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Theoretical Investigation of the Reactivity of Methylcyclopentadiene

Tesi di Laurea Magistrale in
Chemical Engineering - Ingegneria Chimica

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Abstract

The reactivity of methylcyclopentadiene is studied in this thesis through ab initio transition state theory master equation simulations, a method that is purely based on computations and no experimental data. The analyzed reaction classes are: abstraction, beta-scission, and isomerization. The abstraction reactions lead to the production of methylcyclopentadienyl radicals from three different isomers of methylcyclopentadiene. The H-abstraction (removal of H atom) reactions are given by attacks of H, CH_3, OH and OOH molecules on methylcyclopentadiene. The produced radicals undergo isomerization reactions to form other radicals, and finally some of these radicals lose one hydrogen atom by beta-scission and produce benzene or fulvene. In the calculations two different computer programs were used for the electronic structure calculations to find structures and energies of the molecules: Gaussian and Molpro. The software MESS is used for the solution of the master equation to find the reactions rate constants. Finally, OpenSMOKE++ is used for the kinetic simulations performed with the obtained rate parameters to test their predictive capability. Two other codes, namely EStokTP, which is used for making the process less dependent on human intervention, and MEL, which is used to lump the rate constants for molecules with similar reactivities and structures, have been used in the course of this work. Comparison of rate constant values in the literature with those computed in this thesis showed good agreement. Kinetic simulations performed using a kinetic mechanism developed by the CRECK group of Politecnico di Milano were used to study a literature system. The plots of the mole fractions of the outlet species from the reference article and the results of the kinetic simulations of this thesis are compared with each other, exhibiting similar trends. Finally, the evolution of the mole fractions of the main molecules studied in this thesis in the simulated experimental setup are compared with those predicted by the unmodified CRECK mechanism, and the impact of the modifications is discussed.

Keywords: Ab initio; Abstraction; Decomposition; Kinetic simulations; Master equation; Methylcyclopentadiene

Abstract in Lingua Italiana

La presente tesi studia la reattività del metilciclopentadiene utilizzando metodi di simulazione ab initio basati sulla master equation e sulla teoria dello stato di transizione, così da ottenere una procedura puramente basata su calcoli teorici e nessun dato sperimentale. Le classi di reazione analizzate in questa tesi sono: eliminazione, beta-scissione, e isomerizzazione. Le reazioni di eliminazione portano alla produzione di radicali metilciclopentadienilici da tre diversi isomeri del metilciclopentadiene. Le reazioni di H-eliminazione (rimozione dell'atomo H) sono ottenute mediante attacchi di H, CH_3, OH e OOH al metilciclopentadiene. I radicali prodotti subiscono successivamente reazioni di isomerizzazione per produrre altri radicali e infine alcuni di questi perdono uno degli atomi di idrogeno mediante una reazione di beta-scissione e producono benzene o fulvene. Durante i calcoli sono stati utilizzati due diversi software per i calcoli di struttura elettronica per trovare strutture e energie delle molecole: Gaussian e Molpro. Il software MESS viene utilizzato per la soluzione della master equation e trovare le costanti di velocità per le reazioni. Infine, OpenSMOKE++ è stato usato per le simulazioni cinetiche eseguite con i parametri di velocità ottenuti per testare la loro capacità predittiva. Nel corso di questo lavoro sono stati utilizzati altri due codici, vale a dire EStokTP, che viene utilizzato per rendere il processo meno dipendente dall'intervento umano, e MEL, che viene utilizzato per raggruppare le costanti di velocità per molecole con reattività e strutture simili. Il confronto tra i valori delle costanti di velocità in letteratura e questa tesi ha mostrato un buon accordo. Simulazioni cinetiche eseguite utilizzano un meccanismo cinetico sviluppato dal gruppo CRECK del Politecnico di Milano sono state utilizzate per studiare un sistema di letteratura. I grafici delle frazioni molari delle specie in uscita dal reattore nell'articolo di riferimento e i risultati delle simulazioni cinetiche di questa tesi vengono confrontati tra loro, mostrando andamenti coerenti. Infine, l'evoluzione delle frazioni molari delle principali molecole studiate in questa tesi nel setup sperimentale simulato viene confrontata con quelle previste dal meccanismo CRECK non modificato, e viene discusso l'impatto delle modifiche.

Parole chiave: Ab initio; Eliminazione; Decomposizione; Simulazioni cinetiche; Master Equation; Metilciclopentadiene

Contents

1 | Introduction

In order to better understand the aim of the thesis, it may be useful to know some information that led to the existence of a work like this one. Some of the important background information related to the purpose of this work such as the soot growth and oxidation mechanisms, methylcyclopentadiene reactivity and the main aim of the thesis are shortly mentioned in the next sections of this chapter.

1.1. Background

Sciences can be classified by their applications. For example, they can be experimental or theoretical. Scientists that are working on experimental sciences try to understand the nature by experiments, whereas a theoretical scientist tries to do the same thing with a theoretical background (by using equations).

By their nature, engineering applications generally belong to the experimental sciences. For example, a chemical engineer generally works in a factory or a plant that aims to produce a chemical substance from the raw materials. Because of the changing variables (like the air temperature, corrosion etc.) and the differential equations that cannot be easily solved, it is easier for an engineer to modify the process not by theory but by checking the process conditions with a control system. However, there are also some applications of chemical engineering that belong to the theoretical sciences like modeling and simulation.

The part of the theoretical chemical engineering, where the researcher uses a computer to look for the parameters of a reaction, can be named "computational chemistry". Richard P. Feynman tells, the need for using a computer for running some calculations is because the physical laws are not so perfectly known [11]. Computational calculations in general can be used for many different applications, from finding the reaction kinetic parameters to observing the flow of complex fluids. The importance of using computational chemistry instead of experiments for kinetic parameter calculations is that it allows to observe the chemical dynamics of short living molecules like radicals or even transition states. This is almost impossible to observe in most (if not all) cases by experiments. One other very important advantage is, running some experiments with chemicals can be very expensive for some cases. In such a case running computational analysis can be very cost effective. Even for some cases the reactions could be highly exothermic, highly endothermic, or maybe even nuclear when the researcher works with radioactive substances, in which case he has to be very careful. Computational calculations allow the researcher to work safely and easily in such cases. The worst possible thing that can happen is a code that did not converge and has to be run from the beginning, which is for sure much better than having a catastrophic accident.

Kinetic parameters of a reaction can be obtained either by experiments or by computational calculations, as stated above. For computational calculations, a High Performance Computer (HPC) (or at least a computer that has many available cores for the calculations) is preferred to be used since the computations can require many hours (some complex calculations may even require days of computation) for a regular computer. Even for some cases the job may require so much time and cannot be performed by a classical computer due to classical algorithms and hardware. In that situation a quantum computer, which is a promise of the future, may help to obtain results within an acceptable timeframe through what is called "quantum supremacy" or "quantum computational advantage" [35]. For one single particle many computers could be used to solve the Schrödinger equation. However, for a large system with a high number of particles, these computers would not be enough for a complete description of quantum mechanics [11]. Even if they could be used for some cases, it would not be an effective way to run the simulations.

1.2. Mechanism of Soot Growth and Oxidation

The mechanism of soot formation has always been a very important subject of research for both scientific and industrial applications, especially for the designers and the operators of combustion systems. Thanks to the research in the last years, there are major improvements in understanding the mechanisms and the phenomenon behind soot formation. Even though the chemistry and physics are relatively well known, still the elementary aspects of soot formation are not known very well, and debates still continue on this topic in the literature. That causes a huge problem for so many industries, such as the diesel engine designers, who have strict limits for the particulate matter emissions from the engines, as well as for nitro-oxides emissions.

Soot is a substance that mainly contains carbon atoms, with relatively smaller amounts of hydrogen and oxygen. Combustion or pyrolysis of hydrocarbons at high temperature causes formation of soot. It is a very complex and a very rapid process. The competition between the formation and the oxidation of soot determines the extent of emission of carbon particulate from a flame or a combustor. That is why, in order to have a complete model one must take both soot formation and oxidation into account.

Some of the main difficulties for a model are:
- Discrimination of a molecule and a particle during soot nucleation reactions.
- Many unknown elementary reactions.
- Large number of polycyclic aromatic hydrocarbon isomers.
- Not knowing enough about the thermodynamic and kinetic parameters for so many species.

Pyrolysis of hydrocarbons produce acetylene or similar small hydrocarbons. The first step of soot production is the formation of some aromatic species from the aliphatic hydrocarbons. Once the aromatic species are formed, they tend to form larger aromatic species by addition reactions between each other and with some small alkyl species. In the end large polyaromatic hydrocarbons are formed.

In a flame, the soot particles are formed by chemically controlled phenomena, which means just some milliseconds are needed for the gaseous hydrocarbons to form solid carbon. The formation of soot occurs where it is beyond the thermodynamically stable regimes (with respect to the carbon-oxides), hence thermodynamics alone cannot describe the soot formation process. That shows the importance of chemical kinetics for soot formation [21].

To better understand the soot formation mechanism, particle inception (nucleation), coagulation, aggregation, and finally condensation processes need to be taken into account. Currently, three processes that occur in parallel are considered for the formation and growth of soot. They are nucleation, surface growth, and coagulation [28]. An illustration of the soot growth process is reported on Figure 1.1.

Particle inception starts the production of soot, and compared to the chemistry of pre-particles, soot growth and oxidation has some qualitatively different behavior. Even though some of the old models were totally based on inception, they reached the conclusion that there is a linear dependence between the rate of inception of soot and the net amount of soot produced. The explanation behind that conclusion is due to the fact that the surface growth rates depend linearly on the surface area that is available for the molecules, which in fact depends on the total number of the created (by inception or nucleation) particles. That is why for so many years, these processes were researched by so many research groups.

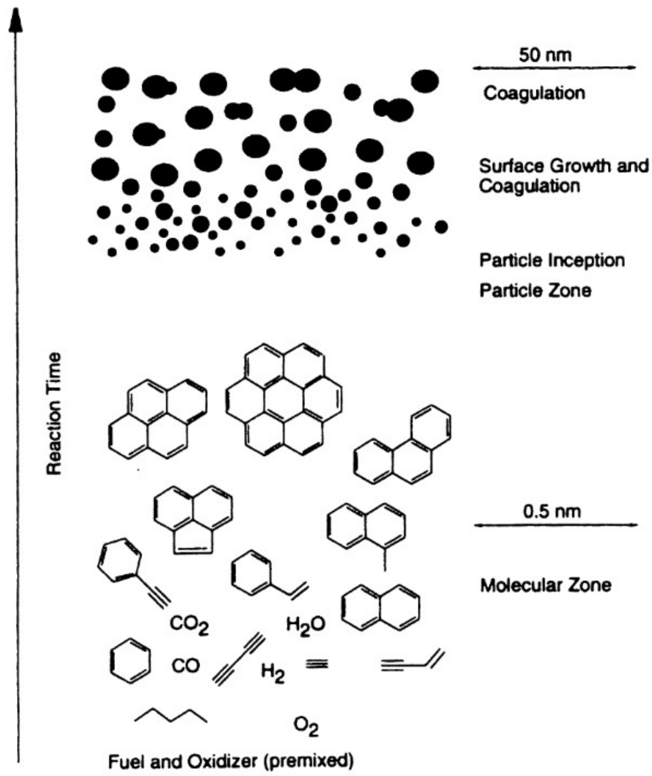


Figure 1.1: An illustration of formation of soot [27].

Surface growth has a very important contribution for soot growth. Even though the surface reactions are not very well known, the following reaction mechanism is suggested by some previous works:

$$C_{soot} - H + H \Rightarrow C_{soot*} + H_2 \tag{1.1}$$

$$C_{soot*} + H_2 \Rightarrow C_{soot} - H + H \tag{1.2}$$

$$C_{soot*} + H \Rightarrow C_{soot} - H \tag{1.3}$$

$$C_{soot*} + C_2H_2 \Rightarrow C_{soot} - H + H \tag{1.4}$$

$$C_{soot*} + O_2 \Rightarrow \text{Products} \tag{1.5}$$

$$C_{soot*} - H + OH \Rightarrow \text{Products} \tag{1.6}$$

The first reaction is the activation of the reactive sites of the surface, caused by hydrogen abstraction. The fourth reaction is soot growth by acetylene addition. The fifth and the sixth reactions (the oxidation reactions) are competing reactions to the other ones.

The last process, namely coagulation, further increases the size of soot by the collisions of other soot particles. Smoluchowski's Brownian coagulation equations can be used to describe particle coagulation [28], which are given below:

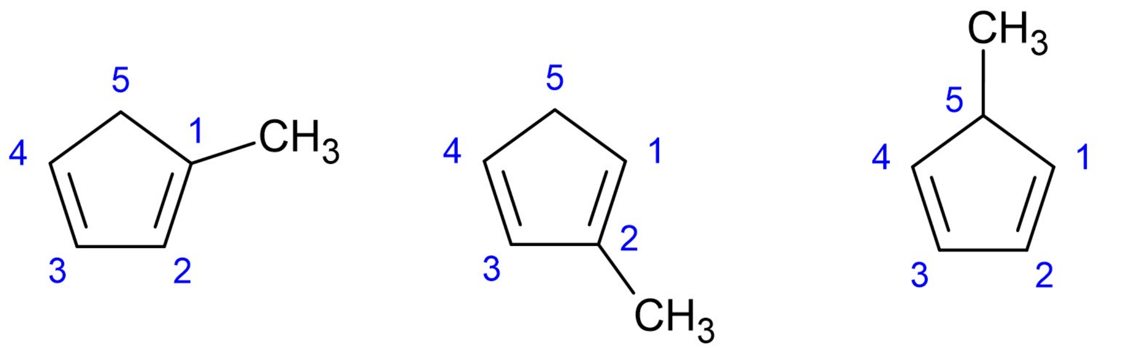
$$\frac{dN_1}{dt} = -N_1 \sum_{j=1}^{\infty} \beta_{1,j} N_j \tag{1.7}$$

$$\frac{dN_i}{dt} = \frac{1}{2} \sum_{j=1}^{i-1} \beta_{j,i-j} N_j N_{i-j} - N_i \sum_{j=1}^{\infty} \beta_{i,j} N_j \quad (i = 2, 3, ..., \infty) \tag{1.8}$$

N_i in the equations above represent the number density of the particles with the size i, $\beta_{i,j}$ represents the frequency of collision between the particles i and j.

1.3. The Reactivity of Methylcyclopentadiene

Methylcyclopentadiene (MCPE), which is a commercially available chemical substance, is formed as a by-product of the thermal cracking reactions of hydrocarbons. It has six carbon atoms and eight hydrogen atoms with two double bonds. Pyrolysis of MCPE dimer forms a mixture that is mainly composed of isomeric MCPEs and little amounts of cyclopentadiene. Depending on the location of the methyl group that is attached to an sp^3 carbon, there are three possible isomers of methylcyclopentadiene: 1-methylcyclopentadiene, 2-methylcyclopentadiene and 5-methylcyclopentadiene [4], as shown in Figure 1.2.



1-methylcyclopentadiene 2-methylcyclopentadiene 5-methylcyclopentadiene

Figure 1.2: Isomers of methylcyclopentadiene.

It is known that MCPE is a highly reactive and a hazardous compound. Some of these hazardous reactions are ring expansion, decomposition, dimerization, oxidation, isomerization, and polymerization [31]. An example of the ring opening reaction, with its steps, can be seen in Figure 1.3, where the radical of 5-methylcyclopentadiene (namely 5-methylcyclopentadienyl) forms cyclohexadienyl.

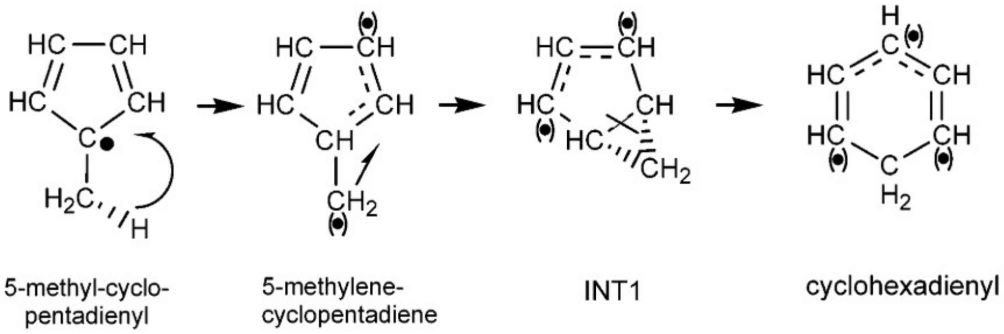


Figure 1.3: Ring opening of 5-methylcyclopentadienyl [7].

Because MCPE is a reactive molecule with three isomers, it is also likely to have isomerization reactions between them. An illustration of the isomerization reactions between them with the relative transition states is reported in Figure 1.4.

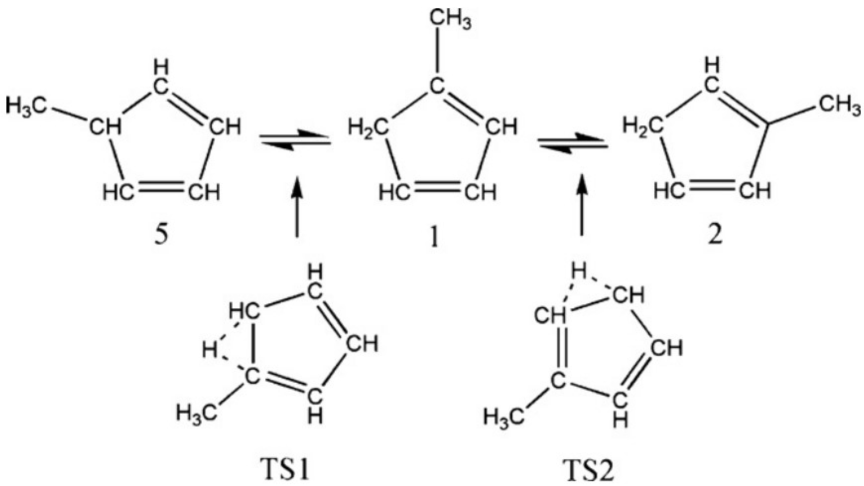


Figure 1.4: Isomerization reactions between MCPE isomers [31].

1.4. Aim of the Thesis

Between the years 1980 and 2001, there were 167 incidents caused by chemical reactions. In average five people lost their lives annually. In 2007 there was also an industrial accident caused by methylcyclopentadiene, which resulted four people to lose their lives and led to some injuries [31]. Most probably, the main reason behind these accidents is not knowing a lot about the chemistry of the reactants, products, and the reaction intermediates. This shows the importance of understanding the chemistry of hazardous compounds and thermal runaway reactions.

For most of the reactions, one can find the information related to the chemical reactivity from the literature or by a simple calorimetric experiment. However, for some reactive chemicals there is not enough experimental data which means literature review cannot provide enough information. Methylcyclopentadiene is one of the chemicals that is not experimentally well known. For a chemical like this one, estimation methods play a crucial role for providing information.

This thesis aims to run molecular simulations completely based on computations (and nothing experimental) for methylcyclopentadiene in order to better understand its reactivity. This can lead to the design of safer processes and safer storage or handling of methylcyclopentadiene in the future, which may prevent other catastrophic incidents caused by MCPE.

The reaction rate parameters are obtained after a series of calculations such as the energies, symmetry numbers, hindered rotor scans of the reactants, products, and transition states. The programs used for the calculation are Gaussian, Molpro and Mess. The first two are used for the electronic structure calculations and the last one is used for the master equation simulations (which provided the reaction rates). These calculations are usually done by separate codes, however Cavallotti et al. [3] provided a code that is available for public use which can combine the calculations. That code is the backbone of this thesis for the calculations. After the rates are determined, to be sure if all the elementary reactions are necessary or their number can be decreased, master equation lumping calculations are done by the code developed by Pratali Maffei et al. [24], which is also available for public use.

2 | Methodology

In a scientific work, understanding the used methods is at least as important as the results of it. This chapter aims to shortly mention the methodology behind the calculations, and be a guide for the following chapters.

The master equation, which focuses on the time-dependent variations of the populations of the energy resolved species, can be used to relate the microscopic processes to the thermal reaction rates. To be able to use the master equation it is necessary to have the knowledge of possible reaction pathways, the rate constants for these reactions, and the possible models for the processes related to the energy transfer.

Ab initio electronic structure theory can be used to map the reaction pathways. The rovibrational properties of the stationary points on a potential energy surface (PES) can be determined with this method. To be able to find the microcanonical rate constants for transformation of a species to another one, these properties can be combined with transition state theory (TST) [22].

The combination of the methods described above, leads to the ab initio transition state theory master equation simulations (AITSTME) method, which is very useful for the determination of the kinetics for reactions that involve gaseous phases. It should be noted that the selected methodologies affect the predictions remarkably [24]. In the recent years, the AITSTME method has been used in a lot of researches for the determination of complex gas-phase reaction kinetics.

AITSTME calculations are achieved in three steps: Ab initio electronic structure calculations are done for the prediction of the molecular properties of the species of interest. The second step is to find the microcanonical reaction rates with transition state theory, in order to find the rates for this step the properties determined from the previous step are used as an input data. The final step is the determination of the phenomenological rate constants by solving the master equation with a software, this step requires the obtained microcanonical rate constants and the energy transfer rates between the molecules as input.

The transition state theory and the master equation calculations are generally done with the same code, however the electronic structure calculations are usually done with a different software [3]. For this thesis, the electronic structure calculations are done by the software Gaussian [13] and Molpro [32–34], and the master equation simulations are done by MESS [14, 15].

To better understand the calculations behind AITSTME, this chapter will mention ab initio calculations, transition state theory, estimation of the reaction rate constant, master equation simulation and the lumping of its results, and kinetic simulations.

2.1. Ab Initio Simulations

According to quantum mechanics, the properties of a molecule (such as its energy) can be obtained from the solution of the Schrödinger equation, which is reported below in its most general time independent formulation:

$$\boldsymbol{H}\Psi = E\Psi \tag{2.1}$$

However, the exact solution of the Schrödinger equation by computation is not so practical. This is the motivation for the development of electronic structure methods. Two of the major electronic structure computational methodologies are the semi-empirical and the ab initio methods.

If some experimental data are used to ease the computations, the calculations are called semi-empirical calculations. They are performed by solving an approximate form of the Schrödinger equation with some parameters tuned to reproduce a selected set of experimental data.

Ab initio calculations refer to the type of calculations that are done purely by computations and with no experimental data. The name ab initio comes from Latin and has the meaning of "from the beginning" [9]. These computations use laws of quantum mechanics as their basis of calculation, with some constants such as the speed of light, Planck's constant, the masses of electrons and so on, and aims to calculate the stationary states that a molecule has as well as characterizing the transitions that happen between these states [16].

The cost of computations and the result accuracy determines which of these two methods to be used. The semi-empirical methods are usually cheaper and give good enough qualitative results for the structures and their energies when well known parameters are used.

On the other hand, ab initio calculations can be used for many more systems with results of high-quality predictions. There are no specific system limits for ab initio calculations. The size of the system was a concern for the early programs, however in today's world that is not a problem at all. Current programs can easily (in a few minutes) compute the required calculations for a system with ten or similar heavy atoms. Even the jobs with hundreds of atoms can be handled computationally (the use of a super computer can be suggested for very high number of atoms). It should be noted that for the small systems the approximation of the Schrödinger equation is much closer to the real value than for the large systems. For a single hydrogen atom, the smallest possible system, an exact solution can even be found.

By using a program such as Gaussian [13], the researcher can work with any atom types (including the metals). Energies, structures and many molecular properties can be calculated by that software, even the molecules in solutions and their excited states can be investigated [12].

There is also a third type of electronic structure method that is called density functional theory (DFT). DFT is very similar to ab initio calculations. The resources required for the computations are similar to those required for Hartree-Fock (HF) calculations, which is not an expensive ab initio method. In order to tell the software how deep the calculations should be done the basis sets and the level of correlation are used together. That is shown on Figure 2.1.

Each molecule has molecular orbitals, and basis sets are basically their mathematical representations. Basis sets consist of a group of basic functions that can be added to each other or stacked to be able to obtain the feature of interest. The word "stacked" means multiplying each term in the equation with its own constant and then adding the obtained values to one another.

$$\gamma = a_1\beta_1 + a_2\beta_2 + ... + a_k\beta_k \tag{2.2}$$

The value of k in Equation 2.2 is the basis set size, $\beta_1, \beta_2, \ldots, \beta_k$ represent the basis functions and $a_1, a_2, \ldots, a_k$ are the constant for each basis function. The first person to use the basis sets for the calculations of the orbital computation is John C. Slater, his work is known as the Slater Type Orbitals [26].

The deeper (meaning lesser number of constraints) you want the calculations to be done, you more accurate and precise the results. However, you would also need more time and additional computational resources. The horizontal axis of Figure 2.1 represents the basis sets, and the accuracy of calculations increases by going from left to right. Similarly, the

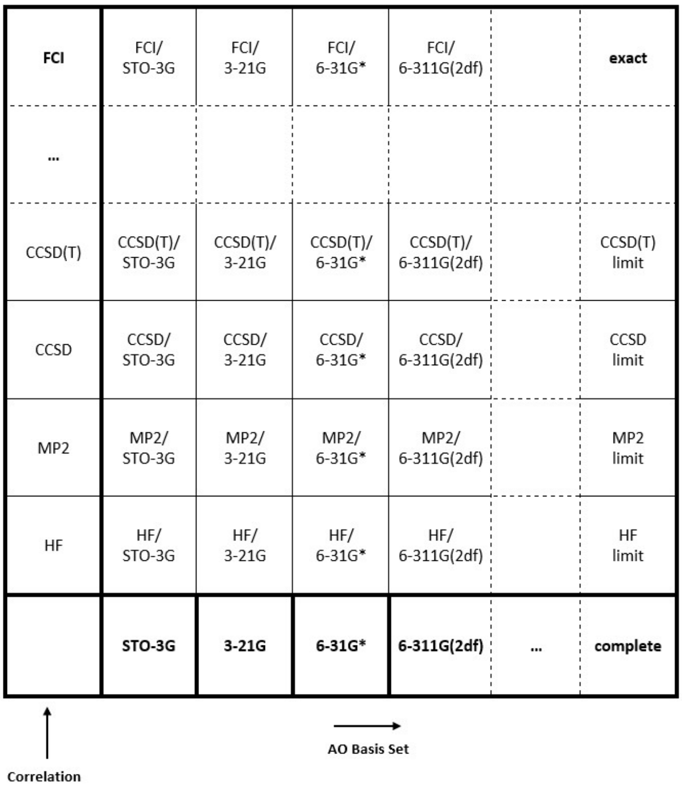


Figure 2.1: Basis sets and the level of theory on the solution of the Schrödinger equation [16].

vertical axis represents the level of correlation and it also increases from bottom to top. In the theoretical highest level of correlation and the basis sets (which is the top right corner) the exact solution of the Schrödinger equation is achieved.

The comparison between the theoretical levels (shown as correlation in Figure 2.1) are shown in Figure 2.2.

Theoretical method	Current computational dependence on molecular size, *M*	Current estimate of maximum feasible molecular size
FCI	factorial	2 atoms
CCSD(T)	M^7	8-12 atoms
CCSD	M^6	10-15 atoms
MP2	M^5	25-50 atoms
HF, KS-DFT	M^2-M^3	50-200 atoms

Figure 2.2: Comparison of theoretical levels [16].

The first column of the Figure 2.2 shows the theoretical method used, the molecular size (shown by M) in the second column shows how longer the computations would take if the size of the molecule is increased by M times. For example, if the size of the molecule gets doubled for a CCSD level calculation, the computations would take 64 times longer than before. The third column shows the maximum number of first-row non-hydrogen atoms that can be handled with the selected method. Again, for a CCSD type calculation, a maximum of 10-15 non-hydrogen atoms can be handled.

Running some simple level calculations before the high-level calculations could be very useful, since they require less time one can observe the shortcomings in the adopted computational procedure (if there is any) rapidly in a cost-effective way.

2.1.1. Density Functional Theory

Density functional theory is based on the Hohenberg and Kohn theorem, which states that the ground state electronic energy of a system is totally determined by its electron density. E. B. Wilson explains why the system can be defined completely by the density with the following statements [20]:

- Number of electrons are defined by the integral of the density.

- The nuclei position is defined by the cusps in the density.

- The nuclear charges are defined by the cusps' heights.

The importance of the Hohenberg-Kohn theorem can be observed when it is compared to the wave function approach. For each electron, the wave function has three spatial coordinates and one spin coordinate. For a system with Q number of electrons, the integration of the square of the wave function over Q-1 electron coordinates is equal to the electron density. Spin density depends just on the spatial coordinates (three per electron) and does not depend on the electron number. As the number of electrons increases, the wave function complexity also increases with an exponential behavior. However, the number of variables for the electron density is still the same, it does not depend on the size of the system. Even though it is known that each density corresponds to a different energy for the ground state, the functional between them is not known. In this framework, the aim of density functional theory can be rationalized in terms of the creation of functionals that connect the energy and the electron density together.

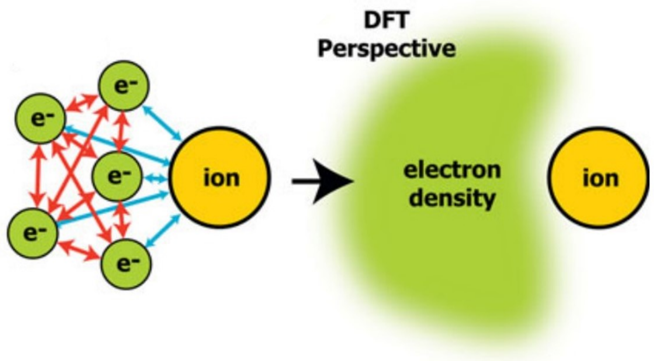


Figure 2.3: Using electron density instead of many-electron system [23].

The first implementations of density functional theory models aimed to use the electron density to express the energies. However, these models could not reach high performance, and researchers preferred wave functional methods over them. The modern density functional theory methods gained importance after the work done by Kohn and Sham in 1965, which states in order to calculate the electron kinetic energy, an auxiliary orbital set should be used to represent the electron density.

Even though Hartree-Fock theory is both computationally and conceptually similar to density functional theory, due to the better results achieved the latter is usually the method of choice. One of the major problems of density functional theory is that the results cannot be improved systematically. Another important problem is that some important properties (like the van der Waals interactions) cannot be successfully described.

2.1.2. Coupled-Cluster Theory

Coupled-cluster theory is used as a reference method. It is used for the electronic structure theory for the molecules that lie between the smallest and the largest systems. The theory first was developed around 1960's and used for the nucleons, then after a few years it started to be used for electron correlation problems. In 1970's it is inserted in computational codes related to quantum chemistry. After the introduction of coupled-cluster theory in quantum chemistry, new methods and new computational strategies have developed very rapidly. Nowadays, the users can select many different options to improve the results depending on the system under investigation [2].

In order to face the main quantum chemistry related problems, analytical high-order derivatives and analytical gradients are two of the most active fields of research in coupled-cluster theory. Some of the described problems are searching and characterizing the critical points that define the local minima and the transition state structures on the potential energy surface, and determining the respective molecular properties. The first and the second derivatives of coupled-cluster theory are developed for both the ground state and the excited state. Coupled-cluster equation-of-motion/linear response theory methods and symmetry-adapted cluster configuration interaction method are used to define these states. The analytical derivatives method of the coupled-cluster are mostly obtained for the isolated molecules.

2.1.3. Multi-Configuration Self-Consistent Field

In quantum chemistry, the word "configuration" stands for the description of the occupation of the molecular orbitals of a system. One way to describe these configurations is the use of Slater determinants. If more than one configuration is used for a calculation, the method is called multi-configurational. The simplest method, Hartree-Fock, is a single-configurational method. Configuration interaction methods use the linear combinations for various Slater determinants, the additional determinants come from the excitations of the determinant of the ground state.

When performing electronic structure calculations, reference configuration or configurations must be selected and excitations, for example in CCSD(T) theory, are generated from the reference configuration. Just like the previous case if more than one reference configuration is used for the calculations, the system is called as a multi-reference system. For the single-reference calculations, the Hartree-Fock configuration is usually selected to generate the excitations.

Sometimes single-reference methods cannot describe the wave-function correctly, in such cases there is a need to use multi-configuration self-consistent field methods (MCSCF). One of the most common approaches for this method is the "complete active space self-consistent field" (CASSCF) method, which is also called as "full optimized reaction space" method. The systems for which single-reference methods can handle the calculations are called weakly correlated (or dynamic) systems, the systems for which multi-reference methods have to be used are called strongly correlated systems, and as already mentioned CASSCF (MCSCF) can be used for strong (or static) correlations.

For the MCSCF method, which is a configuration interaction method, the coefficients of the determinants are optimized using the variational principle just like single-configuration methods, however also the molecular orbitals that are used to construct the determinants are optimized. The optimization process is an iterative one just like the self-consistent field (SCF) optimization. As the number of configurations increases, the number of iterations increases as well.

For the Hartree-Fock method, the first derivative of energies with respect to the molecular orbital expansion coefficients has to be equal to zero. Iterative SCF methods can be used to solve the equations, however the solution may not be the minimum of the energies with respect to the molecular orbital coefficients. To be sure that a minimum is reached, the matrix of the second derivatives can be calculated. Usually that is not necessary for the SCF wave functions, since they mostly converge to a minimum. However, the same cannot be said for the MCSCF wave functions, that is why second-order SCF procedure, which uses Newton-Raphson methods to find convergence, is usually applied.

For the CASSCF method, the molecular orbitals are partitioned into active and inactive spaces to select the configurations. The active molecular orbitals mainly contain the highest occupied molecular orbitals, with some lowest unoccupied molecular orbitals from the restricted Hartree-Fock calculations. The inactive molecular orbitals can be doubly occupied (meaning they contain two electrons) or empty (zero electrons). A full configuration interaction is performed for the active molecular orbitals, and the proper configurations are used for the MCSCF optimization. Depending on the problem and the computational costs, the molecular orbitals to be included in the active space have to be manually decided. In case multiple points on a PES must be analyzed, all of the desired orbitals which has significant changes, or the ones for which there is an expectation for the electron correlation to change must be included in the MCSCF active space [20].

