957   -4.5E-5
H  3.525051   -1.261947   -3.0E-6
H  3.538797   1.206684   7.4E-5
H  1.409123   2.482827   1.05E-4
H  -1.491577   -2.199938   -6.1E-5
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                 1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]         4.00E-1     !do not change
        PotentialPowerExponent         6.70         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
107.2854               197.4040               269.8732
274.4375               423.9136               449.5162
463.4823               488.2501               542.9561
594.9856               600.1944               667.6426
722.3320               750.7749               790.9983
805.9823               815.0955               867.3432
873.6848               888.7209               929.6171
962.6779               981.9853               982.8102
```

```
1037.0743              1117.6931              1165.8559
1169.5088              1188.8115              1196.1402
1223.4811              1276.6787              1325.6325
1344.4708              1383.5600              1409.7392
1452.0208              1477.4612              1502.2124
1538.7312              1605.0493              1624.2556
3029.6281              3057.8460              3138.8472
3157.5643              3163.9492              3175.8573
3187.5787              3197.1411              3227.1005
      ElectronicLevels[1/cm]                   1
                0       2
      ZeroEnergy[kcal/mol]                     -20.4     !equal to the
energy of separated products
   End

# -------bar_i10_p3-----------
Barrier      i10_p3  i10   p3    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -2.066573   -0.06128   2.4E-5
C  -3.43224   -0.100359   1.81E-4
C  -1.228264   1.216647   -2.26E-4
C  0.176804   -0.71253   -5.1E-5
C  0.19347   0.707497   6.1E-5
C  1.386176   -1.428444   -3.9E-5
C  2.584087   -0.722842   1.7E-5
C  2.593242   0.67647   7.2E-5
C  1.39181   1.397701   1.09E-4
C  -1.179944   -1.163091   -7.9E-5
H  -4.026278   0.805659   1.73E-4
H  -3.96502   -1.043959   2.53E-4
H  -1.442789   1.832245   -0.88049
H  -1.443051   1.83277   0.879577
H  1.384342   -2.512957   -4.5E-5
H  3.525051   -1.261947   -3.0E-6
H  3.538797   1.206684   7.4E-5
H  1.409123   2.482827   1.05E-4
H  -1.491577   -2.199938   -6.1E-5
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                 1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]         4.00E-1     !do not change
        PotentialPowerExponent         6.70         !do not change
     End
         Frequencies[1/cm]  51                                    !
product frequencies
107.2854               197.4040               269.8732
274.4375               423.9136               449.5162
463.4823               488.2501               542.9561
594.9856               600.1944               667.6426
722.3320               750.7749               790.9983
```

```
805.9823                815.0955                867.3432
873.6848                888.7209                929.6171
962.6779                981.9853                982.8102
1037.0743               1117.6931               1165.8559
1169.5088               1188.8115               1196.1402
1223.4811               1276.6787               1325.6325
1344.4708               1383.5600               1409.7392
1452.0208               1477.4612               1502.2124
1538.7312               1605.0493               1624.2556
3029.6281               3057.8460               3138.8472
3157.5643               3163.9492               3175.8573
3187.5787               3197.1411               3227.1005
      ElectronicLevels[1/cm]                    1
                0       2
      ZeroEnergy[kcal/mol]                      -20.4     !equal to the
energy of separated products
   End
# -------bar_i3_p4-----------
Barrier i3_p4 i3 p4
        RRHO
                Geometry[angstrom] 20
                        C   0.156151    -0.414769     0.146351
                        C   2.033040     0.938490    -0.091782
                        H   3.057896     1.273015    -0.186070
                        C  -0.317344     0.923090     0.036913
                        C   0.858364     1.869988     0.003895
                        H   0.803988     2.571828    -0.838500
                        C  -0.754900    -1.485196    -0.005384
                        C  -2.111421    -1.206464    -0.073840
                        H  -2.823644    -2.020600    -0.149019
                        C  -2.574199     0.115711    -0.066865
                        H  -3.638919     0.310907    -0.124837
                        C  -1.672783     1.185976    -0.033675
                        H  -0.401183    -2.509616    -0.020010
                        H  -2.037724     2.206472    -0.088947
                        H   0.905324     2.490297     0.912446
                        C   1.642795    -0.401156    -0.021417
                        C   2.458285    -1.513754    -0.092438
                        H   2.061750    -2.517446    -0.011174
                        H   3.527543    -1.408989    -0.227762
                        H   0.237035    -0.467362     1.923336
                Core RigidRotor
                SymmetryFactor 0.5
        End
        Tunneling Eckart
                ImaginaryFrequency[1/cm] 895.0161
                WellDepth[kcal/mol] 15.7
                WellDepth[kcal/mol] 1.4
        End
        Frequencies[1/cm] 53
                  127.2863     189.6990
                  235.5199     256.2677     389.4994
                  411.7608     464.6170     483.2950
                  518.7140     526.1380     551.2408
```

