

The Role of Methylaryl Radicals in the Growth of Polycyclic Aromatic Hydrocarbons: The Formation of Five-Membered Rings

Galiya R. Galimova^{a,b}, Iakov A. Medvedkov^{b,c}, and Alexander M. Mebel^{a,*}

^a*Department of Chemistry and Biochemistry, Florida International University, Miami, FL 33199
(USA)*

^b*Department of Physics, Samara National Research University, Samara 443086
(Russian Federation)*

^c*Lebedev Physical Institute, Samara 443011
(Russian Federation)*

Abstract. The regions of the C₁₃H₁₁ potential energy surface (PES) related to the unimolecular isomerization and decomposition of the 1-methylbiphenyl radical and accessed by the 1-/2-methylnaphthyl + C₂H₂ reactions have been explored by ab initio G3(MP2,CC)//B3LYP/6-311G(d,p) calculations. The kinetics of these reactions relevant to the growth of polycyclic aromatic hydrocarbons (PAH) under high-temperature conditions in circumstellar envelopes and in combustion flames has been studied employing the RRKM-Master Equation approach. The unimolecular reaction of 1-methylbiphenyl proceeding via a five-membered ring closure followed by H elimination is predicted to be very fast, on a sub-microsecond scale above 1000 K and to result in the formation of an embedded five-membered ring in the 9*H*-fluorene product. The 1-/2-methylnaphthyl + C₂H₂ reaction mechanism involves acetylene addition to the radical on the methylene group followed by a six- or five-membered ring closure and aromatization via an H atom loss. Despite of the complexity of the C₁₃H₁₁ PES, these straightforward pathways are dominant in the high-temperature regime (above ~1000 K), with the prevailing products being phenalene, with a significant contribution of 1*H*-cyclopenta(a)naphthalene, for 1-methylnaphthyl + C₂H₂, and 1*H*-cyclopenta(b)naphthalene and 3*H*-cyclopenta(a)naphthalene for 2-methylnaphthyl + C₂H₂. The methylnaphthyl reactions with acetylene represent a clean source of the three-ring PAHs, but they are relatively slow owing to the high entrance barriers of ~10 kcal/mol, with the rate constants of about an order of magnitude lower as compared to those for naphthyl + allene and σ-aryl + C₂H₂. The 1-methylnaphthyl + C₂H₂ and 2-methylnaphthyl + C₂H₂ reactions represent prototypes for PAH growth by an extra six- and five-membered ring on a zigzag

* E-mail: mebela@fiu.edu

edge or a corner of PAH and the generated modified Arrhenius expressions are recommended for kinetic modeling of PAH expansion by the mechanism of acetylene addition to methylaryl radicals.

1. INTRODUCTION

Polycyclic aromatic hydrocarbons (PAHs) – organic molecules composed of fused benzene rings, together with their (de)hydrogenated,¹ alkylated,^{2,3} protonated,⁴ and ionized^{5,6} derivatives, are believed to be omnipresent in the interstellar space and in circumstellar envelopes, with up to 20% of the carbon budget in our galaxy^{7,8} attributed to the molecules of this class. It has been also hypothesized that they represent the missing link between small carbon molecules and carbonaceous nanoparticles (interstellar grains).⁹ The evidence of PAH existence in the outer space comes from the observation of the diffuse interstellar bands (DIBs),^{1,2,4,5,8,10} which are discrete absorption features overlaid on the interstellar extinction curve ranging from ~400 nm (visible) to 1.2 μm (near-infrared) and the unidentified infrared (UIR) emission bands^{9,11,12} in the 3-14 μm range, but most clearly, from the identification of PAHs in carbonaceous chondrites such as Murchison, Allende, and Orgueil,^{13,14} where the $^{13}\text{C}/^{12}\text{C}$ and D/H isotopic analyses¹⁵ corroborate their circumstellar origin. PAHs are conjectured to be formed through eventual growth from small aromatic molecules like benzene and toluene in carbon-rich asymptotic giant branch (AGB) stars and planetary nebulae as the descendants of AGB stars at elevated temperatures of a few 1000 K through molecular mass growth processes involving, among others, hydrogen abstraction–carbon addition (HACA) sequences,^{16,17} which are reminiscent of the PAH growth mechanism on Earth, in combustion flames of hydrocarbon fuels.¹⁷⁻²²

Methyl-substituted and, more generally, alkylated PAHs, with toluene being their prototype molecule, may play a special role in the PAH growth processes. In high temperature environments, such as in circumstellar envelopes or in combustion, they can be produced via methylation/alkylation processes, i.e., via CH_3 /alkyl-radical-for-H exchange reactions, which require significant barriers.²³⁻²⁷ Alternatively, alkylated PAH can be also produced via barrierless reactions feasible even under very low temperature conditions like those in cold molecular clouds. Such reactions are exemplified by the reactions of ethynyl radical C_2H with isoprene (2-methyl-1,3-butadiene)²⁸ and of 1-propynyl radical CH_3CC with 1,3-butadiene²⁹ producing toluene, as has been recently shown by our combined experimental crossed molecular beams and theoretical studies. We have also demonstrated that benzyl radical is the major product of the barrierless

reactions of dicarbon $C_2(X^1\Sigma_g^+/^3\Pi_u)$ with isoprene.³⁰ The C-H bond in the out-of-ring methyl group of a methylated PAH molecule is relatively weak and can be readily cleaved via direct H abstraction by another radical^{27,31,32} or through photodissociation.^{33,34} The methylaryl radical formed as a result is an analog of benzyl radical and represents both a resonantly stabilized and aromatic π radical which leads to its high stability. Radicals of this type tend to accumulate in combustion flames and likely in circumstellar envelopes as well. Consequently, they can react with abundant acetylene molecules thus contributing to the PAH growth. For example, the reaction of benzyl radicals with C_2H_2 has been shown to form indene, a prototype PAH molecule containing a five-membered ring, both theoretically^{27,35} and by experiments in a pyrolytic microreactor under combustion-like conditions at 600 K.³⁶ Interestingly, this reaction was found to form the indene isomer exclusively, which suggests that this pathway could be one of major routes to synthesize cyclopenta-PAHs, i.e., those containing five-membered rings. There also exists a barrierless (low-temperature) pathway to produce indene from toluene involving two consecutive additions of methylidyne radical: $CH + \text{toluene} \rightarrow \text{styrene} + H$ ³⁷ and $CH + \text{styrene} \rightarrow \text{indene} + H$.³⁸ In turn, cyclopenta-PAHs represent a vital molecular building block of non-planar PAHs like corannulene; non-planar PAHs are potential precursors to fullerenes.^{39,40} Five-membered rings in the carbon skeleton are required to curve PAHs out of the plane and thus, to ultimately form three-dimensional carbonaceous nanostructures.⁴¹

In view of the potentially important role of methylated PAHs in the growth processes involved in the formation of an extra five-membered ring, in the present work we theoretically explore the fate of methylaryl radicals, with the methylene group produced after H abstraction/H loss from the methyl moiety located in various positions on a PAH edge. In particular, we consider a unimolecular reaction of the *ortho*-methylbiphenyl radical representing methylaryl with CH_2 on an armchair edge, which results in the formation of fluorene, and bimolecular reactions of 1- and 2-methylnaphthyl radicals standing for methylaryls with CH_2 on a zigzag edge or a corner of PAH, respectively, with acetylene, which can form a new five- or six-membered ring in cyclopentanaphthalene isomers or phenalene. Our studies include electronic structure calculations of the reaction potential energy surfaces (PES) followed by statistical Rice-Ramsperger-Kassel-Marcus Master Equation (RRKM-ME) calculations of temperature- and pressure-dependent rate constants for the overall reactions and individual product channels. As a result, we uncover the reaction mechanisms and generate rate expressions which can be utilized in kinetic models

describing the growth of cyclopenta-PAHs and three-dimensional carbonaceous nanostructures both in combustion flames on Earth and in circumstellar envelopes.

2. CALCULATION METHODS

Geometries of the reactants, products, intermediates, and transition states participating in the unimolecular reaction of the *ortho*-methylbiphenyl radical and the reactions of 1- and 2-methylnaphthyl radicals with acetylene both accessing the C₁₃H₁₁ PES were optimized at the hybrid density functional B3LYP/6-311G(d,p) level of theory^{42,43} with vibrational frequencies computed using the same method. Energies of reactants, products, and various C₁₃H₁₁ species were refined by single-point calculations using the composite G3(MP2,CC) model chemistry scheme⁴⁴⁻⁴⁶ where the energies were computed as

$$E_0[\text{G3(MP2,CC)}] = E[\text{CCSD(T)/6-311**}] + \Delta E_{\text{MP2}} + E(\text{ZPE}),$$

where $\Delta E_{\text{MP2}} = E[\text{MP2/G3Large}] - E[\text{MP2/6-311G**}]$ is the basis set correction and $E(\text{ZPE})$ is the zero-point vibrational energy. Relative energies computed within this scheme are normally accurate within 1-2 kcal/mol. The T1 diagnostics were checked during the coupled clusters calculations to make sure that the wave functions do not exhibit a significant multireference character. The Gaussian 16⁴⁷ and MOLPRO 2021⁴⁸ program packages were used for the electronic structure calculations.

In order to check the performance of the B3LYP DFT method vs. a more recent ω B97XD functional,⁴⁹ for the methylbiphenyl reaction we additionally carried out geometry optimization and vibrational frequencies calculations at the ω B97XD level and recomputed single-point G3(MP2,CC) energies using the ω B97XD geometries and ZPE. The results show that the B3LYP and ω B97XD optimized geometries are nearly identical, whereas the difference in vibrational frequencies does not exceed 4% being on average only ~1%. Moreover, the G3(MP2,CC)//B3LYP and G3(MP2,CC)// ω B97XD relative energies agree with each other within 0.3 kcal/mol. Interestingly, the B3LYP and ω B97XD relative energies with the same 6-311G(d,p) basis set may disagree by up to ~3 kcal/mol but with the single-point energy refinement using the higher-level G3(MP2,CC) approach, the difference practically disappears.

The Rice-Ramsperger-Kassel-Marcus Master Equation (RRKM-ME) theoretical approach was employed to compute phenomenological temperature- and pressure-dependent rate constants by solving the one-dimensional master equation using the MESS program package.^{50,51} Densities of

states for local minima and numbers of states for transition states and partition functions were assessed within the Rigid-Rotor, Harmonic-Oscillator (RRHO) approximation. For rate-controlling entrance transition states of acetylene addition to 1- and 2-methylnaphthyl radicals, low-frequency normal modes corresponding to internal rotations were treated as one-dimensional hindered rotors, where the one-dimensional torsional potentials were evaluated by scanning PESs at the B3LYP/6-311G(d,p) level of theory. Asymmetric Eckart potentials were used to compute tunneling corrections for the rate constants. We employed collision parameters used by us earlier for RRKM-ME calculations on the $C_{13}H_{11}$ PES for the 1- and 2-naphthyl + C_3H_4 reactions^{52,53} and before that, for the prototype $C_7H_7 + C_2H_2$ reaction.⁵⁴ In particular, the Lennard-Jones parameters were taken as $(\epsilon/\text{cm}^{-1}, \sigma/\text{\AA}) = (390, 4.46)$ and the $\alpha(T) = \alpha_{300}(T/300 \text{ K})^n$ expression with $n = 0.62$ and $\alpha_{300} = 424 \text{ cm}^{-1}$ was used for the temperature dependence of the range parameter α for the deactivating wing of the energy transfer function. The input files for the MESS calculations, which include optimized Cartesian coordinates of all species involved, vibrational frequencies, and hindered rotor potentials, are given in Supporting Information. Note that for the 1-/2-methylnaphthyl + C_2H_2 reactions, the MESS input files are based on those published in our previous works on the 1- and 2-naphthyl + C_3H_4 reactions,^{52,53} with inclusion of additional structures accessed via acetylene addition to the $C_{11}H_9$ reactants.

3. RESULTS AND DISCUSSION

3.1. PES for the unimolecular reaction of 1-methylbiphenyl

The process of formation of a five-membered ring on an armchair edge of PAH is simulated here by considering the unimolecular isomerization and decomposition of the *ortho*-methylbiphenyl radical $C_{13}H_{11}$ consisting of two six-membered rings connected to each other by a C-C bond, with the methylene group attached to one of the six-membered rings in *ortho* position. As seen in Figure 1, the five-membered ring closure takes place via the formation of a C-C bond between the methylene group and the *ortho* C atom on the opposite six-membered ring via a transition state (ts1) lying 24.2 kcal/mol above 1-methylbiphenyl (**i1**). The distance between the carbons forming a bond in ts1 is 2.117 Å. The produced intermediate **i2** consisting of two six-membered rings connected by a newly formed five-membered ring lies 1.4 kcal/mol higher in energy than **i1**. The H loss from the CH group in the joint vertex of the five- and six-membered

rings in intermediate **i2** gives the products 9*H*-fluorene + H (**p1**) which lie 20.0 kcal/mol above **i1** via a barrier of 26.5 kcal/mol relative to the initial *ortho*-methylbiphenyl reactant.

3.2. Rate constants for the formation of fluorene

Calculated rate constants for the five-membered ring formation on the armchair edge of 1-methylbiphenyl are illustrated in Figure 2. Isomerization of **i1** to **i2** prevails at temperatures below 1000 K (30 Torr), 900 K (1 atm), 1375 K (10 atm), and 1650 K (100 atm), whereas the formation of 9*H*-fluorene + H (**p1**) takes over at higher temperatures. In fact, the formation of **p1** occurs very quickly above 1000 K, with the rate constant for the unimolecular decomposition reaction **i1** → 9*H*-fluorene + H exceeding 10^6 s^{-1} at 1000 K (1 atm) and 1125 K (0.03, 10, and 100 atm). If intermediate **i2** gets collisionally stabilized, its unimolecular reaction leads either back to **i1** or to dissociation to the same **p1** products. Thus, at relatively low temperatures, **i1** and **i2** may establish an equilibrium and eventually decompose to 9*H*-fluorene + H. The RKKM-ME calculations show that neither **i1** nor **i2** are stable above the temperatures of 1250, 1650, and 2000 K at the pressures of 0.03, 1, and 10 atm, respectively. However, at 100 atm, **i1** can survive in the entire considered 500-2500 K temperature range. In the meantime, the calculated rate constant for **i1** → 9*H*-fluorene + H at 100 atm is higher than 10^9 s^{-1} above 2000 K pointing at the lifetime of **i1** being on a nanosecond scale even at this highest pressure. The rate constant for the reverse 9*H*-fluorene (**p1**) + H → **i1** reaction is computed to be on the order of 10^{-12} - $10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at temperatures above 1000 K. Interestingly, one can notice that the curves representing the $k(\mathbf{p1} + \text{H} \rightarrow \mathbf{i1})$ rate constant computed at different pressures cross as the temperature varies (Fig. 2(b)). This behavior originates from the peculiarity of the PES. The addition of an H atom to 9*H*-fluorene first leads to the intermediate **i2**, which can consequently isomerize to **i1**, where **i1** and **i2** are nearly isoergic. Considering the total rate constant of the collisional stabilization of the two wells on the PES (Fig. 2(b)), $k(\mathbf{p1} + \text{H} \rightarrow \mathbf{i2}) + k(\mathbf{p1} + \text{H} \rightarrow \mathbf{i1})$, one can see that it grows with pressure, as can be anticipated since a higher pressure increases the collision frequency of a complex formed in the bimolecular **p1** + H reaction with bath gas molecules and thus facilitates its deactivation. The rate constant increase with pressure becomes more and more apparent as the temperature rises and the re-dissociation rate of the complex back to **p1** + H, if it is not collisionally deactivated, grows. Similar behavior is also observed for the formation rate constant of the initial complex **i2**, $k(\mathbf{p1} + \text{H} \rightarrow \mathbf{i2})$. However, since **i1** is formed by isomerization of **i2** when the latter cannot be collisionally

stabilized, the dependence of $k(\mathbf{p1} + \text{H} \rightarrow \mathbf{i1})$ on pressure is more complex. At low temperatures, when the formation of $\mathbf{i2}$ prevails, $k(\mathbf{p1} + \text{H} \rightarrow \mathbf{i1})$ decreases with pressure. However, at higher temperatures when the $\mathbf{i2} \rightarrow \mathbf{i1}$ isomerization is fast, $k(\mathbf{p1} + \text{H} \rightarrow \mathbf{i1})$ grows with pressure. This results in the observed curve crossings for this rate constant.

In summary, the presence of a methylaryl radical on a PAH armchair edge is predicted to result in a rapid five-membered ring closure turning this edge into a zigzag. In the reverse direction, the addition of an H atom to a five-membered ring can lead back to a methylaryl radical.

3.3. PES of the 1-methylnaphthyl + C₂H₂ reaction

Now we address the addition of acetylene to the 1-methylnaphthyl radical (1-C₁₁H₉) accessing another region of the C₁₃H₁₁ PES, which is illustrated in Figure 3. This radical is a prototype of methylaryl with the CH₂ group on a zigzag edge of PAH. Note that this region of the surface was investigated in detail in our previous work on the 1-naphthyl + C₃H₄ reaction.⁵³ We keep the same notation for the C₁₃H₁₁ isomers, which were covered in the previous publication and the newly found intermediates of the 1-methylnaphthyl + C₂H₂ reaction are designated as **1mn-ix**. Also, only new transition states located in the present work are denoted as 1tsx in Fig. 3. The reaction begins with the addition of acetylene to the carbon of the methylene group of 1-methylnaphthyl with the formation of the intermediate **1mn-i1** (14.6 kcal/mol below the reactants) through 1ts1, which is 9.8 kcal/mol higher in energy than 1-C₁₁H₉ + C₂H₂ (Fig. 3). Then, **1mn-i1** can immediately lose a hydrogen atom from the β -position in the out-of-ring group through the barrier of 21.8 kcal/mol above the initial reactants and form products **1p6** (1-(prop-2-ynyl)naphthalene) + H. The products **1p6** + H lie 19.0 kcal/mol higher in energy than the initial reactants.

Alternative reaction pathways from **1mn-i1** include the formation of a new five- or six-membered ring. The pathway denoted in red in Fig. 3 is energetically favorable. The intermediate **1mn-i1** can undergo the out-of-ring (-CH₂CHCH) group ring closure on the zigzag edge through the transition state 1ts4 (6.6 kcal/mol below the reactants), which leads to the formation of a new six-membered ring in the **1mn-i2** isomer (42.9 kcal/mol below the reactants) having two common edges with each of the two six-membered rings of the naphthalene moiety. Then, a hydrogen atom sitting in the common vertex of two six-membered rings in **1mn-i2** can fly off via 1ts6 (15.0 kcal/mol below the reactants) forming products **1p1** (phenalene) + H lying 19.8 kcal/mol lower in energy than 1-C₁₁H₉ + C₂H₂. The intermediate **1mn-i2** can also produce **i14** (46.6 below the

reactants) by shifting the hydrogen atom located in the common vertex of two six-membered rings onto the neighboring C atom in the newly formed ring through a barrier at 1ts7 (7.3 kcal/mol below the reactants) and then form the **1p1** + H products by H elimination from one of the two CH₂ groups in the new ring through a transition state residing 15.3 kcal/mol lower in energy than the initial reactants.

The intermediate **1mn-i1** can also undergo the side chain ring closure toward the edge corner (see the pathways shown in blue in Fig. 3) through a barrier at 1ts5 (2.1 kcal/mol below the reactants) leading to **1mn-i3** (32.9 kcal/mol below the 1-C₁₁H₉ + C₂H₂ reactants), which has a new five-membered ring sharing one edge with the six-membered ring. The isomer **1mn-i3** can then form the products **p3** (1*H*-cyclopenta(a)naphthalene) + H (15.6 kcal/mol below the reactants) through a transition state 1ts8 that is located 9.9 kcal/mol below the reactants, losing the hydrogen atom located on the carbon in the vertex shared by the five- and six-membered rings. This H loss can also be fulfilled along the two-step pathway: **1mn-i3** → **i12** (45.3 kcal/mol below the reactants) → **p3** + H through a hydrogen migration (1ts9, 3.0 kcal/mol below the reactants) and its further detachment via a transition state located 11.5 kcal/mol below 1-C₁₁H₉ + C₂H₂. Interestingly, **i12** can dissociate not only to 1*H*-cyclopenta(a)naphthalene (**p3**) but to 3*H*-cyclopenta(a)naphthalene (**p2**) as well, via a transition state also residing 11.5 kcal/mol below the reactants; the formation of both **p3** and **p2** from **i12** should be competitive.

The intermediate **i10** (16.1 kcal/mol below the reactants) can form from **1mn-i1** through a transition state lying 29.5 kcal/mol higher in energy than 1-C₁₁H₉ + C₂H₂, by shifting the hydrogen atom from β - to γ -position in the out-of-ring chain. The intermediate **1mn-i1** can rearrange to **i11** (11.0 kcal/mol below the reactants) by the migration of a hydrogen atom from position 2 in the naphthalene moiety in the six-membered ring linked to the out-of-ring group to the γ -position of the side chain through a barrier at 1ts11 (1.9 kcal/mol below the reactants). **1mn-i1** can also isomerize to **i13** (11.7 kcal/mol below the reactants) by migration of a hydrogen atom sitting on the carbon in position 1 of the six-membered ring in the naphthalene moiety, which is not linked to the out-of-ring group, to the γ -position of the side chain via 1ts12, 0.9 kcal/mol above the reactants). Finally, **1mn-i1** can form **i15** (43.1 kcal/mol below the reactants) through a transition state 1ts10 lying 20.0 kcal/mol higher in energy than the initial reactants, through a 1,3-H shift from the α -position of the out-of-ring group to the γ -position. The subsequent reaction pathways from **i10**, **i11**, **i13**, and **i15** along with the other pathways in this region of the C₁₃H₁₁ PES were

described in detail earlier.⁵³ By comparing the competing channels, we can conclude that most likely, $1\text{-C}_{11}\text{H}_9 + \text{C}_2\text{H}_2 \rightarrow \mathbf{1mn-i1} \rightarrow \mathbf{1mn-i2} \rightarrow \mathbf{1p1} + \text{H}$ (red) and $1\text{-C}_{11}\text{H}_9 + \text{C}_2\text{H}_2 \rightarrow \mathbf{1mn-i1} \rightarrow \mathbf{1mn-i3} \rightarrow \mathbf{p3} + \text{H}$ (blue) should be expected to provide largest contributions in the overall product yield.

3.4. PES of the 2-methylnaphthyl + C₂H₂ reaction

The reaction of 2-methylnaphthyl (2-C₁₁H₉) with C₂H₂ emulates acetylene addition to methylaryl with the methylene group on a corner of a PAH edge. The mechanism of 2-C₁₁H₉ + C₂H₂ appears to be rather similar to that for 1-C₁₁H₉ + C₂H₂ described in the previous section but some details and, in particular, the expected prevailing products differ. The pertinent region of the C₁₃H₉ PES is shown in Figure 4. This region overlaps with the one studied earlier in detail for the 2-naphthyl + C₃H₄ reaction.⁵² As for 1-C₁₁H₉ + C₂H₂, in Fig. 4 we maintain the notation for the C₁₃H₁₁ isomers from the previous publication and designate the newly found intermediates of the 2-methylnaphthyl + C₂H₂ reaction as **2mn-ix**, with the new transition states denoted as 2tsx. The reaction begins with the C₂H₂ addition to the -CH₂ carbon of 2-C₁₁H₉ with the formation of the intermediate **2mn-i1** (14.6 kcal/mol below the reactants) across the barrier at 2ts1 lying 10.1 kcal/mol higher in energy than 2-C₁₁H₉ + C₂H₂ (Fig. 4). The intermediate **2mn-i1** can rearrange to a variety of different isomers through H migrations and five-membered ring closures and form products via a hydrogen atom elimination. The most energetically favorable pathway (shown in red in Fig. 4) involves the formation of **2mn-i2** (37.5 kcal/mol below the initial reactants) through a closure of the -CH₂CHCH side chain to a new five-membered ring via a transition state 2ts4 lying 4.1 kcal/mol below the reactants. Then, intermediate **2mn-i2** can lose a hydrogen atom located on the carbon in the common vertex of the five- and six-membered rings producing 3H-cyclopenta(a)naphthalene (**p2**) + H (15.0 kcal/mol below 2-C₁₁H₉ + C₂H₂) through a transition state 2ts6 lying 10.5 kcal/mol lower in energy than the reactants. The formation of **p2** + H from the isomer **2mn-i2** can also occur through the intermediate **i18** (44.7 kcal/mol below the reactants) obtained by the hydrogen shift from the carbon in the common vertex of the five- and six-membered rings to the neighboring carbon of the five-membered ring through the barrier at 2ts7 that lies 2.0 kcal/mol lower in energy than the initial reactants. This is followed by the loss of this hydrogen via a transition state located 11.0 kcal/mol below the reactants. A nearly isoergic

transition state connects **i18** with the 1*H*-cyclopenta(a)naphthalene (**p3**) + H products, which makes the formation of **p2** and **p3** from **i18** competitive.

The intermediate **2mn-i1** can also isomerize to **2mn-i3** (32.0 kcal/mol below the reactants) through a transition state 2ts5 that is 3.8 kcal/mol lower in energy than the reactants. The intermediate **2mn-i3** can lead to the products 1*H*-cyclopenta(b)naphthalene + H (15.3 kcal/mol below the reactants) either directly through the loss of a hydrogen atom sitting on the carbon in the common vertex of the six- and five-membered rings (2ts8, 9.3 kcal/mol below 2-C₁₁H₉ + C₂H₂ – see the pathway shown in blue in Fig. 4), or through the migration of this hydrogen atom from to the newly formed five-membered ring (2ts9, 1.1 kcal/mol below the reactants) and further loss of one of four hydrogens from the symmetric CH₂ groups in the five-membered ring via a transition state residing 10.9 kcal/mol below the reactants. The intermediate **2mn-i1** can directly decompose to the products 2-(prop-2-ynyl)naphthalene (**2p6**) + H (19.0 kcal/mol higher in energy than the reactants) through a transition state 2ts2 that lies 21.8 kcal/mol above 2-C₁₁H₉ + C₂H₂. There are also four possible alternative pathways where intermediates **i9**, **i14**, **i15**, and **i16** can be formed from the isomer **2mn-i1**. The intermediate **i9** (44.4 kcal/mol below the reactants) can be obtained by the migration of a hydrogen atom from the α - to γ -position in the out-of-ring group (2ts10, 19.7 kcal/mol above the reactants). The formation of isomer **i14** (15.3 kcal/mol below the reactants) occurs through a transition state 2ts3 lying 29.6 kcal/mol higher in energy than the initial reactants through a shift of a hydrogen atom from the β - to γ -position in the out-of-ring group. The isomer **i15** (10.7 kcal/mol below the reactants) is formed through the migration of a hydrogen atom from the position 3 of the six-membered ring in the naphthalene moiety linked to the out-of-ring chain to the γ -position in this chain (2ts11, 0.9 kcal/mol below 2-C₁₁H₉ + C₂H₂). At last, the intermediate **2mn-i1** can isomerize to the intermediate **i16** (10.2 kcal/mol below the reactants) through the migration of the hydrogen sitting in position 1 of the same six-membered ring to the γ -position in the side chain (2ts12, 1.9 kcal/mol below the reactants). The reaction pathways involving **i9**, **i14**, **i15**, and **i16** and the related pathways were described earlier in our work on the 2-naphthyl + C₃H₄ reaction.⁵² Summarizing, we anticipate that the two most favorable competing pathways, 2-C₁₁H₉ + C₂H₂ → **2mn-i1** → **2mn-i2** → **p2** + H (red) and 2-C₁₁H₉ + C₂H₂ → **2mn-i1** → **2mn-i3** → **2p1** + H (blue), should govern the reaction outcome.

3.5. Kinetics of the methylaryl + C₂H₂ reactions

The total rate constant for the 1-C₁₁H₉ (1-methylnaphthyl) + C₂H₂ reaction computed in the high-pressure limit (HP) and at finite pressures is illustrated in Figure 5(a). The total rate constant at finite pressures considered in the present study does not depend on pressure and the values obtained at 0.03, 1, 10, and 100 atm merge into one line. The HP total rate constant shows a typical Arrhenius behavior increasing from 2.3×10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 500 K to 9.5×10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 2500 K. The finite pressure rate constants nearly coincide with the HP values up to ~1000 K and begin to show a fall-off behavior at higher temperatures. For instance, at 1200 K, the computed values at 0.03, 1, 10, and 100 atm are ~30% lower than the HP limit rate constant and the difference increases to ~50% at 1500 K and to a factor of 4.3 at 2500 K. Figure 5(b) shows the rate constants calculated for the prevailing individual channels of the 1-C₁₁H₉ + C₂H₂ reaction. Phenalene (**1p1**) + H is predicted to be the main bimolecular product and its relative yield decreases from 77% to 27% in the 1000-2500 K temperature range at 0.03 atm, from 70% to 27% in the 1200-2500 K temperature range at 1 atm, from 64% to 27% at 10 atm (1400-2500 K), and from 52% to 27% at 100 atm (1700-2500 K) (see Table S1 in Supporting Information). Below the aforementioned temperature intervals, the branching ratio of **1p1** grows as the yield of collisionally stabilized intermediates, mostly **1mn-i1** and **1mn-i2**, drops. 1*H*-cyclopenta(a)naphthalene (**p3**) + H is the second noticeable bimolecular product. For example, at 1 atm, the relative yield of **p3** + H is calculated to be in the 15-24% range reaching maximal values at 1600-1700 K. Alternatively, 3*H*-cyclopenta(a)naphthalene (**p2**) + H is only a minor product with the branching ratio not exceeding ~6%. The product yield to **1p6** (1-(prop-2-ynyl)naphthalene) + H is controlled by a barrier of 36.4 kcal/mol for its formation from the intermediate **1mn-i1**. This product is favored by the entropic factor and the rate constant demonstrates a fast increase with temperature, with the relative yield of **1p6** reaching ~37% at the highest considered temperature of 2500 K and exceeds that of **1p1**. Nevertheless, at typical sooting temperatures (1400-1800 K), the dominant reaction outcome is the formation of phenalene (**1p1**) and 1*H*-cyclopenta(a)naphthalene (**p3**) with the rate constants on the order of 10⁻¹⁴ cm³ molecule⁻¹ s⁻¹.

Figure 6(a) demonstrates the total rate constant for the 2-C₁₁H₉ (2-methylnaphthyl) + C₂H₂ reaction computed in the HP limit and at finite pressures. The finite-pressure total rate constant slightly depends on pressure in the 900-1400 K temperature range and merges into one line at 500-900 K and 1400-2500 K for all considered pressures of 0.03, 1, 10, and 100 atm. The HP limit rate constant is Arrhenius-like and grows from 5.2×10⁻¹⁷ to 3.0×10⁻¹² cm³ molecule⁻¹ s⁻¹ in the 500-

2500 K temperature interval. The fall-off behavior is moderate and similar to the one seen for the $1\text{-C}_{11}\text{H}_9 + \text{C}_2\text{H}_2$ rate constant; for instance, at 900 K the computed values of the finite-pressure rate constant are 5-11% lower than the HP limit value, with the difference increasing to 58-59% at 1500 K and to 77% at 2500 K. The individual channel rate constants for $2\text{-C}_{11}\text{H}_9 + \text{C}_2\text{H}_2$ are illustrated in Fig. 6(b), whereas the product branching ratios are presented in Table S2 in Supporting Information. The main bimolecular products are $1H$ -cyclopenta(b)naphthalene + H (**2p1**) and $3H$ -cyclopenta(a)naphthalene + H (**p2**). At low temperatures, collisional stabilization of intermediates **2mn-i1**, **2mn-i2**, and **2mn-i3** plays the leading role in the reaction but above 1000 K (or higher, 1200 and 1400 K at 10 and 100 atm, respectively) the well-skipping channels to bimolecular products take over. In this high-temperature regime, the relative yields of the **2p1** and **p2** products are close to each other, 37% and 42%, respectively, at 1000 K and 1 atm, and decrease with temperature, to 14-15% each at 2500 K. There is also a minor contribution of the $1H$ -cyclopenta(a)naphthalene + H (**p3**) + H products, which does not exceed ~6%. This decrease in the yield of **2p1** and **p2** with temperature occurs due to the growth of the branching ratio of the entropically favorable 2-(prop-2-ynyl)naphthalene (**2p6**) + H product to as much as 57% at 2500 K. Nevertheless, in the sooting temperature range of 1400-1800 K, the formation of the three cyclopentanaphthalene isomers dominates the reaction with their overall yield being 92-75% at 1 atm.

Figure 7 compares rate constants for three reactions of the same type, benzyl + C_2H_2 , 1-methylnaphthyl + C_2H_2 and 2-methylnaphthyl + C_2H_2 . Here, we included only the channels leading to the PAH growth, i.e., the formation of indene for benzyl + C_2H_2 and the formation of three-ring PAHs, phenalene and cyclopentanaphthalene isomers, for 1-/2-methylnaphthyl + C_2H_2 . One can see that the rate constants for the benzyl + C_2H_2 and 1-methylnaphthyl + C_2H_2 reactions are similar, with a maximal difference of a factor of 1.56 in favor of the latter at 2500 K. The rate constant for 2-methylnaphthyl + C_2H_2 is calculated to be somewhat higher, by factors of 2.2-3.8 as compared to benzyl + C_2H_2 and, nearly uniformly in the entire 500-2500 K range, by factors of 2.2-2.8 (2.2-2.3 at 1400-1800 K) as compared to 1-methylnaphthyl + C_2H_2 . The difference in the 2-methylnaphthyl + C_2H_2 rate constant from that for 1-methylnaphthyl + C_2H_2 is attributed to a more flexible entrance transition state for the former, i.e., lower first few low vibrational frequencies in this transition state, with the reaction barriers being nearly identical. It is also informative to compare the rate constants for 1-/2-methylnaphthyl + C_2H_2 encompassing the

formation of all three-ring PAHs with those for 1-/2-naphthyl + C₃H₄ leading to the same products. The values at 1500 K and 1 atm in cm³ molecule⁻¹ s⁻¹ are 4.5×10⁻¹⁴ (1-methylnaphthyl + C₂H₂), 1.1×10⁻¹³ (2-methylnaphthyl + C₂H₂), 1.8×10⁻¹²/1.2×10⁻¹³ (1-naphthyl + allene/propyne),⁵³ and 9.9×10⁻¹³/3.7×10⁻¹⁴ (2-naphthyl + allene/propyne).⁵² Thus, the formation of the three-ring PAHs is about an order magnitude faster in the naphthyl + allene reactions but comparable in the naphthyl + propyne reactions. Both naphthyl + allene/propyne reactions were calculated to be significantly faster overall as compared to methylnaphthyl + C₂H₂ due to much lower entrance reaction barriers of only 1.2-3.3 kcal/mol.^{52,53} However, the low relative yield of the three-ring PAHs in naphthyl + propyne reactions is reflected in the rate constant for the formation of three-ring PAHs being close for those for methylnaphthyl + C₂H₂. Also, the rate constants for the 1-/2-methylnaphthyl + C₂H₂ reactions are more than or about an order of magnitude lower than the rate constants for C₂H₂ addition to σ PAH radicals, such as those for 1-naphthyl + C₂H₂ → acenaphthylene + H (2.2×10⁻¹² cm³ molecule⁻¹ s⁻¹ at 1500 K and 1 atm) forming an extra five-membered ring on a zigzag PAH edge and for 4-phenanthrenyl + C₂H₂ → pyrene + H (8.9×10⁻¹³ cm³ molecule⁻¹ s⁻¹) producing an additional six-membered ring on an armchair edge.²² Therefore, although the methylaryl + C₂H₂ reactions should predominantly form PAH products with an extra five-membered ring, they are relatively slow as compared to regular C₂H₂ additions in the HACA sequences and hence their overall contribution to the PAH growth at various conditions still needs to be assessed by kinetic modeling.

4. CONCLUSIONS

We explored the regions of the C₁₃H₁₁ PES related to the unimolecular isomerization and decomposition of the 1-methylbiphenylyl radical to 9*H*-fluorene + H and accessed by the 1-/2-methylnaphthyl + C₂H₂ reactions, which predominantly form the three-ring PAHs phenalene and cyclopentanaphthalene isomers under high-temperature conditions, including those occurring in combustion flames and in circumstellar envelopes. The unimolecular reaction of 1-methylbiphenylyl proceeding via a five-membered ring closure followed by H elimination is predicted to be very fast, on a sub-microsecond scale above 1000 K. The reaction results in the formation of an embedded five-membered ring. This reaction is a prototype for the formation of an embedded five-membered ring from a methylaryl radical on an armchair PAH edge. However, the calculated rate constant for 1-methylbiphenylyl → 9*H*-fluorene + H is likely somewhat higher

than those for armchair edge methylaryl radicals because of the high flexibility of the biphenyl moiety. The 1-/2-methylnaphthyl + C₂H₂ reactions proceed by the mechanism involving acetylene addition to the radical on the methylene group followed by a six- or five-membered ring closure and aromatization via an H atom loss. Despite of the complexity of the C₁₃H₉ PES, these straightforward pathways are dominant in the high-temperature regime (above ~1000 K). The prevailing products are phenalene, with a significant contribution of 1*H*-cyclopenta(a)naphthalene, for 1-methylnaphthyl + C₂H₂, and nearly equally 1*H*-cyclopenta(b)naphthalene and 3*H*-cyclopenta(a)naphthalene for 2-methylnaphthyl + C₂H₂. Although the methylnaphthyl reactions with acetylene represent a rather clean source of these three-ring PAHs, they are relatively slow owing to the high entrance barriers of ~10 kcal/mol, with the rate constants being about an order of magnitude lower as compared to those for naphthyl + allene and σ -aryl + C₂H₂. The 1-methylnaphthyl + C₂H₂ and 2-methylnaphthyl + C₂H₂ reactions represent prototypes for PAH growth by an extra six- and five-membered ring on a zigzag edge of PAH or a PAH corner and therefore the modified Arrhenius expressions generated here for these reactions (Table 1) are recommended for kinetic modeling of PAH growth via the mechanism of acetylene addition to methylaryl radicals.

Supporting Information Available

Calculated product branching ratios for the 1-methylnaphthyl + C₂H₂ (Table S1) and 2-methylnaphthyl + C₂H₂ (Table S2) reactions at various temperatures and pressures; input files for RRKM-ME calculations using the MESS code containing optimized Cartesian coordinates, vibrational frequencies, and relative energies for all reactants, products, intermediates, and transition states of the considered reactions. The Supporting Information is available free of charge on the ACS Publications website at DOI: .

Conflicts of interest

There are no conflicts to declare.

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Table 1. Parameters of fitted modified Arrhenius expressions $k = A T^n \exp(-E_a/RT)$ or $k = A_1 T^{n_1} \exp(-E_{a1}/RT) + A_2 T^{n_2} \exp(-E_{a2}/RT)$ for the considered reactions. Pre-exponential factors A are in $\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$ for bimolecular reactions and in s^{-1} for unimolecular reactions, E_a are in cal mol^{-1} .

Reaction	p , atm	A	n	E_a	T range, K
1-methyl-biphenyl → 9H-fluorene + H	PLOG/3.000E-02	5.43E+57	-13.74	48326	500-1250
	PLOG/1.000E+00	1.01E+57	-13.015	54320	500-1650
	PLOG/1.000E+00	1.32E+73	-16.502	91770	
	PLOG/1.000E+01	8.52E+140	-37.427	105710	500-2000
	PLOG/1.000E+01	1.02E+33	-5.7346	46629	
	PLOG/1.000E+02	8.21E+30	-4.9893	49026	500-2500
9H-fluorene + H → 1-methyl-biphenyl	PLOG/3.000E-02	9.05E+55	-12.74	27480	500-1250
	PLOG/1.000E+00	6.85E+55	-12.203	33714	500-1650
	PLOG/1.000E+00	7.35E+72	-16.006	70170	
	PLOG/1.000E+01	2.37E+148	-39.167	89532	500-2000
	PLOG/1.000E+01	7.39E+31	-4.9239	26079	
	PLOG/1.000E+02	1.84E+29	-4.0346	28185	500-2500
1-methyl-naphthyl + C ₂ H ₂ → 1p1 + H	PLOG/3.000E-02	2.44E+24	-3.6178	18089	500-2500
	PLOG/3.000E-02	2.35E-48	16.403	-12795	
	PLOG/1.000E+00	3.15E+44	-9.3026	32646	500-2500
	PLOG/1.000E+00	6.36E+11	-0.02620	15098	
	PLOG/1.000E+01	1.62E+51	-11.008	41363	500-2500
	PLOG/1.000E+01	3.67E+09	0.64162	16758	
	PLOG/1.000E+02	7.53E+49	-10.369	47554	500-2500
	PLOG/1.000E+02	1.75E+04	2.0406	16968	
1p1 + H → 1-methyl-naphthyl + C ₂ H ₂	PLOG/3.000E-02	9.95E+31	-4.7291	40033	500-2500
	PLOG/3.000E-02	8.07E+20	-2.4038	32104	
	PLOG/1.000E+00	5.00E+42	-7.6548	49396	500-2500
	PLOG/1.000E+00	1.56E+98	-27.892	53883	
	PLOG/1.000E+01	2.64E+58	-12.002	63064	500-2500
	PLOG/1.000E+01	2.32E+15	0.021044	37565	
	PLOG/1.000E+02	4.13E+57	-11.519	69517	500-2500
	PLOG/1.000E+02	1.06E+10	1.4293	37782	
1-methyl-naphthyl + C ₂ H ₂ → p3 + H	PLOG/3.000E-02	2.55E+29	-5.1225	24741	500-2500
	PLOG/3.000E-02	2.94E+16	-1.4803	15356	
	PLOG/1.000E+00	3.42E+23	-3.3329	21553	600-2500
	PLOG/1.000E+01	2.17E+37	-7.1249	33258	500-2500
	PLOG/1.000E+01	9.60E+46	-12.172	25761	
	PLOG/1.000E+02	1.14E+48	-9.9678	45917	500-2500
	PLOG/1.000E+02	5.70E+02	2.4834	17644	
p3 + H → 1-methyl-naphthyl + C ₂ H ₂	PLOG/3.000E-02	6.89E+34	-5.6314	40587	500-2500
	PLOG/3.000E-02	1.07E+23	-2.411	31931	
	PLOG/1.000E+00	3.33E+30	-4.3233	38559	600-2500
	PLOG/1.000E+00	1.43E+52	-10.39	54737	500-2500

	PLOG/1.000E+01	8.01E+13	0.3576	33702	
	PLOG/1.000E+01	9.40E+55	-11.218	63534	500-2500
	PLOG/1.000E+02	9.95E+08	1.6914	34257	
1-methyl-naphthyl + C ₂ H ₂ → p ₂ + H	PLOG/3.000E-02	5.20E+22	-3.247	21840	500-2500
	PLOG/1.000E+00	1.46E+50	-10.953	42356	500-2500
	PLOG/1.000E+00	2.90E+07	1.108	18302	
	PLOG/1.000E+01	1.94E+54	-11.898	50377	500-2500
	PLOG/1.000E+01	2.41E+08	0.88497	22190	
	PLOG/1.000E+02	5.68E+50	-10.632	55773	500-2500
	PLOG/1.000E+02	2.57E+00	3.028	22569	
p ₂ + H → 1-methyl-naphthyl + C ₂ H ₂	PLOG/3.000E-02	4.94E+29	-4.2405	38698	600-2500
	PLOG/1.000E+00	2.11E+57	-11.987	59426	500-2500
	PLOG/1.000E+00	3.50E+13	0.35522	34704	
	PLOG/1.000E+01	5.91E+61	-13.03	67583	500-2500
	PLOG/1.000E+01	3.83E+14	0.097083	38639	
	PLOG/1.000E+02	5.12E+58	-11.901	73256	500-2500
	PLOG/1.000E+02	3.23E+06	2.2751	38996	
1-methyl-naphthyl + C ₂ H ₂ → 1p ₆ + H	PLOG/3.000E-02	7.61E+18	-1.4795	37248	500-2500
	PLOG/3.000E-02	9.3462	3.2319	23827	
	PLOG/1.000E+00	2.67E+18	-1.3464	37059	500-2500
	PLOG/1.000E+00	95.579	2.9292	24418	
	PLOG/1.000E+01	9.59E+18	-1.4931	37719	500-2500
	PLOG/1.000E+01	1278.8	2.6301	25750	
	PLOG/1.000E+02	5.49E+21	-2.219	40864	500-2500
	PLOG/1.000E+02	2.9215	3.3692	25901	
p ₆ + H → 1-methyl-naphthyl + C ₂ H ₂	PLOG/3.000E-02	1.44E+25	-2.8313	18767	500-2500
	PLOG/3.000E-02	5.95E+06	2.0102	5099.1	
	PLOG/1.000E+00	5.17E+24	-2.7013	18585	500-2500
	PLOG/1.000E+00	6.02E+07	1.7091	5688.2	
	PLOG/1.000E+01	1.95E+25	-2.8542	19265	500-2500
	PLOG/1.000E+01	7.84E+08	1.4137	7017.7	
	PLOG/1.000E+02	1.18E+28	-3.5864	22436	500-2500
	PLOG/1.000E+02	1.67E+06	2.1644	7165.2	
2-methyl-naphthyl + C ₂ H ₂ → 2p ₁ + H	PLOG/3.000E-02	1.22E+66	-15.616	47153	500-2500
	PLOG/3.000E-02	2.23E+20	-2.4106	15846	
	PLOG/1.000E+00	4.10E+31	-5.5135	24794	500-2500
	PLOG/1.000E+00	3.68E+15	-5.5514	1813.1	
	PLOG/1.000E+01	1.56E+41	-8.0918	34425	500-2500
	PLOG/1.000E+01	1.15E+79	-22.737	33029	
	PLOG/1.000E+02	8.86E+47	-9.7929	45339	500-2500
	PLOG/1.000E+02	1.93E+04	2.125	17715	
2p ₁ + H → 2-methyl-naphthyl + C ₂ H ₂	PLOG/3.000E-02	5.35E+48	-9.6835	47341	500-2500
	PLOG/3.000E-02	1.49E+26	-3.1757	32089	
	PLOG/1.000E+00	8.39E+34	-5.5442	39444	600-2500
	PLOG/1.000E+01	7.76E+48	-9.3626	51837	500-2500

	PLOG/1.000E+01	3.51E+67	-17.658	45343	
	PLOG/1.000E+02	3.84E+55	-11.047	62709	500-2500
	PLOG/1.000E+02	1.16E+10	1.3851	33983	
2-methyl-naphthyl + C ₂ H ₂ → p2 + H	PLOG/3.000E-02	1.50E+29	-4.9329	20925	500-2500
	PLOG/3.000E-02	3.83E+00	3.0793	8429.5	
	PLOG/1.000E+00	1.78E+38	-7.3485	29990	500-2500
	PLOG/1.000E+00	7.95E+162	-50.838	50850	
	PLOG/1.000E+01	5.51E+55	-12.192	45091	500-2500
	PLOG/1.000E+01	6.67E+08	0.97599	18200	
	PLOG/1.000E+02	1.64E+51	-10.621	50099	500-2500
	PLOG/1.000E+02	2.60E+03	2.3422	18209	
p2 + H → 2-methyl-naphthyl + C ₂ H ₂	PLOG/3.000E-02	1.48E+36	-6.0144	37575	500-2500
	PLOG/3.000E-02	7.27E+08	1.5962	25225	
	PLOG/1.000E+00	6.72E+45	-8.6002	46953	500-2500
	PLOG/1.000E+00	6.10E+156	-47.557	64151	
	PLOG/1.000E+01	7.27E+62	-13.309	61812	500-2500
	PLOG/1.000E+01	3.72E+14	0.22959	34096	
	PLOG/1.000E+02	6.15E+58	-11.872	67047	500-2500
	PLOG/1.000E+02	1.45E+09	1.6	34117	
2-methyl-naphthyl + C ₂ H ₂ → p3 + H	PLOG/3.000E-02	1.78E+29	-5.0073	25060	500-2500
	PLOG/3.000E-02	3.89E+166	-53.608	47166	
	PLOG/1.000E+00	3.34E+41	-8.3255	36902	500-2500
	PLOG/1.000E+00	5.65E+48	-12.582	28370	
	PLOG/1.000E+01	9.44E+56	-12.548	51822	500-2500
	PLOG/1.000E+01	2.94E+08	0.98707	22884	
	PLOG/1.000E+02	5.47E+51	-10.765	57415	500-2500
	PLOG/1.000E+02	1.57E-01	3.4604	22655	
p3 + H → 2-methyl-naphthyl + C ₂ H ₂	PLOG/3.000E-02	4.36E+31	-4.7848	38909	600-2500
	PLOG/1.000E+00	8.09E+60	-13.006	60701	500-2500
	PLOG/1.000E+00	9.40E+16	-0.57335	36266	
	PLOG/1.000E+01	1.69E+64	-13.697	68747	500-2500
	PLOG/1.000E+01	1.86E+14	0.23155	38944	
	PLOG/1.000E+02	2.39E+59	-12.028	74556	500-2500
	PLOG/1.000E+02	7.93E+04	2.7378	38695	
2-methyl-naphthyl + C ₂ H ₂ → 2p6 + H	PLOG/3.000E-02	1.60E+27	-3.704	40491	500-2500
	PLOG/3.000E-02	1.24E+01	3.5343	23706	
	PLOG/1.000E+00	1.05E+26	-3.3491	40305	500-2500
	PLOG/1.000E+00	3.86E+02	3.112	24925	
	PLOG/1.000E+01	2.62E+25	-3.1341	40795	500-2500
	PLOG/1.000E+01	5.68E+02	3.0414	26022	
	PLOG/1.000E+02	1.93E+26	-3.2782	43862	500-2500
	PLOG/1.000E+02	1.01E+01	3.436	26303	
2p6 + H → 2-methyl-	PLOG/3.000E-02	3.98E+32	-5.0306	21900	500-2500
	PLOG/3.000E-02	1.32E+06	2.3069	4921.9	
	PLOG/1.000E+00	2.95E+31	-4.6907	21744	500-2500

naphthyl + C ₂ H ₂	PLOG/1.000E+00	4.16E+07	1.8831	6144.1	
	PLOG/1.000E+01	8.78E+30	-4.4977	22289	500-2500
	PLOG/1.000E+01	5.87E+07	1.8191	7236.5	
	PLOG/1.000E+02	5.32E+31	-4.6181	25302	500-2500
	PLOG/1.000E+02	1.32E+06	2.1788	7539.2	

Figure Captions

Figure 1. Potential energy diagram for unimolecular isomerization and decomposition of the *ortho*-methylbiphenyl radical. Relative energies calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.

Figure 2. Rate constants for the *ortho*-methylbiphenyl \rightarrow 9*H*-fluorene + H in the forward, **i1** \rightarrow **p1** + H (a) and reverse, **p1** + H \rightarrow **i1/i2**/total (b) directions calculated at different pressures.

Figure 3. Potential energy diagram for the 1-methylnaphthyl + C₂H₂ reaction. Relative energies calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.

Figure 4. Potential energy diagram for the 2-methylnaphthyl + C₂H₂ reaction. Relative energies calculated at the G3(MP2,CC)//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) level of theory are given in kcal/mol.

Figure 5. Rate constants for the 1-methylnaphthyl + C₂H₂ reaction: (a) the total rate constant at the high-pressure limit (HP) and at finite pressures; (b) rate constants for the prevailing individual well-skipping reaction channels. Dotted, solid, dashed and dash-dotted lines show rate constants calculated at 0.03, 1, 10, and 100 atm, respectively.

Figure 6. Rate constants for the 2-methylnaphthyl + C₂H₂ reaction: (a) the total rate constant at the high-pressure limit (HP) and at finite pressures; (b) rate constants for the prevailing individual well-skipping reaction channels. Dotted, solid, dashed and dash-dotted lines show rate constants calculated at 0.03, 1, 10, and 100 atm, respectively.

Figure 7. Comparison of rate constants of the reactions of benzyl and 1- and 2-naphthyl radicals with C₂H₂ for the channels leading to the PAH growth by an extra five-membered ring.

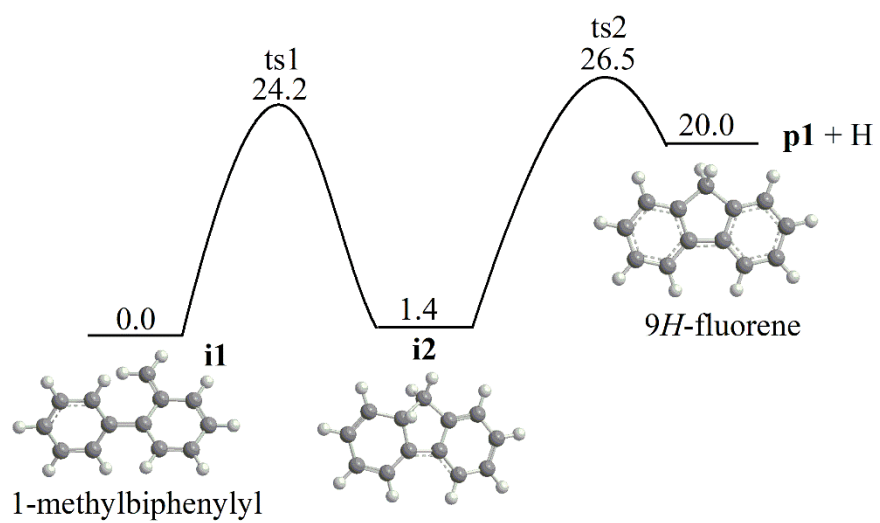


Figure 1

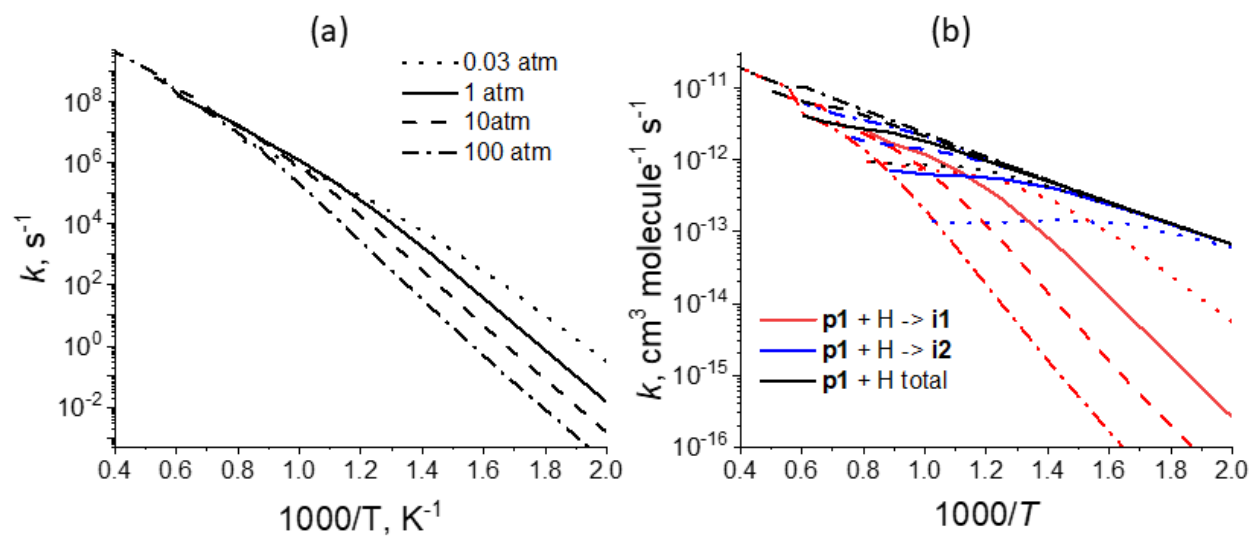


Figure 2

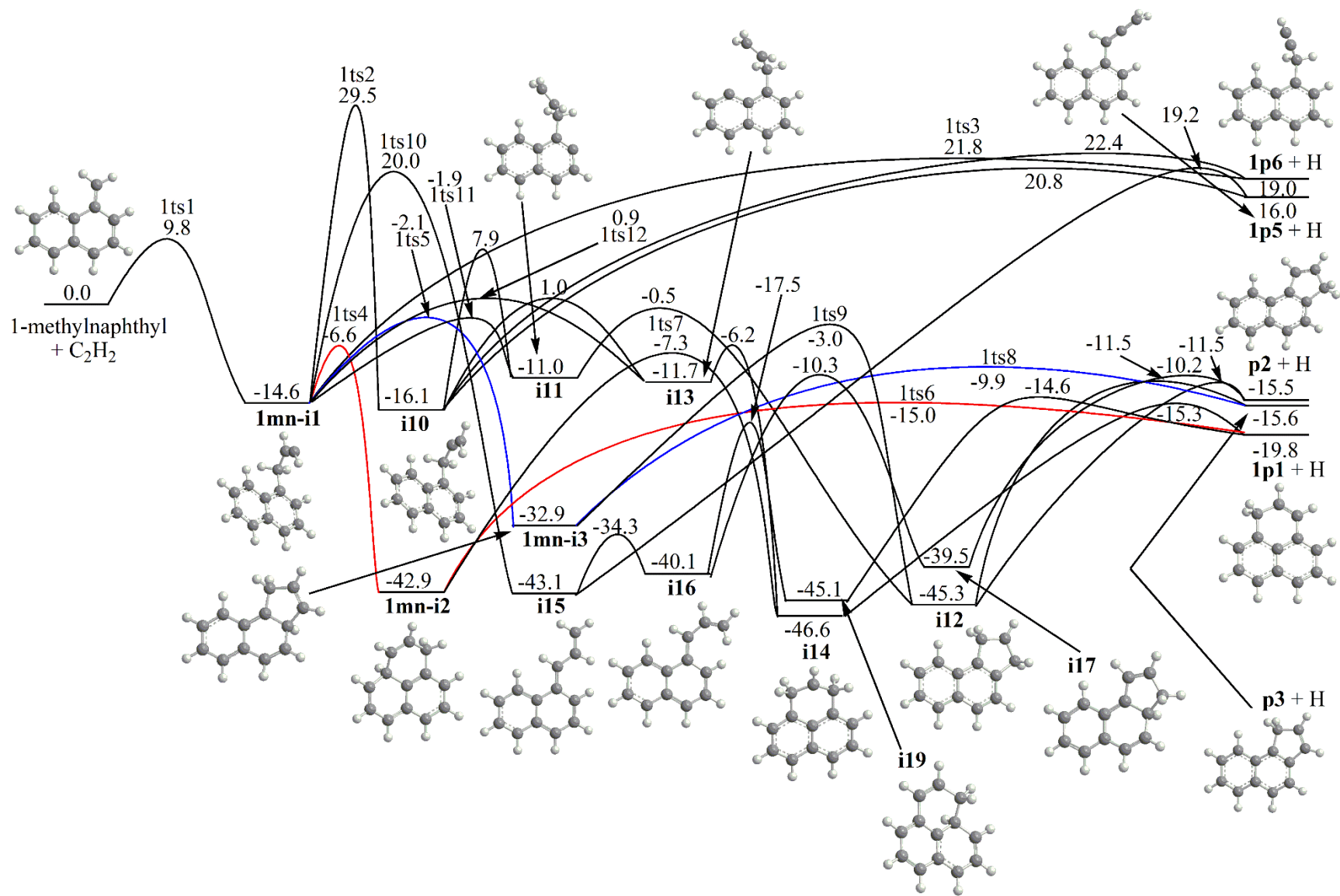


Figure 3

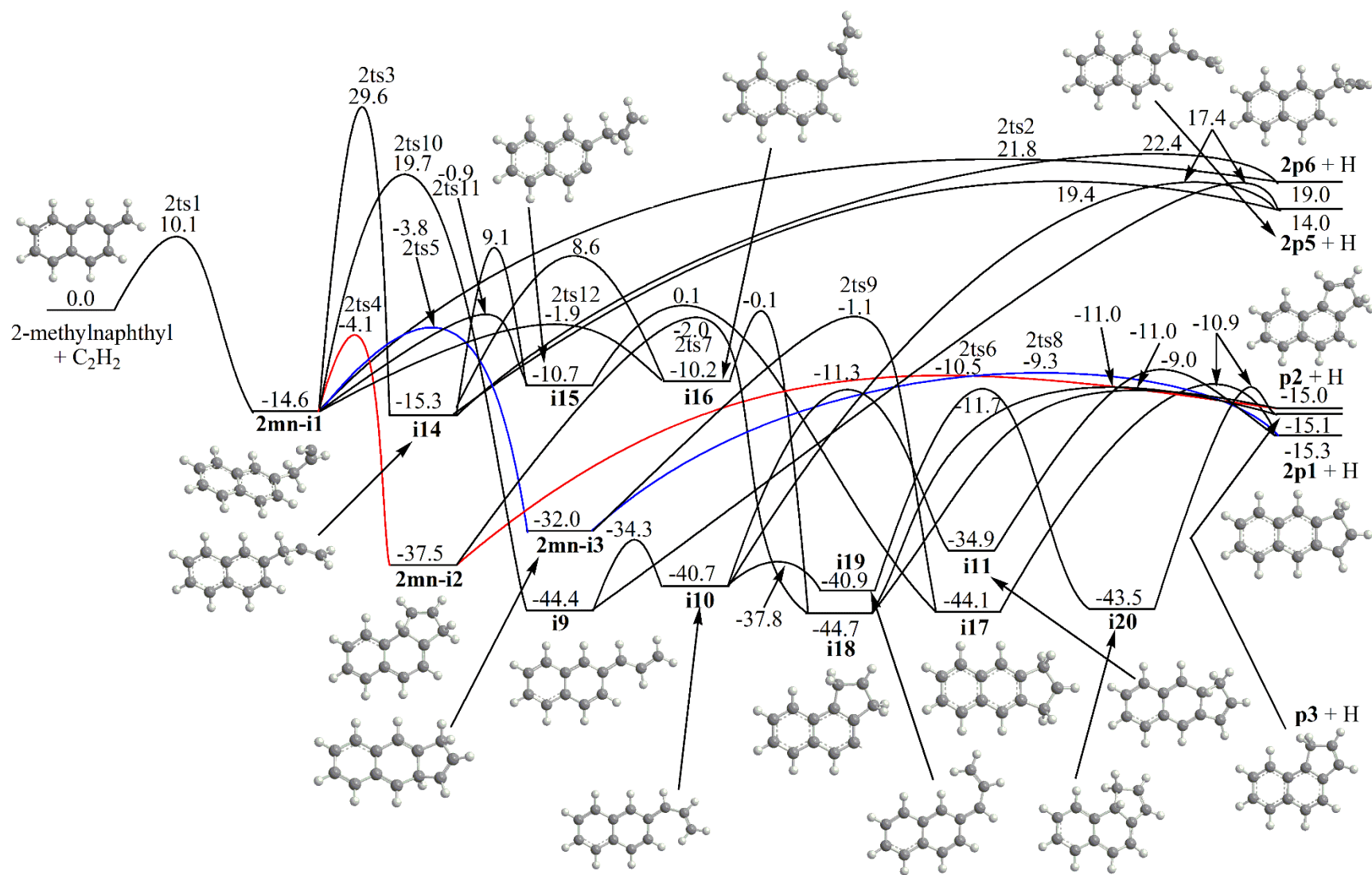


Figure 4

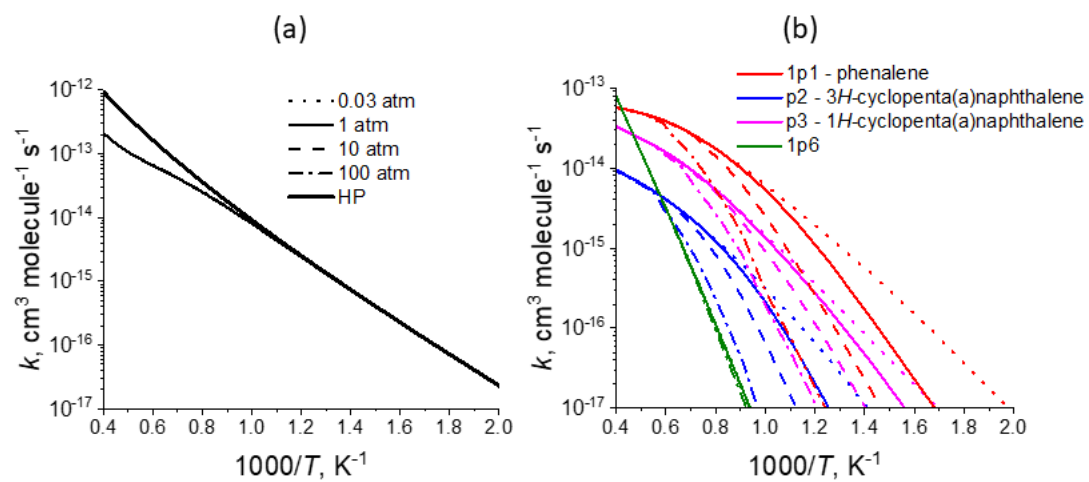


Figure 5

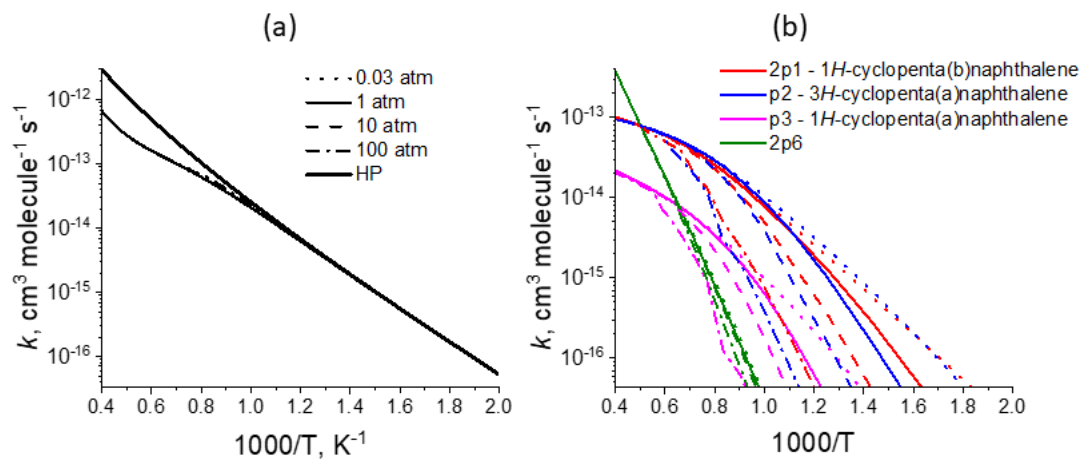


Figure 6

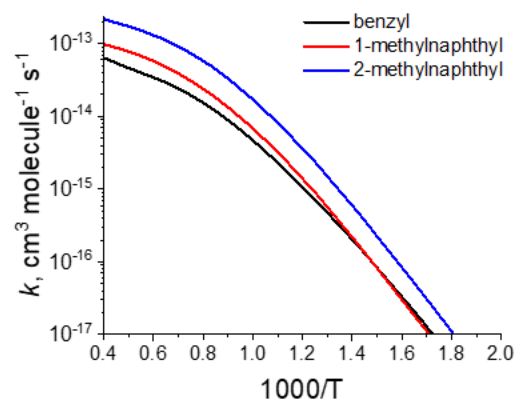


Figure 7

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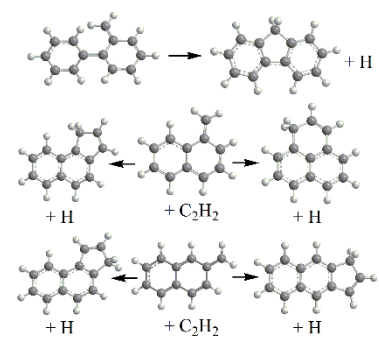
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TOC Graphic



Supporting Information

for

**The Role of Methylaryl Radicals in the Growth of Polycyclic Aromatic
Hydrocarbons: The Formation of Five-Membered Rings**

Galiya R. Galimova^{a,b}, Iakov A. Medvedkov^{b,c}, and Alexander M. Mebel^a

*^aDepartment of Chemistry and Biochemistry, Florida International University, Miami, FL 33199
(USA)*

*^bDepartment of Physics, Samara National Research University, Samara 443086
(Russian Federation)*

*^cLebedev Physical Institute, Samara 443011
(Russian Federation)*

Table S1. Calculated product branching ratios for the 1-methylnaphthyl + C₂H₂ reaction at various temperatures and pressures.