2.2. Transition State Theory

Transition state is a term used for the intermediate states of a reaction, that converts the reactants to the products. It is often associate with the presence of a barrier of energy between the reactants (the initial state) and the products (the final state). The reaction occurs when the reactive flux passes (overcomes) the top of this barrier of energy. Of course, this barrier appears on the reaction path that has the minimum energy on the multidimensional potential energy surface, since that is the easiest path for the reaction to occur. The top of the barrier (i.e. the highest energy point) is called as the transition structure. The relative energy of that point with respect to the reactants strongly affects the rate of the reaction, as predicted by transition state theory (TST) [20].

In a pioneering work about transition state theory, M. G. Evans and M. Polanyi define the probability of a transition state as a layer of a phase space with infinitesimal thickness, that has faces extending to infinity for all the directions orthogonal than the reaction coordinate [10]. One can think of it as a real molecule which has one less degree of freedom, that is the reaction coordinate. In a mathematical approach, transition states are defined with delta functions for the reaction coordinates [30]. If the representative points of a system belong to this layer, the system is considered as a transition state. Whenever, a representative point reaches that layer and passes in any of the two directions a chemical reaction occurs in the direction of the representative point (forward or backward). A representation of a reaction with the transition state is reported in Figure 2.4.

By considering the quasi-equilibrium of the reactants and the transition states, M. G. Evans and M. Polanyi reached the statistical mechanical and quasi-thermodynamic formulation of transition state theory. Even though transition state theory is originally applied to gas phase reactions, nowadays it can be used for many other cases, for example condensed reactions.

TST is a semi classical theory that takes the quantum nature into account by using the quantization of the rotational and the vibrational energy states. Classical treatments are done for the dynamics along the reaction path, whereas quantization is taken into account for the perpendicular directions. One important assumption is that the energy distribution of all the possible quantum states along the reaction coordinate are in equilibrium. Finding a molecule in a specific quantum state has the probability proportional to $e^{-\Delta E/k_B T}$. That

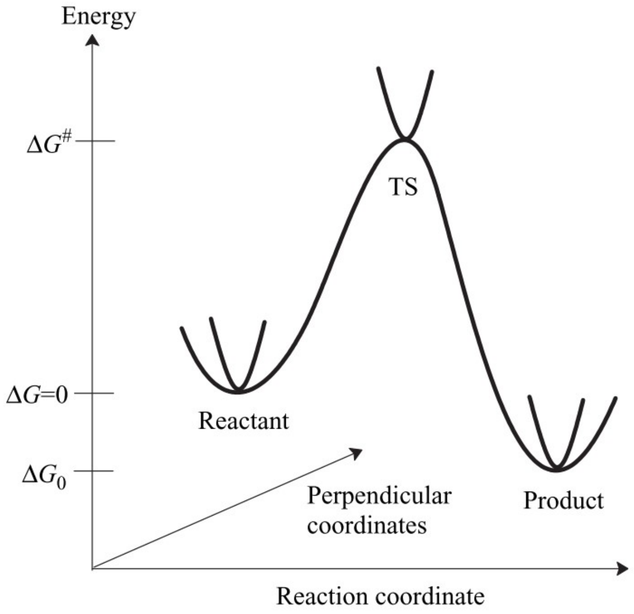


Figure 2.4: Representation of a reaction path [20].

is known as the Boltzmann distribution. If the molecules that appear in the transition state reach the equilibrium with the reactants, the macroscopic rate constant can be evaluated as:

$$k = \frac{k_B T}{h} e^{-\Delta G^{\neq}/RT} \tag{2.3}$$

$$\Delta G^{\neq} = \Delta G_{TS} - \Delta G_{reactant} \tag{2.4}$$

The expressions above can be used only if all of the molecules that are passing through the transition state starting from the reactants form the products. In other words, it is assumed that there is no re-crossing, which means all the molecules passing through the transition state will form the products. Due to this assumption, the rate constant that is calculated using the Equation 2.3 represents the upper limit for the actual rate constant [20].

2.3. Master Equation Rate Constant Estimation

The determination of the rate constants with transition state theory requires two steps, which are calculations related to the electronic structures of the species, and the use of a kinetic solver that can solve the master equation based on transition state theory.

The software called MESS (master equation system solver) can be used to calculate the rate coefficients for temperature and pressure dependent reactions. That is achieved by solving the one-dimensional master equation. A lot of codes, that are used either for electronic structure or master equation calculations can be found in the literature, but not many can do both. Cavallotti et al. [3] wrote a code, named EStokTP, that is able to solve electronic structure, transition state theory, and master equation calculations, and predict the temperature and pressure dependent rate constants. The designed code has two main aims: rate constants for the reactions of interest should be obtained automatically and reliably, and the rate constants should be highly accurate.

The process of finding the rate constants start with a level 0 geometry scan. EStokTP uses Monte Carlo sampling to find the minimum energies for each species. Level 0 scans are then followed by level 1 scans. The difference between them is the increase of accuracy of the calculations performed using the selected electronic structure software, for example by increasing the size of the basis sets or the correlation levels, as described in Section 2.1. Level 0 structures are used as initial guesses for level 1 calculations. The resulting level 1 structures are used as guesses for the future calculations, such as high-level energies or symmetry number calculations. If needed, the researcher can also run hindered rotor calculations after this step. Torsional scans are also possible. They can be done as one, two or three-dimensional scans along selected dihedral angles. The rate constant and the thermodynamic properties linearly depend on the symmetry number. That is why to be able to achieve accurate rate constants, the symmetry numbers should also be calculated before running the rate calculation. High accuracy energy estimations are obtained by high-level calculations performed on level 1 structures. If requested, the evolution around the reaction path can be achieved by intrinsic reaction coordinate scans. These scans are used to make sure the obtained transition state structure connects the desired reactants to the desired products.

Once all the calculations described above are done, the user can finally calculate the reaction rate constants as a function of temperature and pressure. EStokTP can automatically perform the necessary calculation for the following reaction classes: abstraction, addition, beta-scission, isomerization, and barrierless reactions. In order to calculate rates of reactions with ab initio methods, the software needs some parameters related to the system of interest. These parameters have to be reported for both the molecule of interest and a bath gas (in which it is assumed that the reactants are immersed) that must be selected before performing master equation simulations (in this thesis the selected bath gas is argon). The parameters that must be written in the input file are the atomic masses of the molecule and the bath gas, Lennard-Jones potential parameters (σ and ϵ), and the values of the exponent (n) and ΔE_{down} of the following equation:

$$\Delta E_{down} = \Delta E^{0}_{down}\left(\frac{T}{T^{0}}\right)^{n} \tag{2.5}$$

The Lennard-Jones potential [1] is expressed as:

$$V_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{2.6}$$

The mass of the system can simply be calculated by the masses of the elements forming the molecule (six carbon atoms and seven or eight hydrogen atoms for the reactions that are analyzed in this thesis). The values of the Lennard-Jones potential parameters could be found from the literature. However depending on the molecule it may be hard to find these values directly from literature. In that case, other researches that reported some empirical equations to calculate them could be very useful. In particular, Jasper [18] reported an empirical equation that can be used for calculating the parameters for different hydrocarbons (which is the case for this thesis). The following equations are reported to calculate Lennard-Jones potential parameters for hydrocarbons when argon (Ar) is used as the bath gas:

$$\sigma(N) = 3.40N^{0.18} \tag{2.7}$$

$$\epsilon(N) = 113N^{0.31} \tag{2.8}$$

Where N is the number of non-hydrogen (heavy) atoms, and the units of α and ϵ are Å and cm^{-1} respectively.

Once these parameters are calculated, the value of ΔE_{down} can be calculated for different temperature values as suggested by Jasper (a Microsoft Office Excel Sheet is available as a supplementary material). To be able to use Equation 2.5, the values of ΔE^{0}_{down} and n should be known. It is easy to calculate ΔE^{0}_{down} since it is the value of ΔE_{down} at the temperature of interest (300 K for this thesis), which could be calculated using Jasper's work. The calculation of the value of n requires linearization of Equation 2.5, which is:

$$ln\Delta E_{down} = ln\Delta E^{0}_{down} + n \cdot ln\left(\frac{T}{T^{0}}\right) \tag{2.9}$$

Once the values of $ln\left(\frac{T}{T^{0}}\right)$ and $ln\Delta E_{down}$ are known, it is possible to draw the best-fit line and find the slope (which is the exponent "n").

As stated earlier, the atomic masses of the molecule and the bath gas, the values of the Lennard-Jones potential parameters (σ and ϵ), and finally the values of the exponent (n) and ΔE_{down} of the Equation 2.5 are used as some of the input parameters for the calculation of the reaction rates.

2.3.1. Reaction Types

It is possible to find the rate constant for four different types of reactions by using EStokTP. These reactions are abstraction, isomerization, beta-scission, and addition. Once the input parameters that are required for the calculation of the rate constant are fed to the code, the prediction is done completely automatically [3].

Abstraction reactions tend to have three different transition state structures. One of them is the transition state for the abstraction process, the others are for the van der Waals wells. One of them is for the entrance channel formation and the other is for the exit channel decay. The rate constant is obtained by the solution of the master equation for all these three channels. An illustration of the three transition state model is given in Figure 2.5.

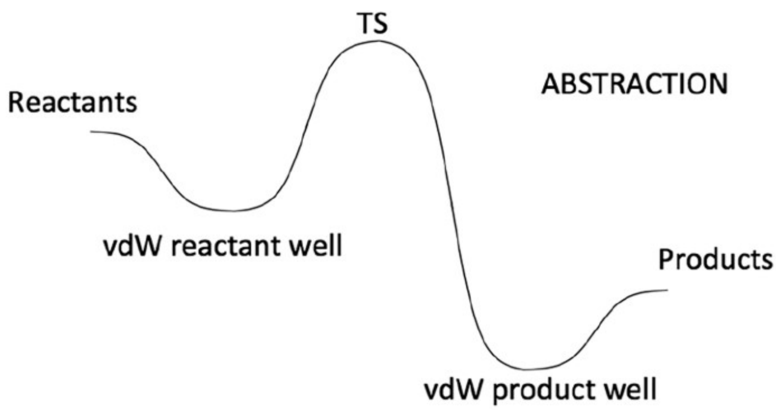


Figure 2.5: Three transition state model for the abstraction reactions [3].

The user does not necessarily need to use the three transition state model, it is possible to have two transition state model (that includes a van der Waals well only on the reactant side) or one transition state model (no van der Waals wells). In the literature it is possible to find a lot of studies that use the one transition state model.

The calculations for isomerization reactions are done as pressure-dependent reactions with one reactant and one product (as a unimolecular process). The algorithm behind isomerization reactions can be used for the elimination reactions however, because of the simple transition state location procedure it is expected to have errors for the rate calculation.

Addition reactions, just like abstraction reactions, are expected to have a van der Waals well at the entrance channel. Hence, for the addition reactions, EStokTP can be run with two different models, the one with two transition states or the one with one transition state. For the two transition state model, just like for abstraction reactions, the rate constant can be found by solving the master equation for both of the channels. An illustration for the two transitions state case is reported in Figure 2.6.

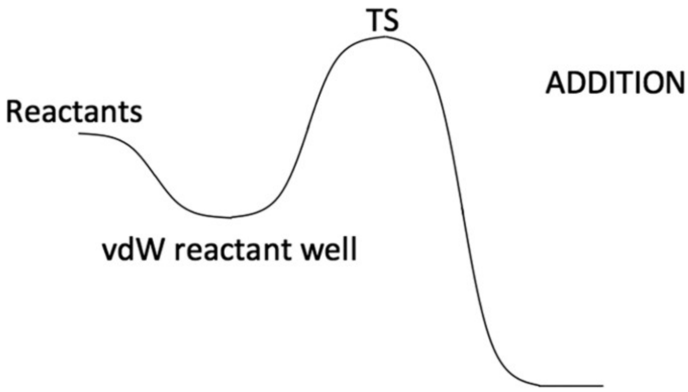


Figure 2.6: Two transition state model for the addition reactions [3].

Beta-scission reactions are the backward version of addition reactions, so the rate constants for these cases can be calculated by a detailed balance that includes the rate constant for the addition reaction. However, EStokTP has an algorithm that allows the user to calculate the rate constants for the beta-scission reactions directly. The described algorithm can work better for some systems than the first method. For example, for the cases with a low decomposition barrier the algorithm provides more effective results.

2.4. Master Equation Lumping

The ab initio transition state theory master equation methodologies became more and more popular for the calculation of the rate constants due to the improvements in the automation of the electronic structure calculations, mechanism and potential energy surfaces generations. The master equation simulation generates rate constants up to the number $S(S-1)$, where S is the number of species at a specific temperature and pressure.

In case of the presence of a complex potential energy surface (many species), there will be a large number of intermediates. Moreover, most of the intermediates will not be present in the kinetic mechanism. If these intermediates are all included, there will be a lot of species and reactions, which will cause the solution of the system to be much longer. Also, the generated rate constants do not necessarily cover the whole temperature and pressure values due to thermodynamic or kinetic instabilities of the reaction channels [24].

In order to avoid the problems described above, lumping of the data can be done. It is known that lumping is widely used for chemical kinetics [24]. Figure 2.7 shows how a detailed scheme can be turned into a lumped scheme.

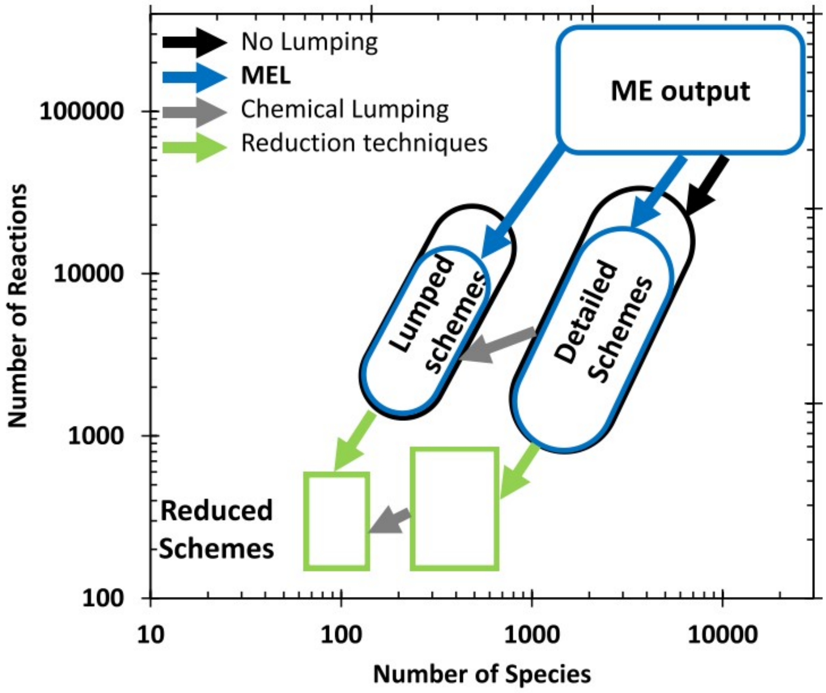


Figure 2.7: Lumping of detailed reaction schemes [24].

Pratali Maffei et al. [24] developed a Python code, named MEL, that takes the output of the master equation simulations as input, and lumps them into a smaller set of reactions without losing accuracy. Even though the methodology for that purpose appeared in some previous works, this code is noted as the first systematic approach to reach that aim. The code aims to reduce $S(S-1)$ reactions to $\tilde{S}(\tilde{S}-1)$ reactions where $S > \tilde{S}$. Another important aim is to eliminate the species that are highly reactive for all the temperature and pressure values, since they will not cause any accumulations. To find the accumulating species, the code uses a software called OpenSMOKE++. It can solve the ordinary differential equations, which are the time evolution of the concentration of different species. Since the number of species decreases after the solution of the ordinary differential equations, the number of rate constants decreases as well. The reduction of the number of species and the reactions are shown on Figure 2.8

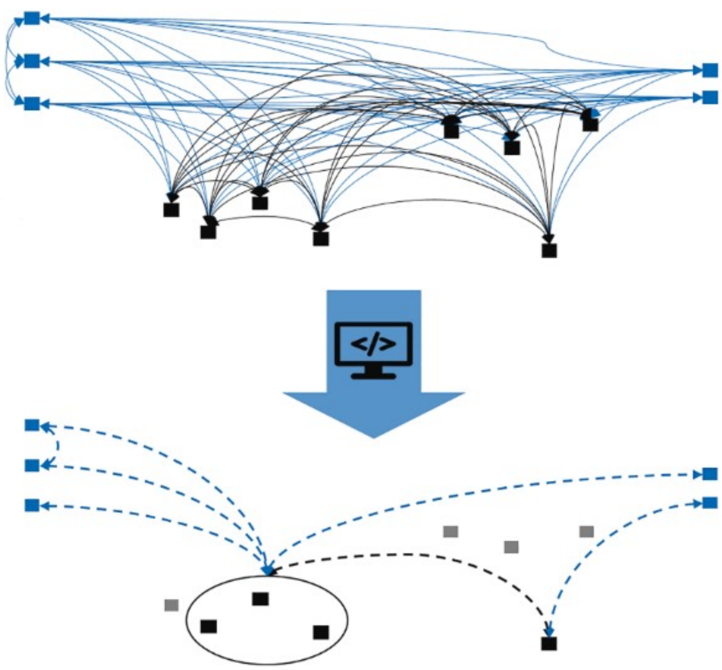


Figure 2.8: Reduction of number of species and reactions [24] following the application of the MEL procedure.

The code requires the input of the master equation simulation and the output rate data from the simulation. Once these two files are used as an input, the user also needs to identify the pseudospecies. These are the species that the user wants to be used for lumping. They can either be one species or species that are combined together due to similar structures (such as isomers), reactivity or energies. This is represented by the circle drawn in the lower part of Figure 2.8.

Initially, the code separates the species as accumulating and non-accumulating species. Because non-accumulating species are formed and disappear fast, they are not used for the lumped pseudospecies since they do not appear in macroscopic simulations. After the list of species are determined, the code can run the simulations for:
- Prescreening: Analyzes the species that are present in the detailed mechanism with respect to their reactivity.
- Lumping: After the accumulating species are determined, based on their reactivity the rate constants are found.
- Validation: Compares the reactivity of both the detailed (input) mechanism and the lumped (output) mechanism.

2.5. Kinetic Simulations

Kinetic simulations correspond to the final step of investigation of the selected reactive system. The researcher is ready to do kinetic simulations after the geometries and the energies of the reactants, products and the transition states, the rate constants between them and the lumping for these rate constants are done. For this thesis, the software OpenSMOKE++ is used to perform the kinetic simulations [5, 6].

To be able to perform an accurate description of the system reactivity there is a need for realistic numerical simulations. As the investigated system involves molecules containing a large number of carbon atoms (the fuel for example), a kinetic model that is able to describe properly its reactivity must include many chemical species and reactions. That means there is a need for kinetic mechanisms with different levels of detail and comprehensiveness. In order to analyze a combustion process, a mechanism often has thousands of reactions and chemicals.

OpenSMOKE++ is a software that is coded with object-oriented C++, it is used for the numerical simulations for the reacting systems involving chemical kinetics, thermodynamics, and transport processes. It includes detailed chemical mechanisms with thousands of chemicals and reactions between them, and it is suitable to perform calculations according to the needs of the user without forcing the user to make major changes in the functionality of the software. The types of the simulations that can be done include ideal reactors (such as a plug-flow, batch or a stirred reactor), which is the type used for this thesis. Other than the ideal reactors the software is also capable of doing simulations for the rapid compression machines or shock-tubes which are useful for the computational fluid dynamics of reactive flows. The software uses high level cost minimization techniques so that the computational costs become lower, but the accuracy and the robustness of the calculations remain almost unchanged [6].

A chemical kinetic model includes three parts, namely: elementary reactions, thermodynamic data for these reactions, and their rate coefficients. The set of the elementary reactions, that include all the relevant reactions, must be present in the kinetic model. The second part of the model is the thermodynamic data set. After the major developments from the research of Benson and Buss, nowadays the systematic prediction of thermodynamic data only by computations is almost at the level of experimental accuracy. Even though for single compounds very high levels of accuracy for the prediction of thermodynamic data can be obtained, to have high accuracy for all the species of a chemical model the costs of computation should be further decreased. The last part of the model is the rate coefficients. Since the work of Arrhenius, the laws used to express reaction rates have not changed a lot. However, major improvements have been achieved for the prediction of the rate constants. These improvements are obtained with methods such as the master equation simulations and Rice-Ramsperger-Kassel-Marcus theory (RRKM), since for these methods the collisions and the energy transfers are taken into account as well as the molecular properties of the species and the transition states [8].

3 | Results

Once the molecules that appear in the reaction mechanism and the reactions between each of them are decided, calculations can be performed to determine thermochemical parameters and rate constants. The first step towards this purpose is the creation of molecular models of each reacting molecule. This means defining bond lengths, bond angles, and dihedral angles in an input file. The automated software used for this thesis then adopts this as an initial guess and tries to converge to an energetically favorable structure.

Once structure and energies of the molecules have been determined, calculations such as transition state energies of the reactions or the reaction rate constants can be done through automated subroutines that allow minimum human interaction. For example, to find the transition state the user needs to tell the software what kind of changes are expected to occur depending on the type of reaction. These changes include bond formation, bond breakage and movements of the atoms from one place to the other one. The software then calculates the energies and tries to find a saddle point. Once that point is found, the software defines that point as the transition state. The only human interaction for that calculation is to create the input file and check if the calculations converged to the correct result.

In this section, the main results of the calculations for both methylcyclopentadienyl decomposition and H-abstraction from methylcyclopentadiene will be reported. The main results are:

- diagrams of the potential energy surfaces;
- reaction rate constants;
- lumped master equation results;
- kinetic simulation predictions for one literature system.

3.1. Methylcyclopentadienyl Decomposition

Methylcyclopentadienyl molecules are the radicals of methylcyclopentadiene. They have six carbon atoms and seven hydrogen atoms. The calculations regarding methylcyclopentadienyl radicals are reported in this section. The first step for the calculations is to determine the species of interest (that is, all the well on the same PES that can be accessed in the course of the reaction) and the reactions between them. For this thesis, six different radicals are selected to be analyzed, between these six radicals, six reactions (isomerization type) took place. Five of these radicals undergo a beta-scission reaction to produce a product molecule and a hydrogen atom. There are two product molecules for this thesis, namely benzene and fulvene, both of them have six carbon and six hydrogen atoms. The radicals that are analyzed are reported in Figure 3.1. Similarly, fulvene and benzene are reported in Figure 3.2. Finally, the scheme of the reactions between the radicals and the products are shown in Figure 3.3. For the reaction scheme, the isomerization reactions are represented with a double-headed arrow, and the beta-scission reactions are represented with a single-headed arrow.

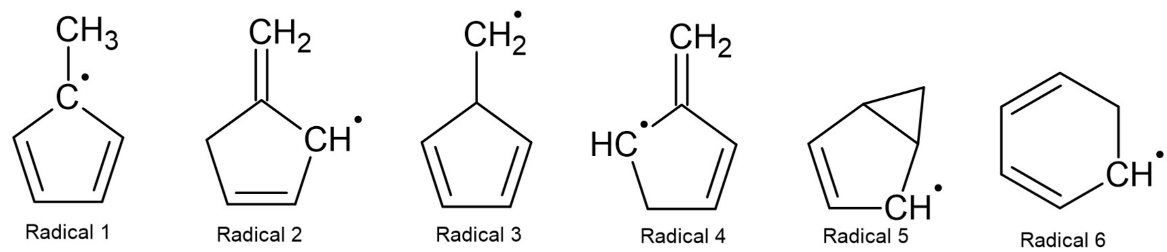


Figure 3.1: Analyzed radicals of methylcyclopentadienyl for the thesis.

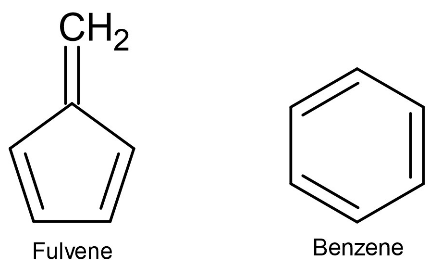


Figure 3.2: Products of the decomposition of methylcyclopentadienyl radicals.

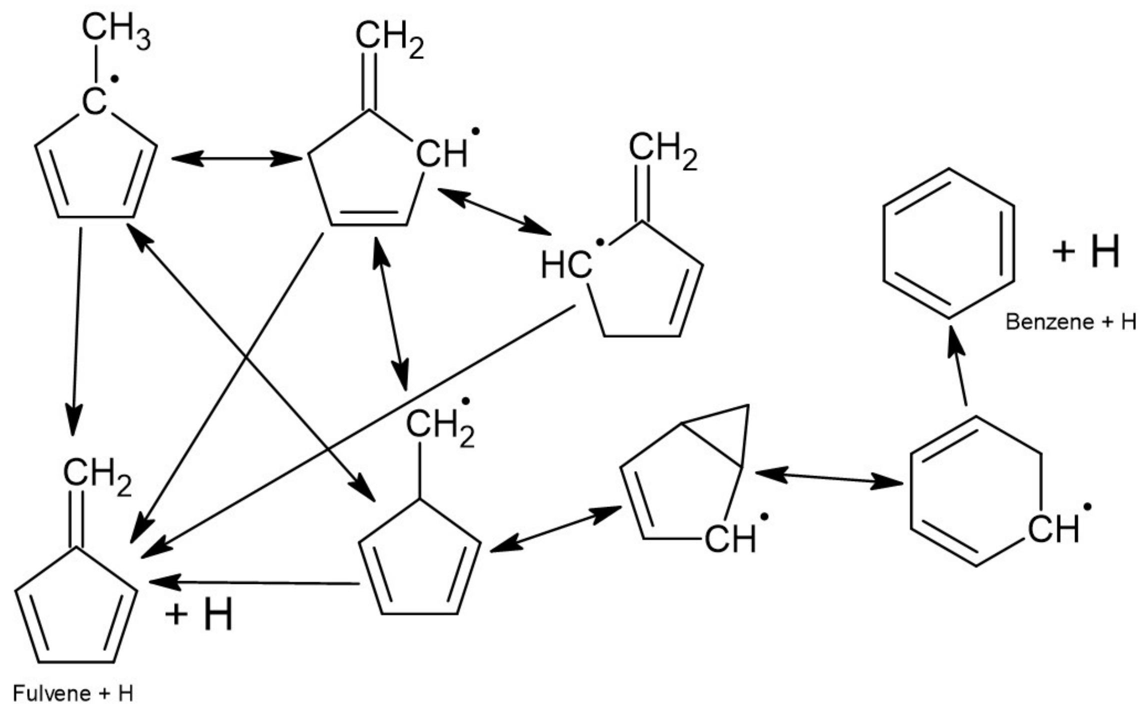


Figure 3.3: Scheme of the reactions for the decomposition of methylcyclopentadiene radicals considered in the investigated PES.

3.1.1. PES

After the determination of the wells and their interconversion reactions, the next step is to obtain the potential energy surface (PES) for these species. The PES is a diagram that has the values of energies on the y-axis and the reaction coordinate along the x-axis. In order to be able to draw the PES diagram, the energies of each species and transition states have to be known. As discussed in previous chapters, this is possible by ab initio calculations.

Level 0, hindered rotor analyses and the symmetry analyses are at the WB97X-D/6-31+g(d,p) theoretical level, while level 1 calculations are done at the WB97X-D/aug-cc-pVTZ level. The high-level calculations are performed at the CCSD(T) level of theory with complete basis sets (CBS), density fitted formalism (DF) at the level of MP2, and corrections for the core electrons. The formula for the calculation of the high-level energies is as follows:

$$E(HL) = E(CCSD(T)/aug-cc-pVTZ) + E(CCSD(T,core)/cc-pVTZ)$$
$$-E(CCSD(T)/cc-pVTZ) + E(DF-MP2/CBS) - E(DF-MP2/aug-cc-pVTZ) \quad (3.1)$$

$E(DF-MP2/CBS)$ is calculated with the following formula, which is obtained by Jan M. L. Martin's two-parameter extrapolation formula [25]:

$$E(DF-MP2/CBS) = E(DF-MP2/aug-cc-pVQZ)$$
$$+0.5772 \cdot [E(DF-MP2/aug-cc-pVQZ) - E(DF-MP2/aug-cc-pVTZ)] \quad (3.2)$$

The PES, determined using the energies obtained from the high-level calculations, is shown in Figure 3.4. The DFT level (level 1) values of the energies are also reported in the figure inside parenthesis. The radicals (wells) are shown with the letter "W" and the products are shown with the letter "P". As it can be seen from the figure, the third radical (W3) is selected as the reference species and all the energies are reported relatively to that molecule.

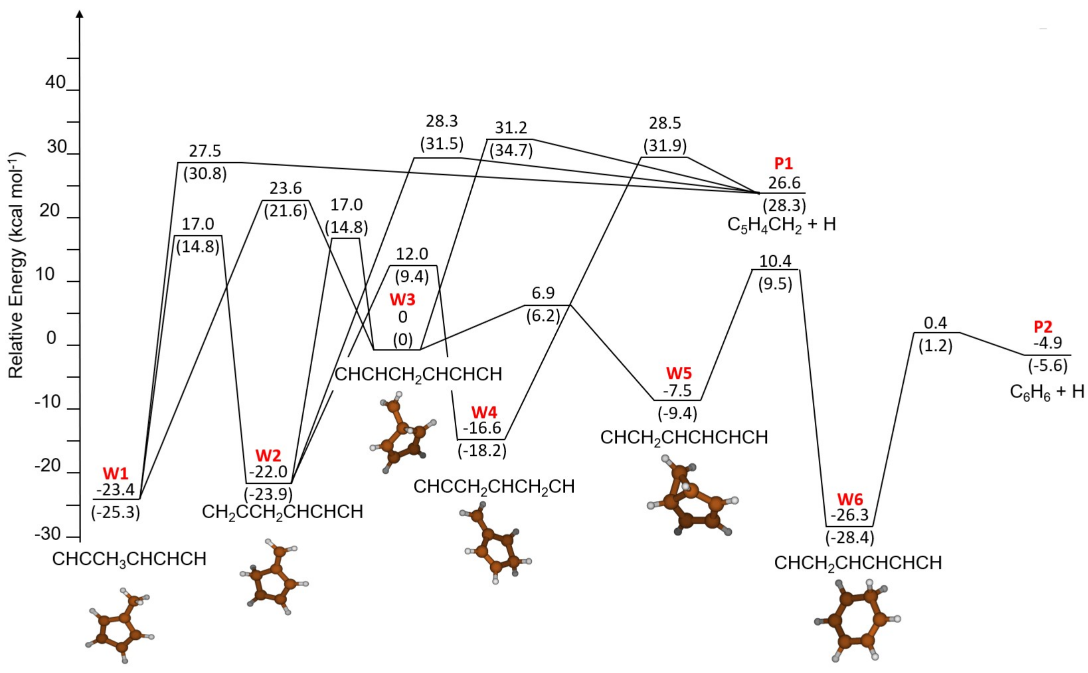


Figure 3.4: The PES for the reactions of methylcyclopentadienyl decomposition.

As already discussed in Section 3.1, there are eleven reactions in total for the analyzed system. Five of them result in a hydrogen loss and produce either fulvene or benzene, the remaining six reactions are isomerization types which causes some changes in the molecule (such as changes of the electron density or bond breakage/formation) but does not change the number of atoms in the molecule. As it can be seen from the PES reported in Figure 3.4, fulvene and the hydrogen atom (P1) has the highest energy level of the eight species, and W6 has the lowest energy level of all the analyzed species. The discussions of the changes in the PES of all the reactions (one-by-one) are reported in the following paragraphs.

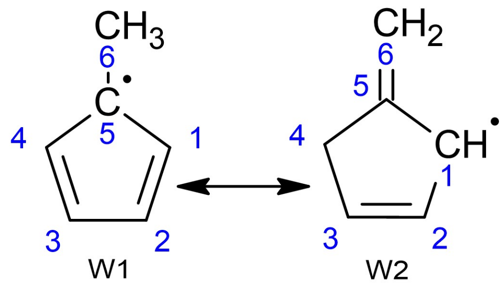


Figure 3.5: Reaction 1 – Isomerization reaction between W1 and W2.

For the isomerization reaction between the wells W1 and W2 (Figure 3.5), one of the first noticeable changes is the migration of the hydrogen atom from C(6) to C(4), that also results in the shift of the radical center from C(5) to C(1). Similarly, the double bonds between C(1)-C(2) and C(3)-C(4) become a single bond and the bonds between C(2)-C(3) and C(5)-C(6) became double bonds. This causes changes in the bonds lengths, for example the length of the bond between C(5)-C(6) changes from 1.48 Å to 1.35 Å due to the formation of the double bond. The reactant and the product have very similar energies, with a difference of 1.4 kcal/mol, but for the reaction to occur there is an energy barrier of 40.4 kcal/mol, which is the energy of the transition state.

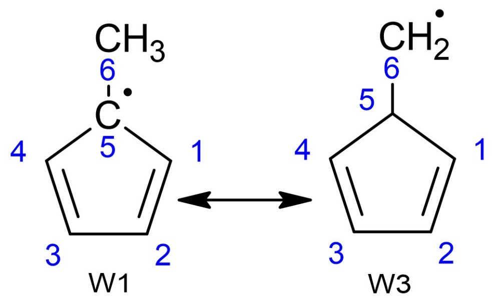


Figure 3.6: Reaction 2 – Isomerization reaction between W1 and W3.

The reaction between W1 and W3 (Figure 3.6) result in the shift of the radical center from C(5) to C(6), and the migration of the hydrogen atom in the opposite direction (from C(6) to C(5)). W3 has higher energy than W1, the difference is 23.4 kcal/mol, which means W1 is 23.4 kcal/mol more stable than W3. This relatively large energy difference comes from the fact that there is no resonance stabilization for W3. The energy barrier for the reaction to occur is just about twice as much as the energy difference between W1 and W3, 47.0 kcal/mol.

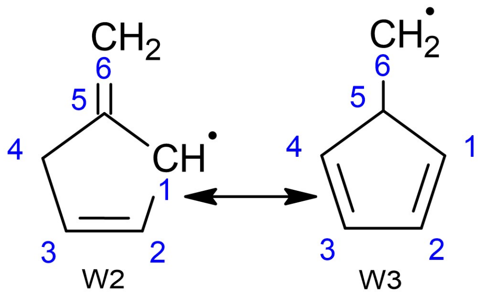


Figure 3.7: Reaction 3 – Isomerization reaction between W2 and W3.