```
                  566.8884     626.4034     674.0841
                  699.6511     719.8214     745.5126
                  763.2948     799.9011     837.0184
                  865.6583     925.5732     944.4150
                  954.2262     984.8216    1016.7487
                 1040.7015    1096.4897    1139.4103
                 1148.6335    1175.8217    1197.0161
                 1234.4777    1250.7265    1315.4455
                 1337.9422    1378.7697    1412.9379
                 1448.3165    1473.7200    1493.7014
                 1516.2152    1589.6907    1628.5707
                 2973.3229    3012.4207    3148.7557
                 3159.3821    3167.3836    3180.4983
                 3190.0200    3202.6811    3240.1525
        ZeroEnergy[kcal/mol] -15.3
        ElectronicLevels[1/cm] 1
        0 1
End
# -------bar_i4_p4-----------
Barrier      i4_p4  i4   p4    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -2.041609   0.931976   -3.4E-5
C  -2.463875   -1.520944   -1.92E-4
C  -0.86193   1.860737   1.64E-4
C  -0.156142   -0.417162   2.33E-4
C  0.311959   0.906579   1.3E-5
C  0.742958   -1.481823   2.18E-4
C  2.110335   -1.209607   -1.8E-5
C  2.573976   0.107751   -1.77E-4
C  1.674347   1.17562   -1.38E-4
C  -1.64119   -0.409053   -1.04E-4
H  -3.070891   1.266475   -3.53E-4
H  -3.541533   -1.414286   -0.00109
H  -2.062618   -2.526183   8.5E-4
H  -0.855762   2.522694   0.87758
H  -0.855691   2.523649   -0.876471
H  0.391915   -2.507982   3.98E-4
H  2.821547   -2.028163   -1.41E-4
H  3.6408   0.301681   -4.16E-4
H  2.039263   2.197671   -1.42E-4
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          4.00E-1     !do not change
        PotentialPowerExponent          6.70         !do not change
        End
          Frequencies[1/cm]  51                                    !
product frequencies
138.8133              190.1179              244.6336
258.4211              412.9391              457.9508
```

```
468.9236              524.0911              537.0384
561.9048              611.8354              677.8857
702.1255              732.3106              755.2261
761.0925              786.0837              841.5495
872.5232              924.7836              944.5991
954.3103              988.7664             1015.9128
1046.3478             1099.5006             1139.1661
1151.8925             1179.2813             1207.7274
1234.2941             1248.9391             1323.6220
1343.8281             1384.6453             1412.2618
1450.1750             1493.8211             1497.3618
1519.2547             1623.5201             1649.8843
2990.4294             3004.1788             3148.0491
3157.0438             3164.5635             3175.2272
3186.9590             3201.5905             3239.1650
      ElectronicLevels[1/cm]                  1
                0       2
      ZeroEnergy[kcal/mol]                    -16.7     !equal to the
energy of separated products
   End

# -------bar_i4_p5-----------
Barrier      i4_p5  i4   p5    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -2.07207   -1.017546   -1.53E-4
C  -2.421267   1.510136   3.79E-4
C  -0.793101   -1.804877   -2.55E-4
C  -0.148346   0.425276   7.0E-6
C  0.305909   -0.935449   1.24E-4
C  0.768874   1.471236   -2.82E-4
C  2.133593   1.184472   -2.16E-4
C  2.587519   -0.148931   1.76E-4
C  1.697234   -1.206402   3.34E-4
C  -1.61382   0.441457   -1.94E-4
H  -2.694311   -1.23903   -0.877325
H  -2.694297   -1.239008   0.877062
H  -3.500268   1.405095   5.11E-4
H  -2.029846   2.520998   8.99E-4
H  -0.742682   -2.885306   -5.0E-4
H  0.43181   2.502261   -6.01E-4
H  2.85458   1.99379   -5.28E-4
H  3.654348   -0.344416   3.28E-4
H  2.053521   -2.230617   6.4E-4
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          4.00E-1     !do not change
        PotentialPowerExponent          6.70         !do not change
          End
```