<i>p</i> = 0.03 atm								
T(K)	1mn-i1	1mn-i2	1mn-i3	C ₁₀ H ₇ +allene	1p1	p2	p3	1p6
500		52.39%	1.47%	0.00%	37.58%	0.11%	4.82%	0.00%
600		22.99%	0.46%	0.00%	63.93%	0.54%	8.16%	0.00%
700		6.69%	0.10%	0.00%	77.69%	1.42%	11.28%	0.00%
800		1.45%	0.02%	0.00%	80.43%	2.44%	14.11%	0.00%
900		0.28%		0.01%	78.91%	3.28%	16.47%	0.01%
1000				0.04%	76.50%	3.93%	18.38%	0.05%
1100				0.11%	73.94%	4.45%	19.94%	0.13%
1200				0.29%	71.46%	4.91%	21.22%	0.31%
1300				0.63%	68.95%	5.30%	22.23%	0.66%
1400				1.17%	66.30%	5.63%	22.99%	1.27%
1500				1.96%	63.50%	5.89%	23.49%	2.22%
1600				3.00%	60.31%	6.08%	23.70%	3.61%
1700				4.25%	56.87%	6.18%	23.63%	5.51%
1800				5.67%	53.19%	6.20%	23.27%	7.99%
1900				7.15%	49.31%	6.13%	22.64%	11.03%
2000				8.60%	45.33%	5.98%	21.77%	14.60%
2100				9.94%	41.31%	5.76%	20.68%	18.61%
2200				11.11%	37.35%	5.47%	19.44%	22.95%
2300				12.07%	33.54%	5.13%	18.09%	27.47%
2400				12.81%	29.95%	4.77%	16.70%	32.04%
2500				13.35%	26.62%	4.40%	15.31%	36.54%
<i>p</i> = 1 atm								
T(K)	1mn-i1	1mn-i2	1mn-i3	C ₁₀ H ₇ +allene	1p1	p2	p3	1p6
500	4.29%	83.88%	5.10%	0.00%	2.00%	0.00%	0.56%	0.00%
600		78.53%	5.55%	0.00%	7.81%	0.03%	2.39%	0.00%
700		60.74%	4.07%	0.00%	21.23%	0.17%	5.99%	0.00%
800		37.98%	2.09%	0.00%	40.35%	0.61%	10.16%	0.00%
900		18.82%	0.86%	0.01%	57.04%	1.51%	13.81%	0.01%
1000		7.84%	0.31%	0.03%	66.35%	2.67%	16.78%	0.04%
1100		2.98%		0.09%	69.53%	3.73%	19.19%	0.12%
1200				0.23%	70.49%	4.53%	20.82%	0.30%
1300				0.51%	68.22%	5.11%	22.02%	0.64%
1400				1.01%	65.82%	5.60%	22.94%	1.23%
1500				1.77%	62.99%	5.86%	23.43%	2.18%
1600				2.81%	59.92%	6.05%	23.65%	3.57%
1700				4.09%	56.59%	6.16%	23.60%	5.48%
1800				5.67%	53.20%	6.20%	23.27%	7.98%
1900				7.15%	49.32%	6.13%	22.64%	11.03%

2000				8.61%	45.33%	5.98%	21.77%	14.60%
2100				9.95%	41.31%	5.76%	20.68%	18.61%
2200				11.11%	37.36%	5.47%	19.44%	22.95%
2300				12.07%	33.55%	5.13%	18.09%	27.47%
2400				12.81%	29.95%	4.77%	16.70%	32.04%
2500				13.35%	26.62%	4.40%	15.31%	36.54%
<i>p</i> = 10 atm								
T(K)	1mn-i1	1mn-i2	1mn-i3	C₁₀H₇+allene	1p1	p2	p3	1p6
500	49.57%	43.05%	2.75%	0.00%	0.10%	0.00%	0.03%	0.00%
600	28.20%	58.69%	5.25%	0.00%	0.63%	0.00%	0.26%	0.00%
700	14.60%	65.11%	7.15%	0.00%	2.63%	0.01%	1.22%	0.00%
800		70.21%	7.76%	0.00%	8.09%	0.08%	3.66%	0.00%
900		55.60%	5.97%	0.01%	18.18%	0.30%	7.38%	0.01%
1000		38.88%	3.81%	0.02%	31.47%	0.82%	11.39%	0.04%
1100		24.09%	2.17%	0.08%	43.97%	1.70%	14.96%	0.12%
1200		13.68%		0.20%	53.06%	2.78%	18.99%	0.29%
1300		7.31%		0.45%	58.06%	3.82%	20.67%	0.62%
1400				0.87%	63.57%	4.66%	21.98%	1.20%
1500				1.52%	62.75%	5.28%	22.84%	2.12%
1600				2.45%	59.62%	5.99%	23.61%	3.49%
1700				3.64%	56.26%	6.09%	23.55%	5.38%
1800				5.05%	52.68%	6.11%	23.21%	7.86%
1900				6.58%	48.91%	6.05%	22.59%	10.91%
2000				8.12%	45.02%	5.90%	21.73%	14.50%
2100				9.98%	41.21%	5.70%	20.68%	18.61%
2200				11.14%	37.37%	5.47%	19.44%	22.95%
2300				12.10%	33.56%	5.14%	18.09%	27.47%
2400				12.83%	29.96%	4.78%	16.70%	32.04%
2500				13.36%	26.62%	4.40%	15.31%	36.54%
<i>p</i> = 100 atm								
T(K)	1mn-i1	1mn-i2	1mn-i3	C₁₀H₇+allene	1p1	p2	p3	1p6
500	91.18%	7.17%	0.47%	0.00%	0.00%	0.00%	0.00%	0.00%
600	81.49%	14.02%	1.36%	0.00%	0.02%	0.00%	0.01%	0.00%
700	68.50%	22.20%	2.94%	0.00%	0.11%	0.00%	0.06%	0.00%
800	54.57%	29.80%	4.88%	0.00%	0.49%	0.00%	0.31%	0.00%
900	41.72%	35.33%	6.55%	0.00%	1.57%	0.02%	1.03%	0.01%
1000	38.43%	38.47%	7.56%	0.01%	3.51%	0.06%	2.34%	0.03%
1100		56.10%	9.89%	0.04%	10.28%	0.27%	5.70%	0.09%
1200		45.28%	8.05%	0.13%	17.40%	0.64%	8.86%	0.24%
1300		34.52%	6.10%	0.32%	25.20%	1.24%	12.05%	0.55%
1400		25.23%	4.43%	0.75%	32.87%	2.05%	15.03%	1.13%
1500		17.62%		1.34%	38.75%	2.93%	20.32%	2.04%
1600		11.78%		2.17%	42.70%	3.75%	21.24%	3.39%

1700				3.22%	51.81%	4.43%	21.88%	5.27%
1800				4.47%	49.29%	5.94%	23.07%	7.72%
1900				5.86%	48.73%	5.95%	22.56%	10.76%
2000				7.29%	44.80%	5.80%	21.70%	14.34%
2100				8.69%	40.85%	5.57%	20.63%	18.38%
2200				9.97%	36.96%	5.29%	19.40%	22.75%
2300				11.09%	33.22%	4.97%	18.07%	27.31%
2400				12.01%	29.69%	4.63%	16.68%	31.91%
2500				13.41%	26.46%	4.29%	15.31%	36.54%

Table S2. Calculated product branching ratios for the 2-methylnaphthyl + C₂H₂ reaction at various temperatures and pressures.

<i>p</i> = 0.03 atm								
T(K)	2mn-i1	2mn-i2	2mn-i3	C ₁₀ H ₇ +allene	2p1	p2	p3	2p6
500	0.17%	37.91%	11.02%	0.00%	27.14%	17.06%	0.16%	0.00%
600		19.13%	2.93%	0.00%	35.40%	34.57%	0.75%	0.00%
700		6.36%	0.55%	0.00%	38.85%	46.49%	1.91%	0.00%
800		1.56%	0.09%	0.00%	40.90%	50.63%	3.16%	0.01%
900		0.34%		0.02%	42.20%	50.99%	4.09%	0.05%
1000				0.08%	42.77%	50.27%	4.74%	0.16%
1100				0.26%	42.90%	49.11%	5.24%	0.45%
1200				0.62%	42.78%	47.88%	5.66%	1.05%
1300				1.22%	42.31%	46.46%	5.99%	2.09%
1400				2.03%	41.49%	44.76%	6.23%	3.70%
1500				2.98%	40.24%	42.72%	6.37%	6.01%
1600				4.07%	38.61%	40.37%	6.41%	9.15%
1700				5.07%	36.47%	37.60%	6.31%	13.07%
1800				6.00%	33.96%	34.57%	6.11%	17.79%
1900				6.81%	31.19%	31.37%	5.81%	23.17%
2000				7.44%	28.26%	28.11%	5.43%	29.00%
2100				7.90%	25.30%	24.91%	5.00%	35.03%
2200				8.20%	22.41%	21.86%	4.54%	41.00%
2300				8.34%	19.70%	19.06%	4.07%	46.72%
2400				8.37%	17.22%	16.53%	3.63%	52.03%
2500				8.32%	15.00%	14.30%	3.21%	56.85%
<i>p</i> = 1 atm								
T(K)	2mn-i1	2mn-i2	2mn-i3	C ₁₀ H ₇ +allene	2p1	p2	p3	2p6
500	27.05%	36.55%	23.84%	0.00%	2.18%	0.61%	0.00%	0.00%
600	11.59%	42.85%	24.40%	0.00%	8.57%	3.24%	0.03%	0.00%
700	5.21%	38.37%	16.45%	0.00%	18.93%	10.53%	0.20%	0.00%
800		27.65%	8.32%	0.00%	28.52%	22.69%	0.72%	0.01%
900		14.88%	3.19%	0.01%	34.00%	34.49%	1.75%	0.04%

1000		6.80%	1.13%	0.05%	37.26%	41.97%	3.06%	0.14%
1100		2.85%		0.15%	39.79%	45.30%	4.24%	0.38%
1200				0.36%	40.76%	47.19%	5.10%	0.88%
1300				0.76%	41.03%	45.94%	5.66%	1.81%
1400				1.42%	41.14%	44.45%	6.12%	3.35%
1500				2.33%	39.94%	42.45%	6.27%	5.64%
1600				3.42%	38.32%	40.11%	6.31%	8.78%
1700				4.56%	36.27%	37.44%	6.24%	12.78%
1800				6.04%	33.95%	34.56%	6.11%	17.79%
1900				6.83%	31.18%	31.36%	5.81%	23.17%
2000				7.46%	28.26%	28.10%	5.43%	29.00%
2100				7.92%	25.29%	24.90%	5.00%	35.02%
2200				8.20%	22.41%	21.86%	4.54%	41.00%
2300				8.35%	19.70%	19.06%	4.07%	46.72%
2400				8.38%	17.22%	16.53%	3.63%	52.03%
2500				8.33%	15.00%	14.30%	3.21%	56.85%
$p = 10 \text{ atm}$								
T(K)	2mn-i1	2mn-i2	2mn-i3	C₁₀H₇+allene	2p1	p2	p3	2p6
500	77.47%	9.30%	6.48%	0.00%	0.07%	0.02%	0.00%	0.00%
600	56.06%	18.27%	12.77%	0.00%	0.59%	0.17%	0.00%	0.00%
700	34.94%	26.53%	17.52%	0.00%	2.76%	0.96%	0.01%	0.00%
800	26.16%	30.72%	17.64%	0.00%	7.83%	3.55%	0.07%	0.01%
900	20.90%	29.95%	14.49%	0.01%	14.03%	8.33%	0.28%	0.03%
1000		28.86%	11.78%	0.03%	23.55%	18.46%	0.85%	0.11%
1100		19.13%	6.53%	0.10%	28.75%	27.12%	1.78%	0.32%
1200		11.74%		0.26%	35.59%	33.78%	2.93%	0.79%
1300		6.76%		0.60%	36.66%	37.94%	4.04%	1.70%
1400				1.10%	37.38%	43.27%	4.92%	3.16%
1500				1.82%	37.35%	41.69%	5.50%	5.37%
1600				2.75%	38.17%	40.04%	6.19%	8.44%
1700				3.81%	36.13%	37.36%	6.11%	12.42%
1800				4.92%	33.71%	34.41%	5.92%	17.25%
1900				5.94%	31.01%	31.27%	5.65%	22.75%
2000				6.80%	28.13%	28.05%	5.30%	28.70%
2100				7.95%	25.24%	24.90%	4.91%	35.01%
2200				8.23%	22.42%	21.86%	4.55%	40.99%
2300				8.36%	19.70%	19.06%	4.08%	46.71%
2400				8.39%	17.22%	16.53%	3.63%	52.03%
2500				8.33%	15.01%	14.30%	3.21%	56.84%
$p = 100 \text{ atm}$								
T(K)	2mn-i1	2mn-i2	2mn-i3	C₁₀H₇+allene	2p1	p2	p3	2p6
500	96.81%	1.17%	0.82%	0.00%	0.00%	0.00%	0.00%	0.00%
600	91.46%	2.95%	2.13%	0.00%	0.01%	0.00%	0.00%	0.00%

700	82.22%	5.87%	4.31%	0.00%	0.09%	0.03%	0.00%	0.00%
800	70.01%	9.51%	6.91%	0.00%	0.43%	0.15%	0.00%	0.00%
900	56.61%	13.09%	9.05%	0.00%	1.44%	0.58%	0.01%	0.01%
1000	55.91%	15.54%	9.87%	0.00%	3.33%	1.65%	0.05%	0.05%
1100	56.03%	17.36%	10.09%	0.02%	5.87%	3.51%	0.14%	0.17%
1200	48.21%	18.34%	9.57%	0.08%	8.16%	5.01%	0.21%	0.46%
1300		27.18%	15.33%	0.27%	17.32%	15.19%	1.17%	1.24%
1400		20.68%	10.91%	0.60%	21.11%	20.21%	1.93%	2.51%
1500		15.31%		1.12%	30.79%	24.46%	2.78%	4.55%
1600		10.81%		2.35%	31.00%	27.49%	3.58%	8.11%
1700				3.28%	30.71%	35.50%	4.19%	12.13%
1800				4.25%	29.61%	34.41%	5.79%	16.94%
1900				5.19%	28.04%	31.26%	5.49%	22.45%
2000				6.05%	28.03%	28.05%	5.12%	28.44%
2100				6.76%	25.10%	24.87%	4.71%	34.60%
2200				7.30%	22.25%	21.84%	4.28%	40.70%
2300				7.67%	19.56%	19.04%	3.86%	46.51%
2400				8.41%	17.12%	16.53%	3.45%	52.01%
2500				8.35%	14.92%	14.30%	3.07%	56.83%

**Input files for RRKM-ME calculations using the MESS code containing optimized
Cartesian coordinates, vibrational frequencies, and relative energies for all reactants,
products, intermediates, and transition states**

1-methylbiphenyl → 9H-fluorene + H

```

TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125.
1250. 1375. 1500. 1650. 1800. 2000. 2250. 2500.
PressureList[atm]          0.01 0.03 0.1 0.3 1. 3. 10. 30. 100.
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discretization energy step to T
ExcessEnergyOverTemperature 100
ModelEnergyLimit[kcal/mol] 1000
WellCutoff                 10
ChemicalEigenvalueMax     0.2
ChemicalEigenvalueMin     1.e-6          #only for direct
diagonalization method
CalculationMethod          low-eigenvalue
EigenvalueOutput           Naphthalene_13p.out
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      Factor[1/cm]          424      ! Jasper calc N2
      Power                 0.62
      ExponentCutoff        15
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  CollisionFrequency
    LennardJones
      Epsilons[1/cm]       390. 390.      ! N2 , A3/A3a/A6 ! from new
      Jasper calc 11/22/15
      Sigmas[angstrom]     4.46 4.46      ! N2 , A3/A3a/A6 ! from new
      Jasper calc 11/22/15
      Masses[amu]          28. 167.08608
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  OutputReferenceEnergy[kcal/mol] 0.
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  Species
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C  1.6220137064 -1.4236937067 -0.0996977234
C  0.4296975857 -0.6906216111 -0.0165172969
C  -0.7762529114 -1.3969834143 0.1064222885
C  0.4601785521 0.7966921726 -0.0076818813
C  1.2442619795 1.4476739774 0.9428102578
C  1.2941448379 2.8396358305 1.032105947
C  0.5381799699 3.6166000866 0.1465086027
C  -0.2371420112 3.003540562 -0.8159674459
C  -0.2973042194 1.5830515766 -0.9468755321
C  -1.0394087256 1.0202973365 -1.9966467686

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H 1.9051843064 3.3120381205 1.7923536947
H 0.5636567535 4.6985826758 0.2137192323
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H -1.5885338136 1.6615315198 -2.6749788253
H -1.0600478561 -0.0436181949 -2.1815076742
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    564.6945 572.7694 628.1409
    635.2121 716.9757 722.2853
    729.2603 747.2491 774.9307
    787.7997 851.2822 861.3337
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    1354.3146 1447.5337 1477.8982
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    1560.5677 1601.9080 1615.7417
    1642.0681 3154.4815 3159.7412
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    3176.2300 3177.1826 3183.0145
    3190.0562 3190.7040 3257.6793
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  ElectronicLevels[1/cm] 1
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  End
  End
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  Species
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C 1.6145624937 -2.8236118385 0.0237330514
C 1.6783318523 -1.4520731106 -0.2706972243
C 0.5228248249 -0.7040042811 -0.3144966289
C -0.8045360692 -1.2852628344 0.1313151489
C 0.2672881512 0.6205127438 -0.8399266887
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```

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C  -1.121851504  0.7753924328  -1.0514436788
C  -1.8551568745  -0.5062340036  -0.7099399964
H  -1.7702923652  -3.2969343595  0.2338439448
H  0.3350470468  -4.5577568765  0.2451514989
H  2.5233473307  -3.4127389041  0.0498215806
H  2.6307656777  -1.0072007169  -0.542183215
H  -0.9558979431  -0.9491166847  1.1782787118
H  2.2122397892  1.5601110708  -0.9892419319
H  1.2974599988  3.6770641326  -1.8890206126
H  -1.1331552045  3.9445065049  -2.2435898332
H  -2.6927363123  2.0861375569  -1.7241022394
H  -2.7930425312  -0.3391001788  -0.1748909094
H  -2.0902080583  -1.0622812323  -1.6261301104
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  SymmetryFactor  0.5
  End
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    613.5385  618.6836  662.0667
    691.7940  728.5141  740.4811
    767.6424  782.1282  813.0965
    854.6472  874.7150  914.7186
    941.9527  967.5705  979.5278
    986.1119  994.4567  1003.0528
    1044.4735  1054.6634  1072.0606
    1114.6339  1125.1750  1160.2152
    1177.6420  1181.5146  1196.5057
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    1309.8899  1326.0491  1327.5636
    1353.7965  1392.5447  1425.2538
    1478.4549  1491.1549  1494.3911
    1536.0986  1594.7974  1608.3764
    1635.4039  2842.3241  3011.3698
    3075.3245  3150.2543  3154.9774
    3157.7109  3164.5896  3169.0037
    3175.7802  3187.3314  3189.0093
  ZeroEnergy[kcal/mol]  1.35
  ElectronicLevels[1/cm]  1
    0  2
  End
  End
  Bimolecular  p1  # 9H-fluorene + H
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  RRHO
  Geometry[angstrom]  23
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C  0.4170543452  -3.1415135829  1.1248697995
C  1.6471512249  -2.4802987206  1.1157827503

```

```

C 1.7055894041 -1.0876168843 1.1117304512
C 0.5142702267 -0.3623063018 1.1169244363
C -0.7251562446 -1.0304050176 1.1260861048
C 0.2659806896 1.0855043795 1.1147119057
C 1.1475639291 2.166286728 1.1067185891
C 0.6284421886 3.4599261119 1.1065818136
C -0.7516835858 3.673531333 1.1143226475
C -1.636794025 2.5927392088 1.1223233178
C -1.1252320973 1.3024911977 1.122470168
C -1.8563715793 -0.0236384455 1.1300186469
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H 2.5657412349 -3.0563338087 1.1118283315
H 2.664991273 -0.581950669 1.1046417118
H 2.2206316168 2.0091528683 1.1006566606
H 1.3026200919 4.3090933465 1.1004174355
H -1.139189471 4.6860820207 1.1141405957
H -2.7080426649 2.7660607507 1.128312936
H -2.4967088442 -0.1321017582 2.0129519147
H -2.5061326457 -0.1364060057 0.2544902447
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 63
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498.8090 553.8100 576.4900
637.0948 645.1440 711.9175
741.2211 754.4592 756.1213
796.3664 813.9210 853.6331
870.8892 879.7876 930.6185
947.8700 972.8917 987.8059
989.8239 1024.6443 1046.1974
1052.2321 1117.4362 1131.0016
1162.4770 1176.1837 1180.1610
1192.1603 1207.3507 1220.5716
1252.7136 1320.1064 1329.5667
1344.5348 1374.7729 1451.2744
1478.6003 1484.8995 1509.4957
1510.8005 1619.7891 1624.1355
1649.0451 1650.1625 3022.6596
3047.4008 3157.5484 3157.9697
3163.6104 3165.3388 3174.7206
3176.0473 3187.4146 3188.1643
ZeroEnergy[kcal/mol] 0.
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2

```

```

      End
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    End
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      RRHO
      Geometry[angstrom]      24      #
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C   0.2394258267  -3.4282888929  -0.212187643
C   1.5342111654  -2.9217040075  -0.0415106967
C   1.7221814614  -1.558617115   0.2317837613
C   0.6355098851  -0.7110320376   0.3626244566
C  -0.7065760188  -1.2219314853   0.2108311316
C   0.683107069   0.7572646416   0.3313951025
C   1.5417213402   1.6105521282   1.0213382883
C   1.3970600146   2.9906414894   0.8818677602
C   0.3967574507   3.5130196242   0.0625097347
C  -0.458033643   2.6631673916  -0.6413824345
C  -0.3113143749   1.2798200555  -0.5300018419
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H   0.1021592842  -4.4829374431  -0.426385407
H   2.391825587  -3.5759414173  -0.1446068714
H   2.7265983227  -1.15158359   0.2851868544
H  -1.500343044  -0.7307542635   0.7663309064
H   2.2937062886   1.2032046733   1.6883542859
H   2.0526837698   3.6598900216   1.4276074896
H   0.2830289455   4.5873557432  -0.0313406761
H  -1.2207330927   3.0770023311  -1.2923602056
H  -2.1706852348   0.4343796437  -1.3858700539
H  -0.6269796882  -0.2364866913  -2.0884484454
      Core      RigidRotor
      SymmetryFactor      0.5
    End
    Tunneling      Eckart
      ImaginaryFrequency[1/cm]      586.5979
      WellDepth[kcal/mol]           24.18
      WellDepth[kcal/mol]           22.83
    End
    Frequencies[1/cm]      65
      93.0941      105.9214
      177.8774      235.1816      284.5646
      364.3257      400.0483      431.8682
      456.9222      517.5303      562.5770
      570.1120      597.8714      612.5944
      627.5484      726.6929      732.2033
      744.2282      750.6558      779.3419
      813.8782      837.0476      843.0132
      881.0256      934.1240      946.3818
      951.2860      975.4968      990.3359
      1007.8471     1018.0724     1030.8997
      1040.9138     1056.6082     1087.3160
      1129.2702     1170.7620     1181.6125
      1185.3014     1219.0868     1256.9985
      1302.4944     1322.3973     1333.0631

```

1340.8961	1441.4426	1452.5831
1485.7271	1489.4347	1509.2171
1556.7184	1598.9480	1604.1708
1634.9529	3098.6198	3120.9270
3157.9152	3158.8408	3163.8649
3166.7365	3176.0548	3177.0098
3181.9594	3187.4131	3189.1256

ZeroEnergy[kcal/mol] 24.18

ElectronicLevels[1/cm] 1

0 2

End

Barrier B2 i2 p1 # ts2

RRHO

Geometry[angstrom] 24 #

C	-0.8045227783	-2.7846391483	0.0453888375
C	0.3857953505	-3.469629654	0.2522775403
C	1.6185608849	-2.8164341748	0.1201628596
C	1.6806817948	-1.4756966784	-0.257855089
C	0.4956826555	-0.777516353	-0.4704003586
C	-0.7598529035	-1.4079781263	-0.2364412586
C	0.2493114408	0.5885208927	-0.9328026593
C	1.1340249747	1.6301897316	-1.2177012022
C	0.6201234187	2.8533966253	-1.6412172687
C	-0.7581400343	3.0377164766	-1.778642484
C	-1.6457366875	1.9970929197	-1.4968554842
C	-1.1396777658	0.7744767429	-1.0771109752
C	-1.8773546383	-0.5019916661	-0.7352477344
H	-1.7575513314	-3.2927979966	0.1448039232
H	0.3634878262	-4.5223346892	0.5104519401
H	2.5359762539	-3.3697103981	0.2865409133
H	2.6418524629	-0.9952432599	-0.4044459737
H	-0.9116477263	-0.8456616216	1.5229847159
H	2.2045546881	1.4958957166	-1.1076501423
H	1.2949686788	3.6725606692	-1.862967235
H	-1.1410624806	3.9977103815	-2.1062308708
H	-2.7147781729	2.1470802989	-1.6068640097
H	-2.6737777672	-0.3503135977	-0.0031048322
H	-2.3374951437	-0.9371750909	-1.6312201521

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 792.1032

WellDepth[kcal/mol] 25.1

WellDepth[kcal/mol] 6.5

End

Frequencies[1/cm] 65

97.8713	133.2966	
216.0137	239.6740	277.3734
389.8661	416.9473	433.6100
463.3833	492.4703	502.0243
518.2826	567.9760	575.0924
634.2377	648.6942	714.8060
744.9939	751.7015	754.1090

794.0119	813.5845	851.0024
871.1598	880.5362	933.8394
949.5517	972.5071	987.5860
990.6331	1021.8834	1043.5938
1050.0475	1118.2458	1130.0355
1165.6165	1173.6757	1179.2910
1191.2535	1206.0734	1219.4343
1247.2662	1322.1636	1328.7026
1340.0826	1366.5937	1453.2752
1467.2271	1483.2625	1503.1216
1507.3753	1595.4537	1619.7290
1630.7342	1647.9924	3019.2361
3076.5119	3158.6084	3161.3917
3165.1048	3168.0929	3175.7520
3178.0810	3187.9198	3189.4768

```

ZeroEnergy[kcal/mol]      26.46
ElectronicLevels[1/cm]   1
0       2

```

```

End
End

```

1-methylnaphthyl + C₂H₂

```

TemperatureList[K]      300 400 500 600 700 800 900 1000
1100 1200 1300 1400 1500 1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
PressureList[atm]      0.03 1. 10. 100.
EnergyStepOverTemperature 0.2          #Ratio of
discretization energy step to T
ExcessEnergyOverTemperature 150
ModelEnergyLimit[kcal/mol] 1000
WellCutoff              10
ChemicalEigenvalueMax  0.2
ChemicalEigenvalueMin  1.e-6          #only for direct
diagonalization method
CalculationMethod      direct
EigenvalueOutput      eigenvalue.out
Model
EnergyRelaxation
Exponential
Factor[1/cm]           424    ! Jasper calc N2
Power                  0.62
ExponentCutoff         15
End
CollisionFrequency
LennardJones
Epsilons[1/cm]        390. 390.    ! N2 , A3/A3a/A6 ! from new Jasper
calc 11/22/15
Sigmas[angstrom]      4.46 4.46    ! N2 , A3/A3a/A6 ! from new Jasper
calc 11/22/15
Masses[amu]           28. 167.
End
OutputTemperatureStep[K] 100

```

```

OutputTemperatureSize 24
OutputReferenceEnergy[kcal/mol] 0.
!-----
-----
!-----well_i1-----
Well      i1
Species
RRHO
Geometry[angstrom] 24
C  -0.1573235108  0.4430953886  0.1489257125
C  -1.455717507  1.0188727104  0.2042976017
C  1.0209763571  1.1100911714  0.6285434368
C  -2.5574995248  0.3501774123  -0.2728690638
C  -2.4268946565  -0.9410329314  -0.8300963615
C  -1.1925261335  -1.5376517026  -0.8858542267
C  -0.0337382685  -0.8768391953  -0.3993043272
C  2.2365986952  0.4503933325  0.5646766592
C  1.2374426741  -1.5023946815  -0.4380372504
C  2.3470840895  -0.8517866124  0.0425854752
H  -1.5875436407  1.9981801563  0.645772126
H  -3.5358453953  0.8143052358  -0.2165311479
H  -3.3027144331  -1.458598105  -1.2049411375
H  -1.0824178647  -2.533538875  -1.302583045
H  3.1249097915  0.9646807379  0.9131999733
H  1.3174252368  -2.5009301042  -0.8545575997
H  3.319106111  -1.3312873464  0.0091717086
C  0.9546473349  2.4839310702  1.1671559878
C  2.034360314  4.3080731572  2.6975906724
C  1.8057278769  3.0336091514  2.0084977053
H  0.1264467783  3.1102775479  0.8192268497
H  2.0226486856  4.1825687145  3.785365749
H  1.2557456363  5.0417024011  2.4359439284
H  3.0039563538  4.7409293662  2.4296665737
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
52.4302          87.5488          121.4754
162.9171         174.9192         210.5186
267.2844         297.4492         324.8855
424.4747         440.0549         479.1888
510.4865         534.6082         552.7954
629.5636         647.7522         740.7137
749.9268         780.1613         799.6634
805.5151         823.2683         862.8333
881.4553         923.0558         950.0551
963.1843         983.3971         994.9396
1031.5112        1044.5573        1047.8990
1067.2826        1106.0541        1168.0807
1187.7829        1192.0996        1231.0718
1259.6603        1265.0072        1310.2747
1372.8735        1388.5976        1398.0806
1423.3880        1452.1399        1470.0565
1473.8768        1492.8733        1547.2534

```

1612.5008	1631.6379	1661.4080
1733.5360	2960.4173	3028.0189
3042.1431	3064.3304	3157.4439
3160.1325	3168.6244	3172.4439
3183.7902	3185.3172	3198.5893

ZeroEnergy[kcal/mol] -39.94

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i2-----

Well i2

Species

RRHO

Geometry[angstrom] 24

C	-3.9716462514	0.5290628747	1.0293387367
H	-3.28845971	1.1785495168	1.5962976901
H	-4.702077427	1.1679553404	0.5216942203
H	-4.5230996305	-0.0849201309	1.7491078037
C	-3.2396735817	-0.3103052102	0.0731978201
C	-2.0553644831	-0.483206237	-0.4750979218
C	-0.8623292904	0.3814287051	-0.264453575
C	-0.9859000007	1.7584652955	-0.2511549448
C	0.1331079069	2.600146802	-0.0768892551
C	1.3873787826	2.0640424473	0.0690972057
C	0.4389099145	-0.2026963539	-0.1001818891
C	1.5737757319	0.6576924677	0.0588151295
C	2.8620714257	0.0816701811	0.2110969935
C	3.033510612	-1.2804534526	0.2172975663
C	0.6535035043	-1.6063823279	-0.0709435109
C	1.9150271786	-2.1316559307	0.0792868454
H	-1.9181521085	-1.3332208075	-1.143960756
H	-1.9609177033	2.2023292557	-0.4140401637
H	-0.0053442043	3.6756196076	-0.0766070885
H	2.2531764477	2.7063004221	0.1910688485
H	3.7147024425	0.7429028288	0.3266782013
H	4.0237158253	-1.7060739629	0.3348780273
H	-0.1951506358	-2.2736481653	-0.1525038556
H	2.0532742547	-3.206917166	0.098483872

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

42.2735	87.8768	136.4419
160.1998	180.5972	223.3749
244.2594	374.3249	392.8798
432.6205	445.9414	480.8198
510.9639	536.2310	554.7665
626.2304	663.3195	737.4691
748.7638	789.4189	799.2751
809.2722	824.8445	859.9272
885.3938	922.4455	926.3534
965.7695	982.8095	996.6789

1035.2265	1038.5090	1044.6602
1054.2184	1099.2856	1168.2936
1183.2084	1189.1448	1231.6391
1253.2343	1276.2703	1301.0625
1372.3072	1389.4254	1394.2218
1420.6350	1458.4557	1467.3218
1470.9361	1491.6067	1544.9071
1611.4148	1632.7519	1661.0809
1734.5659	2972.0473	3044.0034
3063.9135	3088.0838	3157.7277
3160.4495	3168.9337	3174.3289
3183.5970	3187.4022	3196.4680

ZeroEnergy[kcal/mol] -39.43

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i3-----

Well i3

Species

RRHO

Geometry[angstrom] 24

C	0.0108561018	0.5425057255	0.0053570418
C	1.3949064632	1.2309915061	0.0418821584
C	0.3853246135	2.0275843306	0.0676996182
C	2.8365136164	0.9166893997	0.0273963853
C	-0.4614502859	-0.1192789926	1.2334822232
C	-0.474522641	-0.0515979624	-1.2863589902
C	-1.2553936102	-1.2407997011	1.2007697544
C	-1.2934736503	-1.218233297	-1.2614362514
C	-1.6704689283	-1.805645239	-0.0108150478
H	-0.0420368999	3.0170688841	0.0973784691
H	3.0981357082	0.2868719968	0.882997621
H	3.093144529	0.3559128152	-0.8764135176
H	3.4426312283	1.8255309306	0.0609933415
H	-0.1493386697	0.3108227482	2.1791534286
H	-1.5704622622	-1.6975432275	2.1336401879
H	-2.2948174453	-2.6916144847	-0.0172907418
C	-0.1398372221	0.5082864068	-2.5221280989
C	-1.7291902061	-1.7695743852	-2.4864738721
C	-0.581721293	-0.0507149843	-3.7178652956
C	-1.3796672464	-1.1982417444	-3.6976016822
H	0.4759916944	1.4002090523	-2.5485093645
H	-2.3527317204	-2.6575579777	-2.4637423898
H	-0.3068066454	0.4058810671	-4.6620787963
H	-1.7259402287	-1.6379528672	-4.6263981812

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

53.5715	92.8506	144.1585
165.5476	182.0764	254.8803
269.9684	379.9767	404.2973

435.5959	446.5756	503.1854
512.6592	526.9539	550.6847
560.6722	659.6081	688.6327
702.3243	721.9467	764.4998
792.3602	796.2180	798.4983
856.8429	881.6505	920.8665
954.6087	958.8596	974.5610
982.8894	1025.9717	1052.6059
1058.5059	1086.6716	1097.9137
1125.4074	1146.9156	1173.0285
1180.7995	1229.4966	1270.9152
1303.5742	1324.9566	1381.5283
1403.8539	1443.4151	1463.3272
1475.5945	1480.5247	1512.9358
1544.9943	1591.7334	1628.1291
1869.2451	3023.3935	3080.5813
3095.8738	3151.9525	3155.4159
3164.3951	3170.1335	3175.1946
3181.6512	3186.8380	3242.6981

ZeroEnergy[kcal/mol] -22.71
 ElectronicLevels[1/cm] 1
 0 2

End
 End

!-----

!-----well_i4-----

Well i4

Species

RRHO

Geometry[angstrom] 24

C	0.5528364458	-0.9816075716	-0.167231412
C	1.5444904696	0.0464849993	-0.064743573
C	-0.1895529122	1.6518732446	0.5175805335
C	1.1619691315	1.3315865044	0.2603157596
C	-1.15579445	0.6807241075	0.4466242644
C	-0.8154474554	-0.6528854002	0.1014186164
C	3.5640284305	0.0413027414	-1.4284214114
C	3.003535339	-0.2615264143	-0.2800092619
C	3.7576879915	-0.8803107315	0.8785498321
C	-1.4596433708	-2.9535872911	-0.3474117649
C	-0.1127065882	-3.2760124846	-0.6281102909
C	-1.7999284786	-1.6709577245	0.0047719552
C	0.8661586621	-2.3152730059	-0.5422263378
H	-0.4555941423	2.6709523902	0.7749927739
H	1.9181465022	2.1056769694	0.327035287
H	-2.1947885504	0.9198411107	0.6478626289
H	3.2519574484	0.4784967344	-2.3662489015
H	3.2842024293	-1.8130145651	1.1992638182
H	3.7450771766	-0.2035153003	1.7391613498
H	4.7941982812	-1.0846162968	0.6070593392
H	-2.2226006418	-3.7206318402	-0.418042514
H	0.1470228456	-4.2878312876	-0.9186072553
H	-2.8337735473	-1.4142785386	0.2116577373
H	1.8928929837	-2.5648763496	-0.780744173

```

Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
44.6482          93.9982          149.4955
169.1939        183.6421          189.2130
294.5026        320.4277          381.1259
441.6107        479.0297          495.2312
499.4038        555.5961          579.3260
582.5278        660.4298          693.4082
710.7981        747.6614          792.8048
805.5905        813.5983          821.2044
859.0973        880.3005          924.1077
968.0383        985.5753          991.7336
998.4561        1026.5658         1045.3620
1051.0775       1082.5619         1138.9889
1168.5633       1182.6218         1197.7697
1234.2889       1258.1662         1290.1846
1361.4162       1388.9302         1401.3911
1418.9963       1464.8923         1480.8618
1483.3529       1490.9307         1542.7242
1611.0092       1632.3226         1660.7343
1671.7064       3022.3806         3074.1478
3115.3705       3158.0869         3160.7630
3169.0355       3172.6777         3182.9802
3186.3281       3193.0038         3229.2159
ZeroEnergy[kcal/mol] -36.71
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i5-----
Well      i5
Species
RRHO
Geometry[angstrom] 24
C 0.4846848777 -0.9966854697 -0.1814615569
C 1.4741637901 0.0340287874 -0.0933277848
C -0.2656014072 1.6456748715 0.4528031727
C 1.0875464527 1.3232959295 0.206272157
C -1.2294140574 0.6713484672 0.3991216471
C -0.8849386436 -0.6671415068 0.0782217226
C 3.5548603104 0.0725184102 -1.3851013583
C 2.9326939994 -0.2745450526 -0.2831617765
C 3.6442917319 -0.9470444744 0.8843443754
C -1.524725999 -2.9747001089 -0.3420196052
C -0.1770621797 -3.2975846353 -0.6190625375
C -1.8674607064 -1.6883245462 -0.0065555303
C 0.7997370532 -2.3341211128 -0.5427643018
H -0.5348447131 2.6691475453 0.6886527093
H 1.8419950014 2.0998957244 0.2587209633
H -2.2693266689 0.9116373589 0.5941467532
H 4.5542948864 0.008945254 -1.7919996335

```

```

H 3.1465433423 -1.8823468543 1.1557818433
H 3.610613857 -0.295495888 1.7634437987
H 4.6881202214 -1.1606677146 0.6479163468
H -2.2861019409 -3.7440496469 -0.4044822797
H 0.0841314243 -4.3116022568 -0.9005892972
H -2.9021639298 -1.4302843125 0.1942870904
H 1.8260722981 -2.5845427685 -0.782047918
Core RigidRotor
SymmetryFactor 0.5
End
      Rotor      Hindered      ! 46 cm^-1
      Group      7 9 17 18 19 20
      Axis      2 8
      Symmetry    1
      Potential[kcal/mol] 8
0.07509219 3.240905055 5.159036836 0.738948391 0.335457214 0.033901833 0
0.246417368
End
Frequencies[1/cm] 65
                94.7074                148.1626
168.8853        183.5304        191.8989
294.6737        327.6680        379.3976
444.1525        477.5062        479.5041
499.6196        551.6103        582.6395
594.7534        662.1872        690.3142
692.3489        747.7323        793.4618
806.6249        815.6198        844.7734
850.2385        880.3740        923.7703
963.6085        970.4569        985.5837
997.4492        1019.6540        1037.3963
1045.8682       1081.3057        1132.4680
1168.4150       1182.9180        1196.9811
1234.6087       1261.2342        1292.6974
1363.7595       1390.1869        1395.0350
1420.7674       1465.8169        1478.8524
1484.0882       1492.1226        1543.7902
1615.1090       1634.0198        1661.3250
1675.9832       3021.5751        3078.1617
3109.0398       3157.8422        3160.4870
3168.4700       3173.6365        3182.7158
3186.9137       3192.9829        3223.7123
ZeroEnergy[kcal/mol] -35.94
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i7-----
Well      i7
Species
RRHO
Geometry[angstrom] 24
C 0.4746250402 -1.0011427781 0.0253216667
C 1.5123902508 -0.0172627637 -0.1008123113

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C -0.2145046441  1.7047650271  -0.2667740339
C  1.1388729345  1.3098501059  -0.2230532224
C -1.2182131838  0.7743331225   -0.170514716
C -0.9090007861  -0.6004661214   -0.0155869338
C  3.3883258026  -1.5320175907   -0.6575665122
C  2.9495949493  -0.4008443951   -0.0917574892
C  3.9182141938  0.5501649249   0.5750043125
C -1.6190260866  -2.9139159926   0.3028045333
C -0.2603550272  -3.3317629645   0.359248219
C -1.9233517572  -1.5868927283   0.1217166535
C  0.6859362442  -2.3702133879   0.2273339273
H -0.4555196816  2.7558878182   -0.3792406759
H  1.9013753487  2.0737844444   -0.309696931
H -2.2595563309  1.0774900073   -0.2000570218
H  4.4387342222  -1.8000802056   -0.6245413358
H  3.5988948151  0.7884025993   1.5941108382
H  3.9944893663  1.4986535546   0.0335249315
H  4.917961416  0.1151191646   0.6158984273
H -2.4090249297  -3.6499941267   0.407612811
H -0.009186739  -4.3766524018   0.5065944467
H -2.9592596504  -1.2670836982   0.0854847035
H  2.7273032328  -2.2111336143   -1.1803812871

```

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

```

38.4831          101.7593          165.7196
174.7445          192.8646          206.3873
320.8047          364.2097          393.9182
457.1323          469.6650          495.0524
503.8776          548.0520          580.5764
582.9704          630.6609          690.2538
723.9580          754.6836          773.1280
798.9498          825.0375          845.1010
884.0702          918.2311          923.6079
930.1562          971.3100          985.8592
1000.3975         1033.9537         1048.9428
1066.7061         1098.2296         1160.0378
1175.2875         1190.0696         1227.1139
1238.5642         1309.4770         1347.6211
1356.3372         1394.9983         1413.1858
1441.2282         1455.4707         1468.1459
1484.2703         1498.4660         1509.9611
1587.7431         1629.7145         1650.0065
1683.6888         3023.0025         3070.7998
3108.5719         3138.3431         3156.4779
3160.4185         3166.9340         3177.2493
3180.6535         3194.1921         3223.2819

```

ZeroEnergy[kcal/mol] -35.93

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

```

!-----well_i8-----
Well      i8
Species
RRHO
Geometry[angstrom]  24
C  -0.277909   -0.187287   -0.010967
C  1.047942    0.352971    0.027509
C  0.119457    2.603484    0.102121
C  1.221419    1.720806    0.074174
C  -1.160198    2.110573    0.081037
C  -1.39349    0.71272    0.020471
C  2.537494   -1.307222    1.143267
C  2.257395   -0.536536    0.02057
C  3.079758   -0.537156   -1.096936
C  -2.926481   -1.170703   -0.094558
C  -1.828943   -2.059438   -0.142617
C  -2.709888    0.182557   -0.017719
C  -0.541372   -1.581195   -0.103064
H  0.294034    3.672659    0.146447
H  2.22776    2.123236    0.104521
H  -2.011914    2.782257    0.107309
H  3.414618   -1.943739    1.172864
H  1.899871   -1.284503    2.017295
H  2.842717    0.054761   -1.971231
H  3.98056   -1.140175   -1.122321
H  -3.937585   -1.561048   -0.124068
H  -2.006169   -3.126728   -0.215011
H  -3.547281    0.872132    0.011112
H  0.292281   -2.270299   -0.146648
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
33.6177           94.8354           159.2962
171.9887          192.1049          317.5311
338.2136          389.3128          448.4033
480.1284          501.8609          502.8165
546.6121          557.8267          562.3976
588.1096          630.8944          673.0416
699.5150          747.9578          776.6459
794.9349          806.6093          810.4702
818.0749          856.2024          880.3002
925.7461          967.4068          982.8495
985.4702          997.5163          1012.3426
1041.7356         1049.0168         1086.4933
1166.7802         1173.6917         1184.9083
1229.2340         1237.5760         1281.4046
1297.7522         1365.3819         1380.1033
1390.0870         1432.4655         1467.4117
1479.6263         1493.7251         1523.1051
1545.7795         1617.6504         1635.4140
1661.5950         3135.3818         3142.1803
3157.3096         3159.9953         3168.8382
3171.8436         3183.7228         3185.9316

```

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3198.2308          3237.6701          3239.5885
ZeroEnergy[kcal/mol] -60.59
ElectronicLevels[1/cm]      1
0 2
End
End
!-----
!-----well_i9-----
Well      i9
Species
RRHO
Geometry[angstrom]  24
C  -0.273246   -0.224245   0.079015
C  1.16693    0.174606   0.196786
C  0.470093    2.536276  -0.132324
C  1.468149    1.605528   0.012693
C  -0.87989    2.164812  -0.145265
C  -1.263915   0.789015  -0.055022
C  2.893323   -1.411412  -1.098857
C  2.241238   -0.805563  -0.126397
C  2.055124   -0.572138   1.292528
C  -2.996388   -0.925524  -0.07002
C  -2.016835   -1.917614   0.039774
C  -2.622422   0.404918  -0.121276
C  -0.673258   -1.562505   0.108468
H  0.733949    3.583119  -0.240948
H  2.510542    1.903211   0.016857
H  -1.653338    2.916467  -0.251363
H  3.698662   -2.108262  -0.887926
H  2.641308   -1.236578  -2.139268
H  1.53074    -1.311742   1.890217
H  2.76779    0.041856   1.835397
H  -4.0444    -1.19846   -0.123158
H  -2.300091   -2.963653   0.065886
H  -3.375985    1.179595  -0.219058
H  0.077416   -2.342476   0.172741
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
57.3542          101.1206          168.5949
183.5309         238.7150          279.0664
384.3867         390.1099          428.7733
443.7507         494.8447          501.2559
519.1099         546.3505          560.5739
657.3592         684.4954          691.1796
707.6675         760.7256          787.5948
790.2782         798.0569          842.7229
878.4845         895.2252          928.2150
928.7551         954.2541          957.5318
983.4671         1020.8540         1023.6909
1037.4408        1059.3590         1097.1440
1121.7669        1140.0962         1156.0303
1178.4405        1184.3611         1232.2546

```

1284.3905	1318.1903	1331.8320
1386.1391	1433.7369	1444.0179
1462.9019	1467.2126	1516.6051
1550.0404	1591.8662	1629.0183
1819.3689	3094.0011	3121.9060
3156.7840	3158.0718	3165.3998
3174.6633	3176.0725	3181.2748
3185.1380	3188.1312	3205.4716

ZeroEnergy[kcal/mol] -30.41

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i10-----

Well i10

Species

RRHO

Geometry[angstrom] 24

C	0.2484209625	-0.1339621248	-0.2932173862
C	-0.995487167	0.5468098689	-0.4897350552
C	0.047651617	2.6347205469	0.2082062096
C	-1.0738707213	1.8985816806	-0.2328125859
C	1.2540824407	2.0085990924	0.3897987061
C	1.388086057	0.6176765246	0.1442541467
C	-2.8311389194	-1.2275141965	1.3831655816
C	-2.9175886367	-0.9646125108	0.1046536011
C	-2.2387387593	-0.1967546558	-0.9641242678
C	2.7502002571	-1.3952769012	0.0908152667
C	1.6275677527	-2.1410630909	-0.3322256684
C	2.6287442882	-0.048114912	0.3244637232
C	0.4117427523	-1.5278280713	-0.5178107191
H	-0.0522991596	3.6978391074	0.3959893496
H	-2.0183293445	2.4126035512	-0.3789002094
H	2.1223737015	2.5669622225	0.7234567105
H	-2.0295934609	-0.8185565339	2.0042346337
H	-3.5506743668	-1.867166376	1.8880226164
H	-1.9893304619	-0.8706790366	-1.7918110936
H	-2.9465880246	0.5290164041	-1.3781960127
H	3.7040322225	-1.8907623051	0.2326825866
H	1.7265858827	-3.2063676401	-0.5079388822
H	3.484961749	0.5316889515	0.6534645637
H	-0.4402756613	-2.1219605952	-0.8223768149

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

46.1485	76.7145	141.5103
146.0508	175.8974	248.6691
284.2559	386.3108	431.6205
435.6599	462.0407	478.2063
508.4539	522.0077	558.9246
609.6911	664.0629	717.8786
745.1595	792.6506	804.1325

811.7218	864.1262	880.5941
888.1627	903.1385	921.5407
938.8723	964.6127	983.1086
995.5197	1008.2681	1037.8693
1057.2600	1095.4975	1168.3213
1183.5577	1187.3444	1208.8805
1237.9658	1259.1847	1288.0880
1313.0651	1381.3721	1393.5776
1409.3482	1422.5298	1467.5698
1478.7902	1493.8057	1547.3255
1615.0581	1638.7659	1664.0346
1737.9349	3019.4294	3043.5557
3047.8617	3143.8697	3156.8383
3158.4207	3164.8856	3169.7516
3183.4894	3184.3574	3199.7752

ZeroEnergy[kcal/mol] -37.16

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i11-----

Well i11

Species

RRHO

Geometry[angstrom] 24

C	-0.4491447986	-0.7659684195	-0.4039808257
C	-1.3308312859	0.3689659101	-0.5123534765
C	0.6149886039	1.8676551331	-0.2313798404
C	-0.736281958	1.5857561865	-0.4159532033
C	1.4615926672	0.7848026225	-0.13433052
C	0.9568266864	-0.5409197819	-0.2194692856
C	-2.8320686704	0.2331318572	-0.709562219
C	-4.4677930224	-1.1131499821	0.6595469129
C	-3.5752131524	-0.1340134385	0.552782031
C	1.3435747628	-2.9423852549	-0.2111676585
C	-0.0392373221	-3.164501707	-0.3901599783
C	1.8256701713	-1.6595680538	-0.1270618157
C	-0.9119156855	-2.105878004	-0.4827132857
H	0.9861051905	2.8842859264	-0.1690087219
H	2.5275648692	0.9334062419	0.0078580405
H	-3.2021322275	1.2008065987	-1.0641662628
H	-3.0520522855	-0.4949910204	-1.4964218293
H	-4.721006048	-1.7503782261	-0.1830978396
H	-4.983621491	-1.3116426733	1.5921431603
H	-3.3484701817	0.4813606809	1.4209209845
H	2.0204073289	-3.7861363634	-0.1389868466
H	-0.4157672401	-4.1795720187	-0.451391528
H	2.8869586127	-1.4810110082	0.011353096
H	-1.9700065239	-2.2953302054	-0.6037850883

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

51.0600	69.0946	106.8147
172.7584	191.5220	255.1185
296.2623	372.4337	426.4375
436.1319	480.7850	492.9414
520.3717	556.8542	565.7473
623.5784	668.5424	738.1547
742.6379	783.9648	792.2928
802.2545	867.5814	877.4951
916.1841	932.8291	946.0922
951.9860	966.9255	994.8589
1027.0481	1036.2738	1052.7509
1110.0520	1139.1452	1160.0872
1180.6957	1185.9380	1219.1773
1244.8690	1284.8684	1313.9559
1327.3463	1332.2966	1381.3055
1409.0112	1447.9889	1451.0468
1470.4462	1482.7514	1533.5251
1592.1335	1624.0681	1655.4261
1703.3560	3026.0843	3063.9801
3122.2237	3134.2495	3155.2857
3159.9322	3169.6693	3178.1615
3185.3787	3207.5535	3208.2649

ZeroEnergy[kcal/mol] -31.98

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i12-----

Well i12

Species

RRHO

Geometry[angstrom] 24

C	0.1943913493	-1.3242603157	-0.025109683
C	1.4355537785	-0.6506294206	-0.0082297025
C	0.3105604907	1.5104254756	-0.0150867385
C	1.4942519245	0.727056357	-0.0033290084
C	-0.949208093	0.8256464075	-0.0321223328
C	-0.9702526928	-0.595862192	-0.0367408612
C	2.8200223873	-1.2636394145	0.0063945785
C	2.9284101337	1.2164925146	0.0153957947
C	3.7144470772	-0.0608513927	0.0207512141
C	-0.8613572321	3.6397595351	-0.0217474603
C	-2.1032875652	2.9655098649	-0.0386060118
C	0.315791187	2.9295838267	-0.010635104
C	-2.143024338	1.591883006	-0.0440331459
H	0.1623678041	-2.4088454738	-0.0289384892
H	-1.9310277686	-1.1002178099	-0.049870609
H	2.9694074197	-1.9159998975	0.8818320135
H	2.9903536756	-1.9107211368	-0.8691349318
H	3.1375252911	1.8459151084	0.8955507336
H	3.1585557436	1.8514890195	-0.8554405529
H	4.795073097	-0.1067502587	0.0326211302
H	-0.8406745798	4.723925685	-0.0178300282

```

H -3.0244076131  3.5373253286  -0.0472952666
H  1.2642167378  3.4546368863  0.0024514452
H -3.0954672145  1.071829297  -0.0568969836
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
107.0347          128.5822          178.5528
226.0360          235.7459          276.7961
353.2598          420.6255          428.3238
460.9840          507.1061          519.1965
533.6438          603.7883          642.7840
671.0801          744.3952          751.4360
781.2758          788.6921          819.9104
868.7519          873.0958          911.2996
928.9603          930.0905          958.7096
960.1686          970.3396          993.5062
1025.4738         1045.4108         1072.8487
1129.5129         1137.3270         1167.6668
1177.4834         1184.1677         1211.9936
1234.2417         1271.5962         1283.4728
1324.5227         1345.9942         1377.9925
1400.1998         1412.7276         1457.6092
1463.8398         1470.8638         1497.5903
1552.6952         1612.0053         1636.2092
1665.8059         2947.8933         2949.9134
2952.4191         2952.4886         3155.0524
3157.4553         3165.2023         3173.7437
3178.2148         3188.1034         3204.6060
ZeroEnergy[kcal/mol] -66.29
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----well_i13-----
Well      i13
Species
RRHO
Geometry[angstrom]  24
C  0.261049  -0.089069  -0.216966
C -0.79516  0.861023  -0.361462
C  0.788239  2.640725  0.15189
C -0.51286  2.196729  -0.178266
C  1.815878  1.743195  0.29655
C  1.590333  0.354183  0.115933
C -2.199608  0.389941  -0.68833
C -3.416207  -1.424164  0.567835
C -2.916686  -0.194094  0.504951
C  2.39137  -1.950033  0.068606
C  1.08528  -2.41084  -0.260585
C  2.627062  -0.608499  0.249284
C  0.117122  -1.471271  -0.38508
H  0.969263  3.701194  0.287115

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H -1.306717  2.927735  -0.293238
H  2.81536   2.083052  0.547222
H -2.771047  1.246393  -1.064012
H -2.165734  -0.354058  -1.490121
H -3.329557  -2.115735  -0.264468
H -3.926126  -1.785086  1.453983
H -3.013656  0.468116   1.3633
H  3.197352  -2.668232  0.175565
H  0.892153  -3.468698  -0.401518
H  3.623833  -0.261639  0.500021
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
40.2572          67.2218          114.2085
168.6763        189.2897          239.6669
300.7709        377.9173          438.3903
447.0916        469.7792          492.6279
518.9589        564.6048          571.2018
617.4952        669.1613          734.7892
753.0874        774.5818          797.1910
817.9802        870.1966          884.1742
914.7536        920.3708          939.5138
947.1807        970.2855          985.1761
1025.1230       1030.7407         1053.7051
1086.5542       1124.1950         1163.2422
1186.1828       1193.4516         1226.0620
1250.5993       1261.7657         1316.6304
1329.4682       1352.7153         1373.5732
1395.2005       1449.2717         1454.4843
1471.8398       1478.6350         1511.5740
1591.5573       1636.9210         1655.3637
1703.3275       3018.4222         3063.1276
3123.2666       3132.4421         3156.0526
3157.2713       3163.4401         3168.2463
3180.6274       3183.3422         3211.2476
ZeroEnergy[kcal/mol] -32.71
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i14-----
Well          i14
Species
RRHO
Geometry[angstrom] 24
C  1.030888025  -0.4131209403  0.3405528696
C  0.8779823504  0.8141811129  -0.3731879815
C  1.1265063657  2.0492277611  1.7078811452
C  0.9233765303  2.008536835   0.3121456091
C  1.2785487799  0.8844534124  2.4173893752
C  1.2329358268  -0.371275804  1.7603135824
C  0.6783770194  0.8046386159  -1.8782901368

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C 0.7843530895 -1.758999396 -1.8178811619
C 0.2230112014 -0.5113397576 -2.4052423777
C 1.3277772364 -2.7920516625 1.8219671279
C 1.1245878035 -2.8340176431 0.4262282327
C 1.3812509128 -1.5866546142 2.475623363
C 0.9815635246 -1.6811252354 -0.3143862087
H 1.1570343188 3.0068469936 2.2157913136
H 0.7986758005 2.9391313789 -0.2330489695
H 1.4328659221 0.9071315945 3.4910278108
H -0.0205538876 1.5980924879 -2.1621321471
H 1.6396888032 1.0855227674 -2.3521205861
H 1.7663247947 -1.9817604902 -2.2800413308
H 0.1535656039 -2.6197928449 -2.0623701061
H -0.2817882916 -0.5548061034 -3.3633340369
H 1.436662743 -3.7189242004 2.3742265476
H 1.078517859 -3.7963752005 -0.0743094078
H 1.5347696682 -1.5458980674 3.5488424741
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
78.9096 133.8973 164.1190
235.4993 239.1190 388.1462
395.0495 437.3452 452.1558
470.1947 476.0541 477.5626
571.1033 574.5909 598.8709
635.5373 726.9066 759.0918
787.1068 806.5144 808.6198
832.0184 851.0386 911.7637
913.6174 918.1345 967.2240
976.6489 986.1117 1045.8801
1050.1993 1083.7823 1103.6479
1141.4497 1168.4922 1184.4790
1192.6991 1219.2144 1226.0687
1250.3849 1264.7307 1293.0811
1361.4426 1381.9365 1388.3936
1389.9532 1418.2059 1449.8624
1458.4621 1467.3333 1497.5369
1546.6549 1623.9166 1639.3150
1658.3129 2876.6264 2879.8878
3040.1730 3040.3073 3152.1672
3152.2942 3161.2850 3163.9993
3173.7231 3181.0291 3182.5125
ZeroEnergy[kcal/mol] -67.59
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i15-----
Well i15
Species
RRHO
Geometry[angstrom] 24

```

```

C -0.267883467 -1.1131542874 0.0075401891
C -1.3590207195 -0.1463893274 -2.25164E-4
C 0.3080853584 1.6586525622 -0.0233998281
C -1.0184768093 1.2177889608 -0.0154426175
C 1.3473928714 0.7542721909 -0.0163936363
C 1.084399494 -0.6407760245 -8.625729E-4
C -2.7203669229 -0.5710651066 0.007019508
C -5.1459457263 -0.2274635296 0.008614099
C -3.8712360018 0.2505901481 0.001152609
H 0.5135755966 2.7232912719 -0.0352719917
H -1.8053272371 1.9606300103 -0.0214535437
H -2.9191070731 -1.6359327538 0.0180694494
H -5.9996252126 0.438299187 0.0037366832
H -5.3496973425 -1.2931284422 0.0197363051
H -3.7430035464 1.3289735621 -0.0099183379
C 1.9132980082 -2.9280015968 0.0218093937
C 0.5859685555 -3.3992844495 0.0302543985
C 2.1514419629 -1.5754431774 0.0066011962
C -0.4704723032 -2.5147834159 0.0232842589
H 2.7388434743 -3.6306482838 0.0274011924
H 0.3927904731 -4.4660716365 0.0422629456
H 3.168312565 -1.1969382809 2.247798E-4
H -1.474494032 -2.9168353855 0.0303298622
H 2.3774300343 1.0936208044 -0.0226621779

```

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

```

55.7169          66.7403          140.9919
152.4080        173.2745          260.6782
317.9342        360.2731          423.0701
448.7745        478.8529          510.1570
535.2604        543.7539          607.0310
641.2200        643.6401          735.2366
760.8168        775.5787          785.5649
799.9843        825.3613          863.8814
869.4634        875.6316          890.3688
956.5479        973.1059          983.1783
992.7291        998.7572          1044.5701
1059.5033       1118.9906         1161.3729
1185.7507       1188.9434         1209.5502
1221.9230       1252.3429         1274.9857
1313.4882       1334.0721         1373.2637
1391.6244       1422.9515         1464.4765
1484.9173       1494.5595         1533.2962
1558.3801       1592.2324         1606.6464
1652.9966       3135.4157         3148.1814
3159.1674       3163.2331         3169.8635
3177.7327       3179.6291         3186.5014
3199.1524       3207.6014         3229.2060

```

ZeroEnergy[kcal/mol] -64.08

ElectronicLevels[1/cm] 1

0 2

End