The reaction that converts W2 to W3 (Figure 3.7) results in the shift of the radical center from C(1) to C(6). One hydrogen atom moves from C(4) to C(5), and the double bonds between C(5)-C(6) and C(2)-C(3) become single bonds, however the single bonds between C(1)-C(2) and C(3)-C(4) become double bonds. The energy difference between the product and the reactant is 22.0 kcal/mol, and there is a need for 39.0 kcal/mol energy for the reaction to occur. Just like the case described in Figure 3.6, the large energy difference between two molecules is determined by the lack of resonance stabilization of W3.

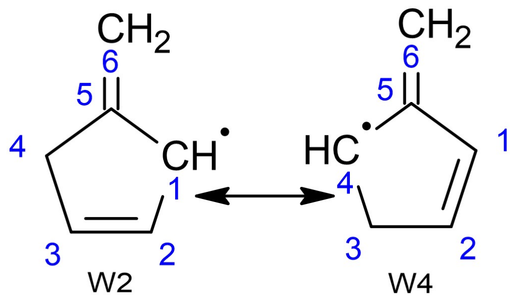


Figure 3.8: Reaction 4 – Isomerization reaction between W2 and W4.

Between the wells W2 and W4, the isomerization reaction (Figure 3.8) causes the hydrogen atom of C(4) to migrate to C(3), and the electron density moves from C(1) to C(4). As a consequence, the double bond between C(2)-C(3) becomes a single bond, and the bond between C(1)-C(2) becomes a double bond. W4 is 5.4 kcal/mol higher in energy than W2, and the barrier of energy for the reaction is 34.0 kcal/mol.

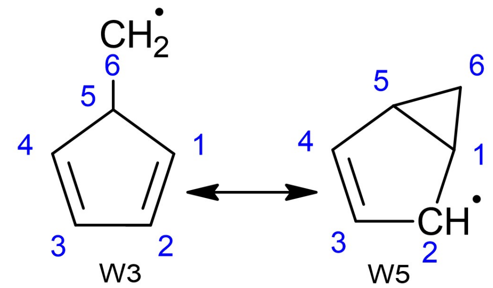


Figure 3.9: Reaction 5 – Isomerization reaction between W3 and W5.

The reaction between W3 and W5 (Figure 3.9) occurs as C(6) moves towards C(1), at one point C(6) creates a bond between C(1) while it is still attached to C(5) resulting a bicyclic molecule. The radical center moves from C(6) to C(2), and the double bond between C(1)-C(2) becomes a single bond. That means the length of that bond has to increase, and indeed an increase from 1.34 Å to 1.48 Å is observed. The energy barrier for the reaction is 6.9 kcal/mol, and the product is 7.5 kcal/mol less energetic than the reactant.

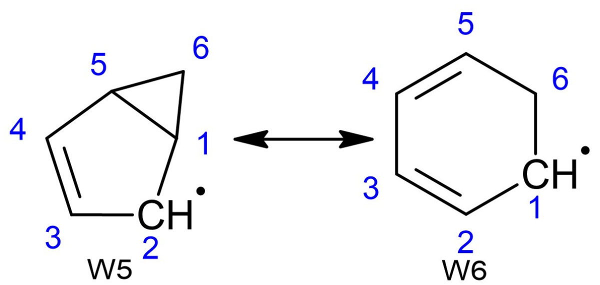


Figure 3.10: Reaction 6 – Isomerization reaction between W5 and W6.

The isomerization reaction between W5 and W6 (Figure 3.10) is a ring opening reaction. The bond between C(1)-C(5) gets stretched, the bond angle between C(1)-(C6)-C(5) gets bent and at one point the bond between C(1)-C(5) gets broken, so that the bicyclic structure becomes a single ring with six carbon atoms. The breakage of the bond causes the angle of the bond between C(5)-C(6)-C(1) to rise from 59.87 degrees to 113.39 degrees. There is no hydrogen transfer, but the electron density moves from C(2) to C(1), and the single bonds between C(2)-C(3) and C(4)-C(5) become double bonds and as a result of that, the double bond between C(3)-C(4) becomes a single bond. The energy of the reactant is 18.8 kcal/mol higher than the energy of the product, and the reaction barrier is 17.9 kcal/mol above the reactant. The energy barrier for this reaction to occur is not very high, the low energy needed to break the bond C(1)-C(5) is due to the large energy releases during the process due to the strain energy.

The reactions that are analyzed from now on are of beta-scissions, where one hydrogen atom is lost to produce fulvene (from Figure 3.11 to Figure 3.14) or benzene (Figure 3.15). Both of the products are planar molecules with six carbon and six hydrogen atoms.

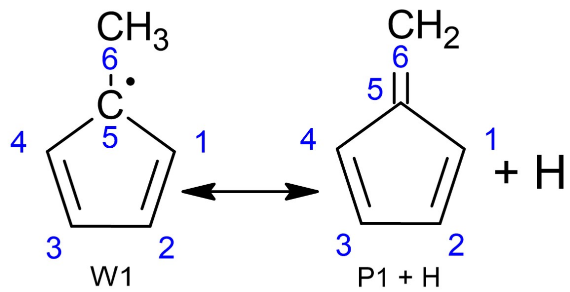


Figure 3.11: Reaction 7 – Beta-scission reaction between W1 and fulvene.

The well W1 is transformed into fulvene by losing one hydrogen atom via the beta scission reaction shown in Figure 3.11. The hydrogen is removed from C(6), and the bond between C(5)-C(6) becomes a double bond. The total energy of the products is 50.0 kcal/mol more than that of the reactant, and the energy barrier for the reaction is 50.9 kcal/mol. The high energy barrier is caused by the difference between the stability of the reactant (much more stable) and the products.

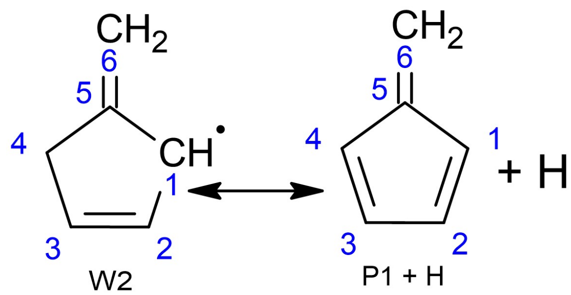


Figure 3.12: Reaction 8 – Beta-scission reaction between W2 and fulvene.

W2 loses a hydrogen atom from C(4) to produce fulvene through the reaction shown in Figure 3.12. The bond between C(2)-C(3) becomes a single bond and, bonds between

C(1)-C(2) and C(3)-C(4) become double bonds. The energy barrier is 50.3 kcal/mol and the energy of the products is 48.6 kcal/mol more than W2.

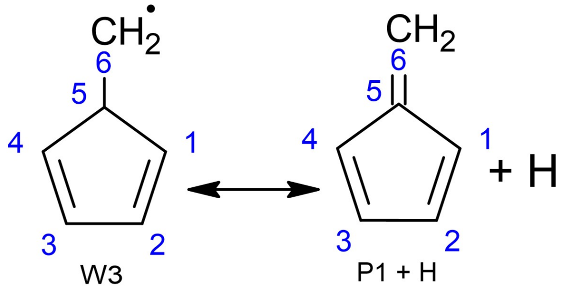


Figure 3.13: Reaction 9 – Beta-scission reaction between W3 and fulvene.

The bond between the hydrogen atom and C(5) gets broken, and W3 forms fulvene by beta-scission (Figure 3.13). As a consequence of that, the single bond between C(5)-C(6) becomes a double bond. The products are 26.6 kcal/mol more energetic than W3, and the energy barrier for the reaction is 31.2 kcal/mol.

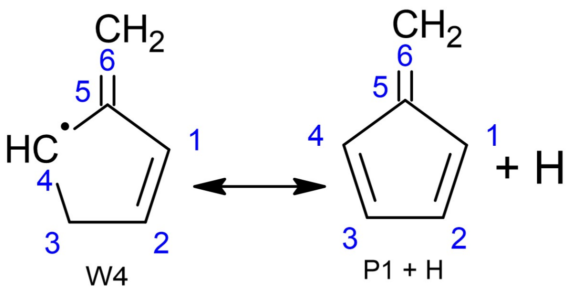


Figure 3.14: Reaction 10 – Beta-scission reaction between W4 and fulvene.

Fulvene is produced from W4 with the loss of hydrogen atom from C(3) (Figure 3.14). A double bond is formed between C(3)-C(4). The length of that bond decreases from 1.49 Å to 1.34 Å. In order to have the reaction, a 45.1 kcal/mol energy barrier must be overcome. The reactant is 43.2 kcal/mol less energetic than fulvene and the hydrogen atom.

In Figure 3.15, the hydrogen attached to C(6) is removed from the molecule W6 to produce the aromatic benzene molecule and a hydrogen atom. The single bond between C(1)-C(6) becomes a double bond. Formation of the double bond causes a change in the length of the bond from 1.49 Å to 1.39 Å. The products have 21.4 kcal/mol more energy than the reactant. The energy of the transition state is 26.7 kcal/mol above W6.

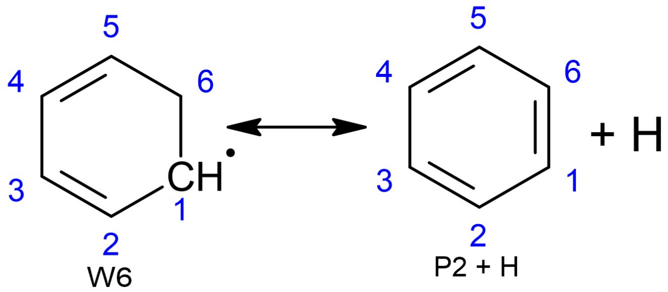


Figure 3.15: Reaction 11 – Beta-scission reaction between W6 and benzene.

3.1.2. Master Equation Simulation / Rate Constant

As described in Section 2.3, in order to have the calculations for the rate constants, some parameters such as the Lennard-Jones potential parameters, the exponent "n" for Equation 2.5 and the value of ΔE_{down} should be written in the input file. The values of the Lennard-Jones potential parameters are found by equations 2.7 and 2.8 as 4.69 Å and 197 cm^{-1} for σ and ϵ, respectively.

After the values of the Lennard-Jones parameters are obtained, the Microsoft Office Excel sheet provided by Jasper [18] can be used to find the value of ΔE^0_{down}. Similarly, the values for ΔE_{down} at all temperatures can be found by interpolating the values of ΔE_{down} from Jasper's Excel document for some of the calculated temperatures. Then, it is possible to use Equation 2.9 to find the value for the exponent "n" using $ln\left(\frac{T}{T^0}\right)$ and $ln\Delta E_{down}$. By interpolating the values that are reported by Jasper for this system, Table 3.1 is obtained. By using the values of Table 3.1 and running a least square analysis, the value of the exponent "n" is found to be 0.535.

The reaction rate constants analyzed for the decomposition reactions include the pressures between 0.001 atm to high-pressure limits, and the temperatures between 300 K and 2500 K. The high-pressures plots of the forward and reverse rate constants are reported in the following. All of the data used to obtain these plots are reported in the appendix. It should be noted that all the figures are reported for a single species, in other words each figure include plots of the rate constants that form or consume the species of interest. For example, all the reactions related to the species W1 are reported in Figure 3.16.

As it can be seen in 3.16, the reaction that mostly consumes W1 is the one shown in 3.16a. That means W1 will tend to form W2 more than P1+H and W3. That is an expected result because the energy barrier of the reaction that produces W2 is relatively lower than that of the other reactions (which was described in Section 3.1.1), meaning it is an easier (and a more favored) reaction.

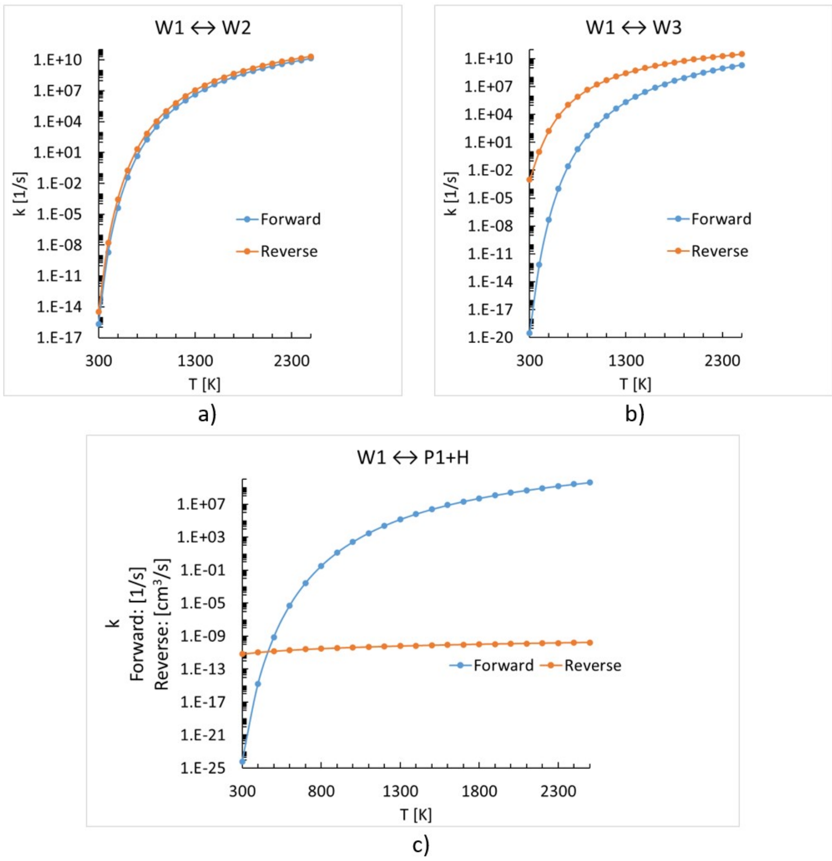


Figure 3.16: W1 reactions to give: a) W2, b) W3 and c) P1+H at high pressure.

Temperature [K]	$\Delta E_{down}[cm^{-1}]$	$ln\Delta E_{down}$	$ln\left(\frac{T}{T^0}\right)$
300	316.000	5.756	0.000
400	353.429	5.868	0.288
500	390.857	5.968	0.511
600	428.286	6.060	0.693
700	465.714	6.144	0.847
800	503.143	6.221	0.981
900	540.571	6.293	1.099
1000	578.000	6.360	1.204
1100	613.588	6.419	1.299
1200	649.176	6.476	1.386
1300	684.765	6.529	1.466
1400	720.353	6.580	1.540
1500	755.941	6.628	1.609
1600	791.529	6.674	1.674
1700	827.118	6.718	1.735
1800	862.706	6.760	1.792
1900	898.294	6.800	1.846
2000	921.000	6.825	1.897

Table 3.1: The Values to Calculate the Exponent "n"

When the backwards reactions are analyzed, it can be seen that W1 is produced mainly from the dissociation of W3, followed by W2. The backwards reaction of P1+H is expected to be much lower than its forward reaction, since P1+H is one of the main products, one would expect it to be stable once it is formed.

Another main conclusion is that both the forward and the backward rate constants tend to increase as temperature increases, which is explained by the dependence of temperature in the exponential term of the modified Arrhenius law. It should also be noted that the gap between the forward and the backward reactions for the reaction between W1 and W2 is relatively smaller than the other two reactions in the observed temperature range. That is caused by their very similar energy values.

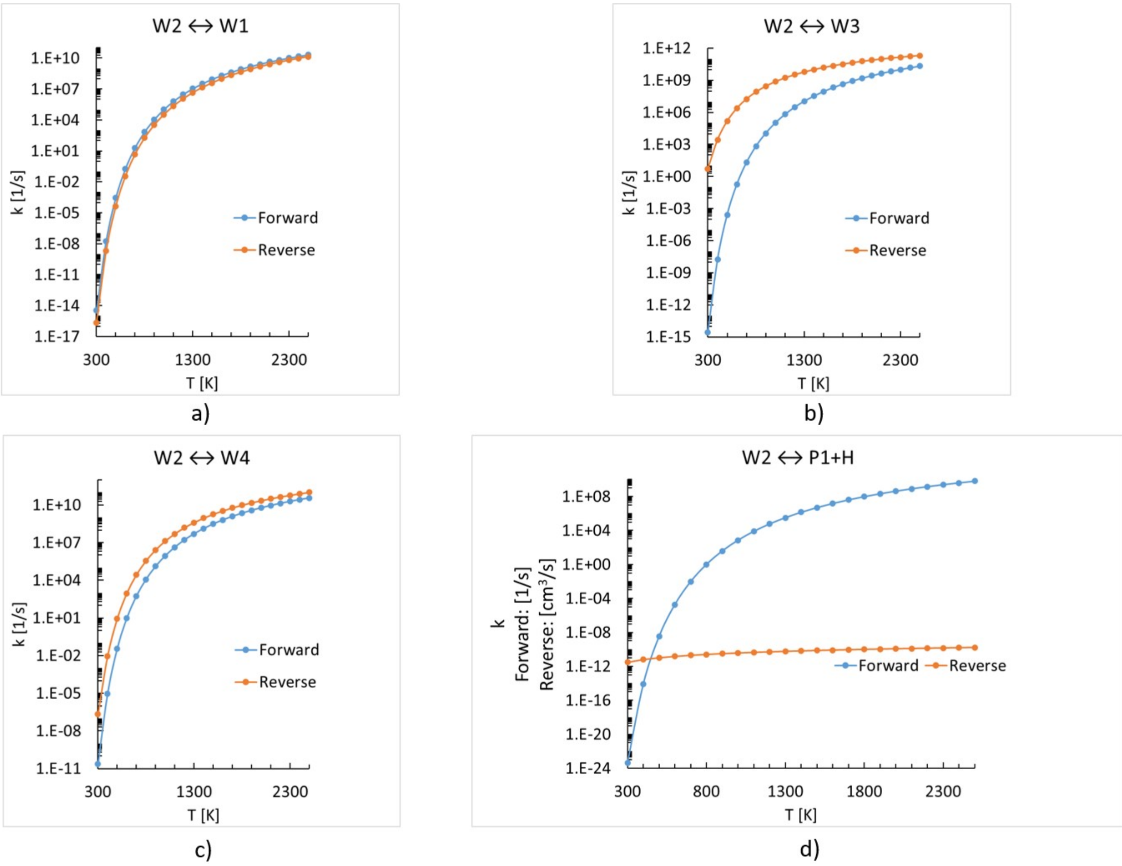


Figure 3.17: The reactions of W2 with species; a) W1, b) W3, c) W4 and d) P1+H at high pressure.

W2 reactions are shown in Figure 3.17. It can be seen that most of W2 is converted to W4, then similar rate constants are achieved for the reactions W2-W1 and W2-W3, finally relatively slower rates are achieved for the production of P1+H. These results are all in good agreement with the PES, which showed that the energy barrier of reaction W2-W4 is lower than the others, the value of the barrier is exactly the same for W2-W1 and W2-W3, and it is much higher for the reaction that produces P1+H.

The product P1+H does not tend to form much more W2 as temperature rises since it has a relatively flat curve. However, the rest of the reactions produce W2 in a high extent. It can be seen that specifically the reactions W3-W2 and W4-W2 tend to produce W2 much more than W1-W2 especially at low temperatures. The rate constants are even a few orders of magnitude greater than all the other rates reported for W2.

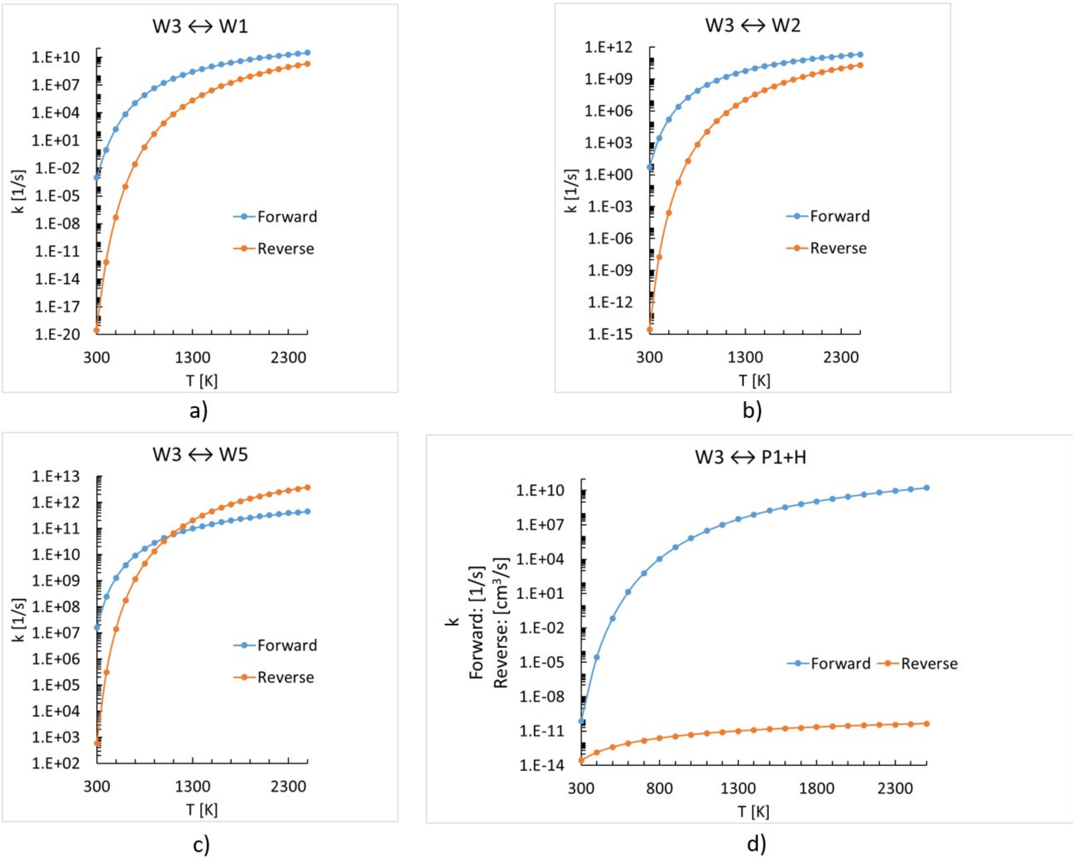


Figure 3.18: W3 reactions to form: a) W1, b) W2, c) W5 and d) P1+H at high pressure.

All of the reactions that include W3 are reported in Figure 3.18. The only reaction that tends to form W3 more than its consumption is the one with W5 (starting from moderate temperatures), however the rate constants for W5-W3 are much higher than all the other cases. In all of the graphs there is a huge gap between the forward and the reverse reaction rate constants at low temperatures, the gap starts to decrease as the temperature increases with the exception of the P1+H case. As already stated, for W5, the reverse rate constants even become larger than the forward ones at higher temperatures.

Compared to the cases that include W2 and W5, the reaction rates for both forward and reverse reactions are much slower for the cases with W1 and P1+H. W3 is mostly used by the reaction with W5 followed by W2. The decomposition rates of W3 for W1 and P1+H production are much slower than W5 and W2, with relatively higher rates for W1 production.

The reason behind having very fast forward and reverse reaction rates for the case with W5 can be explained by the PES. The energy barrier for both ways of the reaction is much smaller than the other cases, that is why the reaction between W3-W5 (in both directions) is much more favored than other reactions. Similarly, the slow reaction rates of W1 and P1+H can also be explained by their high energy barriers.

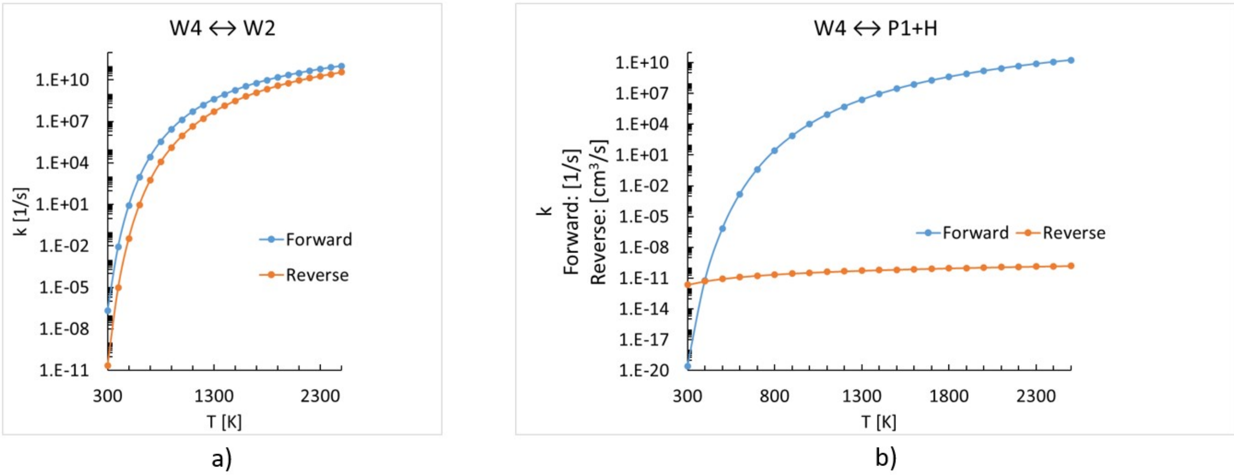


Figure 3.19: The reactions of W4 with species; a) W2 and b) P1+H at high pressure.

W4 appears only in two reactions, which are reported in Figure 3.19. One of them is an isomerization (shown as Figure 3.19a), and the other one is a beta-scission (shown as Figure 3.19b). It can easily be seen that the forward reaction that tend to form W2 is more favored than the reverse reaction. Because of the small number of reactions and slow W4 formation rates, one can assume W4 tends to form other species, and that is why probably it will not accumulate in the system. The rates of both directions of the reactions are faster for the case with W2, which is in agreement with the PES when the activation energies are taken into account.

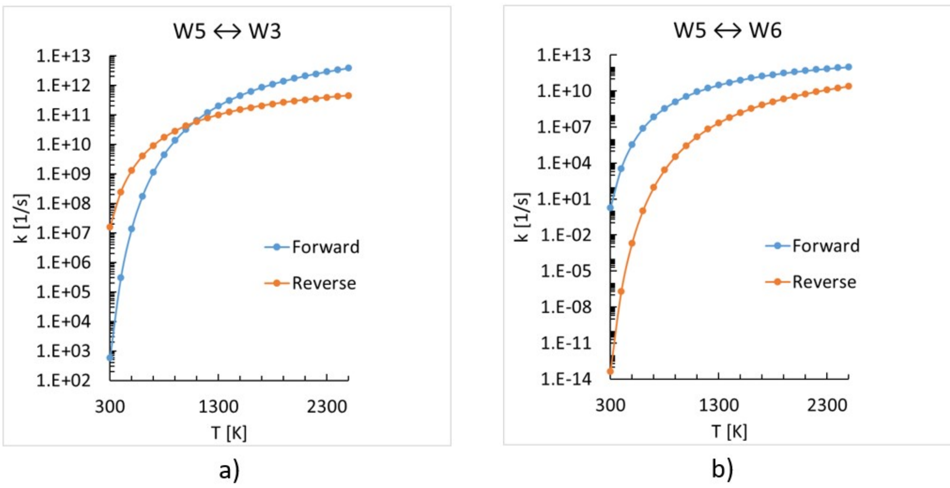


Figure 3.20: W5 reactions to give a) W3 and b) W6 at high pressure.

W5 does not undergo beta-scission, but forms W3 and W6 by isomerization. The rate constants of these reactions are reported in Figure 3.20. It can be seen that the forward rates are faster than the reverse rates for the case that includes W6, that is why W5 mainly tends to form W6. For the case of W3, at low temperatures W5 does not tend to form W3, but the opposite scenario occurs above 1200K. Probably just like observed for the W4 reactions reported above, W5 also does not tend to accumulate and forms other species at high temperature values. This conclusion is reached because in both of the cases, the forward reactions are much faster than the reverse reactions at higher temperatures. Also, it can be seen that the rates in both directions are much faster for the case with W3 than W6. Similar to all other reported cases, this is due to the smaller energy barrier of W5-W3.

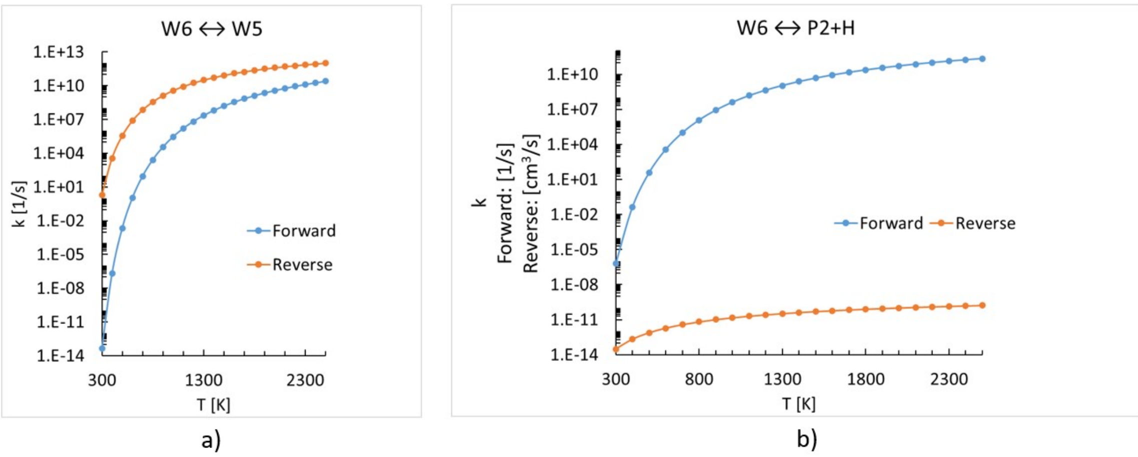


Figure 3.21: The reactions of W6 with species; a) W5 and b) P2+H at high pressure.

Figure 3.21 shows that W6 is produced from the isomerization reaction of W5, and it is converted into P2+H. Both of the reactions have a huge gap between the forward and the reverse rate constants, especially for the case that produces P2+H, which is why that reaction probably could be assumed as almost irreversible. As it can be seen from the PES, for the reaction of formation of W5 from W6 to occur, almost 20 kcal/mol of additional energy must be present than for the reaction from W5 to W6. That is why that reaction is not favored, and reverse rate constants are higher than the forward ones, as can be seen in Figure 3.21a.

The rates for the W5-W6 reaction (reverse reaction in plot in Figure 3.21a) are higher than those leading to P2+H, which means there will be some W6 present in the system. However, most of the produced W6 will tend to form P2+H. Since P2 is a stable product, it would be expected for it not to dissociate, and the results similarly prove this expectation.

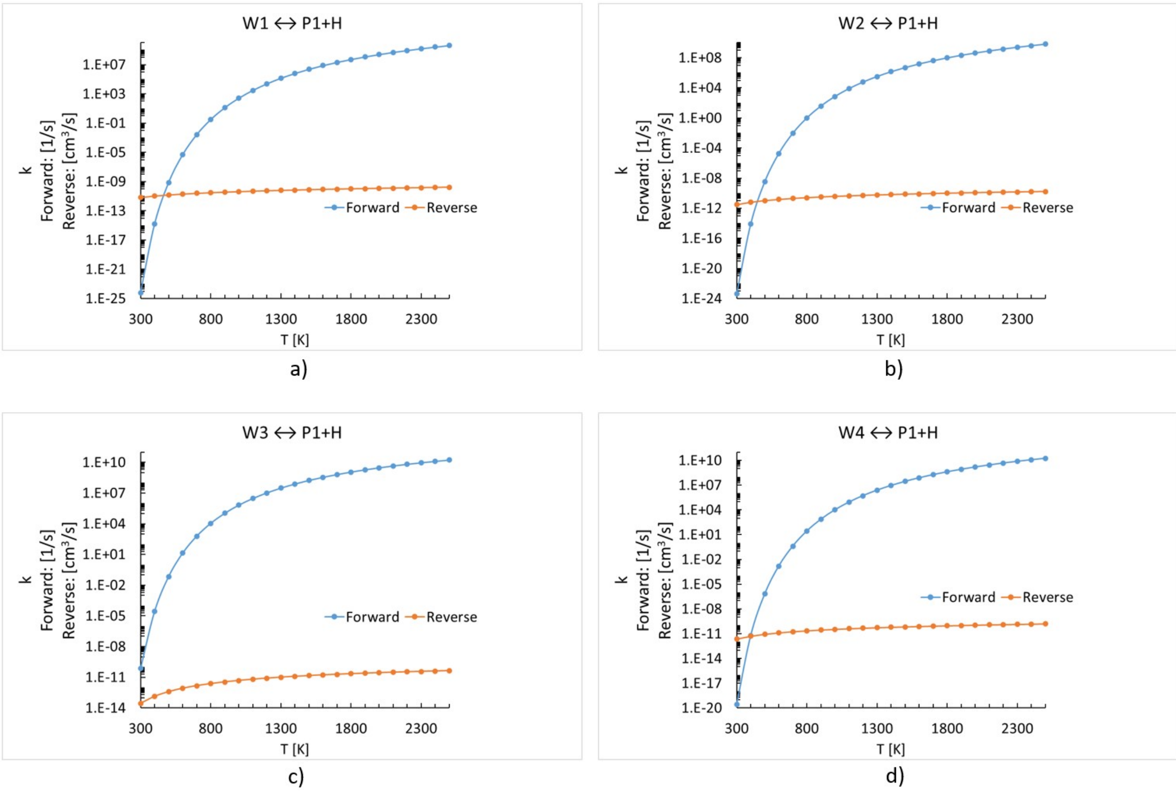


Figure 3.22: The reactions of formation of P1+H from a) W1, b) W2, c) W3 and d) W4 at high pressure.

Figure 3.22 shows all the reactions that lead to the formation of P1+H. When the values of the rate constants are compared with each other it is clear that the fastest reaction is the one starting from W3, followed by W4. The rate constant of the reaction starting from W2 is somewhat comparable to that of the W4, but the last reaction (from W1) is at least one order of magnitude smaller than the other reactions. In the PES, the smallest energy barrier was the one of W3, followed by W4, then W2 and finally the largest energy barrier was the one of W1. Once again, this situation perfectly fits to the rate data reported in the figure.

The products P2+H are only produced by one reaction, which is reported in Figure 3.23. W6 tends to form the stable products P2+H, once they are formed they will not tend to reform W6 with the reverse reaction.