```
          Frequencies[1/cm]  51                                        !
product frequencies
98.2212               180.2672              245.9736
267.0355               399.1984              465.6482
469.0492               534.4811              551.5839
552.4676               608.8821              676.1590
684.0336               745.4599              757.2383
782.3519               860.6388              873.7475
883.1060               899.4699              928.7646
943.6584               979.8313             1000.2384
1032.0211              1098.7469             1130.2355
1145.6364              1164.0718             1197.9530
1242.5857              1275.5889             1312.1139
1332.8773              1386.6327             1444.8391
1451.1361              1454.9932             1503.8168
1578.6663              1602.8567             1673.2544
2997.7826              3013.8864             3136.9465
3160.0775              3166.8756             3177.6129
3188.7980              3208.1615             3217.0914
      ElectronicLevels[1/cm]                   1
                0       2
      ZeroEnergy[kcal/mol]                     -13.4     !equal to the
energy of separated products
   End

# -------bar_i5_p5-----------
Barrier      i5_p5  i5   p5    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -2.07207   -1.017546   -1.53E-4
C  -2.421267   1.510136   3.79E-4
C  -0.793101   -1.804877   -2.55E-4
C  -0.148346   0.425276   7.0E-6
C  0.305909   -0.935449   1.24E-4
C  0.768874   1.471236   -2.82E-4
C  2.133593   1.184472   -2.16E-4
C  2.587519   -0.148931   1.76E-4
C  1.697234   -1.206402   3.34E-4
C  -1.61382   0.441457   -1.94E-4
H  -2.694311   -1.23903   -0.877325
H  -2.694297   -1.239008   0.877062
H  -3.500268   1.405095   5.11E-4
H  -2.029846   2.520998   8.99E-4
H  -0.742682   -2.885306   -5.0E-4
H  0.43181   2.502261   -6.01E-4
H  2.85458   1.99379   -5.28E-4
H  3.654348   -0.344416   3.28E-4
H  2.053521   -2.230617   6.4E-4
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
```

```
        PotentialPrefactor[au]          4.00E-1     !do not change
        PotentialPowerExponent          6.70         !do not change
     End
          Frequencies[1/cm]  51                                      !
product frequencies
98.2212               180.2672              245.9736
267.0355               399.1984              465.6482
469.0492               534.4811              551.5839
552.4676               608.8821              676.1590
684.0336               745.4599              757.2383
782.3519               860.6388              873.7475
883.1060               899.4699              928.7646
943.6584               979.8313             1000.2384
1032.0211              1098.7469             1130.2355
1145.6364              1164.0718             1197.9530
1242.5857              1275.5889             1312.1139
1332.8773              1386.6327             1444.8391
1451.1361              1454.9932             1503.8168
1578.6663              1602.8567             1673.2544
2997.7826              3013.8864             3136.9465
3160.0775              3166.8756             3177.6129
3188.7980              3208.1615             3217.0914
      ElectronicLevels[1/cm]                   1
                0       2
      ZeroEnergy[kcal/mol]                     -13.4     !equal to the
energy of separated products
   End

# -------bar_w22_p5-----------
Barrier      w22_p5  w22   p5    #-----------------
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  -2.07207   -1.017546   -1.53E-4
C  -2.421267   1.510136   3.79E-4
C  -0.793101   -1.804877   -2.55E-4
C  -0.148346   0.425276   7.0E-6
C  0.305909   -0.935449   1.24E-4
C  0.768874   1.471236   -2.82E-4
C  2.133593   1.184472   -2.16E-4
C  2.587519   -0.148931   1.76E-4
C  1.697234   -1.206402   3.34E-4
C  -1.61382   0.441457   -1.94E-4
H  -2.694311   -1.23903   -0.877325
H  -2.694297   -1.239008   0.877062
H  -3.500268   1.405095   5.11E-4
H  -2.029846   2.520998   8.99E-4
H  -0.742682   -2.885306   -5.0E-4
H  0.43181   2.502261   -6.01E-4
H  2.85458   1.99379   -5.28E-4
H  3.654348   -0.344416   3.28E-4
H  2.053521   -2.230617   6.4E-4
        FragmentGeometry[angstrom]    1
```