```

End
!-----
!-----well_i16-----
Well      i16
Species
RRHO
Geometry[angstrom]  24
C  -0.1774061305   -1.2620667521   -0.0893067904
C  -1.3549546384   -0.4235356263   -0.2236631984
C   0.1067759529   1.5454915899   -0.2358048395
C  -1.167842671    0.9614737738   -0.2906364731
C   1.2307700172    0.7617466408   -0.1194201315
C   1.1168514158   -0.6513732969   -0.0473111956
C  -2.6608560836   -1.012345914    -0.3609766131
C  -4.2348311562    0.6733538077    0.6366340117
C  -3.9269574866   -0.4478673597   -0.0813836664
H   0.1993694212   2.6235251706   -0.3075787114
H  -2.0271915497    1.5976708068   -0.4528430573
H  -2.6903098569   -2.024355554    -0.7481332606
H  -5.2682155511    0.9655223085    0.7769390031
H  -3.4838828471    1.2745393269    1.1321507236
H  -4.7696575849   -1.0274457677   -0.4536726813
C   2.1649567316   -2.8353853565    0.1695312955
C   0.8915833848   -3.4401556799    0.153891825
C   2.2695872621   -1.4691085941    0.0768042599
C  -0.2452266471   -2.6724048868    0.0342654418
H   3.0543635993   -3.4479211372    0.2646766552
H   0.8061960928   -4.5171204281    0.2457515682
H   3.2428127482   -0.9899092938    0.1019793772
H  -1.2098838565   -3.1621372652    0.0561401003
H   2.2179354336    1.2101294874   -0.086640643
Core RigidRotor
SymmetryFactor  0.5
End
      Rotor      Hindered      ! 58 cm^-1      CH3
      Group                8 9 12 13 14 15
      Axis                2 7
      Symmetry                1
      Potential[kcal/mol]      8
0      4.01606E-05 2.903614885 3.689028478 3.671993475 9.703104234 3.695189367
      2.892052393
      End
Frequencies[1/cm]  65
                    95.8452                    156.4647
178.3147            202.8461                    268.8782
321.4872            411.1400                    427.8340
445.8091            481.3369                    508.7393
545.1694            547.4310                    568.2200
637.7875            669.2575                    741.3992
764.2918            769.7920                    794.6788
804.0690            817.7148                    856.7810
868.2623            882.7967                    920.2123
964.0025            982.4033                    988.6037
995.4822            1002.6832                   1051.1844

```

1067.1235	1101.3716	1141.6305
1166.3798	1187.2048	1198.6973
1224.6438	1260.9722	1278.5363
1292.7332	1343.6366	1378.1856
1413.3854	1446.4141	1456.5856
1473.5980	1485.5932	1536.5114
1561.4416	1592.8425	1614.7152
1654.9460	3121.0357	3149.9866
3158.7703	3162.3587	3166.9444
3171.4037	3179.2642	3185.2642
3199.9266	3204.8535	3239.2783

ZeroEnergy[kcal/mol] -61.17

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i17-----

Well i17

Species

RRHO

Geometry[angstrom] 24

C	0.2500308018	1.5403092821	-0.0233822633
C	1.4718288692	0.8123331749	-0.0976070745
C	0.2125923459	-1.3594684083	-0.1383547785
C	1.4883868688	-0.6512771951	-0.4848813804
C	-0.9215502726	-0.6664064138	0.0480178094
C	-0.9712352534	0.7926274165	0.0210657126
C	2.7968318161	1.1947235164	0.2286317343
C	2.8344632655	-1.1721746663	0.0904215694
C	3.6150823059	0.1017127491	0.3034241728
H	0.2080759883	-2.4450952958	-0.1160358937
H	1.591017133	-0.6897546637	-1.5870377083
H	3.1103545484	2.2084681003	0.4459269913
H	3.3320253927	-1.8865939309	-0.5715302115
H	2.6752794018	-1.684564201	1.0508592321
H	4.6641907469	0.1229404434	0.5693738706
C	-2.2308392333	2.8667670268	0.1687657163
C	-1.038532339	3.6008669495	0.1445096819
C	-2.1865846158	1.4771205204	0.1161672502
C	0.1804741575	2.9497614135	0.0595802265
H	-3.1842037107	3.377993258	0.2360938328
H	-1.0687660315	4.683902612	0.1896435578
H	-3.108689889	0.9059600047	0.1581720979
H	1.0972192341	3.5279785343	0.0326231139
H	-1.8543115308	-1.1894392269	0.2366527406

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

90.6488	106.4262	189.6997
238.6207	255.0841	361.1524
413.3124	425.0734	445.7761
496.5394	518.0739	541.0825

579.2870	649.8980	683.5008
698.1687	723.7031	747.7860
768.8834	790.7789	824.0169
854.9281	873.9721	921.4270
937.5715	945.3123	950.1509
977.2845	985.1344	989.3134
1047.1039	1061.9216	1075.8915
1104.3607	1137.1859	1152.6790
1170.0712	1181.3741	1204.1635
1228.5702	1261.0226	1279.9605
1292.8037	1331.3527	1339.8356
1351.2277	1416.1883	1424.1420
1458.1698	1477.4136	1488.5870
1513.6667	1573.0875	1618.3977
1666.4525	2873.9468	2978.5334
3058.2917	3144.5500	3155.5668
3163.1079	3165.9099	3176.4631
3185.0641	3188.5998	3205.7889

ZeroEnergy[kcal/mol] -60.54
 ElectronicLevels[1/cm] 1
 0 2

End
 End

!-----
 !-----well_i19-----

Well i19

Species

RRHO

Geometry[angstrom] 24

C	0.6206530597	-0.4605060987	-0.245038274
C	1.3686992392	0.7237224546	-0.1458507559
C	-0.6881829697	1.9907176885	0.0892955037
C	0.7048727928	1.9476301958	0.0096507083
C	-1.4271280982	0.8205314502	0.0290606753
C	-0.787649979	-0.4285957074	-0.1367958281
C	2.8334253611	0.6390742112	-0.1671827856
C	2.7059469953	-1.8116639366	0.1958080674
C	3.4707576879	-0.5253835198	0.0083501027
C	-0.8555370926	-2.8950383505	-0.2167595441
C	0.5048385677	-2.9749061462	-0.3600424105
C	-1.5228941749	-1.6604792704	-0.1544287867
C	1.3547726331	-1.7536774404	-0.5463198513
H	-1.1919547373	2.9433731903	0.2098170031
H	1.2831234812	2.8629541757	0.0793230412
H	-2.5084370612	0.851605256	0.1122309577
H	3.3927524239	1.5641037162	-0.2688551086
H	3.2867571993	-2.6633330546	-0.1712458257
H	2.5376177286	-1.9900775296	1.2683166621
H	4.5544295129	-0.5547153449	0.0614397711
H	-1.4371543339	-3.8086856286	-0.1439405429
H	0.995665784	-3.9416570241	-0.4092602009
H	-2.6022235247	-1.6279343463	-0.0607007792
H	1.6228335048	-1.7055299406	-1.6219277991

Core RigidRotor

```

SymmetryFactor 0.5
End
Frequencies[1/cm] 66
117.6881      138.3197      197.6327
230.3082      361.4098      383.5760
420.6596      448.8591      459.1684
479.5070      489.3342      549.7250
568.3033      599.5874      634.4620
685.3026      713.3897      752.7517
761.4686      775.7725      798.6934
827.5272      836.1899      898.7177
944.5908      964.0838      972.0881
981.4039      990.4356      1015.4540
1044.9562     1077.2726     1101.6610
1104.5623     1174.4498     1177.5722
1187.7393     1197.5879     1212.0714
1236.2883     1254.9207     1274.2591
1322.3698     1324.6317     1362.5004
1379.2632     1414.5105     1433.1006
1475.0850     1477.2481     1493.1682
1548.3550     1600.8551     1609.8554
1684.3810     2857.4538     2982.5854
3053.9036     3148.0724     3149.7639
3157.3805     3165.4177     3166.5317
3169.9098     3181.2858     3183.4637

```

```

ZeroEnergy[kcal/mol] -66.13
ElectronicLevels[1/cm] 1
0 2
End
End

```

```

!-----
!-----well_i20-----
Well      i20

```

```

Species
RRHO
Geometry[angstrom] 24
C -0.3568356392 -0.9503959611 -0.1696642696
C -1.324671389 0.1532618425 -0.2040444128
C 0.5368707297 1.7413513423 0.0200909905
C -0.8244008288 1.4875908002 -0.1060652958
C 1.4581690012 0.7066506856 0.0555999294
C 1.0308027366 -0.6494881643 -0.0385998686
C -2.6583555933 -0.0681370037 -0.322674603
C -3.937415269 -0.2565434166 -0.4600107163
C -4.9328005369 -0.437706308 0.66632406
H 0.8782050994 2.7683813331 0.0911168443
H -1.5342229471 2.3050357638 -0.132555994
H -4.3578187 -0.2903154257 -1.4699997012
H -4.4437345405 -0.3952997853 1.6400540844
H -5.4453729175 -1.4009129349 0.574966908
H -5.7006176081 0.3418961457 0.6274865817
H 2.5173357694 0.9159940126 0.154867535
C 1.5430071383 -3.0279360638 -0.0987068076
C 0.1732635217 -3.3200404463 -0.2286636318

```

```

C  1.9599855722  -1.7185446201  -0.0059151812
C  -0.7544943781  -2.2969136253  -0.2630492692
H  2.2680943829  -3.8336334408  -0.0717386643
H  -0.1552797619  -4.3506097212  -0.3018382768
H  3.0150251829  -1.4856361204  0.0943324407
H  -1.8093920249  -2.5246168884  -0.3644086817

```

```

Core RigidRotor
SymmetryFactor 0.5
End

```

```

Frequencies[1/cm] 66
52.4134          74.5911          124.7622
143.4908        174.8683          214.1369
233.6810        345.2472          380.6539
417.4539        481.3706          485.3626
500.0020        541.5363          556.7608
590.3862        634.3970          696.7137
726.4502        767.2286          782.0196
796.8542        799.3888          850.0816
852.8685        884.5450          933.1043
963.6443        968.7438          992.8568
1042.1795       1053.9296         1061.6849
1075.4953       1101.4720         1153.6398
1166.3883       1183.2988         1186.0348
1233.0620       1281.7745         1316.7667
1343.2225       1362.0033         1400.5062
1407.5653       1462.2382         1468.0289
1484.6354       1492.4315         1519.3916
1554.4512       1589.0504         1643.9989
1915.4934       3018.7667         3038.2257
3068.3592       3117.3523         3157.9489
3162.4189       3168.0479         3177.9747
3179.5281       3189.2598         3192.6879

```

```

ZeroEnergy[kcal/mol] -48.05
ElectronicLevels[1/cm] 1
0 2

```

```

End
End

```

```

!-----

```

```

!-----well_i21-----

```

```

Well      i21

```

```

Species

```

```

RRHO

```

```

Geometry[angstrom] 24
C  -9.2859674738  -0.4309097014  0.2025466707
C  -9.3093779291  -1.8112750965  0.0096190143
C  -8.0525873993  -2.4395706951  -0.1606143026
C  -6.8892815952  -1.6743525483  -0.2061378757
C  -6.9162140681  -0.2713784642  -0.1418346979
C  -8.150585479   0.3593461473  0.0401510575
C  -10.4927937247  0.4203937495  0.4145081482
C  -11.7136493242  -0.2095171246  -0.192457384
C  -11.7349188311  -1.5773758012  -0.3632552993
C  -10.6050098845  -2.4062316166  -0.1801888339
C  -8.608543469   1.7560140073  0.0016687261

```

```

C -9.9535561607 1.8215780677 0.1252845267
C -10.8153879227 3.0417051764 0.1286618887
H -7.9989427615 -3.5140191836 -0.3009201536
H -5.9369287436 -2.1750072515 -0.3437808756
H -6.0003426838 0.2968711291 -0.260566556
H -10.6849177263 0.4430447638 1.5107361755
H -12.6071945604 0.3815265938 -0.3592606281
H -12.66321824 -2.0456989547 -0.6759915699
H -10.6937766701 -3.4768887498 -0.3247120383
H -7.9563445217 2.6116602375 -0.1282390741
H -11.366916219 3.140177008 1.0710839571
H -10.2232647326 3.9482576331 -0.0122112285
H -11.5640448797 2.9997806738 -0.6711136473

```

```

Core RigidRotor
SymmetryFactor 0.5

```

End

```
Frequencies[1/cm] 66
```

```

118.7913 157.0522 160.5839
196.8446 225.4279 292.2623
352.8514 405.1368 469.2695
481.5610 504.5838 530.9203
540.7660 577.8873 598.1561
631.4909 664.7759 711.9780
750.9904 776.6173 797.8826
806.0638 818.6475 875.9718
894.2700 932.5644 956.0805
968.4436 1010.7453 1034.0550
1053.3730 1068.1192 1070.4166
1083.3051 1142.4467 1164.4746
1168.3169 1190.1147 1202.3254
1232.4356 1276.7291 1292.9118
1318.7069 1338.8860 1385.3753
1415.8920 1422.0973 1469.3511
1478.6834 1481.0981 1490.6256
1524.7270 1605.1903 1622.0306
1643.0127 2834.0754 3007.4331
3047.1352 3098.4643 3151.3504
3157.7559 3170.1699 3173.7003
3181.7504 3183.1780 3186.2363

```

```
ZeroEnergy[kcal/mol] -59.27
```

```
ElectronicLevels[1/cm] 1
```

```
0 2
```

End

End

```
!-----
```

```
!-----well_i22-----
```

```
Well i22
```

Species

RRHO

```
Geometry[angstrom] 24
```

```

C -0.201397855 -0.0107686372 0.0818276784
C -1.3411878734 0.780334085 -0.1322769652
C -2.5672534631 0.0768100584 -0.3305487394
C -2.589432867 -1.3156666903 -0.3057527692

```

C	-1.4429859868	-2.0985715069	-0.0916358821
C	-0.2074675918	-1.4488852274	0.1097296708
C	1.0839804802	0.4997692354	0.297365751
C	1.2611648506	1.8700035767	0.2996477147
C	0.1331890844	2.6988631755	0.0851540171
C	-1.1352184829	2.1831922521	-0.1251664169
C	1.1022674094	-1.8720152118	0.3477251779
C	2.032701582	-0.6784872484	0.4898271296
C	3.2212142901	-0.6994988794	-0.4911668386
H	-3.4852722685	0.6285778425	-0.5007395448
H	-3.5376676479	-1.8202769006	-0.4593067671
H	-1.5167130126	-3.1799919026	-0.082316788
H	2.2341790644	2.3212438794	0.4626613361
H	0.2701731024	3.7748851907	0.0872488474
H	-1.9733855292	2.8535026167	-0.2842713202
H	1.4397505948	-2.8973872752	0.4274028469
H	3.8518270616	0.1835335466	-0.3575789565
H	3.8426802993	-1.5841982226	-0.3284117647
H	2.8673262177	-0.7139935601	-1.5246979185
H	2.4411875412	-0.6554541965	1.5116155013

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

93.0384	167.6773	173.7045
235.0537	238.7650	283.1505
387.1133	420.9094	480.7843
495.9576	505.0357	526.6202
546.5100	597.6685	625.3395
654.6819	671.0319	702.1868
755.3628	779.5146	807.3659
818.8732	831.5125	862.0047
904.6750	908.8404	970.0565
975.7381	978.6399	1033.4482
1049.4102	1067.4763	1075.8978
1094.7036	1131.4514	1175.7350
1176.9393	1211.8116	1221.2722
1243.2087	1280.1966	1304.5661
1335.1422	1366.0235	1398.1368
1411.8916	1422.0644	1458.7169
1466.9905	1496.8708	1497.4516
1514.0950	1574.3678	1622.9528
1637.2044	2972.8779	3026.8250
3091.0097	3101.4387	3156.7370
3158.1104	3166.8993	3174.1911
3180.7678	3183.9661	3200.9834

ZeroEnergy[kcal/mol] -76.39

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_mn-il-----

Well mn-il

Species

RRHO

Geometry[angstrom] 24

```
C -0.0732407572 -0.0995987221 -1.7516201268
C 0.0895285362 -1.5237616502 -1.7427856825
C 1.3961999735 -2.0764758097 -1.7503116
C 2.4965215006 -1.2588598499 -1.7708501151
C 2.3367566193 0.1443046489 -1.789943027
C 1.0911301761 0.7347452743 -1.7818680534
C -1.3955945902 0.4217528427 -1.7352493572
C -2.4896883615 -0.4097148024 -1.7191828172
C -2.3243872982 -1.8126762437 -1.7162095194
C -1.0626078234 -2.352959549 -1.7263171146
C 0.9813565513 2.2427050809 -1.8100029663
C 0.6655243 2.9201261373 -0.4758475811
C 0.513351444 2.3416758198 0.6858046387
H 1.5082343037 -3.1555990277 -1.7411722651
H 3.4945231502 -1.682498381 -1.7780617
H 3.2201700086 0.7741698394 -1.8146013952
H -1.5442647741 1.4937663243 -1.7188177711
H -3.4881921153 0.0127101666 -1.7052352872
H -3.1954019205 -2.4581590553 -1.7037477299
H -0.9260717963 -3.4294921597 -1.7216540487
H 1.9261307243 2.660527745 -2.1743743104
H 0.2232197857 2.5588126031 -2.5366534885
H 0.5761520424 4.0067419192 -0.5407695688
H 0.5272413208 1.3497108493 1.1108218867
```

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

```
53.3614 82.9494 119.0196
155.6686 176.4210 263.8030
287.5392 408.0331 435.4376
438.4823 479.1115 512.1609
519.8877 559.7255 614.0518
634.8837 666.9745 716.5035
745.2461 792.4842 803.0203
810.8117 831.3808 860.0383
862.2906 888.6769 923.0979
938.4419 959.5154 965.0696
983.3132 995.3428 1041.3642
1063.8535 1098.8366 1168.2040
1183.2316 1188.7917 1206.4912
1232.5338 1242.7524 1262.2958
1289.4052 1343.3862 1383.0464
1394.6156 1426.5894 1471.2437
1484.0531 1495.3965 1548.4388
1619.6010 1640.5069 1664.4843
1668.5030 3013.9465 3043.6485
3074.5271 3155.7103 3157.7211
3163.8138 3169.1093 3182.9376
3183.8885 3200.2215 3246.4982
```

ZeroEnergy[kcal/mol] -35.64

```

ElectronicLevels[1/cm]      1
0 2
End
End
!-----
!-----well_mn-i2-----
Well      mn-i2
Species
RRHO
Geometry[angstrom]  24
C  -0.0614156877  -0.3888170723  -1.0440878944
C  0.0912647997  -1.8000448296  -1.0458565072
C  1.3930580286  -2.3411281044  -1.0406248664
C  2.5021562481  -1.5113497146  -0.9982722465
C  2.3371981953  -0.1275026739  -0.9426266241
C  1.057727589   0.4397399779  -0.9662560374
C  -1.4491195444  0.2263766599  -1.1464742398
C  -2.5532025591  -0.7343313656  -0.8049311695
C  -2.3478021508  -2.0875695127  -0.7945910383
C  -1.0693676612  -2.6395980129  -0.9789306316
C  0.880256182   1.9435299223  -0.883301256
C  -0.4530181407  2.3352196625  -0.2987631887
C  -1.5189178245  1.5487668792  -0.4069264597
H  1.5153590155  -3.4191421108  -1.0498338318
H  3.4991777151  -1.9377034897  -0.9884291891
H  3.2064336908  0.5188830035  -0.8764577431
H  -1.5968872437  0.476648094   -2.2192633699
H  -3.5457833657  -0.3241862433  -0.6505624073
H  -3.1883086778  -2.7534382937  -0.6264214174
H  -0.9360138808  -3.7152724173  -0.9843590001
H  1.6966184045  2.3775945363  -0.2978745925
H  0.9756919389  2.3819936904  -1.8890423845
H  -0.5227221894  3.2921305305  0.2089054937
H  -2.4777208816  1.8435728844  0.0084946015
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
  73.8282          135.0816          196.1165
 228.6736          333.3816          408.8948
 422.0391          440.2987          461.2935
 472.9847          494.0553          540.5876
 568.6555          578.4549          629.5698
 674.2795          702.9351          753.2463
 760.4692          782.4585          798.0864
 817.2684          860.8828          892.8386
 951.4117          956.8597          961.3913
 973.6289          987.6632          1013.4821
1038.0615          1069.2465          1100.8989
1102.8855          1171.4331          1182.3333
1186.8380          1196.9666          1208.5272
1228.7245          1245.0318          1253.1428
1288.5226          1328.4496          1352.3905
1381.8033          1398.3706          1429.8854

```

```

1470.5125          1474.0839          1495.4950
1549.3595          1608.4451          1611.4796
1713.9972          2830.9147          2967.4399
3047.9995          3144.9646          3151.4419
3155.1017          3163.5031          3166.8916
3169.3724          3180.6716          3182.9415
ZeroEnergy[kcal/mol] -63.95
ElectronicLevels[1/cm]      1
0 2
End
End
!-----
!-----well_mn-i3-----
Well      mn-i3
Species
RRHO
Geometry[angstrom]  24
C  -0.2206232065  -0.1774585555  -0.4407141679
C  -0.0567393331  -1.5962595593  -0.2527121672
C  1.2820133725   -2.1668315464  -0.3113106883
C  2.3595157492   -1.4542974403  -0.6751332458
C  2.2159682657   -0.0409218229  -1.1667918369
C  0.9023821186   0.591579799   -0.7813885419
C  -1.5096647297   0.3818746673  -0.2221849444
C  -2.5887388423   -0.4185673198  0.1029181844
C  -2.4270404526   -1.8042530673  0.2473070844
C  -1.1664535766   -2.3738354801  0.0813353079
C  1.1018390508    2.0747749669  -0.5942850596
C  2.6105259339    2.1765017961  -0.4716108495
C  3.2179884056    1.0238381544  -0.7483736582
H  1.3913844519   -3.207716518  -0.0212995551
H  3.3447128951   -1.9099235908  -0.6983993377
H  2.2783695413   -0.103113461  -2.2770854414
H  -1.6472060533   1.4506512109  -0.3415456847
H  -3.5669061401   0.0277268027  0.2450305424
H  -3.2761511435   -2.4277461794  0.5018720467
H  -1.0337624948   -3.4410029226  0.2300000256
H  0.7380061252    2.6716722262  -1.4472650212
H  0.5768021492    2.4585272989  0.2888400499
H  3.1121395485    3.1010905503  -0.2114641463
H  4.2891673652    0.8593239908  -0.7552538953
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
  78.1236          120.9526          192.4001
 220.6411          241.8846          371.4930
 402.0717          419.5705          449.8211
 487.6927          507.4496          526.6119
 576.0304          647.4431          679.6381
 699.1476          726.4716          753.8288
 781.6647          797.2120          817.5927
 843.6963          863.8824          923.2826
 940.1207          945.6262          962.1627

```

967.3196	974.8294	987.5209
1025.7892	1050.3361	1072.9373
1117.7204	1125.0367	1152.5356
1155.2884	1173.2464	1182.9303
1218.1324	1243.1689	1279.1121
1284.1656	1301.9580	1332.2969
1363.9155	1411.3922	1424.9313
1455.9011	1468.1314	1488.4562
1561.3283	1605.4836	1660.6373
1672.9124	2803.3705	2945.4219
3018.0037	3144.4505	3154.4395
3162.2598	3166.0874	3174.6086
3177.0975	3188.1742	3198.5903

```

ZeroEnergy[kcal/mol] -53.89
ElectronicLevels[1/cm] 1
0 2
End
End

```

```

!-----
!-----c10h7_c3h4_p0p-----
Bimolecular p0p
Fragment c3h4
RRHO

```

```

Geometry[angstrom] 7
C -0.823420841 0.0519880348 -0.0208571707
C 1.824711204 -0.1816552298 1.678957E-4
H -1.8820502847 0.1362504236 -0.0342313517
H 2.1265806386 -1.2327357481 0.0038417281
H 2.2515118512 0.2935470245 0.887798287
H 2.2667123243 0.2920674571 -0.8807572055
C 0.3727611076 -0.0556769621 -0.0121801829

```

```

Core RigidRotor
SymmetryFactor 3.0
End

```

Frequencies[1/cm] 15		
339.4278	339.9763	666.0166
666.0469	943.1202	1056.2902
1056.6567	1416.3162	1479.4028
1479.6937	2229.8067	3026.9185
3085.7411	3086.1443	3478.9987

```

ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End

```

```

Fragment c10h7
RRHO
Geometry[angstrom] 17
C 0.014468 -0.761638 0.0
C 1.273145 -1.416493 0.0
C -1.226649 -1.409071 0.0
C 2.435985 -0.68536 0.0
C 2.394138 0.728582 0.0
C 1.190743 1.391526 0.0
C -0.035299 0.677452 0.0

```

```

C -2.446252 -0.820405 0.0
C -1.301795 1.322885 0.0
C -2.472747 0.604434 0.0
H 1.296576 -2.499829 0.0
H 3.394416 -1.191867 0.0
H 3.321619 1.290112 0.0
H 1.161733 2.476345 0.0
H -3.369305 -1.389453 0.0
H -1.330033 2.407247 0.0
H -3.42943 1.115969 0.0
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 45
169.5513 186.3331 361.7572
400.6956 462.4518 507.3376
508.4714 521.5661 610.9897
631.4357 731.1317 772.9822
773.8392 790.0839 800.0831
865.8314 893.2849 932.4053
964.6946 976.4209 998.9404
1033.6684 1046.5606 1138.8725
1169.0256 1175.9683 1197.8985
1236.3006 1270.8697 1359.7546
1378.0259 1389.4947 1451.5684
1484.0991 1520.9853 1582.9071
1637.0922 1662.7184 3157.5448
3159.0870 3169.4881 3170.4343
3181.2007 3182.1190 3192.4871
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 0.0
End
!-----c10h7_c3h4_p0a-----
Bimolecular p0a
Fragment c3h4
RRHO
Geometry[angstrom] 7
C -0.7953643067 0.0340930197 3.929351E-4
C 1.7999079767 -0.188313622 -0.0384040502
H -1.2789000818 0.9884787247 0.182918491
H -1.4365104427 -0.8255826572 -0.1664284561
H 2.3603730273 -0.4130354538 0.8635083944
H 2.3636835038 -0.0613232862 -0.9572540549
C 0.5024913234 -0.0757887252 -0.0189202593
Core RigidRotor
SymmetryFactor 4.0
End
Frequencies[1/cm] 15
371.2233 371.5183 865.8663
866.2617 884.0403 1016.3687
1016.5866 1109.0953 1422.1712

```

```

1479.1925          2051.9260          3118.9601
3123.0938          3193.6015          3194.4729
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment          c10h7
RRHO
Geometry[angstrom]  17
C  0.014468   -0.761638   0.0
C  1.273145   -1.416493   0.0
C  -1.226649   -1.409071   0.0
C  2.435985   -0.68536    0.0
C  2.394138    0.728582   0.0
C  1.190743    1.391526   0.0
C  -0.035299    0.677452   0.0
C  -2.446252   -0.820405   0.0
C  -1.301795    1.322885   0.0
C  -2.472747    0.604434   0.0
H  1.296576   -2.499829   0.0
H  3.394416   -1.191867   0.0
H  3.321619    1.290112   0.0
H  1.161733    2.476345   0.0
H  -3.369305   -1.389453   0.0
H  -1.330033    2.407247   0.0
H  -3.42943    1.115969   0.0
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  45
169.5513          186.3331          361.7572
400.6956          462.4518          507.3376
508.4714          521.5661          610.9897
631.4357          731.1317          772.9822
773.8392          790.0839          800.0831
865.8314          893.2849          932.4053
964.6946          976.4209          998.9404
1033.6684         1046.5606         1138.8725
1169.0256         1175.9683         1197.8985
1236.3006         1270.8697         1359.7546
1378.0259         1389.4947         1451.5684
1484.0991         1520.9853         1582.9071
1637.0922         1662.7184         3157.5448
3159.0870         3169.4881         3170.4343
3181.2007         3182.1190         3192.4871
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol]  1.14
End
!-----h_c13h10_p1-----
Bimolecular    p1
Fragment          c13h10

```

RRHO

Geometry[angstrom] 23

C	-0.0437500061	0.0123095206	0.0252617316
C	0.6512048508	1.2535293387	0.0674946639
C	-1.4811697898	2.4219864887	0.0295580341
C	-0.0733849906	2.4297205801	0.0689110895
C	-2.1697345502	1.2326288178	-0.0114837262
C	-1.4723860618	4.463414E-4	-0.0147419459
C	2.1674259738	1.2854522682	0.1103769977
C	2.1271302562	-1.2065166299	0.0632193462
C	2.8216565622	-0.0652372226	0.1036075121
C	-1.4482975741	-2.4277915557	-0.0589128135
C	-0.0367694945	-2.4192400451	-0.0194545592
C	-2.1507497801	-1.2494370704	-0.0567039312
C	0.6679100113	-1.2321074712	0.0220911204
H	-2.0199183363	3.3631269993	0.0318430024
H	0.4509615944	3.3800208572	0.1009604327
H	-3.2541168815	1.2229121865	-0.0418266034
H	2.5455514135	1.8722361414	-0.7386036755
H	2.4970134376	1.8399994694	1.0003049323
H	2.6437836564	-2.1614699211	0.0598841027
H	3.9065563461	-0.0871677721	0.1334188125
H	-1.974612129	-3.3752899639	-0.0910812134
H	0.5049714574	-3.3593907628	-0.0217646563
H	-3.2351439657	-1.2535515946	-0.0869256535

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 63

89.1288	159.1117	202.1785
237.0345	378.2836	414.2774
432.7842	473.7832	478.3040
478.8314	504.4393	579.8259
580.2949	608.2522	646.5788
735.8134	763.3361	777.3378
793.2144	815.7311	824.6976
843.4769	897.7987	914.0571
954.4027	964.0034	979.9784
985.7081	1000.7368	1046.2329
1066.7674	1101.4892	1122.1096
1176.2572	1194.7653	1203.5052
1223.3532	1235.1670	1254.7218
1269.2080	1335.9060	1383.4596
1398.0764	1420.1847	1425.2403
1459.3047	1468.0401	1497.3962
1543.1068	1624.3055	1633.1183
1648.5874	1706.5838	2985.7361
2994.5071	3146.5544	3151.2918
3157.2425	3162.3213	3165.6717
3168.3035	3181.0060	3183.5965

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

End

```

Fragment      H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]    1
0  2
End
GroundEnergy[kcal/mol] -40.86
End
!-----h_c13h10_p2-----
Bimolecular  p2
Fragment      c13h10
RRHO
Geometry[angstrom]    23
C  -1.00819315  2.0029815592  -9.632184E-4
C  -1.628409413  0.7423855931  0.0011819134
C  0.5428905122  -0.3896342963  0.0020266231
C  -0.8788425691  -0.4297755539  0.0026152024
C  1.1693880937  0.9011689526  -1.452962E-4
C  0.3673101323  2.0745686408  -0.0016047233
C  -3.0944999782  0.3873861137  0.0023270246
C  -1.8036733799  -1.5679183356  0.0046518783
C  -3.0722254003  -1.1200886322  0.0045556658
C  2.7327038279  -1.4427688499  0.0027903843
C  3.3522129163  -0.1720040495  6.463853E-4
C  1.3622984979  -1.5473954491  0.0034644518
C  2.5875474865  0.9689121875  -7.786774E-4
H  -1.6038118374  2.9100381879  -0.0020854409
H  0.863146506  3.0395146806  -0.0032513242
H  -3.6160970822  0.7898381071  0.8802721015
H  -3.6169442175  0.7873346278  -0.8762454251
H  -1.5058101688  -2.6080462538  0.0064287965
H  -3.9648801754  -1.7311472901  0.0056825131
H  3.3450004555  -2.3376490281  0.0039081922
H  4.4342227121  -0.1023134772  1.303487E-4
H  0.896351355  -2.5261288065  0.0051186234
H  3.0613748766  1.9452413719  -0.002425999
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]    63
113.6369            131.8043            229.2486
241.8624            268.1795            387.6199
432.8761            438.9501            463.5555
506.1622            519.7898            564.9987
613.2146            666.3128            682.0154
723.1259            748.4914            753.1746
798.3392            817.3539            841.0882
879.1071            882.4464            933.1764
950.2629            955.0476            958.7634
966.8115            969.3634            992.8641
1043.8602           1074.0915           1126.0872
1143.1529           1166.9896           1178.4408
1191.9357           1216.8143           1236.5436
1283.2443           1293.4780           1351.7496

```

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1378.3128          1389.2441          1429.9837
1431.5175          1469.3301          1486.4362
1555.0881          1584.8304          1618.7769
1634.2324          1664.4116          3014.4320
3037.0896          3155.8948          3157.6475
3165.4279          3174.7870          3178.0413
3188.0239          3195.8059          3217.7140
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment      H
Atom
Mass[amu]     1
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol] -36.48
End
!-----h_c13h10_p3-----
Bimolecular    p3
Fragment      c13h10
RRHO
Geometry[angstrom]      23
C  0.2079539949  -1.3236037336  -0.0293198595
C  1.4449134189  -0.6402904261  -0.0118366402
C  0.3131038156  1.5259732599  -0.0154327576
C  1.4940034378  0.7494297974  -0.0050686174
C  -0.9423550658  0.8281988632  -0.0331950759
C  -0.9561627666  -0.5939419797  -0.0396786718
C  2.8170545022  -1.1568678191  0.0017974887
C  2.9396634748  1.1836529957  0.013893014
C  3.6841614526  -0.1299061388  0.016655728
C  -0.8786352872  3.6449545064  -0.0196538428
C  -2.1155777833  2.9588961608  -0.0372446822
C  0.3041744388  2.946775239   -0.0091436667
C  -2.1423509347  1.585418576   -0.0439367221
H  0.1795566913  -2.4078678834  -0.0345179255
H  -1.9161098602  -1.0996153168  -0.053153079
H  3.0735818544  -2.2088713166  1.193785E-4
H  3.1813661716  1.7876833877  0.8977900664
H  3.2019767323  1.7956598273  -0.8585622442
H  4.7634660877  -0.2019802964  0.029108642
H  -0.8681963824  4.7293030031  -0.0145329232
H  -3.0418440058  3.5222031879  -0.0454370489
H  1.248232734   3.4801673323  0.0043765793
H  -3.090263721  1.0570647739  -0.05740314
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]      63
111.6568          140.7102          235.6844
237.2977          257.3903          398.3061
432.9100          435.8335          465.2576

```

517.6351	520.4029	551.8127
616.8141	670.8690	681.8542
717.6867	751.4681	760.6125
787.6021	828.8345	839.7059
870.5954	872.9517	937.1086
954.6082	955.6063	959.7776
969.6397	982.1818	991.7866
1043.5437	1060.8248	1117.8038
1144.3104	1166.9374	1179.2839
1185.5663	1233.5486	1244.6810
1263.9404	1288.2738	1363.8797
1378.3823	1398.5186	1416.6139
1434.3843	1470.0655	1487.4275
1552.8417	1587.7447	1621.5463
1637.2740	1664.2119	3014.3619
3037.2215	3156.0943	3158.8407
3163.7816	3176.2621	3177.0994
3187.4040	3191.0726	3215.7707

ZeroEnergy[kcal/mol] 0.0
 ElectronicLevels[1/cm] 1
 0 1

End
 Fragment H
 Atom
 Mass[amu] 1
 ElectronicLevels[1/cm] 1
 0 2

End
 GroundEnergy[kcal/mol] -36.62
 End

!-----h_c13h10_p4-----

Bimolecular p4
 Fragment c13h10
 RRHO

Geometry[angstrom]		23
C	-4.528101345071	-0.932478089845 0.03903978798
C	-3.187158947241	-0.363750657592 0.030039174806
C	-2.079371027764	0.115290359409 0.022527791082
C	-0.774578035774	0.693060520968 0.015885463092
C	-0.630125010456	2.0722604561 0.016198591032
C	0.644027596887	2.672338809846 0.010901996584
C	1.77811576128	1.897491116809 0.005267569479
C	0.397365620117	-0.13906510272 0.009418406193
C	1.686170994385	0.482073929924 0.004299595108
C	2.844080944149	-0.339537765781 -0.001658141
C	2.739457552364	-1.708368281295 -0.002860372657
C	0.324599776749	-1.554847127866 0.007827661382
C	1.465748911976	-2.320726459291 0.00177062926
H	-5.138168961711	-0.490168865641 0.832446511633
H	-5.038913318856	-0.754628808811 -0.912398498724
H	-4.4972196563	-2.013304229311 0.204373445384
H	-1.518324364398	2.692309059022 0.020835451
H	0.721151063548	3.753696311406 0.011450574214
H	2.760519662039	2.357695883854 0.001417712739

```

H 3.818783133071 0.137188944856 -0.005318459891
H 3.632271326669 -2.32354338991 -0.007451649299
H -0.651919836009 -2.023481000559 0.011146352726
H 1.391125160311 -3.402434613576 4.88407428E-4
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 63
6.2293 72.0222 74.4190
163.8638 176.6064 259.7311
265.9221 365.2929 387.5813
396.4508 453.9989 479.1291
499.2776 540.6374 583.2657
589.8083 653.5972 683.9733
747.3335 790.9499 804.9864
815.2779 833.1334 881.3513
922.9556 957.1114 967.7726
985.0968 998.8840 1042.0246
1049.3393 1054.5261 1075.7846
1120.3994 1168.7343 1180.8739
1201.9878 1237.0497 1267.9492
1308.1541 1357.2424 1391.6614
1414.6731 1427.6216 1467.7618
1477.6395 1478.9786 1492.4778
1543.6290 1613.6708 1627.8875
1661.0870 2331.6720 3019.6748
3073.9098 3079.7100 3158.9578
3162.5687 3169.8168 3178.2820
3183.0913 3192.5443 3194.4850
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -10.28
End
!-----h_c13h10_p5-----
Bimolecular p5
Fragment c13h10
RRHO
Geometry[angstrom] 23
C -4.480700820267 -0.629961654177 0.276907240784
H -4.883330543335 -0.845664825687 1.263046932174
H -5.182378932456 -0.281991534865 -0.476753053402
C -3.216106576495 -0.782429591461 0.009512577434
C -1.943993481034 -0.949328611635 -0.259307028182
C -0.89480219054 0.08353548318 -0.135350503304
C -1.235687965293 1.42488744264 -0.109824060823
C -0.261110116228 2.435055562076 -0.013075947999

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C 1.071529710913 2.109124129693 0.045614297446
C 0.491803531292 -0.28464263164 -0.05740954204
C 1.479838130069 0.752454756035 0.024441097473
C 2.853697580304 0.399742852961 0.091141295705
C 3.250807967076 -0.913431174679 0.088752389682
C 0.943782982531 -1.632151665434 -0.041828401882
C 2.281684853197 -1.938829071739 0.026260166657
H -1.646738298276 -1.930062964247 -0.619001087913
H -2.281780747416 1.700704923559 -0.179086995227
H -0.571475388922 3.473836795685 0.001568624797
H 1.829009345928 2.883096848426 0.108308482195
H 3.588846875035 1.195822800966 0.147843018459
H 4.303400944928 -1.167670222384 0.141055046593
H 0.225112265248 -2.440709377754 -0.068875156227
H 2.596312873737 -2.976371269508 0.037280607587
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 63
34.9256 94.5729 134.8635
176.5932 239.6672 258.7652
321.8270 408.7192 413.7803
431.5133 476.8336 509.2602
516.6136 542.7298 607.4089
655.0582 678.4938 744.1389
766.6646 793.9369 805.8972
813.9631 869.5746 877.3258
878.9295 901.5681 925.3020
962.5839 984.9457 995.8558
1011.6259 1016.7775 1052.7399
1100.3751 1128.3501 1169.4513
1190.5669 1197.2151 1233.1650
1264.1030 1280.9695 1339.1628
1383.9795 1393.8708 1424.5484
1463.5509 1484.0357 1496.2001
1550.0010 1613.5941 1634.1732
1662.6119 2033.8783 3104.0534
3144.5264 3158.7888 3161.3806
3169.4659 3173.3218 3173.5683
3184.2770 3186.1441 3198.6078
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -5.04
End
!-----h_c13h10_p6-----
Bimolecular p6

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```

Fragment          c13h10
RRHO
Geometry[angstrom]  23
C  0.2417293017  -0.1231029792  -0.2663292228
C  -0.9998538449  0.5615351061  -0.4565573225
C  0.0708264558  2.6610063627  0.154617934
C  -1.0638962028  1.9203122781  -0.2460227709
C  1.2738839602  2.030357528  0.3377267714
C  1.393403319  0.6312828386  0.1315794027
C  -2.2501629942  -0.185015172  -0.9038100881
C  2.7390925835  -1.3927402926  0.108905572
C  1.6049695864  -2.1402234371  -0.2781734669
C  2.6314490257  -0.0388708254  0.3098826501
C  0.3902309487  -1.5229669912  -0.4593099951
H  -0.018242751  3.7299138517  0.3120805565
H  -2.0068760763  2.4371793268  -0.3906819199
H  2.151755128  2.5909440572  0.6412577803
H  -2.0253973669  -0.8015835174  -1.7819178023
H  -2.9949295799  0.546250848  -1.2317265779
H  3.6912805545  -1.8918978632  0.2489313828
H  1.6937681179  -3.210254916  -0.4289239071
H  3.4972539485  0.5424020194  0.6098342153
H  -0.4705422556  -2.1182979108  -0.7355054762
C  -3.3369946642  -1.7267744707  0.9797615886
C  -2.8467194933  -1.0312891624  0.1316469445
H  -3.7647307007  -2.3388746787  1.7352007517
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  63
53.0973           76.9056           149.9481
175.6043          256.3389           262.6339
344.3904          392.1855           427.5207
434.2643          478.9520           512.5606
522.8119          557.3915           616.0057
664.2892          670.7530           675.1393
724.1538          745.4770           793.0457
804.2224          812.7617           866.3796
886.7231          917.7622           935.9585
957.0324          966.2268           983.7392
996.3317          1040.3698          1061.1259
1097.2954         1168.7413          1184.8333
1188.5373         1216.9966          1240.8398
1261.9381         1289.0032          1334.8405
1383.4957         1397.2626          1424.7856
1469.8395         1481.4292          1495.3975
1548.5129         1618.6270          1641.8188
1665.8494         2221.0616          3020.8864
3059.0888         3158.0483          3159.4820
3165.9205         3170.1972          3184.2919
3185.3131         3198.5910          3477.3261
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1

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End
Fragment          H
Atom
Mass[amu]         1
ElectronicLevels[1/cm]      1
0  2
End
GroundEnergy[kcal/mol] -2.0
End
!-----ch3_c12h8_p7-----
Bimolecular      p7
Fragment          c12h8
RRHO
Geometry[angstrom]  20
C  0.5443045687    0.2005444428    0.8505882989
C  -0.7487312176   0.8012408473    1.0254685357
C  0.1899684447    2.9782201099    0.4807434526
C  -0.9031654786   2.1660967544    0.8395463005
C  1.4365711371    2.4278504078    0.3075436019
C  1.6464170241    1.036488149     0.4860751955
C  -2.8274825718   -0.6655359612   1.6986686947
C  -1.8760325877   0.0054170134    1.3890740191
C  3.1132088224    -0.9005879857   0.4886319094
C  2.0232635745    -1.7249183022   0.8487972933
C  2.9266177105    0.4479222943    0.3120605133
C  0.7705583185    -1.1879268817   1.0253007116
H  0.0378789474    4.0424551849    0.3424740129
H  -1.8831391325   2.6072680104    0.9743656549
H  2.2798709967    3.0518173445    0.0310687068
H  -3.6671176836   -1.2572572886   1.9693598738
H  4.0961079551    -1.3373744707   0.3526289688
H  2.1789602544    -2.7890059356   0.9863991687
H  3.7587351911    1.0869079361    0.0355849516
H  -0.0639252734   -1.8208156691   1.301348136
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  54
102.4513           138.5306           175.2683
202.9107           353.7725           364.1458
445.2477           451.3350           478.8168
495.6215           551.3867           582.9265
593.9030           628.1577           655.4881
690.7284           705.6784           749.1842
791.0004           806.2552           817.0283
872.6489           882.9997           928.0044
970.7953           988.0719           1001.9896
1036.9341          1053.1978          1096.1872
1169.1937          1182.5636          1192.3821
1237.0354          1251.8741          1292.9297
1360.3674          1392.3362          1422.9748
1468.9275          1491.9413          1544.4621
1614.1481          1628.4663          1661.8362
2200.7963          3160.2690          3164.1854

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3171.2083          3180.3108          3184.6645
3194.7060          3196.0618          3476.9162
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment          ch3
RRHO
Geometry[angstrom]    4
C  3.465073663   -1.8287770054   7.55108E-5
H  2.9494866157   -1.9893536196   -0.9357821139
H  2.9493016592   -1.9893430857   0.9358330347
H  4.4960410621   -1.5052722892   1.755672E-4
Core RigidRotor
SymmetryFactor 6.0
End
Frequencies[1/cm]    6
505.5776          1403.1131          1403.3797
3103.7859          3282.6714          3283.0465
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol] -15.82
End
!-----h_c13h10_p8-----
Bimolecular    p8
Fragment          c13h10
RRHO
Geometry[angstrom]    23
C  -0.3922641251   -3.7210691382   -0.7554262317
H  0.2746093546   -4.0794398649   -1.547498267
H  -0.1056249533   -4.2452469846   0.1630690935
H  -1.4103649088   -4.0208934777   -1.0107602649
C  -0.2888064764   -2.2383332731   -0.5887224039
C  -1.2858886378   -1.3174067893   -0.7209568027
C  -0.7520806394   0.0301584592   -0.4716092601
C  -1.2534664645   1.3134238365   -0.4583786661
C  -0.3707375699   2.3912574429   -0.1575458971
C  0.9681699968   2.2010281547   0.1215218544
C  0.6221112346   -0.1452112921   -0.1832868457
C  1.5142132215   0.8835472895   0.1149195091
C  2.8573393181   0.4862980786   0.3749499554
C  3.2051079076   -0.8501991807   0.3225521757
C  0.9582196352   -1.5168399569   -0.2416799826
C  2.2646067242   -1.8739000349   0.0141224001
H  -2.3146302076   -1.5419044156   -0.9713539439
H  -2.2966790271   1.5238680338   -0.6697448321
H  -0.772317769   3.3986876206   -0.1489316319
H  1.6029981452   3.051847095   0.3452455161
H  3.6079263432   1.2323642518   0.6142521081
H  4.2319736923   -1.1355302456   0.5231621048
H  2.5945912054   -2.907291609   -0.0127926876
Core RigidRotor

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SymmetryFactor 1.0
End
Frequencies[1/cm] 63
123.6554          145.0837          165.2801
219.8869          230.4511          299.8964
406.4497          409.7388          461.9884
498.2425          533.6410          547.7805
588.7086          592.9362          630.4302
677.6053          678.8317          764.1281
781.7886          800.5684          816.5086
819.6503          855.7291          919.6885
926.7661          971.3683          973.6004
984.0718          1017.1347         1035.4674
1056.9106         1059.6228         1086.5646
1158.4683         1179.7372         1204.9284
1220.3426         1247.6447         1280.5653
1322.0509         1386.5098         1406.3004
1414.8708         1450.0206         1461.5859
1480.8588         1488.1775         1492.6846
1515.2612         1595.3952         1635.7790
1654.5020         1659.5208         3013.6915
3055.3217         3102.0961         3158.4831
3159.0177         3167.6841         3168.9914
3182.1158         3183.1647         3202.5868
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment          H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -37.58
End
!-----ch3_c12h8_p9-----
Bimolecular      p9
Fragment          c12h8
RRHO
Geometry[angstrom] 20
C 0.2474731132   -0.0017353973   -0.0873576261
C 1.3842839801   0.7912130642    0.0631843178
C 2.6211177064   0.0927337572    0.1769335129
C 2.6397734955   -1.2884002657   0.1345710569
C 1.4571493826   -2.0659726552   -0.0206678822
C 0.2467795828   -1.4157010294   -0.1328995413
C -1.0721757537   0.4912806987    -0.2171557552
C -1.2563572511   1.8573028204    -0.1938781882
C -0.1179086697   2.6987294075    -0.0414534636
C 1.1643548377   2.1989735178    0.0839332276
C -1.1609899217   -1.8133931398   -0.3009625416
C -1.9347504468   -0.694645335    -0.3504080449
H 3.547655231    0.644337076     0.2966603007

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H 3.5891074108 -1.805169376 0.2224427509
H 1.5313070623 -3.1481130452 -0.0474108747
H -2.2402605978 2.3048545329 -0.2881547269
H -0.2686285616 3.7725003934 -0.0237709184
H 2.0025413527 2.8783100067 0.1980333929
H -1.5146548296 -2.8329483454 -0.3726936943
H -3.0095781232 -0.6714536857 -0.4682813022
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 54
160.5077 212.2102 229.3073
375.5763 423.1391 461.5454
470.8274 518.8992 561.3635
583.0543 615.6679 668.6491
675.1331 695.7926 741.1577
766.9659 788.4054 818.0424
848.4967 879.4882 917.5353
929.4159 935.3924 975.8155
985.5792 1027.4923 1034.8022
1056.5181 1102.5586 1113.1093
1176.0904 1203.3361 1224.4432
1246.4128 1273.1232 1331.5419
1385.4527 1419.4808 1447.3262
1457.4011 1489.6834 1515.4936
1540.3868 1636.3596 1652.3436
1660.5778 3159.6761 3160.0774
3168.9918 3169.7302 3183.0860
3184.0689 3201.8299 3221.8770
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment ch3
RRHO
Geometry[angstrom] 4
C 3.465073663 -1.8287770054 7.55108E-5
H 2.9494866157 -1.9893536196 -0.9357821139
H 2.9493016592 -1.9893430857 0.9358330347
H 4.4960410621 -1.5052722892 1.755672E-4
Core RigidRotor
SymmetryFactor 6.0
End
Frequencies[1/cm] 6
505.5776 1403.1131 1403.3797
3103.7859 3282.6714 3283.0465
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -43.96
End
Bimolecular r1
Fragment c11h9

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RRHO
Geometry[angstrom] 20
C -0.0860161383 0.2728083414 0.
C 0.0803134218 -1.1458414363 0.
C 1.388236214 -1.7087247236 0.
C 2.5050743775 -0.8928774166 0.
C 2.3700522885 0.4930498187 0.
C 1.1009775518 1.130630046 0.
C -1.3992400432 0.7880733446 0.
C -2.5005562018 -0.0441538381 0.
C -2.3345638626 -1.4413663935 0.
C -1.0674419947 -1.9773179971 0.
C 1.0372544261 2.5192757209 0.
H 1.492407143 -2.7880277328 0.
H 3.4963606177 -1.3323824809 0.
H 3.2560707502 1.1183891607 0.
H -1.5547502329 1.8592661893 0.
H -3.4977148005 0.3811795953 0.
H -3.2030829565 -2.090119627 0.
H -0.9274834338 -3.0532365411 0.
H 1.9498074578 3.1020906782 0.
H 0.1073944159 3.0692532918 0.
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 54
 98.9377 171.3251 237.6948
313.6055 412.2016 448.9643
452.3687 480.9357 507.9409
512.3484 564.4777 584.6091
639.0810 719.9857 732.2534
750.3155 778.2477 799.0960
807.9600 866.9870 884.2934
888.7662 956.6052 968.7268
972.1724 991.3835 1050.7828
1104.0508 1115.1133 1160.0199
1176.9196 1191.6434 1228.3037
1253.5569 1310.3353 1355.8564
1368.0915 1417.9514 1466.8005
1474.4230 1514.8920 1528.4432
1569.1587 1593.2349 1648.1360
3157.0771 3159.2971 3161.9742
3170.4916 3171.8755 3184.3321
3185.6533 3197.0693 3251.3289
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment c2h2
RRHO
Geometry[angstrom] 4
C 0.0 0.0 0.5990703976
C 0.0 0.0 -0.5990703976
H 0.0 0.0 1.6619081422

```

```

H 0.0 0.0 -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 7
642.0679 642.0679 772.6955
772.6955 2069.5209 3420.9273
3523.7963
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] -21.02
End
!-----bar_ts0-1-----
Barrier ts0-1 i1 p0p
RRHO
Geometry[angstrom] 24
C 0.470333 -0.151755 -0.227133
C 0.449763 -1.563667 -0.377451
C -0.644568 0.682915 -0.423588
C 1.586643 -2.306482 -0.170219
C 2.798294 -1.675591 0.197213
C 2.852382 -0.311765 0.353075
C 1.701052 0.492696 0.149145
C -0.634277 2.03374 -0.269051
C 1.719711 1.904931 0.304404
C 0.588517 2.658055 0.103
H -0.483637 -2.038988 -0.653952
H 1.55915 -3.384126 -0.287332
H 3.687271 -2.275671 0.356724
H 3.782358 0.171412 0.635841
H -1.526587 2.631415 -0.424013
H 2.651089 2.383703 0.588309
H 0.620519 3.735669 0.22709
C -2.706114 -0.229668 -1.107978
C -4.016101 -0.780731 1.143374
C -3.385692 -0.514233 -0.139583
H -2.417312 -0.099501 -2.124349
H -4.280436 -1.837516 1.24136
H -4.931025 -0.193191 1.261822
H -3.34106 -0.52387 1.967251
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 299.7862
WellDepth[kcal/mol] 41.68
WellDepth[kcal/mol] 1.74
End
Rotor Hindered ! 57 cm^-1 CH3
Group 22 23 24
Axis 19 20
Symmetry 3

```

```

    Potential[kcal/mol]      4
0  0.071106877 0.179382401 0.070254091
End
Rotor      Hindered      ! 17 cm^-1
  Group      19 20 21 22 23 24
  Axis      3 18
  Symmetry      1
  Potential[kcal/mol]      8
0  0.534680841 1.8736721 0.477881183 0.001157755 0.456316189 1.721036667
0.406609899
End

```

```

Frequencies[1/cm]  63
                   35.6533
                   89.6241
                   101.7003
171.2419           193.3488           316.2767
350.8434           372.2125           405.7979
469.0672           499.7525           511.3195
519.9559           595.3877           621.3856
658.8588           704.9756           737.3383
777.2651           784.1230           797.3976
802.6777           869.5187           898.8601
926.2114           939.4749           965.1524
976.3497           997.7390          1035.0451
1039.8818          1050.7858          1057.8464
1135.8799          1167.7238          1176.2465
1201.3652          1234.8784          1269.8281
1362.2137          1381.3859          1385.4874
1411.6407          1452.7598          1473.9049
1474.4423          1482.6103          1522.9826
1582.3819          1634.4438          1659.9137
2111.4609          3015.3060          3070.5633
3083.8860          3151.3024          3154.9701
3162.0807          3166.9013          3175.9532
3181.0882          3192.6782          3431.3587

```

```
ZeroEnergy[kcal/mol] 1.74
```

```
ElectronicLevels[1/cm] 1
```

```
0 2
```

```
End
```

```
!-----
```

```
!-----bar_ts0-5-----
```

```
Barrier      ts0-5  i5  p0p
```

```
RRHO
```

```
Geometry[angstrom]  24
```

```

C  -0.6298601875  0.0377674688  -0.0719979277
C  0.6524726573  0.6163319424  -0.0342907811
C  -0.2240210352  2.8312377667  0.1473707096
C  0.890209868  1.9527618813  0.0529792832
C  -1.5040290197  2.3326274155  0.1361907611
C  -1.7487313472  0.937545357  0.0256020902
C  2.8147164319  -0.8320574423  -1.2552498255
C  2.5290544979  -0.731770059  -0.0723467724
C  2.6596728171  -0.9381032217  1.3779468423
C  -3.2624602123  -0.9589616646  -0.1159436465
C  -2.1612039688  -1.8405598022  -0.2199636389

```

```

C -3.0598275207 0.3945533937 0.0021578808
C -0.8761645236 -1.3550883225 -0.1987224665
H -0.0546922104 3.90014717 0.226893282
H 1.8992866473 2.3523564785 0.0535294324
H -2.3527837499 3.0047361659 0.2074443514
H 2.8682482804 -0.7806970661 -2.3162997093
H 1.7653771684 -1.4104024513 1.7903527459
H 2.7965500558 0.0124034107 1.8979172139
H 3.5214934568 -1.5783249885 1.5848130852
H -4.2707351611 -1.3574885825 -0.1330246105
H -2.3366332497 -2.9058945244 -0.3199529839
H -3.9052547508 1.071117136 0.0779359683
H -0.028704944 -2.0236464614 -0.291911284
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 373.6138
WellDepth[kcal/mol] 38.61
WellDepth[kcal/mol] 2.67
End
Rotor Hindered ! 153 cm^-1 CH3
Group 18 19 20
Axis 8 9
Symmetry 3
Potential[kcal/mol] 4
0 0.445792225 1.291397166 0.480834243
End
Rotor Hindered ! 33 cm^-1
Group 7 9 17 18 19 20
Axis 2 8
Symmetry 1
Potential[kcal/mol] 8
0 1.670964539 5.143005849 1.476119674 0.004166664 1.095134757 3.594033566
0.980218298
End
Frequencies[1/cm] 63
50.8858
76.0292 156.6214
174.3989 221.9524 237.7945
361.1689 385.4939 409.6355
469.4145 506.9269 515.8877
520.8724 562.1984 620.7239
623.2516 681.9563 738.4206
766.2118 777.7233 797.7613
802.9552 869.9148 899.1608
911.4459 933.0302 966.2199
977.4450 997.8735 1035.1833
1041.0399 1052.5316 1066.9174
1136.4488 1168.2513 1177.0022
1202.0869 1235.0661 1270.1387
1362.8351 1382.0931 1384.8985
1414.8405 1453.1780 1477.1258
1482.0330 1482.7686 1523.6535

```

1582.4641	1634.2063	1659.6334
2062.3549	3034.1763	3098.9727
3101.3672	3150.7134	3155.2397
3161.0345	3167.3229	3176.1997
3181.3630	3192.6561	3452.9220

ZeroEnergy[kcal/mol] 2.67

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts1-2-----

Barrier ts1-2 i1 i2

RRHO

Geometry[angstrom] 24

C	-4.5171805107	-0.8423526916	-0.5353990485
H	-4.7670491551	-0.2983009596	0.3868636789
H	-4.98681165	-0.3047960468	-1.3670284715
H	-5.0063700026	-1.8261491921	-0.4683528024
C	-3.0857439214	-0.9442775989	-0.7319065319
C	-1.7885548436	-1.0293076712	-0.8633874057
H	-1.3580366323	-1.9556462355	-1.2601938247
C	-0.8038046579	0.0409341123	-0.5446700341
C	-1.1853856996	1.3697769287	-0.5936793284
C	-0.2800739202	2.4131064203	-0.3210380258
C	1.0269044138	2.1316968983	-0.0084163719
C	0.5532743867	-0.2795648919	-0.2016918141
C	1.4750417529	0.7885842149	0.0585459799
C	2.8209905469	0.4790737042	0.3882136212
C	3.2502910025	-0.8215238615	0.4727040284
C	1.0327020368	-1.6128410652	-0.0858371102
C	2.3419601151	-1.8773535544	0.2380185155
H	-2.2061134412	1.6083580449	-0.871373871
H	-0.6198587695	3.4415174478	-0.3757164831
H	1.7337638369	2.9304312955	0.1897890674
H	3.5080850959	1.2975093691	0.5771341176
H	4.2810361923	-1.0424791596	0.726228087
H	0.3523199436	-2.4401252826	-0.2398861439
H	2.6798968807	-2.9044012251	0.3202711713

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 245.6869

WellDepth[kcal/mol] 5.45

WellDepth[kcal/mol] 4.94

End

Frequencies[1/cm] 65

38.6772	75.7988	
96.6580	174.3311	178.3561
250.0129	287.6780	317.1825
419.7192	428.7456	479.1015
498.5213	530.6029	544.4188
612.8207	643.3423	727.8498
742.9960	776.4607	798.2513

806.2131	823.0574	846.3765
880.8846	917.5401	924.2758
963.5913	981.4319	986.7625
994.9548	1036.6889	1039.1692
1053.4624	1102.7993	1168.6065
1187.0623	1189.5157	1231.4727
1246.3664	1274.0143	1302.5161
1378.0923	1389.3009	1405.5653
1420.2367	1451.3958	1468.1461
1470.2281	1491.8040	1546.7016
1611.1012	1632.8419	1661.5621
1810.6603	2951.9893	2985.5872
3003.3333	3046.2402	3156.8249
3158.5773	3167.6715	3169.3056
3182.3441	3183.4266	3198.3909

ZeroEnergy[kcal/mol] -34.49

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts2-3-----

Barrier ts2-3 i2 i3

RRHO

Geometry[angstrom] 24

C	-1.1218021334	0.2086494433	0.348449078
C	-2.3969774405	-0.8527578207	-0.4601107843
C	-2.1715580343	-0.7543548436	0.8016824568
C	-3.0048554205	-1.2987292436	-1.7136671143
C	-1.4047429382	1.6082236847	0.2692723695
C	0.2759941379	-0.2139281695	0.1911423142
C	-0.4223067318	2.5280794904	-0.0776604043
C	1.2597999954	0.7588849606	-0.1662042588
C	0.8851510671	2.1269922451	-0.3133599734
C	0.6819574389	-1.5472251264	0.3796318549
C	2.6001289996	0.3382004529	-0.3422338252
C	2.0022444399	-1.9288389089	0.2124711343
C	2.9676020175	-0.9782344756	-0.1573595718
H	-2.4991489278	-1.1332283808	1.7661324197
H	-3.403347227	-0.4497805407	-2.2773251936
H	-2.2620148796	-1.7931983731	-2.3471603454
H	-3.82585664	-2.0062392082	-1.5335172961
H	-2.4202034118	1.9369532958	0.4587786241
H	-0.6838363306	3.5782589975	-0.1553601415
H	1.6439610109	2.8517388037	-0.5861235171
H	-0.0596685679	-2.2893116052	0.651287869
H	3.3430705863	1.0781277252	-0.6221505121
H	2.2902759012	-2.9628990473	0.3653735247
H	4.0002660887	-1.2795093553	-0.2945717073

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 527.591

WellDepth[kcal/mol] 22.28

```

WellDepth[kcal/mol]  5.56
End
Frequencies[1/cm]   65
72.0040              79.0329
125.0441             152.5167           187.4163
248.3727             267.8324           305.6232
397.2511             439.9563           463.0052
490.4843             513.0152           522.3483
561.1917             614.2876           699.6667
716.2729             751.6211           770.8325
783.0948             800.7536           827.2984
871.8468             874.3250           880.6119
955.6688             959.9654           985.6399
1019.4823            1033.9774          1052.2172
1058.5672            1095.3235          1122.8887
1154.8165            1175.6522          1181.2612
1216.2226            1232.7161          1286.2288
1323.2070            1345.9205          1393.6696
1399.4417            1461.0555          1465.4299
1466.5200            1468.9988          1522.0634
1552.1682            1587.0143          1637.6655
1869.0831            2983.4018          3054.6990
3077.9842            3121.6978          3155.0061
3156.7397            3165.5034          3172.8406
3177.4463            3182.9760          3187.9248

```

```
ZeroEnergy[kcal/mol] -17.15
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```
ElectronicLevels[1/cm] 1
```

```
0 2
```

```
End
```

```
!-----
```

```
!-----bar_ts2-15-----
```

```
Barrier      ts2-15  i2  i15
```

```
RRHO
```

```
Geometry[angstrom]  24
```

```

C  -4.1959291577  -0.2252471692  0.3388039885
C  -3.1674028602  -0.9852853422  -0.2641068791
C  -1.8233969966  -1.1131474823  -0.2029014073
C  -0.8457646924  -0.0302498501  -0.1020489159
C  -1.2504555554  1.3017658  -0.0706587521
C  -0.3325347172  2.360992005  0.0151523527
C  1.0173508613  2.1109812341  0.0687683367
C  0.571941155  -0.3133985888  -0.0555737193
C  1.4986585742  0.7783905143  0.034297865
C  2.8917320101  0.5085145902  0.0883372481
C  3.3696287355  -0.7770910628  0.0581258909
C  1.1090255179  -1.6280803978  -0.0820791165
C  2.4640890361  -1.855887274  -0.0274049809
H  -4.0308108141  0.4105063042  1.2132877013
H  -5.149803819  -0.1232342486  -0.170052949
H  -1.4322367777  -2.1149305809  -0.3355645429
H  -2.3055431687  1.5359215044  -0.1323935865
H  -0.6999231389  3.3811400636  0.0349561244
H  1.7309804049  2.925100376  0.1353852062
H  3.5765786947  1.3476338658  0.1551913079