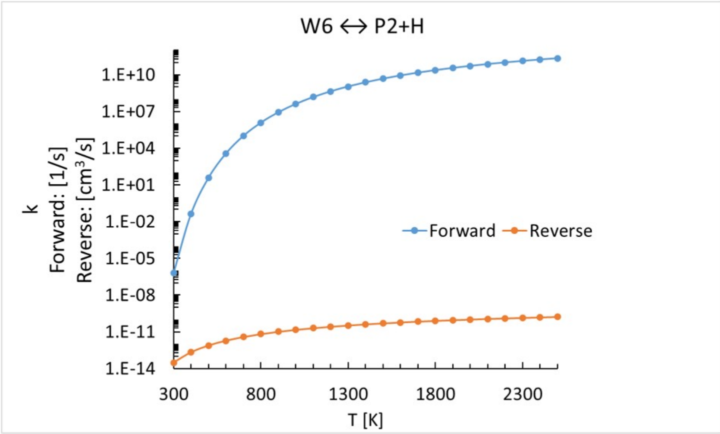
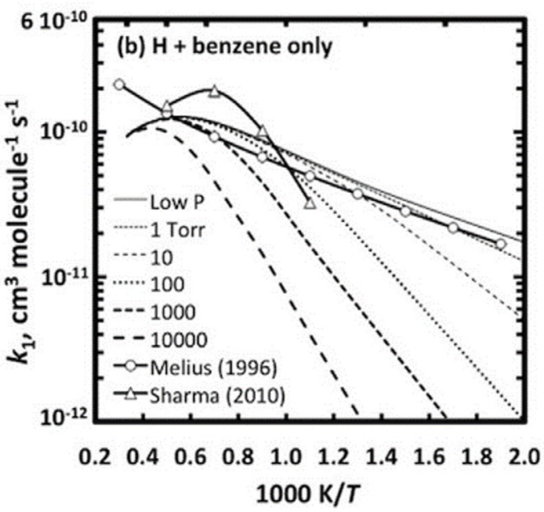


Figure 3.23: The reaction of P2+H with W6 at high pressure.

Besides the reactions reported above, in the literature it is found that the reaction of Fulvene + H → Benzene + H is also analyzed in some previous works [19]. In order to make a comparison with the values found in this thesis and the literature values, the rate constants for the reaction of interest at different temperature and pressure values are plotted and compared with the plots found in the literature. Both plots are reported in Figure 3.24, it should be noted that all the curves represent a different pressure value, the y-axis of the curves is the rate constant, and the x-axis is 1000 K divided by the temperature in Kelvin.



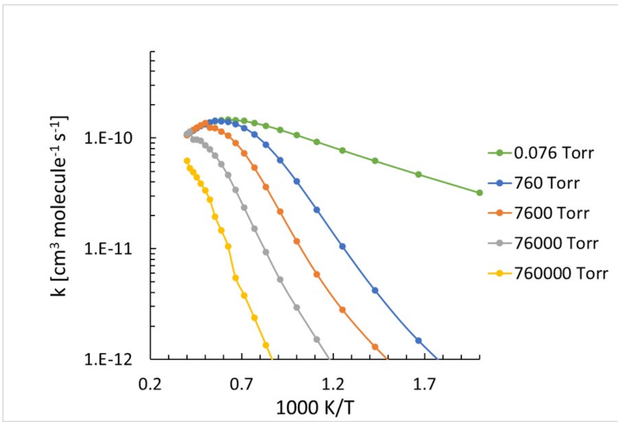


Figure 3.24: Reaction rate constants for Fulvene + H → Benzene + H at different temperature and pressure values; a) plot obtained from the literature [19] b) plot obtained from this thesis.

By looking at Figure 3.24, it is possible to compare the obtained values with the literature values. However, a better comparison is achieved if both plots were reported in one single graph, as done in Figure 3.25.

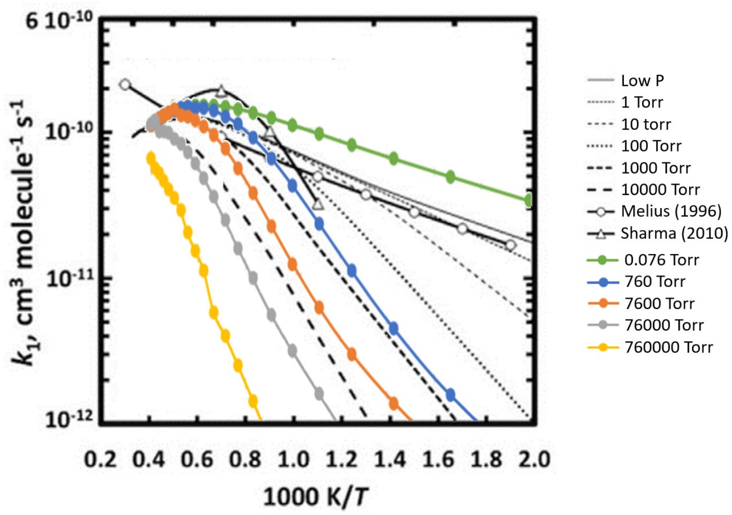


Figure 3.25: Comparison of the rate constants of Fulvene + H → Benzene + H.

By looking at Figure 3.25, it is possible to see the values and the shapes of the calculated curves are similar to the curves found in the literature. One important conclusion is that at high temperature values, all the rate constants tend to approach each other no matter what the pressure is, and they diverge from each other at lower temperatures.

It should be noted that the analysis in this thesis and the other work used different pressure values, that is why differences in the plots were expected. It was important to observe similar shapes, no major crossings of the lines and similar values at similar pressures, which is the case achieved in Figure 3.25. All of the rate constant values obtained in this thesis are reported in the appendix.

3.1.3. Master Equation Lumping

The results of the master equation calculations consist in a long list of reactions and rate constants. However, to simplify the system, some of the species can be merged into each other. The code described in Section 2.4 is used for this purpose, which is called master equation lumping. Two main input files are required for the code to run, which are the input and the output (the reaction rate constants) files for the master equation simulations. Besides these files, the user has to specify which substances has to be grouped together in order to reduce the number of wells and the reactions.

Because of the similar structures and energy values, three species (namely W1, W2 and W4) are selected to be merged together to simplify the calculations. The merged species are shown inside a red rectangle on the potential energy surface in Figure 3.26.

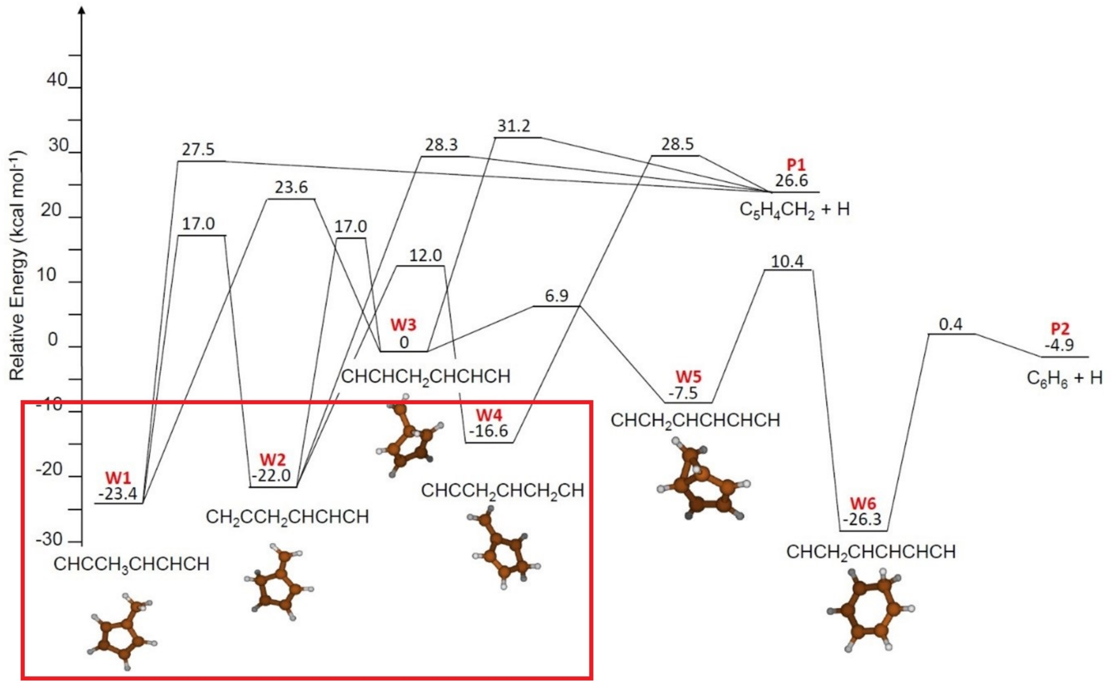


Figure 3.26: Merged species shown on the potential energy surface.

The output of the calculations are the plots for the mole fractions of the species with respect to time, which include the comparison of the fractions with the lumped and the not lumped (input) data, the steady state values of the molar fractions, and the rate parameters for each reaction in terms of the modified Arrhenius equation form (k_0, α, E_a):

$$k = k_0 T^{\alpha} exp(-E_a/RT) \tag{3.3}$$

The code first runs some kinetic simulations in order to determine the change of the mole fractions with respect to time. The composition selection step then runs some tests with the species that are selected to be lumped. The code randomly assigns some composition values to run the tests, and tries to find a suitable composition so that these species can act as a group and have a single rate constant. The code finally plots the molar fractions with respect to time for different temperature and pressure values. As an example, the output of the composition selection step at 1 atm is reported in Figure 3.27.

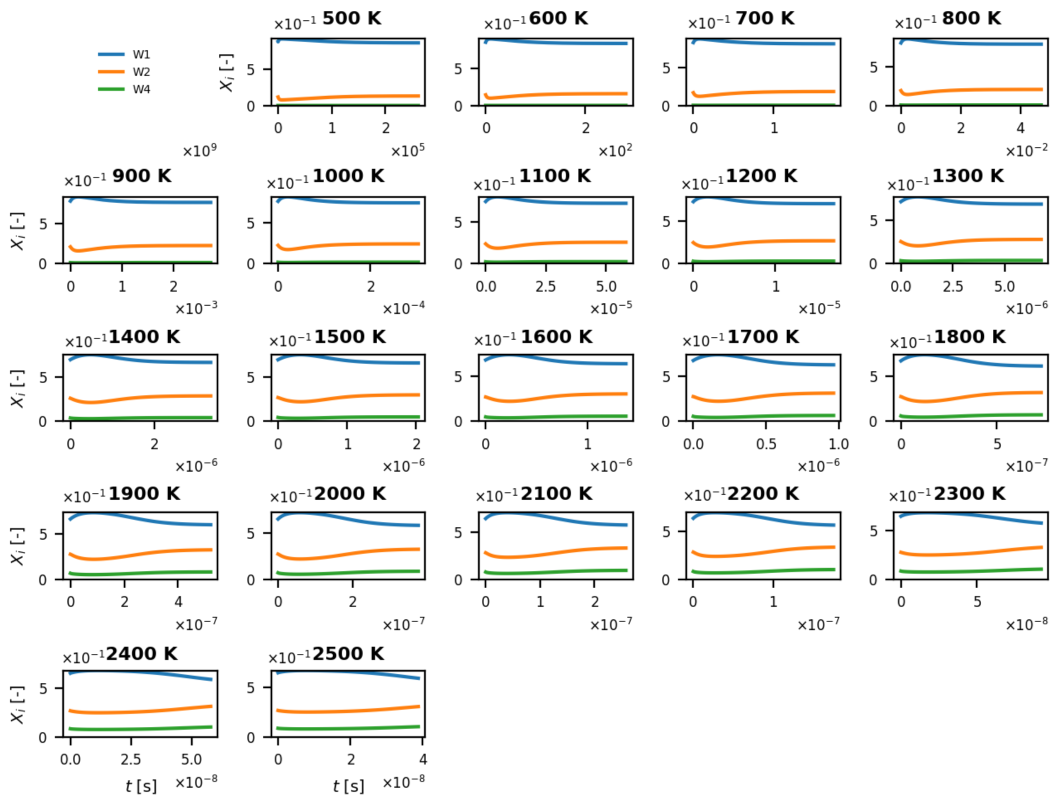


Figure 3.27: Selection of compositions of W1, W2 and W4 for the lumped species at 1 atm.

It is possible to see the changes in the molar fractions of the species W1, W2 and W4. The initial compositions are randomly selected, and the progression of the plots are obtained according to minimization of the possible errors caused by lumping. The composition that is used for the validation of the lumped system is the steady state (the final) composition achieved from the plots. These plots are also done for different pressure values (0.01, 10, 10, 100 and 1000 atm), however similar plots are obtained, and the figure above is used as an example of how the output looks like. After the compositions are selected, the lumped system can be validated with the validation step.

In the validation step of the calculations, the code runs the simulations using the rate parameters that are reported in the detailed (input) mechanism, and then runs the simulations for the same system parameters but using the rate parameters obtained from the lumping step for the lumped species. Because of the changes in the number of species and reactions, small differences are obtained when the comparison of both plots are done. The graphs obtained from the validation calculations for the lumped species, that compares the detailed rate constants with the lumped rate constants are reported in the following figures at different temperature and pressure values. It should be noted that H is not reported in the graphs, that is why the sum of final mole fractions does not tend to approach unity. It is known from the stoichiometries of the reactions that the moles of produced H is equal to the moles of P1 and P2.

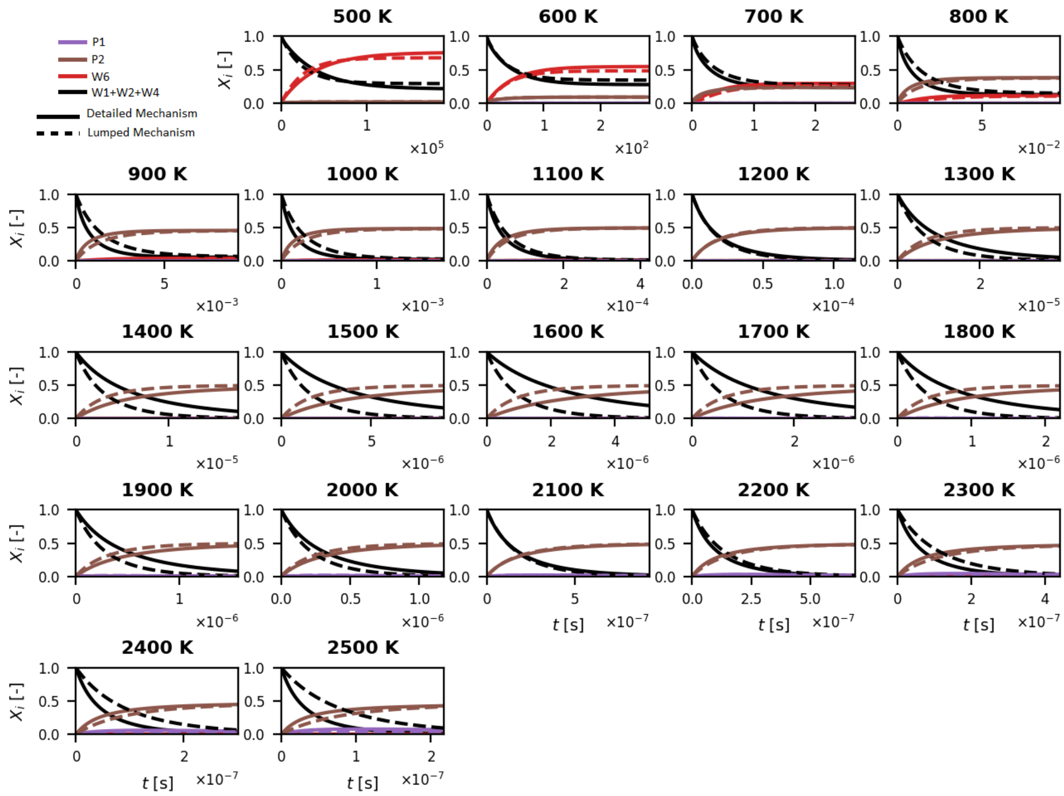


Figure 3.28: Comparison of the lumped and the detailed mechanisms at 0.01 atm.

As the graphs for 0.01 atm are analyzed, it can be seen that the lumped species tend to produce mainly W6 at very small temperatures (between 500-700 K), while at higher temperatures almost all the produced W6 tends to turn into P2+H. That is caused by the relatively faster reaction rates between W6 to P2+H compared to the smaller temperature values. P1+H only appears at very high temperatures (above 2000 K) however, even at that temperature they are not produced in a significant amount. The explanation of these plots can be done by the PES, for the production of P1+H all the reactions have a huge energy barrier, which is why W1 tends to form W2, W2 tends to form W3 and W4, W4 tends to reform W2 and finally W3 tends to form W5, W6 and P2+H in this order. It is obvious that W5 produces W6 rapidly, and depending on the temperature value W6 may accumulate or immediately produce P2+H. Because of the huge energy barrier, the reactions that produce P1+H are only occurring at very high temperatures.

The detailed and the lumped mechanisms produce very similar results up to 1300 K, after that temperature the two mechanisms tend to have different values for the molar fractions. The reason for that is the reduction of reactions from the detailed to the lumped mechanism. Even though some very similar values are achieved at some high temperatures (2000-2300 K) it can be concluded that the lumping of W1+W2+W4 produces differences in the reaction rates at moderate and very high temperatures. One interesting fact is that the lumped mechanism shows the lumped species is consumed faster than the detailed mechanism before 2100 K, and the opposite scenario happens above 2200 K. This is because of the composition and the overall rate constant of the lumped species. In other words, the overall rate constant causes the lumped species to be consumed faster compared to the individual rates of each of these species at moderate temperatures, and at high temperatures the individual rates consume the lumped species more than the overall rate.

It is also worth to mention that all of the curves tend to diverge from each other but arrive to the same fraction in the end. That value is approaching 0.5 in the cases above 900 K, the reason is the absence of H, as already described above. For example, if the final molar fraction of P2 is 0.5, the remaining part (again with a fraction of 0.5) stands for H.

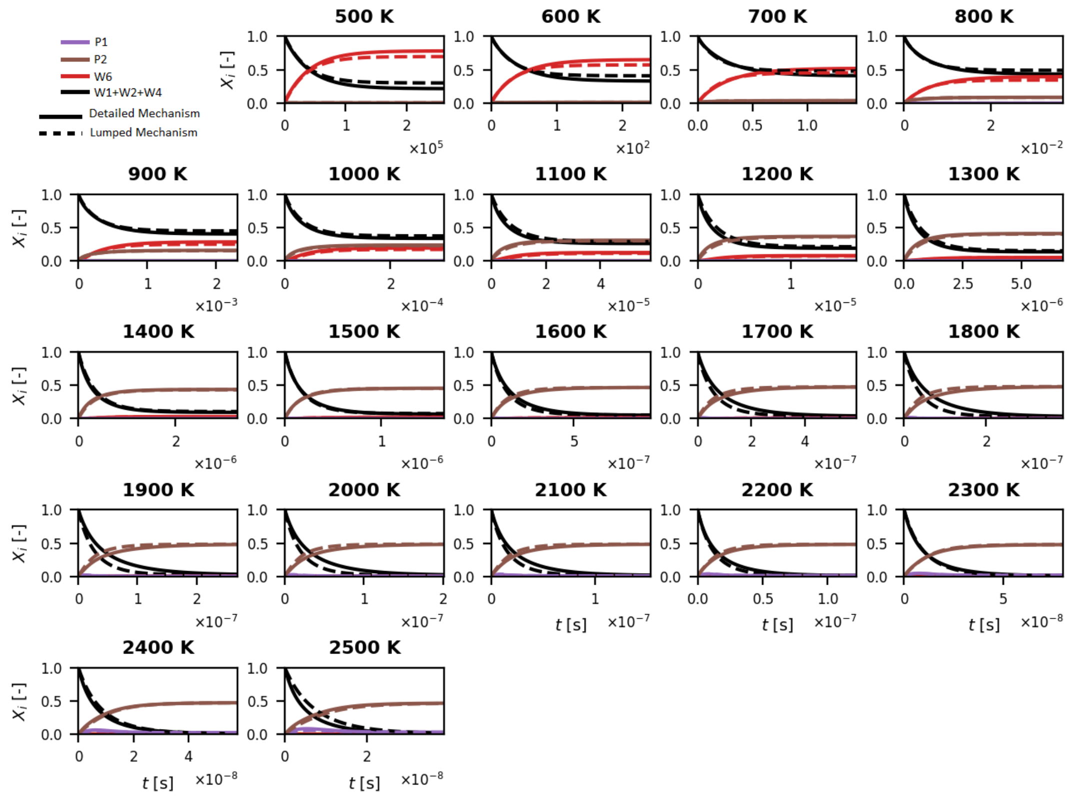


Figure 3.29: Comparison of the lumped and the detailed mechanisms at 1 atm.

Similar to the case at 0.01 atm, W6 tends to be the major product at lower temperatures, the difference is significant amount of W6 are produced for a larger range of temperatures (up to 1100 K). As already described for the previous case, at moderate temperatures P2+H becomes the main product and very small amounts of P1+H are produced at very high temperatures (above 2000 K).

One very important difference between the figures for 0.01 atm and 1 atm is the accuracy of the lumping, similar to the previous case the composition profiles tend to diverge from each other at moderate temperatures. However, the difference between the curves for the detailed and the lumped mechanisms are much smaller for this case. This shows that lumping of W1+W2+W4 becomes a relatively more reasonable assumption at 1 atm. In other words, as the pressure increases, the effects of all the single reactions of W1, W2 and W4 are not really necessary for the kinetic mechanism, grouping them together also provides accurate results.

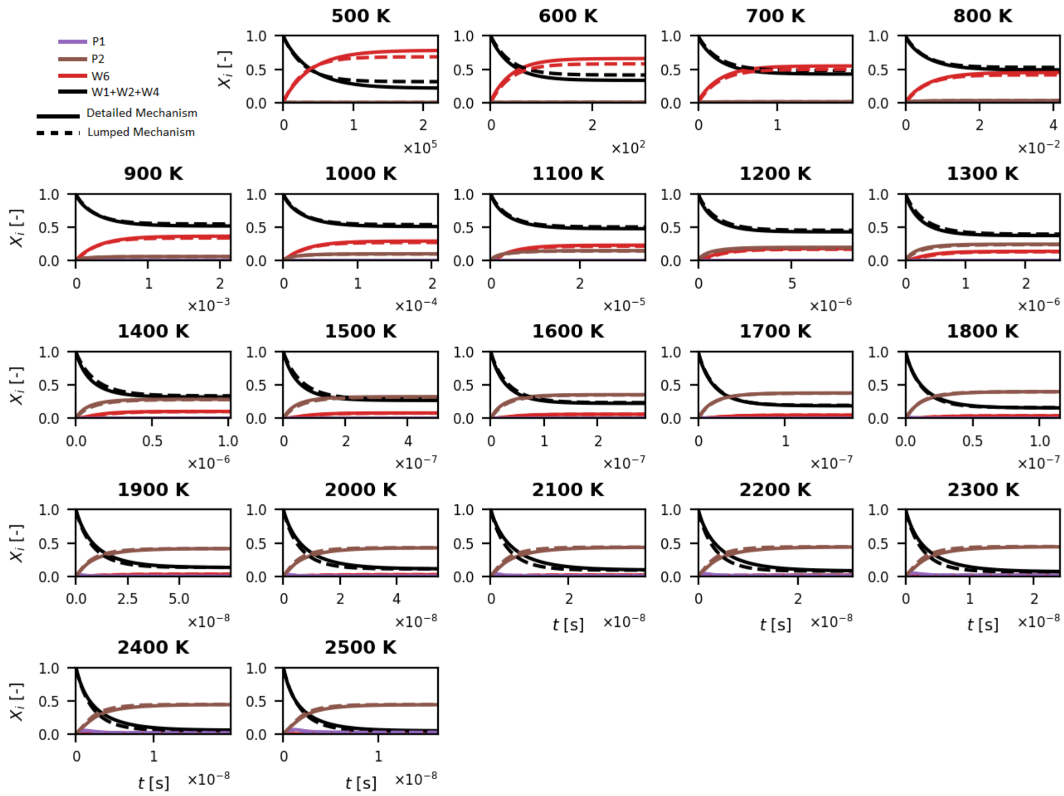


Figure 3.30: Comparison of the lumped and the detailed mechanisms at 10 atm.

Almost the same results that are achieved for 1 atm can be observed for 10 atm. There are two major differences; W6 tends to accumulate in significant amounts up to 1300 K (a larger range) and the curves of detailed and lumped mechanisms get much closer to each other. They are almost overlapping in the 800-1900 K temperature range. This shows that the results obtained from lumping are getting even better compared to 1 atm.

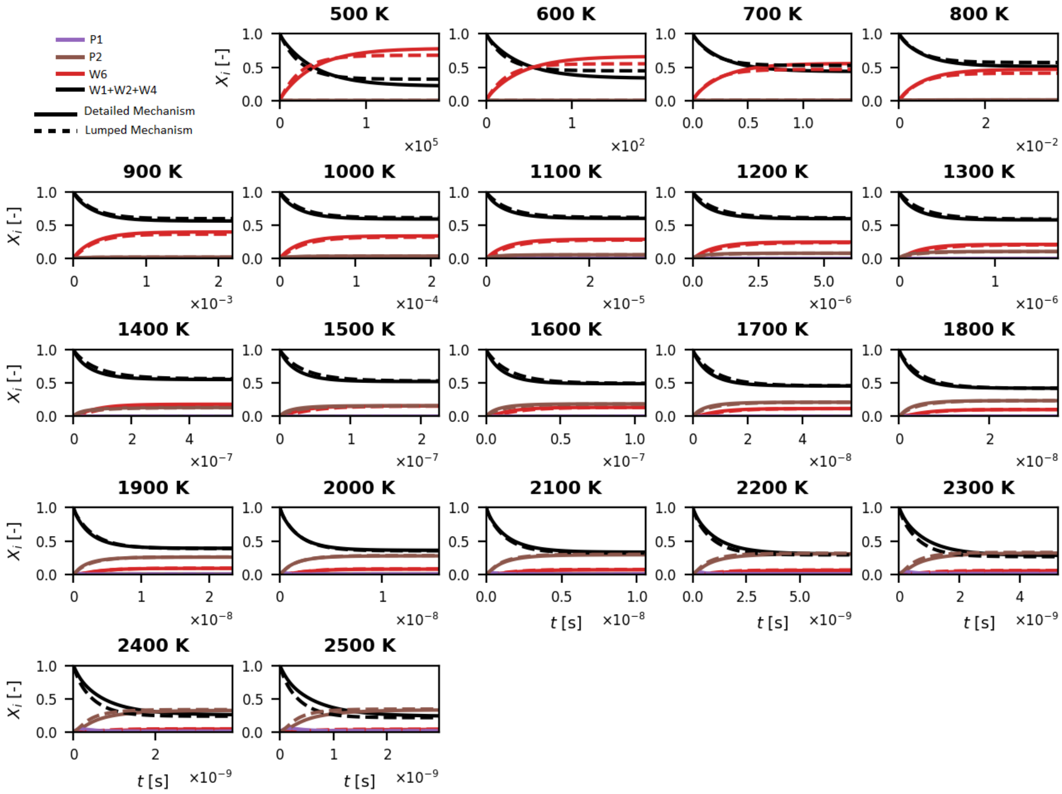


Figure 3.31: Comparison of the lumped and the detailed mechanisms at 100 atm.

The findings for the previous cases are still valid for 100 atm. Namely, the larger range of W6 production (up to 1800 K), and accurate lumping results (perfect overlapping between 800-2200 K). However, there is a very important difference for this case. In all the previously analyzed pressures, the molar fraction of the lumped species (W1+W2+W4) tends to approach zero (i.e. fully consumed) as the temperature increases, but for this case it reaches just around the molar fraction of 0.3. That means the rate of production of it becomes equal to the rate of consumption, it reaches equilibrium and becomes an accumulating species. That is a major difference from the previous cases.

For the case with the pressure of 1000 atm, the results for the case of 100 atm are still the same. The mole fraction of the lumped species never approaches zero, not only that but does not even go below 0.5 at high temperatures, thus it becomes the major accumulating species in the system. As it can be seen, for 1000 atm, the plots at different temperatures have very similar behavior, it is thus hard to distinguish them after 1800K. One very important note is that, lumping again produces very accurate results. Except at small (up to 700 K) and very high temperatures (above 2400 K), the curves of the detailed mechanism and the lumped mechanism are almost the same as each other.

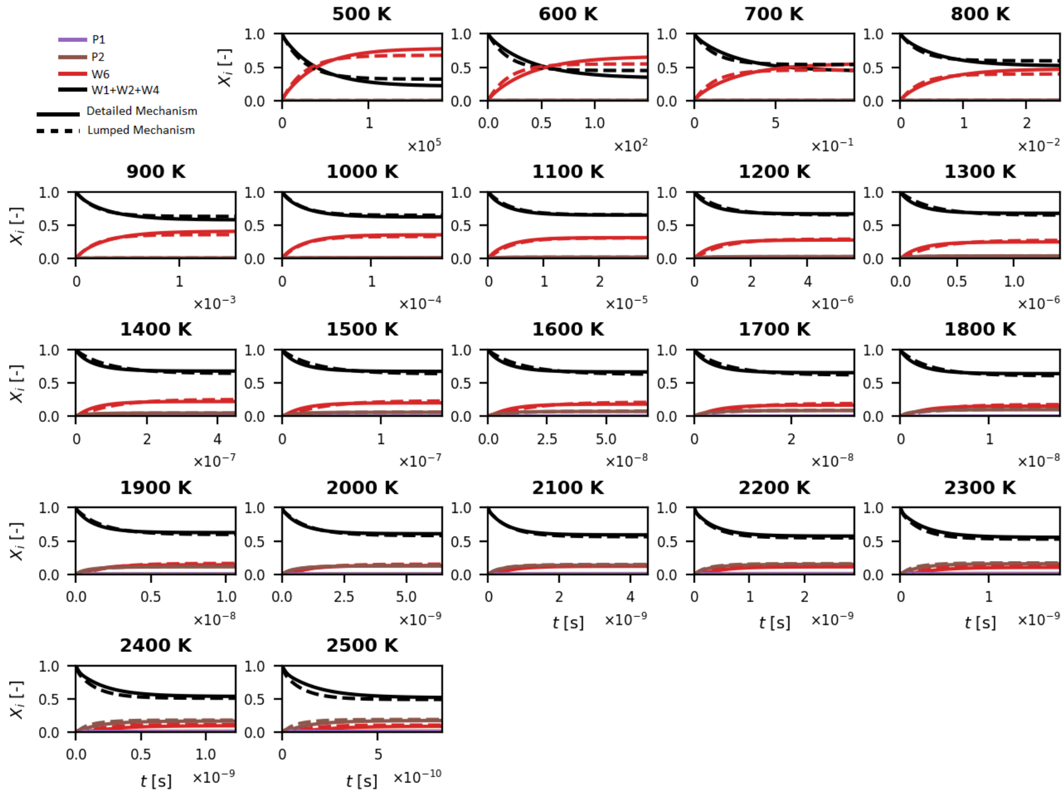


Figure 3.32: Comparison of the lumped and the detailed mechanisms at 1000 atm.

3.2. H-Abstraction from Methylcyclopentadiene by H, CH_3, OH and OOH

In this section different types of abstraction reactions, namely, the attacks of H, CH_3, OH and OOH to the methylcyclopentadiene (MCPE) molecules will be analyzed. As the reactant molecules, all of the three methylcyclopentadiene isomers described in Section 1.3 are included in the calculations. In abstraction reactions, one molecule approaches the other, breaks the bond of an atom (the hydrogen atom for all the calculations in this thesis), and creates a bond with the atom that has been removed.

In the calculations, the attacking atom can remove a hydrogen atom either from the CH_3 group of the MCPE molecule, or from the carbon that has two hydrogen atoms. That means for 1-methylcyclopentadiene and 2-methylcyclopentadiene two different cases needs to be analyzed, while for 5-methylcyclopentadiene only one case (for the carbon with two hydrogen atoms). After the free hydrogen atom is captured by the attacking H, CH_3, OH and OOH molecules, H_2, CH_4, H_2O, H_2O_2 will be formed, respectively. Depending on the site of the attack of the MCPE isomers, they will turn into some of the radicals (or their resonance structures) which are analyzed in Section 3.1.

As already mentioned in Section 2.3.1 the abstraction reactions could be analyzed with different models depending on the number of transition states (for the process and for the van der Waals wells). In this thesis, the abstraction reactions are analyzed with two different models, namely the three transition state model and the one transition state model. The latter model is used only for the cases where there is the attack of the OH molecule. The reason behind using a one transition state model for that specific case is, the computations did not converge to a van der Waals well. Hence, the well structures are excluded from the calculations and the only transition state structure is the one for abstraction. This does not cause any problems for the calculations, as already mentioned in Section 2.3.1 there are lots of studies in the literature that use the one transition state model.

The reactions that are analyzed in this section are reported in the following. Specifically the reactions with 1-methylcyclopentadiene are shown in figures 3.33 and 3.34, the reactions with 2-methylcyclopentadiene are shown in figures 3.35 and 3.36, finally the reactions with 5-methylcyclopentadiene are shown in Figure 3.37.

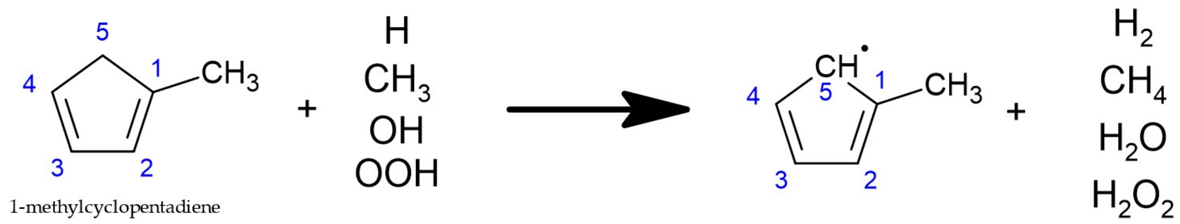


Figure 3.33: H-abstraction of 1-methylcyclopentadiene from the carbon with two hydrogen atoms.