```
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          4.00E-1     !do not change
        PotentialPowerExponent          6.70         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
98.2212               180.2672              245.9736
267.0355               399.1984              465.6482
469.0492               534.4811              551.5839
552.4676               608.8821              676.1590
684.0336               745.4599              757.2383
782.3519               860.6388              873.7475
883.1060               899.4699              928.7646
943.6584               979.8313             1000.2384
1032.0211              1098.7469             1130.2355
1145.6364              1164.0718             1197.9530
1242.5857              1275.5889             1312.1139
1332.8773              1386.6327             1444.8391
1451.1361              1454.9932             1503.8168
1578.6663              1602.8567             1673.2544
2997.7826              3013.8864             3136.9465
3160.0775              3166.8756             3177.6129
3188.7980              3208.1615             3217.0914
      ElectronicLevels[1/cm]                  1
                0       2
      ZeroEnergy[kcal/mol]                    -13.4     !equal to the
energy of separated products
   End

# -------bar_w24_p13-----------
Barrier      w24_p13  w24   p13    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  2.498545   -0.697531   -5.2E-5
C  1.17813   -1.396929   -7.1E-5
C  2.385467   0.799183   9.0E-6
C  -0.064016   0.722015   1.1E-5
C  -0.043264   -0.718056   8.0E-6
C  -1.287696   1.3915   -2.6E-5
C  -2.493813   0.693714   -6.7E-5
C  -2.486404   -0.711099   6.0E-6
C  -1.292869   -1.40351   8.1E-5
C  1.202832   1.433007   6.8E-5
H  3.101925   -1.022986   0.866013
H  3.1019   -1.022913   -0.866158
H  1.177837   -2.482266   2.6E-5
H  3.309313   1.368937   5.2E-5
H  -1.292165   2.477103   6.0E-6
H  -3.43404   1.232557   -1.93E-4
H  -3.425132   -1.254209   5.7E-5
```

```
H  -1.290007   -2.488594   2.05E-4
H  1.168895   2.5186   1.84E-4
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          4.00E-1     !do not change
        PotentialPowerExponent          6.70         !do not change
         End
          Frequencies[1/cm]  51                                    !
product frequencies
123.3347              173.0144              257.7164
357.9903              393.8082              459.7952
498.4553              504.2186              542.9712
615.2203              687.2613              700.4505
750.4204              759.2844              784.9193
788.2145              863.5324              900.9898
926.8348              927.8706              942.5778
974.6647              995.4948             1036.7673
1053.1506             1139.3661             1163.2684
1177.7355             1183.5210             1202.7389
1249.9945             1294.9554             1340.6531
1358.5897             1413.0465             1436.2870
1446.8400             1459.4012             1504.7200
1562.2803             1603.7669             1676.1235
2913.0958             2926.1623             3145.4274
3154.6715             3157.5034             3160.5475
3167.8210             3173.6738             3188.6360
      ElectronicLevels[1/cm]                  1
                0       2
      ZeroEnergy[kcal/mol]                    -18.9     !equal to the
energy of separated products
   End

# -------bar_w24_p12-----------
Barrier      w24_p12  w24   p12    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  2.446641   -0.513347   -6.2E-5
C  1.226407   -1.381968   8.5E-5
C  2.365945   0.8532   -6.2E-5
C  -0.104388   0.792469   7.0E-6
C  -0.088258   -0.626739   -6.0E-6
C  -1.350583   1.456385   1.8E-5
C  -2.540146   0.7477   -8.0E-6
C  -2.517484   -0.649799   -4.6E-5
C  -1.296438   -1.320513   -4.9E-5
C  1.130728   1.521757   2.8E-5
H  3.413405   -1.004856   -1.44E-4
H  1.257745   -2.059255   0.868609
H  1.257769   -2.059587   -0.868164
H  3.27952   1.439327   -1.44E-4
```