```

```

H 4.4362171779 -0.967109334 0.0997064467
H 0.4468564638 -2.4808794549 -0.144580033
H 2.8394554983 -2.8728533149 -0.0504803147
H -4.1270184335 -1.5436691571 0.4146927288
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1821.0623
WellDepth[kcal/mol] 42.85
WellDepth[kcal/mol] 67.5
End
Frequencies[1/cm] 65
24.5570 88.5183
138.6199 173.0926 222.7249
231.6450 337.0042 371.4037
429.4101 439.4516 448.1297
480.5899 513.9683 546.3480
570.6956 652.4600 658.0382
738.6691 764.2337 784.7169
796.8756 802.5624 832.7083
868.5124 872.1961 889.7324
911.6693 956.5716 978.6669
992.2053 1004.3906 1034.7307
1055.0035 1074.8652 1114.5311
1137.9787 1167.7300 1191.2353
1199.3517 1228.9580 1257.7121
1280.9828 1335.9036 1381.0205
1402.3980 1423.8258 1459.6559
1471.1287 1490.5226 1544.6356
1561.1442 1615.6520 1627.0746
1658.7431 2176.4022 3027.1524
3157.2697 3160.9658 3163.2910
3168.4863 3169.9198 3177.4308
3184.7206 3195.1024 3206.7257
ZeroEnergy[kcal/mol] 3.42
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-20-----
Barrier ts2-20 i2 i20
RRHO
Geometry[angstrom] 24
C -4.1318147367 -1.5680126573 0.7498767696
C -3.1326913707 -1.1543414517 -0.2768956784
C -2.0580317228 -0.4751988407 -0.4945959933
C -0.9615467859 0.4226627712 -0.3191741303
C -1.1586963869 1.7978519204 -0.4614783251
C -0.0850531897 2.6976436895 -0.3679699554
C 1.1956381057 2.2457576193 -0.1414994539
C 0.3728687356 -0.076443014 -0.0845850832
C 1.4532868976 0.8565370038 0.0047458183
C 2.7628145368 0.3642570799 0.2425752307

```

```

C  3.0018036934   -0.9816274712    0.384906089
C  0.6526082452   -1.4552554607    0.0676465297
C  1.9348847672   -1.9007108938    0.2962405437
H  -3.9163587493   -1.0814048295    1.7107363875
H  -5.14377441    -1.2988139289    0.437906544
H  -4.1088076866   -2.6508240116    0.8956506201
H  -2.1601118129    2.1689181918   -0.6441557131
H  -0.2758583468    3.7599938128   -0.473382864
H  2.0234939523    2.9428626097   -0.0717751229
H  3.5790992956    1.0761070302    0.3096646539
H  4.0089699748   -1.3403183869    0.5655420717
H  -0.164298935   -2.1647026469    0.0021793698
H  2.1274432248   -2.9616973274    0.409332644
H  -2.4943872957   -1.1899008079   -1.4424499525
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  2065.9969
WellDepth[kcal/mol]  44.24
WellDepth[kcal/mol]  52.86
End
Frequencies[1/cm]  65
44.3047          67.4441
108.5518         149.7766          173.2941
211.3223         244.1321          248.3056
366.5553         390.2747          418.7057
451.3949         480.8590          496.5940
542.3458         568.8739          589.9472
643.1330         685.5769          741.3225
784.6179         802.2427          806.3972
822.9596         874.1045          895.3511
923.2403         963.6458          974.3860
993.7160         1021.6229         1029.8288
1043.1492        1065.2080         1101.3867
1165.6561        1179.6643         1191.5957
1224.9092        1237.8435         1289.2888
1344.6786        1378.6522         1384.7855
1414.0733        1464.7212         1465.9989
1475.7461        1481.7120         1537.7997
1588.5422        1609.9906         1653.3699
1969.4389        2293.0449         2986.4971
3073.9564        3095.7218         3157.2810
3161.0997        3166.9927         3175.6156
3178.7686        3187.9517         3189.0465
ZeroEnergy[kcal/mol]  4.81
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts2-21-----
Barrier      ts2-21  i2  i21
RRHO
Geometry[angstrom]  24

```

C	-0.7958293728	-3.749870677	-1.0778023626
H	-0.1953539919	-4.0418612044	-1.945333378
H	-0.4871733416	-4.3920960093	-0.2447667368
H	-1.8488738152	-3.9759224459	-1.2977062858
C	-0.6081061341	-2.3269432153	-0.7466296921
C	-1.3862366938	-1.2610213579	-0.5919350204
C	-0.7415491146	-0.0115188233	-0.1801947424
C	-1.2501231472	1.272406747	-0.3031100582
C	-0.3876304372	2.3777622044	-0.1582727206
C	0.9698452795	2.1999077611	0.0212539457
C	0.6129531957	-0.1942617615	0.1900568567
C	1.5137361415	0.8957411505	0.1582447007
C	2.9114769076	0.6099575926	0.1742997295
C	3.3581780226	-0.6996636655	0.2012431878
C	1.0785556184	-1.5418152603	0.4092438832
C	2.4668573228	-1.7740991606	0.3569096359
H	-2.4513519299	-1.2777894469	-0.8303256476
H	-2.2864785755	1.4278055981	-0.5832017975
H	-0.7882086069	3.3800836137	-0.2631388018
H	1.6377934124	3.0547113617	0.0256765956
H	3.6200124925	1.4297992866	0.1282638023
H	4.4243717623	-0.8990252399	0.1784405729
H	0.4954368111	-2.1902436873	1.0580643017
H	2.8564541942	-2.7690233606	0.5408360319

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 526.0228
WellDepth[kcal/mol] 15.2
WellDepth[kcal/mol] 35.04
End
Frequencies[1/cm] 65

104.4394	141.2395	
163.9178	184.7534	208.0470
275.7736	333.9873	379.3355
417.5868	469.2378	480.3732
515.3011	538.7697	582.1135
613.2457	640.1586	693.9858
743.2674	766.3065	778.1941
800.6839	814.1341	837.2865
865.7739	896.1273	908.6810
960.5699	967.1173	975.0022
1030.5138	1043.7442	1053.4717
1081.2541	1095.5883	1144.2360
1171.8212	1184.3216	1202.7859
1221.0353	1245.8291	1294.3537
1356.7593	1380.7674	1398.0694
1401.0162	1448.4761	1458.4621
1475.4991	1476.7469	1518.2838
1563.2066	1598.1268	1630.6378
1688.8901	2978.8909	3041.7983
3060.2654	3081.6924	3107.1283
3157.2454	3158.1524	3168.0082

```

3171.8584          3181.6637          3182.9745
ZeroEnergy[kcal/mol] -24.23
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts3-4-----
Barrier      ts3-4  i3  i4
RRHO
Geometry[angstrom]  24
C  0.3187108343  -0.1767089183  -0.0272686108
C  -1.0459028795  0.3622690251  -0.0800842402
C  -0.1012498593  2.6324108134  -0.137362571
C  -1.1973528981  1.7780956308  -0.1862135001
C  1.188377714  2.1357442002  -0.0259585365
C  1.4216864212  0.7298818768  0.017361579
C  -2.3029059511  -0.4462703255  1.0109368992
C  -2.2294484174  -0.539296435  -0.2706857418
C  -2.8653082689  -1.1429383809  -1.4764817969
C  2.9601101483  -1.156209376  0.1005815252
C  1.873999943  -2.0461843509  0.046053004
C  2.7345050154  0.2034418585  0.0883205608
C  0.5807035826  -1.5592944546  -0.0134272501
H  -0.2616124613  3.7038333992  -0.1951805235
H  -2.199863189  2.1801385629  -0.2779274848
H  2.0373618104  2.8089627412  0.0123823453
H  -2.7159616178  -0.6344747042  1.9860153803
H  -2.1462959345  -1.761790188  -2.0214974597
H  -3.1975824312  -0.3571447505  -2.1620649818
H  -3.724580196  -1.7571752654  -1.2004776792
H  3.9729517275  -1.539827518  0.1535069638
H  2.049229227  -3.1160977252  0.0556543457
H  3.5688269559  0.8961072105  0.1311155504
H  -0.2513222752  -2.2532889261  -0.0297297774
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  604.1172
WellDepth[kcal/mol]  6.46
WellDepth[kcal/mol]  20.46
End
Frequencies[1/cm]  65
81.0246          91.5021
134.3827         168.4294         183.3953
226.3361         276.1962         369.7836
397.4020         470.9722         472.7723
493.7575         522.7610         536.9735
561.3816         605.7633         639.3156
647.7566         691.3615         722.1578
771.6290         784.6987         799.1007
826.5922         841.7650         880.8534
908.7783         958.3105         962.4797
987.6116         1014.4673        1040.3793

```

1051.8062	1085.9397	1115.3429
1156.7620	1176.3407	1182.6957
1231.7724	1238.6704	1288.6103
1324.6277	1349.2580	1393.4134
1399.3780	1461.0697	1467.3328
1475.8596	1483.2000	1521.8367
1554.4534	1587.6479	1640.3774
1814.0237	3024.5870	3078.5508
3109.5238	3156.2613	3158.2804
3166.9640	3173.7544	3179.4834
3183.9743	3189.8070	3286.0267

ZeroEnergy[kcal/mol] -16.25

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts4-5-----

Barrier ts4-5 i4 i5

RRHO

Geometry[angstrom] 24

C	-0.2728869063	-0.1794948736	-0.0715451777
C	1.0403223592	0.3891326112	-0.088185117
C	0.0709062394	2.6154031337	0.0661597993
C	1.1898275879	1.7584599978	-0.029558364
C	-1.1978759071	2.095084759	0.1023544476
C	-1.4046300406	0.6932157549	0.0312940929
C	2.9121784187	-0.6597035052	-1.2574169759
C	2.2673293278	-0.491788879	-0.1387064153
C	2.696547237	-1.1051290867	1.1898744885
C	-2.8956842907	-1.2259944637	-0.0374825004
C	-1.7814699602	-2.0874687052	-0.1545198561
C	-2.7082116846	0.1312570396	0.0491130246
C	-0.5056976478	-1.5772907055	-0.1732491708
H	0.2240717663	3.6878003104	0.1136932551
H	2.1878621357	2.1815582819	-0.0532207015
H	-2.0609278038	2.7479779391	0.1802607539
H	3.4537218091	-0.815344814	-2.1606594751
H	1.8793221816	-1.6838072835	1.6306368504
H	2.9480782208	-0.3111934886	1.900724377
H	3.5641940931	-1.7538506253	1.0638893366
H	-3.897458693	-1.6404639889	-0.0235202584
H	-1.937219154	-3.1574291562	-0.2360814719
H	-3.5598628534	0.7990815508	0.128678734
H	0.3416045648	-2.2427618029	-0.285805676

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 710.1939

WellDepth[kcal/mol] 4.66

WellDepth[kcal/mol] 3.89

End

Frequencies[1/cm] 65

42.5911	94.2169
---------	---------

147.8980	168.6124	174.3170
189.3461	299.8491	327.9163
380.7559	443.7658	478.6877
497.9453	500.7314	557.0123
584.3111	587.1113	641.3337
663.5846	694.9807	747.3138
793.5222	805.6236	815.1449
842.6506	879.5232	921.2243
952.1095	968.3694	984.3516
997.3084	1015.3916	1035.2289
1044.9419	1078.9626	1115.1994
1167.9818	1181.9849	1190.1677
1233.7553	1252.2229	1287.6074
1362.1785	1389.0889	1391.5558
1418.5800	1465.0498	1479.5251
1481.6929	1491.1070	1542.9816
1612.3824	1633.1191	1660.9463
1673.4829	3020.7469	3075.7576
3115.9315	3157.2995	3159.8189
3168.1880	3171.4658	3182.4042
3185.1551	3192.6877	3435.1637

ZeroEnergy[kcal/mol] -32.05

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts5-7-----

Barrier ts5-7 i5 i7

RRHO

Geometry[angstrom] 24

C	-0.3214924007	-0.1477460768	0.0393666974
C	1.0385202238	0.3076420197	-0.0172515398
C	0.1969231152	2.5924467213	-0.1684579409
C	1.2654894469	1.667206225	-0.119833952
C	-1.1071705302	2.1678107953	-0.1150519121
C	-1.4035138685	0.7830727992	-0.0094309101
C	-2.977922561	-1.0692811879	0.1522855961
C	-1.9054735973	-1.9969381459	0.2010275078
C	-2.7300522733	0.2803123025	0.050044089
C	-0.6288334843	-1.5134332735	0.1438112454
H	0.4202205908	3.6504033254	-0.2490945978
H	2.278506514	2.0473242869	-0.1649604582
H	-1.9231774719	2.8818804015	-0.1527313984
H	-3.9992413512	-1.4324387735	0.1963405081
H	-2.1094129074	-3.0592600795	0.2816644641
H	-3.5551964316	0.9839180882	0.0132809065
C	1.8544389772	-1.9851094198	0.135019243
C	2.1392611086	-0.687183183	0.035866783
C	3.5716178816	-0.1969530522	-0.0245430492
H	2.534220374	-2.8278912751	0.1843938732
H	3.7935887902	0.4781034206	0.8080062462
H	3.7630087534	0.3504841787	-0.952868809
H	4.2671431955	-1.0352332373	0.0241304002
H	0.5341429061	-2.1578318598	0.1704540074

```

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 1618.6465
WellDepth[kcal/mol] 8.92
WellDepth[kcal/mol] 8.91
End
Frequencies[1/cm] 65
91.5438          155.0625
178.3413         214.3170          220.2743
266.7426         354.0256          394.8654
458.3114         466.8088          467.4779
506.2533         519.8291          561.9771
591.8543         612.8501          643.1957
696.5611         722.1389          754.9205
782.0968         806.3781          825.5849
865.3707         898.4603          921.9498
960.6959         975.4195          986.9299
990.2819         1023.4004         1030.0156
1049.4184        1056.1112         1091.3990
1167.4744        1170.5969         1217.5366
1224.0975        1242.2008         1291.1239
1357.8408        1380.7492         1404.3939
1408.0878        1452.9985         1474.5921
1485.4757        1488.8274         1517.0213
1577.7994        1592.9711         1633.7815
1642.8269        1688.5869         3021.8643
3073.2333        3114.3371         3155.5331
3160.5483        3166.5555         3177.0521
3179.4874        3181.6004         3193.5496
ZeroEnergy[kcal/mol] -27.02
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts7-8-----
Barrier      ts7-8  i7  i8
RRHO
Geometry[angstrom] 24
C -0.3254724974 -0.1742138486 -0.0223713799
C 1.0351062139 0.28083458 -0.0193136404
C 0.2169462753 2.5700855852 0.1049894304
C 1.2766401695 1.6386975316 0.0611453868
C -1.0920800148 2.1521907797 0.0719925657
C -1.4023736546 0.770150578 0.0091769164
C -2.9992150512 -1.0705608232 -0.0428218947
C -1.9366462725 -2.0140944873 -0.0640394194
C -2.7354289685 0.2779666425 -0.0061559612
C -0.6585905285 -1.5404349534 -0.0625594066
H 0.4460384116 3.6278869921 0.1708380276
H 2.2987087605 1.996593219 0.1043600954
H -1.9021513739 2.8731550508 0.108154516
H -4.0249270525 -1.4240753041 -0.0522749022

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H -2.1537142959 -3.0767363779 -0.0852087562
H -3.552300534 0.9916412913 0.0168722651
C 3.2450206285 -0.4793382251 -0.8393629914
C 2.1182037148 -0.7296078538 -0.1535671386
H 4.0157885844 -1.2343519745 -0.9435295585
H 3.4233137306 0.4761059253 -1.3182387583
C 1.8178638886 -2.0689436584 0.41636178
H 1.7401920961 -2.0924820645 1.5051281256
H 2.4178326838 -2.8890396348 0.0253129941
H 0.5944940864 -2.2244329698 0.0863437045
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1546.5932
WellDepth[kcal/mol] 7.57
WellDepth[kcal/mol] 32.23
End
Frequencies[1/cm] 65
91.9233 127.1667
176.5707 208.3510 283.8831
351.9265 397.5545 405.7644
463.4072 475.3999 496.6039
508.5375 549.6622 565.4009
588.6311 626.6960 637.9787
718.3839 726.3157 760.4659
786.6744 805.4182 832.4306
870.5335 896.2646 908.3704
925.9550 946.6200 976.1335
987.9089 1015.7012 1047.5989
1058.0831 1073.1203 1088.4866
1165.3315 1174.5001 1212.5955
1217.5962 1238.7022 1302.6665
1317.0487 1358.7184 1373.0926
1400.9795 1429.5776 1455.4412
1459.8232 1467.5657 1513.8395
1564.9151 1593.5657 1629.4450
1650.8943 1660.3468 3062.9622
3138.2760 3145.6685 3154.7455
3159.4783 3165.6074 3173.8271
3178.7223 3187.2570 3222.7124
ZeroEnergy[kcal/mol] -28.36
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts8-9-----
Barrier ts8-9 i8 i9
RRHO
Geometry[angstrom] 24
C -0.2343235937 -0.2474583139 0.0448693616
C 1.1826828393 0.1442193298 0.1163855599
C 0.5076585572 2.4957394436 -0.1213783103
C 1.5043645592 1.53400043 -0.0539681774

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C	-0.8359252466	2.1452363342	-0.0739768852
C	-1.2276261399	0.7751243809	-0.0110990405
C	3.0168015688	-1.512279841	-0.7432689316
C	2.2555475344	-0.8631549003	0.1215448833
C	2.0829951683	-0.6342795311	1.5399233957
C	-2.9642782811	-0.9326540462	-0.0284734355
C	-1.9820984945	-1.9354866262	3.20617E-4
C	-2.5912135544	0.3952694591	-0.038945613
C	-0.640461488	-1.5923326039	0.0319517043
H	0.7865111118	3.5393140255	-0.2210846892
H	2.5490250396	1.8190730792	-0.0998651538
H	-1.6051084845	2.9077042024	-0.1195443838
H	3.8002072258	-2.1823375242	-0.4055106436
H	2.8753862851	-1.3950813802	-1.8117766945
H	1.3918510569	-1.2339089866	2.1181506096
H	2.7478572996	0.0327166295	2.0758984732
H	-4.01408714	-1.2030111816	-0.0514556145
H	-2.2725352783	-2.9799110948	-0.0079757336
H	-3.3455727778	1.1744326208	-0.075805202
H	0.1131952326	-2.3717519052	0.0410029039

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 527.5157
WellDepth[kcal/mol] 32.6
WellDepth[kcal/mol] 2.42
End
Frequencies[1/cm] 65

83.8037	87.9406	
156.8416	191.3936	212.4967
293.5545	364.3537	387.2803
436.5984	473.1645	495.7832
499.1882	519.4853	562.0430
605.4042	647.8815	694.4712
715.1016	725.8550	761.7327
773.7603	802.8424	807.0948
831.6882	865.2739	882.0326
931.8923	958.0647	960.3596
962.1068	989.0570	1017.6192
1025.2346	1052.4578	1094.3964
1129.1472	1154.9949	1176.4612
1183.6363	1212.8615	1234.1721
1287.9674	1325.2809	1344.8315
1390.5692	1423.7171	1458.5931
1462.8509	1464.9851	1522.1713
1548.4294	1587.2459	1636.6569
1800.3540	3128.6502	3131.6025
3157.4601	3160.3729	3166.7806
3175.7366	3177.3689	3185.9360
3188.3226	3218.4461	3233.0557

ZeroEnergy[kcal/mol] -27.99
ElectronicLevels[1/cm] 1
0 2

```

End
!-----
!-----bar_ts9-10-----
Barrier      ts9-10   i9   i10
RRHO
Geometry[angstrom]  24
C  0.3813595401   -0.1625442929   -0.3045860264
C  -0.9221762555    0.4871285395   -0.4069860656
C  0.1122199133    2.6189152021    0.2172810774
C  -0.9995152681    1.8878751263   -0.1936465416
C  1.3434618027    2.0090272435    0.384505822
C  1.5040359823    0.6203932166    0.1113554841
C  -2.7757566494   -0.8437846506    1.6445792787
C  -2.2979143751   -0.4602055329    0.493437405
C  -2.147995194    -0.2527617192   -0.9189616271
C  2.9363201705   -1.3421608339   -0.0692675833
C  1.8328854149   -2.1102345575   -0.4793093691
C  2.7701757732   -0.0060955914    0.2206721815
C  0.584465069    -1.5277750678   -0.5907527818
H  0.0096783338    3.6848024994    0.3903461858
H  -1.9532814052    2.3846563074   -0.3337123763
H  2.2065861406    2.5837996556    0.7003773303
H  -2.2896402491   -0.59440594     2.5857203259
H  -3.6896574509   -1.4404616725    1.7200574481
H  -1.9562761285   -1.1294204578   -1.5390383108
H  -2.887510595    0.396543187     -1.392472632
H  3.9140082266   -1.8024322999    0.0198669964
H  1.9587987763   -3.163303272     -0.7038647478
H  3.6172056816    0.5937271794    0.5373685364
H  -0.2536402542   -2.1474222684   -0.8851210096
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  554.0274
WellDepth[kcal/mol]  13.42
WellDepth[kcal/mol]  20.17
End
Frequencies[1/cm]  65
66.7900          72.2580
143.5806         177.5793         235.6246
265.1868         326.2018         393.8315
419.0436         460.5338         480.2076
487.5819         509.3165         522.3780
561.2409         614.7866         698.2004
719.8195         768.9232         781.7030
800.2420         829.2506         855.5641
873.4457         905.3043         919.8081
931.9982         948.7144         959.4926
984.8778         1003.0798        1034.2985
1061.3482        1092.8397        1117.8189
1161.0717        1176.7441        1186.4041
1195.5724        1217.6068        1237.8866
1290.7419        1350.9133        1357.9356

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1405.3306          1432.9317          1460.4835
1468.2415          1475.5719          1530.8640
1566.5219          1589.0399          1642.7188
1816.9615          3029.7562          3042.9735
3102.4365          3124.1631          3156.9564
3158.4818          3168.3768          3170.6086
3180.5063          3183.4255          3191.9733
ZeroEnergy[kcal/mol] -16.99
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts10-11-----
Barrier      ts10-11  i10  i11
RRHO
Geometry[angstrom] 24
C 0.2347665409 -0.2262891961 -0.2946780018
C -1.027216237 0.3962883076 -0.5059845728
C -0.0980972527 2.5815101413 0.0924330575
C -1.1486279502 1.7459608134 -0.3102537539
C 1.1332673466 2.0002808114 0.3030074374
C 1.3310638548 0.6032051174 0.118437322
C 2.7785118216 -1.3512714457 0.1530065705
C 1.6981511913 -2.1660483424 -0.2536579851
C 2.5966675096 -0.001270828 0.3336787604
C 0.4569465119 -1.6166131268 -0.472018971
H -0.2419066253 3.6467372668 0.2349176546
H 1.9775056443 2.6070201353 0.6157749188
H 3.7525254567 -1.7963966331 0.3220203986
H 1.8523594402 -3.230209866 -0.3933580509
H 3.4260443358 0.6249845301 0.6459959151
H -0.3673025869 -2.2480805409 -0.7839239776
C -4.5879613441 0.9869901539 -1.2971710123
C -3.3117528571 0.8693460469 -0.9979463219
C -2.322861548 -0.2652045645 -0.9407810705
H -5.098406967 1.9445704586 -1.2643719135
H -5.1921356609 0.1277845541 -1.5920552563
H -2.6438119367 -1.0376801246 -0.2307712943
H -2.2220832077 -0.7550566839 -1.9173738907
H -2.4860734803 1.8615850151 -0.6253309625
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 1833.0551
WellDepth[kcal/mol] 24.03
WellDepth[kcal/mol] 18.85
End
Frequencies[1/cm] 65
50.9686          132.0657
165.0610          165.8899          230.6505
270.2842          299.7142          402.2211
413.4286          477.7128          486.0750
507.4578          525.3486          562.0049

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569.3533	636.6257	641.0730
746.2028	748.0058	783.6219
810.0418	812.3970	867.3448
876.4532	902.4877	910.7373
955.5949	957.1595	971.2516
995.6617	1029.5780	1045.8982
1052.8331	1093.5681	1137.8956
1163.1177	1168.3030	1178.4497
1196.5920	1228.9233	1260.0945
1289.7426	1365.2701	1390.4807
1399.5570	1424.2806	1459.1406
1462.8010	1473.0831	1541.0193
1600.7317	1613.8429	1658.7002
1727.2821	1745.4615	3003.7837
3028.6754	3075.0453	3153.5676
3158.5476	3166.1206	3169.2225
3176.1923	3178.3035	3188.8393

ZeroEnergy[kcal/mol] -13.13

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts11-12-----

Barrier ts11-12 i11 i12

RRHO

Geometry[angstrom] 24

C	1.5731967121	0.7393682913	0.0343768815
C	3.0873832812	0.5254960066	0.0672469418
C	3.2858994963	-0.918112022	-0.3129234979
C	2.5070072885	-1.8500763997	0.3053898789
C	0.7892339261	-0.3777623067	-0.0120221203
C	-0.608268829	-0.38016287	-0.0390181819
C	-1.2484692568	0.8409717418	-0.0320360623
C	-0.5086500528	2.0535465467	0.0180636171
C	0.926235513	2.0134803235	0.0578236672
H	3.6046091396	1.1966251731	-0.6231574781
H	3.4751767169	0.7473486036	1.0712315667
H	3.7580311199	-1.1464207115	-1.2627364524
H	2.1876014597	-1.725886996	1.334160279
H	2.4185089874	-2.8560121247	-0.0917512877
C	-0.4392407239	4.4842041537	0.0952623118
C	0.972213183	4.4449337179	0.1403512983
C	-1.1582383314	3.3152771713	0.0357695203
C	1.6367291839	3.2414121094	0.1219691808
H	-0.9515358577	5.4395809183	0.1089276036
H	1.532973978	5.3718173714	0.1896416775
H	-2.2426651082	3.3412914691	0.0032065456
H	2.7195731928	3.2258180831	0.1590201058
H	-1.1745220088	-1.3048386035	-0.0705441186
H	-2.33275101	0.8916563534	-0.0631638767

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

```

ImaginaryFrequency[1/cm] 430.6211
WellDepth[kcal/mol] 10.51
WellDepth[kcal/mol] 44.82
End
Frequencies[1/cm] 65
76.2656 126.0891
191.8347 214.9594 220.0327
282.7316 414.2004 437.2419
444.2483 478.5834 491.9855
519.0362 536.4077 594.0266
627.0391 671.2436 742.4772
747.4524 779.1685 781.5584
807.8639 860.7825 872.4651
898.2019 919.6443 938.7477
952.2561 958.5119 967.0725
993.8520 1015.5241 1046.7745
1085.3975 1121.8683 1161.7864
1178.5042 1184.3502 1200.7156
1229.1145 1268.7050 1283.5513
1298.7740 1354.7271 1383.9578
1397.8017 1424.9884 1452.2609
1465.2323 1483.9789 1534.1954
1568.4587 1593.9945 1615.4399
1656.6957 2991.5055 3066.7773
3126.5677 3149.7292 3157.8216
3161.5619 3166.3667 3169.7498
3180.5622 3189.8157 3206.7585
ZeroEnergy[kcal/mol] -21.47
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts10-13-----
Barrier ts10-13 i10 i13
RRHO
Geometry[angstrom] 24
C 0.2276865416 -0.1368191378 -0.1011589787
C -0.8583758916 0.7819681878 -0.2274376871
C 0.7293658056 2.6174575637 -0.0657581646
C -0.5900047632 2.1324199041 -0.21678688
C 1.784806276 1.7501530865 0.0764757615
C 1.5667290022 0.3492729756 0.0598896058
C -2.2899461786 0.2653610479 -0.3077824605
C -3.2980605992 -1.7584695429 -1.5365353711
C -2.396202337 -1.1417723175 -0.7976044712
C 2.3709903771 -1.9500383216 0.1478715783
C 1.0494038582 -2.438461719 -0.0308763438
C 2.6177381968 -0.5979860418 0.1871673195
C 0.036001791 -1.531888074 -0.1425074456
H 0.9021492384 3.687943093 -0.0611467723
H -1.4051772424 2.8418993133 -0.3189985382
H 2.795553502 2.125645375 0.1972790358
H -2.7169829561 0.3090913729 0.7048239037
H -2.8941121155 0.9387202402 -0.9273401736

```

```

H -4.1834157373 -1.2419240906 -1.9095687424
H -3.2033731062 -2.8060640377 -1.8037869775
H 3.1901214702 -2.6546974448 0.2459192581
H 0.8669973098 -3.5066651246 -0.0786049586
H 3.6320636048 -0.2338393267 0.3129826091
H -1.2867890467 -1.7281069809 -0.4345301068
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1612.9218
WellDepth[kcal/mol] 17.14
WellDepth[kcal/mol] 12.69
End
Frequencies[1/cm] 65
64.0491 121.4037
167.2366 214.2931 237.1582
263.3501 361.5032 405.2792
431.7413 450.6593 468.7786
501.7915 549.4655 567.6019
571.3980 627.6223 634.2803
739.9182 754.3754 778.8162
806.8934 816.8009 879.5719
887.5257 908.8948 913.2310
931.5828 945.6762 975.8842
985.3594 1028.9105 1061.5163
1084.7478 1106.1838 1126.3204
1166.9548 1188.0727 1210.8467
1219.7882 1238.8482 1253.1837
1292.2772 1365.3427 1375.0004
1401.7320 1431.9973 1451.0381
1456.4723 1477.8489 1517.3203
1588.3498 1603.1943 1635.1404
1655.8295 1720.0860 2981.3017
3028.0518 3077.1092 3154.0513
3154.3779 3162.4304 3165.6962
3173.4882 3177.9762 3181.9837
ZeroEnergy[kcal/mol] -20.02
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts13-14-----
Barrier ts13-14 i13 i14
RRHO
Geometry[angstrom] 24
C -0.0085582509 -0.0313097756 0.0936804925
C 0.7122419613 1.2067109396 0.1341886638
C -1.3870138455 2.4152899397 -0.1253502284
C 0.018841552 2.3906223259 0.0129703445
C -2.1021917764 1.2449815294 -0.1476289278
C -1.4418250703 -0.0062930049 -0.0438608633
C 2.2238591442 1.217940462 0.3476724272
C 2.9572791977 -1.1280854198 0.0641812957

```

```

C  2.8793797084   0.1220698329  -0.4392269466
C -1.5076563667  -2.4415306314   0.0177158884
C -0.0924629071  -2.483534609    0.1410502425
C -2.1558615408  -1.2344431304  -0.0751524597
C  0.5867731252  -1.3056462162   0.1762009779
H -1.896712834   3.3684772914   -0.2117944867
H  0.5636526829   3.329091558    0.0338437339
H -3.182561488    1.2596185125   -0.2485134282
H  2.6119455021   2.203160822    0.0757059999
H  2.4289349892   1.0718224708   1.4155084075
H  2.8932608705   -1.3065974772   1.1315322983
H  3.2815336755   -1.965056277    -0.544211557
H  3.043285813    0.2925319525   -1.4995169849
H -2.0707456688   -3.3688572849   -0.0090602278
H  0.4176956809   -3.4399455996   0.2013172511
H -3.2354561544   -1.2012842108   -0.177495913
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  307.9882
WellDepth[kcal/mol]  5.43
WellDepth[kcal/mol]  40.31
End
Frequencies[1/cm]  65
86.2408          127.1758
171.8267         237.8031          257.8402
330.1055         407.6493          440.0152
454.4478         469.3721          483.6747
515.7923         558.8908          578.4343
623.4799         644.7406          741.6489
755.3921         776.1504          801.3225
816.6011         854.9871          882.9753
902.1229         923.6859          936.4560
956.1878         971.4011          973.7813
983.6439         1022.0629         1055.3707
1090.3419        1109.3951         1161.5448
1184.8730        1199.0582         1231.1661
1244.1374        1256.9500         1292.1740
1301.5092        1358.4898         1374.5380
1387.5333        1435.3263         1455.0553
1467.6640        1482.3781         1513.0873
1588.8843        1608.9243         1634.9399
1650.2733        3008.7264         3067.8606
3132.3336        3146.7346         3150.1920
3154.0850        3158.1474         3161.5179
3175.0032        3181.4977         3217.1804
ZeroEnergy[kcal/mol]  -27.28
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts15-16-----
Barrier      ts15-16  i15  i16

```

RRHO

```
Geometry[angstrom] 24
C 0.5554711997 -0.3337005282 -0.0664577434
C -0.8875260392 -0.0846260171 -0.1254075513
C -0.4251604613 2.3306542306 -0.0223778563
C -1.3211570578 1.2649731139 -0.0946789254
C 0.9368101785 2.1055030195 0.0268519162
C 1.4506861036 0.7784420515 0.0081203838
C -1.8211690958 -1.1244910167 -0.2136520239
C 3.3570707277 -0.733149371 0.0494181295
C 2.4793686903 -1.8301244223 -0.0211008194
C 2.8474083058 0.5442233742 0.0637767881
C 1.1148894193 -1.6297234311 -0.0775159027
H -0.8068873087 3.3456577371 -0.0044307882
H -2.3852023106 1.4631583644 -0.1244400887
H 1.6330714372 2.9350016354 0.0830074726
H -1.4730172186 -2.1501982971 -0.2649217473
H 4.4279763584 -0.8962789065 0.0930173814
H 2.8755932625 -2.8392701543 -0.0308971088
H 3.5130209686 1.3993830645 0.1192067277
H 0.4681509175 -2.4959165061 -0.1287575579
C -4.1403613334 -0.9253340279 0.6875192537
C -3.2825449743 -0.9397766717 -0.3307945015
H -5.2068555759 -0.8142361403 0.5240567266
H -3.8052514531 -1.0243434202 1.7148241701
H -3.6782997405 -0.8391416807 -1.3441943347
```

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 178.3067

WellDepth[kcal/mol] 8.8

WellDepth[kcal/mol] 5.89

End

Frequencies[1/cm] 65

```
70.0450 86.4537
161.7942 182.6467 231.8001
277.5198 399.5872 417.7644
448.7769 473.8670 489.4586
520.9606 529.4487 563.7424
623.5875 675.1314 695.5232
733.9795 779.2380 788.1655
801.3506 807.3677 869.2729
878.1920 888.0023 954.8812
957.5465 967.4235 976.5757
990.6159 1013.3486 1049.2723
1062.9121 1106.8866 1122.8839
1160.1980 1180.3261 1192.2259
1222.9197 1258.4767 1274.9988
1315.3575 1327.2311 1366.1326
1396.3965 1434.4340 1461.4595
1475.8556 1477.5601 1528.9563
1572.4719 1594.6614 1648.8104
1686.6048 3070.8139 3128.6306
```

```

3158.6536          3162.0999          3162.2558
3170.2973          3178.2366          3184.8418
3193.6998          3199.7146          3212.9798
ZeroEnergy[kcal/mol] -55.28
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts16-17-----
Barrier      ts16-17  i16  i17
RRHO
Geometry[angstrom] 24
C  -0.2504511843  -0.326586861  0.5146476007
C  1.1294051074  -0.3705697921  0.1873108387
C  1.0988825107  2.0469859584  -0.2957189866
C  1.824424441  0.8126869892  -0.2047701493
C  -0.2315972034  2.0904867783  0.0017991766
C  -0.9429635911  0.9300248124  0.4381806123
C  1.8935961184  -1.5826154192  -0.109330575
C  2.6169709281  -0.19383494  -1.9476385141
C  2.6796539034  -1.464704157  -1.1977473599
C  -2.9978626142  -0.1452728785  1.1656265232
C  -2.3275197996  -1.3855766839  1.2232892629
C  -2.3124680287  0.9855084176  0.7736751341
C  -0.9936862465  -1.4772770258  0.8986438908
H  1.6285374209  2.9532019281  -0.5678737873
H  2.8806142659  0.8787221043  0.0335268384
H  -0.7713845545  3.0307601115  -0.0547509197
H  1.8027397495  -2.5027625925  0.455660528
H  3.544023444  0.2513386716  -2.3006092182
H  1.7754838237  -0.0580379538  -2.6234309039
H  3.3332093172  -2.2722073863  -1.5204133512
H  -4.0491977628  -0.0860687971  1.4224094465
H  -2.8709678378  -2.2748891377  1.5231680301
H  -2.8245206807  1.9406363888  0.7127143391
H  -0.4967975265  -2.4391665354  0.940753544
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 638.9894
WellDepth[kcal/mol] 29.89
WellDepth[kcal/mol] 29.26
End
Frequencies[1/cm] 65
87.1305          118.1877
188.7124          221.0112          247.1189
361.7480          430.8089          453.6761
465.4662          477.0079          487.3062
550.2862          555.5941          565.9527
652.6072          680.3497          723.9664
741.1664          755.5491          788.0304
790.3671          814.6247          844.1904
868.7334          878.4520          919.1932

```

950.4209	961.4855	976.4356
985.1273	1009.3608	1040.3130
1054.5038	1062.6004	1097.1515
1152.3983	1158.5208	1178.9352
1187.0448	1219.4395	1234.8126
1287.0703	1356.7609	1368.5685
1384.4543	1424.1980	1449.3518
1452.2211	1477.2910	1527.7850
1557.8524	1605.0039	1617.3051
1636.6673	3091.6994	3127.9531
3136.7910	3154.1144	3157.4472
3165.1164	3173.4710	3178.1989
3180.0678	3186.3668	3191.6573

ZeroEnergy[kcal/mol] -31.28

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts16-19-----

Barrier ts16-19 i16 i19

RRHO

Geometry[angstrom] 24

C	-0.2507039602	0.0180002894	-0.4623630246
C	0.8383192003	0.9386011455	-0.5360926765
C	-0.6512737157	2.7155770917	0.1961437115
C	0.6091291609	2.2765390893	-0.2504427427
C	-1.6699496166	1.8122717421	0.3974227895
C	-1.4905526144	0.4400366687	0.0856975756
C	2.1896150675	0.4308079296	-0.8045558689
C	1.6720977994	-1.7343400823	0.2590729872
C	2.567094073	-0.8146339919	-0.4301185239
C	-2.3151966563	-1.8552111762	-0.0041796641
C	-1.1440739052	-2.2677156129	-0.654319929
C	-2.5103589853	-0.5283830204	0.3271188658
C	-0.079963309	-1.3733388201	-0.8732913003
H	-0.8019582306	3.7651237302	0.4230710985
H	1.4285263235	2.9840229478	-0.3233005888
H	-2.6216664875	2.1373532672	0.8043133898
H	2.9032756571	1.0956322964	-1.2806125389
H	1.9013477372	-2.7949011859	0.2136052112
H	1.226813302	-1.4174105823	1.1960871212
H	3.5553436128	-1.1711691699	-0.7121286303
H	-3.104488502	-2.5762304224	0.1803155674
H	-1.0660485626	-3.2838055346	-1.0250380378
H	-3.446234987	-0.2032340171	0.7681248294
H	0.5611565987	-1.5613975821	-1.7264466213

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 688.5853

WellDepth[kcal/mol] 22.63

WellDepth[kcal/mol] 27.59

End

```

Frequencies[1/cm] 65
135.8869          141.3535
185.9715          243.0352          310.8670
361.0165          412.7008          457.6790
469.1912          490.3113          504.6763
558.2994          567.7446          630.6723
639.0723          687.9795          705.0774
729.2566          766.4812          771.3669
800.5419          811.6540          843.7867
866.4548          895.8233          911.3173
944.5004          970.1342          980.1015
988.8157          1007.8306         1036.3488
1065.9161         1089.8702         1106.2390
1148.3335         1177.0570         1187.3347
1208.3370         1220.2956         1239.6934
1262.6145         1353.7025         1372.2863
1396.9944         1413.7495         1443.6882
1469.0565         1479.5661         1515.5788
1577.4307         1586.5189         1600.9472
1638.4690         3112.6181         3125.6165
3147.4975         3157.3305         3158.6564
3163.1880         3166.5872         3171.4042
3182.1083         3183.7341         3196.5064

```

ZeroEnergy[kcal/mol] -38.54

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts21-22-----

Barrier ts21-22 i21 i22

RRHO

Geometry[angstrom] 24

```

C  -0.4669755963  -3.701610993  -0.7560042591
C  -0.364658677   -2.2380042685  -0.4431040042
C  -1.3640496721  -1.2537253662  -0.5628174146
C  -0.7973304566   0.0406128192  -0.3653411155
C  -1.3009585392   1.3643330878  -0.3403581275
C  -0.406241838   2.4127602614  -0.1124781808
C  0.9648263413   2.2136192807   0.09387206
C  0.5781252599  -0.1335175259  -0.1138547409
C  1.5019984483   0.9014135934   0.0965529322
C  2.8641641787   0.5110653771   0.2370575235
C  3.2280388973  -0.8394577274   0.1267637061
C  0.9207842022  -1.5223831006  -0.1299950314
C  2.3127304635  -1.8690650968  -0.0792158496
H  0.198005059   -4.3009096379  -0.1285987292
H  -1.4855089415  -4.067114074   -0.6094754263
H  -0.1863958334  -3.8883830579  -1.7983647747
H  -2.4088271522  -1.4741510029  -0.7347272831
H  -2.3519040625   1.5708474573  -0.5082078687
H  -0.787265167   3.4286581874  -0.1052444201
H  1.6171206965   3.0672972954   0.242300734
H  3.6295614802   1.261909983    0.3975647804
H  4.2802344038  -1.0959708939   0.193772702

```

```

H 0.2199655632 -2.0546391529 0.8068349307
H 2.6464559421 -2.8960414448 -0.1663301432
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1321.6917
WellDepth[kcal/mol] 19.62
WellDepth[kcal/mol] 36.74
End
Frequencies[1/cm] 65
129.3272 152.6303
186.2525 207.1028 228.3477
294.3726 384.5954 412.2917
487.4940 492.2843 521.1271
543.3617 563.8827 588.3376
620.0803 664.1652 683.2639
724.3769 742.1932 783.9967
788.9082 813.0639 826.0473
830.9283 867.1503 954.1646
957.1588 967.8940 1013.5285
1053.7376 1057.0375 1073.3256
1097.4201 1134.5796 1153.4463
1170.3095 1186.1486 1202.6743
1237.2615 1285.0202 1320.0586
1358.2714 1375.4241 1396.4872
1422.2314 1446.8197 1460.6445
1483.1567 1490.1960 1509.1882
1515.3927 1541.8323 1577.5859
1618.5504 1910.4369 3020.3598
3074.3564 3101.6903 3157.2610
3158.7205 3172.4807 3177.4032
3182.9537 3187.4991 3207.9837
ZeroEnergy[kcal/mol] -39.65
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts14-p1-----
Barrier ts14-p1 i14 p1
RRHO
Geometry[angstrom] 24
C -0.0633239864 0.0011982866 0.0475940345
C 0.6354222909 1.2415683388 0.0320952331
C -1.4910121067 2.4143721182 -0.0938669567
C -0.083454048 2.4184258167 -0.0353308166
C -2.1838336617 1.227416816 -0.0780496278
C -1.4921025928 -0.0061103217 -0.0042810531
C 2.1508318985 1.2713800704 0.0871729332
C 2.1040697552 -1.226165482 0.1974829814
C 2.7961111871 -0.0660522168 0.2726262744
C -1.4810653956 -2.4322994519 0.0995798982
C -0.0704999792 -2.4276580534 0.1524851239
C -2.1765794633 -1.252130742 0.0215199557

```

```

C  0.6380732665   -1.2441267028    0.1258599353
H  -2.025193034    3.3564597626   -0.1481553979
H  0.4444698481    3.3672043936   -0.0429499113
H  -3.2677929119    1.2200903054   -0.1200801506
H  2.539872688     1.72343872    -0.8384739367
H  2.4794481366    1.949054969    0.8862416868
H  2.6032854961   -2.1668361833    0.4027675117
H  3.8728443929   -0.086140795    0.4046431939
H  -2.0120784395   -3.3773574274    0.1200799783
H  0.4666997481   -3.3685923269    0.2085011021
H  -3.2605685526   -1.2526300658   -0.0208715052
H  2.4957754636   -1.7021548282   -1.6753144868
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  654.3176
WellDepth[kcal/mol]  31.32
WellDepth[kcal/mol]  4.59
End
Frequencies[1/cm]  65
77.7429          155.9644
198.1064         233.7055          257.4250
360.2480         402.2492          432.1628
439.3368         474.0601          476.7943
478.4899         519.8273          577.5389
594.6595         607.5869          655.2759
735.6529         764.1114          778.1287
792.9817         815.1477          823.4318
842.9291         899.3350          915.9988
951.4987         962.5704          979.9930
987.3014         1005.3515         1047.2960
1064.5692        1102.4606         1118.2720
1173.2163        1193.5163         1199.9750
1219.1200        1234.1637         1252.8575
1267.6933        1333.7497         1384.2505
1397.0186        1418.5977         1421.6223
1452.5798        1467.2531         1497.4050
1541.1712        1609.8521         1625.3637
1637.3509        1666.0553         2966.7481
3003.8122        3152.0865         3156.9158
3159.1933        3163.5131         3167.4729
3174.7765        3181.8740         3184.8758
ZeroEnergy[kcal/mol]  -36.27
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts19-p1-----
Barrier      ts19-p1  i19  p1
RRHO
Geometry[angstrom]  24
C  -0.0600934276   -0.0174735345    0.0518734566
C  -0.3769357849    1.374639625     0.0311127042

```

C	-2.743538218	0.8144064086	0.0243139557
C	-1.7045859051	1.7669342216	0.0197339062
C	-2.4569720293	-0.5293962913	0.0263373068
C	-1.1097725428	-0.9810922141	0.033550237
C	0.7143267301	2.3437945619	-0.0200189424
C	2.4104737639	0.5549284235	0.3125314137
C	1.9973223002	1.9804433174	0.0834334294
C	0.539697061	-2.7663281199	0.0550856968
C	1.576756005	-1.8228697483	0.0792932656
C	-0.7772440932	-2.3601445397	0.0301536221
C	1.3084298328	-0.453094308	0.0332110393
H	-3.7745798994	1.1499179892	0.0171181651
H	-1.9465417219	2.8243674824	-2.592871E-4
H	-3.2552227202	-1.263826085	0.0188919633
H	0.4491304755	3.3884551963	-0.1498992824
H	3.3015553587	0.3138268448	-0.2743769678
H	2.7155578341	0.4487798055	1.3658468218
H	2.7826942036	2.7284083657	0.0474992951
H	0.7807730633	-3.8234677302	0.0643254589
H	2.6080013049	-2.1586547869	0.1125955078
H	-1.5775064875	-3.0923162562	0.0180927538
H	1.4968378966	-0.2568276279	-1.8785255192

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 721.9896
WellDepth[kcal/mol] 30.54
WellDepth[kcal/mol] 5.27
End
Frequencies[1/cm] 65

113.9477	156.4338	
202.2847	239.7456	372.9049
387.4188	415.7992	425.8074
450.6250	476.5690	483.0602
503.7095	509.2932	573.3572
596.0444	613.1110	645.7605
729.0293	761.3059	779.4538
788.8410	815.9835	822.4566
846.2760	895.6429	913.7229
955.9012	959.5731	979.7623
985.8237	997.0472	1048.4061
1066.3522	1104.3991	1122.1488
1175.7537	1193.0175	1204.0232
1217.5079	1229.0593	1251.9467
1267.3358	1331.2121	1381.5721
1390.8294	1410.1336	1424.3944
1461.3140	1465.1456	1487.8280
1535.2097	1605.6250	1616.8584
1636.7616	1699.3217	2961.6450
3050.8807	3150.7025	3158.1255
3159.2497	3166.1013	3168.1987
3172.3959	3183.2037	3184.7577

ZeroEnergy[kcal/mol] -35.59

```

ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts12-p2-----
Barrier      ts12-p2  i12  p2
RRHO
Geometry[angstrom]  24
C  -1.010282092    2.0058058373   -0.0457078139
C  -1.631988179    0.7469614412    0.0278370486
C   0.5370052173   -0.3862457896    0.0672678421
C  -0.8833740316   -0.4213140832    0.0855424869
C   1.1655400551    0.9012081522   -0.0010847807
C   0.3646477745    2.0744814579   -0.0565369427
C  -3.100341405    0.4005773588    0.0604700451
C  -1.8094401942   -1.5638077869    0.1491350655
C  -3.0869152013   -1.0983933583    0.1833029486
C   2.7232350207   -1.4438801175    0.0900224226
C   3.3454007186   -0.1760612918    0.0293783262
C   1.3526103652   -1.5454766794    0.1083049247
C   2.5834554701    0.9659543857   -0.0158623113
H  -1.6049386933    2.9122416263   -0.0901424898
H   0.8618007313    3.0373264661   -0.1089773222
H  -3.6240750117    0.8754577253    0.9001385685
H  -3.6203950271    0.7292562801   -0.850031292
H  -1.516940653    -2.5876792857    0.3349157806
H  -1.6848304688   -2.2060767569   -1.7564388697
H  -3.9795911463   -1.7039685769    0.2592689758
H   3.3336633179   -2.3394579301    0.1203413484
H   4.4274800622   -0.1094053724    0.0162535667
H   0.8840637682   -2.5219185658    0.1493675803
H   3.0593896019    1.9399188638   -0.0660121082
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  586.3837
WellDepth[kcal/mol]  33.77
WellDepth[kcal/mol]  3.96
End
Frequencies[1/cm]  65
112.3577          129.5063
220.1278          236.9661          257.1050
277.2873          325.6929          411.5057
432.8427          459.7626          465.0112
506.8749          520.0614          573.5601
612.4584          680.1111          681.7438
715.7034          749.0580          752.7241
795.8303          818.3469          838.5436
878.6747          881.4479          931.3597
955.4761          958.4054          964.1298
968.9099          971.0319          994.0632
1044.3349         1071.3736         1118.2310
1141.5153         1167.5446         1178.7616

```

1190.5546	1216.4718	1236.7107
1283.2014	1295.0506	1351.1799
1378.1811	1391.3769	1426.5539
1430.1135	1469.1562	1486.5530
1534.1178	1559.4663	1606.6464
1630.8977	1665.1776	3005.2631
3029.5507	3156.8165	3158.7557
3166.8129	3175.6793	3179.5578
3189.4202	3204.2843	3222.7327

ZeroEnergy[kcal/mol] -32.52

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts17-p2-----

Barrier ts17-p2 i17 p2

RRHO

Geometry[angstrom] 24

C	-0.5561474778	-0.4019702496	0.0025529198
C	0.8616160091	-0.4996742827	0.0030965122
C	1.0807770774	1.9419054508	-0.0590289665
C	1.6649861946	0.6530355615	0.0561873677
C	-0.2838614868	2.0577425177	-0.0830675805
C	-1.1319258617	0.9113793989	-0.0325388803
C	1.7367799817	-1.6648227637	-0.0658740081
C	3.1104251811	0.2377641315	-0.1349828799
C	3.0218781382	-1.2660410179	-0.1320312758
C	-3.3533813084	-0.0769684086	-0.0161561656
C	-2.7851599281	-1.3692876533	0.0119276572
C	-2.5430781562	1.0345273777	-0.0395183665
C	-1.4188658633	-1.5269266759	0.0185972128
H	1.7112020163	2.8237367234	-0.0932258704
H	-0.7466058838	3.0371288215	-0.1424322493
H	1.3995320219	-2.6927083253	-0.0691049124
H	3.7874954055	0.6279818047	0.6300731319
H	3.4825740189	0.602265051	-1.1026942759
H	3.8864417149	-1.9137899466	-0.1889421224
H	-4.4316515397	0.0358812165	-0.0204457732
H	-3.4315844058	-2.2395147415	0.0304107135
H	-2.9789429034	2.0279557598	-0.0639863919
H	-0.9910599616	-2.5224518711	0.0440398481
H	1.8032910169	0.6888871213	1.9727033556

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 702.9684

WellDepth[kcal/mol] 29.37

WellDepth[kcal/mol] 5.31

End

Frequencies[1/cm] 65

111.0437	128.7695	
224.3494	241.8118	274.3638
370.0890	401.9669	422.8161

441.9605	458.8567	504.7338
515.1000	521.2554	567.5127
611.3282	674.3077	684.2630
726.0641	748.9940	752.3363
801.3682	815.6097	840.6904
879.1104	881.2481	932.1632
952.0595	954.6435	959.7125
966.9878	971.0966	993.3931
1045.5647	1076.6118	1126.2267
1144.7269	1168.1011	1177.8986
1192.3943	1211.6341	1234.0192
1284.4908	1286.4325	1353.0052
1372.6451	1385.3220	1430.7513
1435.4219	1467.9125	1475.0613
1544.8633	1567.5875	1611.2070
1625.8175	1654.9415	3007.8916
3067.7580	3158.1861	3160.9656
3167.2543	3178.5258	3179.7087
3189.4376	3197.2353	3218.5505

ZeroEnergy[kcal/mol] -31.17

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts12-p3-----

Barrier ts12-p3 i12 p3

RRHO

Geometry[angstrom] 24

C	0.2003578984	-1.3234899668	0.136586655
C	1.4365421729	-0.6405377373	0.1382952226
C	0.3117157251	1.5227823086	0.0091383506
C	1.4910471609	0.744908703	0.0769664475
C	-0.9444560277	0.8272974254	0.0108376283
C	-0.9616660409	-0.5936215939	0.0762809094
C	2.8114396447	-1.164291235	0.1882705451
C	2.9359723366	1.1835303956	0.0972011125
C	3.6808114085	-0.1202680357	0.2140317415
C	-0.8736010771	3.6406916603	-0.1205880972
C	-2.1115934464	2.9569993091	-0.1185404464
C	0.307290221	2.9414983542	-0.0579673274
C	-2.142258741	1.5849618059	-0.0541637426
H	0.1712759852	-2.4066401231	0.179347513
H	-1.9223616559	-1.0978963345	0.0752810747
H	3.0635780645	-2.200727516	0.3682863244
H	3.0015989967	-1.7655012927	-1.7225285686
H	3.1609382573	1.8548369618	0.9358912383
H	3.2169517918	1.7281032542	-0.8148535544
H	4.7579041462	-0.1909570867	0.2793120534
H	-0.8603989731	4.7237261563	-0.1721997829
H	-3.0361847524	3.5208865179	-0.1682701045
H	1.2523864646	3.4731765806	-0.060545173
H	-3.0912735597	1.0585864888	-0.0528560193

Core RigidRotor

SymmetryFactor 0.5

```

End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  589.7493
WellDepth[kcal/mol]  33.74
WellDepth[kcal/mol]  4.07
End
Frequencies[1/cm]  65
109.5949          136.2490
229.1342          235.9127          245.0849
272.8001          327.5149          415.3074
433.4025          456.8020          466.0928
520.4309          520.7384          559.3707
616.6653          680.9680          682.6272
714.6219          751.3348          759.5826
787.1020          827.9301          837.1024
870.3640          873.6152          934.1113
956.0219          958.5093          969.0526
972.1631          981.2720          993.1048
1044.0550         1059.1820         1110.1578
1143.6833         1167.3814         1179.3699
1185.0116         1232.9099         1241.4073
1266.3998         1288.5925         1361.1544
1377.9750         1397.9458         1415.9543
1432.6410         1467.9526         1488.4605
1535.2006         1561.8214         1611.9018
1630.6206         1663.3786         3004.8701
3029.4209         3157.2641         3160.7871
3164.7169         3177.0352         3179.4718
3188.0144         3199.0250         3219.6406
ZeroEnergy[kcal/mol]  -32.55
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts2-p4-----
Barrier      ts2-p4  i2  p4
RRHO
Geometry[angstrom]  24
C  -4.5390052317  -0.8030966877  1.2088351288
C  -3.3033248329  -0.0830534569  0.9520765945
C  -2.2577195624  0.407898198   0.5613023452
C  -1.0846751629  1.2333794144  0.443326404
C  -1.2303169031  2.5863996177  0.1896150277
C  -0.1070998138  3.4301188299  0.0785020157
C  1.1604165731   2.9206485732  0.2174975872
C  0.2279592833   0.674670959   0.5908751939
C  1.3612134041   1.5403908702  0.4759177954
C  2.6621144938   0.9922907649  0.6258909583
C  2.8402757991   -0.345702983  0.8764262444
C  0.4466459083   -0.7017540546  0.8511194816
C  1.7200873632   -1.1997389549  0.9896282625
H  -4.4870531479  -1.3604217575  2.1486745126
H  -5.3901411027  -0.119039386   1.2692286679
H  -4.7396101864  -1.5194781777  0.4031419616

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H -2.0667112493 -0.5860483885 -1.0532299332
H -2.2264647278 2.995735038 0.0744647706
H -0.2538554153 4.4857713178 -0.1193814423
H 2.0268493094 3.5678281748 0.1312236487
H 3.5175524821 1.6539898329 0.5385550641
H 3.8395227877 -0.7512298899 0.9884234791
H -0.4103729283 -1.3580447518 0.9375724877
H 1.8688868603 -2.2553881023 1.1871447441
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 706.1139
WellDepth[kcal/mol] 34.95
WellDepth[kcal/mol] 5.8
End
Frequencies[1/cm] 65
47.2621 71.2991
77.9395 158.2765 160.5429
175.8722 243.7666 262.4663
354.5689 385.1569 404.1424
446.5882 478.7933 500.2188
531.7432 542.8026 587.8280
604.3266 655.6980 690.1442
747.0397 791.1077 805.6297
815.3470 833.1670 881.1620
924.9642 957.6110 967.6782
985.7296 999.3818 1037.0870
1042.5812 1055.2557 1076.3271
1119.6429 1168.7724 1182.3772
1200.9802 1237.4349 1266.4944
1301.8607 1360.7203 1392.6782
1410.0495 1425.6910 1468.1055
1470.7639 1475.1882 1492.8365
1544.3146 1613.0113 1629.5928
1661.8480 2233.5965 3009.1703
3065.0897 3083.3039 3159.0145
3162.7282 3170.3651 3178.9945
3183.9017 3193.7088 3196.3476
ZeroEnergy[kcal/mol] -4.48
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts20-p4-----
Barrier ts20-p4 i20 p4
RRHO
Geometry[angstrom] 24
C 0.4520731587 -0.1396946256 0.0489447314
C -0.7313529035 0.6771046821 0.0908504394
C 0.653443589 2.6771367973 -0.0178134153
C -0.6089948422 2.0599245685 0.0561191636
C 1.7978500366 1.9173188091 -0.0567929246
C 1.7288753378 0.5008599407 -0.0250094438

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C -2.0211037092    0.0856361416    0.17097991
C -3.1293631686   -0.4097830462    0.1715293908
C -4.4439857854   -0.9851948334    0.4465317425
C  2.8159267234   -1.6724564073   -0.0376823875
C  1.5537734265   -2.3036610244    0.0339431731
C  2.898694939    -0.3023610221   -0.0666668323
C  0.4013505912   -1.5554862665    0.0761377859
H  0.7148016262    3.7590586819   -0.0442296543
H -1.5060427274    2.6661828817    0.0861893784
H  2.7718877237    2.3915679103   -0.113396253
H -3.3160901902   -0.5398815694   -1.94390215
H -4.6175625497   -1.039450619    1.5256539983
H -4.5267045554   -1.9945444975    0.0355879922
H -5.2384843092   -0.3801260853    0.0025126681
H  3.7172684155   -2.2740681777   -0.0705485431
H  1.4962931318   -3.3861454189    0.0546658651
H  3.8643561515    0.1890884778   -0.1228030275
H -0.5659721101   -2.0398162975    0.1290973928
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  415.8985
WellDepth[kcal/mol]  40.99
WellDepth[kcal/mol]  3.22
End
Frequencies[1/cm]  65
52.1117          71.5811
74.2595          136.6391          163.9678
177.7013         274.4205          275.0017
343.8571         378.8381          407.6289
413.8758         471.5166          480.4276
499.2670         541.0993          584.0272
590.4129         653.0752          684.6341
747.6880         790.3669          804.7850
816.1606         833.0399          882.1945
924.2946         954.6183          968.9802
986.6926         1000.4394         1042.4203
1044.2063        1060.3610         1076.4707
1119.7825        1168.8892         1181.6404
1202.2683        1237.6208         1266.9255
1308.3161        1356.5778         1390.7028
1412.8599        1426.8259         1467.7051
1475.9276        1480.3572         1491.4179
1543.0525        1609.3770         1625.2395
1660.4924        2273.6239         3025.6362
3084.5928        3091.8607         3160.1195
3163.8492        3171.0304         3179.7801
3184.0883        3194.1663         3195.4235
ZeroEnergy[kcal/mol]  -7.06
ElectronicLevels[1/cm]  1
0  2
End
!-----

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!-----bar_ts2-p5-----
Barrier      ts2-p5  i2  p5
RRHO
Geometry[angstrom]  24
C  -4.3533905647   -0.510217511   0.7115720434
C  -3.0960738432   -0.6412416486   0.366557573
C  -1.8514758722   -0.8399528623   0.0139571871
C  -0.7892730529    0.1865534873   -0.0290127347
C  -1.120637176    1.5278962867   -0.1101516262
C  -0.1357979158    2.5307868687   -0.1736809098
C  1.1955262252    2.1947722284   -0.1706891053
C  0.5963815082   -0.1907539421   -0.0062650429
C  1.5936761139    0.8371814216   -0.0888164127
C  2.9665426659    0.4751931314   -0.0791434077
C  3.3539202529   -0.8373994481   0.0177328775
C  1.0389113462   -1.5364319616   0.1089756506
C  2.3764572011   -1.8519150801   0.1176788559
H  -4.6677026442   -0.6057173723   1.7468641072
H  -5.1026304174   -0.1778603507   -0.0013047094
H  -5.1935841979   -2.47824175    0.4417353164
H  -1.5895589785   -1.8511865692   -0.2880318055
H  -2.1674352452    1.8082729112   -0.1397561491
H  -0.437895536    3.5699850032   -0.2389020697
H  1.9602030139    2.9617318777   -0.231908376
H  3.7089582875    1.2635426847   -0.1472649925
H  4.4059487231   -1.0990187375   0.0246578049
H  0.3142141633   -2.3341449402   0.2075924748
H  2.6847589428   -2.887488727    0.2074594508
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  357.7577
WellDepth[kcal/mol]  37.23
WellDepth[kcal/mol]  2.84
End
Frequencies[1/cm]  65
36.5788          87.5914
120.6938         166.0537         176.6909
226.0967         259.4551         262.9401
357.1700         419.0076         426.2693
432.6091         478.2649         513.7969
526.7005         543.5507         618.0513
655.6935         689.0048         744.7060
764.2745         794.1602         805.9207
814.8087         868.3656         878.9819
893.2214         902.7002         925.7164
963.5513         985.2184         996.8898
1014.0947        1017.3089        1052.4984
1096.0389        1121.7256        1169.6668
1190.1902        1195.5037        1232.9137
1264.0128        1279.5211        1336.4346
1383.1544        1392.8609        1424.7388
1461.7609        1481.0422        1495.7246

```

1549.7271	1613.5587	1634.3695
1662.6503	2001.0535	3109.0217
3130.5323	3159.3992	3161.9891
3169.8897	3173.6210	3181.6871
3184.6032	3186.5446	3197.9931

ZeroEnergy[kcal/mol] -2.2

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts10-p5-----

Barrier ts10-p5 i10 p5

RRHO

Geometry[angstrom] 24

C	0.5309185348	-0.2657386867	-0.0753144147
C	-0.7985186755	0.1257935313	0.2986957771
C	0.0093839876	2.3745358718	0.7769453768
C	-1.0280535418	1.4257778577	0.7093561671
C	1.2925574219	2.0214237515	0.4407146444
C	1.5850810199	0.7034241452	0.0101309446
C	-4.4453552875	-0.2995739385	0.6635403999
C	-3.1820621867	-0.5677681401	0.5261797128
C	-1.9132453141	-0.8542730711	0.2650589486
C	3.1903564296	-0.9442542477	-0.7782528275
C	2.1536223629	-1.8975340483	-0.8799019952
C	2.9068337133	0.3265089503	-0.3458211343
C	0.8635281169	-1.5666834169	-0.5403281807
H	-0.2130688051	3.3832882179	1.1060230554
H	-2.0320336983	1.7173912821	0.9958943211
H	2.099382528	2.7441471822	0.4992907601
H	-4.9138197105	-0.2197927623	1.641534438
H	-5.0861436337	-0.1464494866	-0.2034027446
H	-1.652129541	-1.9076481666	0.2729519072
H	4.2040811671	-1.2179476179	-1.0479059028
H	2.3768062772	-2.897604279	-1.2342164057
H	3.6934849713	1.0701464437	-0.2717187024
H	0.0895992284	-2.3145036132	-0.649341079
H	-2.0233763648	-1.1249307587	-1.6749450662

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 670.7499

WellDepth[kcal/mol] 36.95

WellDepth[kcal/mol] 4.83

End

Frequencies[1/cm] 65

45.2001	106.0587	
123.5117	176.4943	213.9752
248.5106	260.4308	364.9655
403.3492	422.1199	434.4510
452.1806	478.4215	514.5551
523.8723	542.1603	602.0572
652.1209	673.5545	743.1356

765.8695	792.9350	806.3842
812.9614	868.3921	876.3565
881.1238	926.5930	943.6714
962.2858	986.5699	994.4425
996.3063	1011.2629	1053.0150
1096.6676	1119.7558	1169.6641
1191.7536	1196.6841	1233.8341
1262.4955	1280.6567	1335.6908
1384.0842	1394.4412	1424.1116
1454.0661	1480.0666	1496.0628
1550.6472	1613.7095	1636.1978
1663.4989	1981.2230	3088.7629
3151.7328	3157.7635	3159.5346
3162.3227	3170.6475	3173.8011
3185.1720	3186.7880	3203.1758