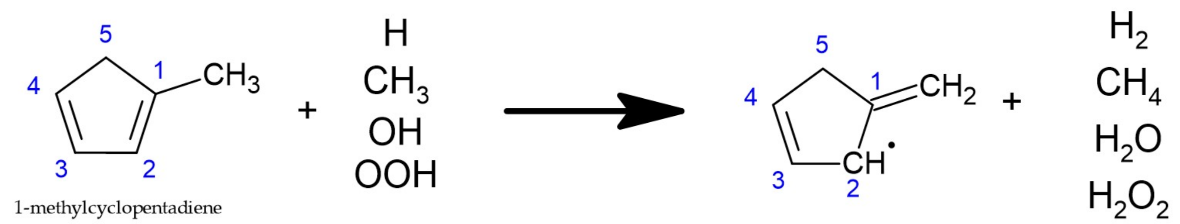


Figure 3.34: H-abstraction of 1-methylcyclopentadiene from the CH_3 group.

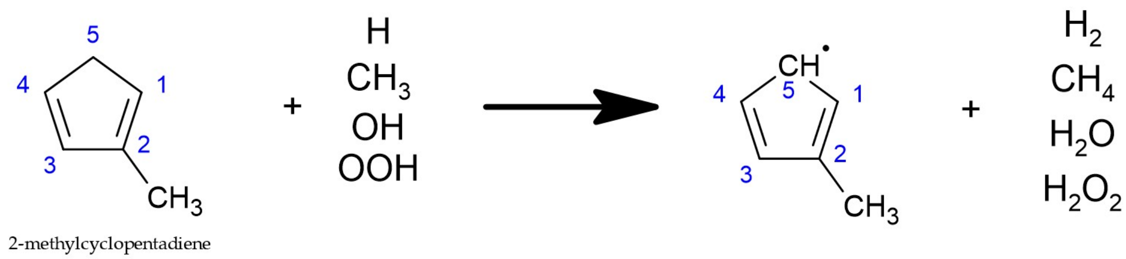


Figure 3.35: H-abstraction of 2-methylcyclopentadiene from the carbon with two hydrogen atoms.

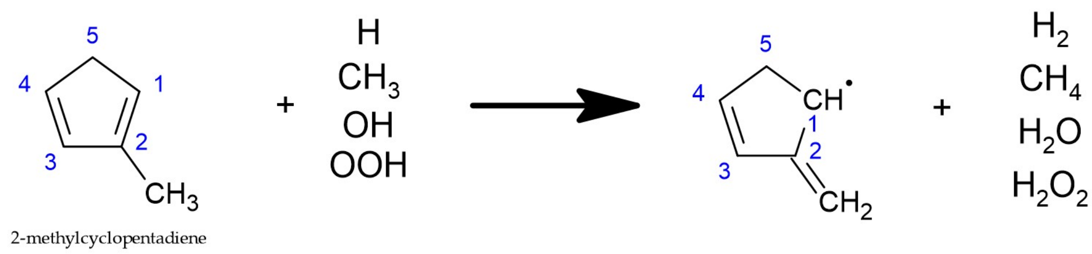


Figure 3.36: H-abstraction of 2-methylcyclopentadiene from the CH_3 group.

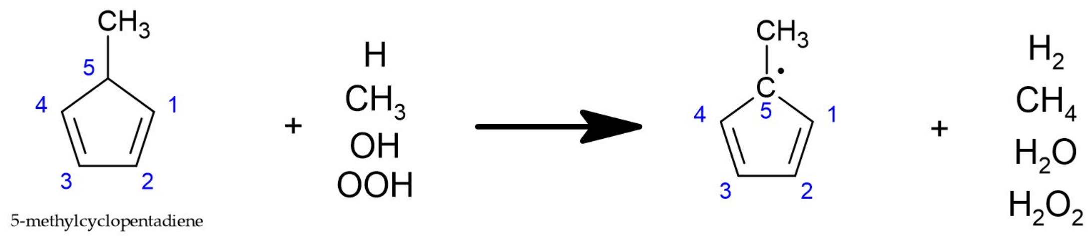


Figure 3.37: H-abstraction of 5-methylcyclopentadiene.

3.2.1. PES

The graphs for the potential energy surfaces of the abstraction reactions are reported in this section. The reactants are selected as the reference and are assumed to have an energy of zero. The energies of the products, transition states and the van der Waals wells are reported with respect to the energies of the reactants.

Level 0 calculations are performed at the WB97X-D/6-31+g(d,p) level of theory, which is used also for hindered rotor, symmetry, and IRC analyses. The hindered rotor analysis for the transition state are done with at the UWB97X-D/6-31+g(d,p) level of theory. For level 1 calculations, the WB97X-D/aug-cc-pVTZ level of theory is used. As described in Section 3.1.1, the high-level calculations are obtained at the CCSD(T) level of theory combined with CBS and DF at the MP2 level, taking the core electron corrections into account. The equations 3.1 and 3.2 (that are used for the previous case) are used to calculate the high-level energies.

The following potential energy surface diagrams are obtained from the high-level energy calculations, while also DFT (level 1) energies are reported in the parenthesis. The energies correspond to the reactants, transition states, products and two van der Waals wells. The wells are not reported for the cases with the OH attack since the calculations did not converge to a van der Waals well, as already mentioned before. One other important thing to mention about the calculations is that the high-level calculations are not performed for the wells, that is why for the wells only the DFT energies are reported. The reason of not running the high-level calculations for the wells comes from the fact that they will not be used for the rate analysis and the cost of having high-level calculations is quite high, and it is not worthwhile to run expensive calculations if they will not be used for the analysis in the next steps.

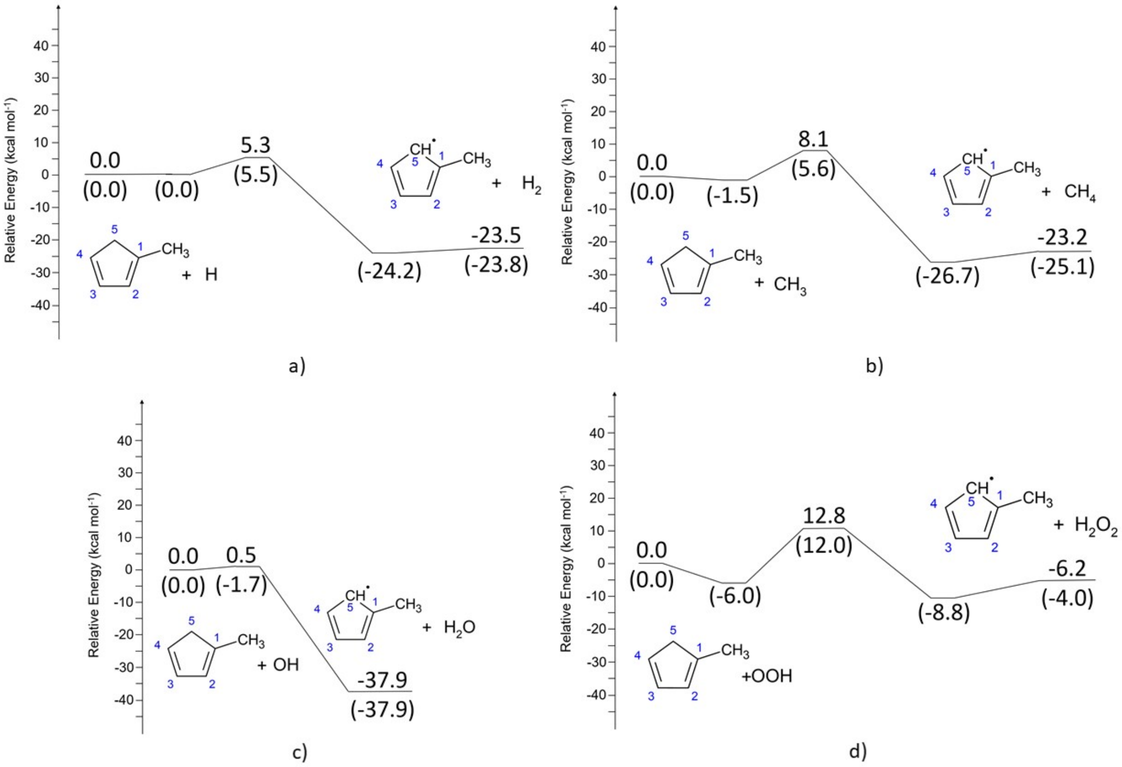


Figure 3.38: Hydrogen abstraction reactions from C(5) of 1-methylcyclopentadiene by a) H, b) CH_3, c) OH, d) OOH molecules.

The reactions shown in Figure 3.38 are hydrogen abstraction reactions of the molecule

1-methylcyclopentadiene from the carbon that has two hydrogen atoms (C(5)). As it can be seen from the plots, all of the reactions starting from 1-methylcyclopentadiene are exothermic and since the abstractions are done from the same site, the major product is exactly the same for all the cases. The most exothermic case is the one with an OH attack, the products are 37.9 kcal/mol less energetic than the reactants. That reaction also has the lowest energy barrier compared to other three reactions. This means the reaction with OH can occur more easily than the others.

The shape of the PES and the values of the energies are very similar for the cases with H and CH_3 attacks. Both the reactions have an energy barrier that is less than 10 kcal/mol and the products are about 20 kcal/mol less energetic than the reactants.

For all the reactions that include the van der Waals wells, the energies of the reactants and the first well, and similarly the energies of the products and the second well are very close to each other. The case with H attack has the smallest difference between them, the first well is exactly equal to the energy of the reactants and the second well is just 0.4 kcal/mol less energetic compared to the products. This occurs because the attacking atom (H) is the smallest possible atom, and it does not cause huge differences in the energetic values of the system. Similarly, for the case with OOH attack the opposite can be observed, there is a difference of 6.0 kcal/mol energy between the reactants and the first well, and 4.8 kcal/mol difference between the products and the second well. Opposite to the case explained for the case with hydrogen, this happens because OOH is a large molecule with respect to other molecules analyzed in this thesis, and it changes energetic values more compared to other reported cases. Also, the energy barrier for the reaction of OOH is relatively higher than the other cases. This means it is relatively harder for this reaction to occur than the others.

The potential energy surfaces reported in Figure 3.39 are very similar to the ones in Figure 3.38. The same comments can be written for this case too, as even the values of energies do not change a lot. That was expected since they have the exact same reactants with the previous case, the only difference is the carbon that is attacked by the attacking species. Therefore, it may be better to compare the cases with the same reacting species reported in figures 3.38 and 3.39.

When the energies are compared between the two figures, it can be seen that the values are larger for the cases with the attack of the methyl group. In other words, the energy barrier, which shows how easy the reaction occurs, is larger for the case with an attack to methyl. On the other hand, the reactions are less exothermic for the methyl attack compared to the hydrogen attack. For example, for the cases where CH_3 attacks the

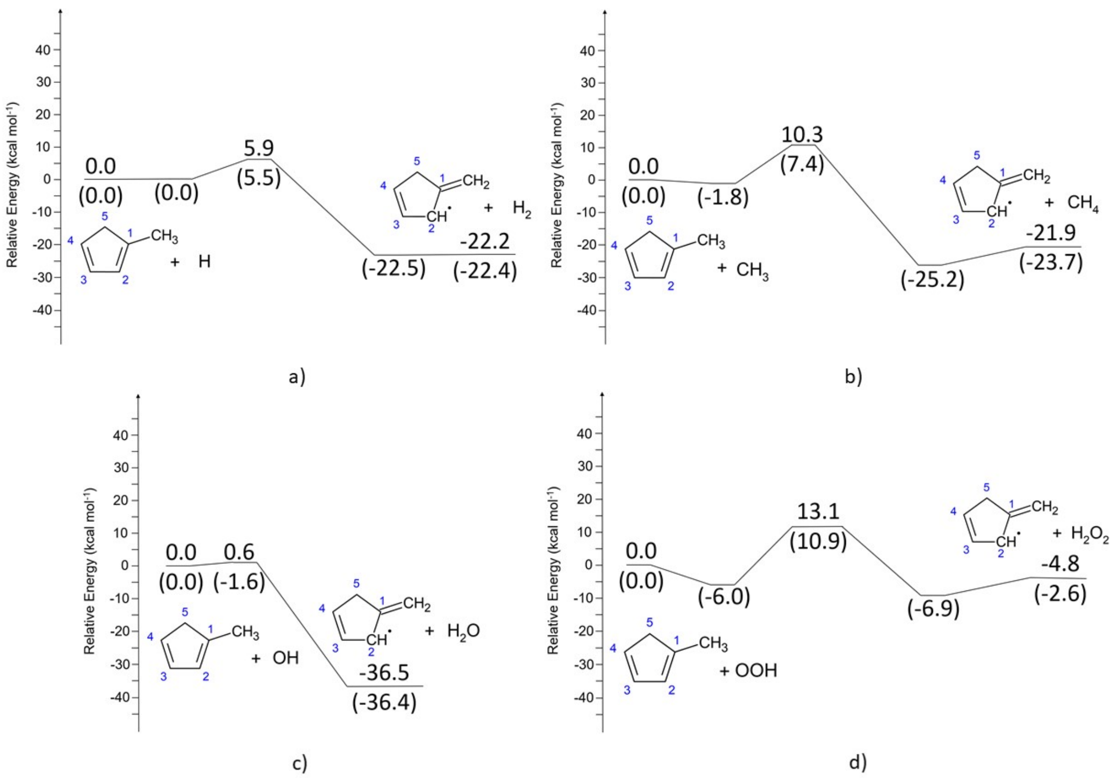


Figure 3.39: Hydrogen abstraction reactions from the methyl group of 1-methylcyclopentadiene by a) H, b) CH_3, c) OH, d) OOH molecules.

molecule, one can see that the energy barrier increases from 8.1 to 10.3 kcal/mol, while the enthalpy of the reaction decreases from -23.2 to -21.9 kcal/mol when the methyl group is attacked.

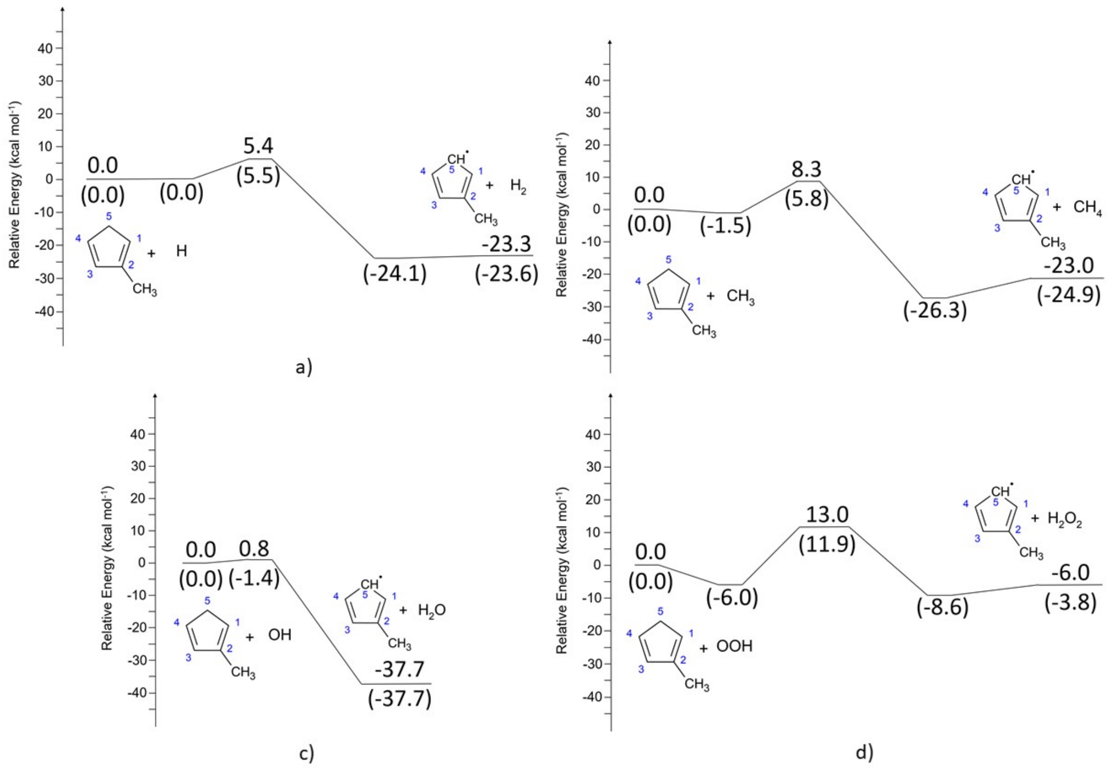


Figure 3.40: Hydrogen abstraction reactions from C(5) of 2-methylcyclopentadiene by a) H, b) CH_3, c) OH, d) OOH molecules.

2-methylcyclopentadiene and 1-methylcyclopentadiene are two similar isomers. When the values in figures 3.38 and 3.40 are compared, it can be seen that the values are close (almost the same) to each other. Moreover, the values mostly changed 0.1 or 0.2 kcal/mol, with the highest difference for the energy being 0.4 kcal/mol. That is why the exact same comments can be reported for the abstraction reactions from the carbon with two hydrogen atoms of 1-methylcyclopentadiene and 2-methylcyclopentadiene.

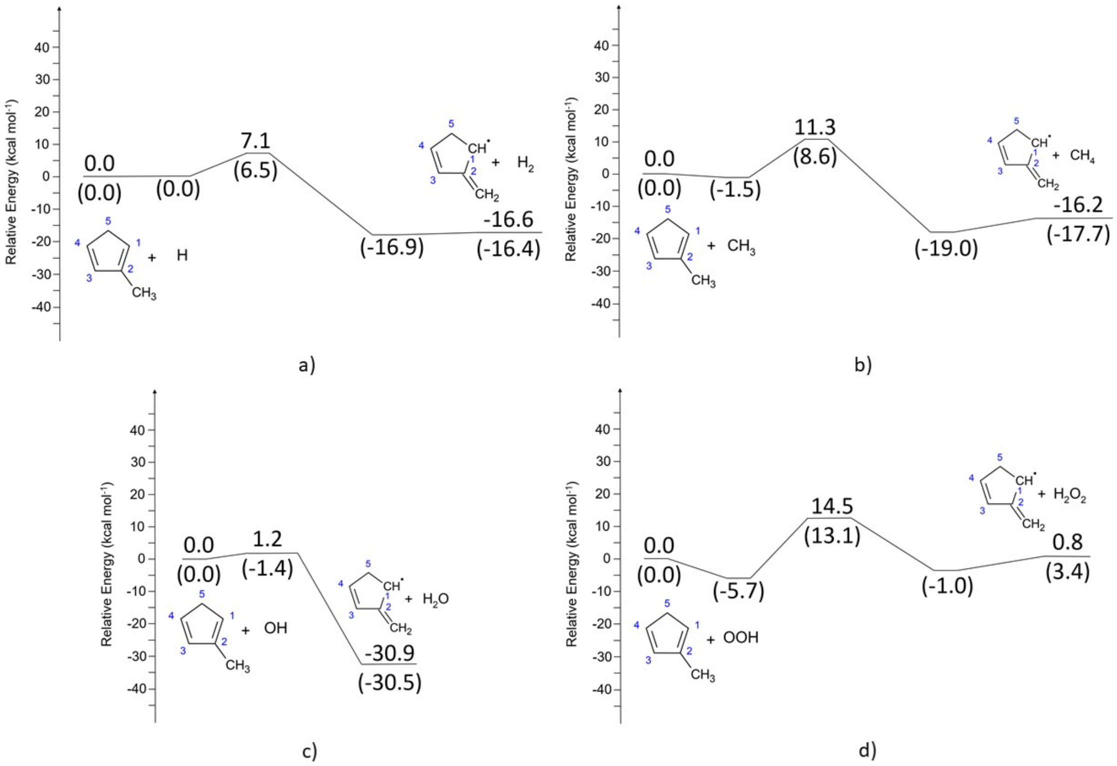


Figure 3.41: Hydrogen abstraction reactions from the methyl group of 2-methylcyclopentadiene by a) H, b) CH_3, c) OH, d) OOH molecules.

Unlike the previous case, when the methyl group of the isomers are attacked, relatively larger differences in the energies can be obtained between 1-methylcyclopentadiene and 2-methylcyclopentadiene. When the values are compared between figures 3.39 and 3.41, it can be seen that the values of the energies are larger when the reactant is 2-methylcyclopentadiene, however it should be mentioned that the shapes of the potential energy surfaces remained similar. As already mentioned in one of the previous cases, this means the barrier of energy is larger but the exothermicity of the reaction is smaller for 2-methylcyclopentadiene compared to 1-methylcyclopentadiene.

One interesting difference can be seen when the plots of the OOH attack are compared with each other. The reaction becomes endothermic when the reactant is 2-methylcyclopentadiene, this is the only case for all of the analyzed abstraction reactions in this thesis. It should be mentioned that the enthalpy of the reaction is 0.8 kcal/mol, therefore it is not so true to call it an (highly) endothermic reaction, but still it is slightly endothermic and it is the only case with a positive value for the products.

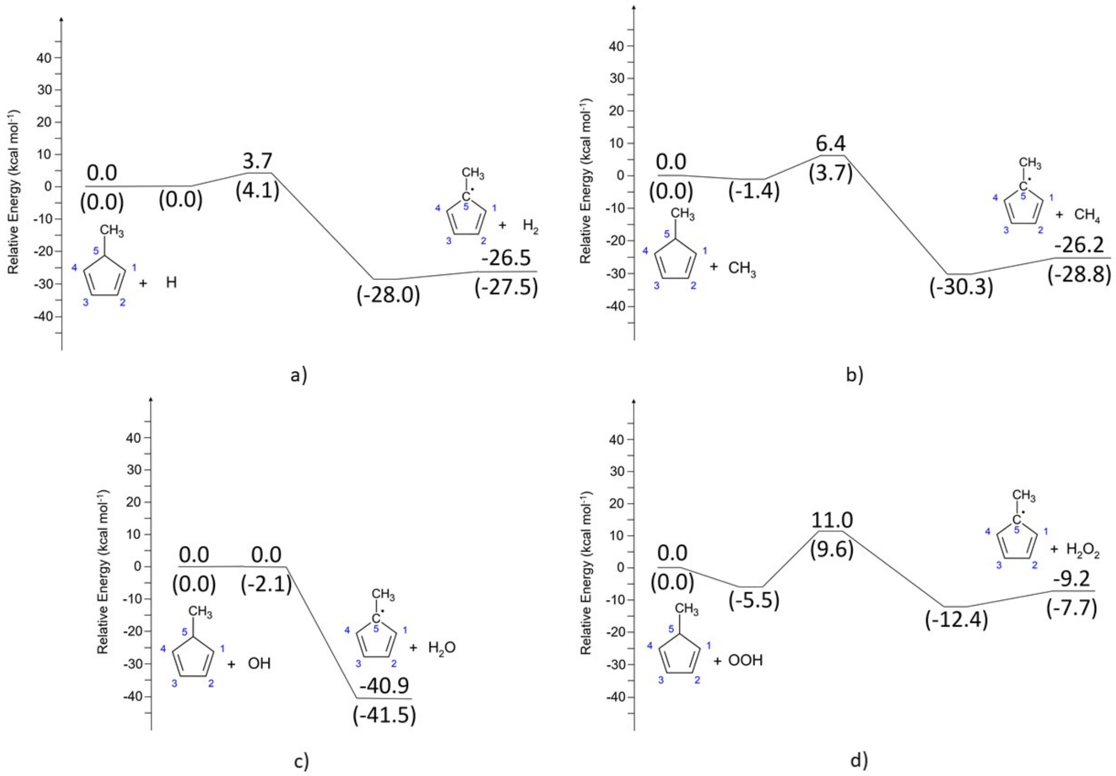


Figure 3.42: Hydrogen abstraction reactions of 5-methylcyclopentadiene by a) H, b) CH_3, c) OH, d) OOH molecules.

Unlike the previously analyzed cases the abstraction reactions of 5-methylcyclopentadiene are only analyzed for one case, where the carbon that contains one hydrogen and one methyl group (C(5)) is attacked. The reason is, the methyl group and the hydrogen are so close to each other and methyl would act as a more stable group, that is why when a molecule approaches to attack the hydrogen would tend to be removed from the molecule rather than a hydrogen of the methyl group.

Even though the shapes of the potential energy surfaces are similar to the cases analyzed before, one important change is that the values of the energies are smaller when 5-methylcyclopentadiene is the reactant, for example the enthalpy of the reaction of the OH attack on 5-methylcyclopentadiene is around -41 kcal/mol, that is the only case where the energy of the products is below -40 kcal/mol.

3.2.2. Master Equation Simulation / Rate Constant

As described in Section 3.1.2, the rate constant analysis needs some parameters as input. The exact same values calculated for the decomposition of methylcyclopentadienyl radical using Jasper's work [18] are calculated for the abstraction reactions too due to the similarity of the system. Once the input file is created, the software MESS is used to calculate the rate constants just as done for the decomposition reactions.

The same pressure and temperature values are used for the rate constant analysis, which means the pressures are between 0.001 atm and the high-pressure limits, and the temperature values are between 300 K to 2500 K. However, to improve the fitting the values calculated at 300 and 400 K are excluded from the rate constant regression. The rate constants are reported in the following are those computed at the lowest pressure (0.001 atm). The reason is that at higher pressures the van der Waals wells become stable and affect the reaction rate constants for the net reaction. However, for the cases with an OH attack, as described before, the one transition state model is used, since there is no van der Waals wells, and thus the high-pressure limits could be used for the rate constant analysis without any problems.

The species that are present for the abstraction reactions are reported in Figure 3.43. In the following figures the plots of the rate constants are reported, while the data that is used to determine these plots are reported in the appendix.

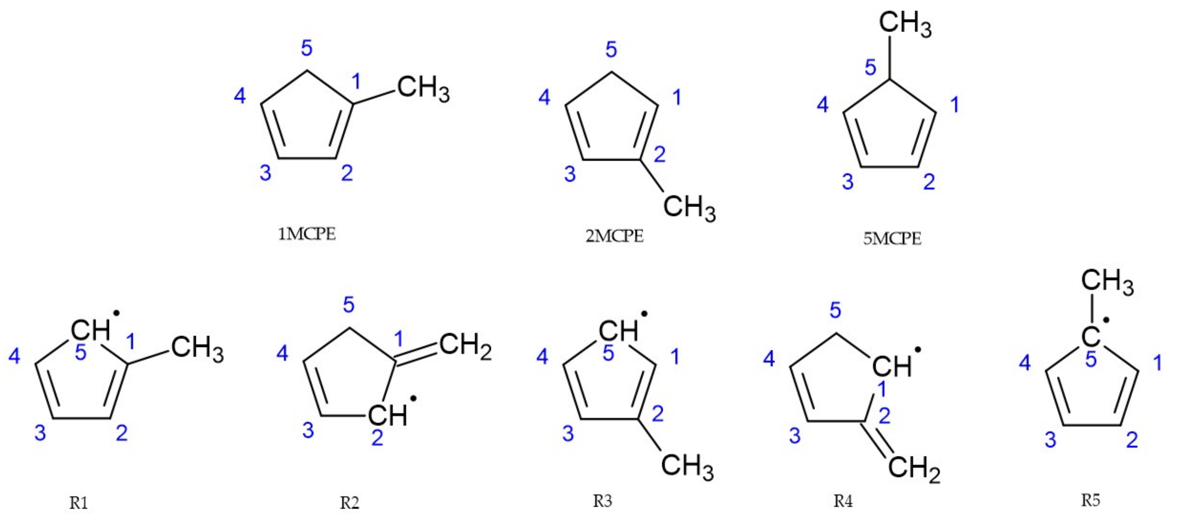


Figure 3.43: List of the species that have been considered as reactants (above) and products (below) for the abstraction reaction study.

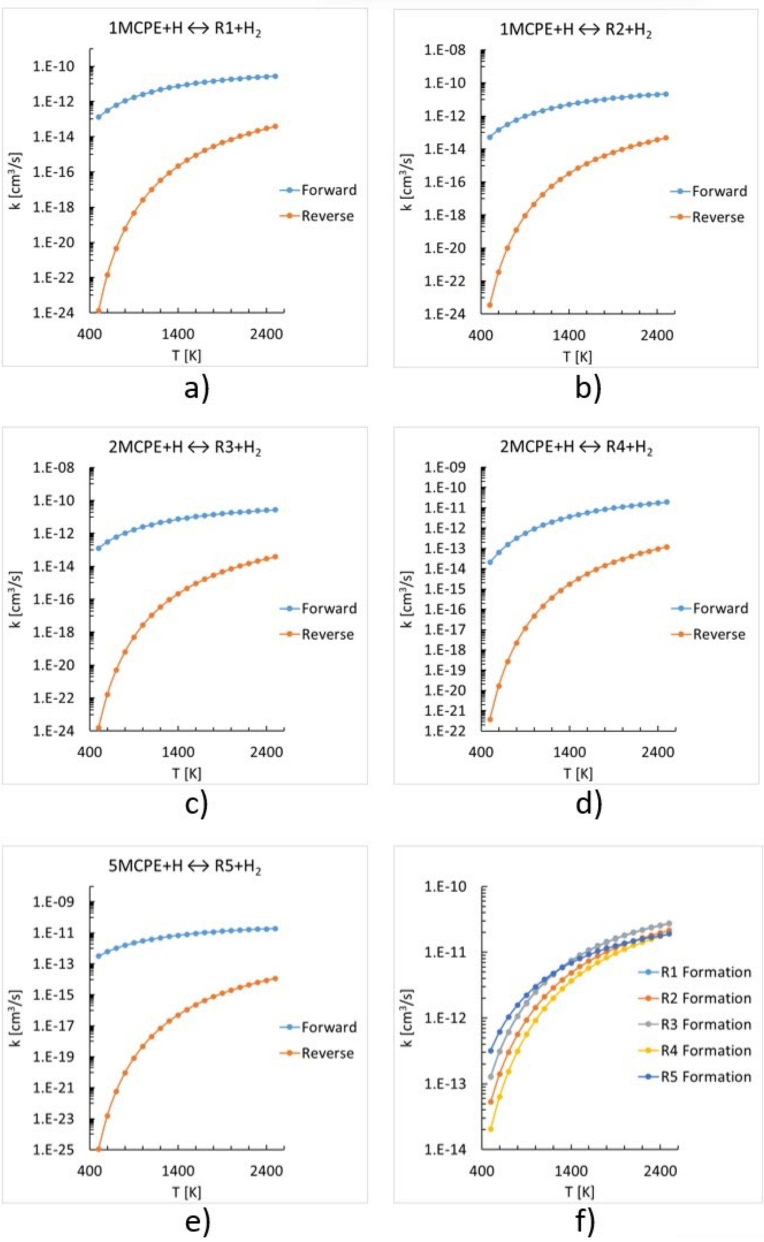


Figure 3.44: Plots of the abstraction rate constants for the H attack for different cases (a-e) and comparison of forward rate constants for the different channels (f) at 0.001 atm.

When the rate constant are analyzed, the first obvious result is the slowness of the reverse reaction rate compared to the forward rate for each case. Hence, the reactions can almost be thought as if they are only going in one direction, the one that forms methylcyclopentadienyl. One other important conclusion is about the value of the rate constants, they all are at very similar order of magnitudes. To be able to compare all the cases and comment on them, a log plot (with a base of ten) is used for the forward rates of all reactions. As shown in Figure 3.44f, the rate constants between the cases reported in Figure 3.44a and Figure 3.44c cannot be distinguished, which means they have very similar rates for all the temperature range. That could be expected when the PES of both reactions are compared with each other. The energy barrier of Figure 3.44a was 5.3 kcal/mol and that of Figure 3.44c was 5.4 kcal/mol, also the energy of the products of Figure 3.44a was -23.5 kcal/mol and it was -23.3 kcal/mol for Figure 3.44c. Because of the similar values, one could expect similar reaction rates, and this is the case observed when they are compared graphically.

Another important result is that the rate constants at high temperatures tend to approach to each other even though they started from very different values. The diversity at the low temperatures is caused by different reactivities of the radicals and the sites they attack, however at high temperatures they become highly reactive and don't have that much of a difference in their rates.

Except the case reported in Figure 3.44e, none of the forward rate constants intersect the other, but that is very clearly observed in Figure 3.44f. The reaction rates start at a relatively higher value for Figure 3.44e and reach a relatively smaller value at higher temperatures. Which means it loses some reactivity compared to other cases at higher temperatures. It should be noted that the values still increase as temperature increases thus, its reactivity increases but not as much as the increase in other cases.

Compared to the cases of H attack (Figure 3.44), by looking at Figure 3.45 it can be seen that all the reactions have smaller rate constants. It can be seen that the rate constants of the reverse reactions show an increasing trend too, however they are still at least one order of magnitude smaller than the forward rate constants. That means the reactions still tend to follow the forward path. Except for the trends of the plots, there are some major differences between the cases with H and CH_3 attack.

The rates between Figure 3.45a and Figure 3.45c were very similar for H attacks, however this cannot be observed for the CH_3 attack, this can be seen from the fact that all of the curves are clearly identifiable in Figure 3.45f. In fact, the reactions have relatively similar values for their rate constants at lower temperatures and they diverge from each other as the temperature increases. This is caused by the changes in the reactivities of the radicals and the methyl molecule (which is relatively bulkier than hydrogen) that is attacking the radicals.