```
H  -1.363349   2.541544   2.7E-5
H  -3.486921   1.276263   5.0E-6
H  -3.444921   -1.211049   -7.3E-5
H  -1.282882   -2.40662   -7.9E-5
H  1.097203   2.60508   5.3E-5
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          4.00E-1     !do not change
        PotentialPowerExponent          6.70         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
86.0667               172.1344              251.0656
357.5737               429.6094              471.5310
485.5430               506.4692              541.6557
612.7051               660.3964              713.9658
747.7418               751.4459              791.8633
794.5749               871.2099              920.8227
931.9666               954.5132              959.5321
966.5833               984.7572             1056.8223
1092.6382              1139.3179             1175.6202
1179.3283              1201.8461             1202.5165
1234.0543              1277.4316             1309.2880
1356.0487              1393.8304             1439.2594
1445.6397              1473.6849             1515.7469
1559.5059              1599.1827             1629.7487
2952.2734              2952.4859             3148.8035
3152.5568              3158.0580             3171.2889
3172.5326              3182.9429             3187.1206
      ElectronicLevels[1/cm]                  1
                0       2
      ZeroEnergy[kcal/mol]                    -24.0     !equal to the
energy of separated products
   End

# -------bar_w25_p12-----------
Barrier      w25_p12  w25   p12    #
   RRHO
     Stoichiometry  C10H10
      Core      PhaseSpaceTheory
        FragmentGeometry[angstrom]    19
C  2.446641   -0.513347   -6.2E-5
C  1.226407   -1.381968   8.5E-5
C  2.365945   0.8532   -6.2E-5
C  -0.104388   0.792469   7.0E-6
C  -0.088258   -0.626739   -6.0E-6
C  -1.350583   1.456385   1.8E-5
C  -2.540146   0.7477   -8.0E-6
C  -2.517484   -0.649799   -4.6E-5
C  -1.296438   -1.320513   -4.9E-5
C  1.130728   1.521757   2.8E-5
H  3.413405   -1.004856   -1.44E-4
```

```
H  1.257745   -2.059255   0.868609
H  1.257769   -2.059587   -0.868164
H  3.27952   1.439327   -1.44E-4
H  -1.363349   2.541544   2.7E-5
H  -3.486921   1.276263   5.0E-6
H  -3.444921   -1.211049   -7.3E-5
H  -1.282882   -2.40662   -7.9E-5
H  1.097203   2.60508   5.3E-5
        FragmentGeometry[angstrom]    1
H  0.0   0.0   0.0
        SymmetryFactor                  1.0          !symmetry factor of
the heavy fragment
        PotentialPrefactor[au]          4.00E-1     !do not change
        PotentialPowerExponent          6.70         !do not change
     End
          Frequencies[1/cm]  51                                    !
product frequencies
86.0667               172.1344              251.0656
357.5737               429.6094               471.5310
485.5430               506.4692               541.6557
612.7051               660.3964               713.9658
747.7418               751.4459               791.8633
794.5749               871.2099               920.8227
931.9666               954.5132               959.5321
966.5833               984.7572              1056.8223
1092.6382              1139.3179               1175.6202
1179.3283              1201.8461               1202.5165
1234.0543              1277.4316               1309.2880
1356.0487              1393.8304               1439.2594
1445.6397              1473.6849               1515.7469
1559.5059              1599.1827               1629.7487
2952.2734              2952.4859               3148.8035
3152.5568              3158.0580               3171.2889
3172.5326              3182.9429               3187.1206
      ElectronicLevels[1/cm]                    1
                0       2
      ZeroEnergy[kcal/mol]                      -24.0     !equal to the
energy of separated products
   End