ZeroEnergy[kcal/mol] -0.21

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts15-p5-----

Barrier ts15-p5 i15 p5

RRHO

Geometry[angstrom] 24

C	-0.4992521186	-0.3173368125	0.0360054166
C	0.8677635987	0.1275956826	-0.035949809
C	0.0904951842	2.4141345947	-0.3820826249
C	1.1255676839	1.4747015725	-0.2408756352
C	-1.2221700869	2.0144520038	-0.3125362156
C	-1.5482950685	0.6518321978	-0.1033278873
C	1.9776101285	-0.8236662059	0.1074769089
C	4.4866602882	-0.3426509916	-0.4539766453
C	3.2609972461	-0.5485819913	-0.0599675768
C	-3.2246409713	-1.0897721972	0.1643276716
C	-2.1971307686	-2.0494721032	0.2939119512
C	-2.9019892078	0.2289010242	-0.0314020072
C	-0.8767051281	-1.6735135784	0.2295621983
H	0.3370955262	3.45819914	-0.5385481812
H	2.1555891322	1.8094930067	-0.2827983495
H	-2.026425725	2.7351317055	-0.414651778
H	1.7456373412	-1.8328637116	0.4318019424
H	5.2618616203	0.0119338117	0.2159030981
H	4.7675314841	-0.5298896375	-1.4878564823
H	-4.262440105	-1.3985559019	0.2171763826
H	-2.4523140371	-3.0925604624	0.4433656711
H	-3.6819328896	0.975810855	-0.1366120588
H	-0.1174878926	-2.4385749536	0.3229799643
H	3.5674247656	-0.1685980477	2.031474046

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 487.7839

WellDepth[kcal/mol] 62.28

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WellDepth[kcal/mol]  3.24
End
Frequencies[1/cm]   65
22.2570              84.0729
120.3893             126.6883           175.9574
241.5962             259.5355           365.3472
396.1572             415.3698           420.1932
440.5641             477.0014           511.7776
520.0771             543.4342           609.2635
655.1899             681.3478           742.9924
767.5304             792.4481           805.3679
812.5573             871.7810           876.7425
885.5229             892.1358           926.4910
961.1696             987.1901           996.5448
1005.9913            1016.2488          1053.6649
1101.4745            1123.9559          1169.6763
1192.1512            1201.5932          1233.1387
1263.7761            1280.1672          1337.9869
1384.4245            1396.4665          1424.7521
1460.3564            1481.9424          1494.6993
1550.2335            1609.9485          1631.7369
1662.2742            1983.6281          3109.5037
3156.6846            3160.0260          3162.9532
3170.8221            3175.3703          3185.4935
3187.6683            3190.5477          3201.8766
ZeroEnergy[kcal/mol] -1.8
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts16-p5-----
Barrier      ts16-p5  i16  p5
RRHO
Geometry[angstrom]  24
C  -0.2575223884   -0.0327404005    0.0125427607
C   0.825947297    0.9138760084    0.0952173987
C  -0.78633698     2.7484089674   -0.1005644519
C   0.5295583296    2.2698387762    0.0254309557
C  -1.8324840221    1.8636545875   -0.1666536197
C  -1.5969970731    0.4657942569   -0.1164377692
C   2.2445628669    0.5833878307    0.2575752938
C   3.5733677237   -1.5961900978    0.8222620816
C   2.8792282491   -0.5679667891    0.416476637
C  -2.4623929723   -1.805907651    -0.1613751048
C  -1.1468993181   -2.3005912968   -0.0455516856
C  -2.6770725885   -0.4506933897   -0.1975708934
C  -0.0770877227   -1.4391236626    0.039300432
H  -0.964521794    3.8166911951   -0.1447923025
H   1.343998641    2.9844159702    0.0778356983
H  -2.8531871289    2.2182053496   -0.2622973587
H   2.9009534179    1.4516880208    0.2017195583
H   4.0329177506   -2.2969737576    0.1344059223
H   3.6959040607   -1.7876787752    1.8857162048
H  -3.296938441    -2.4949590168   -0.2255926194

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H -0.975468948 -3.371077151 -0.025511718
H -3.6831609659 -0.0557207424 -0.2926183541
H 0.9193520826 -1.8446443842 0.124170638
H 3.061903924 -0.9186618483 -1.6895657037
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 487.0267
WellDepth[kcal/mol] 60.08
WellDepth[kcal/mol] 3.95
End
Frequencies[1/cm] 65
36.7032 101.8680
136.5124 142.3226 176.9138
247.5559 277.4011 366.0295
386.1574 415.3938 424.7488
442.2608 480.0651 512.0620
520.7546 551.3736 612.7407
646.0492 680.4563 722.6458
744.9662 791.3461 808.3120
815.6813 877.3851 888.6322
892.9783 895.4110 926.3566
967.8929 984.5027 999.8032
1009.8839 1041.9383 1052.8918
1088.8628 1143.9365 1169.9407
1189.4866 1206.3704 1236.0389
1245.0021 1293.9863 1349.6380
1385.3061 1398.4769 1427.7581
1465.1950 1482.4649 1494.3745
1550.0954 1606.3177 1630.5263
1661.6893 1978.0754 3102.3256
3109.4832 3159.5480 3161.2205
3168.2370 3171.2228 3186.0919
3187.3094 3190.1109 3233.6803
ZeroEnergy[kcal/mol] -1.09
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts10-p6-----
Barrier ts10-p6 i10 p6
RRHO
Geometry[angstrom] 24
C 0.2733794815 -0.0339281707 -0.199476254
C -0.9506643831 0.6971958561 -0.3134957167
C 0.2720271911 2.7826300708 -0.0289962974
C -0.9322942859 2.0709471388 -0.2277297554
C 1.4596925313 2.1068924915 0.0785217716
C 1.4945361831 0.6905871246 -0.0053748263
C -3.2090669399 -1.4059689712 1.5340873346
C -2.7835779738 -0.7311735397 0.6264061795
C -2.2765390436 -0.0173118198 -0.5434382197
C 2.7403171669 -1.3961595399 0.0155630268

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C 1.5382402053 -2.1135299977 -0.1713741208
C 2.7149728765 -0.0258916295 0.0975931583
C 0.3381022059 -1.4513477543 -0.2747717997
H 0.2480718535 3.8645551592 0.0344912088
H -1.8626813376 2.6224493258 -0.3151670295
H 2.3899994267 2.6447063612 0.2278160997
H -3.5728158374 -1.8279747949 2.4392796715
H -2.1854301432 -0.7279651155 -1.3747617084
H -3.0229577603 0.7188258875 -0.8563185424
H 3.679894875 -1.9309926513 0.0962038589
H 1.5628025864 -3.1958604896 -0.2293866286
H 3.6336226721 0.5328958534 0.2431988528
H -0.5721104661 -2.0239098974 -0.3987446594
H -3.3786230843 -3.2987528974 0.6880063957
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 449.3232
WellDepth[kcal/mol] 38.5
WellDepth[kcal/mol] 3.34
End
Frequencies[1/cm] 65
45.3091 54.0144
78.8575 150.9509 176.8174
217.7525 262.1258 275.6250
378.5677 416.1950 433.2491
436.0754 478.8597 513.7825
523.8740 557.5711 616.5222
663.2079 664.9663 724.1107
746.8152 755.0295 793.0110
804.7137 813.3714 867.0211
886.4878 918.0674 933.3033
956.2360 967.6476 984.6778
998.0466 1040.2011 1061.4485
1097.8132 1169.2296 1185.2944
1188.8542 1214.6533 1240.7487
1262.0586 1289.3159 1332.5679
1383.7810 1397.5236 1425.2570
1467.6405 1479.7013 1495.8324
1549.3139 1618.7591 1641.9892
1665.9763 2169.9616 3010.5530
3058.5398 3158.3558 3159.9913
3166.1673 3171.1324 3184.9135
3185.7463 3200.5033 3463.2959
ZeroEnergy[kcal/mol] 1.34
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts4-p7-----
Barrier ts4-p7 i4 p7
RRHO
Geometry[angstrom] 24

```

```

C 0.4733024465 0.0997196019 0.7155802006
C -0.8425080651 0.6611477346 0.8072935849
C 0.0685944495 2.8673674122 0.3452159867
C -1.0234603465 2.0193967281 0.6219845344
C 1.33874363 2.3555758824 0.2484351748
C 1.5743306778 0.9686286297 0.4310940699
C -2.8088162408 -0.6732143015 1.8665730106
C -1.9875548715 -0.1810973492 1.0934394503
C -2.4578444954 -0.85177211 -1.0056752447
C 3.0922564 -0.927580627 0.5261057751
C 2.0047905412 -1.7842883588 0.8100776686
C 2.8791722197 0.4163017939 0.3430870955
C 0.7285648092 -1.2828861688 0.903866978
H -0.1052154634 3.9287948236 0.2096805175
H -2.0222771683 2.4325409415 0.6949653922
H 2.1803573932 3.0053274159 0.0330980248
H -3.6332702381 -1.2254076828 2.2532151272
H -1.4844315021 -1.2159221724 -1.3101648229
H -2.7703179148 0.1031966194 -1.4093093048
H -3.2318577128 -1.5941749772 -0.8585820985
H 4.0944228581 -1.3352446808 0.4560924311
H 2.1813981395 -2.8437920745 0.9578040698
H 3.7101856495 1.0801722176 0.1286305403
H -0.1026691954 -1.9392532977 1.1306058386
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 541.7243
WellDepth[kcal/mol] 31.85
WellDepth[kcal/mol] 10.96
End
Frequencies[1/cm] 65
41.8345 83.7354
89.4065 136.3084 155.5747
173.8321 229.1338 316.2761
355.7762 433.5588 447.1053
474.8120 479.0291 508.3359
518.1158 546.0993 562.8477
575.5390 606.9517 650.0449
697.0455 705.4575 747.3657
791.4012 806.0677 815.4793
864.7867 881.3995 893.8615
924.0189 969.6221 985.5888
999.6514 1032.5655 1049.1644
1091.7810 1167.9840 1179.8628
1188.0629 1234.2161 1245.8766
1288.1620 1359.9581 1391.5726
1417.2908 1419.7836 1422.6493
1467.3793 1490.7375 1543.3199
1611.9100 1629.8501 1661.1185
1989.8059 3087.1778 3159.2705
3163.0248 3170.1622 3178.1029
3183.8262 3191.6227 3194.8727

```

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3247.3856          3248.2445          3431.7594
ZeroEnergy[kcal/mol] -4.86
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts21-p8-----
Barrier      ts21-p8  i21  p8
RRHO
Geometry[angstrom] 24
C  -0.2685444226  -0.0159566706  0.0445457761
C  -1.4119320204  0.7803454707  0.068592984
C  -2.6550056245  0.0895963888  -0.0139253368
C  -2.6696860752  -1.2866014028  -0.1444101104
C  -1.4793929387  -2.0610081463  -0.2176768969
C  -0.261492027  -1.4158266789  -0.1273919233
C  1.0668275347  0.4763195031  0.1031904946
C  1.2424306945  1.8579244066  0.0301351653
C  0.0988020339  2.6908521192  0.071559232
C  -1.1921172522  2.188224707  0.1123251468
C  1.1511912282  -1.810906949  -0.2110220878
C  1.9483414701  -0.7145130771  -0.0918308336
C  3.4407584963  -0.6570256505  -0.129097286
H  -3.5874474379  0.6433283639  0.0115224748
H  -3.623445682  -1.7984147826  -0.2119619237
H  -1.5491744827  -3.1345527465  -0.3571504401
H  1.3306216829  0.2881211789  1.9650792311
H  2.2297705331  2.304886656  -0.0090031388
H  0.2430279045  3.7656775626  0.0652536079
H  -2.0365200117  2.8685693053  0.1422798743
H  1.504461339  -2.8249403368  -0.3461779679
H  3.7929931404  -0.0175882981  -0.9463818334
H  3.8423546062  -0.2400960439  0.8007009304
H  3.870847311  -1.6503588789  -0.2694431384
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 813.9111
WellDepth[kcal/mol] 27.56
WellDepth[kcal/mol] 5.87
End
Frequencies[1/cm] 65
125.6299          150.6479
170.2657          215.9667          229.9769
294.6746          322.1176          409.8960
414.5657          432.5569          474.3070
496.4841          533.5039          548.3305
584.8000          592.3271          623.4650
664.0912          684.7728          761.3242
774.8164          799.2438          816.4866
818.3943          858.1695          909.1416
920.0877          968.4812          974.2899
982.7933          1018.9768         1040.5504

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1058.4725	1062.6814	1088.5472
1155.7303	1178.6472	1202.6261
1211.2809	1245.6208	1282.6925
1315.2457	1381.5807	1396.3056
1412.5757	1443.2018	1452.3463
1476.8563	1480.6916	1489.6370
1514.0051	1597.0222	1611.6854
1643.6810	1649.9083	3014.3549
3057.7275	3103.8709	3160.1606
3161.0276	3170.4641	3172.2479
3183.4047	3184.5564	3202.5384

ZeroEnergy[kcal/mol] -31.71

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts22-p8-----

Barrier ts22-p8 i22 p8

RRHO

Geometry[angstrom] 24

C	0.4596999626	-0.0183589649	0.4175197111
C	1.5993581458	0.7843306008	0.363755708
C	2.8451419883	0.0952015744	0.2926452893
C	2.8689078063	-1.2867114876	0.2777272108
C	1.6856429174	-2.074909556	0.3333464389
C	0.4648694479	-1.434378789	0.4070908001
C	-0.8640105199	0.465199561	0.4893984071
C	-1.0573375567	1.8288063507	0.5203184295
C	0.0823648942	2.6800417444	0.4745191026
C	1.3722606356	2.1897051035	0.3959509845
C	-0.9353498537	-1.8450330095	0.4884158675
C	-1.7462440351	-0.7311861993	0.5085135282
C	-3.2202220064	-0.6929038928	0.7824287613
H	3.773901483	0.6543241624	0.2523022516
H	3.8250480935	-1.7954922552	0.2228478507
H	1.7645193097	-3.1567685853	0.3193062201
H	-2.0477802163	2.2684466571	0.5718091455
H	-0.0728280021	3.752984529	0.4990198247
H	2.2114929567	2.876375058	0.3596947228
H	-1.2867343278	-2.8679142242	0.5169706193
H	-2.0243974714	-0.7487585974	-1.5712597031
H	-3.7298748221	0.0433020683	0.1562789334
H	-3.6806703925	-1.666146407	0.6035300275
H	-3.4040824369	-0.4182334413	1.8276578686

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 529.6788

WellDepth[kcal/mol] 42.21

WellDepth[kcal/mol] 3.4

End

Frequencies[1/cm] 65

129.1800	160.1892
----------	----------

170.2600	211.3810	233.4819
280.1370	299.9895	383.4010
413.6668	425.2039	463.2951
502.1416	534.0570	548.7563
584.0311	594.2354	628.9343
670.8247	678.7660	763.9168
782.0881	800.1689	815.6987
819.2675	852.8184	918.9508
927.2557	969.3909	975.7484
985.8815	1014.9023	1037.4315
1052.0649	1058.3718	1090.1006
1157.5797	1179.6633	1205.6641
1219.0924	1248.2245	1283.6499
1316.8059	1381.8489	1404.4596
1414.6630	1449.7032	1457.7280
1481.4118	1489.0792	1490.2839
1516.4341	1544.0966	1631.8043
1649.1711	1658.0720	3017.7763
3074.5312	3109.0404	3160.2465
3160.7976	3169.8678	3171.0169
3183.6104	3184.5386	3207.6626

ZeroEnergy[kcal/mol] -34.18

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts22-p9-----

Barrier ts22-p9 i22 p9

RRHO

Geometry[angstrom] 24

C	0.5159982963	-7.20132E-5	-0.492847879
C	1.6246888237	0.77993161	-0.1585828951
C	2.8330455757	0.0696490158	0.1026460013
C	2.8557721935	-1.3102872775	0.0119825928
C	1.7110987601	-2.0756943787	-0.3391567481
C	0.5225899311	-1.4158977375	-0.5980261158
C	-0.7653836025	0.5098428114	-0.795533479
C	-0.9418346742	1.8768506647	-0.7753471284
C	0.1673403279	2.7032519682	-0.4445058696
C	1.4131703033	2.1873295104	-0.1390182748
C	-0.8231926698	-1.8018016645	-0.9986836261
C	-1.6191574688	-0.6703723803	-1.0668858292
C	-2.8753224937	-0.652257174	1.0217696321
H	3.7352329762	0.6113258669	0.3662141733
H	3.7843172074	-1.8340171593	0.2118533658
H	1.7900625038	-3.1557995275	-0.4021506108
H	-1.8995433072	2.3347677917	-0.9995109479
H	0.0246866342	3.7782548051	-0.4308534677
H	2.230716367	2.8557241048	0.1099092874
H	-1.151796581	-2.8128175142	-1.1961222996
H	-2.5989953108	-0.6265727707	-1.5189363886
H	-3.4309188724	0.2660073111	0.8808617741
H	-3.4109582641	-1.5872949824	0.9235686246
H	-2.0177906557	-0.6265468803	1.679491108

```

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 366.3596
WellDepth[kcal/mol] 37.84
WellDepth[kcal/mol] 5.42
End
Frequencies[1/cm] 65
74.4637          91.3835
94.0092          165.6382          222.6769
240.2713         371.7494          421.0985
437.7108         462.5129          465.7981
482.5491         517.7196          558.1013
566.9208         621.3854          657.1732
670.6948         698.7810          735.4363
765.4992         772.1013          787.8468
815.5952         841.9975          870.8753
891.3854         910.3856          922.5380
973.7400         983.4085          1027.5981
1037.4318        1058.2189          1082.8727
1113.8368        1175.2964          1203.3418
1218.0263        1245.2760          1270.4810
1326.8448        1356.2402          1411.8834
1412.8360        1414.7422          1426.4946
1450.6166        1469.3841          1484.6337
1515.5058        1623.2050          1643.6288
1654.7724        3093.3538          3158.6149
3159.0151        3168.2901          3169.7184
3182.0155        3183.1360          3208.1301
3226.9033        3256.3208          3267.0270
ZeroEnergy[kcal/mol] -38.54
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsa-8-----
Barrier      tsa-8  i8  p0a
RRHO
Geometry[angstrom] 24
C -0.0181814664  0.7086009756  -0.0048916025
C -1.2903001756  1.33872805   -0.0330515354
C 1.2100558863  1.394494446  0.0041781266
C -2.4426251461  0.5908698687  -0.0395232797
C -2.3806262132  -0.8221104634  -0.0221893513
C -1.1663094148  -1.4637452734  8.1073336E-4
C 0.0480672705  -0.7292696573  0.0109171847
C 2.4299195646  0.7953695331  0.0440965981
C 1.319970436   -1.3615207251  0.0363254043
C 2.4799340579  -0.6258240453  0.0500725768
H -1.3316059004  2.4209673019  -0.0565685152
H -3.408271412  1.0835346955  -0.0607792734
H -3.2990535726  -1.3984184129  -0.0291818624
H -1.1189085843  -2.548100694   0.0112946722

```

```

H 3.3487683685 1.3719312671 0.0665537011
H 1.360755325 -2.4456417762 0.0477109089
H 3.443504797 -1.1243818272 0.0701490883
C 1.3359900477 3.9895442144 1.2973392299
C 1.1737136609 3.9922747978 -1.296714175
C 1.2455681988 3.7621918736 -0.0088784955
H 0.4550293852 3.9818281243 1.9309740742
H 2.3012587 4.0399706367 1.7908060048
H 1.1418117511 3.204729807 -2.036806635
H 1.1419924357 5.0198932828 -1.6500885779
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 379.4546
WellDepth[kcal/mol] 63.89
WellDepth[kcal/mol] 2.16
End
Rotor Hindered ! 25 cm^-1
Group 18 19 21 22 23 24
Axis 3 20
Symmetry 2
Potential[kcal/mol] 4
0 0.67478177 3.46828441 0.453420232
End
Frequencies[1/cm] 64
50.9563
72.8522 110.7348 157.2665
174.6022 223.1429 243.3183
366.9442 393.2684 410.0668
469.0025 508.9215 516.9695
521.3382 617.7680 620.6303
737.0222 762.4501 776.3415
796.1755 802.4918 808.4932
811.1414 868.1593 895.2839
897.1112 919.6938 964.9512
976.3016 997.3881 1006.6860
1021.4819 1036.4483 1051.1197
1062.5129 1137.4093 1168.4723
1177.4855 1202.2841 1235.3393
1270.8517 1362.3854 1381.9267
1384.6280 1427.9280 1452.7938
1471.3812 1483.2696 1523.5377
1582.4280 1634.6617 1659.8925
1927.3981 3118.5100 3122.0573
3152.6952 3155.4395 3163.2401
3167.7575 3177.0998 3181.7773
3193.2148 3198.4771 3222.0054
ZeroEnergy[kcal/mol] 3.3
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsa-10-----

```

```

Barrier      tsa-10  i10  p0a
RRHO
Geometry[angstrom]  24
C  0.161836292  0.7384373026  0.0516065949
C  -1.0500266585  1.4604970248  0.2171078634
C  1.4355393165  1.3291468619  -0.0413813256
C  -2.253959728  0.8030650913  0.2932224941
C  -2.3076971853  -0.6075188134  0.208540251
C  -1.1546917662  -1.337377914  0.0515097563
C  0.1094437509  -0.6979066546  -0.0312063754
C  2.59606856  0.6361650901  -0.1883498522
C  1.3194700393  -1.4250942737  -0.1908353975
C  2.5304902076  -0.7823093466  -0.266993503
H  -1.0079937871  2.5400976998  0.2915559036
H  -3.1713755613  1.3667306415  0.4207612139
H  -3.2656355822  -1.1117342138  0.2700093302
H  -1.1952839182  -2.420176956  -0.0118545971
H  3.5588848491  1.1343136475  -0.2480282659
H  1.2707214292  -2.5072680694  -0.2510267029
H  3.4459783692  -1.3521598504  -0.3875283968
C  1.6872242817  3.6776823202  0.0084696252
C  0.8296465628  4.4970124473  2.3454445861
C  1.2712855741  4.1578672728  1.1702269984
H  2.7454227244  3.5158029027  -0.1649932936
H  1.0586753231  3.7491266132  -0.8725951159
H  0.4387812513  3.75231135  3.0362316198
H  0.8355206558  5.5291928264  2.6857295889
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  259.2179
WellDepth[kcal/mol]  39.65
WellDepth[kcal/mol]  1.35
End
      Rotor      Hindered      ! 23 cm^-1
      Group      19 20 21 22 23 24
      Axis      3 18
      Symmetry    1
      Potential[kcal/mol]  8
0      0.431762366 0.46246641 0.447822219 0.495196683 0.024928446 0.404301919
      0.633293973
      End
Frequencies[1/cm]  64
      35.3008
88.0958      118.9646      170.9919
192.4061      330.1983      340.4464
367.6939      381.2228      406.4605
468.1632      501.3107      512.2570
521.7083      603.8213      619.8811
735.1939      749.6154      777.2654
794.3458      801.9431      855.0737
865.4989      874.6043      875.1544
895.2766      936.6288      963.9005

```

975.5462	996.0347	998.1067
1033.8730	1037.3348	1054.6759
1064.7385	1138.5142	1168.1506
1178.3226	1204.6261	1234.7166
1270.6161	1362.1951	1383.4993
1386.3815	1420.1487	1453.5688
1466.0069	1483.5514	1524.0002
1582.7839	1635.4745	1659.9757
1969.6019	3092.9368	3124.8194
3146.7906	3155.5575	3159.5184
3162.9212	3168.1407	3176.4823
3182.1328	3194.9055	3200.5618

ZeroEnergy[kcal/mol] 2.49

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsmn-1-----

Barrier tsmn-1 r1 mn-il

RRHO

Geometry[angstrom] 24

C	0.0719533483	-0.1725285204	-1.690763323
C	0.2943215648	-1.5796859814	-1.8376698082
C	1.6072049438	-2.0626963039	-2.082805852
C	2.6675448137	-1.1881401868	-2.1724854308
C	2.4642641421	0.1911127046	-2.0304622989
C	1.1939923758	0.7357980283	-1.8081112041
C	-1.2488721098	0.2683668026	-1.4293568063
C	-2.2961024743	-0.6212158216	-1.324516601
C	-2.0741605985	-2.004579399	-1.4779729476
C	-0.8052543458	-2.4690720374	-1.7290212923
C	1.0506959488	2.152494996	-1.6460756147
C	0.9706705842	2.5324937306	0.4639155272
C	1.5254390479	3.5530217	0.8722629738
H	1.7602586866	-3.1308023789	-2.1926528683
H	3.6681059193	-1.5634803518	-2.3564172118
H	3.3113529349	0.8645399471	-2.1041043924
H	-1.4470545028	1.3257527327	-1.3072376453
H	-3.296631856	-0.2550234387	-1.123771417
H	-2.9038693931	-2.6975955561	-1.3960876926
H	-0.6241383238	-3.5325467529	-1.8458846717
H	1.90951468	2.7658658058	-1.885496068
H	0.0963201525	2.6256833829	-1.8339799638
H	0.4031366485	1.6572391423	0.711598521
H	2.079416813	4.4622057559	0.9104970877

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 613.4889

WellDepth[kcal/mol] 9.79

WellDepth[kcal/mol] 24.405

End

Rotor Hindered ! 37.2713 cm⁻¹

```

Group          13 23 24
Axis           11 12
Symmetry       1
Potential[kcal/mol] 8
0  0.194527973 0.251003836 0.7655617  0.909888905 1.436996961 1.669175509
0.822037563

```

```

End
Frequencies[1/cm] 64

```

```

57.5689
86.1610          145.3181          179.5781
241.7025         271.5273          323.4554
424.5216         444.5895          479.6873
488.9935         511.3439          514.3458
558.4599         585.5610          625.7422
652.1358         711.8201          721.4795
742.9496         777.8346          786.3565
802.4390         807.2362          838.8031
875.0926         888.9809          899.7066
945.0501         962.2376          977.0387
993.2380         998.4427          1049.2744
1097.3715        1112.7612         1165.8825
1185.9230        1199.2070         1229.2164
1254.4977        1298.8251         1366.4104
1377.4081        1421.4540         1469.3796
1481.6981        1500.2371         1539.1085
1585.8135        1610.4879         1652.8214
1843.4869        3151.6560         3158.5186
3160.3447        3169.1146         3170.0651
3183.6816        3184.5139         3195.5603
3237.1954        3311.8769         3436.3328

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ZeroEnergy[kcal/mol] -11.24

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ElectronicLevels[1/cm] 1

```

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0 2

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End

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!-----

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!-----bar_tsmn-2-----

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Barrier      tsmn-2  mn-i1 i10

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RRHO

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Geometry[angstrom] 24

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```

C -0.0554752008 -0.1187635897 -1.7710110292
C  0.0956033008 -1.5443176236 -1.7832004051
C  1.3971400756 -2.1078689722 -1.8198154677
C  2.5048474396 -1.2995143448 -1.8462521913
C  2.3585704908  0.1045249955 -1.8430596616
C  1.1165387855  0.7035184734 -1.8130965073
C -1.3722006912  0.4137649464 -1.7240758085
C -2.4733307212 -0.408671937 -1.6999508248
C -2.3200939291 -1.8126001593 -1.7185610651
C -1.0632933741 -2.3635190181 -1.7574878176
C  1.0193768528  2.2157198601 -1.7925478163
C  0.7266490219  2.7623243358 -0.4203902899
C  0.4858416626  2.5074651027  0.822749604
H  1.4998924848 -3.1878754437 -1.8264143022
H  3.4985661226 -1.7322908453 -1.8751744782

```

```

H 3.2468499672 0.7273252514 -1.871530289
H -1.5130516779 1.4865540264 -1.6917511465
H -3.4676551783 0.0221002817 -1.6627638581
H -3.1963416406 -2.4508111612 -1.6993304855
H -0.9363071652 -3.4411624767 -1.7687050953
H 1.9624856671 2.6464641121 -2.1394096403
H 0.2513609817 2.5754596102 -2.4841696933
H 0.5314651004 3.7293589679 0.4027304581
H 0.3505666252 1.7302356081 1.5749978108
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 2098.3629
WellDepth[kcal/mol] 44.1
WellDepth[kcal/mol] 45.6
End
Frequencies[1/cm] 65
 40.7812 74.9665
136.3939 146.3664 176.0311
193.9740 253.8438 287.7282
404.1117 433.8654 435.8306
479.0881 513.9958 520.4766
559.1999 604.8750 617.4653
669.6253 724.4872 744.9892
791.9180 801.3106 805.4783
818.3635 858.5928 884.2032
886.4754 915.1370 928.2451
963.3795 981.7460 994.5329
1039.2133 1058.6925 1097.0193
1168.3764 1182.7225 1187.7990
1204.7128 1238.3321 1260.4444
1286.6361 1304.1236 1381.2306
1393.0815 1423.2208 1466.3403
1477.9948 1493.8442 1547.6990
1614.9937 1637.8751 1663.4330
1834.7993 2351.3909 3037.6006
3069.4561 3072.0025 3155.9856
3157.8025 3164.2607 3169.0576
3182.8353 3183.7997 3198.5177
ZeroEnergy[kcal/mol] 8.45
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-3-----
Barrier tsmn-3 mn-il p6
RRHO
Geometry[angstrom] 24
C -0.0679663494 -0.0960725448 -1.7643356919
C 0.0833387932 -1.5209946697 -1.7423891159
C 1.3858800499 -2.0843634015 -1.7404572794
C 2.4940200906 -1.2779062166 -1.7641527037
C 2.3472008377 0.1269213997 -1.7936922593

```

```

C  1.1055548861  0.7217355856  -1.7944995824
C  -1.3843218508  0.4387803371  -1.7605581355
C  -2.4855567673  -0.3835919519  -1.7437284764
C  -2.3325957879  -1.7875754993  -1.7268524949
C  -1.0756530748  -2.3396752172  -1.7247708424
C  1.0073836179  2.2393850487  -1.8439986184
C  0.6246078695  2.8424199494  -0.5553899478
C  0.3217390383  3.04107306  0.6011287322
H  1.4881768878  -3.1642710691  -1.7216507407
H  3.4880105763  -1.7105619926  -1.7639053701
H  3.2353018415  0.749794143  -1.8165689015
H  -1.5252620807  1.511973464  -1.7547206482
H  -3.4803284005  0.0476269371  -1.739767842
H  -3.2094870671  -2.4249529989  -1.7134364021
H  -0.9491200336  -3.4172528355  -1.7101264891
H  1.9734906126  2.6510662599  -2.1476427911
H  0.2946537298  2.5549842401  -2.6125809327
H  0.0548051341  3.3425627396  1.5847734389
H  0.6169644467  4.6773032329  -1.2319049056
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  622.3424
WellDepth[kcal/mol]  36.37
WellDepth[kcal/mol]  2.8
End
Frequencies[1/cm]  65
  51.1211          79.0555
 104.4709         156.1257         176.3838
 267.4318         276.4015         361.0312
 410.8720         424.0384         435.3801
 467.4507         479.7068         516.8494
 525.7689         558.9053         619.0657
 650.9358         672.1667         672.2740
 726.1047         745.5692         793.0119
 804.3184         812.8731         866.6690
 886.5202         918.0867         932.2563
 947.4450         964.8638         984.1771
 996.3961         1040.3274        1060.9184
1097.4631         1168.8804        1185.1831
1188.7118         1219.9415        1241.4748
1262.7166         1288.3237        1332.1532
1383.2874         1396.6167        1424.6975
1470.1821         1481.7502        1495.4238
1548.4894         1618.4433        1641.5721
1665.6847         2134.9431        3037.1742
3071.5651         3158.5492        3159.9805
3166.3692         3170.5328        3184.6177
3185.7513         3198.3285        3467.5398
ZeroEnergy[kcal/mol]  0.73
ElectronicLevels[1/cm]  1
0  2
End

```

```

!-----
!-----bar_tsmn-4-----
Barrier      tsmn-4  mn-i1 mn-i2
RRHO
Geometry[angstrom]  24
C  -0.0837210264  -0.4342557841  -1.2670820435
C   0.1019172901  -1.8310060765  -1.0447963126
C   1.4214926632  -2.3445112616  -0.9809727929
C   2.5040194451  -1.5036743625  -1.0933147448
C   2.313039493   -0.1139568083  -1.2274396163
C   1.0430905318   0.4283977583  -1.3014744383
C  -1.4218678772   0.0853889077  -1.365924402
C  -2.5125057747  -0.776924571  -1.2188950939
C  -2.3143455922  -2.1368069564  -0.9343478112
C  -1.0402062805  -2.6622470339  -0.8731267833
C   0.8207040651   1.9213090861  -1.2667440357
C  -0.0824328217   2.3424816438  -0.1012704284
C  -1.1620854664   1.6902835135   0.2549917051
H   1.5636510049  -3.4091237043  -0.8277272778
H   3.5112460046  -1.9021954581  -1.0435174234
H   3.1766340925   0.5429576726  -1.2433428529
H  -1.5817707575   1.0283068267  -1.8716113526
H  -3.5181889354  -0.3936964643  -1.3486568578
H  -3.1729770858  -2.7864492239  -0.8035926879
H  -0.891878972   -3.7215363309  -0.6924360464
H   1.7814020556   2.4339983722  -1.1892401069
H   0.3630683178   2.2695366781  -2.2032017622
H   0.2276418773   3.2411953221   0.4381499905
H  -1.9168142511   1.8264162549   1.016326175
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  380.2352
WellDepth[kcal/mol]  8.04
WellDepth[kcal/mol]  36.35
End
Frequencies[1/cm]  65
  123.5251          141.7360
  186.1480          224.4607          261.0727
  296.3044          419.7202          435.7281
  464.4845          482.4267          508.2554
  529.2449          558.7548          587.4339
  626.3435          653.6971          716.4005
  747.1618          771.3389          802.1853
  804.4853          814.4646          854.3679
  861.7482          885.3526          897.3008
  917.7012          937.0265          972.0549
  980.6401          991.2173          1041.4610
 1069.6919          1095.3792          1152.0041
 1176.2126          1187.1721          1193.1808
 1228.7365          1235.9354          1250.6240
 1273.7762          1321.8237          1370.2938
 1385.0897          1415.6348          1457.3537

```

1481.9451	1486.9283	1532.7079
1590.0673	1608.2652	1642.8221
1655.5587	2991.9835	3051.7725
3082.6192	3155.9196	3158.3357
3164.0293	3169.9286	3179.2521
3182.3312	3188.8696	3225.9958

ZeroEnergy[kcal/mol] -27.6

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsmn-5-----

Barrier tsmn-5 mn-i1 mn-i3

RRHO

Geometry[angstrom] 24

C	-0.0852902612	-0.388033507	-1.2303633325
C	0.0954605794	-1.7998372974	-1.0215477987
C	1.4108015437	-2.3502657212	-1.0583082861
C	2.4951048765	-1.5660243683	-1.3197682326
C	2.3401237101	-0.1571964198	-1.5166020303
C	1.0509492572	0.4221297214	-1.4844516045
C	-1.4132287366	0.1242241476	-1.1815286994
C	-2.4895705122	-0.6983728808	-0.9458350046
C	-2.3031558117	-2.0815809397	-0.7387696885
C	-1.033430661	-2.613724205	-0.7775117279
C	1.0625457732	1.9306463319	-1.3818975623
C	2.1200924779	2.2405858842	-0.3263007953
C	2.9362880888	1.2742198269	0.0332310755
H	1.5287531838	-3.4173344921	-0.89937506
H	3.4852773888	-2.0026307111	-1.3877188487
H	3.1334980334	0.3618327614	-2.0435546328
H	-1.5828377396	1.1800320688	-1.3512626978
H	-3.4904896462	-0.2819756354	-0.9205365928
H	-3.1584906484	-2.7207056818	-0.5516931398
H	-0.8814214186	-3.6765624351	-0.6187818699
H	1.3270175564	2.4112580091	-2.3345486112
H	0.095229762	2.3411456541	-1.0872033874
H	2.1661614568	3.2461383208	0.0935626549
H	3.7727407478	1.1930085682	0.7136918725

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 487.5680

WellDepth[kcal/mol] 12.56

WellDepth[kcal/mol] 30.81

End

Frequencies[1/cm] 65

78.5650	120.1334	
191.1166	234.8247	254.5468
305.4746	416.1779	439.6278
461.8676	480.1667	514.3241
543.3954	558.6549	615.4887
629.0440	673.7269	726.3228

747.2192	779.5267	794.5031
811.7586	839.6121	867.0898
870.0625	875.3156	888.1278
950.3426	955.5327	967.5666
976.7321	988.3780	1037.7795
1051.1847	1085.4173	1161.1926
1169.0439	1182.5796	1185.4590
1208.1420	1229.7876	1248.4799
1278.6762	1307.8277	1368.0866
1391.9137	1419.4243	1457.4721
1478.0894	1482.8174	1535.5213
1572.1868	1622.2324	1641.2630
1649.2991	2989.4870	3080.9365
3092.6286	3144.7024	3156.3792
3159.4106	3167.5126	3180.2053
3183.7602	3195.1379	3219.8091

ZeroEnergy[kcal/mol] -23.08

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsmn-6-----

Barrier tsmn-6 mn-i2 p1

RRHO

Geometry[angstrom] 24

C	-0.0558661976	-0.1888409051	0.1044775516
C	0.1034865372	-1.6021122238	-0.0034865444
C	1.4087974083	-2.1382698117	-0.1065183623
C	2.5061454205	-1.3078628708	-0.0802538466
C	2.3421703958	0.0830275467	0.047290013
C	1.0832196787	0.6527074596	0.1299889158
C	-1.3900197045	0.3676195438	0.1863018898
C	-2.4775014704	-0.5073632164	0.3143405088
C	-2.3068070877	-1.8947748911	0.1978230111
C	-1.0520268889	-2.4340076841	0.0232783296
C	0.9242383622	2.1570488763	0.2324084528
C	-0.4684702657	2.612273296	0.5599726114
C	-1.5222436741	1.7959100314	0.5114627128
H	1.53083882	-3.2123256268	-0.1967932547
H	3.5051155207	-1.7235618758	-0.1513697671
H	3.219824829	0.7212306503	0.0790209632
H	-1.6297119541	0.6278374548	-1.6304599158
H	-3.4691525029	-0.0934759746	0.4606414385
H	-3.1730039069	-2.5445656168	0.253199551
H	-0.9229914929	-3.5072162078	-0.0662953966
H	1.6306828874	2.5537541917	0.9716714822
H	1.2245343719	2.61636277	-0.7221386035
H	-0.6017052589	3.6595443193	0.8117733646
H	-2.5205238269	2.1666717648	0.720271895

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 888.4127

```

WellDepth[kcal/mol] 27.9
WellDepth[kcal/mol] 4.8
End
Frequencies[1/cm] 65
 86.0569          153.3068
209.9487          231.4717          352.1774
401.2197          418.2545          436.1362
448.7962          475.7837          482.9780
503.4951          511.0431          571.1198
586.1211          606.9068          647.6572
729.2820          754.2431          778.5545
787.1594          811.4541          822.2483
842.7818          893.0342          909.7243
955.0979          962.0775          977.7194
985.0053          997.5269          1046.4098
1064.9899         1106.3744          1120.4556
1174.7468         1194.8080          1199.6942
1219.8962         1227.0692          1252.6030
1265.0691         1334.8784          1377.8277
1378.6424         1411.4657          1420.4535
1458.8043         1465.5634          1485.9797
1532.3804         1600.3472          1615.3459
1640.0958         1708.8209          2969.3716
3018.6628         3151.8552          3153.6117
3161.3101         3165.1043          3170.8262
3173.4108         3183.0622          3185.9048
ZeroEnergy[kcal/mol] -36.05
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-7-----
Barrier      tsmn-7  mn-i2 i14
RRHO
Geometry[angstrom] 24
C -0.0478369259 -0.1807894815 0.1253272767
C 0.1035761141 -1.5959755877 0.0010907969
C 1.4097164243 -2.1299407913 -0.1059243805
C 2.5106715538 -1.3037945211 -0.0681621819
C 2.3517920346 0.0847447642 0.0719042054
C 1.0916831791 0.6563835781 0.1610848086
C -1.3933414104 0.3709882828 0.2422282577
C -2.4931481547 -0.5189052359 0.344825103
C -2.3081904469 -1.8926132071 0.205528342
C -1.0473853815 -2.4340160032 0.0201901536
C 0.9653158314 2.1711432506 0.252063974
C -0.412778955 2.6543134727 0.59269847
C -1.5118645587 1.8328795551 0.4931142699
H 1.5293328237 -3.2033152399 -0.207630012
H 3.5078889458 -1.7235891359 -0.1432484485
H 3.2293396329 0.7226479099 0.1050543893
H -1.6601580994 1.2575646059 -0.7594861649
H -3.4865639381 -0.1136827887 0.505067165
H -3.1713866457 -2.5470989225 0.26073655

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```

H -0.9171015226 -3.5051326675 -0.0818979725
H 1.6923399598 2.5530529656 0.9801424754
H 1.2813840072 2.6053629902 -0.7123518577
H -0.5539265508 3.7076113014 0.8020916255
H -2.5044609167 2.1974449058 0.7345751551
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1729.0474
WellDepth[kcal/mol] 35.6
WellDepth[kcal/mol] 39.3
End
Frequencies[1/cm] 65
 78.0119 148.5260
210.3419 230.3502 344.6950
413.7611 430.4937 460.7962
471.8608 478.3867 489.0910
565.4655 579.0597 595.5439
627.5938 673.2041 725.1174
759.2555 774.6576 796.8347
810.0203 823.9487 829.6995
895.7033 904.2899 947.8885
958.7819 960.5656 980.9155
1034.0656 1056.9182 1096.9022
1105.9156 1111.6178 1161.9118
1190.5090 1190.7527 1213.7031
1219.7779 1252.0177 1259.5847
1320.5818 1338.3782 1369.3117
1389.5623 1402.9872 1450.3087
1466.3521 1473.3495 1493.3277
1546.1877 1556.0689 1585.4519
1610.6286 1635.7312 2923.4475
3002.4873 3153.9297 3157.2862
3163.6026 3165.6566 3170.2356
3180.4750 3184.2841 3185.6058
ZeroEnergy[kcal/mol] -28.35
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-8-----
Barrier tsmn-8 mn-i3 p3
RRHO
Geometry[angstrom] 24
C -0.198916014 -0.1847575224 -0.3187544851
C -0.0475058432 -1.6106079473 -0.2224062912
C 1.2525982311 -2.1923946278 -0.3354093628
C 2.3598829202 -1.4336371811 -0.5853068399
C 2.2088949528 -0.0223274756 -0.7761961417
C 0.9600958378 0.5857354928 -0.5483996374
C -1.4942355068 0.3757402172 -0.155982697
C -2.5868668193 -0.4266429562 0.07331248
C -2.4389575461 -1.8286557505 0.1584193703

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C -1.1952863623 -2.4022633614 0.0158019479
C 1.1381965299 2.0823594852 -0.5636654977
C 2.636237304 2.2406011274 -0.6776713379
C 3.2319804105 1.0461112157 -0.7934635833
H 1.345658294 -3.2664802097 -0.2132303348
H 3.3395940316 -1.8891088584 -0.6748437262
H 2.1926502233 -0.1573764657 -2.5696813935
H -1.6162261461 1.4509422508 -0.2243111457
H -3.5698956963 0.0163805096 0.1879581121
H -3.3079571223 -2.4510227378 0.3390657731
H -1.0798439938 -3.4789699554 0.0868122059
H 0.6254298573 2.5516652238 -1.4161251538
H 0.7358503518 2.5601151318 0.3378308678
H 3.1309895091 3.2026780314 -0.6896767405
H 4.2919955968 0.8645663636 -0.9143753888
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 901.2332
WellDepth[kcal/mol] 22.93
WellDepth[kcal/mol] 5.7
End
Frequencies[1/cm] 65
108.4725 137.5793
225.6831 236.5333 266.4766
346.8737 416.3416 427.9883
436.5113 466.9899 507.1994
516.6419 522.5173 557.3804
612.8517 675.8390 684.5113
724.0348 747.5342 761.6869
787.4137 824.7797 835.4200
865.8698 874.5265 938.0435
953.9165 958.9827 961.2951
973.9086 977.2990 991.2333
1045.4709 1059.0170 1119.9419
1148.3420 1167.1540 1177.0389
1186.2871 1228.9139 1232.4229
1267.8321 1289.2479 1352.7763
1370.1801 1393.0208 1418.6971
1436.4963 1468.3762 1473.5614
1538.7295 1575.1994 1622.4152
1635.7880 1650.4234 2993.9461
3033.9024 3157.6699 3161.1455
3165.4381 3178.0628 3181.6143
3188.7308 3195.1058 3217.5920
ZeroEnergy[kcal/mol] -30.96
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-9-----
Barrier tsmn-9 mn-i3 il2
RRHO

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```

Geometry[angstrom]    24
C  -0.1721516733  -0.1854663371  -0.297736008
C  -0.0349615181  -1.6154962828  -0.2084512601
C  1.2676640245  -2.2036206403  -0.3135274239
C  2.3877527456  -1.4580713964  -0.5310142675
C  2.2512639553  -0.0378561723  -0.6910490956
C  0.9885873194  0.5842504421  -0.5023575035
C  -1.4688869185  0.3782640062  -0.1485206143
C  -2.5688539163  -0.422695509  0.0622722074
C  -2.4327007495  -1.8239980217  0.1391429143
C  -1.1854290747  -2.4013883321  0.0074449252
C  1.1551089636  2.0871257282  -0.545558345
C  2.6516585316  2.2670955953  -0.6471830847
C  3.2762599701  1.0464873521  -0.7772824156
H  1.35196893  -3.2797795666  -0.2014998024
H  3.3641418474  -1.9241579521  -0.6047168887
H  2.7676535352  0.3328901067  -1.9139246391
H  -1.5864180698  1.4543699484  -0.2089986885
H  -3.5502069257  0.0266473017  0.1693044219
H  -3.3062694645  -2.4437451717  0.3051129089
H  -1.0752410139  -3.4793025586  0.0732467949
H  0.6320870184  2.5347094148  -1.411320859
H  0.7234946041  2.5863933026  0.3356390809
H  3.1392978239  3.2275480824  -0.7324363568
H  4.3399350552  0.8525946602  -0.8096430011
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 1652.1546
WellDepth[kcal/mol] 29.83
WellDepth[kcal/mol] 42.3
End
Frequencies[1/cm] 65
103.3330      140.3702
224.5044      234.0389      257.3528
358.8843      423.7517      429.3058
460.6154      513.9426      516.2616
551.0592      598.1966      627.8071
672.0619      682.4024      739.3559
752.7448      774.6539      800.0122
808.9989      859.9713      863.8808
883.1702      918.7421      933.2346
946.9108      963.5667      966.5480
983.4598      1015.3341     1046.8685
1060.5392     1108.4263     1127.8120
1155.6225     1171.0005     1175.3762
1191.9452     1229.4939     1243.5726
1271.0395     1286.5370     1325.9785
1363.8132     1393.5496     1422.5168
1442.7833     1463.6615     1472.2552
1502.2881     1535.3267     1570.8715
1626.6100     1644.3473     2898.9125
2958.1973     3154.3595     3158.0156

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3162.3297          3177.0746          3177.5829
3187.7040          3204.4976          3222.4545
ZeroEnergy[kcal/mol] -24.06
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-10-----
Barrier      tsmn-10  mn-i1 i15
RRHO
Geometry[angstrom] 24
C -0.3319094662 -0.484721663 -0.8153785399
C  0.0002413252 -1.8544835854 -1.0682725752
C  1.3222880753 -2.3118658357 -0.8259555885
C  2.2829396733 -1.4484748784 -0.3592632224
C  1.9643479092 -0.1024233764 -0.1002667386
C  0.6834810959  0.3979343967 -0.2943806529
C -1.6539617645 -0.0572606988 -1.1011096147
C -2.5987617666 -0.9302870975 -1.5897977371
C -2.2718270154 -2.2831393746 -1.8210633667
C -0.9984602178 -2.7302821789 -1.5669594801
C  0.3840611533  1.8033101678  0.00337855
C  1.420564789  2.7420188174  0.5641976412
C  1.5595414255  3.5687778812 -0.4569037167
H  1.5608119353 -3.3515538891 -1.023183615
H  3.2935882525 -1.7995511701 -0.1829936432
H  2.7389134661  0.5622194072  0.2638053591
H -1.9263929472  0.9789401542 -0.947336146
H -3.6011970098 -0.5758682231 -1.8023587252
H -3.0245996722 -2.9630577874 -2.20372097
H -0.7339642778 -3.7667678562 -1.7491542177
H  0.545418516  2.6687310769 -1.0553927008
H -0.6306432273  2.0159548462  0.336690013
H  1.885460949  2.7254038848  1.5454687299
H  2.1289237993  4.4619179823 -0.7010300427
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 2121.7072
WellDepth[kcal/mol] 34.6
WellDepth[kcal/mol] 63.1
End
Frequencies[1/cm] 65
  63.5091          89.3149
 162.2565          181.0791          200.5138
 260.4458          333.8658          420.5009
 436.6330          481.6270          486.3588
 532.8349          557.5640          574.2566
 644.4485          656.1232          681.4732
 742.6588          754.6705          787.7240
 804.8249          808.1897          857.3913
 873.2320          905.1742          912.8905
 917.8137          946.7256          965.0664

```

983.4836	995.7718	1003.1025
1050.8734	1077.2911	1110.9120
1152.2062	1168.6468	1187.5905
1192.6253	1213.7292	1229.7047
1259.7270	1277.3901	1330.2440
1377.2796	1390.2347	1427.0461
1471.0837	1490.1769	1544.0556
1601.3123	1622.4646	1628.3497
1659.0248	1784.6035	3105.1691
3131.9143	3158.3611	3161.1484
3168.9096	3170.1154	3175.1117
3183.9094	3187.4190	3197.8867

ZeroEnergy[kcal/mol] -1.04

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsmn-11-----

Barrier tsmn-11 mn-11 i11

RRHO

Geometry[angstrom] 24

C	-0.1082678493	-0.3649937273	-1.0623221397
C	0.0917520481	-1.7846199915	-1.0352564829
C	1.4107939757	-2.3138570777	-1.0640418799
C	2.5007604089	-1.4788709185	-1.1176732007
C	2.2764945442	-0.0934866374	-1.1431726849
C	1.0420160907	0.4929566758	-1.1183896239
C	-1.4396311485	0.1275017568	-1.0322838139
C	-2.5143886786	-0.72906764	-0.9786064661
C	-2.3154239015	-2.1264499251	-0.9520358172
C	-1.0407727432	-2.6375939618	-0.979862939
C	0.9061222963	2.0014563229	-1.1496097851
C	2.2120462172	2.7581987024	-1.2081820214
C	3.3952519395	2.1737124248	-1.2313121165
H	1.5421697657	-3.3912743325	-1.0428759329
H	3.5080603028	-1.8802133645	-1.1397270668
H	3.2080123819	0.8703580825	-1.1947797691
H	-1.6138501368	1.1964120063	-1.0519191566
H	-3.5224472343	-0.3300169679	-0.9564729415
H	-3.1701536045	-2.791999307	-0.9097177755
H	-0.8805844291	-3.7106742364	-0.9596878318
H	0.2902033626	2.2996077343	-2.0088181249
H	0.3445340769	2.3405274863	-0.2686229905
H	2.123612624	3.8457709399	-1.2310425862
H	4.3826766917	2.6178719557	-1.2725608529

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1587.0819

WellDepth[kcal/mol] 12.68

WellDepth[kcal/mol] 9.1

End

Frequencies[1/cm] 65

76.9244	128.0461	
189.2002	206.9709	223.7465
283.1704	380.4071	415.5525
439.1248	474.4090	484.9975
531.4962	552.5643	593.5002
600.4207	633.3385	677.1269
747.4541	761.6289	780.1498
811.6865	816.4363	857.8973
871.6903	900.1098	924.9581
955.1201	958.8698	973.9385
994.3379	1027.8455	1043.0498
1044.5275	1051.4486	1144.6220
1165.7360	1180.8379	1199.4738
1225.1036	1230.9286	1276.0165
1286.7420	1312.4099	1372.9772
1387.1916	1407.4820	1455.8403
1456.3973	1477.5762	1539.5609
1566.7317	1605.9091	1628.8156
1657.1043	1706.6148	2998.0111
3012.7731	3082.2522	3153.2554
3158.5162	3167.4677	3173.8661
3182.2816	3187.7742	3191.9250

ZeroEnergy[kcal/mol] -22.96

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsmn-12-----

Barrier tsmn-12 mn-11 i13

RRHO

Geometry[angstrom] 24

C	-0.1320362677	-0.3919316663	-1.1697992003
C	0.0583081341	-1.805157141	-0.9940769438
C	1.3682768928	-2.3066935085	-0.7829356125
C	2.4393287691	-1.4516698879	-0.7445013434
C	2.2532418841	-0.0662580565	-0.9485689197
C	1.0066424289	0.4780914543	-1.1762982438
C	-1.4628716564	0.0572057945	-1.3246498778
C	-2.5472153173	-0.7741746431	-1.331507653
C	-2.3412185574	-2.1708045569	-1.2093749412
C	-1.0718518981	-2.6648530606	-1.0325680383
C	0.9002983366	1.9530217312	-1.5344095879
C	-0.0766477944	2.8150882854	-0.7455506415
C	-1.3606900839	2.5403967757	-0.6240854108
H	1.5061438559	-3.3746412821	-0.6498973467
H	3.4391430549	-1.8342875619	-0.5723005473
H	3.1217540641	0.5842612599	-0.9472678465
H	-1.6444482781	1.3693435094	-1.1552707436
H	-3.554356967	-0.3797631613	-1.4192340723
H	-3.1918300493	-2.843475124	-1.2353642564
H	-0.9135780134	-3.7312436103	-0.9100784607
H	1.8977588349	2.3895451467	-1.4567547448
H	0.6240921339	2.0213370479	-2.5951476444
H	0.3321213238	3.724488726	-0.3036717512

```

H -2.1292198303 3.0750545294 -0.0786971717
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1557.5198
WellDepth[kcal/mol] 15.5
WellDepth[kcal/mol] 12.6
End
Frequencies[1/cm] 65
 90.5420 118.2061
171.1477 236.5939 243.2043
277.0094 359.2690 424.9652
438.6660 459.3089 472.2434
522.8437 554.8179 579.1857
592.5769 632.4607 693.2174
739.1866 760.5738 781.3562
804.8509 822.9790 868.4900
896.1137 908.7513 915.6490
926.8327 951.5957 975.5501
985.6932 1023.1745 1062.9956
1089.9893 1096.4420 1130.3952
1168.2409 1187.9493 1213.5520
1222.7183 1245.0136 1260.6661
1292.5095 1331.2047 1363.2882
1381.0615 1390.6371 1446.3125
1470.7362 1482.7811 1497.8122
1532.3619 1598.5710 1635.2665
1654.2210 1683.8565 3000.5955
3076.7494 3094.6503 3154.1433
3156.2058 3162.5105 3164.6667
3179.1609 3183.2801 3190.0313
ZeroEnergy[kcal/mol] -20.14
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```

2-methylnaphthyl + C₂H₂

```

TemperatureList[K] 300 400 500 600 700 800 900 1000
1100 1200 1300 1400 1500 1600 1700 1800 1900 2000 2100 2200 2300 2400 2500
PressureList[atm] 0.03 0.1 1. 10. 100.
EnergyStepOverTemperature 0.2 #Ratio of
discretization energy step to T
ExcessEnergyOverTemperature 150
ModelEnergyLimit[kcal/mol] 1000
WellCutoff 10
ChemicalEigenvalueMax 0.2
ChemicalEigenvalueMin 1.e-6 #only for direct
diagonalization method
CalculationMethod direct

```

```

EigenvalueOutput                               eigenvalue.out
!EigenvectorNumber                             0
!ReductionNumber                               5
!Reactant          #ground energy of bimolecular species will be used as a
reference.
Model
  EnergyRelaxation
    Exponential
      Factor[1/cm]                             424      ! Jasper calc N2
      Power                                     0.62
      ExponentCutoff                           15
    End
  CollisionFrequency
    LennardJones
      Epsilons[1/cm]                           390.  390.    ! N2 , A3/A3a/A6 ! from new
Jasper calc 11/22/15
      Sigmas[angstrom]                         4.46  4.46    ! N2 , A3/A3a/A6 ! from new
Jasper calc 11/22/15
      Masses[amu]                              28.  167.
    End
  OutputTemperatureStep[K] 100
  OutputTemperatureSize 24
  OutputReferenceEnergy[kcal/mol] 0.

```

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!-----
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!-----well_i1-----

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```

Well      i1
Species
RRHO
Geometry[angstrom] 24
C  -4.4777142276 -0.6486773981 0.184095337
C  -0.643267704  1.1448981024 0.233670301
C  -4.3592885865 0.7583631571 0.2517568763
C   0.5011430224 0.3727956056 0.1844988145
C  -0.8695677831 -1.6347076872 0.0999264085
C   0.36476292  -1.0449362217 0.1164853626
C  -3.3514422107 -1.4362669028 0.1343514717
C  -3.1191610612  1.3506792237 0.2683909289
C  -2.0588351866 -0.8566396777 0.1498438218
C  -1.9372767143  0.5664608935 0.2182614767
H  -5.4615165179 -1.1041667545 0.1716012833
H  -0.5597106685  2.2264525587 0.2857489882
H  -5.2539049442  1.3697978992 0.2905726412
H  -0.9558158355 -2.7153911209 0.047914661
H   1.2630220638 -1.6507982573 0.0778839669
H  -3.4392576975 -2.5166927067 0.0823547779
H  -3.0281746264  2.4308018779 0.3203313989
C   1.8251784027  1.0115980975 0.2024722994
C   4.4278226483  0.742209432  0.1629601676
C   2.998811764  0.4149577487 0.1614261091
H   1.813414753  2.1080453063 0.2562930286
H   4.923777426  0.3786980411 -0.7432650413
H   4.9416624563  0.2924044195  1.0190863948

```

```

H 4.5810473073 1.8315843636 0.2146845255
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
51.2649 100.0666 119.0897
165.4383 182.2119 224.4902
275.1951 310.4884 315.8372
404.7125 407.4164 484.6069
526.0085 529.0816 574.2920
639.2679 647.4856 750.5594
753.6545 780.9732 781.1417
806.2483 836.2559 876.7060
877.8728 911.6601 954.2107
962.4604 982.2070 983.9236
994.4393 1042.4954 1043.9529
1051.5545 1147.0890 1172.6987
1177.0458 1195.6919 1239.9529
1271.7124 1284.2597 1294.6683
1384.2680 1393.7262 1398.1411
1412.2687 1452.0944 1470.0870
1474.3053 1501.3830 1542.0316
1608.4188 1643.0532 1667.4938
1735.2331 2960.7487 3003.0358
3041.4834 3063.4485 3153.3223
3156.3465 3158.3124 3161.8870
3174.1966 3180.1689 3187.1391
ZeroEnergy[kcal/mol] -42.12
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i2-----
Well i2
Species
RRHO
Geometry[angstrom] 24
C -3.7685085569 0.3162841332 0.1095875958
C 0.2425431262 -1.0224603811 -0.0729925242
C -3.4865030987 -1.0695151488 0.1292213127
C 1.2918507634 -0.124241909 -0.1453977948
C -0.3068117665 1.7119122983 -0.119187446
C 0.9881657417 1.2681985549 -0.1770470289
C -2.744431032 1.2297651957 0.0307665076
C -2.1882754817 -1.5150817931 0.0696942526
C -1.3941622674 0.8028666155 -0.0305623304
C -1.1071299383 -0.5978960696 -0.0110504274
C 2.67925489 -0.6340720119 -0.1933110311
C 3.8077459159 0.0302758083 -0.0497169847
H -4.7974610346 0.654533399 0.1570208867
H 0.452091923 -2.0878144684 -0.0566180181
H -4.3024918708 -1.7808242354 0.1913675077
H -0.5178429421 2.7761004466 -0.1492002026

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H 1.7930855397 1.9863473004 -0.2676749216
H -2.958035731 2.2936267212 0.0146461238
H -1.9718822389 -2.5782951365 0.0844407903
H 2.7508480758 -1.7115002986 -0.3562439157
C 4.421803946 1.334564912 0.2222343687
H 3.7985584832 1.9494104854 0.8866524564
H 4.5914021351 1.8964819324 -0.7035418513
H 5.3952734188 1.2179286496 0.7107226747
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
28.0073 83.5010 109.1892
133.5065 186.7240 218.9466
259.5024 380.5428 387.0248
394.0610 410.8365 485.4407
524.2916 526.6618 601.8770
636.8480 648.3648 738.7510
752.3383 780.5739 781.7454
810.0416 835.0317 866.0476
877.0535 914.9444 940.3285
962.6356 974.2734 975.8261
995.1570 1013.2985 1030.9135
1041.9786 1146.1289 1173.7207
1181.0345 1189.9129 1237.2826
1279.0685 1284.8456 1294.2975
1385.9239 1394.0085 1399.3125
1405.9301 1456.8673 1470.0948
1473.6468 1499.1801 1542.9988
1606.3307 1639.2229 1665.1396
1736.2357 2977.4980 3038.6055
3054.4557 3070.7042 3154.4580
3157.0102 3160.0068 3162.9261
3174.6304 3187.4110 3196.9874
ZeroEnergy[kcal/mol] -40.05
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i3-----
Well i3
Species
RRHO
Geometry[angstrom] 24
C -3.7793940786 0.6161594701 0.0318477038
C 0.0576709913 -1.1615330245 -0.1010372283
C -3.6516766954 -0.7828643422 0.0758194527
C 1.2803251925 -0.3568229779 -0.184743143
C -0.1645889384 1.6502669927 -0.2018095308
C 1.0666181449 1.1038378028 -0.2432883466
C -2.6400236834 1.4099034167 -0.0575496682
C -2.4057431346 -1.3740149902 0.0320677579
C -1.3633241034 0.8433031365 -0.1033352434

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C   -1.2210409763  -0.5885314532  -0.0566560185
H   -4.7610905525  1.0739688532  0.0663799734
H    0.1611075674  -2.2417241099  -0.0726527985
H   -4.5397865955  -1.4017679916  0.1444129595
H   -0.2822350844  2.7289620081  -0.2463466364
H    1.9484145839  1.7322293921  -0.3224725178
H   -2.7352761005  2.4907902008  -0.0937091463
H   -2.3121070729  -2.4546222013  0.0659210831
C    2.5475857392  -0.9621836024  -0.8215462765
C    2.5849932845  -0.8995191783  0.4619733053
C    3.2030618912  -1.136089944  1.7813843889
H    2.973097597  -1.2501644062  -1.7697788167
H    2.5587744903  -1.7747520673  2.3929914636
H    3.3278691764  -0.1928453573  2.3217862867
H    4.1802343573  -1.615662627  1.6815129961
Core   RigidRotor
SymmetryFactor   0.5
End
Frequencies[1/cm]   66
53.6692              99.3419              136.2830
169.6039             188.5506              255.3686
273.0203             353.4577              387.1398
424.7420             453.1640              465.6777
506.0938             514.6512              544.0269
619.5734             648.0808              673.7482
713.0608             724.2616              753.1318
758.8917             783.7029              809.5167
863.3294             873.9743              915.3368
924.9123             936.9861              972.2732
974.3715             985.5712             1043.2889
1050.9864            1055.8924            1103.1618
1142.8850            1157.7741            1167.1657
1206.2495            1249.5984            1280.9256
1293.7802            1343.5520            1404.5401
1409.7077            1427.8375            1457.5673
1475.1088            1480.0472            1504.6639
1560.2095            1608.0117            1646.2465
1869.7904            3022.5336            3079.9639
3094.5328            3145.6523            3152.9567
3156.3551            3159.1904            3167.4024
3171.8447            3187.0607            3239.0798
ZeroEnergy[kcal/mol] -17.76
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----well_i4-----
Well      i4
Species
RRHO
Geometry[angstrom]   24
C   -3.870470236  0.5830193474  -0.025368228
C    0.0695888063  -0.9098790155  0.3964388525

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C   -3.6580103489  -0.7002010763  0.5284728125
C   1.16220445   -0.1654181838  -0.0055306459
C   -0.3413237244  1.6259937322  -0.6939989349
C   0.9263983041  1.1308389594  -0.5527997258
C   -2.8019378876  1.3490798996  -0.4275934364
C   -2.3827115884  -1.1927205717  0.6697927982
C   -1.475490344   0.8683640424  -0.2965206873
C   -1.2584606125  -0.4275017085  0.2636258666
H   -4.8813052812  0.9603666761  -0.1313587087
H   0.2054951291  -1.8970599626  0.8214994218
H   -4.5081097895  -1.2954728034  0.8423421124
H   -0.4939119141  2.6176357217  -1.1076454675
H   1.7721771771  1.7406861987  -0.8463102923
H   -2.9621785674  2.3347312214  -0.8523205507
H   -2.219472657  -2.1777074151  1.0949668958
C   3.577606494   -0.1594639932  -0.5093234002
C   2.5523785016  -0.6957838146  0.1238644501
C   2.7802841463  -1.9119922424  1.0040082127
H   3.7975826289  0.6406300124  -1.1984165277
H   2.2716124227  -2.7920846708  0.5982994163
H   2.396422121  -1.7415739328  2.0143057615
H   3.84391677   -2.1392974205  1.0687740052
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
25.1565           87.2535           169.1652
181.2959          218.6508           241.1144
321.5525          348.9185           396.9149
444.4098          471.2418           485.7804
497.0971          527.7866           553.4063
631.9661          636.6692           677.4083
690.3952          760.3538           781.9014
784.3128          802.1004           830.0262
872.0110          887.8667           907.7711
961.3933          963.2628           976.4720
996.2120          1004.8849          1042.6245
1048.9676         1084.9699          1151.8553
1174.8429         1184.0666          1210.4781
1242.8092         1282.6947          1292.8570
1372.2286         1394.9065          1403.0848
1408.9817         1466.2942          1484.3235
1489.5704         1500.0564          1540.2911
1606.7357         1640.4797          1647.5405
1667.2374         3024.2219          3077.0074
3122.7573         3156.6554          3159.6615
3162.3911         3174.7330          3183.1604
3187.3135         3188.1533          3249.1780
ZeroEnergy[kcal/mol] -37.32
ElectronicLevels[1/cm] 1
0 2
End
End
!-----

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!-----well_i5-----
Well      i5
Species
RRHO
Geometry[angstrom]  24
C   -3.9077387148  0.6773913178  -0.0905455934
C   -0.1157330663  -1.194551157  -0.15462891
C   -3.8034629132  -0.6967954535  -0.4163876059
C   1.0377973322  -0.4864489743  0.1364697832
C   -0.3120751464  1.5115850361  0.4907242459
C   0.9130447211  0.891646305  0.4680288666
C   -2.7823314  1.4067393009  0.2050695535
C   -2.577428896  -1.3131178029  -0.4400617135
C   -1.4993468667  0.8006455902  0.1888744338
C   -1.3915031252  -0.5878995434  -0.1410284182
H   -4.8828470415  1.1511871366  -0.075436649
H   -0.0417423059  -2.2501089002  -0.3948466904
H   -4.7001208543  -1.2608675678  -0.6474669053
H   -0.3817680912  2.564657098  0.7433214518
H   1.7973240013  1.4700324271  0.703699412
H   -2.8601575431  2.4597880474  0.4554536116
H   -2.4961434741  -2.3659900317  -0.6891995248
C   2.5515754297  -2.3432553558  -0.4287218497
C   2.3709778599  -1.1499521889  0.1042913409
C   3.5632110714  -0.4165653754  0.7070209975
H   3.3741168957  -3.0263141644  -0.5798586853
H   3.3629655842  -0.1376119685  1.7460374489
H   3.7816576607  0.4993770289  0.1493477984
H   4.4554928825  -1.0426408039  0.6854476014
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
21.3639           87.3776           168.0427
181.6143          221.0295          239.9350
310.6918          348.8985          394.6243
450.8998          463.7035          483.6950
504.5956          528.9001          564.0251
627.5050          641.2032          671.5498
672.7411          760.1144          780.5829
782.1215          829.1879          856.8731
865.1149          873.4814          921.3393
957.8148          963.2429          974.2890
996.1019          1009.3399         1030.2812
1039.7822         1079.2824         1155.2555
1173.6721         1185.6305         1211.0896
1245.7709         1282.0305         1290.6028
1377.1647         1391.1528         1401.1921
1405.2552         1465.6271         1484.3200
1486.3646         1500.7994         1543.2323
1602.9012         1633.5919         1649.5806
1672.5192         3022.0316         3077.6746
3115.4392         3156.5546         3161.0087
3161.9346         3164.8390         3174.8103

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3187.2700          3194.0418          3237.5227
ZeroEnergy[kcal/mol] -37.12
ElectronicLevels[1/cm]      1
0 2
End
End
!-----
!-----well_i6-----
Well      i6
Species
RRHO
Geometry[angstrom]  24
C   -3.6711917155  0.3237348412  0.0146535213
C    0.3296297363 -0.9485507976  0.1032394351
C   -3.3952110283 -1.0608305392  0.1264846896
C    1.4219704157 -0.129863259  0.0323605833
C   -0.1960377272  1.7080570688 -0.1113440887
C    1.1035865176  1.2633462841 -0.0800062813
C   -2.6465483238  1.2352910613 -0.0635352145
C   -2.1002497998 -1.5139020216  0.1585240916
C   -1.2930693069  0.8126609823 -0.0342014643
C   -1.0169243803 -0.5965173273  0.0796364433
H   -4.7008483573  0.6621874026 -0.0090435915
H   -4.216881031 -1.7654168848  0.187031929
H   -0.3977823681  2.770490626 -0.1971908771
H    1.9097486765  1.9846192245 -0.14185622
H   -2.8601471504  2.2958832771 -0.1491889444
H   -1.8819927987 -2.5718136573  0.2439435489
H    2.3005106025 -2.6713794329  0.23600189
C    3.091013656 -1.9324714097  0.1728804469
C    2.8215874396 -0.6251688465  0.0674441829
C    3.9367162663  0.3884073265 -0.0192815744
H    4.1117004246 -2.2954507404  0.198610594
H    3.8859807829  0.9632921655 -0.9499212054
H    4.9075371785 -0.1070822644  0.0174539555
H    3.8925342907  1.1063609206  0.8063971499
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
16.8782          84.0209          160.4246
179.5530         228.7675          240.6793
316.6528         336.5418          402.5950
450.2503         477.6864          501.5406
507.1230         522.5373          546.5240
626.3906         632.9779          680.9454
725.1192         760.9675          772.6681
780.9788         826.0563          867.7764
874.5786         923.9828          932.6932
955.7678         963.1212          969.2093
996.8588         1026.3847         1037.0278
1068.4136        1135.7535         1155.6998
1175.4046        1186.8487         1238.6802
1266.1911        1286.1081         1353.5943