For this case, even at high temperatures the curves do not tend to approach each other, which means the reactivities of the molecules do not become similar, they are different both at low and high temperatures. However, around 1000 K all of the reactions have similar rate constants, which was not observed in the case of H attack. Also, one other

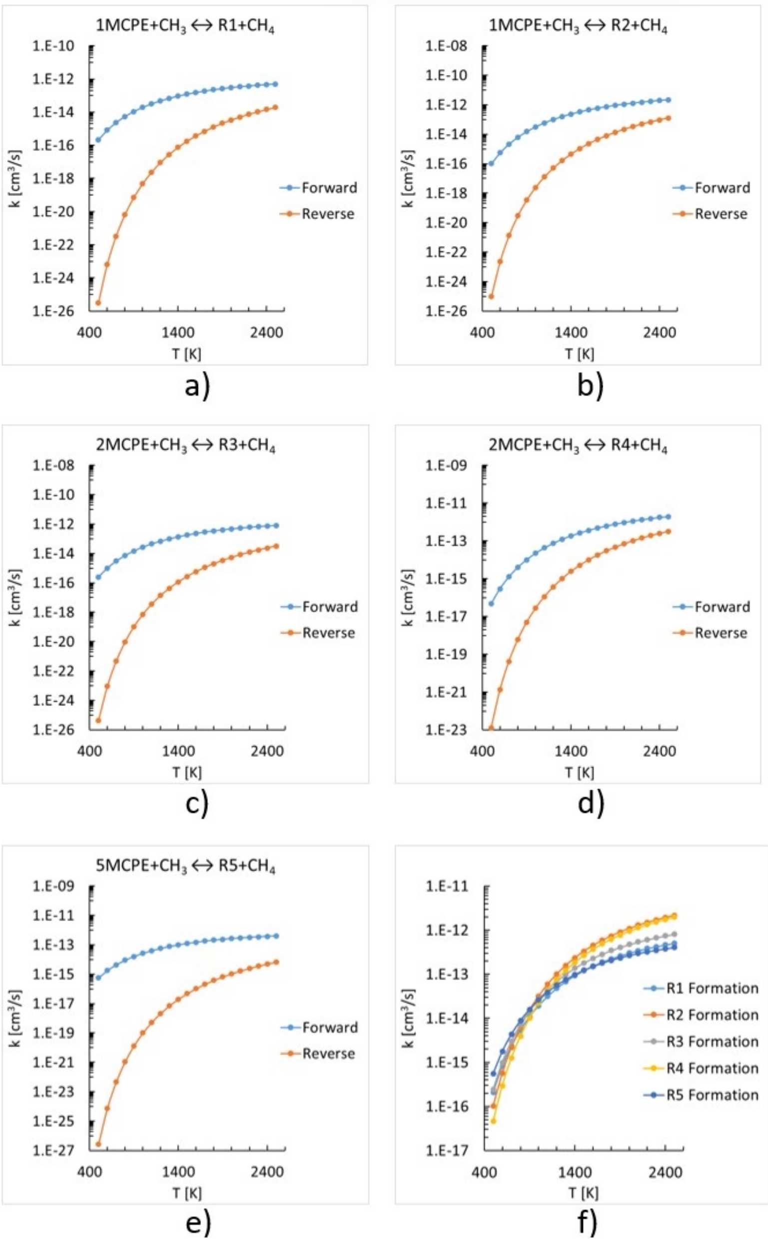


Figure 3.45: Plots of the abstraction rate constants for the CH_3 attack for different cases (a-e) and comparison among all forward rate constants (f) at 0.001 atm.

difference is, for CH_3 attack, not only the reaction shown in Figure 3.45e but also Figure 3.45a and Figure 3.45c crosses the other curves. That also shows the changes in the rates of the growth of the rate constants for different reactions at low and high temperatures for this case.

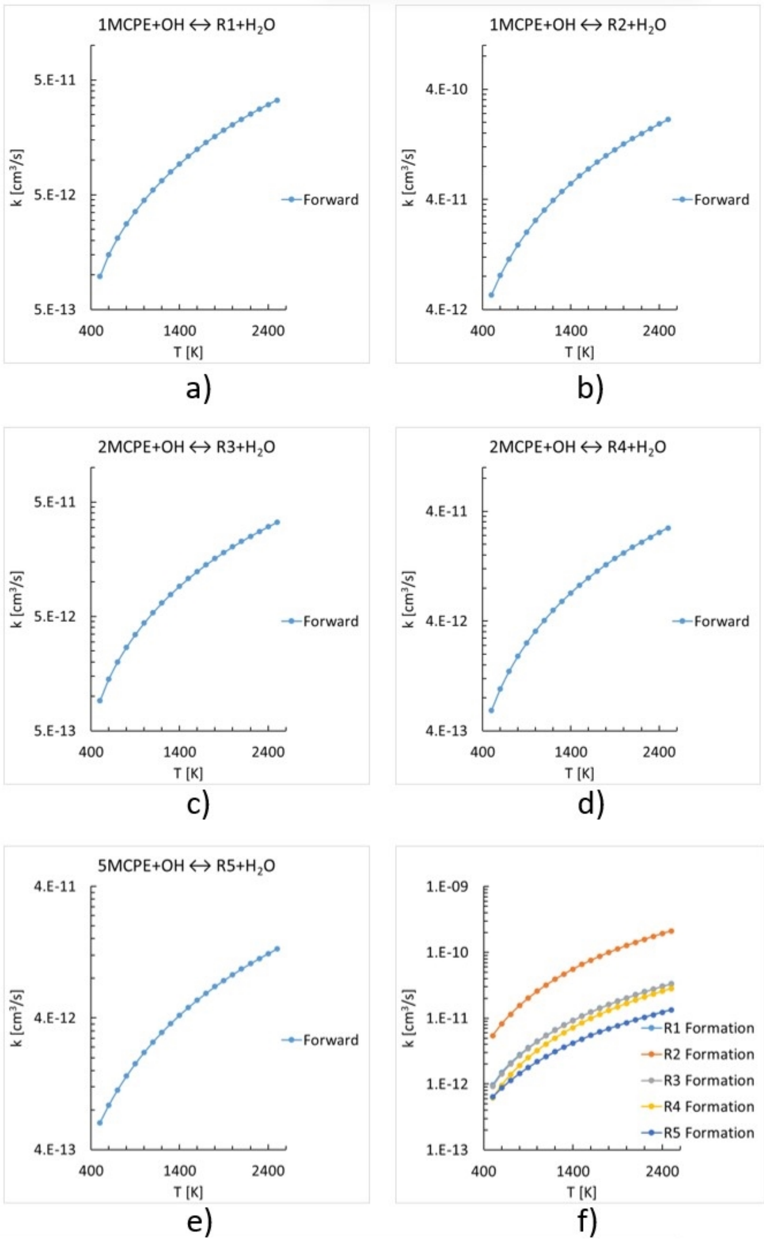


Figure 3.46: Plots of the abstraction rate constants for the OH attack for different cases (a-e) and the comparison of the forward rate constants (f) at high pressure.

As already mentioned, the OH attack calculations are done by using the one transition state model. When this model is used the results of the rate constant calculations do not report the reverse reaction rates from products to the reactants, but only from the transition state to the reactants, which occurs too fast. Because of that reason the plots do not include the reverse (transition state to the reactants) reaction rate constants. The input files for these calculations are also reported in the appendix.

By looking at Figure 3.46f, a trend that has not been observed for the other cases can be seen. None of the curves majorly cross each other, and neither at low nor at high temperatures do they converge to a common value. Similar to the case of H attack, the curves reported at Figure 3.46a and Figure 3.46c are so close to each other at all the temperatures, that is why it is so hard to identify them from one another on Figure 3.46f. Also, for the H and CH_3 attacks, the orders of magnitudes of the rate constants were comparable with each other, there was not a major reaction that is much faster than the other ones at all the temperature range. However, for the OH attack, the curve reported at Figure 3.46b is much faster than all of the other reactions at every analyzed temperature. One other result is that the curves do not tend to approach each other and converge to a specific value. They have different values at the low and the high temperatures with respect to each other.

When the plots of the OOH attack (Figure 3.47) are analyzed, it is once again possible to see some increase in the reverse rates, due to the temperature dependent modified Arrhenius law. However, just like found for the other cases the order of magnitude of the reverse rate constants are smaller than those of the forward rates except for case Figure 3.47d. The forward and the backward reaction rate constants of Figure 3.47d are very similar to each other. This behavior is not observed in any of the analyzed cases. This odd behavior can be perfectly explained by the energies of the species. The products have an energetic value of 0.8 kcal/mol, which was never the case for the other analyzed reactions. That means the products and the reactants are so energetically close to each other, and thus the energy barrier for the forward and the backward reactions are so close to each other too. This is the reason of the very similar forward and backward rate constants. Also, in general the forward rates are comparable with each other, this can perfectly be seen when the curves at Figure 3.47f are analyzed.

Like most of the cases, the curves of Figure 3.47a and Figure 3.47c almost perfectly coincide with each other and form a single indistinguishable line on the plot Figure 3.47f. At higher temperatures not only these two but all of the curves approach each other, and they tend to converge to a specific value. This means their reactivities (even though different at low temperatures) become very similar. It is clearly observable that for the cases with OOH attack, it is very hard to differentiate the curves from each other above 1500 K. This was not the case for any other attacking molecules.

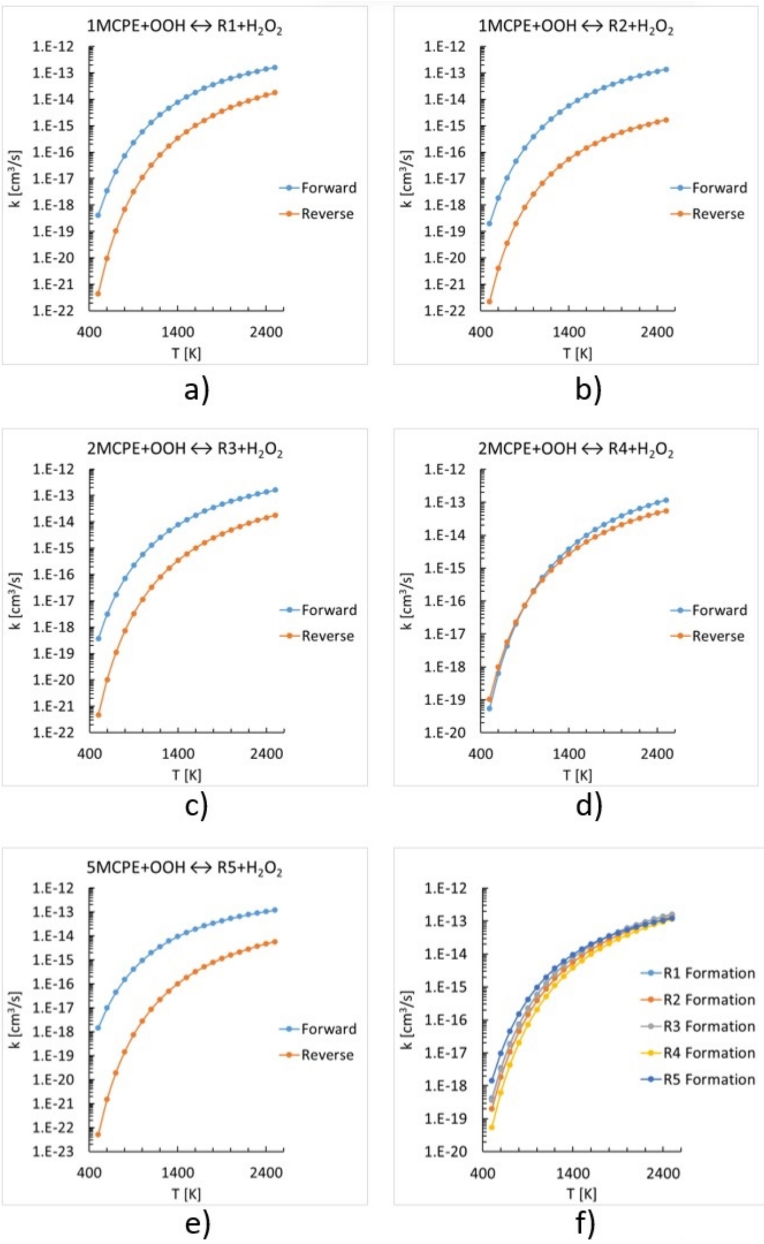


Figure 3.47: Plots of the abstraction rate constants for the OOH attack for different cases (a-e) and the comparison of the forward rate constants (f) at 0.001 atm.

Like the case of OH attack, for this case the curves also do not tend to majorly cross, they just approach to each other and continue to have similar values for the rate constants at different temperatures. This is another way of observing the changes in their reactivities at different temperatures.

3.3. Kinetic Simulations

Kinetic simulations are the final part of the thesis, which allows to compare the findings with the literature. Also, they show the expected chemical composition of an outlet feed from a reactor by taking hundreds (or thousands) of reactions into account. To perform the computational simulations, the software OpenSMOKE++ is used. As described in Section 2.5, it solves equations related to chemical kinetics by numerical methods. The user does not have to change any of the codes of the software, only the input file has to be modified according to the interests.

A few chemical mechanisms that are available in the scientific literature can be used to describe the reactivity of streams containing methylcyclopentadiene. For this thesis the mechanisms created by the CRECK group of Politecnico di Milano [29] are used. The kinetic simulations are done using their mechanisms (without any modifications) and their mechanisms with the modifications of the kinetic parameters obtained in this thesis. This helps to compare the effects of the reactions obtained during this thesis and the reactions that were already present in the CRECK mechanism. It should be noted that the mechanisms include so many reactions, some of them are not even necessary for many of the cases. For example, if a system that does not have any atoms except carbon and hydrogen is analyzed, the reactions that include other atoms such as oxygen do not affect the results. Also, because of the very large number of reactions, even a small change in the production of a species can cause (somewhat) a chain effect, in other words the produced species will form other ones and the new species will form a totally different molecule and the concentration of the analyzed species change. That results in obtaining different values between the simulations performed with CRECK parameters and those determined in this thesis.

The changes that are done in the mechanism are as follows:

- The rate parameters obtained from the lumping of the decomposition reactions of methylcyclopentadienyl radicals are added to the mechanism.
- The abstraction rate parameters are added to the mechanism.
- All the present reactions that include the reactions obtained from this thesis are removed to have a better comparison.

One important thing should be mentioned, the present CRECK mechanism uses only one type of methylcyclopentadienyl radical and one type of methylcyclopentadiene isomer. However, the reactions obtained in this thesis included many different radicals and isomers that is why using the mechanism of CRECK may not provide perfect results for the analyzed system. Although the results may not be perfect, they can be used as a comparison for now, and in the future different isomers and radicals could be added to the mechanism to provide more accurate results.

To be able to modify the reactions that include different isomers, somehow a weighted average of the isomers is used. To have the average values some parameters such as partition functions (translational, rotational, vibrational, etc.) are needed. They are obtained (or calculated) from the output files of the Gaussian calculations. Then, by using these parameters the Gibbs free energy change between different isomers are calculated. Finally, the weighting factors for each isomer and the net rates of abstraction reactions are found by using the following averaging equations:

$$\frac{\theta_i}{\theta_j} = exp\left(-\frac{\Delta G_{i \to j}}{RT}\right) \tag{3.4}$$

$$\sum_{i=1}^{\infty} \theta_i = 1 \quad (i = 1, 2, ..., \infty) \tag{3.5}$$

$$k = \sum_{i=1}^{\infty} k_i \theta_i \tag{3.6}$$

Where i and j represent different isomers.

To be able to compare the findings with the literature, it is necessary to find a reference experimental study that provides the information necessary to be used as input data. The information includes the pressure, temperature, inlet species with their fractions, reactor type, fractions of the outlet species and so on. Of course, it is possible to select a random system, however it would not allow the researcher to compare their findings with the literature.

When literature review is done to find an article that includes a system similar to the one described in this thesis, the article of Herbinet et al. [17] is found. They used a perfectly stirred reactor with a volume of 90 cm^3 and a residence time of 1 s. The pressure of the system was constant at 106.7 kPa, and the temperature ranged from 773 to 1073 K. The inlet species was diluted cyclopentene with a mole fraction of 0.04, and the remaining part consisted of noble gas (helium or argon). They analyzed the molar fractions of 25 outlet species. The reaction scheme they suggested in the article is reported in Figure 3.48.

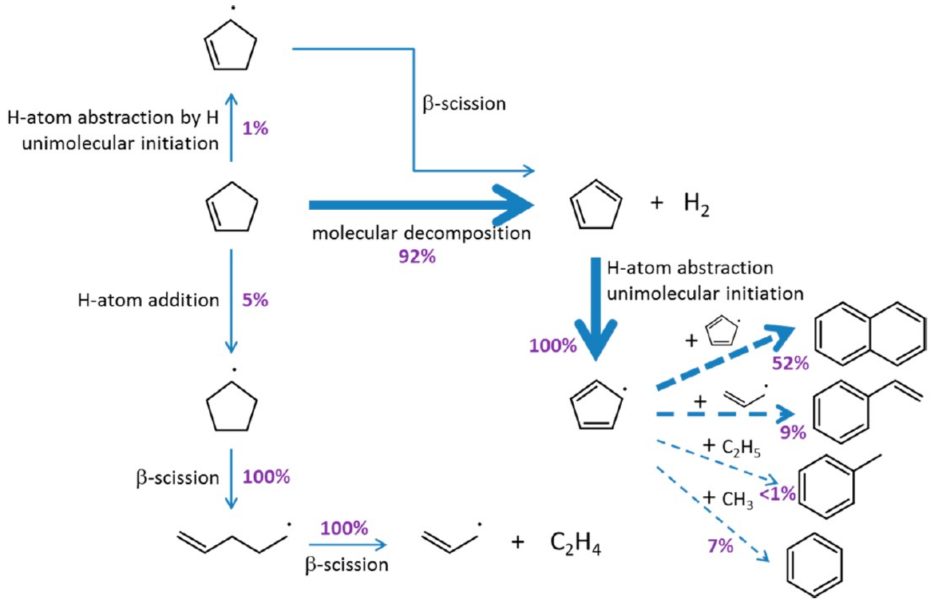
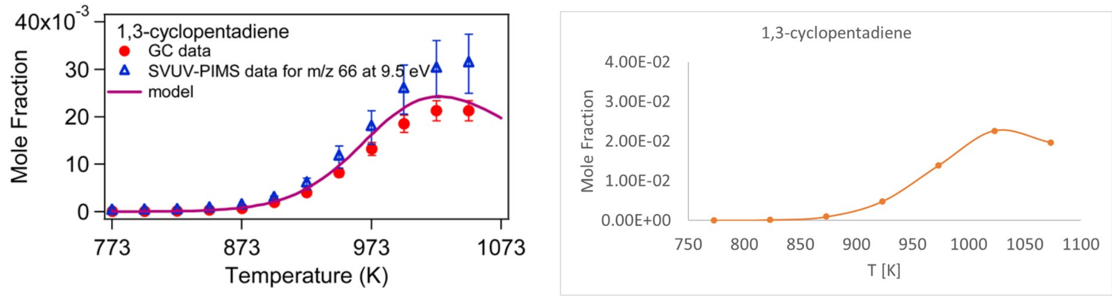


Figure 3.48: Main reaction routes starting from cyclopentene at 1000 K according to the literature [17].

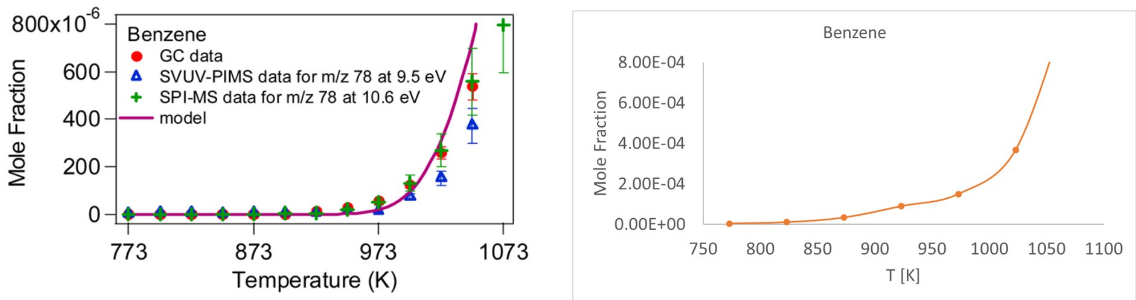
After the input file for OpenSMOKE++ is modified with the system parameters described in the article, it is possible to run the kinetic simulations. For the comparison of the findings of Herbinet et al., the CRECK mechanism modified with the rate constants found in this thesis is used. The following figures include the graphs of the mole fractions reported in the article and the values obtained from the kinetic simulations of this thesis for some of the species. The first plot in all the figures correspond to the findings of Herbinet et al., they reported experimental data as well as the model they suggest. To report the experimental data, they used three different methods, namely gas chromatography, single photon laser ionization mass spectrometry, and synchrotron vacuum ultraviolet photoionization mass spectrometry.

By looking at Figure 3.49, it is possible to conclude that the CRECK mechanism perfectly fits the literature, not only the shape but also the values obtained from the simulations almost perfectly coincide with the model suggested in the literature.



a) b)

Figure 3.49: Comparison of the mole fractions of 1,3-cyclopentadiene in a) literature [17], b) this thesis.



a) b)

Figure 3.50: Comparison of the mole fractions of benzene in a) literature [17], b) this thesis.

Figure 3.50 shows the comparison of the mole fractions with respect to benzene, it can easily be seen that the two plots have very similar trends, not only the trends but the values are close to each other (except some small differences). This shows the mechanism of CRECK provides similar values for benzene when compared with the literature. This actually plays an important role for this thesis since benzene is the main product for the methylcyclopentadiene decomposition reactions analyzed in this thesis. Similar values with the literature show that the obtained rate constants can be used in the mechanism of CRECK.

In Figure 3.51 naphthalene does not show a huge increase in the plot obtained from the literature. This can also be seen in the CRECK mechanism, the trends of the mole fractions of naphthalene are very similar in both plots. The main difference between the two models is that at high temperatures the CRECK mechanism reaches a slightly higher value. However, the order of magnitude is still the same in both plots.

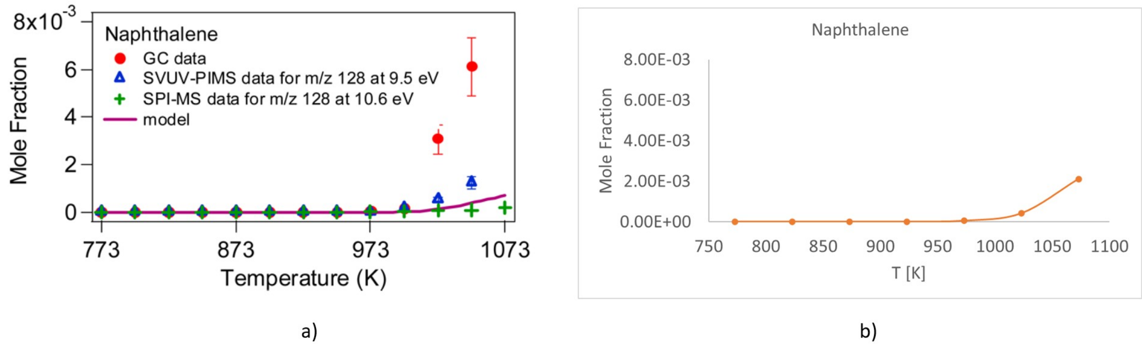


Figure 3.51: Comparison of the mole fractions of naphthalene in a) literature [17], b) this thesis.

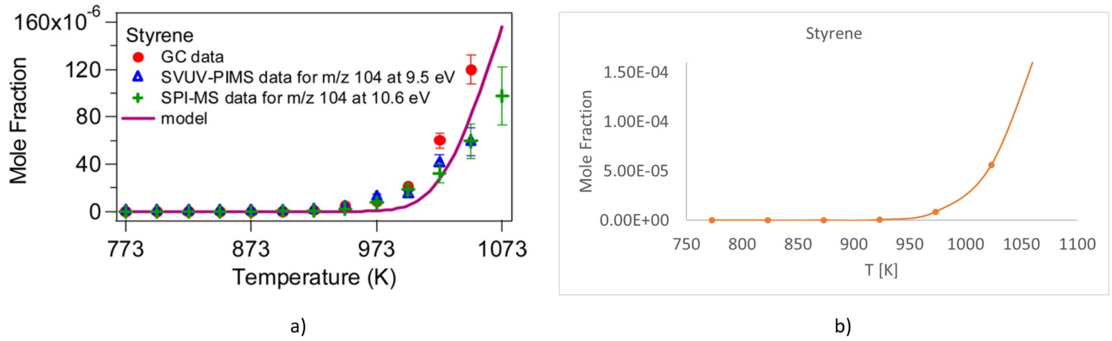


Figure 3.52: Comparison of the mole fractions of styrene in a) literature [17], b) this thesis.

When the plots for styrene are compared, just like the previous cases it is possible to conclude that the model of Herbinet et al. is in good agreement with the model of CRECK, both the trend and the values are very close to each other.

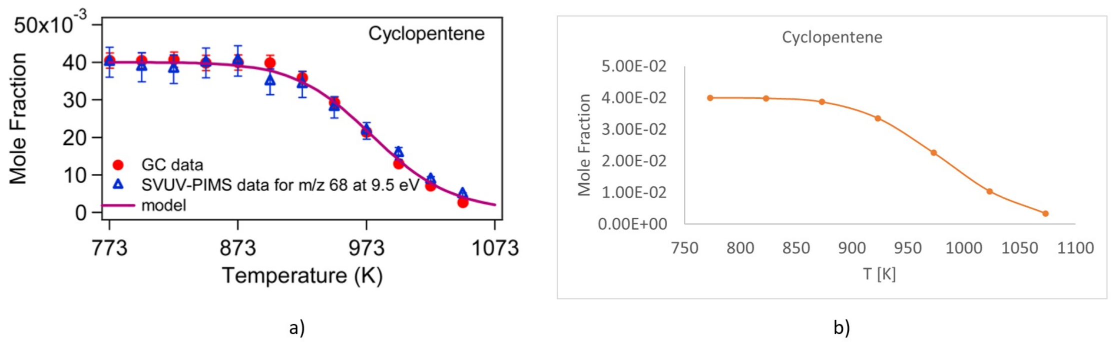


Figure 3.53: Comparison of the mole fractions of cyclopentene in a) literature [17], b) this thesis.

The only reactive inlet molecule, cyclopentene, has a change of mole fractions as shown in Figure 3.53. Both plots are almost perfectly equal to each other, the values, trends, major changes in the molar fractions occur at very similar places. Once again, this shows how accurate the CRECK model is.

None of the comparison figures reported above include methylcyclopentadiene or methylcyclopentadienyl radicals, the reason is they were not analyzed in the article that is used for comparison. To be able to see the changes it is possible to use kinetic simulations with and without the modifications (from this thesis) of the parameters of the CRECK mechanism.

In the original CRECK mechanism, the methylcyclopentadienyl decomposition reactions are not present, while the abstraction reactions of methylcyclopentadiene are included. To see if changing the values of the rate parameters affect the mole fractions or not, two separate simulations are done. One with the original mechanism, then with the modified mechanism. For the modification, only the abstraction reactions are changed to the new parameters, the decomposition parameters are not yet added to the mechanism. The simulations are done for the system described in the article of Herbinet et al. The mole fractions of methylcyclopentadiene, methylcyclopentadienyl, benzene, fulvene and hydrogen obtained from both simulations are reported in tables 3.2 and 3.3. Also, the comparison of the rate constants in the present CRECK mechanism and this thesis at different temperatures are reported in Figure 3.54. It should be noted that different rate parameters for a single reaction are reported as "CRECK 1", "CRECK 2" and "CRECK 3" in the figures.

One thing to mention about Figure 3.54 is that, except the case with H attack, the rate constants in different parts of the CRECK mechanism (for the same abstraction reaction) have different values from each other. The rate constants obtained from this thesis are either close to one of the values reported in CRECK, such as the plot in Figure 3.54d, or somewhere in between the CRECK values and one of other proposed rate constant values, like in Figure 3.54b or Figure 3.54c. This is a good sign, as it shows the values from this thesis are consistent with the values reported in the literature. Specifically, for the case with H attack, all of the curves are in perfect agreement with each other, so that it is hard to distinguish them, especially at intermediate temperatures.

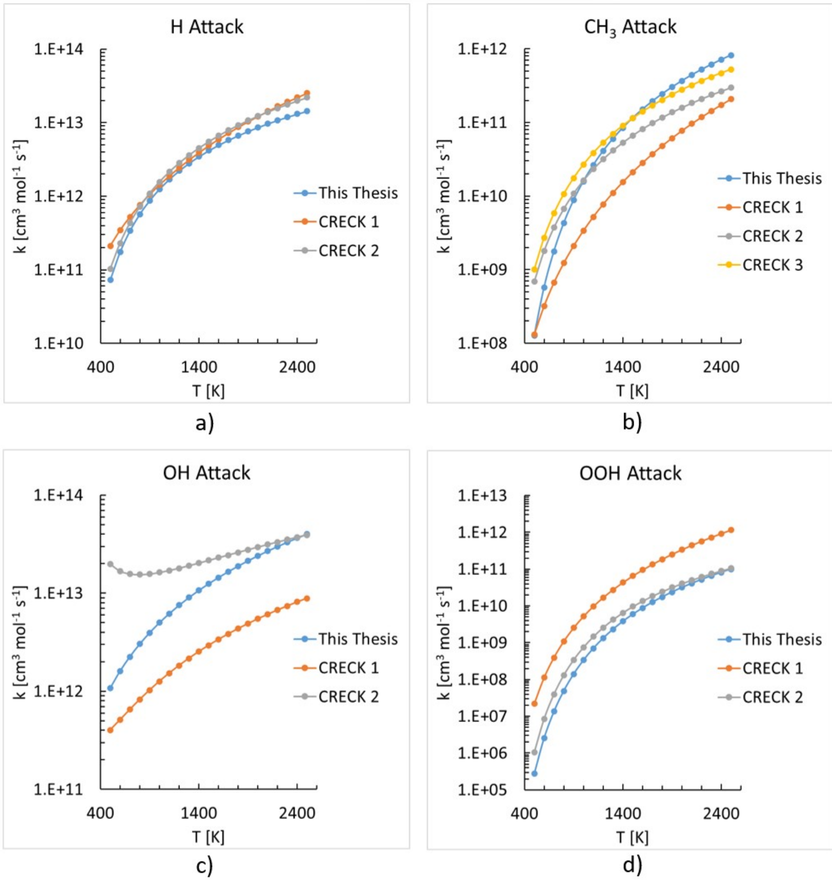


Figure 3.54: Comparison of the rate constants obtained from this thesis and the CRECK mechanism for a) H attack, b) CH_3 attack, c) OH attack, d) OOH attack.

Temperature [K]	Benzene	Fulvene	Methylcyclopentadienyl	H	MCPE
773	3.56E-06	4.63E-14	6.59E-15	6.84E-13	1.56E-11
823	1.02E-05	6.18E-12	2.19E-12	5.49E-12	1.40E-09
873	3.30E-05	1.10E-09	6.78E-10	3.97E-11	8.84E-08
923	8.93E-05	8.46E-08	4.24E-08	2.18E-10	1.20E-06
973	1.49E-04	1.13E-06	2.69E-07	6.27E-10	2.77E-06
1023	3.66E-04	5.38E-06	1.34E-06	1.58E-09	5.31E-06
1073	1.14E-03	1.11E-05	9.07E-06	6.72E-09	9.91E-06

Table 3.2: Mole Fractions According to the Original CRECK Mechanism

Temperature [K]	Benzene	Fulvene	Methylcyclopentadienyl	H	MCPE
773	3.56E-06	4.63E-14	5.56E-15	6.84E-13	1.56E-11
823	1.02E-05	6.18E-12	1.67E-12	5.49E-12	1.40E-09
873	3.30E-05	1.10E-09	5.08E-10	3.97E-11	8.85E-08
923	8.93E-05	8.47E-08	3.23E-08	2.18E-10	1.20E-06
973	1.49E-04	1.13E-06	2.02E-07	6.27E-10	2.78E-06
1023	3.66E-04	5.38E-06	9.27E-07	1.59E-09	5.33E-06
1073	1.14E-03	1.11E-05	5.79E-06	6.73E-09	9.96E-06

Table 3.3: Mole Fractions According to the CRECK Mechanism Modified with the Abstraction Rates

By comparing the values from tables 3.2 and 3.3, it is possible to see that the modifications have some impact, though there is no major change in the orders of magnitudes of the molar fractions of any of the species at any temperature. The species that shows the most different values between two tables is methylcyclopentadienyl, but that was expected since the abstraction reactions are mainly about methylcyclopentadienyl and methylcyclopentadiene. The reason of not seeing major changes in methylcyclopentadiene is because of the relatively higher order of magnitude of its mole fraction. The changes in methylcyclopentadienyl affects methylcyclopentadiene too, but they are too small to change its mole fraction significantly.

Just like Figure 3.54, this also shows how close the parameters obtained from this thesis are to the literature values. One other very important conclusion is that, even though CRECK mechanism used experimental or estimated data for most of the rate parameters, their values are very close to the ab initio calculations of this thesis. This shows their mechanism can be used for a system similar to the one of this thesis without any problems.

There is one more very important comparison to be made, as already stated the values obtained in Table 3.3 did not include the decomposition reactions, however they play a very important role in this thesis. A third simulation is done with the modified rate parameters, this time all of the reactions analyzed in this thesis are included in the mechanism and the values reported in Table 3.4 are obtained.

Temperature [K]	Benzene	Fulvene	Methylcyclopentadienyl	H	MCPE
773	3.56E-06	4.64E-14	1.97E-16	6.84E-13	1.56E-11
823	1.02E-05	6.16E-12	1.81E-15	5.49E-12	1.40E-09
873	3.30E-05	1.08E-09	1.94E-14	3.97E-11	8.85E-08
923	8.94E-05	7.93E-08	1.57E-13	2.18E-10	1.20E-06
973	1.50E-04	1.02E-06	4.72E-13	6.27E-10	2.78E-06
1023	3.68E-04	4.93E-06	1.77E-12	1.59E-09	5.33E-06
1073	1.15E-03	1.10E-05	1.19E-11	6.74E-09	9.97E-06

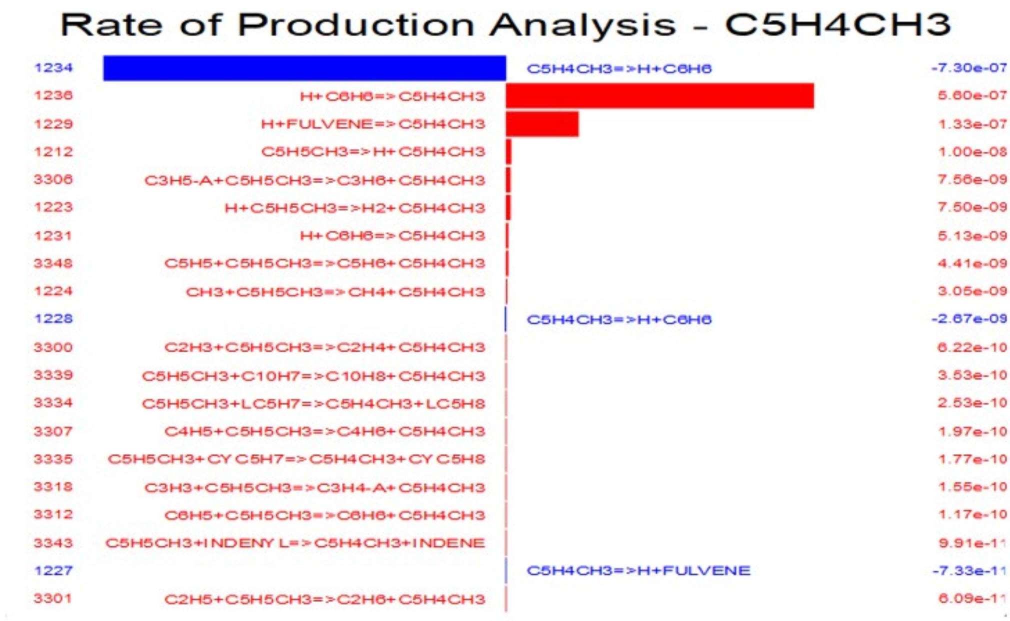
Table 3.4: Mole Fractions According to the CRECK Mechanism Modified with the Abstraction and Decomposition Rates

When the values reported in tables 3.3 and 3.4 are compared, it is seen that the values of mole fractions are almost the same except the values for methylcyclopentadienyl radical, which decreased a lot after the addition of the decomposition reactions. That was an expected result, as already analyzed in Section 3.1 the decomposition reactions tend to form mostly benzene and some fulvene, and once these molecules are formed, they do not tend to form methylcyclopentadienyl radicals again. In other words, addition of the decomposition reactions results in forming benzene and fulvene from the methylcyclopentadienyl radicals. The reason of not having major changes in the mole fractions of benzene and fulvene can be explained from the order of magnitudes. Benzene and fulvene they both have higher fractions than methylcyclopentadienyl at all temperatures, especially benzene (the main product) has at least three orders of magnitude difference from methylcyclopentadienyl, this means even though large percentage of methylcyclopentadienyl is decomposed to form benzene, it does not affect the mole fraction due to the large amount of benzene with respect to methylcyclopentadienyl. The same is also valid for fulvene, even though its fraction is not as high as benzene, since it is not produced as much as benzene the decomposition of methylcyclopentadienyl does not affect its fraction a lot too.