End
```

## References


1. L. Zhao, R. I. Kaiser, W. Lu, B. Xu, M. Ahmed, A. N. Morozov, A. M. Mebel, A. H. Howlader and S. F. Wnuk, Molecular Mass Growth through Ring Expansion in Polycyclic Aromatic Hydrocarbons via Radical–Radical Reactions, *Nat. Commun.*, 2019, **10**, 3689.
2. D. S. N. Parker, R. I. Kaiser, T. P. Troy and M. Ahmed, Hydrogen Abstraction/Acetylene Addition Revealed, *Angew. Chem. Int. Ed.*, 2014, **53**, 7740-7744.
3. L. Zhao, W. Lu, M. Ahmed, M. V. Zagidullin, V. N. Azyazov, A. N. Morozov, A. M. Mebel and R. I. Kaiser, Gas-Phase Synthesis of Benzene via the Propargyl Radical Self-Reaction, *Sci. Adv.*, 2021, **7**, eabf0360.
4. R. I. Kaiser, L. Zhao, W. Lu, M. Ahmed, V. S. Krasnoukhov, V. N. Azyazov and A. M. Mebel, Unconventional Excited-State Dynamics in the Concerted Benzyl ($C_7H_7$) Radical Self-Reaction to Anthracene ($C_{14}H_{10}$), *Nat. Commun.*, 2022, **13**, 786.
5. F. Qi, Combustion Chemistry Probed by Synchrotron VUV Photoionization Mass Spectrometry, *Proc. Combust. Inst.*, 2013, **34**, 33-63.
6. Q. Guan, K. N. Urness, T. K. Ormond, D. E. David, G. Barney Ellison and J. W. Daily, The Properties of a Micro-Reactor for the Study of the Unimolecular Decomposition of Large Molecules, *Int. Rev. Phys. Chem.*, 2014, **33**, 447-487.
7. M. V. Zagidullin, R. I. Kaiser, D. P. Porfiriev, I. P. Zavershinskiy, M. Ahmed, V. N. Azyazov and A. M. Mebel, Functional Relationships between Kinetic, Flow, and Geometrical Parameters in a High-Temperature Chemical Microreactor, *J. Phys. Chem. A*, 2018, **122**, 8819-8827.
8. R. I. Kaiser, L. Zhao, W. Lu, M. Ahmed, M. V. Zagidullin, V. N. Azyazov and A. M. Mebel, Formation of Benzene and Naphthalene through Cyclopentadienyl-Mediated Radical–Radical Reactions, *J. Phys. Chem. Lett.*, 2022, **13**, 208-213.
9. C. Lee, W. Yang and R. G. Parr, Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density, *Phys. Rev. B*, 1988, **37**, 785-789.
10. A. D. Becke, Density-Functional Thermochemistry. III The Role of Exact Exchange, *J. Chem. Phys.*, 1993, **98**, 5648–5652.
11. R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, Self‐Consistent Molecular Orbital Methods. XX. A Basis Set for Correlated Wave Functions, *J. Chem. Phys.*, 1980, **72**, 650-654.
12. L. A. Curtiss, K. Raghavachari, P. C. Redfern, V. Rassolov and J. A. Pople, Gaussian-3 (G3) Theory for Molecules Containing First and Second-Row Atoms, *J. Chem. Phys.*, 1998, **109**, 7764-7776.
13. L. A. Curtiss, K. Raghavachari, P. C. Redfern, A. G. Baboul and J. A. Pople, Gaussian-3 Theory using Coupled Cluster Energies, *Chem. Phys. Lett.*, 1999, **314**, 101-107.
14. A. G. Baboul, L. A. Curtiss, P. C. Redfern and K. Raghavachari, Gaussian-3 Theory Using Density Functional Geometries and Zero-Point Energies, *J. Chem. Phys.*, 1999, **110**, 7650-7657.
15. J. A. Miller, S. J. Klippenstein, Y. Georgievskii, L. B. Harding, W. D. Allen and A. C. Simmonett, Reactions between Resonance-Stabilized Radicals: Propargyl+ Allyl, *J. Phys. Chem. A*, 2010, **114**, 4881-4890.
16. A. Matsugi and A. Miyoshi, Computational Study on the Recombination Reaction between Benzyl and Propargyl Radicals, *International Journal of Chemical Kinetics*, 2012, **44**, 206-218.
17. P. Celani and H.-J. Werner, Multireference perturbation theory for large restricted and selected active space reference wave functions, *J. Chem. Phys.*, 2000, **112**, 5546-5557.
18. T. Shiozaki, W. Győrffy, P. Celani and H.-J. Werner, Communication: extended multi-state complete active space second-order perturbation theory: energy and nuclear gradients, *J. Chem. Phys.*, 2011, **135**, 081106.
19. T. H. Dunning, Gaussian Basis Sets for Use in Correlated Molecular Calculations. I. the Atoms Boron through Neon and Hydrogen, *J. Chem. Phys.*, 1989, **90**, 1007-1023.
20. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A.

Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision A. 01, Gaussian, *Gaussian Inc.: Wallingford, CT, 2009*.

21. H. J. Werner, P. J. Knowles, G. Knizia, F. R. Manby and M. Schütz, Molpro: A General‐Purpose Quantum Chemistry Program Package, *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 2012, **2**, 242-253.
22. R. A. Marcus, Unimolecular Dissociations and Free Radical Recombination Reactions, *J. Chem. Phys.*, 1952, **20**, 359-364.
23. Y. Georgievskii, J. A. Miller, M. P. Burke and S. J. Klippenstein, Reformulation and Solution of the Master Equation for Multiple-well Chemical Reactions, *J. Phys. Chem. A*, 2013, **117**, 12146-12154.
24. Y. Georgievskii and S. J. Klippenstein, *Master Equation System Solver (MESS)*, URl: https://tcg.cse.anl.gov/papr/codes/mess.html, 2015.
25. W. H. Miller, Tunneling Corrections to Unimolecular Rate Constants, with Application to Formaldehyde, *J. Am. Chem. Soc.*, 1979, **101**, 6810-6814.
26. S. J. Klippenstein, Variational Optimizations in the Rice–Ramsperger–Kassel–Marcus Theory Calculations for Unimolecular Dissociations with No Reverse Barrier, *J. Chem. Phys.*, 1992, **96**, 367-371.
27. Y. Georgievskii, J. A. Miller and S. J. Klippenstein, Association Rate Constants for Reactions between Resonance-stabilized Radicals: $C_3H_3 + C_3H_3$, $C_3H_3 + C_3H_5$, and $C_3H_5 + C_3H_5$, *Phys. Chem. Chem. Phys.*, 2007, **9**, 4259-4268.
28. Y. Georgievskii and S. J. Klippenstein, Variable Reaction Coordinate Transition State Theory: Analytic Results and Application to the $C_2H_3 + H \rightarrow C_2H_4$ Reaction, *J. Chem. Phys.*, 2003, **118**, 5442-5455.
29. V. S. Krasnoukhov, P. S. Pivovarov, M. V. Zagidullin, V. N. Azyazov, A. M. Mebel and A. N. Morozov, Formation of Two-ring Polycyclic Aromatic Hydrocarbons via the Recombination of Benzyl and Propargyl Radicals under the Circumstellar Envelopes Conditions of Asymptotic Giant Branch Stars, *Astronomy Reports*, 2022, **66**, 811-826.
30. S. J. Klippenstein and J. I. Cline, Classical Phase Space Theory for Product State Distributions with Application to the *v–j* Vector Correlation, *J. Chem. Phys.*, 1995, **103**, 5451-5460.
31. L. B. Harding, S. J. Klippenstein and Y. Georgievskii, On the Combination Reactions of Hydrogen Atoms with Resonance-Stabilized Hydrocarbon Radicals, *J. Phys. Chem. A*, 2007, **111**, 3789-3801.
32. A. N. Morozov and A. M. Mebel, Theoretical Study of the Reaction Mechanism and Kinetics of the Phenyl+ Allyl and Related Benzyl + Vinyl Associations, *J. Phys. Chem. A*, 2019, **123**, 1720-1729.
33. A. M. Mebel, Y. Georgievskii, A. W. Jasper and S. J. Klippenstein, Pressure-Dependent Rate Constants for PAH Growth: Formation of Indene and Its Conversion to Naphthalene, *Faraday Discuss.*, 2016, **195**, 637-670.
34. J. Troe, Theory of Thermal Unimolecular Reactions at Low Pressures. I. Solutions of the Master Equation, *J. Chem. Phys.* , 1977, **66**, 4745-4757.
35. S. J. Klippenstein, Y. C. Yang, V. Ryzhov and R. C. Dunbar, Theory and Modeling of Ion–Molecule Radiative Association Kinetics, *J. Chem. Phys.*, 1996, **104**, 4502-4516.
36. C. Multiphysics.
37. L. Zhao, R. I. Kaiser, B. Xu, U. Ablikim, M. Ahmed, M. V. Zagidullin, V. N. Azyazov, A. H. Howlader, S. F. Wnuk and A. M. Mebel, VUV Photoionization Study of the Formation of the

Simplest Polycyclic Aromatic Hydrocarbon: Naphthalene ($C_{10}H_8$), *J. Phys. Chem. Lett.*, 2018, **9**, 2620-2626.
38. M. Szwarc, B. N. Ghosh and A. H. Sehon, The C–Br Bond Dissociation Energy in Benzyl Bromide and Allyl Bromide, *J. Chem. Phys.*, 1950, **18**, 1142-1149.
39. M. Levy, M. Szwarc and J. Throssell, Mechanism of Formation of the Quinonoid Hydrocarbon $CH_2$: $C_6H_4$: $CH_2$, *J. Chem. Phys.*, 1954, **22**, 1904-1911.