```

1366.7527	1387.5668	1411.1263
1435.6492	1450.3254	1485.3823
1491.3467	1500.5098	1520.6085
1577.2365	1631.7715	1654.6484
1688.9047	3018.7091	3064.9541
3110.8572	3137.2342	3157.1235
3163.7139	3168.7362	3181.0877
3186.4817	3191.4341	3221.4757

ZeroEnergy[kcal/mol] -36.45

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i7-----

Well i7

Species

RRHO

Geometry[angstrom] 24

C	3.6155696094	-0.1105140056	0.0190093877
C	-0.5014845523	0.8638744548	-0.1264613836
C	3.2148322678	1.2317834313	-0.1795161485
C	-1.4656384707	-0.1139073783	0.0113272358
C	0.2836470276	-1.788071777	0.2597047661
C	-1.0470144889	-1.4595786063	0.2062011377
C	2.6738239428	-1.1001716871	0.1639867863
C	1.8814776885	1.5578362258	-0.2281132392
C	1.2887240308	-0.7969376672	0.1176230604
C	0.8823957851	0.5597003729	-0.07970408
H	4.6713830311	-0.3542730487	0.0556010842
H	3.9676634304	2.0037194015	-0.2932799642
H	0.5836003498	-2.8185776427	0.4200256721
H	-1.7989636965	-2.229588406	0.3350151459
H	2.9787842648	-2.1304401022	0.3159337914
H	1.5733454042	2.5869980599	-0.3808280808
C	-3.7792884114	-0.595818933	-0.7752427608
C	-2.9212703888	0.2218569167	-0.0477851862
C	-3.3919115557	1.344493205	0.6242130182
H	-3.4160525017	-1.4474464032	-1.335204311
H	-4.8403819072	-0.3814458461	-0.8194363277
H	-4.437843164	1.622019224	0.5694096001
H	-2.7404478041	1.9546097758	1.2356517491
H	-0.799667891	1.8927784359	-0.298334953

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

61.5257	83.7845	162.6394
185.2409	221.9911	315.7415
357.6780	392.8183	435.6403
486.3373	493.4387	525.2572
537.1731	545.4619	554.8259
598.2343	632.8777	679.8387
685.1655	761.2647	770.9907

781.7611	785.9993	803.3766
835.9515	875.6318	885.3958
920.2442	964.6880	964.7314
979.9108	982.8435	995.9836
1035.5727	1041.5489	1121.4455
1160.4613	1172.2825	1180.4777
1223.9415	1267.2190	1288.6271
1289.4845	1373.9898	1386.1491
1398.8525	1409.3421	1463.9660
1484.7258	1501.1796	1524.7840
1542.3290	1607.2459	1642.8188
1669.6550	3141.4305	3148.5334
3156.9577	3160.0793	3162.4895
3167.2797	3174.8597	3181.7476
3187.2782	3240.7412	3242.6521

ZeroEnergy[kcal/mol] -60.6

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i8-----

Well i8

Species

RRHO

Geometry[angstrom] 24

C	-3.6069916063	0.0933806358	-0.014399582
C	0.5232274086	-0.8404488152	0.0338217063
C	-3.1899025062	-1.2568891675	-0.0068253034
C	1.4784895278	0.1570933746	0.0423482363
C	-0.2929262425	1.8300884249	0.0189298477
C	1.0371361099	1.5144865183	0.0344967368
C	-2.6760639873	1.1057333976	-0.0061665353
C	-1.8512260393	-1.5692468126	0.0088292287
C	-1.2895990978	0.8158598092	0.00996429
C	-0.8659863833	-0.5481749345	0.017649851
C	3.8491366344	0.8012376427	0.0674349468
C	2.9316624237	-0.1482223866	0.0592883826
C	3.3718327764	-1.6063109785	0.0674458013
H	-4.6655371871	0.3274870649	-0.0267436435
H	0.8171564505	-1.8833483741	0.0393652129
H	-3.9322153279	-2.0471411743	-0.0134284284
H	-0.6054076669	2.8693977329	0.0131960327
H	1.7844344467	2.299791198	0.0411659233
H	-2.9939069739	2.1433117662	-0.0119527367
H	-1.5305682111	-2.6060499414	0.0146519437
H	4.9274036997	0.8586785425	0.0792815085
H	3.0019323615	-2.1281980513	-0.8204528702
H	2.9819598016	-2.1243441365	0.9490296296
H	4.4590835886	-1.6846233349	0.0798918213

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

43.0655	88.5825	166.7133
182.4922	229.0412	242.0227
319.7288	349.1879	396.9751
454.5990	456.4615	486.2481
496.6197	526.9496	566.6385
630.1026	644.7449	673.3770
674.9245	761.2891	782.8811
783.7264	835.7384	859.1722
873.6733	882.1750	906.9230
957.3329	963.6825	985.1207
987.8938	995.7416	1031.7494
1043.1632	1084.3517	1151.8602
1174.4745	1178.8677	1215.9186
1247.1430	1288.6722	1294.3394
1373.8350	1393.7401	1399.5345
1412.8511	1467.2449	1486.3453
1487.3755	1500.7769	1539.7891
1608.0798	1639.9450	1649.1674
1667.8393	3022.9812	3078.6409
3116.4845	3155.6792	3157.9078
3161.2399	3174.0728	3179.3240
3180.8739	3187.4966	3237.4109

ZeroEnergy[kcal/mol] -38.25

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i9-----

Well i9

Species

RRHO

Geometry[angstrom] 24

C	-3.6224535805	0.5374817594	0.0100480652
C	0.2266136829	-1.2130305838	0.0096705889
C	-3.4895000006	-0.8691735627	0.0050148338
C	1.3852976328	-0.4288133917	0.0144288793
C	-0.0224199211	1.5670425176	0.0196320969
C	1.2180035992	0.9979902801	0.0194897513
C	-2.5020873053	1.3394486925	0.0148269549
C	-2.2432904943	-1.4493120826	0.0048408971
C	-1.2070171246	0.7743088153	0.0147812142
C	-1.0681050083	-0.6505541978	0.0096940827
C	2.6669993235	-1.0646723852	0.0141545649
C	5.1178511815	-1.1130041012	0.0172824154
C	3.9287779547	-0.4413560672	0.0182280034
H	-4.6105737925	0.983382751	0.0101300005
H	0.3223056565	-2.2945379609	0.0058070231
H	-4.3777207126	-1.4909526893	0.0012890767
H	-0.1224811306	2.6477651041	0.0235061236
H	2.092112531	1.6371475835	0.023283836
H	-2.6022398457	2.4200179961	0.0187008956
H	-2.1409804526	-2.5295201029	0.000986898
H	2.6599877602	-2.1520791973	0.010010755

```

H   6.0641821341 -0.5874439922 0.0201508282
H   5.1524837976 -2.1973141562 0.0137964275
H   3.9668111146 0.6446549716 0.0219097878
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
59.6049          129.6801          133.0886
166.1036         184.7885          309.7656
311.0694         327.2713          402.5542
433.6023         478.3128          524.7586
528.0305         582.4115          602.1255
639.2645         649.7429          755.4975
766.2610         775.0454          778.9246
815.1026         822.4663          849.9191
870.4852         892.0951          896.6836
955.8556         958.9410          973.9116
992.8064         999.8935          1003.2637
1042.5727        1142.5128         1170.8248
1174.9943        1198.7471         1213.2405
1238.6962        1274.4540         1290.5746
1308.6539        1334.1260         1388.0987
1392.5295        1416.2159         1461.5694
1489.7663        1500.2629         1537.2217
1542.1253        1590.1533         1629.9968
1650.4433        3132.5741         3138.5891
3146.7678        3156.2313         3157.9789
3160.1835        3163.3071         3175.3986
3188.2571        3191.9895         3230.7649
ZeroEnergy[kcal/mol] -65.69
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i10-----
Well      i10
Species
RRHO
Geometry[angstrom] 24
C   -3.6493242995 0.5735470844 -0.1452412478
C    0.1809207835 -1.2019959828 0.079553051
C   -3.5216361778 -0.8333728293 -0.1985002434
C    1.3406804466 -0.4282139952 0.1853955444
C   -0.0596668419 1.5731744203 0.204270295
C    1.1774496942 0.9952579726 0.2662459192
C   -2.5311445483 1.3667699793 -0.0187907227
C   -2.2820470186 -1.4216085918 -0.1246777867
C   -1.240711587 0.7928549858 0.0572170653
C   -1.1076678019 -0.6312806704 0.0035604134
C    2.6121716974 -1.0955864181 0.2487196049
C    4.3509703305 0.6066362315 -0.407460719
C    3.9236128874 -0.5959007033 0.0829132066
H   -4.6330422153 1.0253001321 -0.2040189147

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H  0.2712340122 -2.2832308288 0.038002107
H  -4.4092827237 -1.448001286 -0.297792788
H  -0.1566908321 2.6513600344 0.2826448993
H  2.046088422 1.6185423064 0.4251708504
H  -2.6275207971 2.446790116 0.0242682724
H  -2.1835360815 -2.5014318466 -0.1652823162
H  2.5490085545 -2.16270503 0.4431777195
H  5.4106395434 0.8196466966 -0.4758513948
H  3.6783615348 1.3606686303 -0.7923895868
H  4.7049340184 -1.3060974076 0.3476217717
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
49.8806 100.8988 136.5411
188.5402 216.3213 264.2685
333.3133 392.2019 406.7560
419.3030 479.6661 522.8956
528.0985 569.3201 623.4643
639.6441 656.2147 752.6535
760.1797 775.7416 780.5665
792.5792 831.4076 850.2815
871.3939 884.9528 901.7047
958.4768 962.3715 987.0937
992.5674 994.8571 1034.3766
1042.5503 1107.3842 1153.4326
1174.0998 1177.6220 1206.8484
1245.8912 1279.9150 1288.1722
1297.5482 1355.8983 1392.0175
1406.4136 1442.6882 1454.2988
1483.1624 1488.8671 1536.5418
1559.9195 1589.8976 1628.1535
1651.8929 3118.0955 3145.5017
3153.8292 3156.2958 3158.2009
3160.3063 3163.6236 3175.4937
3188.3735 3212.2464 3242.8691
ZeroEnergy[kcal/mol] -62.0
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i11-----
Well i11
Species
RRHO
Geometry[angstrom] 24
C 3.6489124218 0.5462303942 0.279666327
C -0.2253820534 -1.176294578 -0.1967710789
C 3.4984420562 -0.8516308353 0.2346061825
C -1.3049162502 -0.3892283221 -0.3943679749
C 0.1336824125 1.660064152 -0.2709344993
C -1.1751775015 1.0908781965 -0.6952668057
C 2.5523386477 1.367443927 0.1279441993

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C  2.2379882254 -1.4073677017 0.0499155108
C  1.248794483 0.8328980068 -0.0894673394
C  1.1014324422 -0.6058878223 -0.1112722853
C  -2.7232426078 -0.6687318257 -0.260697086
C  -2.509260277 1.6901266267 -0.1676270008
C  -3.4162953648 0.4793982327 -0.1447262979
H  4.6315956843 0.9781046525 0.4335349508
H  -0.3396752158 -2.2410764643 -0.0149442174
H  4.3630023996 -1.4944450668 0.3534179008
H  0.25849285 2.7381414412 -0.2402238959
H  -1.2353859948 1.1786115823 -1.7996515015
H  2.6695280764 2.445853943 0.1586251751
H  2.1213466026 -2.4865459009 0.037506886
H  -3.1426619725 -1.6657253035 -0.2003013665
H  -2.8873300539 2.5051902111 -0.7909769832
H  -2.3846357953 2.0912038271 0.8475475889
H  -4.4857942147 0.5480956275 0.0138176116
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
88.7557 111.4088 221.6221
249.3454 263.2087 371.1532
382.9945 404.5914 442.4998
468.1022 544.6548 560.5294
617.5827 660.3913 680.3771
705.0729 734.4981 744.4632
758.0152 776.1114 793.5343
827.0968 857.7670 891.5433
906.8091 945.0236 948.5227
967.9861 974.8884 984.4600
1023.8964 1042.6206 1098.6760
1120.7635 1138.6980 1147.9340
1162.2393 1175.6791 1202.9893
1244.4230 1252.2983 1281.8236
1284.9774 1318.5806 1339.8018
1367.1966 1382.6140 1403.8226
1451.3332 1483.0098 1499.8606
1555.3529 1599.9997 1616.1923
1661.5229 2851.0055 2997.4510
3062.1087 3150.0163 3154.0831
3155.9141 3159.7789 3173.4004
3180.2784 3187.8540 3202.0502
ZeroEnergy[kcal/mol] -56.18
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i12-----
Well i12
Species
RRHO
Geometry[angstrom] 24

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```

C 3.7958464732 0.002016814 0.1551284761
C -0.335209756 -0.8435048613 -0.1687935044
C 3.3546229925 -1.335141674 0.0640714803
C -1.2945851304 0.2020163812 -0.1896048346
C 0.5227503231 1.8262721716 0.0121930197
C -0.8063841133 1.5646605101 -0.0921562446
C 2.8790927224 1.0351814552 0.1391539862
C 2.0128468972 -1.620189182 -0.0409053412
C 1.4982261234 0.778098786 0.0324580247
C 1.0437000667 -0.5792230517 -0.0604418117
C -2.6326989415 -0.0490332179 -0.2936398237
C -3.9013756404 -0.2811289568 -0.4532963297
C -4.9113461349 -0.5048382684 0.6524096259
H 4.8553392855 0.2155460661 0.2374818904
H -0.6765435939 -1.8698182258 -0.2395840618
H 4.0799303168 -2.1410827918 0.0770188481
H 0.8675407771 2.853108177 0.0819526648
H -1.5306383625 2.3701864706 -0.1064515651
H 3.2160416689 2.0645198702 0.2088617342
H 1.6747100557 -2.6487634924 -0.1110817195
H -4.4434942211 -0.4503930677 1.6359354096
H -5.3854318929 -1.4859720993 0.5454053367
H -5.706649319 0.2460407347 0.6023461393
H -4.3035465966 -0.3250115478 -1.4709133998
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
43.4020 77.4461 117.3978
143.8946 179.2768 213.0037
261.6343 341.6312 351.2802
399.1634 467.5913 486.6121
510.7458 524.2664 552.5185
627.9539 638.8825 677.8971
751.1375 759.4565 768.1959
773.3555 818.1814 839.1897
871.0952 877.9623 939.1176
953.0870 955.2411 979.1128
987.5019 1042.9277 1054.0182
1066.4858 1123.6996 1158.9187
1170.9823 1177.3219 1220.1437
1263.2429 1288.4621 1323.3021
1345.9394 1373.0002 1400.4762
1409.9999 1451.5929 1471.3351
1485.2102 1492.3596 1517.6141
1563.9701 1621.3503 1632.9135
1908.4732 3018.4898 3030.1147
3068.4928 3117.0163 3156.3672
3158.9481 3162.0155 3174.7754
3178.2790 3188.4199 3189.4102
ZeroEnergy[kcal/mol] -45.94
ElectronicLevels[1/cm] 1
0 2
End

```

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End
!-----
!-----well_i13-----
Well      i13
Species
RRHO
Geometry[angstrom]  24
C   3.6029795805 -0.1269478816 0.107728744
C  -0.4986047026 0.8190909805 -0.2780256337
C   3.2040079132 1.2081762145 -0.0805987972
C  -1.5338252759 -0.2171523031 -0.2067396262
C   0.2680364828 -1.8758306599 0.0836080401
C  -1.0445957716 -1.6002345685 -0.03169383
C   2.6439119896 -1.1329028773 0.1627618451
C   1.8687447557 1.5276286926 -0.2092203153
C   1.2823254272 -0.8438296835 0.0363930577
C   0.8629250269 0.5199561436 -0.1531969
H   4.6541220248 -0.3707866466 0.207807106
H  -0.811314682 1.8457408001 -0.4360746031
H   3.9525152017 1.9917147259 -0.1251291191
H   0.5944788765 -2.9030813786 0.2135501971
H  -1.7832100057 -2.3943596903 -0.0030686509
H   2.9497925334 -2.1646758189 0.3053099105
H   1.5646459273 2.5590706404 -0.3540673282
C  -3.4112884385 0.0332181973 -2.1037522386
C  -2.8301644552 -0.0001759359 -0.9214705655
C  -2.911122135 0.1540537564 0.5166084087
H  -2.8522750089 -0.1701877203 -3.0108056065
H  -4.4671248147 0.2649436354 -2.206583905
H  -3.3558239582 -0.6343452663 1.1168790595
H  -2.9684244912 1.1494996443 0.9466957506
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
53.4873           92.6295           177.3986
182.7825          233.7767           280.2562
362.8145          372.6432           412.2195
442.0220          466.4859           502.4190
510.5536          547.3933           617.3095
648.3904          668.9138           689.9380
719.1838          750.2947           757.7492
779.7213          801.5927           849.3599
863.9052          893.3926           921.5139
927.8405          933.0050           939.7836
974.4720          982.1289           1017.4368
1026.5969         1043.7682           1078.7331
1121.8761         1146.3172           1166.0118
1171.2531         1208.6799           1254.2587
1293.2818         1318.0808           1345.2619
1414.7238         1425.9777           1437.6208
1459.4771         1465.3239           1506.0680
1560.1938         1608.6869           1651.9473
1817.8471         3094.7741           3120.4536

```

```

3151.6867          3155.4207          3159.3249
3166.2944          3173.8913          3174.2490
3181.5657          3188.6372          3204.0166
ZeroEnergy[kcal/mol] -25.7
ElectronicLevels[1/cm]      1
0 2
End
End
!-----
!-----well_i14-----
Well      i14
Species
RRHO
Geometry[angstrom]  24
C   -2.1708788549 -0.9260967149 -0.3726883959
C    1.0893593865  1.6631920972  0.4039510152
C   -2.4095324054  0.429497517  -0.04822489
C    2.3823548735  1.1992362363  0.3447741261
C    1.5648182311 -1.0121357589 -0.2392953773
C    2.6110617828 -0.1625122941  0.0134201264
C   -0.8849899129 -1.4061850374 -0.4371938672
C   -1.3588532039  1.2779392342  0.2054928637
C    0.2213700651 -0.556428538 -0.1807569801
C   -0.0191870874  0.8138277575  0.1475376935
H   -3.0086640883 -1.585144026 -0.5707759611
H    0.8975361375  2.7029599906  0.65215143
H   -3.4284324362  0.7971739777 -0.0006126874
H    1.7542526675 -2.0505915347 -0.491121139
H    3.6315121077 -0.5249128491 -0.0474037239
H   -0.6988288669 -2.4458287662 -0.6863204474
H   -1.5418755997  2.3182701253  0.4541486208
C    3.5587054705  2.1136065638  0.6502071931
C    5.8446403113  1.9199410102 -0.6014353623
C    4.5744444236  2.1773205664 -0.4187825047
H    3.1846346811  3.1215119617  0.8583038611
H    4.0529764614  1.7719585207  1.5773791701
H    6.4706545243  1.5275977338  0.2068777162
H    6.3419573316  2.0842372269 -1.5535534798
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
23.5293          71.2218          106.2674
179.2895         197.7096          241.6284
306.8364         324.0052          403.2800
406.3950         447.4936          487.0145
514.1745         526.7582          581.2887
636.3853         658.5397          735.8589
763.9667         781.1979          786.6345
832.6449         864.3947          878.5778
883.7540         889.7888          913.4227
947.6315         963.8884          977.5358
979.6539         996.2394          1042.1791
1042.5549        1147.5463         1172.2849

```

1177.9235	1188.0492	1204.4470
1237.0804	1277.1098	1288.2727
1303.1735	1391.7054	1396.5431
1406.7277	1413.4844	1447.3755
1474.0169	1502.4998	1545.8055
1612.3082	1645.6789	1673.1690
1734.1983	2923.2560	3025.6637
3044.3966	3148.0055	3152.9757
3157.0511	3158.8097	3162.5382
3174.7730	3178.2433	3187.6229

ZeroEnergy[kcal/mol] -36.53

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i15-----

Well i15

Species

RRHO

Geometry[angstrom] 24

C	-3.6853081126	0.3132365987	0.1702103376
C	0.3608289559	-0.8464602687	-0.331969764
C	-3.3694510029	-1.0152460623	-0.1960618228
C	1.3966585044	0.0491667037	-0.14136726
C	-0.2546159212	1.8011835045	0.3969886337
C	1.005369486	1.3450591001	0.2165516366
C	-2.6855099659	1.2359034637	0.3652824467
C	-2.0597060833	-1.3964940546	-0.3597603906
C	-1.3247278148	0.8732493513	0.2031617884
C	-1.0000621699	-0.4714203142	-0.1676652918
C	2.8527805263	-0.3334369186	-0.3291945064
C	3.9744330945	-0.6029692777	-2.5658237144
C	3.4180528077	0.1662710387	-1.6360944049
H	-4.7226549234	0.6021367903	0.2969927092
H	0.5871443192	-1.8713395262	-0.6141663866
H	-4.1673864743	-1.7333902279	-0.3472912581
H	-0.4728050859	2.8260688121	0.680144627
H	-2.9258272111	2.2558780549	0.6463617595
H	-1.8173984251	-2.4161315094	-0.6407623727
H	3.4330494535	0.091660233	0.4985215128
H	2.9570784298	-1.4202179574	-0.2727942107
H	4.0594557285	-1.6784160801	-2.4402428471
H	4.3673190168	-0.1865484719	-3.4864509305
H	3.3445228682	1.2394080179	-1.7995902909

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

23.6820	59.0243	101.6365
181.5633	191.6930	248.0398
317.3843	372.9903	397.9920
411.1026	476.6877	480.2778
530.8658	541.4642	617.4221

633.9593	657.9506	746.8350
762.7680	766.9880	777.8534
838.1710	870.9931	875.9615
894.8381	935.2553	940.2048
949.8672	954.7086	964.7459
994.1871	1032.2668	1041.9649
1106.3999	1148.5986	1169.3863
1180.3087	1217.6022	1222.1123
1253.9220	1275.1993	1310.5901
1325.9500	1342.1294	1387.3455
1399.3607	1432.6102	1453.6459
1473.9690	1479.0407	1528.4245
1595.7633	1626.4345	1655.7364
1705.8503	3015.9238	3072.6714
3123.8773	3134.8424	3144.8492
3157.3214	3158.6700	3163.8622
3175.8249	3188.2097	3209.2217

ZeroEnergy[kcal/mol] -32.01

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i16-----

Well i16

Species

RRHO

Geometry[angstrom] 24

C	-3.7134868502	0.4626528905	0.2739172892
C	0.214288241	-1.0043733187	-0.0577859539
C	-3.494811008	-0.9322214027	0.3574026028
C	1.3142881011	-0.2303580259	-0.2438987554
C	-0.20765562	1.6827450688	-0.2205981714
C	1.0628592481	1.1754979655	-0.3286915892
C	-2.6583811093	1.3234110898	0.0870521733
C	-2.2252660656	-1.4470199529	0.2526507402
C	-1.3319692981	0.835237156	-0.0255415656
C	-1.1155562205	-0.5842220609	0.0596164515
H	-4.7219473444	0.851509706	0.3586365615
H	-4.3380476807	-1.5973856008	0.5053309714
H	-0.3701676676	2.7532198088	-0.2890533193
H	1.9037839135	1.8457739559	-0.4828550945
H	-2.8279753478	2.3935127984	0.0230310287
H	-2.0501141594	-2.514519772	0.3160451783
H	2.3223365968	-2.4955322298	-1.654109045
C	2.7280854243	-0.7750165058	-0.3358122069
C	3.3978033994	-3.1730374526	0.0059400542
C	2.8010804537	-2.2288520731	-0.7140786691
H	3.276661245	-0.1786533269	-1.0765969219
H	3.2394342126	-0.6177228668	0.6213419624
H	3.8776145937	-2.9485565711	0.9539739199
H	3.4273659427	-4.20543428	-0.3236126411

Core RigidRotor

SymmetryFactor 0.5

```

End
Frequencies[1/cm] 66
29.4750          63.7939          98.6585
154.7319        180.3027        259.2692
303.6574        371.7089        408.3747
432.7212        474.9463        502.2206
509.5688        520.0494        613.6675
626.7124        648.4669        742.2549
755.5953        771.3618        779.8885
815.5489        875.6975        903.4153
928.6905        943.7640        951.9850
958.1390        969.3808        974.3603
997.1942        1029.9790       1039.7471
1127.6701       1139.4412       1161.7711
1171.0638       1195.6947       1236.1080
1245.6112       1265.1242       1311.1170
1325.8133       1359.6068       1364.7015
1394.7834       1447.4229       1450.8237
1471.1123       1496.4028       1520.5586
1583.0241       1643.1138       1664.7373
1709.9389       3001.8781       3033.6926
3124.0430       3133.4331       3146.7504
3157.4233       3168.5484       3172.1509
3181.6314       3191.7745       3209.6418
ZeroEnergy[kcal/mol] -31.49
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i17-----
Well      i17
Species
RRHO
Geometry[angstrom] 24
C  3.7558777361 -0.0540624488 0.3680328436
C  -0.3416996382 -0.7685246127 -0.4463485298
C  3.3030906976 -1.3720213857 0.1260750898
C  -1.216707186 0.2870671651 -0.4720146886
C  0.5608043689 1.8583828 0.0358069038
C  -0.7618178876 1.611174834 -0.2290842351
C  2.8721260868 0.9971502426 0.3402203165
C  1.9763841959 -1.6101524827 -0.1384665874
C  1.4941543391 0.7879163108 0.0701566683
C  1.0352441678 -0.5478781782 -0.1750846005
C  -2.7093623931 0.2752732546 -0.7383053172
C  -1.9121632934 2.59519271 -0.3129352415
C  -3.0893650794 1.7217014013 -0.6289583335
H  4.8052619337 0.1227704547 0.5758652948
H  -0.6837840657 -1.7825540832 -0.6313961324
H  4.009143534 -2.1945588955 0.1504175309
H  0.9140986772 2.8683126525 0.2222260121
H  3.2183818029 2.0088651526 0.525735636
H  1.6277763572 -2.6210058112 -0.32427399

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H   -2.9431969492 -0.1491363648 -1.727291071
H   -3.2470865904 -0.3582004996 -0.0155048744
H   -1.7366498704  3.3620844441 -1.0836504992
H   -2.0408605404  3.152806685  0.6280032609
H   -4.0973234032  2.0920946549 -0.7594894562
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
94.3256           122.3123           152.5677
256.8166         258.4568           286.3775
366.4610         404.7816           405.2049
411.6028         486.6988           535.1487
575.3483         629.0985           649.8059
718.4084         724.6065           756.7602
779.4559         785.5189           829.0436
858.7876         869.9437           889.3510
912.8743         920.9225           929.0231
942.2427         965.1186           992.4063
1025.1768        1042.2542          1088.4897
1133.7233        1134.6911          1168.5879
1172.1536        1181.5257          1222.9891
1245.4172        1265.9690          1283.2206
1308.2046        1349.1397          1368.7828
1392.9369        1418.0195          1455.5254
1459.8124        1485.0784          1487.7814
1537.5065        1614.4639          1652.0068
1678.1141        2954.9278          2958.3026
2959.3328        2959.3826          3152.4401
3154.2132        3155.7817          3160.5562
3173.3421        3186.4986          3204.3097
ZeroEnergy[kcal/mol] -65.35
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----well_i18-----
Well      i18
Species
RRHO
Geometry[angstrom]  24
C   -3.607062069 -0.4605740743 -0.0318252876
C    0.6292210744 -0.3906776281  0.0277618079
C   -2.8882487414 -1.6773337816 -0.046284512
C    1.2868335286  0.8210121746  0.0610070201
C   -0.805030168  2.0109928583  0.0561101079
C    0.5683326982  2.036618594  0.0754479664
C   -2.9353082483  0.7377778544  0.0013687349
C   -1.5135397761 -1.6733497794 -0.0272977677
C   -1.5174417576  0.7812486353  0.0217280292
C   -0.7887686853 -0.4535965745  0.0070463758
C    2.7894119791  0.6349755857  0.0776853037
C    1.6080635607 -1.5476234172  0.0179128255

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C   2.9386691442 -0.8562776438 0.0494437806
H  -4.6910512064 -0.4770673972 -0.0470524222
H  -3.4275925484 -2.617699124 -0.072494086
H  -1.3698888888 2.9374094166 0.0668786518
H   1.0981762608 2.9832118707 0.1016345141
H  -3.4852400794 1.6733450155 0.0125482626
H  -0.9695478063 -2.6110225926 -0.0385263585
H   3.2723483421 1.1276919034 -0.7815371326
H   3.2485491479 1.0920899577 0.9690463158
H   1.4599913509 -2.2199256023 0.87850768
H   1.4834254148 -2.1853272914 -0.8721972472
H   3.8892594724 -1.3724059599 0.0520514372
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
107.0698          128.5708          178.4724
225.9664          235.7410          276.7820
353.3120          420.6603          428.3135
460.9729          507.0879          519.1917
533.6427          603.8140          642.7945
671.0885          744.3922          751.3863
781.2880          788.6778          819.8450
868.7788          873.0729          911.2819
928.9227          930.0882          958.7208
960.1594          970.2790          993.5074
1025.4853         1045.3607         1072.8194
1129.5222         1137.3259         1167.6873
1177.4641         1184.1963         1212.0690
1234.2226         1271.5683         1283.4381
1324.5049         1346.0158         1377.9853
1400.1540         1412.7110         1457.5895
1463.8005         1470.8255         1497.5447
1552.7075         1612.0443         1636.1373
1665.6815         2948.0004         2950.1224
2952.4369         2952.5572         3155.2200
3157.3450         3165.1983         3173.9764
3178.2905         3188.1393         3204.5390
ZeroEnergy[kcal/mol] -66.0
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i19-----
Well          i19
Species
RRHO
Geometry[angstrom] 24
C   3.6318810329 0.4807542745 0.0164837667
C  -0.2434383243 -1.2107040763 0.1715009654
C   3.4731057942 -0.897396964 0.2869243159
C  -1.3837031239 -0.4316568618 -0.0393356273
C   0.0552111971 1.5277580953 -0.330193233

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C   -1.1903361535  0.9723244628 -0.2716870932
C   2.5285366997  1.2777531678 -0.1910255182
C   2.2177639331 -1.4537653676  0.3414043115
C   1.2231825373  0.7358196657 -0.1410187339
C   1.0581642944 -0.660774276  0.1251246419
H   4.6272643362  0.9083445479 -0.0243518639
H  -0.3439809883 -2.2578012139  0.424775612
H   4.3486207288 -1.5151830757  0.4522842615
H   0.1703771649  2.5900976259 -0.5195887297
H  -2.066656421  1.5949285609 -0.4185021695
H   2.6483304895  2.3369353075 -0.3945287055
H   2.0951971186 -2.5116851041  0.5493027687
C  -2.7325403717 -0.9266761192  0.0003385113
C  -2.5849411392 -3.3960708672 -0.4579690801
C  -3.2260580323 -2.2484996023 -0.0851142619
H  -3.4928412555 -0.1568802084  0.1001777134
H  -3.1214040518 -4.3366536794 -0.4808369014
H  -1.5578416823 -3.4130030955 -0.7959543381
H  -4.2868677829 -2.3439631969  0.1390253873
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
58.9015           101.5076           129.9387
189.0148          215.3316           278.4754
332.1181          389.6537           410.0791
432.0402          481.8984           523.5196
526.6313          569.6826           605.0500
646.2998          656.8319           739.4751
751.9518          773.1264           779.2752
794.0026          833.6479           854.9327
873.1235          906.7269           924.4219
961.5779          965.1367           978.2899
991.8832          993.5742          1020.8295
1042.5393         1112.0085          1153.8579
1171.0841         1179.3984          1211.4510
1229.4784         1267.6219          1286.0095
1293.7944         1367.4051          1389.9154
1411.1832         1442.4774          1453.8730
1478.7488         1489.1216          1534.9779
1561.9633         1592.1557          1632.4830
1651.8740         3119.1245          3145.6842
3154.2215         3155.9985          3157.5469
3161.9987         3174.4123          3175.3508
3187.9911         3197.8435          3243.0872
ZeroEnergy[kcal/mol] -62.2
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----well_i20-----
Well      i20
Species

```

RRHO

Geometry[angstrom] 24

C 3.6230700817 0.4619957723 -0.0842389153
C -0.3031069253 -1.2250619843 0.5110391305
C 3.4846128781 -0.9173547634 0.0738051482
C -1.4265864514 -0.345334985 0.002846485
C 0.0309431114 1.564962644 -0.0513082859
C -1.2438720213 1.0249336922 -0.1416123886
C 2.4972689638 1.2729330543 -0.0993943822
C 2.2137579479 -1.4728422414 0.2311596715
C 1.205775024 0.7294117857 0.0451732
C 1.0745113243 -0.6742348158 0.2252395833
C -2.5378683456 -1.184410105 -0.3056176019
C -0.6972323073 -2.6447765608 0.0209552627
C -2.171488828 -2.4938495309 -0.2745764711
H 4.6079761391 0.9004444951 -0.2002591312
H -0.4108451995 -1.2340230922 1.6114296777
H 4.3598001422 -1.5570681438 0.0808093914
H 0.1760726786 2.6330330374 -0.1708482773
H -2.0855113347 1.6644272303 -0.3897136437
H 2.6027307471 2.3442710184 -0.2374252175
H 2.11440712 -2.544390969 0.3699087987
H -3.5226658597 -0.8182249332 -0.5708291764
H -0.4824639782 -3.4278222972 0.7536584406
H -0.1496975418 -2.9074488569 -0.8955033665
H -2.8191913655 -3.3310424509 -0.5025069317

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

95.7042	110.4329	211.0156
234.1449	251.2703	394.0126
415.9914	425.1121	437.8193
504.0759	519.7746	539.3193
604.9982	654.0605	690.8255
716.1939	724.9124	750.4712
775.3882	796.1987	814.4065
859.2284	880.9569	921.4952
924.5328	946.7092	948.3532
952.4561	979.6145	983.2397
1024.6200	1058.9219	1095.7327
1118.8624	1139.2165	1159.6583
1180.5462	1216.7607	1227.0960
1238.9974	1247.5655	1282.7061
1298.3331	1315.9616	1321.0889
1345.9526	1387.8781	1407.0705
1463.7064	1481.3539	1511.7609
1531.3195	1551.4635	1600.2444
1630.8057	2899.7681	2988.1683
3058.2107	3152.5933	3155.1394
3160.4981	3172.3421	3174.9839
3181.3335	3186.8673	3203.2937

ZeroEnergy[kcal/mol] -64.72

ElectronicLevels[1/cm] 1

```

0 2
End
End
!-----
!-----well_mn-il-----
Well          mn-il
Species
RRHO
Geometry[angstrom]  24
C  -0.6004416988  0.3544455869  -1.1757810566
C  -0.390057768  -1.0438970506  -0.9650399553
C  0.9418382585  -1.5125784277  -0.8173353867
C  2.0046746674  -0.6473609443  -0.8740681772
C  1.8092192504  0.7447345768  -1.084267283
C  0.525115115  1.2179847317  -1.2292345509
C  -1.9289488373  0.8304877473  -1.3263720608
C  -2.9968629569  -0.0322697124  -1.2707189775
C  -2.787794841  -1.4155124195  -1.0626238733
C  -1.5137940088  -1.9081691867  -0.9138244338
C  3.0000122174  1.6722201083  -1.1316146857
C  3.607414477  2.0243156209  0.2262319778
C  3.1623639561  1.6674800824  1.4021881403
H  1.1089536267  -2.5734516462  -0.6612707377
H  3.0155540359  -1.024345155  -0.7585291672
H  0.3555793743  2.2786106332  -1.3902026545
H  -2.0891306219  1.8918080451  -1.4861363438
H  -4.0067342131  0.3449751459  -1.3866890395
H  -3.6389549355  -2.0857709801  -1.0210906319
H  -1.3504493685  -2.9690556307  -0.7543630674
H  2.7243182238  2.6077942353  -1.6310649738
H  3.7928912315  1.2274575829  -1.7461115467
H  4.5033943312  2.645846437  0.1665835856
H  2.3545114844  1.0918026192  1.8275238995
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
   33.7818           71.2911           120.1561
  154.5524          182.9636           263.3985
  296.1082          391.3945           402.9616
  417.5659          485.0298           498.9661
  527.0770          577.7792           633.2026
  636.9695          666.0867           724.7768
  760.1191          780.7970           785.6686
  829.1099          830.4017           858.4278
  879.0855          885.8286           916.9674
  937.3125          960.9562           963.4311
  977.1205          989.0295           995.4340
 1042.0822         1147.9961          1171.2122
 1175.5088         1190.7302          1200.7094
 1233.6451         1242.6642          1277.9424
 1288.8761         1341.5987          1391.4951
 1396.2938         1405.5923          1470.3283
 1478.3036         1503.7384          1544.9609

```

1611.1041	1646.0593	1666.7627
1673.8430	3008.8220	3042.5631
3076.2693	3152.8627	3155.7829
3157.3717	3162.1621	3174.0332
3174.9327	3187.3865	3244.9961

ZeroEnergy[kcal/mol] -35.89
 ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_mn-i2-----

Well mn-i2

Species

RRHO

Geometry[angstrom] 24

C	-0.5495401567	0.2940637649	-1.0884892313
C	-0.3797028821	-1.1178338415	-1.0711612379
C	0.9392451837	-1.6885172283	-1.0929796892
C	2.0743731093	-0.8869664908	-1.2989695002
C	1.974739564	0.4778399058	-1.2954928909
C	0.6805574566	1.1674389614	-0.9240389654
C	-1.8331734895	0.8273321235	-1.1482938573
C	-2.9571539958	0.0015011386	-1.1856578125
C	-2.8001386839	-1.3855903438	-1.1513596366
C	-1.5292942739	-1.9356568814	-1.0951246614
C	2.9547770353	1.504727167	-1.8065358618
C	2.0422972111	2.6719699186	-2.1284094907
C	0.8027900951	2.4831133172	-1.6769910163
H	1.0341924393	-2.7683061432	-1.0768525379
H	3.0234421722	-1.3635235998	-1.5284744931
H	0.723792466	1.4117456158	0.1584316175
H	-1.9669982383	1.903904332	-1.1570158
H	-3.948177376	0.4380797727	-1.2349944874
H	-3.6702161414	-2.0323443284	-1.1725273218
H	-1.404216134	-3.0136369127	-1.0806702696
H	3.5213523474	1.1477773613	-2.6740514383
H	3.7013139557	1.7929059894	-1.0489082491
H	2.3897160468	3.5605331436	-2.6420775058
H	-0.0069597109	3.196718258	-1.7641206631

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

71.2842	111.0258	194.0204
242.9796	260.0683	359.2783
413.5684	423.0046	435.9274
472.3224	520.7721	533.6345
603.5704	644.8904	684.5219
713.6039	729.3775	738.5037
776.5964	799.0565	817.0425
861.9620	883.8090	896.6859
913.3055	947.2670	951.0729
957.2956	972.3581	981.4465

1017.9619	1057.1473	1098.6393
1126.1182	1135.8943	1154.3699
1179.8017	1185.1110	1214.7785
1221.3983	1230.9035	1268.7294
1281.8422	1297.8752	1328.0782
1353.5711	1369.5182	1418.1716
1465.4455	1468.8912	1511.3915
1559.4710	1595.3045	1626.9951
1670.3770	2842.7365	2957.1388
3029.4867	3144.6835	3154.9671
3160.5759	3172.4473	3176.5967
3178.8769	3187.0053	3203.2521

ZeroEnergy[kcal/mol] -58.75

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_mn-i3-----

Well mn-i3

Species

RRHO

Geometry[angstrom] 24

C	-0.6595082354	0.3461917609	-1.1007835026
C	-0.5055997663	-1.0876782676	-1.1497295649
C	0.7743190379	-1.6559122024	-1.1632880324
C	1.9913214326	-0.808882044	-1.3423080726
C	1.7595604796	0.6506337953	-1.0061122591
C	0.5272381677	1.1709049101	-0.9309612214
C	-1.9427772165	0.8949435708	-1.1102525821
C	-3.0770788458	0.0880113285	-1.1625109591
C	-2.9396122004	-1.3093285592	-1.1861325802
C	-1.6855545692	-1.8852597097	-1.1723570971
C	3.0769629786	1.2563727003	-0.5748290649
C	3.8623039192	0.0216309903	-0.1706819018
C	3.2646108239	-1.1038356896	-0.5607540325
H	0.8806413896	-2.7361613717	-1.1813900479
H	2.2683531299	-0.8783915913	-2.4192605807
H	0.3827973143	2.2129069387	-0.6574443227
H	-2.0515168247	1.974223669	-1.066932477
H	-4.0631569742	0.5376954768	-1.1739594265
H	-3.8227475655	-1.9379990526	-1.2157450907
H	-1.5805228828	-2.9651141673	-1.1935373122
H	2.9580738287	1.9821692596	0.2358067871
H	3.5847138269	1.7836408104	-1.397224914
H	4.813108948	0.0773075135	0.3460857795
H	3.648066804	-2.1068710689	-0.4156305243

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

80.3757	110.9969	203.8995
260.9463	267.1762	343.1721
389.5315	412.0929	426.5781

452.4649	536.5813	561.0392
617.1090	652.8559	674.6876
699.1598	718.4971	741.8587
758.6949	788.9357	791.0394
836.1272	862.5058	889.9802
908.1877	943.8040	947.5158
962.5953	974.2332	978.3042
1005.9601	1044.5224	1082.7330
1117.6355	1126.4180	1150.9412
1164.7943	1168.6118	1193.3985
1228.0738	1251.6698	1262.6837
1286.9158	1300.5209	1332.8733
1347.9952	1388.4116	1411.5281
1453.9343	1471.8421	1499.4239
1560.6208	1603.8053	1664.7353
1701.3520	2799.0815	2970.8258
3047.2475	3141.7846	3154.0185
3156.0428	3159.6893	3173.0843
3175.1865	3187.7230	3199.0050

ZeroEnergy[kcal/mol] -53.24
ElectronicLevels[1/cm] 1
0 2

End
End

!-----
!-----c10h7_c3h4_p0p-----

Bimolecular p0p
Fragment c3h4
RRHO

Geometry[angstrom] 7
C -0.823420841 0.0519880348 -0.0208571707
C 1.824711204 -0.1816552298 0.0001678957
H -1.8820502847 0.1362504236 -0.0342313517
H 2.1265806386 -1.2327357481 0.0038417281
H 2.2515118512 0.2935470245 0.887798287
H 2.2667123243 0.2920674571 -0.8807572055
C 0.3727611076 -0.0556769621 -0.0121801829

Core RigidRotor
SymmetryFactor 3.0
End

Frequencies[1/cm] 15		
339.4278	339.9763	666.0166
666.0469	943.1202	1056.2902
1056.6567	1416.3162	1479.4028
1479.6937	2229.8067	3026.9185
3085.7411	3086.1443	3478.9987

ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1

End

Fragment c10h7
RRHO

Geometry[angstrom] 17
C -2.342087 -0.789687 0.000182

```

C  1.23599 1.492987 -0.00007
C  -2.406991 0.622556 -0.000082
C  2.395952 0.795395 -0.00008
C  1.355609 -1.327182 0.000189
C  2.524369 -0.593594 0.000023
C  -1.124987 -1.426414 -0.000392
C  -1.255124 1.371674 0.000158
C  0.086626 -0.68687 -0.00012
C  0.017308 0.74503 0.000139
H  -3.258566 -1.368743 0.000087
H  1.201705 2.577724 -0.00028
H  -3.373351 1.114428 0.000661
H  1.39504 -2.412201 0.000526
H  3.493202 -1.079675 0.000221
H  -1.073657 -2.510327 -0.000363
H  -1.30436 2.455421 -0.000531
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 45
174.5523 191.9823 368.8691
386.9856 471.7499 485.5864
511.3155 520.6059 611.1652
628.1914 745.0901 754.9555
767.1418 793.9645 805.9451
845.2289 888.1353 936.1904
956.7704 970.6818 996.7989
1040.0912 1049.2482 1141.2669
1161.1784 1172.2344 1208.1577
1250.0871 1276.7535 1334.8589
1385.5649 1394.0363 1457.0524
1468.7884 1530.4230 1592.5026
1620.1890 1656.5683 3155.0771
3158.4833 3159.6258 3164.2142
3175.9226 3179.5633 3188.1262
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] 0.0
End
!-----c10h7_c3h4_p0a-----
Bimolecular p0a
Fragment c3h4
RRHO
Geometry[angstrom] 7
C -0.7953643067 0.0340930197 0.0003929351
C 1.7999079767 -0.188313622 -0.0384040502
H -1.2789000818 0.9884787247 0.182918491
H -1.4365104427 -0.8255826572 -0.1664284561
H 2.3603730273 -0.4130354538 0.8635083944
H 2.3636835038 -0.0613232862 -0.9572540549
C 0.5024913234 -0.0757887252 -0.0189202593
Core RigidRotor

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SymmetryFactor 4.0
End
Frequencies[1/cm] 15
371.2233          371.5183          865.8663
866.2617          884.0403          1016.3687
1016.5866         1109.0953         1422.1712
1479.1925         2051.9260         3118.9601
3123.0938         3193.6015         3194.4729
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment          c10h7
RRHO
Geometry[angstrom] 17
C  -2.342087 -0.789687 0.000182
C  1.23599 1.492987 -0.00007
C  -2.406991 0.622556 -0.000082
C  2.395952 0.795395 -0.00008
C  1.355609 -1.327182 0.000189
C  2.524369 -0.593594 0.000023
C  -1.124987 -1.426414 -0.000392
C  -1.255124 1.371674 0.000158
C  0.086626 -0.68687 -0.00012
C  0.017308 0.74503 0.000139
H  -3.258566 -1.368743 0.000087
H  1.201705 2.577724 -0.00028
H  -3.373351 1.114428 0.000661
H  1.39504 -2.412201 0.000526
H  3.493202 -1.079675 0.000221
H  -1.073657 -2.510327 -0.000363
H  -1.30436 2.455421 -0.000531
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 45
174.5523          191.9823          368.8691
386.9856          471.7499          485.5864
511.3155          520.6059          611.1652
628.1914          745.0901          754.9555
767.1418          793.9645          805.9451
845.2289          888.1353          936.1904
956.7704          970.6818          996.7989
1040.0912         1049.2482         1141.2669
1161.1784         1172.2344         1208.1577
1250.0871         1276.7535         1334.8589
1385.5649         1394.0363         1457.0524
1468.7884         1530.4230         1592.5026
1620.1890         1656.5683         3155.0771
3158.4833         3159.6258         3164.2142
3175.9226         3179.5633         3188.1262
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2

```

```

End
GroundEnergy[kcal/mol] 1.1
End
!-----h_c10h6_p1-----
Bimolecular    p1
Fragment        c10h6
RRHO
Geometry[angstrom] 23
C   -3.4297275383  0.6926828295  0.0039083678
C    0.2561865651 -1.4034018581 -0.0085023831
C   -3.4192071452 -0.7206557811 -0.0006487593
C    1.4301622887 -0.6884204437 -0.0080385742
C    0.2375332283  1.4304945887  0.0005892895
C    1.4176697405  0.7420283073 -0.0034772169
C   -2.2463676634  1.3923572342  0.0043120379
C   -2.2271153712 -1.4039826096 -0.0046946993
C   -0.9977522925  0.7205311113  0.0002165193
C   -0.9860464949 -0.7144502301 -0.0044032352
C    2.8281081359 -1.1220833093 -0.0116269207
C    2.8483269174  1.2348432817 -0.004056437
C    3.6409965108 -0.0519460444 -0.0095010525
H   -4.3754448604  1.222915632  0.0070883174
H    0.2599391198 -2.4888289276 -0.0119952953
H   -4.3573702871 -1.2643043552 -0.0009374379
H    0.217623734  2.5163608324  0.0041197655
H   -2.2529829395  2.477688416  0.0078122976
H   -2.2185160279 -2.4892073171 -0.0081914894
H    3.1434835396 -2.157922306 -0.0153885217
H    3.0748527551  1.8496933954  0.8759822814
H    3.072160391  1.8553276045 -0.8808330576
H    4.7229266941 -0.0789710526 -0.0107867963
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 63
102.2294          134.8645          251.8437
263.5800          278.6570          394.6986
405.8898          417.1671          426.3605
487.3719          559.6989          578.1974
628.8197          686.4746          732.6775
738.6653          751.4693          764.7804
783.4099          806.1723          857.4753
858.7720          890.3014          902.4118
913.7707          955.6878          957.5792
963.1137          970.5211          991.6628
1043.4534         1077.4282         1121.2771
1155.6730         1169.2853         1174.4788
1180.6497         1244.5385         1251.5039
1268.6960         1282.1901         1347.9739
1373.3697         1387.7710         1434.9787
1446.5223         1470.3410         1486.9167
1537.3526         1611.9868         1627.0456
1655.0763         1677.6805         3013.8854
3035.4208         3153.1920         3155.6051

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3159.0651          3162.4123          3173.3962
3186.6618          3189.2638          3212.1926
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment          H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol] -36.51
End
!-----h_c10h6_p2-----
Bimolecular    p2
Fragment          c10h6
RRHO
Geometry[angstrom]    23
C   3.3470139691 -0.1784239349 -0.001643978
C   -0.8842205267 -0.4325083205 -0.0072564037
C   2.726429771 -1.4486079448 -0.0077584959
C   -1.6327602416 0.7404671779 -0.0032145561
C   0.3640781219 2.0708040892 0.0046323389
C   -1.0114628758 2.0005023316 0.0027143091
C   2.5833180704 0.9631720545 0.0024139944
C   1.355902182 -1.5520334827 -0.0096475295
C   1.165120296 0.8966729154 0.0005939313
C   0.537531976 -0.3935695503 -0.0055813048
C   -3.0990961767 0.3869034187 -0.0067243045
C   -1.8099242179 -1.5696327613 -0.0128348109
C   -3.0780386636 -1.1207224362 -0.0124526263
H   4.4290830247 -0.1096456294 -0.0001791325
H   3.3379375392 -2.3440222559 -0.0109806364
H   0.860868578 3.0352454583 0.0093447647
H   -1.6062808473 2.908085251 0.0057784256
H   3.0580407341 1.9390508141 0.007080557
H   0.8891185 -2.5303532928 -0.01442073
H   -3.6221352851 0.7853374153 0.8721696031
H   -3.6190854475 0.7919835703 -0.8844308124
H   -1.5129772577 -2.6101143399 -0.0173138716
H   -3.9711972226 -1.7309105476 -0.0167237316
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]    63
113.5257          131.9163          229.2535
241.8649          268.1291          387.6530
432.9010          438.9526          463.5719
506.1584          519.7956          565.0100
613.2436          666.3208          682.0518
723.0441          748.4811          753.1903
798.3278          817.3537          841.0725
879.0965          882.4712          933.2309

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950.4010	954.8911	958.7597
966.8124	969.3282	992.8559
1043.9091	1074.2166	1126.1545
1143.1105	1166.9833	1178.4415
1192.0183	1216.8068	1236.5320
1283.2710	1293.5284	1351.7454
1378.3222	1389.1206	1430.1706
1431.5184	1469.3722	1486.3917
1555.1522	1584.8304	1618.8469
1634.2323	1664.3623	3014.4097
3037.1196	3155.8991	3157.6508
3165.4471	3174.7872	3178.0459
3188.0059	3195.5734	3217.7099

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

End

Fragment H

Atom

Mass[amu] 1

ElectronicLevels[1/cm] 1

0 2

End

GroundEnergy[kcal/mol] -36.19

End

!-----h_c10h6_p3-----

Bimolecular p3

Fragment c10h6

RRHO

Geometry[angstrom] 23

C	3.3589805782	-0.1589532841	-0.0052741521
C	-0.8626124942	-0.4592216299	0.0061451685
C	2.7512244302	-1.4362419127	-0.0057558711
C	-1.6304316353	0.7002778521	0.0104255245
C	0.3504445096	2.0582620245	0.0073112859
C	-1.0208972146	1.9753841923	0.0110703316
C	2.58240266	0.9743296087	-0.0010636067
C	1.3828455855	-1.5556845697	-0.0020600345
C	1.1658232353	0.8928735063	0.0028576508
C	0.5497812064	-0.4047593755	0.0022898527
C	-3.0471181043	0.3231433831	0.013518318
C	-1.786615793	-1.65287093	0.0068930735
C	-3.1559300206	-1.0165005908	0.0115352725
H	4.4401442599	-0.0787740034	-0.00823888
H	3.372925776	-2.3247255603	-0.0090822067
H	0.8378607683	3.0277237362	0.0077226495
H	-1.6280620211	2.8741736402	0.0144845493
H	3.0467756867	1.9552584003	-0.0006703734
H	0.9246806356	-2.5385591873	-0.0024656456
H	-3.8673579721	1.0301984874	0.0178637838
H	-1.6405804813	-2.2929696258	-0.8725833972
H	-1.6357579267	-2.2952054346	0.8839587431
H	-4.0761106684	-1.5851637269	0.0138329637

Core RigidRotor

```

SymmetryFactor 1.0
End
Frequencies[1/cm] 63
111.6057          140.7443          235.7064
237.2840          257.3698          398.3460
432.9203          435.8184          465.2515
517.6631          520.4055          551.8391
616.8391          670.8841          681.8888
717.6433          751.4780          760.5919
787.6060          828.8756          839.7089
870.5955          872.9566          937.1401
954.7419          955.4339          959.8592
969.6851          982.2343          991.7663
1043.6091         1060.8926         1117.9424
1144.2864         1166.9366         1179.2631
1185.6203         1233.5150         1244.7639
1263.9305         1288.3090         1363.9889
1378.3244         1398.4726         1416.6215
1434.3888         1470.0882         1487.4172
1552.8699         1587.7715         1621.6410
1637.3459         1664.1362         3014.2828
3037.1636         3156.0941         3158.7295
3163.7980         3176.1937         3177.0078
3187.4191         3190.5460         3215.9190
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment          H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End
GroundEnergy[kcal/mol] -36.33
End
!-----h_c10h6_p4-----
Bimolecular      p4
Fragment          c10h6
RRHO
Geometry[angstrom] 23
C  3.7695852196 -0.0064018801 0.1624634079
C -0.3681027934 -0.8226648439 -0.1754219653
C  3.3187500647 -1.3444696048 0.0757045779
C -1.2899850887 0.2105062445 -0.2022003511
C  0.51585409 1.8271389281 -0.004209719
C -0.8220659745 1.5561515634 -0.1137952259
C  2.8687958828 1.0311253417 0.1375131586
C  1.9775783278 -1.6190602397 -0.0341907195
C  1.4774799929 0.7826568887 0.0249353278
C  1.0200273942 -0.5701457584 -0.0628983946
C -2.6885215071 -0.0499966899 -0.3160526462
C -3.8738171039 -0.2543236385 -0.412071668
C -5.3035998711 -0.5068617608 -0.5273154055

```

```

H   4.8310747361  0.1965152437  0.2488677317
H  -0.7141061282 -1.8479727961 -0.2418500721
H   4.0392322254 -2.154399737  0.0964489004
H   0.8579800055  2.8547663717  0.0622144114
H  -1.5472635443  2.3605226794 -0.1350036066
H   3.2126102001  2.0581942628  0.2039493882
H   1.6305100804 -2.6449192567 -0.1008133461
H  -5.7209994588 -0.8553331929  0.4225559236
H  -5.5092767819 -1.2719180664 -1.2819815849
H  -5.8417039676  0.4008889412 -0.8153441225
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  63
13.2466           62.5761           74.7243
164.4456          182.3529          269.4018
284.4434          345.5747          373.0123
393.0782          436.4623          485.1788
515.9132          552.1632          557.9209
616.2315          658.6678          661.8111
760.2520          779.5747          781.0217
833.6909          858.7340          874.8436
913.6325          952.6072          964.9148
979.7661          996.7664          1014.7086
1042.2834         1049.7956         1054.1792
1152.0061         1172.8489         1178.1938
1211.5509         1249.9931         1286.9966
1298.8516         1371.5645         1395.9116
1403.2038         1416.5169         1464.4389
1478.0379         1479.1806         1502.0790
1537.4508         1603.0487         1641.3785
1666.7591         2336.3606         3019.6932
3073.9064         3079.7539         3157.6695
3161.4205         3163.8674         3175.3187
3178.1638         3188.2924         3191.9414
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment           H
Atom
Mass[amu]  1
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol] -9.62
End
!-----h_c10h6_p5-----
Bimolecular  p5
Fragment      c10h6
RRHO
Geometry[angstrom]  23
C              3.674981    0.497930   -0.000270
C             -0.219804   -1.159771    0.000398

```

C	3.507073	-0.905745	-0.000471
C	-1.335316	-0.344858	0.000639
C	0.104371	1.613217	0.000265
C	-1.150805	1.068039	0.000508
C	2.577411	1.326248	-0.000042
C	2.247044	-1.454470	-0.000300
C	1.265061	0.792212	0.000092
C	1.093658	-0.627265	0.000071
C	-2.678275	-0.945911	0.000639
C	-4.953878	0.338200	-0.001024
C	-3.818184	-0.297671	-0.000173
H	4.674304	0.918331	-0.000291
H	-0.342425	-2.238727	0.000371
H	4.379634	-1.549380	-0.000766
H	0.228583	2.691348	0.000169
H	-2.024495	1.709749	0.000604
H	2.703431	2.404084	0.000102
H	2.118144	-2.531928	-0.000473
H	-2.716374	-2.033955	0.001034
H	-5.449819	0.614651	-0.927951
H	-5.451004	0.614896	0.925210

Core RigidRotor
SymmetryFactor 1.0
End

Frequencies[1/cm] 63

46.2339	103.8385	125.7138
182.5167	253.5967	276.1306
328.7230	379.4763	401.6511
411.5401	480.6687	497.2674
525.9436	594.2023	604.9617
644.7759	684.6387	761.7100
766.4329	782.3325	784.1895
836.0403	872.7358	881.4050
888.9360	896.1518	922.2063
963.8350	967.0643	983.3427
995.5075	1012.7378	1042.5921
1102.8136	1151.4380	1174.0129
1179.9562	1197.0911	1240.8038
1280.4937	1289.0527	1327.6220
1393.1879	1397.8004	1412.9141
1461.6268	1483.9705	1506.4370
1544.0494	1609.8810	1643.4084
1667.4288	2033.5041	3102.7160
3118.8576	3154.6031	3157.3764
3159.5801	3162.9618	3171.8426
3174.7675	3182.2671	3187.6613

ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1

```

0 2
End
GroundEnergy[kcal/mol] -7.24
End
!-----h_c10h6_p6-----
Bimolecular p6
Fragment c10h6
RRHO
Geometry[angstrom] 23
C -3.601815 0.383900 0.302093
C 0.331336 -1.086775 -0.247675
C -3.363878 -1.009966 0.307200
C 1.382170 -0.220264 -0.431775
C -0.134704 1.666895 -0.258174
C 1.134016 1.177774 -0.433294
C -2.561681 1.263041 0.118863
C -2.091489 -1.497572 0.129425
C -1.236971 0.792021 -0.067861
C -0.995906 -0.616759 -0.062344
C 2.794036 -0.741286 -0.658787
C 4.583078 0.196625 1.078480
C 3.776591 -0.228610 0.296433
H -4.610267 0.755805 0.444027
H 0.506299 -2.158545 -0.239833
H -4.192432 -1.694002 0.452640
H -0.311403 2.737565 -0.261235
H 1.966220 1.860584 -0.565497
H -2.741326 2.333194 0.115215
H -1.908480 -2.567183 0.133933
H 2.788502 -1.834732 -0.616378
H 3.120378 -0.476294 -1.672758
H 5.293819 0.569455 1.774398
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 63
21.6630 74.6359 142.6424
180.7269 243.9161 286.6814
331.4442 373.4920 402.0165
408.0951 485.4417 503.1293
526.7069 576.4951 635.5364
658.0474 667.8370 678.5675
737.5344 764.6428 781.4020
786.3882 832.1626 868.5120
878.8089 903.6712 946.9423
958.7772 965.8670 979.7131
985.0094 996.4644 1042.5726
1148.0008 1172.5342 1179.0625
1188.9602 1216.9373 1239.4898
1277.2317 1289.1479 1325.1916
1392.2986 1396.8940 1408.1882
1466.5377 1474.9665 1503.1218
1545.9904 1612.9193 1646.3300
1674.0852 2223.3362 3008.3643

```

```

3056.3908          3153.8497          3157.5197
3159.6598          3162.9819          3175.1434
3179.1100          3187.9599          3476.1676
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment          H
Atom
Mass[amu]    1
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol] -2.25
End
!-----ch3_c12h8_p7-----
Bimolecular    p7
Fragment          c12h8
RRHO
Geometry[angstrom]    20
C          3.236624    0.172310    0.00
C          -0.841043    -0.948009    0.00
C          2.881179    -1.197039    0.00
C          -1.833267    0.017271    0.00
C          -0.145939    1.764012    0.00
C          -1.464948    1.395382    0.00
C          2.263177    1.142223    0.00
C          1.559667    -1.569997    0.00
C          0.889207    0.791807    0.00
C          0.528778    -0.592960    0.00
C          -4.379851    -0.646290    0.00
C          -3.212685    -0.349389    0.00
H          4.283729    0.453226    0.00
H          -1.115580    -1.996676    0.00
H          3.659088    -1.952091    0.00
H          0.123389    2.814985    0.00
H          -2.247821    2.143774    0.00
H          2.535296    2.192583    0.00
H          1.284563    -2.619418    0.00
H          -5.408056    -0.912317    0.00
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]    54
  87.9880          133.1440          181.2468
 218.2255          352.1262          383.4870
 401.5587          429.5214          484.5990
 516.8219          552.4624          559.6133
 629.3281          632.9808          663.6020
 685.9742          691.9308          760.9473
 779.8212          780.6114          834.1419
 876.3712          899.3207          915.5693
 966.6536          971.2117          980.9216
 999.0278          1041.9866         1145.5746

```

1172.8883	1177.9761	1185.7844
1233.3388	1277.2123	1289.8811
1371.2885	1395.2179	1403.3569
1465.1985	1499.2505	1537.6500
1603.6481	1640.9279	1667.3435
2205.9189	3158.8057	3163.5226
3165.7769	3176.3887	3179.5926
3189.0981	3194.5312	3477.6126
ZeroEnergy[kcal/mol]	0.0	
ElectronicLevels[1/cm]	1	
0 1		
End		
Fragment	ch3	
RRHO		
Geometry[angstrom]	4	
C	0.000000	0.0000 0.000
H	-0.9358075	-0.5401365 0.000
H	0.9358075	-0.5401365 0.000
H	0.0000	1.080495 0.000
Core RigidRotor		
SymmetryFactor	6.0	
End		
Frequencies[1/cm]	6	
505.5776	1403.1131	1403.3797
3103.7859	3282.6714	3283.0465
ZeroEnergy[kcal/mol]	0.0	
ElectronicLevels[1/cm]	1	
0 1		
End		
GroundEnergy[kcal/mol]	-15.3	
End		
Bimolecular	r2	
Fragment	c11h9	
RRHO		
Geometry[angstrom]	20	
C	-0.5705822553	0.6970066241 0.
C	-0.4125226152	-0.7279899448 0.
C	0.9128551718	-1.2656999057 0.
C	2.0070353258	-0.45703719 0.
C	1.8810831094	0.9815480713 0.
C	0.5756113348	1.5170080955 0.
C	-1.8873089913	1.2338626675 0.
C	-2.9869144214	0.4080004165 0.
C	-2.8256210067	-0.9945522511 0.
C	-1.5606899212	-1.5465760108 0.
C	3.0145460064	1.800349873 0.
H	1.0320747119	-2.344511011 0.
H	3.0033769984	-0.8859987303 0.
H	0.4487943654	2.5950843601 0.
H	-2.0109036329	2.3118408917 0.
H	-3.9845376282	0.8326752473 0.
H	-3.699230863	-1.6362778549 0.
H	-1.4354126097	-2.6245435177 0.
H	2.9251822947	2.8794625965 0.

```

H 4.0110346262 1.376988573 0.
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 54
111.7166 177.5685 271.5958
276.9936 390.2742 411.8802
463.0161 466.9013 515.5862
522.5963 525.1087 633.3787
643.2431 730.2838 733.9902
757.7004 772.0531 772.7165
822.3097 853.6877 883.2000
902.3852 952.6616 956.1898
978.7958 989.8120 1006.1465
1043.4045 1142.9014 1166.6632
1174.4793 1207.9210 1240.5356
1289.3027 1302.3650 1373.4214
1378.6831 1413.2425 1462.0308
1477.8488 1495.5665 1530.2794
1572.1531 1623.5710 1639.6542
3145.1334 3155.2985 3157.2591
3159.5081 3162.7597 3175.3738
3175.9804 3188.7682 3241.2206
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
Fragment c2h2
RRHO
Geometry[angstrom] 4
C 0.0 0.0 0.5990703976
C 0.0 0.0 -0.5990703976
H 0.0 0.0 1.6619081422
H 0.0 0.0 -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 7
642.0679 642.0679 772.6955
772.6955 2069.5209 3420.9273
3523.7963
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End
GroundEnergy[kcal/mol] -21.26
End
!-----bar_ts0-1-----
Barrier ts0-1 i1 p0p
RRHO
Geometry[angstrom] 24
C 3.76994 0.01624 0.41853
C -0.28693 -0.8287 -0.49631
C 3.3644 -1.31764 0.18061

```

```

C -1.14991  0.2194  -0.55546
C  0.52793  1.82404 -0.02216
C -0.79045  1.55162 -0.31983
C  2.85519  1.03897  0.35397
C  2.05341 -1.60222 -0.11632
C  1.49237  0.78284  0.04936
C  1.08338 -0.56924 -0.19119
H  4.80736  0.22767  0.65208
H -0.60794 -1.85086 -0.67459
H  4.09504 -2.1172  0.23374
H  0.84704  2.84558  0.16309
H -1.52524  2.3479  -0.37143
H  3.16487  2.06311  0.5357
H  1.7413  -2.62538 -0.29887
C -3.41112 -0.22226 -1.06748
C -4.62584 -0.43934  1.2916
C -4.0514  -0.33822 -0.04039
H -3.17228 -0.18452 -2.10395
H -5.38494  0.33146  1.45299
H -3.85218 -0.31702  2.05762
H -5.09881 -1.41373  1.44402

```

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 290.3817

WellDepth[kcal/mol] 44.44

WellDepth[kcal/mol] 2.31

End

```

Rotor      Hindered      ! 63 cm^-1    CH3
Group                22 23 24
Axis                19 20
Symmetry           3
Potential[kcal/mol] 4
0 0.103333259 0.223148058 0.123061533

```

End

```

Rotor      Hindered      ! 10 cm^-1
Group                19 20 21 22 23 24
Axis                4 18
Symmetry           1
Potential[kcal/mol] 8
0.01195343  0.2797124  0.631229467  0.187441507  0
0.321374644  0.77244548  0.210585943

```

End

Frequencies[1/cm] 63

```

                28.7912
                79.0441                97.7220
176.6484                203.3793                316.3168
348.4021                371.6784                389.1046
477.7321                485.4667                496.9637
515.3030                619.9604                627.8965
657.2454                691.5528                746.3446
768.6028                768.8787                799.7490
813.3370                853.1219                892.6143

```

931.4543	939.8204	956.9292
969.1551	993.7361	1037.8501
1040.2588	1046.6855	1057.5648
1144.3211	1161.4569	1172.6711
1210.1482	1252.8749	1277.2623
1344.1359	1385.5919	1393.0761
1411.4232	1459.0165	1467.3266
1474.0957	1475.1044	1530.7447
1595.4413	1614.3671	1657.0523
2118.1022	3015.3446	3070.3195
3083.2119	3148.1046	3149.9389
3155.9823	3161.1578	3168.8979
3173.6564	3186.4070	3434.7944

ZeroEnergy[kcal/mol] 2.31

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts1-2-----

Barrier ts1-2 i1 i2

RRHO

Geometry[angstrom] 24

C	-3.6991765103	0.5715589621	-0.0082453105
C	0.1412514365	-1.2106173568	0.0327111227
C	-3.5763759946	-0.8357747581	0.0464690616
C	1.2827136024	-0.4344546731	-0.0067634796
C	-0.0942592816	1.5692186668	-0.0754008448
C	1.141906261	0.9817961058	-0.061676544
C	-2.575384954	1.3628969559	-0.0481742656
C	-2.3345984626	-1.4245449156	0.0602129842
C	-1.2807581212	0.7870198245	-0.035349062
C	-1.1546949389	-0.6363933284	0.0199760934
C	2.6168229722	-1.0781892239	0.0083981313
C	3.7826247139	-0.4882426904	-0.0238812471
H	-4.6844319796	1.0239303845	-0.0185614809
H	0.230468771	-2.2923208175	0.0747818701
H	-4.4691669214	-1.4503635938	0.0776323695
H	-0.1838343731	2.6501202707	-0.1174460867
H	2.0367119703	1.5938408085	-0.0927604265
H	-2.6666824861	2.4434966891	-0.0901971912
H	-2.2404081653	-2.5048094314	0.102203717
H	2.5732668394	-2.1752784008	0.0520625286
C	5.0414404221	0.2282552977	-0.0618788086
H	5.1407854075	0.9053855994	0.7958748657
H	5.1270558111	0.8357976334	-0.9716494972
H	5.914361981	-0.4431220088	-0.0422314993

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 229.9263

WellDepth[kcal/mol] 5.28

WellDepth[kcal/mol] 3.21

End

```

Frequencies[1/cm] 65
32.4267          45.3432
123.3654         129.9946         182.4128
276.3873         298.6003         324.7371
387.8631         403.0819         484.6640
518.9512         524.5410         555.7427
633.5105         639.9821         720.2631
750.9756         780.1446         780.1914
804.5984         835.5812         855.5777
876.7152         914.5850         939.2407
962.3259         974.9320         977.5220
994.1034         996.9307         1025.9402
1042.5261        1142.9842        1171.5683
1175.9770        1188.0821        1234.6328
1272.1696        1281.4879        1289.9437
1387.6760        1394.0300        1405.0048
1410.2414        1450.2695        1469.4698
1471.9188        1498.1351        1542.8688
1608.7994        1640.5962        1665.5352
1808.6714        2945.0512        2974.1684
3003.2755        3037.8531        3151.1478
3155.2547        3156.6042        3161.4629
3173.7696        3175.1765        3186.8189

```

ZeroEnergy[kcal/mol] -36.84

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts2-3-----

Barrier ts2-3 i2 i3

RRHO

Geometry[angstrom] 24

```

C   -3.7629695558  0.6187902644  0.0901283413
C    0.0613021541 -1.1672522323 -0.2465481121
C   -3.6387474128 -0.7844949302  0.0842648782
C    1.2475395941 -0.369187977  -0.306068572
C   -0.1637565081  1.6365150515 -0.2621663749
C    1.0661523857  1.0740636388 -0.3582126774
C   -2.631566612  1.4104581951 -0.0176304622
C   -2.3994513246 -1.376313116 -0.0238572519
C   -1.3531654281  0.8393343516 -0.1307505668
C   -1.2178009487 -0.5909423866 -0.1307184082
H   -4.7422058805  1.0755312048  0.1754992386
H    0.1580801056 -2.2477405926 -0.2657275746
H   -4.5267343771 -1.4020330856  0.1651521412
H   -0.2702168308  2.7166411924 -0.2914041657
H    1.9509012625  1.6933909769 -0.4601152407
H   -2.7230668305  2.492224576 -0.0182171189
H   -2.3082859116 -2.4577130919 -0.027692139
C    2.5879104849 -0.985082728 -0.5781508719
C    2.639688458 -0.9098194274  0.7033827115
C    3.162197569 -1.0948416378  2.0598288668
H    3.1218415515 -1.3280317191 -1.458820599
H    2.4790890913 -1.7095863024  2.6537527585

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H 3.2664767087 -0.1342502979 2.5730375167
H 4.1433452553 -1.5875149266 2.0473526825
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 495.1615
WellDepth[kcal/mol] 25.79
WellDepth[kcal/mol] 3.5
End
Frequencies[1/cm] 65
62.2443 91.5754
118.2179 161.5623 194.5210
270.8300 277.1322 300.4171
397.2849 407.0803 439.4227
464.1436 506.0859 520.2349
615.7716 626.1579 692.0752
735.6551 738.5551 756.9831
767.0231 800.1802 808.1683
869.9224 875.5091 889.1462
941.2330 943.5352 975.3791
980.5673 1030.5817 1043.5005
1052.5966 1084.5417 1136.5193
1162.6746 1168.6093 1178.3825
1223.2672 1261.2727 1287.4782
1318.9034 1359.8637 1400.3080
1409.2167 1443.8233 1464.7616
1466.5469 1471.3205 1512.4906
1562.4004 1622.8429 1627.6005
1871.8071 2990.3910 3058.9271
3079.1189 3138.1998 3150.4539
3152.9858 3156.7598 3163.0449
3171.3112 3174.3565 3185.9312
ZeroEnergy[kcal/mol] -14.26
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts3-4-----
Barrier ts3-4 i3 i4
RRHO
Geometry[angstrom] 24
C -3.588856 0.122578 0.121594
C 0.5109 -0.902898 -0.116362
C -3.205125 -1.230563 0.033565
C 1.522477 0.104935 -0.158968
C -0.230558 1.802808 0.074402
C 1.084787 1.484662 -0.015039
C -2.622571 1.113757 0.131701
C -1.874153 -1.575346 -0.045863
C -1.255581 0.796286 0.05372
C -0.857324 -0.580313 -0.041192
C 2.864984 -0.137972 -1.347655
C 2.980895 -0.250293 -0.071725

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```

C   3.901439 -0.570084  1.053345
H  -4.638878  0.384176  0.183566
H   0.808722 -1.944424 -0.177585
H  -3.964958 -2.00443  0.028266
H  -0.532204  2.841617  0.166991
H   1.843119  2.260113 -0.003478
H  -2.914288  2.156993  0.202358
H  -1.582434 -2.618257 -0.115334
H   3.200947 -0.18694 -2.368721
H   3.523613 -1.425401  1.621847
H   3.965558  0.274568  1.74634
H   4.90293 -0.803355  0.6866
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  570.0222
WellDepth[kcal/mol]  3.44
WellDepth[kcal/mol]  23.0
End
Frequencies[1/cm]  65
68.3130          90.9103
135.7836         175.1180          189.4649
229.6581         282.2002          360.5092
393.4619         437.0928          470.7090
483.3880         509.2137          525.1297
611.6183         625.9095          646.3562
673.2161         675.6279          742.8164
756.0611         766.8413          806.8120
810.8880         856.2090          871.9601
912.5533         942.3865          946.0790
976.6454         982.3229         1041.4592
1043.5102        1048.4261         1143.1021
1165.7297        1170.0055         1198.5001
1231.4236        1264.7386         1288.2376
1322.7751        1362.4314         1399.0796
1408.7208        1444.5854         1463.7789
1474.9741        1481.4892         1513.9820
1562.4192        1623.3206         1626.8263
1825.8167        3024.1267         3078.2003
3108.8651        3151.9224         3154.3890
3158.1467        3163.5234         3172.4994
3175.6066        3186.7827         3277.6845
ZeroEnergy[kcal/mol]  -14.32
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts4-8-----
Barrier      ts4-8  i4  i8
RRHO
Geometry[angstrom]  24
C   -3.5991862122  0.0838823616 -0.0039122946
C   0.538119891 -0.8206544558  0.0259658928

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C   -3.1723207626  -1.2633334935  0.013741405
C   1.4866326755  0.1832019129  0.0187110137
C   -0.2971992837  1.8434256057  -0.0089367875
C   1.0351436248  1.5359567998  0.0008662729
C   -2.6755906493  1.1028045443  -0.0114376403
C   -1.8314229446  -1.5660343577  0.0235304556
C   -1.2869106653  0.8228115271  -0.0016979724
C   -0.8533876674  -0.5379379516  0.0161543919
C   3.8602772288  0.8290852736  0.0214032237
C   2.9516612048  -0.1147731752  0.0290153244
C   3.3778196213  -1.5803221062  0.0490953584
H   -4.6594589387  0.3102848513  -0.0115032775
H   0.8384409503  -1.861364111  0.0394844995
H   -3.9090002751  -2.0588508247  0.0195433399
H   -0.6164677883  2.880639283  -0.0224693057
H   1.7758669965  2.3275304058  -0.0048431655
H   -3.000916506  2.1380108047  -0.0249923855
H   -1.5032851361  -2.60040362  0.0370921427
H   4.5929647932  1.6013873145  0.015165185
H   2.9972475911  -2.1083938116  -0.8307764769
H   2.9888185212  -2.0865931635  0.9380497031
H   4.4640377308  -1.6606256136  0.0552370973
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  695.1996
WellDepth[kcal/mol]  3.39
WellDepth[kcal/mol]  4.32
End
Frequencies[1/cm]  65
35.6166          88.8854
169.7470        181.8903        228.3699
242.1694        323.1540        351.1277
397.1980        454.1500        462.7956
485.6657        520.7131        527.3926
559.1763        599.6794        631.8000
664.2612        677.1194        759.8259
782.1021        784.0398        833.9823
872.3881        879.8362        906.8406
952.8431        963.4863        978.1540
982.5105        995.5790        1033.5354
1042.9559       1076.0430       1147.9570
1173.7809       1178.6307       1200.6489
1235.0106       1278.8742       1292.3319
1372.8444       1392.9063       1397.2116
1411.1815       1466.7757       1486.0202
1488.8302       1498.7849       1539.8911
1608.4020       1640.8842       1642.7027
1667.4036       3022.4354       3077.3784
3125.4385       3155.5317       3157.3057
3160.9501       3173.9631       3178.6169
3183.7206       3187.4239       3433.6649
ZeroEnergy[kcal/mol]  -33.93

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ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts8-5-----
Barrier      ts8-5  i8  i5
RRHO
Geometry[angstrom]  24
C   -3.6229139835  0.1254589992 -0.1487551243
C    0.492534337  -0.8708180601 -0.1514305063
C   -3.2260497326 -1.2325584397 -0.147919074
C    1.451112727  0.118177294 -0.1575335261
C   -0.2880730604  1.81363935 -0.156478315
C    1.0429805797  1.478673951 -0.1586966369
C   -2.6784136739  1.1227665965 -0.1504211046
C   -1.8935617418 -1.5658281249 -0.1483257059
C   -1.2935399736  0.812801459 -0.1506887401
C   -0.8917634241 -0.5597901186 -0.1488017975
H   -4.6780050917  0.3750496036 -0.1486756222
H    0.7938141988 -1.9135074658 -0.1594900417
H   -3.9809711277 -2.0108113645 -0.1474588602
H   -0.5874406141  2.8567209169 -0.1642129859
H    1.8013978412  2.253377243 -0.1727249466
H   -2.9806231679  2.1650182298 -0.152171675
H   -1.5883234782 -2.6071290608 -0.149033932
C    3.5981658021 -0.3195703531 -1.2521282798
C    2.9149108669 -0.222765308 -0.1369733865
C    3.5372039084 -0.4305327376  1.2361094387
H    4.6135848062 -0.5348088167 -1.5530933383
H    3.0380186322 -1.2550941071  1.7552476449
H    3.4052238069  0.4660385189  1.8505151336
H    4.6031265631 -0.6539422049  1.1662243815
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  51.6384
WellDepth[kcal/mol]  2.93
WellDepth[kcal/mol]  1.8
End
Frequencies[1/cm]  65
78.2882          146.0952
177.5632         191.7488          197.8492
281.1523         359.1626          367.5052
416.7248         455.3583          486.7135
521.1060         552.4550          566.0342
628.0350         667.3857          676.6094
689.7832         759.6893          780.1439
785.3934         833.4025          847.7952
867.7927         875.5322          913.6508
956.2948         964.4081          977.9071
995.5809         996.9793          1030.1313
1041.4268        1080.7433          1152.6069
1170.6366        1178.3973          1207.4966

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1239.8122	1278.2677	1289.4884
1371.8731	1392.8005	1395.2862
1399.7809	1463.8124	1477.8621
1481.0579	1499.5389	1539.2534
1606.2294	1640.5164	1669.2044
1681.0619	3017.2047	3071.9064
3108.4073	3156.2750	3158.9152
3160.7786	3163.5322	3174.5731
3180.9691	3187.4198	3226.3700

ZeroEnergy[kcal/mol] -35.32

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts5-6-----

Barrier ts5-6 i5 i6

RRHO

Geometry[angstrom] 24

C	-3.5868007287	0.1656043728	0.0328652642
C	0.4962542766	-0.8477742354	0.0885484196
C	-3.2180560395	-1.199705721	0.1329780007
C	1.4812807335	0.1100526309	0.0122036154
C	-0.2284410914	1.7997883558	-0.1054918526
C	1.1114833455	1.4674920496	-0.0872638534
C	-2.6256160055	1.1419242913	-0.0446899109
C	-1.8966791662	-1.5645846663	0.15377219
C	-1.2435331204	0.8132022824	-0.0268967231
C	-0.8728317639	-0.579377391	0.0752319874
H	-4.6368347465	0.4350405238	0.0178748325
H	-3.9909944228	-1.9576770002	0.1933243775
H	-0.5263919417	2.8402826501	-0.1816778522
H	1.8663983841	2.2443435952	-0.1489419957
H	-2.9108135279	2.186400228	-0.1212499223
H	-1.6094241885	-2.6071199718	0.2301857504
H	1.3450155156	-1.9361773992	0.1654995985
C	2.7271350607	-1.842069564	0.151555867
C	2.8335815299	-0.5184033741	0.0523264933
C	4.0997433089	0.2848571204	-0.013886646
H	3.4452440758	-2.6486044844	0.2080917088
H	4.1424660291	0.8666267681	-0.9411254313
H	4.9818237331	-0.355336955	0.0290392019
H	4.1516227501	0.997099894	0.8168198804

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1985.2121

WellDepth[kcal/mol] 25.29

WellDepth[kcal/mol] 24.62

End

Frequencies[1/cm] 65

83.0835	114.5526	
172.0516	179.5260	192.1321
232.2582	297.5574	397.9343

412.8113	453.0482	496.1916
503.6096	521.5282	563.0390
590.0119	647.6322	653.9617
668.4693	681.1581	758.0986
772.6170	794.1662	827.4686
873.1960	883.8911	941.0324
956.3463	968.5779	971.3883
996.0425	1012.6210	1028.2150
1035.7240	1052.2204	1141.3626
1150.4893	1166.2496	1179.4708
1235.2980	1262.1929	1315.1887
1364.0168	1373.0521	1381.0400
1408.6919	1459.2558	1480.5364
1482.5561	1485.5146	1540.0407
1586.8152	1617.4600	1647.4988
1664.4650	1748.3887	3016.1140
3063.2640	3111.2313	3155.2683
3158.4119	3166.4028	3175.3351
3178.4144	3189.1271	3217.9214

ZeroEnergy[kcal/mol] -11.83

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts6-7-----

Barrier ts6-7 i6 i7

RRHO

Geometry[angstrom] 24

```

C   -3.8818416507  0.5179733922  0.0923410731
C    0.0741927685 -0.9302104366  0.1943046931
C   -3.6585137401 -0.8453630549  0.3919063271
C    1.151769329  -0.1158667559 -0.0550590859
C   -0.3707225263  1.7239440514 -0.3883020509
C    0.917571213  1.2531200518 -0.3552836936
C   -2.822473284  1.3574020294 -0.1617008093
C   -2.3803696401 -1.3490019296  0.4330485359
C   -1.4891219579  0.8787371969 -0.1294961783
C   -1.266413474  -0.5094202077  0.1757941663
H   -4.8959384498  0.9002799798  0.063662942
H   -4.5038238843 -1.4947681526  0.5899382653
H   -0.5601300746  2.7677725647 -0.6165947774
H    1.7474658767  1.9217874169 -0.5568547851
H   -2.9962719413  2.4038156684 -0.3914889555
H   -2.2036174823 -2.3937801107  0.6622920259
C    3.6537604375 -0.3501508193 -0.1466545171
C    2.4288790482 -0.8501674395  0.0390090904
C    2.1182552688 -2.2868225905  0.386210609
H    3.8112829623  0.6937992234 -0.3949797362
H    4.5391913843 -0.9684291323 -0.0564018362
H    0.7927644011 -2.1048798059  0.421767446
H    2.4250169699 -2.6211281404  1.376749166
H    2.3219994461 -3.0254069989 -0.3883959146

```

Core RigidRotor

SymmetryFactor 0.5

```

End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1823.649
WellDepth[kcal/mol]  15.79
WellDepth[kcal/mol]  39.94
End
Frequencies[1/cm]  65
47.7513          87.7916
173.7757         192.6830         230.9306
325.2686         348.6520         410.0579
418.5192         452.1716         500.9919
519.5031         521.4468         563.9605
588.0975         639.3369         652.3654
681.8384         728.0673         765.8900
789.1911         797.9509         831.1932
879.0055         894.9549         901.4062
929.8091         961.4452         962.0070
972.8280         997.2662        1033.2269
1040.9221        1041.7961        1132.1362
1147.4397        1170.0022        1179.7117
1234.5315        1238.8738        1263.3445
1306.4911        1362.7349        1365.9334
1397.0405        1426.3130        1448.4897
1462.3296        1486.0932        1537.8860
1590.1835        1628.7694        1652.8016
1669.4116        1725.9372        3077.6711
3135.6816        3152.3194        3156.3528
3159.4385        3167.1740        3177.3461
3178.9267        3189.6819        3216.1468
ZeroEnergy[kcal/mol]  -20.66
ElectronicLevels[1/cm]  1
0 2
End
!-----
!-----bar_ts7-13-----
Barrier      ts7-13  i7  i13
RRHO
Geometry[angstrom]  24
C   3.496209878 -0.1220731838 0.2180543474
C  -0.5732033246 0.819472081 -0.451355826
C   3.1143552293 1.2088839637 -0.0409411006
C  -1.5893702111 -0.1932854716 -0.368837583
C   0.1674718034 -1.8545888379 0.0326831837
C  -1.14041576 -1.5677191837 -0.1634028552
C   2.5369156533 -1.1213979568 0.2482604109
C   1.7920545247 1.5261034674 -0.2599896875
C   1.1806194349 -0.8326065356 0.0295641358
C   0.7821098206 0.5237919145 -0.2264656626
H   4.5390546653 -0.3625249751 0.3892399904
H  -0.8685431355 1.838499976 -0.6767660329
H   3.8681409114 1.9881173278 -0.0675560166
H   0.4769941627 -2.8833864957 0.187842106
H  -1.8860439914 -2.3552210278 -0.1700134991
H   2.8289967749 -2.1489539283 0.4410674462

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H  1.5012659596  2.5525149392 -0.4583282594
C  -3.7001633683  0.1627687834 -1.8896956486
C  -2.9762190131  0.0809796308 -0.7877320508
C  -3.0206917399  0.2259665457  0.6503183481
H  -3.2596673201  -0.0194816072 -2.8635047524
H  -4.7547550255  0.4143518004 -1.8493454461
H  -3.3401620241  -0.5953684095  1.2807291615
H  -2.9452599045  1.2054871832  1.1070932908
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  481.4375
WellDepth[kcal/mol]  36.15
WellDepth[kcal/mol]  1.25
End
Frequencies[1/cm]  65
70.6040          81.7781
165.3074        199.3003          216.1263
292.7356        358.3916          384.9391
432.5199        435.8733          471.9568
506.7616        517.7512          609.0075
623.5365        668.2990          680.3744
719.9347        735.9969          751.3387
764.7324        789.0169          804.2074
836.4330        869.8436          887.4860
930.3889        936.4967          945.8746
960.9091        976.0436          982.2137
1023.0293       1043.8504         1065.8244
1144.2980       1167.6400         1169.9547
1187.4746       1219.6871         1261.6100
1290.3120       1325.5805         1358.7842
1409.8013       1422.7320         1441.9452
1457.9992       1467.0189         1511.3242
1561.3221       1622.1047         1631.6396
1808.6025       3124.1581         3129.3008
3153.4607       3155.6758         3158.9932
3167.0223       3173.2533         3177.2957
3187.4416       3215.9356         3224.7769
ZeroEnergy[kcal/mol]  -24.45
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts13-14-----
Barrier      ts13-14  i13  i14
RRHO
Geometry[angstrom]  24
C  3.4805307629 -0.1527829224 -0.1861075741
C  -0.6315102777  0.8184780489  0.0933407319
C  3.0692772748  1.1949528733 -0.2307313119
C  -1.6107947538 -0.2027369024  0.1792064448
C  0.1689594007 -1.8732369969  0.2109416319
C  -1.152893435 -1.5711252737  0.2853278084

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C  2.5383477977 -1.1554857783 -0.0484209388
C  1.7347082737 1.5219682508 -0.1426634622
C  1.1665061997 -0.8560356645 0.0446072353
C  0.7407653961 0.5138233795 -0.0084559145
C  -3.3416272281 -0.0484791572 -2.298364245
C  -2.9982652784 -0.04662194 -1.0387060602
C  -3.0829969278 0.1274810344 0.3836803633
H  4.5335916481 -0.3995628148 -0.2564625067
H  -0.9461301792 1.8567989636 0.0750719871
H  3.8114378901 1.9787740558 -0.335969267
H  0.4927970828 -2.9063217581 0.2877933244
H  -1.890592686 -2.356776972 0.4104940596
H  2.8505152402 -2.1943804762 -0.0078603588
H  1.4225593593 2.5606619345 -0.1789643151
H  -2.6373521891 -0.3004198448 -3.0882558684
H  -4.3568615897 0.2007112584 -2.619098669
H  -3.6465657918 -0.6237365714 0.9395597868
H  -3.2862999894 1.1340782735 0.7547191179
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 552.2467
WellDepth[kcal/mol] 9.21
WellDepth[kcal/mol] 20.04
End
Frequencies[1/cm] 65
63.4556 72.2755
154.3139 183.2280 246.7529
265.8908 315.1035 391.7663
401.3315 424.1417 464.1634
500.8942 503.9604 521.3806
613.4106 627.9594 689.1816
739.7619 755.0382 768.6371
802.6995 806.8571 867.4681
872.1982 908.5553 921.7956
943.1635 946.2164 948.2678
970.4691 981.6406 1012.8384
1043.6707 1083.9274 1132.4137
1166.5901 1171.7804 1174.1159
1182.9455 1225.3112 1266.6996
1288.9568 1365.3991 1370.4587
1413.5830 1431.9182 1455.5328
1456.5815 1473.0919 1520.9153
1567.3872 1625.9140 1630.9200
1811.6093 3036.3845 3041.2117
3104.6345 3131.5910 3152.9021
3154.6817 3157.6731 3161.2967
3172.1744 3174.0049 3186.5421
ZeroEnergy[kcal/mol] -16.49
ElectronicLevels[1/cm] 1
0 2
End
!-----

```

```

!-----bar_ts14-15-----
Barrier      ts14-15  i14  i15
RRHO
Geometry[angstrom]  24
C   -3.6381931796  0.5687237009  0.438517266
C    0.1086092049 -1.2963855932 -0.2580781774
C   -3.4897495493 -0.8232137723  0.6383797838
C    1.1758806348 -0.541035156  -0.6785407351
C   -0.1821778085  1.4942891566 -0.6606334797
C    0.9947235226  0.8437696795 -0.8682791983
C   -2.5711305541  1.3248510116  0.0179777706
C   -2.2781904782 -1.430313433  0.413820573
C   -1.3055008572  0.7303245679 -0.2234488197
C   -1.1526135048 -0.6820794744 -0.021262363
H   -4.5992462097  1.0371571451  0.6189135446
H    0.2064613301 -2.3670039374 -0.099916244
H   -4.3384995487 -1.4105221848  0.9704436025
H   -0.2926050192  2.5630899782 -0.8150634318
H    2.2830883593  1.1325774002 -1.2683276063
H   -2.6824793217  2.3931825947 -0.1361212454
H   -2.1649023472 -2.4985935589  0.5673835323
C    2.5957591964 -0.9871643407 -0.9875072348
C    4.5307710461  0.5799157753 -1.783919393
C    3.3099192901  0.2734267616 -1.3991753297
H    3.0719098176 -1.4451841582 -0.1125049994
H    2.6160803878 -1.7345750636 -1.7894390802
H    5.3157620643 -0.1730881796 -1.8673473504
H    4.8128075268  1.5974880821 -2.0361883757
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1834.8619
WellDepth[kcal/mol]  24.36
WellDepth[kcal/mol]  19.84
End
Frequencies[1/cm]  65
43.4119          113.4332
173.9459         175.4407         258.3364
264.8237         312.4579         373.2318
391.9182         432.6302         480.7253
509.9273         557.7966         562.8356
590.0260         643.6265         648.3027
751.9746         754.8638         776.3413
778.0881         854.5739         871.1259
885.2161         902.1320         909.4661
912.1373         955.0632         956.0757
966.7788         994.4498         1042.4529
1067.0546        1089.7318        1143.1655
1168.7106        1171.6662        1174.9726
1217.6649        1243.0028        1257.6968
1277.2043        1348.2516        1388.2974
1402.1123        1424.6846        1445.3244
1461.9967        1476.0287        1533.8072

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1609.1104          1631.9751          1658.1793
1726.1091          1735.4890          3012.2901
3039.3973          3074.8563          3146.4066
3156.3643          3157.6699          3162.2286
3169.0387          3174.4428          3187.1480
ZeroEnergy[kcal/mol] -12.17
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts14-16-----
Barrier      ts14-16  i14  i16
RRHO
Geometry[angstrom]  24
C   -3.6459303061  0.3230051641  0.1580253701
C    0.3754595695 -0.9238724811 -0.087141799
C   -3.3514322537 -1.05987104  0.1904304491
C    1.401513926  -0.0247031358 -0.1971672571
C   -0.2089165568  1.7683341399 -0.1494275888
C    1.1013245341  1.3585911173 -0.2291765041
C   -2.634125522  1.246392728  0.0481034817
C   -2.051229674 -1.4975717583  0.1125113166
C   -1.2783993394  0.8368775049 -0.034972831
C   -0.9838222409 -0.5705900573 -0.0016134867
H   -4.6770442965  0.6521617996  0.2205194984
H    1.1355589518 -2.0763165895 -0.0977127075
H   -4.1603596966 -1.7765889647  0.2774726712
H   -0.4485398853  2.826419091 -0.1731780575
H    1.898583925  2.0903439909 -0.3159574306
H   -2.8610115827  2.3075144725  0.0233028168
H   -1.8208692868 -2.5566997036  0.1369804433
C    2.7694145679 -0.6778641634 -0.2716356019
C    3.1927995221 -3.2566515417 -0.2017457813
C    2.4760760041 -2.1529356478 -0.1925955825
H    3.2891449887 -0.4225630412 -1.2033698168
H    3.4174687349 -0.3540068633  0.5521164173
H    4.2806245565 -3.2366277474 -0.2819046249
H    2.7346453601 -4.2383002731 -0.1299433947
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1836.7489
WellDepth[kcal/mol]  23.83
WellDepth[kcal/mol]  18.79
End
Frequencies[1/cm]  65
51.7861          111.7265
157.2918          169.1925          250.8709
262.2797          313.8908          387.6156
412.2045          471.5348          495.4771
509.5303          514.9701          554.1863
563.4579          641.5179          651.7169
736.5858          753.1768          778.7085

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797.7136	820.7294	877.0657
895.1438	910.7621	936.1128
950.7713	962.5021	972.3043
973.2643	996.2412	1040.5871
1040.7551	1095.4464	1140.9118
1164.1746	1167.6574	1172.8969
1202.8400	1234.6950	1259.1305
1292.4016	1365.0604	1371.5734
1390.0518	1424.4849	1458.5661
1463.3997	1489.9967	1538.1530
1589.6900	1633.7118	1661.5994
1726.4216	1740.0278	3006.4598
3031.8991	3075.0358	3152.3173
3156.4389	3166.1261	3168.6207
3171.7061	3178.1978	3188.9897

ZeroEnergy[kcal/mol] -12.7

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts15-17-----

Barrier ts15-17 i15 i17

RRHO

Geometry[angstrom] 24

C	-0.1009863622	-0.6413943597	0.0669605441
C	-1.5129241897	-1.2262975441	0.1267092102
C	-2.4155360612	-0.1221574557	-0.3574847198
C	-2.2634148373	1.106196934	0.2133992338
C	-0.0087189753	0.7610705448	0.0066957474
C	1.1526743152	1.4603441893	-0.05428818
C	2.3808112705	0.7291264758	-0.0653410143
C	2.3327539715	-0.7020911808	-0.0041662042
C	1.0729504015	-1.3597941914	0.0624784523
H	-1.597819414	-2.130975847	-0.4792668577
H	-1.7474871924	-1.5108562502	1.1611680519
H	-2.8890653677	-0.2191664988	-1.3289162558
H	-1.9712464	1.2105556944	1.2527646311
H	-2.6893116855	1.9938916416	-0.2421935133
H	1.1796229439	2.5450874774	-0.0982697091
H	1.0550571205	-2.445973121	0.1059018237
C	4.8071527991	0.6405354966	-0.1445388556
C	4.7625885319	-0.7711624461	-0.0837349118
C	3.643276487	1.371444268	-0.1363225644
C	3.5552173234	-1.4235760108	-0.0160450132
H	5.7654486779	1.1451482157	-0.1978387542
H	5.6870300693	-1.3376775139	-0.0910316061
H	3.6753796694	2.4551251874	-0.1832530562
H	3.5208389041	-2.5073267054	0.0297765213

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 417.0066

WellDepth[kcal/mol] 10.83

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WellDepth[kcal/mol]  44.17
End
Frequencies[1/cm]   65
69.9086             114.4662
191.6696           233.6131           254.5551
297.7749           393.8645           397.4929
421.2474           479.6463           489.8505
524.6141           555.5788           623.1846
635.0302           681.5692           723.2970
753.9803           771.6017           775.2417
848.9654           853.7004           867.7043
894.4591           903.4378           921.3709
940.6993           954.7401           960.4611
964.4494           992.7961           1042.3821
1081.0420          1138.4413          1167.7780
1169.5527          1203.9975          1215.6754
1237.2066          1266.1656          1274.8515
1289.2590          1344.2389          1387.4071
1398.8457          1421.1839          1439.0030
1472.6548          1480.2958          1531.5712
1564.2559          1604.6850          1622.7128
1655.8238          2999.2021          3078.7614
3126.1363          3139.5968          3149.9249
3155.8352          3160.9781          3161.3104
3173.5632          3186.4111          3207.2985
ZeroEnergy[kcal/mol] -21.18
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts16-18-----
Barrier      ts16-18  i16  i18
RRHO
Geometry[angstrom]  24
C   -0.1432039942 -0.5803318662 0.0369707311
C   -1.5258759072 -1.2307635757 0.0427413195
C   -2.4726788448 -0.1294462158 -0.3552930455
C   -2.342219832  1.0723776643 0.2771326436
C   -0.0912721248 0.7834708035 0.0173503292
C   1.0867804783  1.5468484064 0.0240267514
C   2.3245309056  0.8117621713 0.0401411363
C   2.2806716151 -0.6088887133 0.056613786
C   1.0865904957 -1.290353917 0.0572334104
H   -1.5710322967 -2.0802564178 -0.6437429668
H   -1.7477003216 -1.6223971428 1.0450277988
H   -2.9679621436 -0.1875103007 -1.3189181701
H   -2.0380610529 1.1320414566 1.3162709889
H   -2.8073067917 1.9668516734 -0.1241473645
H   3.2178408947 -1.1556065919 0.0690265699
H   1.0804011567 -2.3764876717 0.0724394522
C   2.3283340649  3.631668952  0.0140752384
C   3.5466079174  2.9127852157  0.0280086362
C   1.1268429987  2.9656000087  0.0112082135
C   3.5429412978  1.5387163977  0.0397604594

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H 2.347459705 4.7157533709 0.004274987
H 4.4866416842 3.4530724896 0.0290494597
H 0.1898455737 3.5104110502 -0.0032974899
H 4.4786345217 0.9885627527 0.0505591255
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 424.2524
WellDepth[kcal/mol] 10.17
WellDepth[kcal/mol] 44.68
End
Frequencies[1/cm] 65
81.8095 111.2943
185.4572 206.1254 243.1694
290.5527 408.2988 414.5569
448.0430 493.3601 501.4352
516.3327 531.8734 606.8830
637.5621 654.9188 739.3103
753.0058 765.1792 776.1009
817.2667 874.8398 876.1157
911.7520 925.5851 943.5622
956.1049 958.5528 967.1779
969.3345 995.0029 1039.4755
1083.8976 1136.0867 1166.2766
1170.2372 1199.0524 1202.9898
1234.3784 1259.6136 1275.0374
1294.2257 1360.9109 1364.6547
1388.2157 1421.9694 1453.4587
1479.4952 1490.1698 1528.0272
1564.6986 1583.7174 1635.9549
1661.1497 2994.0570 3067.2195
3126.7929 3146.4089 3155.1423
3161.4757 3165.5927 3170.3377
3178.7808 3188.9098 3207.0571
ZeroEnergy[kcal/mol] -21.32
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-9-----
Barrier ts2-9 i2 i9
RRHO
Geometry[angstrom] 24
C -3.670911 0.563115 -0.055287
C 0.172469 -1.207409 0.028436
C -3.542428 -0.844515 -0.090372
C 1.32134 -0.429923 0.077482
C -0.071491 1.570716 0.103473
C 1.167602 0.990582 0.124772
C -2.550161 1.358218 0.006523
C -2.299602 -1.430047 -0.062941
C -1.255085 0.786221 0.035457
C -1.12213 -0.637798 -0.000211

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C  2.630173 -1.079581 0.099849
C  4.514936 0.664363 -0.282089
C  3.832494 -0.479426 0.200913
H  -4.657241 1.012598 -0.077245
H  0.263411 -2.289273 0.005079
H  -4.43239 -1.462099 -0.138919
H  -0.165013 2.65142 0.141785
H  2.047898 1.617492 0.190634
H  -2.645441 2.438968 0.034107
H  -2.201707 -2.510448 -0.089445
H  2.602942 -2.16698 0.122732
H  5.355744 1.05674 0.281791
H  4.136162 1.280112 -1.1017
H  4.932392 -0.57563 -0.484838
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 1840.5094
WellDepth[kcal/mol] 42.2
WellDepth[kcal/mol] 67.84
End
Frequencies[1/cm] 65
44.8884          111.0161
123.5777          182.7056          224.6447
246.0666          356.9728          386.0985
394.5739          419.0170          436.2324
485.3116          525.4288          548.8213
614.9455          643.7327          661.0778
756.9064          762.4833          780.7614
781.6549          829.8254          837.5241
872.5340          877.8592          893.1396
908.0433          960.9959          963.1615
977.7526          992.8993          1033.0360
1041.6315         1047.5297          1130.4938
1147.9022         1174.0803          1181.2397
1197.2480         1242.6988          1285.0576
1289.5353         1327.3065          1391.8523
1398.0698         1411.1548          1457.9116
1470.9604         1498.4362          1539.7948
1592.2819         1602.0953          1637.3727
1663.0839         2179.2987          3034.8536
3120.0971         3153.4469          3156.1211
3158.6145         3161.8742          3171.5300
3173.9154         3186.9488          3193.0413
ZeroEnergy[kcal/mol] 2.15
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-12-----
Barrier      ts2-12  i2  i12
RRHO
Geometry[angstrom] 24

```

```

C   -3.7727890263  0.2863751064 -0.2136799032
C   0.3336324293 -0.7156336317  0.0321040207
C   -3.3335043518 -0.9973423667 -0.6094816565
C   1.2626176909  0.2124099837  0.4961132915
C   -0.5247868595  1.8319269816  0.8202901151
C   0.799667178  1.5048519581  0.9021841118
C   -2.867068717  1.2121330215  0.2529721114
C   -2.0029240536 -1.332697886 -0.5317519429
C   -1.4902022405  0.8999692345  0.3444887581
C   -1.0421561725 -0.4004880431 -0.0547093461
C   2.6433183229 -0.1334831167  0.650630221
C   3.8723105991 -0.3911901764  0.353809568
C   4.9019770383 -0.3701022832 -0.7246392218
H   -4.8250348671  0.5385701437 -0.27969995
H   0.6685998008 -1.7013982441 -0.2710215211
H   -4.053973872 -1.7200153239 -0.9763335487
H   -0.858124332  2.820345851  1.1198967706
H   1.5212559947  2.2248087565  1.2706196442
H   -3.2002604955  2.1992094138  0.5572894806
H   -1.6673931483 -2.3188809422 -0.8355715168
H   3.4271098279 -0.4468974138  1.598360145
H   4.4527746578 -0.057731903 -1.6769636705
H   5.3497737299 -1.358364457 -0.8540998213
H   5.7064378665  0.3263253369 -0.4753191393
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  2063.8455
WellDepth[kcal/mol]  45.52
WellDepth[kcal/mol]  51.41
End
Frequencies[1/cm]  65
38.3242          56.5027
106.5917         143.9561         179.3810
210.7578         234.0482         277.6966
359.0963         381.0999         396.6021
436.9417         478.7727         515.3278
541.5490         551.0481         621.7835
650.9750         659.2419         754.2864
775.9563         776.6025         824.8125
848.5920         861.7357         892.1744
933.2267         956.2777         974.3634
975.2726         989.6517         1026.3258
1029.9818        1042.2281        1139.2416
1170.5084        1175.2967        1181.7476
1229.0756        1273.5844        1287.6262
1356.9008        1383.8837        1388.1801
1403.5557        1460.6388        1465.8389
1475.4320        1487.9764        1530.7444
1588.1034        1629.3027        1653.1133
1967.3961        2298.2520        2987.1793
3073.4829        3094.9856        3155.6344
3158.7775        3161.2537        3171.9116

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3174.4061          3183.1341          3187.2601
ZeroEnergy[kcal/mol]  5.47
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts9-10-----
Barrier      ts9-10  i9  i10
RRHO
Geometry[angstrom]  24
C   0.0643016429 -0.4228854266 -0.1237875015
C   1.3897298712 -0.8910148288 -0.2028115431
C   2.582806753  -0.0456520088 -0.4043629242
C   3.3507965018  0.444956116  0.5667686131
C   -0.2534541888  0.9831233054 -0.1767453424
C   -1.5412375719  1.420319688  -0.1021463528
C   -2.6347284779  0.5108781109  0.0348348289
C   -2.3489414783 -0.8926718316  0.0936355221
C   -1.0104680552 -1.3254259313  0.0121772803
H   1.5448951689 -1.9671888212 -0.1738278164
H   2.8588381221  0.1674953458 -1.4400551945
H   3.1290161417  0.2642375623  1.6134684153
H   4.2278332655  1.0429326546  0.3436366448
H   0.5593168297  1.6930348805 -0.2715068389
H   -1.7567356226  2.4833585  -0.1447654678
H   -0.8011555407 -2.3899006145  0.0553860384
C   -3.9752839429  0.9432762239  0.1148327007
C   -5.0061510846  0.0360926901  0.2478909686
C   -4.7298087586 -1.3474923105  0.3063337141
C   -3.4339968816 -1.8013990241  0.23118785
H   -4.1859588077  2.0069435583  0.0697634652
H   -6.0315449284  0.3825866228  0.3080214394
H   -5.5464570533 -2.0530680102  0.4109277826
H   -3.2218749043 -2.8646144509  0.2759017181
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  176.0874
WellDepth[kcal/mol]  10.16
WellDepth[kcal/mol]  6.47
End
Frequencies[1/cm]  65
58.9884          118.1762
143.3594          186.5372          265.7495
284.2813          380.4698          392.5955
449.1184          474.9843          493.4555
516.1377          522.6251          617.3919
630.5494          660.8328          696.4010
756.6212          772.2065          772.8247
795.0997          827.3279          857.3025
885.7284          886.2816          951.1393
957.6710          959.9595          985.7775
989.4040          991.4129          1014.6431

```

1042.4218	1097.0442	1145.4287
1165.3729	1172.6588	1202.2104
1235.9989	1275.2230	1290.7650
1315.1615	1339.4717	1380.6597
1403.6935	1420.7562	1452.0834
1471.4569	1482.3140	1529.4492
1573.0427	1622.1227	1640.3165
1685.8856	3066.8506	3127.4896
3131.0439	3155.6143	3157.5864
3158.6182	3162.7295	3174.8984
3188.0176	3188.9740	3212.8347

ZeroEnergy[kcal/mol] -55.53

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts10-11-----

Barrier ts10-11 i10 i11

RRHO

Geometry[angstrom] 24

C	-3.3739532523	-0.704195826	0.2102618768
C	0.3321079162	1.3453331891	-0.1274975412
C	-3.3244095633	0.6919479127	0.3921330466
C	1.4797690611	0.6620262567	-0.4065720699
C	0.2077095433	-1.4411678799	-0.5677662002
C	1.4417111064	-0.7754455026	-0.6686786223
C	-2.2266103601	-1.4074286318	-0.0859313278
C	-2.1221946551	1.3630651738	0.2714399208
C	-0.9752521461	-0.7497610903	-0.2101411625
C	-0.9307625381	0.6745010228	-0.0319171198
C	2.8471559923	1.1543615733	-0.2297821526
C	3.0331010124	-1.0420290375	0.7008520554
C	3.6638662686	0.2283695206	0.3088550897
H	-4.3199098866	-1.2257236294	0.3051636068
H	0.3737292178	2.4053531832	0.1043445728
H	-4.2312230356	1.2384837711	0.6247705428
H	0.1403130886	-2.4928423342	-0.8258961787
H	2.1584629406	-1.1621295561	-1.3868609753
H	-2.2655680998	-2.4826500851	-0.2273757269
H	-2.0830576113	2.4388723645	0.4097172439
H	3.1452496515	2.1689305874	-0.4672785354
H	3.5757319853	-1.9712426586	0.5439125781
H	2.4233495128	-1.0356124382	1.60002074
H	4.7296158513	0.3954821143	0.444608339

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 621.5095

WellDepth[kcal/mol] 29.46

WellDepth[kcal/mol] 23.64

End

Frequencies[1/cm] 65

87.0073	120.4135
---------	----------

193.8175	237.5361	286.0566
373.3478	390.9271	415.7222
457.4084	477.5963	526.8128
550.8634	597.2274	625.7282
645.7777	697.3885	731.8933
746.7738	758.7195	767.0185
793.4221	815.4478	818.7634
867.6585	890.9094	907.7001
942.8676	946.9894	952.1300
978.6937	983.1936	1018.6405
1045.8767	1071.5331	1131.4842
1146.3334	1160.5607	1173.5546
1182.2031	1223.0369	1264.8283
1286.9847	1340.4356	1367.7386
1377.3147	1409.3005	1447.9204
1463.4458	1481.7870	1515.1094
1571.4150	1601.4991	1628.7793
1633.2321	3098.7111	3127.7735
3134.1847	3153.4812	3155.7699
3159.5911	3164.9142	3173.2998
3179.1937	3186.5178	3187.2287

ZeroEnergy[kcal/mol] -32.54

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts11-p1-----

Barrier ts11-p1 i11 p1

RRHO

Geometry[angstrom] 24

C	-3.4161438987	-0.7006126056	0.0442542038
C	0.2505748051	1.4366481775	0.0112789432
C	-3.4182470513	0.7118164046	0.002333923
C	1.4318570431	0.7422279309	0.0134792004
C	0.2518916741	-1.4022025397	0.0602640149
C	1.4405948539	-0.7013218814	-0.0420101523
C	-2.2266650169	-1.3890986047	0.0625873534
C	-2.2315107672	1.407009672	-0.0173981907
C	-0.9831193735	-0.7052893886	0.0385278868
C	-0.9855906829	0.7313394804	0.0002815872
C	2.8189811523	1.1890458287	0.0952635723
C	2.8717797653	-1.1704433589	0.1746376969
C	3.6419402452	0.1291895689	0.1758934097
H	-4.3569356707	-1.2391150222	0.0603955891
H	0.2388938465	2.5216348836	0.036533428
H	-4.3611342106	1.2468451352	-0.012689904
H	0.2465869783	-2.4867971317	0.1031272278
H	1.5799159402	-0.7667877778	-1.908343318
H	-2.2225555069	-2.4738791022	0.0918442281
H	-2.2342754444	2.4917755546	-0.0462141572
H	3.1224621046	2.2282584996	0.0988003843
H	3.2233463442	-1.8717554671	-0.5870037976
H	2.9650742172	-1.6799011958	1.1431078996
H	4.720848653	0.1725469397	0.2497909715

```

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 781.0149
WellDepth[kcal/mol] 25.88
WellDepth[kcal/mol] 6.21
End
Frequencies[1/cm] 65
102.2842          131.8339
249.2988          262.0147          280.6743
382.1412          390.5720          413.0913
424.7886          470.9704          482.5557
528.8816          558.2109          578.6936
627.6745          694.4021          732.3464
745.8256          748.1660          765.1017
779.6125          805.6296          853.4539
856.6266          884.5213          902.9943
913.6281          954.6612          957.2314
963.2458          971.9009          991.9228
1043.3690         1074.9416         1122.2664
1160.3921         1167.4599         1172.5039
1179.3466         1241.3644         1249.0100
1270.9740         1282.9909         1348.9356
1372.5964         1383.9238         1427.8524
1444.8274         1459.0676         1484.4678
1531.9691         1601.2034         1617.7054
1649.5553         1653.7774         3010.0272
3065.3924         3156.6358         3160.1185
3161.4879         3164.2620         3175.0274
3188.0466         3190.5188         3212.6235
ZeroEnergy[kcal/mol] -30.3
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts17-p1-----
Barrier      ts17-p1  i17  p1
RRHO
Geometry[angstrom] 24
C   -3.4369578331 0.699696125 -0.0486182351
C    0.2402614229 -1.4032714515 0.11476639
C   -3.431640392 -0.7118613356 0.0271930958
C    1.4145539726 -0.6917912282 0.0959723728
C    0.2316509305 1.4259228209 -0.0349559104
C    1.4093791552 0.7342530315 0.0219705851
C   -2.2518320656 1.3955101098 -0.0694397383
C   -2.2423500575 -1.3975733853 0.080737623
C   -1.0054560598 0.7209352702 -0.0162292488
C   -0.9992869648 -0.7119312129 0.0614334405
C    2.8159995184 -1.1352648554 0.140940076
C    2.8400136329 1.2280571847 0.033322442
C    3.6314907978 -0.0481038022 0.1639045731
H   -4.3808073277 1.2315641793 -0.0906769188

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```

H 0.2411595473 -2.4873322443 0.1651261945
H -4.3716991825 -1.2519015628 0.0425885025
H 0.2164642023 2.5103606366 -0.0899849907
H -2.2548793033 2.4792355334 -0.1276599684
H -2.2373209736 -2.4812230356 0.1383096626
H 3.1242375647 -2.154704391 0.3305457
H 3.0377996964 -1.7191708869 -1.7517158024
H 3.0381401978 1.9179435674 0.8631555812
H 3.0967958085 1.7714954761 -0.8861628943
H 4.7109197126 -0.0740495431 0.2313574681
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 622.3339
WellDepth[kcal/mol] 33.17
WellDepth[kcal/mol] 4.33
End
Frequencies[1/cm] 65
101.0191 130.6583
238.5014 260.5263 267.6723
284.0391 339.3300 400.4518
407.3612 419.4070 464.9340
487.9126 565.1893 578.5002
628.8708 703.1001 730.0184
732.6100 750.6896 761.8662
782.9217 804.6804 856.1237
859.4452 888.6001 904.6448
913.7844 953.8285 957.7055
965.4928 978.3205 992.9148
1043.3144 1073.1750 1114.9212
1152.3385 1169.4191 1173.8758
1179.5237 1244.0658 1250.0400
1267.9018 1282.4122 1346.3839
1371.7265 1388.7757 1431.1763
1443.3502 1471.5625 1485.1794
1533.1696 1555.5160 1620.3513
1654.1445 1678.4667 3004.3221
3028.6417 3154.5124 3156.7573
3160.4458 3164.8346 3174.1907
3187.2735 3197.5379 3216.2095
ZeroEnergy[kcal/mol] -32.18
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts18-p2-----
Barrier ts18-p2 i18 p2
RRHO
Geometry[angstrom] 24
C 3.3467707902 -0.1785645617 0.0283128244
C -0.8816778736 -0.4308823346 0.0772987843
C 2.7266341807 -1.4474179326 0.0880953707
C -1.6321784739 0.736130503 0.0179818621

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C 0.3623896443 2.0670396569 -0.0625745804
C -1.0124464836 1.9960327066 -0.0543042517
C 2.5830000004 0.962201947 -0.0181305528
C 1.356140247 -1.5512903354 0.1040311628
C 1.1651668353 0.895098189 -0.005705428
C 0.5386850548 -0.3934255842 0.0615287619
C -3.1000284955 0.3871655742 0.0465062112
C -1.8059199662 -1.5749763316 0.1380467099
C -3.084326966 -1.1118664159 0.1685428543
H 4.4287631125 -0.1100948359 0.0169816551
H 3.3385110245 -2.3419746037 0.1195807407
H 0.8580145605 3.0307197271 -0.1141791825
H -1.60855089 2.9014505345 -0.0999804279
H 3.0574186703 1.9369425639 -0.0676418429
H 0.8891385175 -2.5285052108 0.1443867391
H -3.6267749799 0.8603741702 0.8852338262
H -3.6182466881 0.7157557167 -0.8650690172
H -1.676550226 -2.21782164 -1.7679862611
H -1.511687486 -2.5982159243 0.3245781513
H -3.9761071127 -1.7189895784 0.2426998906
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 584.6788
WellDepth[kcal/mol] 33.76
WellDepth[kcal/mol] 3.95
End
Frequencies[1/cm] 65
112.4164 129.4980
220.0739 236.9861 257.0120
277.0483 325.2868 411.4650
432.8203 459.6675 465.0089
506.9468 520.0546 573.4841
612.4456 680.1152 681.7616
715.6635 749.0727 752.7342
795.8643 818.3622 838.5234
878.6929 881.4388 931.3389
955.4615 958.3760 964.0995
968.9134 970.9573 994.0877
1044.3388 1071.3674 1118.2353
1141.5589 1167.5365 1178.7593
1190.5671 1216.4532 1236.6844
1283.2221 1295.0235 1351.1644
1378.1271 1391.3406 1426.5056
1430.1058 1469.1431 1486.5262
1534.1385 1559.4398 1606.6074
1630.8603 1665.1349 3005.3037
3029.5644 3156.7955 3158.7443
3166.7688 3175.6821 3179.5194
3189.3967 3204.2806 3222.7236
ZeroEnergy[kcal/mol] -32.24
ElectronicLevels[1/cm] 1
0 2

```

```

End
!-----
!-----bar_ts18-p3-----
Barrier      ts18-p3  i18  p3
RRHO
Geometry[angstrom]  24
C   3.349603819 -0.1594102526 0.0679420742
C   -0.8707816038 -0.4482471378 -0.0565759073
C   2.7378703675 -1.4343031043 0.0898152056
C   -1.6309329152 0.7114966643 -0.1145524203
C   0.3505332656 2.0645921519 -0.0952555357
C   -1.0201847235 1.9847794732 -0.1326320294
C   2.5777738292 0.9755630688 0.0073462511
C   1.3695355147 -1.550060269 0.050393885
C   1.1617005376 0.8976080754 -0.0339763704
C   0.5420048961 -0.3974444147 -0.0121681545
C   -3.0553133895 0.3404122391 -0.1384823921
C   -1.793557454 -1.643687926 -0.0524545841
C   -3.158287826 -1.0144518751 -0.1519753011
H   4.4305061182 -0.0821729935 0.0994283084
H   3.3560972073 -2.323824692 0.1382419823
H   0.8405272018 3.0325394855 -0.1097156133
H   -1.6254114514 2.8836673056 -0.172484604
H   3.0453978028 1.9547221748 -0.0091659716
H   0.9082011463 -2.5312612362 0.0680849631
H   -3.5279554691 0.7342791839 1.777385027
H   -3.8647175197 1.0371023739 -0.3106965168
H   -1.6010891699 -2.3276028261 -0.8890391808
H   -1.6917225942 -2.2430939383 0.8628032418
H   -4.0776085899 -1.5820215306 -0.1978263569
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  589.455
WellDepth[kcal/mol]  33.74
WellDepth[kcal/mol]  4.06
End
Frequencies[1/cm]  65
109.5879          136.2343
229.1242          235.9090          245.0631
272.7382          327.4880          415.3083
433.3986          456.8034          466.0924
520.4280          520.7401          559.3633
616.6651          680.9692          682.6230
714.6209          751.3308          759.5856
787.1069          827.9317          837.1055
870.3633          873.6078          934.1078
956.0166          958.5071          969.0396
972.1533          981.2748          993.1017
1044.0631         1059.1819         1110.1577
1143.6812         1167.3835         1179.3712
1185.0134         1232.9051         1241.4102
1266.3958         1288.5925         1361.1555

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1377.9802          1397.9462          1415.9582
1432.6389          1467.9509          1488.4644
1535.2150          1561.8297          1611.9057
1630.6281          1663.3817          3004.8694
3029.4418          3157.2792          3160.8015
3164.7244          3177.0407          3179.4833
3188.0262          3199.0570          3219.6524
ZeroEnergy[kcal/mol] -32.27
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts12-p4-----
Barrier      ts12-p4  i12  p4
RRHO
Geometry[angstrom]  24
C   3.8494578241  0.0133955988 -0.0961380097
C   -0.2911225313 -0.8265479342  0.0948842842
C   3.4021715112 -1.3283169831 -0.0691067797
C   -1.2174944552  0.204481585  0.1310021555
C   0.5859118177  1.8319946724  0.0403996317
C   -0.7531367127  1.5549402461  0.102302238
C   2.9443252415  1.0471454419 -0.0607866765
C   2.059655448  -1.6108033656 -0.0071516199
C   1.5517938601  0.7908698527  0.0032861888
C   1.0977969537 -0.5660036235  0.0310897513
C   -2.6119376481 -0.0645497721  0.1980216906
C   -3.8064177326 -0.2793046881  0.1818474905
C   -5.2210016373 -0.5379921904  0.4408899057
H   4.9120872249  0.2224954824 -0.1453491184
H   -0.635976408 -1.8540768318  0.1148228041
H   4.1263542287 -2.1345973167 -0.097955158
H   0.926694903  2.8618680895  0.0177568432
H   -1.4820615265  2.3556052228  0.1287871922
H   3.2860561589  2.0767512387 -0.0819579015
H   1.7147407221 -2.6392681578  0.0131765332
H   -3.9955378372 -0.3148420439 -1.924446239
H   -5.4091081128 -0.5775786362  1.5181810984
H   -5.5337759884 -1.4895547788  0.003768454
H   -5.8492683039  0.2471568919  0.0127612413
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  425.5057
WellDepth[kcal/mol]  39.64
WellDepth[kcal/mol]  3.32
End
Frequencies[1/cm]  65
53.4538          62.5422
74.9951          136.8194          165.3837
183.0263          279.2070          305.6283
328.0119          373.6550          391.5432
402.1043          466.4501          485.3588

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515.7630	557.2344	558.8004
617.5982	659.0138	661.7259
760.7467	779.0749	781.0812
833.6406	858.2031	875.6439
914.2711	951.5970	966.1441
981.2822	998.0836	1011.2170
1042.2855	1045.2865	1061.1751
1151.9282	1173.3863	1178.4243
1211.2272	1249.5762	1287.5086
1298.8388	1371.2273	1395.5124
1403.9579	1414.9346	1464.3868
1476.3920	1480.5800	1500.7272
1536.6110	1601.4894	1639.2873
1664.2171	2277.5550	3026.1221
3085.0693	3092.5693	3158.8822
3162.8109	3165.2170	3176.4407
3180.0431	3189.1717	3193.7348