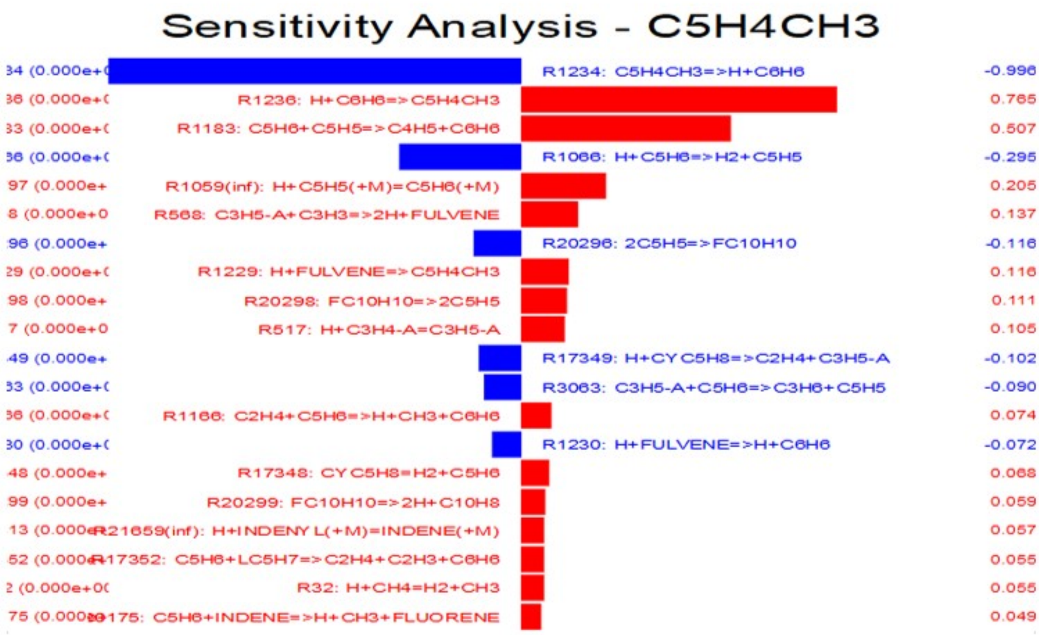
As it can be seen from the results, the mechanism suggested by CRECK group simulates the analyzed system very well. One of the weaknesses of the model was the absence of decomposition reactions. If the parameters obtained from this thesis are added to the mechanism in the future, the model will be more complete for the cases where methylcyclopentadiene or methylcyclopentadienyl radicals are present.

There is one last analysis that can be done using OpenSMOKE++ for this thesis. It is the analysis of the reactions for the production or consumption of the species reported in the tables above. This analysis is done in two different methods, the first one is called "rate of production analysis" and the second one is "sensitivity analysis". They are very similar to each other, the only difference is for the former one only the reactions that include the analyzed species is reported, whereas for the latter one any reaction that affect the flux of the formation or consumption of that species (the species not necessarily involved in these reactions) is reported.

The figures between Figure 3.55 and Figure 3.58 include the graphs of sensitivity and rate of production analysis for the main species analyzed in this thesis. Namely, methylcyclopentadienyl, methylcyclopentadiene, benzene, and fulvene. The red bars on the right side of the figures show the species is produced by the reaction written next to it, and the blue bars on the left show that species is consumed by that reaction. In all of the figures, the reactions that include methylcyclopentadienyl (written as C5H4CH3) and methylcyclopentadiene (written as C5H5CH3) are mostly the reactions obtained from the ab initio calculations of this thesis. These reactions appear more for the analysis of methylcyclopentadienyl and methylcyclopentadiene, and they do not appear a lot for benzene and fulvene. The reason is benzene and fulvene appear in so many other reactions in the mechanism of CRECK, and the rates of other reactions are usually faster than the ones starting from methylcyclopentadienyl radical.



a)



b)

Figure 3.55: Analysis of the production or consumption of methylcyclopentadienyl radical by a) Rate of Production Analysis, b) Sensitivity Analysis.

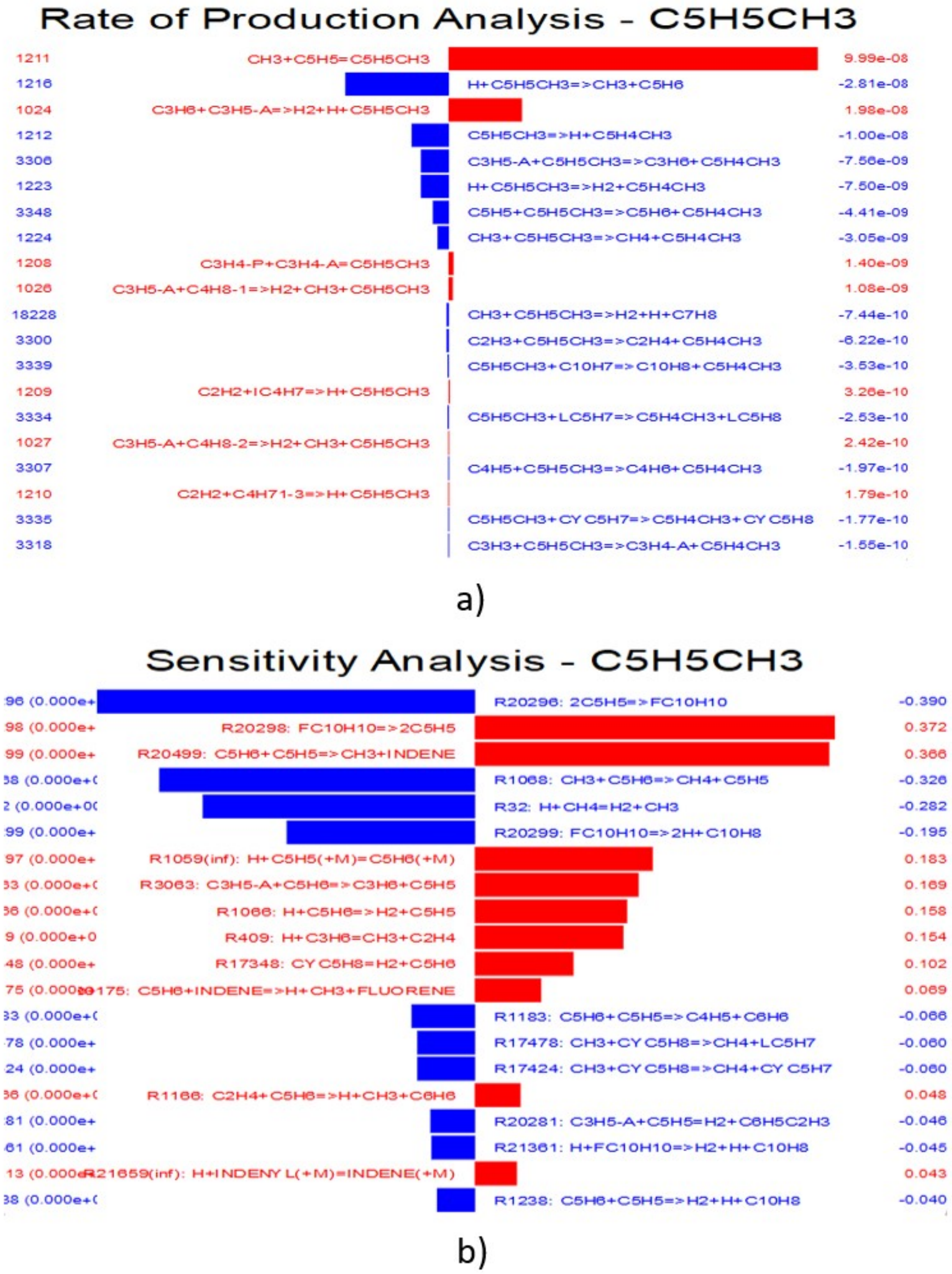


Figure 3.56: Analysis of the production or consumption of methylcyclopentadiene by a) Rate of Production Analysis, b) Sensitivity Analysis.

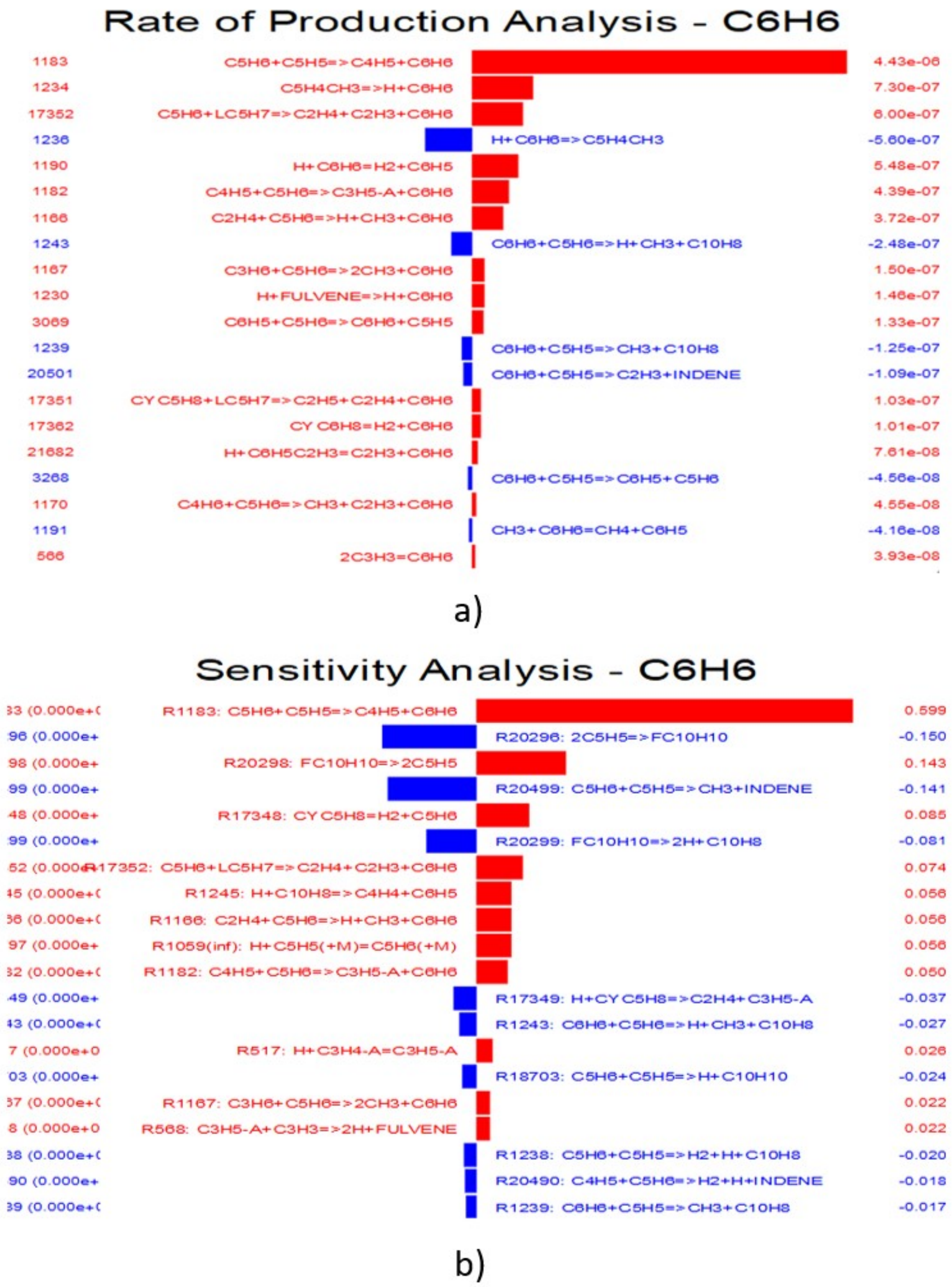


Figure 3.57: Analysis of the production or consumption of benzene by a) Rate of Production Analysis, b) Sensitivity Analysis.

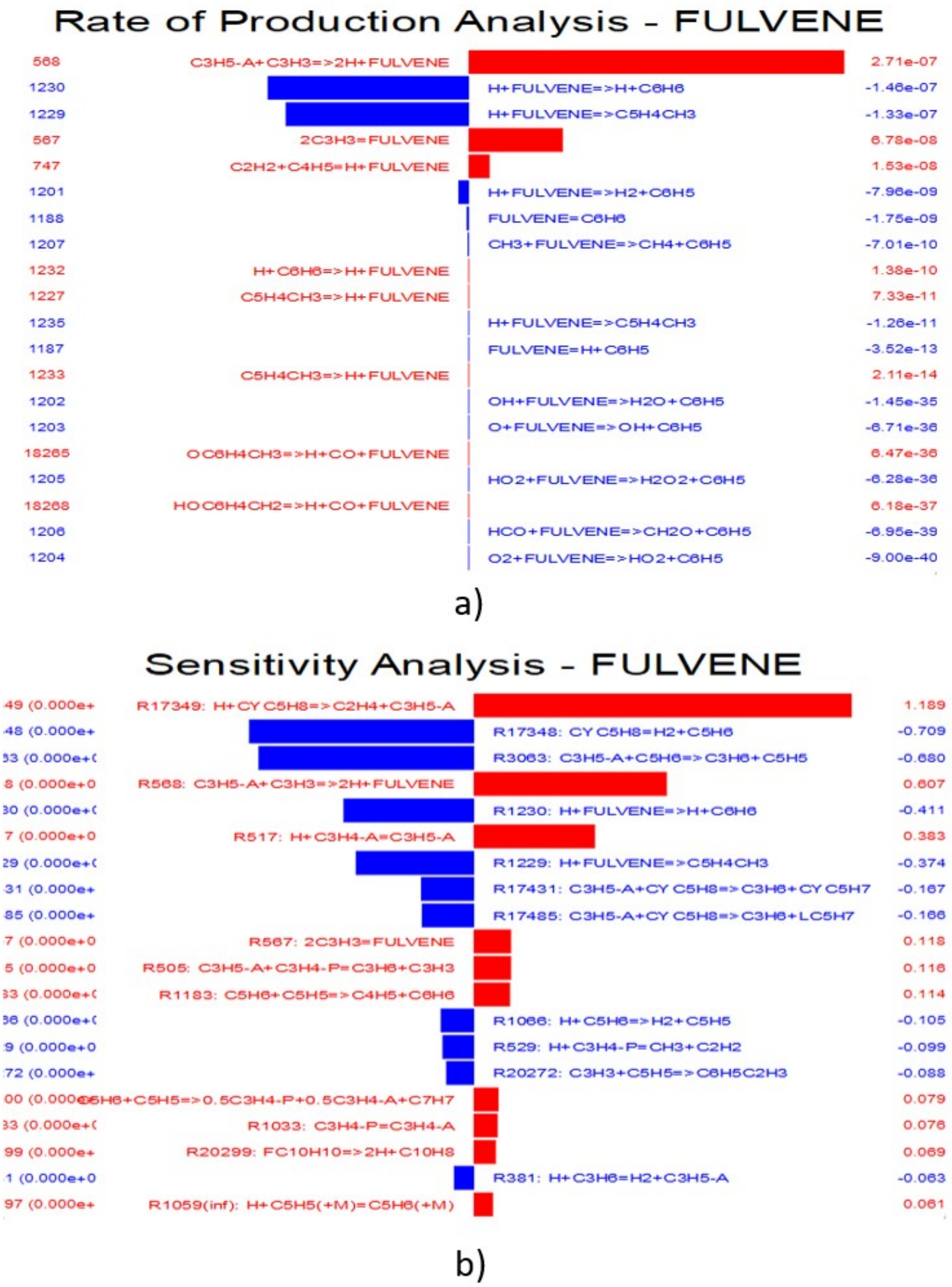


Figure 3.58: Analysis of the production or consumption of fulvene by a) Rate of Production Analysis, b) Sensitivity Analysis.

4 | Conclusions

The reactivity of methylcyclopentadiene is analyzed using theoretical methodologies in this thesis. The main motivation behind this study is the lack of experimental data for the reactions including methylcyclopentadiene, which is an important reaction intermediate in the reactivity of aromatics and, more specifically, a hazardous and a highly reactive substance. Not knowing much about the chemistry of a reactive substance welcomes problems when it is used in an industrial plant. There was even a recorded accident caused by methylcyclopentadiene in 2007, which caused death of four people. The reactivity of methylcyclopentadiene is analyzed using the ab initio transition state theory based master equation methodology, which is a powerful theoretical tool for predicting the reactivity of unknown molecules.

During the investigation of the reactivity, different computer programs are used. Namely, Gaussian and Molpro for the electronic structure calculations, MESS for the master equation simulations and OpenSMOKE++ for kinetic simulations. Besides these programs, some useful source codes are used, for example EStokTP is used to prepare and post process the electronic structure and master equation simulation calculations so that the user can use predefined protocols that are known to work properly for many systems. In these protocols the calculations are automatically done, and the results are collected. MEL is another code which is used for lumping of the results. Most of the reactions found in the master equation analysis in fact are not necessary for kinetic mechanisms. In particular the radicals that have similar reactivities and structures are lumped using MEL so that the number of species and reactions can be reduced, which in the end reduces the model complexity and saves computational time.

As mentioned, to be able find the microcanonical rate constants, ab initio transition state theory master equation simulations method is used. With that method, the calculations are done in three steps: electronic structure calculations, microcanonical reaction rate calculations, and determination of phenomenological rate constants.

The energies and some other properties of the molecules are obtained by numerical solutions of the Schrödinger equation, which is one of the most important equations in quantum mechanics. The computations can be done at different theory levels with different basis sets. The researcher determines the necessary level by taking in consideration how precise the calculations should be, in relation to the computational time and costs required by each level of theory.

Simulations are performed for two sets of systems, one of them starts from methylcyclopentadiene molecule, which has three isomers and consists of six carbon and eight hydrogen atoms. The isomers are attacked by H, CH_3, OH and OOH radicals and undergo an abstraction reaction to lose one hydrogen atom. The products of the reactions include methylcyclopentadienyl radicals, that has six carbon and seven hydrogen atoms. The second set of calculations are done starting from the methylcyclopentadienyl radicals, they undergo isomerization reactions to produce other radicals and some of these radicals form stable species, namely benzene and fulvene by beta-scission reactions, by which the radicals lose one H atom.

The results section starts with the values of the energies of all the species that are present for the calculations, and potential energy surfaces are reported for both systems. The electronic structure calculations were performed with Gaussian and Molpro. The second part of the results include the rate constant calculations, in other words master equation simulation calculations. For these calculations, the software MESS is used, which takes the output files of the electronic structure calculations as input and generates the rate parameters for a range of temperature and pressure values. The rate constants of different reactions are compared by using plots that has logarithmic scale for the values of the rate constants. The values of the rate constants for most of the reactions are also compared with literature values. It is found that the calculated data have similar values with the literature. Different plots are used for showing the similarities of the literature values and the values obtained in this thesis.

Until this point, the results were collected with similar methods for both of the decomposition and abstraction systems. However, for the decomposition system, there is also an extra step that is necessary. Because the reactions include so many isomerization type reactions and similar molecules, some of the reactions may not be necessary. This is why the lumping of some of these molecules is done in order to reduce the number of molecules and reactions. Comparison of concentration profiles produced before and after lumping are reported for different temperature and pressure values. It is found that the suggested lumping of the reactions can be very useful for a wide range of temperatures and for pressures above 1 atm.

The final part of the results section concerns kinetic simulations, performed with the

OpenSMOKE++ software, which is another user-friendly software. The researcher has to change some input files but does not need to modify anything related to the software source codes. Many different types of reactors and systems can be analyzed. Besides OpenSMOKE++, the user also has to use some kinetic mechanisms, for that purpose the freely available mechanisms developed by the CRECK group of Politecnico di Milano are used. Three different simulations are performed and compared with a literature study. The input file is modified according to the system described in that article. The three different simulations are:

- no modifications to the mechanism suggested by CRECK
- modification of the abstraction rates only, and no modifications about the decomposition rates
- modification of both of the abstraction and the decomposition rates.

The modifications of the isomers are done by using a weighted average of the isomers, since the CRECK mechanism only includes one of the isomers. The values of the abstraction reactions that are already present and the values from this thesis are compared both by kinetic simulations and by plotting them in the same graph. Both methods show very similar values.

The results obtained from the simulations that uses the CRECK mechanism which is modified with both the abstraction and the decomposition rates are compared to the plots of the scientific article that is taken as the reference. Both the trends and the values are found to be very similar with the literature. Hence, the rate parameters of this thesis are in good agreement with the literature and the experimental work and can be considered in the future as a useful contribution to the CRECK kinetic mechanism.

Finally, to be able to see which reactions produce and which ones consume the main species analyzed in this thesis (which are methylcyclopentadiene, methylcyclopentadienyl, benzene and fulvene), rate of production and sensitivity analyses are done and the effects of the added reactions on the production of the specified species are analyzed.

It can be concluded that, the ab initio calculations provide similar values with the literature. It is also found that, the current version of the CRECK mechanism contains very similar values to the ones obtained from this thesis. However, some of the reactions were missing in the mechanism, for these reactions the obtained rate constant parameters can be added to the kinetic mechanism of the CRECK group, so that more reactions will be present in the mechanism which will be useful to provide accurate results for a system similar to the one of this thesis. One other comment for future applications is, it is found that different isomers have different reactivities and hence different rate parameters however, they had to be written as a weighted average of the isomers since the mechanism included only one of these isomers. In the future, different isomers can be added to the mechanism so that the difference between the rate parameters for different isomers can be added, and hence the simulations can be done by taking more details into account for a system that includes methylcyclopentadiene.

Bibliography

[1] P. Atkins and J. De Paula. *Elements of physical chemistry*. Oxford University Press, USA, 2013.

[2] R. Cammi. Recent advances in the coupled-cluster analytical derivatives theory for molecules in solution described with the polarizable continuum model (pcm). *Advances in Quantum Chemistry*, 64:1–29, 2012.

[3] C. Cavallotti, M. Pelucchi, Y. Georgievskii, and S. Klippenstein. Estoktp: electronic structure to temperature-and pressure-dependent rate constants—a code for automatically predicting the thermal kinetics of reactions. *Journal of chemical theory and computation*, 15(2):1122–1145, 2018.

[4] S. M. Csicsery. Methylcyclopentadiene isomers. *The Journal of Organic Chemistry*, 25(4):518–521, 1960.

[5] A. Cuoci, A. Frassoldati, T. Faravelli, and E. Ranzi. Numerical modeling of laminar flames with detailed kinetics based on the operator-splitting method. *Energy & fuels*, 27(12):7730–7753, 2013.

[6] A. Cuoci, A. Frassoldati, T. Faravelli, and E. Ranzi. Opensmoke++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms. *Computer Physics Communications*, 192:237–264, 2015.

[7] F. Dubnikova and A. Lifshitz. Ring expansion in methylcyclopentadiene radicals. quantum chemical and kinetics calculations. *The Journal of Physical Chemistry A*, 106(35):8173–8183, 2002.

[8] M. Döntgen, F. Schmalz, W. A. Kopp, L. C. Kröger, and K. Leonhard. Automated chemical kinetic modeling via hybrid reactive molecular dynamics and quantum chemistry simulations. *Journal of chemical information and modeling*, 58(7): 1343–1355, 2018.

[9] Editors of the American Heritage Dictionaries, editor. *The American Heritage Abbreviations Dictionary*. Houghton Mifflin Company, 2002.

[10] M. G. Evans and M. Polanyi. Some applications of the transition state method to the calculation of reaction velocities, especially in solution. *Transactions of the Faraday Society*, 31:875–894, 1935.

[11] R. P. Feynman. Simulating physics with computers. *International Journal of Theoretical Physics*, 21(6):467–488, 1982.

[12] J. Foresman and Æ. Frisch. *Exploring Chemistry with Electronic Structure Methods*. Gaussian Inc., Pittsburg, USA, 1996.

[13] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox. Gaussian 16 Revision C.01, 2016. Gaussian Inc. Wallingford CT.

[14] Y. Georgievskii and S. J. Klippenstein. Mess.2016.3.23, 2016.

[15] Y. Georgievskii, J. A. Miller, M. P. Burke, and S. J. Klippenstein. Reformulation and solution of the master equation for multiple-well chemical reactions. *The Journal of Physical Chemistry A*, 117(46):12146–12154, 2013.

[16] M. Head-Gordon. Quantum chemistry and molecular processes. *The Journal of Physical Chemistry*, 100(31):13213–13225, 1996.

[17] O. Herbinet, A. Rodriguez, B. Husson, F. Battin-Leclerc, Z. Wang, Z. Cheng, and F. Qi. Study of the formation of the first aromatic rings in the pyrolysis of cyclopentene. *The Journal of Physical Chemistry A*, 120(5):668–682, 2016.

[18] A. W. Jasper. "third-body" collision parameters for hydrocarbons, alcohols, and hydroperoxides and an effective internal rotor approach for estimating them. *International Journal of Chemical Kinetics*, 52(6):387–402, 2020.

[19] A. W. Jasper and N. Hansen. Hydrogen-assisted isomerizations of fulvene to benzene

and of larger cyclic aromatic hydrocarbons. *Proceedings of the Combustion Institute*, 34(1):279–287, 2013.

[20] F. Jensen. *Introduction to computational chemistry*. John Wiley & Sons, 2017.

[21] I. M. Kennedy. Models of soot formation and oxidation. *Progress in Energy and Combustion Science*, 23(2):95–132, 1997.

[22] S. J. Klippenstein and C. Cavallotti. Ab initio kinetics for pyrolysis and combustion systems. In *Computer Aided Chemical Engineering*, volume 45, pages 115–167. Elsevier, 2019.

[23] M. T. Lusk and A. E. Mattsson. High-performance computing for materials design to advance energy science. *MRS Bulletin*, 36(3):169–174, 2011.

[24] L. P. Maffei, M. Pelucchi, C. Cavallotti, A. Bertolino, and T. Faravelli. Master equation lumping for multi-well potential energy surfaces: A bridge between ab initio based rate constant calculations and large kinetic mechanisms. *Chemical Engineering Journal*, 422:129954, 2021.

[25] J. M. Martin. Ab initio total atomization energies of small molecules—towards the basis set limit. *Chemical physics letters*, 259(5-6):669–678, 1996.

[26] K. I. Ramachandran, D. Gopakumar, and K. Namboori. Basis sets. *Computational Chemistry and Molecular Modeling: Principles and Applications*, pages 115–138, 2008.

[27] H. Richter and J. B. Howard. Formation of polycyclic aromatic hydrocarbons and their growth to soot—a review of chemical reaction pathways. *Progress in Energy and Combustion science*, 26(4-6):565–608, 2000.

[28] B. Shukla, A. Miyoshi, and M. Koshi. Chemical kinetic mechanism of polycyclic aromatic hydrocarbon growth and soot formation. *Journal of the Combustion Society of Japan*, 50(151):8–18, 2008.

[29] The Creck Modelling Group. Detailed kinetic mechanisms, 2020. URL `http://creckmodeling.chem.polimi.it/menu-kinetics/menu-kinetics-detailed-mechanisms`. Online. Last accessed March 2022.

[30] D. G. Truhlar. Transition state theory for enzyme kinetics. *Archives of biochemistry and biophysics*, 582:10–17, 2015.

[31] Q. Wang, Y. Zhang, W. J. Rogers, and M. S. Mannan. Molecular simulation studies

on chemical reactivity of methylcyclopentadiene. *Journal of hazardous materials*, 165 (1-3):141–147, 2009.

[32] H.-J. Werner, P. J. Knowles, G. Knizia, F. R. Manby, and M. Schütz. Molpro: a general-purpose quantum chemistry program package. *WIREs Comput Mol Sci*, 2: 242–253, 2012.

[33] H.-J. Werner, P. J. Knowles, G. Knizia, F. R. Manby, M. Schütz, P. Celani, W. Györffy, D. Kats, T. Korona, R. Lindh, A. Mitrushenkov, G. Rauhut, K. R. Shamasundar, T. B. Adler, R. D. Amos, S. J. Bennie, A. Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, E. Goll, C. Hampel, A. Hesselmann, G. Hetzer, T. Hrenar, G. Jansen, C. Köppl, S. J. R. Lee, Y. Liu, A. W. Lloyd, Q. Ma, R. A. Mata, A. J. May, S. J. McNicholas, W. Meyer, T. F. Miller III, M. E. Mura, A. Nicklass, D. P. O'Neill, P. Palmieri, D. Peng, K. Pflüger, R. Pitzer, M. Reiher, T. Shiozaki, H. Stoll, A. J. Stone, R. Tarroni, T. Thorsteinsson, M. Wang, and M. Welborn. Molpro, version , a package of ab initio programs, 2012.

[34] H.-J. Werner, P. J. Knowles, F. R. Manby, J. A. Black, K. Doll, A. Heßelmann, D. Kats, A. Köhn, T. Korona, D. A. Kreplin, et al. The molpro quantum chemistry package. *The Journal of Chemical Physics*, 152(14):144107, 2020.

[35] H.-S. Zhong, H. Wang, Y.-H. Deng, M.-C. Chen, L.-C. Peng, Y.-H. Luo, J. Qin, D. Wu, X. Ding, Y. Hu, et al. Quantum computational advantage using photons. *Science*, 370(6523):1460–1463, 2020.