ZeroEnergy[kcal/mol] -6.3

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts10-p5-----

Barrier ts10-p5 i10 p5

RRHO

Geometry[angstrom] 24

```

C 3.7176063655 0.4397991611 -0.2198045521
C -0.1810126658 -1.1477607017 0.206516409
C 3.539714603 -0.9513492883 -0.0423743251
C -1.2892244623 -0.3201350659 0.178268639
C 0.1626547981 1.601637467 -0.1432067191
C -1.094376738 1.080552585 -0.0035420782
C 2.6285222929 1.2789324974 -0.2538351213
C 2.2779855606 -1.4775418628 0.0976633787
C 1.3148682553 0.7685076619 -0.112225737
C 1.133255225 -0.6386370002 0.0673025448
C -2.6255804039 -0.8950244064 0.3427409195
C -4.8613534202 0.4490275384 0.5319987218
C -3.7707293302 -0.231896156 0.3133457752
H 4.7182309799 0.8424189608 -0.3292011187
H -0.3127829333 -2.2171552134 0.3406848292
H 4.4058317397 -1.603049824 -0.0175392785
H 0.2957855625 2.6695796129 -0.2824282136
H -1.9615121089 1.7300243229 -0.0326005969
H 2.7629443913 2.3469994616 -0.3902593249
H 2.140791899 -2.5453262961 0.2333449753
H -2.6757052484 -1.9771450066 0.4486507682
H -5.5489430404 0.7185291699 -0.2615885092
H -5.11455657 0.7655256172 1.5412174422
H -4.0835297514 -0.6113502345 -1.7575938286

```

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

```

ImaginaryFrequency[1/cm]  500.7306
WellDepth[kcal/mol]  58.13
WellDepth[kcal/mol]  3.37
End
Frequencies[1/cm]  65
47.6557                85.2762
110.5325               137.5091           183.2667
254.4873               284.0922           373.2322
383.3305               404.4625           413.4310
427.1121               483.5446           503.6452
525.5981               599.3716           609.1604
644.5790               685.7759           761.2275
767.5694               782.0567           784.0150
835.9268               871.8041           888.9631
891.7821               895.8046           919.4966
964.8807               966.7452           985.1021
996.7166               1009.3820          1042.6344
1094.6169              1150.5578          1174.4815
1179.9030              1197.2920          1241.5470
1281.7074              1289.4384          1327.8247
1393.1864              1398.3897          1413.5533
1458.3294              1481.7288          1503.4538
1543.4078              1607.9909          1641.1639
1664.3641              1982.7975          3110.0526
3123.2332              3156.1935          3158.5898
3161.0835              3164.1597          3175.6998
3185.1014              3188.4279          3192.0679
ZeroEnergy[kcal/mol]  -3.87
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts14-p5-----
Barrier      ts14-p5  i14  p5
RRHO
Geometry[angstrom]  24
C   -3.7006996718  0.459886483  0.0768176268
C    0.2225030897 -1.121154173 -0.068785298
C   -3.5068556878 -0.939719976  0.0256416308
C    1.3187265175 -0.283849154 -0.0648231172
C   -0.1534246469  1.6437441538  0.0305525446
C    1.111888968  1.1224979334 -0.0162025219
C   -2.6195967402  1.3090930962  0.0792347463
C   -2.2374050245 -1.463651412 -0.0218478524
C   -1.2974988004  0.8008471187  0.0310678402
C   -1.1002134688 -0.614362694 -0.0202641297
C    2.6818347582 -0.861209845 -0.1087571485
C    4.9143658784  0.4717882255  0.2385615272
C    3.8002221262 -0.1876530465  0.133598917
H   -4.7074667793  0.860399578  0.1138955162
H    0.3655001602 -2.1965403764 -0.1140279636
H   -4.3671409224 -1.5996052412  0.0236682876
H   -0.2972818636  2.7186957887  0.0674532692
H    1.9731792802  1.7805748493 -0.0160351039

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H   -2.765748666  2.3836386144  0.117907282
H   -2.0883700685 -2.5377086581 -0.0619484471
H    2.740514863 -1.9469482194 -0.0824859129
H    2.8253553792 -1.0988441689 -2.0142144548
H    5.454303015  0.80883063  -0.645162875
H    5.3541113045  0.7105224936  1.203796637
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  717.5388
WellDepth[kcal/mol]  34.68
WellDepth[kcal/mol]  5.39
End
Frequencies[1/cm]  65
42.7687          100.0024
116.5452         182.0797          222.2443
251.0710         268.1260          369.5522
383.0397         407.9560          410.2979
464.0060         485.2776          507.5019
526.1080         586.5718          608.2310
644.3548         678.5813          761.0165
765.4852         782.4542          784.4510
835.2266         873.7566          883.8304
886.9472         907.2581          955.2278
964.8236         967.1568          982.8166
995.6373         996.4339         1042.3969
1086.0679        1150.4375         1173.8510
1180.7377        1192.5428         1238.9812
1278.6955        1288.9328         1320.3166
1393.2198        1397.1820         1410.4812
1452.3378        1479.5000         1504.2094
1545.2929        1610.7479         1643.6301
1668.5182        1979.6187         3087.7720
3127.5976        3155.8410         3157.8430
3158.1680        3160.7331         3163.7437
3175.3896        3183.6475         3188.1502
ZeroEnergy[kcal/mol]  -1.85
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts14-p6-----
Barrier      ts14-p6  i14  p6
RRHO
Geometry[angstrom]  24
C            -3.665301      0.426868      0.288838
C             0.245669     -1.108675     -0.239035
C            -3.450897     -0.970833      0.292792
C             1.311310     -0.258726     -0.414552
C            -0.173803      1.652802     -0.245336
C             1.087790      1.143283     -0.414048
C            -2.609477      1.288831      0.114358
C            -2.185887     -1.479576      0.122096

```

C	-1.291623	0.795913	-0.064367
C	-1.074540	-0.616801	-0.060727
C	2.715577	-0.803206	-0.634902
C	4.561672	0.147183	1.036704
C	3.699283	-0.314026	0.326861
H	-4.668321	0.815341	0.424559
H	0.402674	-2.183234	-0.233529
H	-4.291779	-1.641024	0.431569
H	-0.332500	2.726229	-0.247084
H	1.931839	1.812489	-0.540645
H	-2.771190	2.361802	0.111328
H	-2.021051	-2.552120	0.125470
H	2.693149	-1.896820	-0.602991
H	3.059086	-0.533390	-1.643168
H	5.221754	0.454269	1.811200
H	5.757696	1.218238	-0.288805

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 450.6795
WellDepth[kcal/mol] 37.63
WellDepth[kcal/mol] 3.35
End
Frequencies[1/cm] 65

23.0358	43.3061	
77.1121	143.5213	180.8725
215.6388	250.6938	290.0201
366.9439	402.0135	407.3253
411.0428	485.9321	503.9890
526.6255	577.6872	635.5863
658.3751	667.8629	737.4287
752.2448	765.0766	781.3207
786.5692	832.8690	868.9186
878.5749	903.0521	941.7408
958.8030	966.0046	980.7192
985.1612	997.3401	1042.6079
1148.1454	1172.7595	1179.1794
1188.7823	1213.4614	1238.5026
1277.1847	1289.1681	1322.2129
1392.5186	1397.1355	1408.2386
1461.3924	1474.6256	1503.1973
1546.1495	1613.0883	1646.3885
1674.1010	2170.9902	2997.7885
3055.9136	3153.9269	3158.0270
3160.4406	3163.5144	3175.5814
3179.6240	3188.3237	3463.2031

ZeroEnergy[kcal/mol] 1.1
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-p4-----
Barrier ts2-p4 i2 p4

RRHO

Geometry[angstrom] 24

C -3.9020997809 0.2518136142 -0.0488626414
C 0.1947809317 -0.7950470074 0.0744444134
C -3.5232082297 -1.1075865264 0.0453710048
C 1.1731976037 0.1803459961 0.0238456178
C -0.5453529917 1.8972738776 -0.1117533893
C 0.7781465902 1.5505298235 -0.0711355949
C -2.9447922606 1.2367210887 -0.1006697586
C -2.1951889477 -1.4561389203 0.085965346
C -1.5658762768 0.9107770484 -0.0607558918
C -1.181086136 -0.4633006839 0.0344739606
C 2.5770100181 -0.1178816178 0.0672593491
C 3.7894124901 -0.0124709791 0.1046758511
C 5.2385880491 -0.1021591758 0.1486882169
H -4.9537245897 0.5136497042 -0.0801175676
H 0.4874348821 -1.8362983541 0.145223437
H -4.2879648048 -1.8749937328 0.0853931494
H -0.8298544407 2.9418534365 -0.1842607142
H 1.5484002863 2.3109411586 -0.1105104358
H -3.2341859092 2.2800262842 -0.1730215343
H -1.9023487045 -2.4982522787 0.1580729554
H 2.6136624354 -2.1234064065 0.0321745949
H 5.6404529314 0.3788701268 1.0455004212
H 5.6939306305 0.3762658804 -0.7235357686
H 5.5531362236 -1.1516853564 0.159890979

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 558.1328

WellDepth[kcal/mol] 35.51

WellDepth[kcal/mol] 5.08

End

Frequencies[1/cm] 65

19.9912	68.5063	
93.1169	97.0580	170.4822
182.4707	266.4483	284.8931
337.4801	395.9449	397.9627
444.5423	484.9825	518.7388
525.6564	554.8158	581.7702
617.0338	660.2545	668.3550
761.0202	780.3007	781.6594
832.6040	855.5958	876.7714
921.7636	953.3995	966.0228
979.4538	997.9412	1017.4385
1041.9349	1043.1509	1052.1448
1152.2320	1173.3088	1179.0925
1209.1156	1243.5111	1282.7710
1291.4211	1374.4422	1394.5864
1406.2107	1412.8189	1464.0474
1470.6395	1476.0896	1501.0236
1535.3366	1604.8772	1641.7016
1667.2802	2248.1687	3013.6115

```

3069.5251          3077.6418          3157.8036
3162.4745          3164.2868          3173.7743
3176.1097          3188.3850          3192.9934
ZeroEnergy[kcal/mol] -4.54
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-p5-----
Barrier      ts2-p5  i2  p5
RRHO
Geometry[angstrom] 24
C           -3.758652    0.450192    0.000004
C            0.165116   -1.136492   -0.000003
C           -3.565308   -0.950229    0.000004
C            1.264976   -0.300905   -0.000004
C           -0.209363    1.630692   -0.000003
C            1.055457    1.108402   -0.000004
C           -2.676547    1.298557    0.000001
C           -2.295604   -1.476035    0.000001
C           -1.354738    0.788413   -0.000001
C           -1.157696   -0.627760   -0.000001
C            2.618742   -0.877437   -0.000004
C            3.748950   -0.216297    0.000001
C            4.913022    0.385477    0.000008
H           -4.765473    0.852246    0.000005
H            0.307448   -2.212952   -0.000003
H           -4.426056   -1.609520    0.000005
H           -0.353262    2.706317   -0.000003
H            1.917258    1.766154   -0.000006
H           -2.822195    2.373871    0.000001
H           -2.147055   -2.550920    0.000001
H            2.676951   -1.965726   -0.000008
H            5.385854    0.700969    0.925771
H            5.385861    0.700978   -0.925750
H            6.350538   -1.220885    0.000006
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 364.4727
WellDepth[kcal/mol] 35.69
WellDepth[kcal/mol] 2.88
End
Frequencies[1/cm] 65
45.8409          93.7806
118.9777         168.8815          183.6629
218.6258         266.4369          289.1780
360.9017         387.4330          402.5178
421.3181         484.0472          509.5588
526.0192         605.1940          612.8658
644.4237         694.4512          762.6646
763.7477         782.1298          784.1393
835.4413         873.3269          887.3219

```

896.5254	897.0431	921.9579
964.3822	966.7676	982.5125
996.4094	1017.2344	1042.6303
1091.0918	1150.7966	1174.1896
1180.0138	1196.0201	1240.3339
1279.8506	1289.0112	1323.7799
1393.0392	1397.3946	1412.7416
1460.2518	1481.2507	1505.3257
1543.8836	1609.8265	1643.4395
1667.6830	2000.1882	3105.2836
3109.1033	3155.8287	3158.2324
3160.1051	3163.5986	3175.4678
3180.3865	3181.3439	3188.2396

ZeroEnergy[kcal/mol] -4.36

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsa-7-----

Barrier tsa-7 i7 p0a

RRHO

Geometry[angstrom] 24

C	-4.0000109749	0.4033492002	-0.4659012376
C	-0.0367350294	-0.9925940733	0.1238179299
C	-3.6903460802	-0.9571717598	-0.6964008755
C	0.8911719755	-0.0883163644	0.5317801026
C	-0.6612899427	1.7137689997	0.5862191771
C	0.6257167597	1.261695255	0.7844921381
C	-3.0223550294	1.2747416149	-0.0514365825
C	-2.4102269012	-1.419602457	-0.508506621
C	-1.6888891965	0.8328453842	0.1533865017
C	-1.3772557879	-0.5457537556	-0.0812950446
H	-5.0140129902	0.7555027833	-0.6182281862
H	0.2115953324	-2.0350302603	-0.0511365777
H	-4.4702205032	-1.6359856912	-1.0233140694
H	-0.9066725754	2.7568413428	0.762753119
H	1.4073192655	1.9320798944	1.1241670705
H	-3.258589672	2.3189395608	0.1258756438
H	-2.171836953	-2.4633413023	-0.6849040882
C	3.3185568028	-0.3849476197	2.1125522344
C	3.3065430915	-1.5202479849	-0.2243054859
C	3.1016973696	-0.8782222627	0.9009846148
H	4.0387601981	0.4132090402	2.264454946
H	2.7151229539	-0.6825948091	2.9630029756
H	2.7153919709	-1.3514933305	-1.1143074048
H	4.093290916	-2.2681324047	-0.27542328

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 370.7338

WellDepth[kcal/mol] 64.34

WellDepth[kcal/mol] 2.61

End

```

Rotor      Hindered      ! 25 cm^-1
  Group      18 19 21 22 23 24
  Axis      4 20
  Symmetry      2
  Potential[kcal/mol]      4
0  0.082433425 0.062369433 0.880468746
  End
Frequencies[1/cm]  64
                    43.2367
75.5997              94.8366              165.6363
181.3044            230.5669              242.4409
372.3333            389.3906              393.6208
477.5358            490.1562              514.3201
515.5837            619.8558              629.9287
746.8745            763.7663              765.9630
775.6131            807.8901              813.1685
827.6224            853.3466              884.7754
891.9249            930.4192              957.8761
969.6901            994.7007              1006.6454
1020.7432           1038.0773              1045.6731
1072.4831           1144.0000              1161.2406
1172.4382           1210.3374              1252.0985
1277.2443           1343.8608              1385.6497
1393.7395           1427.1614              1459.1857
1464.5729           1475.4377              1531.6100
1595.7472           1614.8263              1656.9876
1927.9493           3119.6821              3123.7609
3151.0548           3153.4389              3156.9892
3162.4044           3174.2672              3174.7098
3186.7835           3201.1444              3218.0625
ZeroEnergy[kcal/mol]  3.74
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_tsa-14-----
Barrier      tsa-14  i14  p0a
RRHO
Geometry[angstrom]  24
C   -1.9710088797 -0.9466165477  0.4306779248
C    1.1959351256  1.7891338222 -0.2715424956
C   -2.2356031472  0.4420268274  0.3890991995
C    2.4410617339  1.2765203027 -0.4517012704
C    1.7154587641 -0.9759124684 -0.1856843299
C    2.745620596  -0.0886533986 -0.4127137875
C   -0.6923308972 -1.4126912569  0.2446953618
C   -1.2177673516  1.3366883096  0.1623214106
C    0.3842337481 -0.5180749075  0.0080776596
C    0.1139396663  0.8883010499 -0.0339010793
H   -2.7831645927 -1.6419879703  0.610260077
H    0.9958493558  2.8566314802 -0.3038299099
H   -3.2488627225  0.7986900812  0.5373145868
H    1.9112644605 -2.0435985584 -0.1512697909
H    3.7616263477 -0.4404131491 -0.5571939067

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H   -0.4872408557 -2.4778484983 0.2763707923
H   -1.4204890636 2.4022353139 0.1302347381
C    4.2429634293 2.7581772852 -0.8840468176
C    6.2022085117 2.0387064747 0.7004465884
C    5.2650428174 2.4366880665 -0.1086874157
H    4.2109021539 2.4288297687 -1.9168011999
H    3.5927066754 3.5834087266 -0.6143456439
H    6.0461667943 1.203596124 1.3802700633
H    7.1737653302 2.5248161223 0.7350642451
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 239.2847
WellDepth[kcal/mol] 39.53
WellDepth[kcal/mol] 1.87
End
      Rotor      Hindered      ! 12 cm^-1
      Group              19 20 21 22 23 24
      Axis              4 18
      Symmetry          1
      Potential[kcal/mol] 8
0     0.130493757 0.291590529 0.001067394 0.031020309 0.031012151 0.0346812
      0.046290127
      End
Frequencies[1/cm] 64
                    33.8973
67.1787              113.9326              177.2693
200.3338             321.2507              343.7576
367.5468             378.6628              388.6248
476.7878             487.5111              496.7706
515.4107             620.1171              628.9492
745.7566             751.1684              766.8062
771.3702             814.1119              847.2915
859.3780             870.2684              872.8879
889.8419             936.8604              957.9717
969.7716             994.6538              999.1959
1031.9700            1038.6551             1047.2935
1069.9930            1145.3106             1161.8744
1173.1998            1211.6244             1254.0434
1277.5746            1345.8875             1386.1275
1393.5996            1420.4004             1460.4570
1465.8396            1469.4568             1531.7856
1596.0864            1615.2271             1657.2332
1974.8042            3094.2402             3124.3435
3141.2065            3149.9294             3156.6926
3161.7556            3162.5280             3169.8006
3174.3456            3187.1507             3200.9196
ZeroEnergy[kcal/mol] 3.0
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts10-19-----

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Barrier      ts10-19  i10  i19
RRHO
Geometry[angstrom]  24
C   3.5415655422  0.5283386696  0.2733729652
C   -0.2259627703 -1.3430225814 -0.2112450856
C   3.4561468646 -0.8829936358  0.2219898673
C   -1.3781369885 -0.5919289578 -0.3187504277
C   -0.0620915103  1.4451886333 -0.1081694856
C   -1.2775810347  0.8270625198 -0.2635909044
C   2.4067809566  1.2949609284  0.1664333304
C   2.2386563227 -1.4990984632  0.0643704881
C   1.1336080441  0.6898524102  0.0033112709
C   1.0464922809 -0.7364524395 -0.0492698765
H   4.5087560592  1.0022063251  0.3979478556
H   -0.2856665859 -2.4259598523 -0.2493873093
H   4.3589768496 -1.477233825  0.307848525
H   -0.0032375459  2.5280922446 -0.0669001322
H   -2.1828332748  1.4181952395 -0.3448480862
H   2.4695952522  2.3775908133  0.2058998034
H   2.1721212128 -2.5814538623  0.0249340176
C   -2.7023644831 -1.2365984092 -0.5102657461
C   -3.312386698  -1.4278392428  1.8749855409
C   -3.5570950851 -1.5960873129  0.5257641781
H   -3.0199044303 -1.4243458817 -1.5324897277
H   -4.0387751364 -1.7370653649  2.6155820568
H   -2.3901904109 -0.9843338105  2.230277194
H   -4.5026204307 -2.0513101447  0.2391216883
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  69.8626
WellDepth[kcal/mol]  2.9
WellDepth[kcal/mol]  3.1
End
Frequencies[1/cm]  65
67.8243          157.5799
173.8269         175.4641          298.4633
326.1858         398.5906          403.4319
444.2652         485.4007          505.6832
521.8203         525.4738          598.6160
634.6266         667.9718          697.4769
738.1726         769.5193          780.6064
789.7737         809.6093          835.5701
872.8868         900.1543          919.7046
963.4460         970.8201          977.8654
994.6662         995.5600          1027.9459
1041.3933        1112.2176         1153.1265
1170.4738        1177.8639         1194.9317
1221.7119        1243.1394         1275.9898
1288.7286        1364.4843         1390.7664
1398.2672        1425.2334         1447.9288
1461.6116        1501.8120         1520.7968
1536.8603        1603.8413         1640.6813

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1668.9666          3126.5557          3143.3211
3150.0833          3156.5052          3158.7634
3161.5035          3164.5559          3174.6728
3180.8674          3187.2827          3240.7940
ZeroEnergy[kcal/mol] -59.1
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts19-20-----
Barrier      ts19-20  i19  i20
RRHO
Geometry[angstrom] 24
C  3.647561846 0.4742217112 -0.0683128381
C  -0.1900111136 -1.2428831077 0.5713021381
C  3.5402275859 -0.8338738872 0.4468775145
C  -1.3460372568 -0.4600387513 0.2832909219
C  0.0388804033 1.416453359 -0.3736958093
C  -1.2111349783 0.8585592113 -0.1719907623
C  2.5151136907 1.2052175852 -0.3500542077
C  2.2961116209 -1.3897685978 0.6600836017
C  1.2230286832 0.6614184698 -0.1410424807
C  1.1175237974 -0.6739143666 0.3601843735
C  -2.5724928599 -1.2530473695 0.2090619345
C  -1.0021588934 -2.8679854125 -0.6539121014
C  -2.3731052131 -2.5050053367 -0.2473524862
H  4.6276836859 0.9066101794 -0.2365727672
H  -0.2701715624 -2.0070908108 1.3365869438
H  4.4364440226 -1.3991801317 0.6756597957
H  0.1309331789 2.4361770607 -0.7308996052
H  -2.1027800908 1.4297632635 -0.4093134374
H  2.59921526 2.2159468708 -0.7359448562
H  2.2097756921 -2.3980617937 1.0524741486
H  -3.5514684428 -0.8453521087 0.4357719172
H  -0.6090836016 -3.8421234182 -0.3743216485
H  -0.656995998 -2.5091501384 -1.6205425886
H  -3.1876304563 -3.2219034798 -0.3258647006
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 638.8802
WellDepth[kcal/mol] 29.22
WellDepth[kcal/mol] 31.74
End
Frequencies[1/cm] 65
99.4242          107.1809
167.1875          221.8877          266.6939
356.0410          410.7650          429.5283
455.5837          487.7448          518.9563
541.0534          556.3296          613.4703
653.6072          674.5092          711.8163
731.6470          750.3336          774.4498
786.7626          802.8058          828.5291

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877.8900	889.1340	942.1589
955.2309	956.4267	962.3481
975.4885	989.7994	1009.0763
1046.2136	1061.0969	1132.1317
1154.9764	1158.3829	1175.3983
1196.1748	1227.4254	1261.9997
1283.5966	1334.7080	1365.5998
1373.5134	1390.1160	1450.4765
1453.0605	1487.8586	1534.7365
1561.4917	1589.8197	1610.4898
1645.8394	3095.9836	3126.8734
3145.0017	3155.8541	3158.1965
3160.7622	3173.8081	3177.1672
3177.8425	3179.3364	3187.4929

ZeroEnergy[kcal/mol] -32.98

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts20-p3-----

Barrier ts20-p3 i20 p3

RRHO

Geometry[angstrom] 24

C	3.6199469131	0.4847184479	0.0398827217
C	-0.2668666042	-1.2105180837	0.0730829471
C	3.4727822653	-0.9169862608	0.1301720974
C	-1.3752133056	-0.3744111308	-0.1384633342
C	0.0458975145	1.5594576995	-0.1726072525
C	-1.2189194353	1.0236567708	-0.2306178432
C	2.5091003313	1.2903794219	-0.0478438886
C	2.2203001493	-1.4868341109	0.1373585158
C	1.2034872791	0.7377878694	-0.0523311489
C	1.0580473972	-0.6840765418	0.0474282532
C	-2.5705671344	-1.2053947201	-0.2458517453
C	-0.7319891516	-2.6494565398	-0.0260095753
C	-2.226414709	-2.5042539886	-0.1737677195
H	4.6117977494	0.9222579997	0.0396901635
H	-0.4449688671	-1.140227121	2.0482195302
H	4.353994101	-1.545183066	0.197556559
H	0.1843971033	2.6332552076	-0.2438399718
H	-2.0839624148	1.6650645803	-0.3586987705
H	2.6189805435	2.3676102889	-0.1193916885
H	2.1149463933	-2.5629224648	0.2179732322
H	-3.5739525608	-0.8175536304	-0.3678706685
H	-0.4531628582	-3.2639330328	0.8353147178
H	-0.2994482909	-3.133923589	-0.91213115
H	-2.9022024086	-3.3477480054	-0.2201399811

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 629.0042

WellDepth[kcal/mol] 32.58

WellDepth[kcal/mol] 4.19

```

End
Frequencies[1/cm] 65
114.2836      133.5814
233.9749      238.8545      255.4998
376.7410      399.8687      425.0452
432.8509      444.1231      480.3414
521.0521      529.5830      553.3525
618.1347      673.7523      684.4805
720.3311      751.2028      761.9177
792.1620      830.7460      839.3761
868.7640      876.4799      933.3138
955.7548      958.0825      960.3169
971.3406      984.5602      992.7733
1046.1015     1059.9232     1118.6689
1149.6490     1165.8012     1178.8203
1183.7411     1233.7718     1246.1699
1267.3775     1289.7339     1357.1926
1372.8745     1394.7314     1407.6994
1436.2232     1464.2200     1481.3264
1551.6801     1575.3398     1609.3041
1627.9994     1657.6823     3011.3370
3062.2763     3157.7390     3160.7227
3165.7743     3177.8975     3178.8533
3188.7192     3193.0592     3216.6704
ZeroEnergy[kcal/mol] -32.14
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts9-p5-----
Barrier      ts9-p5  i9  p5
RRHO
Geometry[angstrom] 24
C  3.7230963898 0.3981884795 0.1045934107
C  -0.216180129 -1.1175823297 -0.1884371107
C  3.5151860596 -0.9733334296 -0.1676603909
C  -1.3088632159 -0.2865729714 -0.0170807913
C  0.18677235 1.5929910821 0.3501019211
C  -1.083631181 1.0948264111 0.2548604106
C  2.6500150916 1.2413097881 0.2750336787
C  2.2399992557 -1.4763172288 -0.2643822681
C  1.3231311327 0.7544945998 0.181955641
C  1.1111540402 -0.6327620513 -0.0934616396
C  -2.6606909348 -0.8410031893 -0.109626281
C  -4.8845183661 0.4499800769 0.3688468306
C  -3.7925025814 -0.1648290416 0.0076824997
H  4.7340862502 0.7826144415 0.1783233404
H  -0.3709009592 -2.171364307 -0.399563067
H  4.3689319656 -1.6282897929 -0.3004737177
H  0.343134266 2.6469077092 0.5560571035
H  -1.9381712902 1.7489997033 0.3829223818
H  2.8074994988 2.2944400198 0.4837518173
H  2.0797967047 -2.5288606624 -0.4738640978
H  -2.7324035411 -1.9007820247 -0.3471977539

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H   -5.5193148677  0.9731901762 -0.3371813665
H   -5.1933610988  0.4474609274  1.4116388906
H   -3.9857548395  0.1236356139 -2.0923104416
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  500.7546
WellDepth[kcal/mol]  61.82
WellDepth[kcal/mol]  3.37
End
Frequencies[1/cm]  65
47.6575          85.2753
110.5319         137.5114          183.2656
254.4871         284.0916          373.2378
383.3285         404.4638          413.4317
427.1200         483.5448          503.6453
525.5979         599.3704          609.1608
644.5793         685.7748          761.2283
767.5703         782.0584          784.0121
835.9263         871.8056          888.9636
891.7817         895.8024          919.4968
964.8809         966.7458          985.1017
996.7165         1009.3821         1042.6348
1094.6155        1150.5576         1174.4822
1179.9034        1197.2921         1241.5485
1281.7073        1289.4390         1327.8259
1393.1880        1398.3901         1413.5540
1458.3241        1481.7277         1503.4535
1543.4082        1607.9912         1641.1641
1664.3633        1982.7973         3110.0547
3123.2356        3156.1934         3158.5940
3161.0843        3164.1602         3175.6998
3185.1052        3188.4277         3192.0692
ZeroEnergy[kcal/mol]  -3.87
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts0-8-----
Barrier      ts0-8  i8  p0p
RRHO
Geometry[angstrom]  24
C   3.8633115301 -0.0440794168  0.4589066793
C   -0.1956131419 -0.7757107773 -0.5388711269
C   3.4331506641 -1.3620297341  0.1795217729
C   -1.0414716307  0.2880749698 -0.5628159708
C   0.668462941  1.8448319925  0.0146385202
C   -0.6504672173  1.6087075605 -0.3092268926
C   2.9716528658  0.9996604004  0.408381422
C   2.1210308113 -1.6102190511 -0.1440281117
C   1.608394198  0.7810114319  0.0780979564
C   1.1742369898 -0.5549596173 -0.2040016007
H   4.9013193597  0.1385398753  0.7131708494

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H   -0.5321951423  -1.7831201044  -0.7661123371
H   4.1457055042  -2.1783558897  0.2218830273
H   1.007673679   2.8552741353  0.223363542
H   -1.3620721668  2.4258458162  -0.365116992
H   3.3006028557   2.0116177142  0.6217135451
H   1.7903092524  -2.6211873369  -0.358771022
C   -3.2751057825  -0.066080178  -2.3254303348
C   -3.785972882  -0.1910688378  0.2627838996
C   -3.2600711642  -0.0820984077  -1.1056494094
H   -3.0630822686  -0.0142089083  -3.3662440418
H   -4.8656251739  -0.3611160585  0.2330390177
H   -3.5921150827  0.7205690926  0.8324180175
H   -3.3154969982  -1.0178686707  0.7991515905
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 364.7857
WellDepth[kcal/mol] 41.71
WellDepth[kcal/mol] 3.46
End
      Rotor      Hindered      ! 158 cm^-1      CH3
      Group                22 23 24
      Axis                19 20
      Symmetry            3
      Potential[kcal/mol] 4
0     0.67872755 1.281321244 0.644327475
End
      Rotor      Hindered      ! 22 cm^-1
      Group                18 19 21 22 23 24
      Axis                4 20
      Symmetry            1
      Potential[kcal/mol] 8
0     0.004344876 1.044571916 0.368266553 0.041007124 0.520076811 0.745740554
      0.385257003
End
Frequencies[1/cm] 63
                    44.1099
66.9173              152.6870
179.4465             224.6088              245.0673
360.6165             382.9342              390.1903
478.8857             491.0492              509.9220
515.8088             571.6787              623.9236
631.3283             679.4860              747.2507
766.8444             768.2011              781.7072
812.9915             854.3476              892.4799
917.9061             935.0115              957.4057
969.2578             994.7451              1029.4248
1041.5414            1053.8436              1065.4472
1144.9833            1162.1065              1172.9189
1210.9202            1253.9223              1277.7853
1346.1862            1385.5650              1393.6082
1414.4197            1459.3954              1467.7252
1477.0597            1481.2383              1531.2536

```

1596.1948	1614.1237	1657.1665
2070.3004	3033.7439	3097.6832
3100.8197	3146.7032	3147.9644
3155.6171	3160.5144	3167.2053
3173.3798	3186.3646	3454.9822

ZeroEnergy[kcal/mol] 3.46

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts8-p7-----

Barrier ts8-p7 i8 p7

RRHO

Geometry[angstrom] 24

C	-3.607398	0.177020	0.152335
C	0.460048	-0.951104	-0.151188
C	-3.247648	-1.189527	0.213804
C	1.441269	0.007563	-0.310815
C	-0.244628	1.753846	-0.273876
C	1.070530	1.381312	-0.366920
C	-2.641319	1.141496	-0.005446
C	-1.929975	-1.565153	0.116598
C	-1.272109	0.787733	-0.108779
C	-0.907222	-0.593792	-0.046290
C	3.778198	-0.850127	-1.064184
C	2.833363	-0.377225	-0.435119
C	3.540936	0.188144	1.635808
H	-4.651026	0.460175	0.230020
H	0.737239	-1.998382	-0.109269
H	-4.019142	-1.941098	0.337834
H	-0.516729	2.802833	-0.327641
H	1.845292	2.127387	-0.496294
H	-2.915632	2.190252	-0.053746
H	-1.652781	-2.613097	0.162854
H	4.746340	-1.198606	-1.337691
H	2.885754	-0.458225	2.206385
H	3.306610	1.245493	1.639920
H	4.589797	-0.077848	1.612070

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 532.2373

WellDepth[kcal/mol] 34.3

WellDepth[kcal/mol] 11.3

End

Frequencies[1/cm] 65

	27.7948		70.6610
77.6506	136.2543		154.8382
182.8958	239.8253		340.6894
356.8632	409.6971		409.9841
477.4442	485.2458		512.6473
521.5793	535.5788		559.8827

580.7187	633.6376	659.6130
688.4179	696.3183	759.1767
780.2217	782.3936	832.5819
873.5417	878.7338	902.0204
916.0132	964.9340	970.4237
980.3804	996.9217	1042.1040
1141.4150	1171.4461	1174.5510
1179.7892	1229.6648	1273.2195
1288.7322	1369.7715	1393.8886
1401.8953	1416.5141	1421.1694
1465.1758	1497.2007	1538.4098
1604.4867	1639.6767	1666.9434
1997.4584	3087.3002	3157.8222
3162.1219	3164.2455	3175.2643
3177.4559	3188.0410	3189.1667
3246.8920	3249.0233	3436.0875

ZeroEnergy[kcal/mol] -4.

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsmn-1-----

Barrier tsmn-1 r2 mn-1l

RRHO

Geometry[angstrom] 24

C	-0.6389986892	0.3692391033	-1.2801548731
C	-0.601579025	-1.0207399343	-0.9353612341
C	0.6533660484	-1.6002391902	-0.5942534005
C	1.8001804153	-0.8563636082	-0.5951031196
C	1.7875838308	0.5341831963	-0.9418565707
C	0.5615800214	1.1137911717	-1.268559774
C	-1.889629132	0.9515364968	-1.622445136
C	-3.04049936	0.2008132819	-1.623509571
C	-2.9999049562	-1.1705420383	-1.282691572
C	-1.8046534725	-1.7649528429	-0.9465599553
C	2.9984011289	1.3061000924	-0.8898617066
C	3.2336615476	1.9673138493	1.1476429554
C	3.8885732813	2.9938708911	1.3307408906
H	0.6866891625	-2.6538914693	-0.3360610131
H	2.7475527546	-1.3200626288	-0.3394498872
H	0.5240747855	2.1678945422	-1.5257054884
H	-1.9208744044	2.0041354469	-1.8840481532
H	-3.9872111809	0.6591213247	-1.8868319726
H	-3.9147774675	-1.7521022401	-1.2873128821
H	-1.7710768983	-2.817598417	-0.6847580986
H	3.002976315	2.2839159953	-1.3535728391
H	3.9448967437	0.7791577932	-0.9101191617
H	2.6683827284	1.1702693619	1.5873991533
H	4.4717048226	3.8695678219	1.1628274095

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 605.0258

```

WellDepth[kcal/mol] 10.09
WellDepth[kcal/mol] 24.73
End
  Rotor      Hindered      ! 20.6211 cm^-1
  Group      13 23 24
  Axis       11 12
  Symmetry   1
  Potential[kcal/mol] 8
0.13805211 0.564758631 1.267569372 1.098141783 1.25501918 1.261294276
0.24472874 0
End
Frequencies[1/cm] 64
 59.1401
 61.5064          144.6175          185.9499
246.7784          277.9663          303.8418
406.5284          410.4818          467.0712
481.8602          513.4999          525.3576
536.0586          616.7691          635.4578
659.2314          719.6623          734.5795
757.0187          775.1622          777.0309
780.0098          821.5655          829.2598
864.9599          895.0210          906.8460
941.4467          960.3659          965.2899
977.5935          992.5695          1032.9042
1043.6118         1146.1386         1171.1773
1178.0583         1199.8113         1239.6713
1287.6706         1289.5300         1383.2213
1389.8704         1407.9949         1467.4888
1481.5232         1495.7750         1536.4387
1590.7968         1627.9195         1651.4316
1840.8000         3140.3110         3153.7524
3156.7876         3158.7057         3162.5496
3172.4897         3175.1930         3188.0189
3232.2678         3318.2857         3436.2964
ZeroEnergy[kcal/mol] -11.16
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-2-----
Barrier      tsmn-2  mn-il  p6
RRHO
Geometry[angstrom] 24
C -0.949610531 0.4827335222 -1.2768744875
C -0.7330735802 -0.9123653483 -1.0538335951
C 0.5920137039 -1.3624808871 -0.8122787273
C 1.6439631497 -0.4836261064 -0.7926431338
C 1.4383437027 0.9035001491 -1.0159690887
C 0.1643730257 1.3631136174 -1.2504129878
C -2.2707419976 0.9403783592 -1.5178098886
C -3.3271260841 0.0617884376 -1.5377078987
C -3.112344705 -1.3184149218 -1.3176852689
C -1.8445467701 -1.7929443277 -1.081351938
C 2.6237257591 1.8552754638 -1.0116658794

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C  3.2631370147  1.9692295728  0.3098820746
C  3.5634652616  1.8573711767  1.4786502104
H  0.7621052144  -2.4206928604  -0.6426762255
H  2.6486094582  -0.84404082  -0.5994122069
H  -0.0081318476  2.4216370955  -1.4205244522
H  -2.4350559831  1.9996500972  -1.6864825123
H  -4.3319935859  0.4244302623  -1.7227735494
H  -3.9542979671  -2.0011914428  -1.3361115598
H  -1.677196044  -2.8515737851  -0.9117255264
H  2.3051919989  2.84778564  -1.341300392
H  3.3739582135  1.5209535617  -1.7372432255
H  4.6468418224  3.2172873438  -0.2853870924
H  3.9240037708  1.8480792005  2.4784493511
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  624.1305
WellDepth[kcal/mol]  36.4
WellDepth[kcal/mol]  2.8
End
Frequencies[1/cm]  65
  24.7714          72.4486
 109.5428         154.1196         181.2838
 253.0342         301.5283         351.7724
 383.7426         402.6246         415.6860
 464.3471         486.8895         508.1523
 526.8640         578.7459         636.5564
 652.2970         666.5684         671.9716
 739.5474         765.9545         781.3426
 787.6036         832.0249         869.4420
 879.9948         905.3636         944.9485
 950.0288         964.9519         977.9617
 979.9274         996.7217        1042.6382
1148.0577        1172.5005        1178.5426
1189.5417        1216.8459        1240.8888
1277.6252        1289.1872        1325.2412
1391.8643        1396.4297        1408.0138
1467.7060        1474.8653        1503.1880
1545.8818        1612.8787        1646.2070
1673.7260        2135.8734        3026.6537
3070.3082        3154.9384        3157.7416
3159.3163        3163.0361        3175.3200
3177.8495        3188.1362        3466.7810
ZeroEnergy[kcal/mol]  0.51
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_tsmn-3-----
Barrier      tsmn-3  mn-i1  i14
RRHO
Geometry[angstrom]  24
C  -0.6362089922  0.3346755835  -1.2274141317

```

C -0.412391283 -1.0559731236 -0.9794825603
 C 0.9226204213 -1.5059064863 -0.8042072262
 C 1.9768755467 -0.6310933717 -0.8702035951
 C 1.766960568 0.7514083609 -1.1217940198
 C 0.479032319 1.2095256762 -1.2892795875
 C -1.9686856352 0.7910044445 -1.4047607417
 C -3.0269675763 -0.0826346904 -1.3392802559
 C -2.8045956358 -1.4577980669 -1.0940203537
 C -1.5266925128 -1.9314810155 -0.9188669111
 C 2.9472569767 1.6985027419 -1.1474833239
 C 3.4070125929 2.05853459 0.2405398163
 C 3.2390751431 1.9011730372 1.511636095
 H 1.0991733125 -2.5604793175 -0.6186012192
 H 2.9903314687 -0.9932070516 -0.731615163
 H 0.3002598441 2.2642709182 -1.476662013
 H -2.1393029514 1.8461058771 -1.5924952681
 H -4.0397579002 0.2797109378 -1.4757801315
 H -3.6484601325 -2.1367258644 -1.045050266
 H -1.3530220728 -2.9860731439 -0.7309555749
 H 2.6904583502 2.6175072294 -1.6818221054
 H 3.7893580968 1.2518388158 -1.6861155173
 H 4.2049246565 2.6364285102 1.0654307203
 H 2.6605063954 1.4037964091 2.2903073337

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 2097.1150

WellDepth[kcal/mol] 44.2

WellDepth[kcal/mol] 44.9

End

Frequencies[1/cm] 65

26.0537	66.1572	
139.2234	145.3083	181.9257
206.9432	262.9083	286.6626
387.9592	402.8341	417.4265
484.0761	499.7438	526.7622
578.9405	605.4766	636.3640
666.4255	737.2542	764.4456
780.1790	787.3914	806.6637
833.9289	859.7972	877.2156
890.6235	912.0208	940.0204
962.3997	974.8245	975.8839
994.8873	1041.8304	1146.3639
1171.2697	1174.2692	1187.0200
1199.2341	1237.8815	1276.9933
1288.4755	1300.0740	1390.7228
1396.0645	1403.7207	1466.2900
1473.0094	1500.6325	1544.3549
1609.9926	1643.2902	1669.3337
1835.0960	2350.0291	3033.7509
3068.9785	3070.4742	3152.9156
3155.4180	3157.1283	3161.9988
3173.5712	3174.6418	3187.0869

```

ZeroEnergy[kcal/mol]  8.305
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-4-----
Barrier      tsmn-4  mn-i1  mn-i2
RRHO
Geometry[angstrom]  24
C  -0.4790295555  0.3069356129  -0.6689567885
C  -0.3287392414  -1.0063747335  -1.2108689607
C  0.9802609577  -1.5227643849  -1.4080266336
C  2.096787849  -0.7628407273  -1.1105390997
C  1.9771415555  0.5277210358  -0.5820137938
C  0.6956556921  1.0850743511  -0.3831723949
C  -1.7796394778  0.7996618145  -0.423101403
C  -2.8930126207  0.0426489003  -0.718762901
C  -2.7468692352  -1.2477480536  -1.2704302621
C  -1.4921512164  -1.7606029429  -1.5075379001
H  1.0933557801  -2.5235969887  -1.8108499383
H  3.0864537328  -1.1609725756  -1.3109127916
H  0.5767401554  1.9179544094  0.3015105951
H  -1.8919322474  1.7942083923  -0.0032774074
H  -3.8847887725  0.4370806624  -0.5282599518
H  -3.6276504185  -1.8357041903  -1.5031699457
H  -1.3768669907  -2.7560178903  -1.9241228324
C  3.1220988885  1.5081449441  -0.5425968609
C  2.6499743962  2.6854514216  -1.3910834407
C  1.3742753234  2.7451235831  -1.7054008626
H  4.0404839516  1.0686741969  -0.9431163126
H  3.3539876903  1.8477356573  0.4766406954
H  3.3759134298  3.4369190436  -1.7045757201
H  0.7492543736  3.4376584621  -2.252151089
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  475.2799
WellDepth[kcal/mol]  10.48
WellDepth[kcal/mol]  33.34
End
Frequencies[1/cm]  65
  92.3950          107.0654
 185.2105          222.9056          275.1700
 320.2466          393.0389          415.3753
 441.6260          503.3534          523.2359
 533.6426          605.8499          615.6057
 636.4648          665.5065          731.1497
 755.1392          764.8582          779.5092
 809.0104          832.6205          865.5919
 874.3605          877.7947          917.7902
 945.0018          955.7926          964.0567
 971.5221          984.7187          990.7801
1045.2911          1136.8374          1159.0389

```

1167.7610	1175.8887	1180.7567
1211.1648	1232.6915	1264.3820
1282.4989	1307.0283	1373.1645
1375.7422	1381.3252	1458.1468
1480.2077	1492.1996	1541.3613
1580.2646	1597.6864	1645.3784
1650.0171	2991.3736	3056.6726
3089.1219	3148.2944	3154.9261
3156.0342	3160.5082	3173.4303
3174.9447	3187.2040	3220.4014

ZeroEnergy[kcal/mol] -25.4

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsmn-5-----

Barrier tsmn-5 mn-i1 mn-i3

RRHO

Geometry[angstrom] 24

C	-0.6461584117	0.3978334291	-1.1995990802
C	-0.4415566816	-1.0198754535	-1.2252744105
C	0.8620718025	-1.5187328654	-1.4565592774
C	1.9585562921	-0.6583961971	-1.5862452748
C	1.7426966299	0.7723561669	-1.5291439573
C	0.4876712405	1.2614821242	-1.3361054616
C	-1.951659085	0.8964299149	-1.0061105976
C	-3.0233247909	0.0410516039	-0.848600169
C	-2.8262085512	-1.3553526432	-0.8787793579
C	-1.5643128136	-1.873074254	-1.0631318744
H	1.0022822786	-2.5896112621	-1.5608866121
H	2.8338680136	-1.0329422798	-2.106766113
H	0.3342565523	2.3315991494	-1.2297386545
H	-2.1037198572	1.9708204804	-0.9829644181
H	-4.0204735257	0.4407616436	-0.7027150738
H	-3.673678691	-2.0203814369	-0.7555710912
H	-1.4109502717	-2.9471224571	-1.0869629518
C	3.0016077848	1.5866707792	-1.3702140483
C	3.800265847	0.8456318915	-0.3042901052
C	3.4239465542	-0.3770800953	0.0015746609
H	2.7809769909	2.6144337074	-1.0684401277
H	3.583444162	1.6461664319	-2.3011057701
H	4.6519133378	1.3412070542	0.1637144182
H	3.7841521933	-1.1465834321	0.6700193474

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 484.9946

WellDepth[kcal/mol] 10.87

WellDepth[kcal/mol] 28.21

End

Frequencies[1/cm] 65

81.1076	122.8036	
198.9949	231.1270	289.3935

318.5343	392.0737	411.0484
436.9937	478.9848	524.8428
533.2215	603.9466	611.9573
629.7003	692.8485	735.0294
753.3704	767.6090	769.6908
819.6878	837.8671	867.7489
871.2519	878.8852	900.2651
919.0232	955.9608	963.0853
967.1598	985.4385	987.8107
1044.4720	1131.2542	1147.0060
1168.6268	1174.0644	1180.1658
1215.5694	1230.6181	1269.6016
1287.1172	1302.8591	1367.1305
1377.3714	1410.8545	1456.0338
1478.5397	1493.7478	1525.1069
1579.6208	1637.8297	1644.2099
1647.6862	2989.3310	3061.2303
3088.1306	3141.0730	3149.4127
3155.4267	3159.7451	3166.3164
3173.3667	3186.7659	3222.8247

ZeroEnergy[kcal/mol] -25.02

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsmn-6-----

Barrier tsmn-6 mn-i2 p2

RRHO

Geometry[angstrom] 24

C	-0.5431585318	0.28444469608	-1.254314169
C	-0.3750585149	-1.130347784	-1.1224270463
C	0.9321576871	-1.6942411106	-1.1443661879
C	2.0532685138	-0.9125634617	-1.3395208569
C	1.9081227941	0.4715879219	-1.4746627991
C	0.6478941254	1.0871595022	-1.3414813933
C	-1.8482911164	0.8228409839	-1.2671713452
C	-2.9504579439	0.0042559054	-1.1536644025
C	-2.7904207761	-1.3906050843	-1.0137627926
C	-1.5310224197	-1.9425644899	-0.9973946683
C	2.9377743328	1.5266424764	-1.7844383981
C	2.1011966299	2.7709930644	-1.9505243181
C	0.8092436716	2.511259235	-1.7008972565
H	1.0310655496	-2.7694829611	-1.0407732817
H	3.033853726	-1.3722992028	-1.4061917469
H	0.7341436927	1.3923050317	0.4763054388
H	-1.9804391838	1.8944366097	-1.3619510354
H	-3.9466208472	0.4319335051	-1.1684742103
H	-3.6642426892	-2.0254301132	-0.9196431389
H	-1.4048585134	-3.0152161701	-0.8925811261
H	3.5210878308	1.2871294931	-2.6818172329
H	3.663184563	1.6418217586	-0.9660536311
H	2.5157544668	3.7364258451	-2.2085552996
H	0.0034789527	3.2321430843	-1.7242731021

Core RigidRotor

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SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 854.6313
WellDepth[kcal/mol] 26.94
WellDepth[kcal/mol] 4.6
End
Frequencies[1/cm] 65
 116.4365          122.5008
 223.2674          241.3883          265.4556
 358.0528          415.6313          431.0966
 437.4702          453.4707          476.6655
 519.4125          528.4797          563.2209
 613.9871          670.7765          685.2471
 729.7133          748.6334          752.1415
 798.6184          817.3495          838.0568
 876.8011          882.4173          933.0253
 950.6989          955.2966          960.5532
 965.3510          971.4390          992.6117
1046.9314          1070.6594          1128.2978
1146.0464          1164.2136          1178.3772
1188.3982          1220.4813          1236.1316
1283.5718          1287.8093          1343.3324
1370.3028          1379.8085          1412.2898
1432.6903          1463.5931          1480.7814
1553.4122          1577.0900          1608.2204
1629.1320          1655.7440          2998.6132
3035.1895          3157.7020          3159.4328
3167.2225          3176.5199          3179.2687
3189.3955          3198.6157          3220.8770
ZeroEnergy[kcal/mol] -31.8
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-7-----
Barrier      tsmn-7  mn-i2  i18
RRHO
Geometry[angstrom] 24
C -0.5587257519  0.2878708873  -1.2891773475
C -0.3780754238  -1.1229679605  -1.1318322895
C 0.930708032   -1.6878309641  -1.1593276164
C 2.0484312923  -0.8972553338  -1.3725714189
C 1.9145580032  0.4815636867  -1.5202156089
C 0.6346811116  1.0952034419  -1.4039340014
C -1.8631280188  0.8209813915  -1.3039209946
C -2.9655474667  0.0037185522  -1.1569121078
C -2.7963773355  -1.3845574543  -0.9894865387
C -1.5327451352  -1.9314347049  -0.9791691333
C 2.9601576614  1.5377248796  -1.812123924
C 2.1434298315  2.7973191587  -1.9810356467
C 0.8156482106  2.5512707245  -1.6868172611
H 1.0345626781  -2.7606903674  -1.0442110692
H 3.0286254145  -1.3579045931  -1.4475182344

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H  0.6995046393  2.0211486481  -0.3886081962
H -2.0023178926  1.8891655475  -1.4313907123
H -3.9624879639  0.4291620553  -1.1723282001
H -3.6651647114  -2.0226295239  -0.8721427715
H -1.4030194248  -3.001818233  -0.8566854088
H  3.5685252769  1.2966494348  -2.69653942
H  3.6845351243  1.6325610414  -0.9825010603
H  2.5682019804  3.7751495786  -2.1561918724
H -0.0055601313  3.2490041069  -1.7721401659
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1736.8753
WellDepth[kcal/mol]  35.5
WellDepth[kcal/mol]  42.7
End
Frequencies[1/cm]  65
  113.2919          116.3001
  208.7717          238.4120          276.9393
  348.5072          425.3786          429.6242
  453.0556          505.4522          518.6148
  557.0659          604.0619          614.6114
  670.6636          690.2612          738.2702
  747.0695          777.8744          797.2688
  817.5498          869.5403          871.6568
  893.3202          911.2574          937.0683
  948.8953          950.3326          958.8519
  986.7463          1034.4467          1052.9464
 1070.1044          1115.4732          1128.8055
 1157.9448          1172.6341          1182.9639
 1218.8348          1234.7324          1272.2841
 1274.1053          1289.4410          1322.8982
 1358.5996          1378.8946          1412.7542
 1449.7064          1459.3494          1481.5952
 1494.4821          1557.7716          1568.8158
 1599.1869          1647.3383          2906.3973
 2966.3113          3155.1357          3157.0388
 3162.6648          3174.6082          3179.0758
 3187.7702          3209.1003          3225.4687
ZeroEnergy[kcal/mol]  -23.25
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_tsmn-8-----
Barrier      tsmn-8  mn-i3  p1
RRHO
Geometry[angstrom]  24
C -0.6649750685  0.3498241785  -1.0438599196
C -0.5151214502  -1.078413859  -1.0868134034
C  0.7758299291  -1.6489532472  -0.9930029601
C  1.8975160299  -0.8193479568  -0.9607667449
C  1.7281654333  0.6100295364  -0.8107919995

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C  0.4918530426  1.1728022134  -0.8717473397
C  -1.9638329859  0.901388626  -1.1325335775
C  -3.0734838518  0.0948799967  -1.2582196636
C  -2.9294809065  -1.3092898254  -1.2947259147
C  -1.6817348516  -1.8798695673  -1.209209098
C  3.0821947953  1.2261111078  -0.5426067858
C  3.9718514379  0.0140210495  -0.3819661731
C  3.3030485587  -1.1218280689  -0.6209842303
H  0.8863650387  -2.7280086979  -1.0095260641
H  2.2058660925  -0.8400926233  -2.7161480226
H  0.3564809204  2.2451425095  -0.7656180288
H  -2.0749242616  1.9804317416  -1.0989062857
H  -4.0612575646  0.5362698315  -1.3271511293
H  -3.8081846997  -1.9369014352  -1.3923133522
H  -1.569801227  -2.9587378099  -1.2399439795
H  3.0791099184  1.8678595517  0.3457688243
H  3.4191135302  1.8539175587  -1.3795260797
H  5.0223667616  0.084469679  -0.1310274904
H  3.713620379  -2.1228974894  -0.5979175816
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  936.8455
WellDepth[kcal/mol]  22.72
WellDepth[kcal/mol]  6.0
End
Frequencies[1/cm]  65
100.7747          127.8661
246.0540          265.2670          274.6117
367.4844          386.7345          412.7468
417.0324          458.5308          480.6069
529.6491          557.0359          580.6545
627.2206          692.4116          730.6713
736.2687          748.5734          764.7916
777.4309          804.8009          847.5371
856.8348          887.3842          898.4819
913.4696          955.0251          956.8007
962.2296          972.9807          990.7558
1044.2092         1072.6971         1123.0515
1158.4589         1167.0487         1173.2080
1175.0963         1236.8100         1250.6091
1270.4424         1282.8555         1337.3224
1369.8774         1379.7235         1430.0866
1443.1412         1456.8825         1481.3482
1530.8031         1591.5961         1633.5964
1648.4333         1661.7177         2999.2288
3039.3563         3153.7716         3157.2237
3161.4542         3168.2137         3174.9873
3188.0665         3192.2697         3214.4007
ZeroEnergy[kcal/mol]  -30.52
ElectronicLevels[1/cm]  1
0  2
End

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!-----
!-----bar_tsmn-9-----
Barrier      tsmn-9  mn-i3  i17
RRHO
Geometry[angstrom]  24
C  -0.6583616616  0.3390080985  -1.0239705207
C  -0.5081754083  -1.0907963225  -1.066925169
C   0.7743810646  -1.6703414695  -0.9477951003
C   1.9054767399  -0.8388828478  -0.8748246502
C   1.7403372295  0.6029238367  -0.7587866294
C   0.5042876856  1.1577553653  -0.8382652921
C  -1.9488470596  0.8966705115  -1.1320339592
C  -3.0654441268  0.0977987088  -1.2770870256
C  -2.924100894  -1.3049910603  -1.3130073985
C  -1.6801055962  -1.8837272802  -1.2087229562
C   3.093799043  1.2405728617  -0.5007196955
C   4.0150075598  0.053727334  -0.3300446974
C   3.3474462557  -1.1201306746  -0.6069109973
H   0.8783303298  -2.749993048  -0.9575411706
H   2.7641611065  -1.0587794915  -1.9225052066
H   0.3700331599  2.2307779837  -0.7344332388
H  -2.0532595226  1.9766531403  -1.0972469279
H  -4.0493912538  0.544813958  -1.3597942061
H  -3.8031544475  -1.9304257975  -1.4240047226
H  -1.5762541007  -2.9635997942  -1.2375402273
H   3.0811925811  1.9043984233  0.3735073422
H   3.4067364358  1.8720888669  -1.348898163
H   5.0804337398  0.1373959761  -0.1710312181
H   3.7425161402  -2.124959279  -0.5382541695
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1655.3310
WellDepth[kcal/mol]  30.92
WellDepth[kcal/mol]  43.0
End
Frequencies[1/cm]  65
  98.7920          123.7897
 230.3323          260.5557          290.0181
 365.5999          399.5327          406.5101
 416.6014          474.7979          553.1663
 573.5465          617.4006          626.4955
 691.8892          720.1288          729.0775
 749.8922          766.3660          790.8640
 811.3074          827.3898          863.0042
 880.6688          907.5446          911.3384
 934.2643          946.6110          954.9870
 981.7713          1010.0694          1044.7023
1061.3917          1111.0032          1144.0401
1160.1134          1167.7206          1171.6951
1202.2499          1229.5259          1244.5482
1269.3754          1282.7355          1320.2745
1361.1446          1372.4546          1430.2358

```

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1436.2856          1457.6756          1472.9618
1504.1864          1531.4304          1584.5236
1638.0755          1665.8993          2943.4659
3000.5294          3150.2912          3153.9760
3157.8941          3166.1033          3172.4671
3186.8611          3203.6708          3222.3346
ZeroEnergy[kcal/mol] -22.32
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-10-----
Barrier      tsmn-10  mn-11  i9
RRHO
Geometry[angstrom] 24
C -0.9473752436  0.0852881993  -0.368348483
C -0.7039030592  -1.275688744  -0.666055519
C  0.619439176  -1.7961693769  -0.502014226
C  1.6392041334  -0.9176155089  -0.0466259375
C  1.3722635941  0.3963015777  0.2326595721
C  0.0579230235  0.929105667  0.0812822552
C -0.2281337521  2.3447418571  0.3538116141
C  0.7240073992  3.2352382234  1.1066085787
C  1.0911906179  4.0566558902  0.1378185244
C  0.8635976206  -3.1597190714  -0.7993435566
C -1.7286784483  -2.1481333225  -1.1214700497
C -1.4588704742  -3.4655339539  -1.4015744972
C -0.1503933264  -3.9776664804  -1.2392845413
H -1.954441739  0.4722313022  -0.4935246663
H  2.6447306777  -1.3066602929  0.0777534783
H  2.1667459887  1.0519886903  0.5693134392
H -1.2848877773  2.580337562  0.4882177891
H  0.9997584024  3.1916096255  2.156256782
H  1.7424672715  4.918927207  0.016909945
H  1.8682503568  -3.5502894886  -0.6738768885
H -2.7324123957  -1.7550640823  -1.2459758852
H -2.250376944  -4.1201056815  -1.748970852
H  0.0490470512  -5.0194128701  -1.463658521
H  0.1669278469  3.2048730716  -0.6469363547
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 2122.5216
WellDepth[kcal/mol] 34.29
WellDepth[kcal/mol] 64.1
End
Frequencies[1/cm] 65
                    54.3056                    94.0947
138.6540          184.6765          200.0693
278.5528          347.0347          383.7281
408.1124          482.3517          506.6690
525.9362          542.2272          606.1634
648.0751          656.9472          684.0016

```

749.6175	760.9583	779.0098
781.6866	832.9367	864.1872
876.1244	893.9116	915.5970
917.9764	948.9285	963.5626
968.7118	983.5000	995.0404
1039.4707	1043.8102	1144.1199
1151.8888	1172.9264	1178.8161
1190.3300	1212.5603	1241.2019
1276.0086	1289.1218	1317.9242
1393.8477	1396.2964	1406.5067
1471.3514	1497.4289	1540.6742
1599.9580	1623.0898	1635.9646
1659.5215	1786.2614	3088.2568
3128.7007	3153.0534	3157.3754
3159.5966	3163.0921	3168.2145
3175.1098	3184.6336	3187.9315

```

ZeroEnergy[kcal/mol] -1.6
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-11-----

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Barrier      tsmn-11  mn-11  i15
RRHO

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```

Geometry[angstrom] 24
C -1.3401066434 0.5935392212 -0.4693204595
C -1.2440736979 -0.8164815965 -0.3476715246
C 0.0432994645 -1.4427476688 -0.4088521847
C 1.1911851928 -0.6220573723 -0.5910491223
C 1.0280848018 0.7274019288 -0.7009281029
C -0.2177510987 1.3783918503 -0.6458919273
C -0.3019866652 2.8877708178 -0.7778623527
C 1.0251337452 3.5862888842 -0.9652825348
C 2.1855513521 2.9582828047 -1.0145167261
C 0.1282063158 -2.8544166989 -0.285995364
C -2.3907155372 -1.635692009 -0.1656001604
C -2.2741954386 -2.9988456016 -0.0501452848
C -1.0016412577 -3.6149653327 -0.1109543323
H -2.3244376106 1.0523196908 -0.420692937
H 2.1726209996 -1.0839202533 -0.6390986904
H -0.9580240383 3.1453873151 -1.6196684812
H -0.7982589761 3.305359052 0.1079815989
H 0.9747583739 4.672432048 -1.0611670585
H 3.1815777423 3.3646233884 -1.144291498
H 1.1051486708 -3.3243964708 -0.3330716273
H -3.3667257376 -1.1635602921 -0.1189769366
H -3.1588927679 -3.6101577807 0.0884089788
H -0.9231579617 -4.6924470688 -0.0185072979
H 1.9714607722 1.663144144 -0.8748299744

```

```

Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 1596.8574

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WellDepth[kcal/mol] 13.74
WellDepth[kcal/mol] 9.8
End
Frequencies[1/cm] 65
  57.6932          109.4457
 184.3476          211.0461          254.4947
 279.7375          362.2620          394.3791
 395.2767          480.7697          505.9581
 522.3337          580.1375          593.1312
 626.9119          641.9950          647.3408
 754.9206          772.5429          775.6939
 785.2831          853.4719          867.5964
 876.1914          897.8665          909.7460
 937.7603          964.1830          968.1538
 974.0550          994.1834          1036.9667
1040.9473          1048.8049          1150.0193
1170.1355          1181.6803          1219.8714
1224.9577          1248.2629          1279.8404
1286.1231          1306.6344          1359.5529
1393.5968          1397.5978          1445.8340
1466.8118          1471.5814          1529.0301
1584.1821          1603.5666          1629.8055
1659.3300          1702.2222          3002.6494
3018.0040          3081.0025          3141.3914
3154.4063          3156.5486          3161.7540
3174.0858          3186.7529          3188.2215
ZeroEnergy[kcal/mol] -22.16
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_tsmn-12-----
Barrier      tsmn-12  mn-i1  i16
RRHO
Geometry[angstrom] 24
C -1.9318290509  0.1144192363  -0.6136800027
C -1.8301357676  -1.2457385598  -0.4677721374
C -0.5651303371  -1.8883554765  -0.37446389
C 0.6220489304  -1.0847724956  -0.4357006713
C 0.4492703131  0.3070275904  -0.5863947294
C -0.763903447  0.9282123181  -0.6763955173
C -0.8692929912  2.4296092882  -0.8374210856
C 0.4542011067  3.1541386193  -0.8869123483
C 1.6210946715  2.5427051283  -0.7987679252
C -0.4298423882  -3.2918372729  -0.2232647338
C 1.8878710101  -1.7182055073  -0.3433478329
C 0.8115261003  -3.8756651817  -0.1366041606
C 1.9798124635  -3.0817128623  -0.1972189814
H -2.9099335673  0.5814121658  -0.6826455806
H -2.7265982049  -1.8553504751  -0.4212287932
H -1.4366898192  2.6604378661  -1.749420506
H -1.4723818985  2.843719347  -0.0178229947
H 0.3972869345  4.2379633656  -1.0023821819
H 2.6204902425  2.960839904  -0.8225939867

```

```

H -1.3267641938 -3.9013349352 -0.1767522395
H 2.7821498358 -1.1067974782 -0.3902064448
H 0.8996760622 -4.9501066882 -0.0211555418
H 2.9527004303 -3.5552798667 -0.1276246204
H 1.4064745647 1.2453929703 -0.6661830943
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1605.1580
WellDepth[kcal/mol] 12.73
WellDepth[kcal/mol] 8.3
End
Frequencies[1/cm] 65
 75.6390 108.9106
182.4327 187.3607 244.2509
284.4285 385.0871 412.0070
438.0837 474.7319 503.9353
504.8831 533.4497 593.8664
618.3254 639.0435 682.1187
736.0109 752.3495 776.7306
809.7794 819.2441 875.3598
895.8486 923.3088 929.8456
955.4875 961.6389 968.1924
972.8955 995.0600 1036.9993
1040.4680 1052.9065 1143.8845
1168.6140 1172.1886 1198.8494
1216.8894 1236.3143 1271.1815
1279.9402 1334.2589 1367.3675
1380.7978 1398.9629 1453.1441
1457.6417 1492.7089 1532.2342
1564.1857 1601.1206 1641.1430
1661.2136 1705.7271 2997.6000
3011.6660 3081.8144 3148.5331
3156.0814 3165.1489 3170.7521
3177.3739 3186.5593 3188.2699
ZeroEnergy[kcal/mol] -23.17
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```