A | Appendices

A.1. Inputs of the Master Equation System Solver (MESS) Calculations

A.1.1. Decomposition of Methylcyclopentadienyl Reactions

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                    0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                      direct     ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                        diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                   10
!ChemicalEigenvalueMin                 1.e-6         #only for direct
diagonalization method
!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                  1.3
!!
RateOutput                             rate.out                      ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                                  ! Default collisional
energy relaxation kernel
    Exponential                                                  ! Currently the only
possible energy relaxation model
       Factor[1/cm]               316                           ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                 0.535                         ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff                  10                            ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                                  ! Collision frequency
model
    LennardJones                                                  ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                90.58  281.367                 ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]                3.54    4.694                  ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                 39.948  79.05478               ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


Well W1
 Species
 RRHO
 Geometry[angstrom]            13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.41503
 C    1.18545   0.00000   2.30567
 C   -1.37935  -0.00012   1.86252
 C   -2.17206  -0.00015   0.76521
 C   -1.30655  -0.00009  -0.41768
 H    0.87961   0.00007  -0.62336
 H    2.11567  -0.00004   1.74107
 H    1.17602   0.87599   2.95930
 H    1.17594  -0.87588   2.95944
 H   -1.69362  -0.00013   2.89437
 H   -3.25040  -0.00031   0.74341
 H   -1.65477  -0.00006  -1.43922
        Core    RigidRotor
             SymmetryFactor    2.0000000000000000
        End
 Rotor                        Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
    0.00    0.02    0.06    0.08    0.06    0.02    0.00    0.02    0.06    0.08    0.06
0.02
 End
    Frequencies[1/cm]          32
   3255.2      3246.9      3232.4      3224.7      3138.8      3086.7      3034.0
1584.3      1503.0      1481.1
   1477.8      1438.4      1407.4      1311.4      1292.6      1178.7      1098.2
1049.4      1023.5      1013.1
   953.35      930.03      922.99      899.42      740.50      727.85      638.46
604.76      528.85      520.92
   329.51      215.83
  ZeroEnergy[kcal/mol]             0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000       2.0000000000000000
 End
 End
!**********************************
Well W2
 Species
 RRHO
 Geometry[angstrom]            13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.51707
 C    1.09871   0.00000   2.30732
 C   -1.35802  -0.00027   1.92821
 C   -2.19980  -0.00035   0.79318
 C   -1.45655  -0.00014  -0.34828
 H    0.51637  -0.87674  -0.39927
 H    0.51623   0.87681  -0.39930
 H    1.00918   0.00006   3.38497
 H    2.09550   0.00028   1.88850
 H   -1.68722  -0.00031   2.95632
 H   -3.27933  -0.00054   0.83101
 H   -1.83831  -0.00017  -1.35720
        Core    RigidRotor
             SymmetryFactor    1.0000000000000000
        End
    Frequencies[1/cm]          33
   181.99      356.91      395.63      533.43      629.59      643.37      680.31
793.04      824.97      845.94
```

```
  866.96    937.31    954.62    969.83    992.65    1040.3    1116.9
1156.5    1270.0    1282.1
  1316.0    1407.1    1426.9    1447.0    1530.1    1581.8    3052.2
3085.2    3159.4    3215.6
  3230.8    3244.9    3250.2
ZeroEnergy[kcal/mol] 1.36207652215235
 ElectronicLevels[1/cm]          1
  0.0000000000000000    2.0000000000000000
 End
 End
!************************************
Well W3
 Species
 RRHO
 Geometry[angstrom]       13
 C   0.00000   0.00000   0.00000
 C   0.00000   0.00000   1.51349
 C   1.37415   0.00000   2.09021
 C  -0.79641   1.23944   1.82521
 C  -1.17885   1.83267   0.68958
 C  -0.67966   1.05983  -0.45019
 H   0.49634  -0.75551  -0.58874
 H  -0.54681  -0.88208   1.86663
 H   1.98328   0.88845   2.00399
 H   1.83176  -0.91171   2.44398
 H  -1.00030   1.57032   2.83174
 H  -1.76419   2.73667   0.60934
 H  -0.84595   1.31560  -1.48624
      Core   RigidRotor
           SymmetryFactor   0.50000000000000000
      End
 Rotor                  Hindered
 Group   9  10
 Axis        3       2
 Symmetry        2
 Potential[kcal/mol]       12
   0.00   0.16   0.47   0.78   0.98   1.05   1.05   0.90   0.62   0.28   0.03
-0.01
 End
    Frequencies[1/cm]        32
  3271.6    3250.1    3243.8    3224.3    3214.0    3161.0    3035.8
1666.7    1584.2    1461.4
  1409.1    1319.2    1291.2    1219.8    1152.9    1117.3    1103.6
1041.0    1014.0    995.71
  984.30    976.27    879.12    816.42    787.93    746.46    729.49
577.56    556.56    502.86
  284.52    156.41
ZeroEnergy[kcal/mol] 23.38295381311957
 ElectronicLevels[1/cm]          1
  0.0000000000000000    2.0000000000000000
 End
 End
!************************************
Well W4
 Species
 RRHO
 Geometry[angstrom]       13
 C   0.00000   0.00000   0.00000
 C   0.00000   0.00000   1.39444
 C   1.08995   0.00000   2.23526
 C  -1.41350   0.00016   1.81733
 C  -2.21401   0.00023   0.75171
 C  -1.40210   0.00007  -0.51210
 H   0.87982  -0.00002  -0.62471
 H   2.09628  -0.00024   1.84135
 H   0.96823   0.00006   3.30896
 H  -1.72745   0.00003   2.85121
 H  -3.29344   0.00030   0.76601
 H  -1.61730  -0.87447  -1.13625
 H  -1.61709   0.87466  -1.13627
      Core   RigidRotor
           SymmetryFactor   1.0000000000000000
      End
    Frequencies[1/cm]        33
  219.93    352.34    359.02    544.38    592.39    660.77    666.29
754.57    795.61    796.67
  925.37    925.97    951.93    962.74    984.94    1025.3    1111.8
1138.0    1259.1    1288.5
  1330.9    1389.2    1438.9    1448.7    1522.1    1659.0    3024.2
3048.4    3164.7    3213.5
  3232.2    3239.1    3260.1
ZeroEnergy[kcal/mol] 6.77884705811602
 ElectronicLevels[1/cm]          1
  0.0000000000000000    2.0000000000000000
 End
 End
!************************************
Well W5
 Species
 RRHO
 Geometry[angstrom]       13
 C   0.00000   0.00000   0.00000
 C   0.00000   0.00000   1.51738
 C   1.31229   0.00000   0.75575
 C   1.90719   1.32457   0.48884
 C   1.05272   2.06754  -0.31059
 C  -0.06768   1.32462  -0.64851
 H  -0.37596  -0.88218  -0.49787
 H  -0.28085  -0.92276   2.00492
 H  -0.29315   0.90749   2.02638
 H   1.93164  -0.88219   0.83073
 H   2.84800   1.66150   0.89565
 H   1.22207   3.09303  -0.60452
 H  -0.89115   1.66109  -1.25909
      Core   RigidRotor
           SymmetryFactor   1.0000000000000000
      End
    Frequencies[1/cm]        33
  342.93    370.36    543.90    683.70    697.74    721.93    784.67
794.58    825.88    902.58
  946.52    946.87    988.81    1015.1    1048.6    1063.2    1084.6
1099.3    1101.9    1191.0
  1299.5    1342.7    1344.4    1410.4    1466.7    1498.7    3145.0
3187.8    3195.5    3215.6
  3232.1    3240.6    3244.4
ZeroEnergy[kcal/mol] 15.85555168503187
 ElectronicLevels[1/cm]          1
  0.0000000000000000    2.0000000000000000
 End
 End
!************************************
Well W6
 Species
 RRHO
 Geometry[angstrom]       13
 C   0.00000   0.00000   0.00000
 C   0.00000   0.00000   1.35575
 C   1.26585   0.00000   2.14964
 C   2.49703   0.00067   1.30296
 C   2.43979   0.00065  -0.05160
 C   1.20488   0.00023  -0.73720
 H  -0.94266  -0.00008  -0.53214
 H  -0.93532  -0.00009   1.89984
 H   1.28042  -0.86434   2.83010
 H   1.27999   0.86355   2.83107
 H   3.45452   0.00106   1.80702
 H   3.35916   0.00106  -0.62303
 H   1.18203   0.00016  -1.81705
      Core   RigidRotor
           SymmetryFactor   2.0000000000000000
      End
    Frequencies[1/cm]        33
  171.52    390.17    530.85    568.19    596.05    644.94    742.12
793.27    883.44    942.12
  979.59    993.37    996.12    996.26    1006.6    1109.9    1176.4
1194.7    1206.5    1319.1
  1376.4    1428.7    1444.8    1466.6    1564.3    1631.4    2962.6
2963.6    3180.3    3182.2
```

```
  3199.6     3201.5     3221.3
ZeroEnergy[kcal/mol] -2.94706020686205
 ElectronicLevels[1/cm]          1
  0.0000000000000000      2.0000000000000000
 End
 End
!************************************
Bimolecular Pr1
 Fragment PROD1
 RRHO
 Geometry[angstrom]          12
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.46944
 C    1.06401   0.00000   2.27072
 C   -1.41228   0.00022   1.87529
 C   -2.16165   0.00033   0.76165
 C   -1.27731   0.00018  -0.41255
 H    0.88868  -0.00011  -0.61091
 H    2.06932  -0.00005   1.87011
 H    0.95671   0.00010   3.34759
 H   -1.75398   0.00026   2.89814
 H   -3.24003   0.00049   0.71568
 H   -1.61929   0.00025  -1.43630
       Core    RigidRotor
            SymmetryFactor    2.0000000000000000
       End
    Frequencies[1/cm]          30
  206.64     345.63     501.65     641.58     683.35     704.62     797.67
809.15     812.82     916.44
  963.19     971.90     971.98     995.22     1008.0     1108.5     1112.2
1266.9     1356.5     1382.7
  1464.0     1564.1     1649.7     1739.8     3158.0     3221.8     3231.3
3247.1     3248.6     3254.8
 ZeroEnergy[kcal/mol]          0.
 ElectronicLevels[1/cm]          1
  0.0000000000000000      1.0000000000000000

 End
!************************************
 Fragment PROD2
  Atom
  Name H
  ElectronicLevels[1/cm]          1
  0.0000000000000000      2.0000000000000000

 End
 GroundEnergy[kcal/mol]    50.00
 End
!************************************
Bimolecular Pr2
 Fragment PROD1
 RRHO
 Geometry[angstrom]          12
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.38716
 C    1.20141   0.00000   2.08070
 C    2.40281   0.00000   1.38715
 C    2.40281   0.00000  -0.00003
 C    1.20142   0.00000  -0.69357
 H   -0.93666  -0.00000  -0.54090
 H   -0.93665  -0.00000   1.92807
 H    1.20141  -0.00000   3.16231
 H    3.33947   0.00000   1.92804
 H    3.33948   0.00000  -0.54092
 H    1.20141   0.00000  -1.77518
       Core    RigidRotor
            SymmetryFactor    12.000000000000000
       End
    Frequencies[1/cm]          30
  413.87     414.00     626.09     626.32     700.30     724.75     883.10
883.61     1010.0     1010.5
  1028.9     1033.4     1034.1     1072.7     1072.9     1176.6     1207.6
1207.6     1338.3     1389.9
  1528.0     1528.0     1667.7     1668.0     3183.9     3193.7     3194.4
3209.9     3210.6     3220.8
 ZeroEnergy[kcal/mol]          0.
 ElectronicLevels[1/cm]          1
  0.0000000000000000      1.0000000000000000

 End
!************************************
 Fragment PROD2
  Atom
  Name H
  ElectronicLevels[1/cm]          1
  0.0000000000000000      2.0000000000000000

 End
GroundEnergy[kcal/mol] 18.45999480644160
 End
!************************************
Barrier TS1 W1 W2
 RRHO     ! transition state
 Geometry[angstrom]          13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.49079
 C    1.14938   0.00000   2.34024
 C   -1.34498   0.34751   1.85836
 C   -2.08568   0.53550   0.71826
 C   -1.27951   0.31812  -0.42010
 H    0.88370  -0.17444  -0.59242
 H    2.13557  -0.18832   1.94392
 H    1.03151   0.12632   3.40493
 H   -0.10991  -1.09019   0.88637
 H   -1.69025   0.42708   2.87666
 H   -3.14110   0.76019   0.69095
 H   -1.60949   0.34327  -1.44584
       Core    RigidRotor
            SymmetryFactor    0.50000000000000000
       End
    Frequencies[1/cm]          32
  275.79     322.18     330.35     551.96     598.79     645.05     692.55
776.79     785.53     849.96
  906.67     920.29     961.21     965.79     1082.7     1088.8     1097.7
1151.4     1264.0     1324.6
  1331.4     1462.0     1473.9     1501.9     1549.9     2086.1     3177.6
3224.8     3241.2     3249.2
  3259.7     3282.7
 ZeroEnergy[kcal/mol]          40.37
 ElectronicLevels[1/cm]          1
  0.0000000000000000      2.0000000000000000
    Tunneling    Eckart
   ImaginaryFrequency[1/cm]      1224.8105000000000
   WellDepth[kcal/mol]        40.37
   WellDepth[kcal/mol]        39.01
 End
 End
!************************************
Barrier TS2 W1 W3
 RRHO     ! transition state
 Geometry[angstrom]          13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.45684
 C    1.18329   0.00000   2.32455
 C   -1.37279   0.25510   1.87203
 C   -2.12118   0.39709   0.75010
 C   -1.27031   0.23906  -0.41022
 H    0.87080  -0.16255  -0.61477
 H    2.16452  -0.10874   1.89166
 H    1.06460   0.09557   3.39169
 H    0.37057  -1.08174   1.87571
 H   -1.70392   0.31611   2.89638
 H   -3.18256   0.58795   0.71764
 H   -1.60434   0.29476  -1.43458
       Core    RigidRotor
            SymmetryFactor    1.0000000000000000
       End
```

```
   Frequencies[1/cm]         32
  229.50    322.82    411.11    583.32    595.62    652.72    666.80
718.91    784.30    825.24
  914.51    920.52    929.15    941.69    1033.0    1040.2    1099.7
1104.2    1261.6    1313.3
  1342.3    1433.1    1447.1    1537.9    1596.5    2298.3    3185.2
3224.7    3233.9    3247.9
  3255.6    3305.2
 ZeroEnergy[kcal/mol]            46.98
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
    Tunneling    Eckart
  ImaginaryFrequency[1/cm]     1647.2607000000000
  WellDepth[kcal/mol]        46.98
  WellDepth[kcal/mol]        23.59
 End
 End
!************************************
Barrier TS3 W1 Pr1
 Variational
 RRHO        !        1
 Geometry[angstrom]        13
 C   0.58797  0.03458  -1.02571
 C   0.58917  0.03603   0.44233
 C   1.65692  0.04571   1.24378
 C  -0.82068  0.02193   0.85143
 C  -1.57253  0.01611  -0.26085
 C  -0.69004  0.02402  -1.43678
 H   1.47605  0.04135  -1.63738
 H   2.66120  0.07094   0.84196
 H   1.55148  0.06084   2.32051
 H   2.12261 -2.34345   1.57703
 H  -1.15972  0.01771   1.87511
 H  -2.65090  0.00709  -0.30496
 H  -1.03367  0.02158  -2.45993
          Core          RigidRotor
       SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]         32
  3255.3    3249.8    3248.8    3232.0    3222.6    3159.4    1717.0
1647.2    1562.6    1462.3
  1381.3    1355.2    1266.9    1112.1    1108.2    1007.4    991.95
972.46    971.61    962.68
  917.29    811.24    809.41    807.85    715.01    682.77    643.34
511.60    346.49    226.53
  99.590    87.550
 ZeroEnergy[kcal/mol]    50.498472635285417
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
 End
!*********************************************
 RRHO        !        2
 Geometry[angstrom]        13
 C   0.58800  0.03453  -1.02566
 C   0.58913  0.03582   0.44231
 C   1.65711  0.04465   1.24392
 C  -0.82063  0.02188   0.85144
 C  -1.57252  0.01615  -0.26084
 C  -0.69002  0.02407  -1.43678
 H   1.47610  0.04121  -1.63730
 H   2.66135  0.07085   0.84208
 H   1.55163  0.06073   2.32062
 H   2.11912 -2.32803   1.57453
 H  -1.15965  0.01758   1.87512
 H  -2.65089  0.00720  -0.30494
 H  -1.03364  0.02169  -2.45993
          Core          RigidRotor
       SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]         32
  3255.3    3249.9    3248.9    3232.0    3222.6    3159.5    1715.0
1647.0    1562.5    1462.1
  1381.2    1355.1    1266.8    1112.1    1108.1    1007.4    991.46
972.40    971.55    962.57
  917.33    811.09    809.35    808.23    715.36    682.71    643.44
512.07    346.54    228.21
  106.39    94.660
 ZeroEnergy[kcal/mol]    50.548932891010821
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
 End
!*********************************************
 RRHO        !        3
 Geometry[angstrom]        13
 C   0.58804  0.03449  -1.02561
 C   0.58908  0.03562   0.44227
 C   1.65730  0.04358   1.24407
 C  -0.82058  0.02184   0.85145
 C  -1.57252  0.01620  -0.26084
 C  -0.69000  0.02412  -1.43678
 H   1.47615  0.04107  -1.63722
 H   2.66150  0.07079   0.84222
 H   1.55178  0.06068   2.32074
 H   2.11565 -2.31263   1.57203
 H  -1.15958  0.01744   1.87513
 H  -2.65088  0.00731  -0.30493
 H  -1.03360  0.02181  -2.45994
          Core          RigidRotor
       SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]         32
  3255.4    3250.0    3248.9    3232.1    3222.6    3159.5    1712.8
1646.7    1562.3    1461.9
  1381.0    1354.9    1266.8    1112.1    1108.1    1007.4    991.00
972.34    971.50    962.46
  917.36    810.92    809.30    808.64    715.72    682.65    643.54
512.56    346.60    230.18
  113.03    101.72
 ZeroEnergy[kcal/mol]    50.593032277827398
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
 End
!*********************************************
 RRHO        !        4
 Geometry[angstrom]        13
 C   0.58807  0.03444  -1.02555
 C   0.58902  0.03542   0.44223
 C   1.65751  0.04248   1.24423
 C  -0.82053  0.02179   0.85145
 C  -1.57251  0.01624  -0.26084
 C  -0.68999  0.02416  -1.43679
 H   1.47620  0.04093  -1.63713
 H   2.66166  0.07078   0.84236
 H   1.55194  0.06071   2.32087
 H   2.11218 -2.29725   1.56952
 H  -1.15950  0.01731   1.87515
 H  -2.65088  0.00742  -0.30491
 H  -1.03356  0.02192  -2.45995
          Core          RigidRotor
       SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]         32
  3255.4    3250.1    3249.0    3232.1    3222.7    3159.6    1710.5
1646.4    1562.2    1461.7
  1380.9    1354.7    1266.8    1112.1    1108.0    1007.3    990.51
972.27    971.43    962.34
  917.40    810.75    809.33    808.94    716.09    682.58    643.64
513.06    346.66    232.49
  119.33    108.66
 ZeroEnergy[kcal/mol]    50.636588427383558
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
 End
!*********************************************
 RRHO        !        5
 Geometry[angstrom]        13
 C   0.58810  0.03440  -1.02549
 C   0.58896  0.03522   0.44219
```

```
C   1.65772   0.04137   1.24439
C  -0.82047   0.02176   0.85146
C  -1.57251   0.01628  -0.26084
C  -0.68998   0.02420  -1.43679
H   1.47625   0.04080  -1.63704
H   2.66182   0.07083   0.84251
H   1.55211   0.06080   2.32100
H   2.10872  -2.28187   1.56700
H  -1.15942   0.01717   1.87516
H  -2.65088   0.00752  -0.30490
H  -1.03352   0.02203  -2.45996
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]          32
  3255.4    3250.3    3249.0    3232.1    3222.7    3159.6    1708.1
1646.1    1562.0    1461.5
  1380.7    1354.5    1266.8    1112.0    1108.0    1007.3    990.09
972.20    971.38    962.22
  917.45    810.58    809.64    809.05    716.52    682.51    643.77
513.62    346.73    235.15
  125.35    115.55
ZeroEnergy[kcal/mol]    50.674269762421858
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           6
Geometry[angstrom]          13
C   0.58812   0.03437  -1.02544
C   0.58889   0.03504   0.44214
C   1.65795   0.04024   1.24457
C  -0.82042   0.02173   0.85146
C  -1.57252   0.01632  -0.26084
C  -0.68997   0.02424  -1.43680
H   1.47630   0.04067  -1.63695
H   2.66199   0.07095   0.84266
H   1.55228   0.06096   2.32113
H   2.10529  -2.26652   1.56450
H  -1.15934   0.01704   1.87516
H  -2.65088   0.00762  -0.30489
H  -1.03348   0.02213  -2.45997
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]          32
  3255.4    3250.5    3249.1    3232.2    3222.8    3159.8    1705.5
1645.8    1561.9    1461.3
  1380.6    1354.3    1266.7    1112.0    1107.9    1007.3    989.88
972.13    971.32    962.10
  917.50    810.57    810.06    809.05    717.04    682.44    643.91
514.29    346.81    238.08
  131.30    122.61
ZeroEnergy[kcal/mol]    50.719355553737714
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           7
Geometry[angstrom]          13
C   0.58815   0.03433  -1.02537
C   0.58881   0.03487   0.44209
C   1.65820   0.03909   1.24476
C  -0.82037   0.02170   0.85146
C  -1.57252   0.01636  -0.26085
C  -0.68996   0.02427  -1.43681
H   1.47635   0.04055  -1.63685
H   2.66216   0.07115   0.84282
H   1.55246   0.06118   2.32127
H   2.10188  -2.25118   1.56202
H  -1.15926   0.01692   1.87517
H  -2.65088   0.00771  -0.30488
H  -1.03344   0.02222  -2.45999
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]          32
  3255.5    3250.7    3249.1    3232.2    3222.8    3159.9    1702.8
1645.4    1561.7    1461.1
  1380.4    1354.0    1266.7    1112.0    1107.9    1007.3    989.74
972.05    971.27    961.97
  917.56    811.16    810.00    808.99    717.61    682.37    644.05
515.01    346.90    241.31
  137.42    130.18
ZeroEnergy[kcal/mol]    50.753277840430485
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           8
Geometry[angstrom]          13
C   0.58818   0.03431  -1.02531
C   0.58871   0.03470   0.44203
C   1.65845   0.03791   1.24496
C  -0.82032   0.02167   0.85146
C  -1.57253   0.01639  -0.26087
C  -0.68995   0.02431  -1.43682
H   1.47640   0.04043  -1.63675
H   2.66234   0.07141   0.84298
H   1.55263   0.06147   2.32142
H   2.09851  -2.23585   1.55954
H  -1.15919   0.01680   1.87517
H  -2.65089   0.00779  -0.30488
H  -1.03340   0.02231  -2.46001
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]          32
  3255.5    3250.9    3249.2    3232.3    3222.9    3160.0    1699.8
1645.0    1561.5    1460.9
  1380.2    1353.8    1266.6    1112.0    1107.8    1007.3    989.52
971.96    971.22    961.82
  917.61    811.87    809.77    808.91    718.17    682.31    644.20
515.74    347.01    245.00
  143.75    138.44
ZeroEnergy[kcal/mol]    50.794819019161501
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           9
Geometry[angstrom]          13
C   0.58821   0.03429  -1.02524
C   0.58861   0.03454   0.44196
C   1.65871   0.03671   1.24517
C  -0.82027   0.02165   0.85145
C  -1.57254   0.01642  -0.26089
C  -0.68994   0.02434  -1.43684
H   1.47645   0.04032  -1.63664
H   2.66251   0.07173   0.84314
H   1.55281   0.06182   2.32157
H   2.09518  -2.22055   1.55706
H  -1.15912   0.01668   1.87517
H  -2.65089   0.00787  -0.30489
H  -1.03336   0.02239  -2.46003
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]          32
  3255.6    3251.1    3249.2    3232.3    3222.9    3160.1    1696.7
1644.5    1561.3    1460.6
  1380.0    1353.4    1266.5    1111.9    1107.7    1007.3    989.22
971.88    971.15    961.66
  917.67    812.58    809.51    808.81    718.72    682.25    644.35
516.48    347.13    249.29
  149.93    147.19
ZeroEnergy[kcal/mol]    50.830685523418026
 ElectronicLevels[1/cm]                 1
```

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 0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 10
Geometry[angstrom] 13
C 0.58829 0.03427 -1.02515
C 0.58844 0.03440 0.44191
C 1.65899 0.03549 1.24542
C -0.82024 0.02163 0.85147
C -1.57257 0.01645 -0.26094
C -0.68990 0.02437 -1.43691
H 1.47657 0.04021 -1.63643
H 2.66264 0.07211 0.84332
H 1.55305 0.06221 2.32171
H 2.09198 -2.20529 1.55463
H -1.15905 0.01657 1.87515
H -2.65095 0.00795 -0.30496
H -1.03330 0.02247 -2.46012
 Core RigidRotor
 SymmetryFactor 1.0000000000000000
End
 Frequencies[1/cm] 32
 3255.7 3251.8 3249.5 3232.4 3222.9 3160.6 1693.2
1643.9 1561.0 1460.3
 1379.8 1353.1 1266.5 1111.8 1107.6 1007.3 988.74
971.77 971.00 961.43
 917.76 813.14 809.20 808.69 719.12 682.17 644.48
517.25 347.21 254.29
 156.03 155.61
ZeroEnergy[kcal/mol] 50.859605034353166
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 11
Geometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.46689
C 1.07096 0.00000 2.27070
C -1.40848 -0.01264 1.87655
C -2.16088 -0.01777 0.76415
C -1.27823 -0.00985 -0.41178
H 0.88830 0.00584 -0.61129
H 2.07454 0.03841 1.86852
H 0.96491 0.02850 3.34696
H 1.50023 -2.22434 2.57721
H -1.74727 -0.01780 2.90028
H -3.23923 -0.02623 0.72017
H -1.62159 -0.01171 -1.43499
 Core RigidRotor
 SymmetryFactor 1.0000000000000000
End
 Frequencies[1/cm] 32
 3255.8 3252.1 3249.5 3232.4 3223.0 3160.7 1689.6
1643.4 1560.7 1460.0
 1379.5 1352.8 1266.4 1111.8 1107.5 1007.3 988.44
971.67 970.92 961.24
 917.84 813.88 808.89 808.56 719.70 682.11 644.66
518.06 347.35 259.84
 164.79 160.86
ZeroEnergy[kcal/mol] 50.882635435053061
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 12
Geometry[angstrom] 13
C 0.58833 0.03423 -1.02502
C 0.58818 0.03411 0.44172
C 1.65962 0.03301 1.24588
C -0.82010 0.02159 0.85147
C -1.57261 0.01651 -0.26097
C -0.68993 0.02443 -1.43694
H 1.47665 0.03998 -1.63623
H 2.66304 0.07322 0.84365
H 1.55347 0.06329 2.32201
H 2.08517 -2.17484 1.54967
H -1.15884 0.01634 1.87516
H -2.65098 0.00810 -0.30493
H -1.03327 0.02261 -2.46016
 Core RigidRotor
 SymmetryFactor 1.0000000000000000
End
 Frequencies[1/cm] 32
 3255.8 3252.4 3249.6 3232.5 3223.0 3160.8 1686.0
1642.8 1560.5 1459.7
 1379.3 1352.4 1266.3 1111.7 1107.4 1007.3 988.19
971.58 970.83 961.03
 917.92 814.66 808.53 808.42 720.30 682.07 644.84
518.91 347.48 266.07
 173.72 165.91
ZeroEnergy[kcal/mol] 50.906480691643708
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 13
Geometry[angstrom] 13
C 0.58829 0.03421 -1.02497
C 0.58809 0.03397 0.44159
C 1.65996 0.03175 1.24609
C -0.82000 0.02157 0.85145
C -1.57262 0.01653 -0.26094
C -0.69000 0.02445 -1.43690
H 1.47661 0.03986 -1.63622
H 2.66330 0.07396 0.84378
H 1.55366 0.06397 2.32218
H 2.08167 -2.15969 1.54718
H -1.15871 0.01624 1.87520
H -2.65096 0.00817 -0.30484
H -1.03330 0.02268 -2.46012
 Core RigidRotor
 SymmetryFactor 1.0000000000000000
End
 Frequencies[1/cm] 32
 3255.7 3252.2 3249.4 3232.5 3223.2 3160.6 1682.4
1642.3 1560.4 1459.5
 1379.1 1351.9 1266.2 1111.7 1107.4 1007.4 988.13
971.56 970.75 960.86
 917.98 815.66 808.27 808.15 721.09 682.07 645.07
519.81 347.69 273.20
 183.01 170.69
ZeroEnergy[kcal/mol] 50.919562723697851
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 14
Geometry[angstrom] 13
C 0.58830 0.03420 -1.02490
C 0.58793 0.03386 0.44145
C 1.66033 0.03046 1.24634
C -0.81991 0.02156 0.85145
C -1.57265 0.01656 -0.26095
C -0.69003 0.02447 -1.43692
H 1.47664 0.03976 -1.63614
H 2.66352 0.07474 0.84395
H 1.55389 0.06469 2.32233
H 2.07826 -2.14455 1.54477
H -1.15858 0.01613 1.87521
H -2.65098 0.00823 -0.30480
H -1.03331 0.02274 -2.46014
 Core RigidRotor
 SymmetryFactor 1.0000000000000000
End
 Frequencies[1/cm] 32
 3255.7 3252.5 3249.4 3232.6 3223.2 3160.7 1678.4
1641.7 1560.1 1459.1
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  1378.8    1351.5    1266.1    1111.6    1107.3    1007.5    988.01
971.50    970.59    960.62
  918.07    816.60    808.08    807.73    721.77    682.06    645.28
520.79    347.85    281.34
  192.60    175.15
 ZeroEnergy[kcal/mol]    50.933330950186296
  ElectronicLevels[1/cm]            1
  0.0000000000000000    2.0000000000000000
 End
!***********************************************
 RRHO       !     15
 Geometry[angstrom]       13
 C   0.58831   0.03419  -1.02483
 C   0.58776   0.03374   0.44132
 C   1.66071   0.02915   1.24660
 C  -0.81983   0.02155   0.85145
 C  -1.57268   0.01658  -0.26096
 C  -0.69007   0.02449  -1.43694
 H   1.47666   0.03966  -1.63604
 H   2.66373   0.07558   0.84411
 H   1.55412   0.06549   2.32249
 H   2.07488  -2.12944   1.54238
 H  -1.15845   0.01603   1.87522
 H  -2.65101   0.00830  -0.30478
 H  -1.03333   0.02280  -2.46016
           Core        RigidRotor
      SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]       32
  3255.8    3252.9    3249.4    3232.6    3223.3    3160.9    1674.3
1640.9    1559.8    1458.8
  1378.5    1350.9    1266.0    1111.6    1107.2    1007.5    988.05
971.46    970.41    960.37
  918.16    817.69    807.88    807.28    722.50    682.07    645.50
521.83    348.04    290.25
  202.30    179.15
 ZeroEnergy[kcal/mol]    50.935449617660758
  ElectronicLevels[1/cm]            1
  0.0000000000000000    2.0000000000000000
 End
!***********************************************
 RRHO       !     16
 Geometry[angstrom]       13
 C   0.58833   0.03419  -1.02475
 C   0.58757   0.03364   0.44117
 C   1.66110   0.02782   1.24687
 C  -0.81974   0.02154   0.85145
 C  -1.57271   0.01660  -0.26098
 C  -0.69011   0.02451  -1.43696
 H   1.47669   0.03956  -1.63593
 H   2.66395   0.07649   0.84428
 H   1.55436   0.06636   2.32265
 H   2.07153  -2.11436   1.53999
 H  -1.15832   0.01593   1.87522
 H  -2.65104   0.00835  -0.30476
 H  -1.03334   0.02285  -2.46018
           Core        RigidRotor
      SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]       32
  3255.8    3253.2    3249.5    3232.7    3223.3    3161.0    1670.0
1640.2    1559.5    1458.4
  1378.2    1350.4    1265.9    1111.5    1107.0    1007.6    988.16
971.43    970.20    960.09
  918.26    818.81    807.65    806.78    723.24    682.10    645.74
522.91    348.24    299.86
  212.11    182.73
 ZeroEnergy[kcal/mol]    50.931507626291378
  ElectronicLevels[1/cm]            1
  0.0000000000000000    2.0000000000000000
 End
!***********************************************
 RRHO       !     17
 Geometry[angstrom]       13
 C   0.58834   0.03418  -1.02467
 C   0.58737   0.03354   0.44101
 C   1.66151   0.02647   1.24717
 C  -0.81965   0.02154   0.85144
 C  -1.57274   0.01662  -0.26100
 C  -0.69015   0.02453  -1.43698
 H   1.47673   0.03946  -1.63582
 H   2.66417   0.07747   0.84446
 H   1.55459   0.06732   2.32281
 H   2.06819  -2.09932   1.53762
 H  -1.15819   0.01583   1.87523
 H  -2.65107   0.00841  -0.30474
 H  -1.03335   0.02290  -2.46021
           Core        RigidRotor
      SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]       32
  3255.9    3253.6    3249.5    3232.7    3223.4    3161.2    1665.6
1639.3    1559.2    1458.0
  1377.8    1349.8    1265.7    1111.4    1106.9    1007.6    988.20
971.41    969.96    959.79
  918.36    819.91    807.40    806.24    723.98    682.15    645.99
524.02    348.48    310.22
  222.16    185.94
 ZeroEnergy[kcal/mol]    50.921533567513009
  ElectronicLevels[1/cm]            1
  0.0000000000000000    2.0000000000000000
 End
!***********************************************
 RRHO       !     18
 Geometry[angstrom]       13
 C   0.58836   0.03418  -1.02459
 C   0.58715   0.03345   0.44084
 C   1.66194   0.02510   1.24747
 C  -0.81956   0.02153   0.85144
 C  -1.57278   0.01663  -0.26103
 C  -0.69020   0.02455  -1.43701
 H   1.47676   0.03937  -1.63571
 H   2.66439   0.07852   0.84465
 H   1.55483   0.06837   2.32297
 H   2.06488  -2.08432   1.53525
 H  -1.15806   0.01574   1.87523
 H  -2.65110   0.00846  -0.30473
 H  -1.03336   0.02295  -2.46024
           Core        RigidRotor
      SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]       32
  3255.9    3254.0    3249.6    3232.8    3223.5    3161.4    1661.0
1638.4    1558.8    1457.5
  1377.5    1349.1    1265.5    1111.3    1106.8    1007.7    988.18
971.38    969.69    959.45
  918.46    821.05    807.11    805.65    724.73    682.23    646.25
525.19    348.77    321.41
  232.54    188.87
 ZeroEnergy[kcal/mol]    50.899652626807764
  ElectronicLevels[1/cm]            1
  0.0000000000000000    2.0000000000000000
 End
!***********************************************
 RRHO       !     19
 Geometry[angstrom]       13
 C   0.58838   0.03418  -1.02450
 C   0.58691   0.03337   0.44066
 C   1.66238   0.02371   1.24779
 C  -0.81947   0.02153   0.85143
 C  -1.57282   0.01665  -0.26106
 C  -0.69025   0.02457  -1.43703
 H   1.47679   0.03928  -1.63559
 H   2.66461   0.07964   0.84483
 H   1.55507   0.06949   2.32313
 H   2.06158  -2.06936   1.53289
 H  -1.15793   0.01565   1.87524
 H  -2.65114   0.00851  -0.30473
```

H -1.03337 0.02300 -2.46027
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3255.9 3254.4 3249.6 3232.8 3223.6 3161.6 1656.3
1637.4 1558.5 1457.0
1377.1 1348.3 1265.3 1111.2 1106.7 1007.8 988.19
971.38 969.40 959.08
918.56 822.32 806.80 805.01 725.53 682.34 646.53
526.44 349.15 333.37
243.19 191.53
ZeroEnergy[kcal/mol] 50.872654544605830
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 20
Geometry[angstrom] 13
C 0.58839 0.03418 -1.02441
C 0.58665 0.03329 0.44046
C 1.66284 0.02231 1.24812
C -0.81937 0.02153 0.85143
C -1.57287 0.01667 -0.26110
C -0.69030 0.02458 -1.43706
H 1.47682 0.03919 -1.63547
H 2.66484 0.08083 0.84502
H 1.55532 0.07068 2.32330
H 2.05830 -2.05444 1.53054
H -1.15780 0.01556 1.87524
H -2.65118 0.00855 -0.30472
H -1.03339 0.02304 -2.46030
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3256.0 3254.8 3249.6 3232.9 3223.6 3161.8 1651.5
1636.4 1558.1 1456.5
1376.7 1347.6 1265.1 1111.1 1106.5 1007.9 988.37
971.40 969.07 958.69
918.66 823.78 806.47 804.32 726.37 682.50 646.83
527.76 349.64 345.96
253.90 193.95
ZeroEnergy[kcal/mol] 50.827989131698274
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 21
Geometry[angstrom] 13
C 0.58841 0.03419 -1.02431
C 0.58638 0.03323 0.44026
C 1.66332 0.02089 1.24847
C -0.81927 0.02153 0.85142
C -1.57291 0.01668 -0.26114
C -0.69035 0.02460 -1.43709
H 1.47686 0.03911 -1.63535
H 2.66506 0.08208 0.84521
H 1.55556 0.07194 2.32346
H 2.05504 -2.03955 1.52820
H -1.15766 0.01548 1.87524
H -2.65122 0.00859 -0.30472
H -1.03340 0.02309 -2.46034
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3256.0 3255.2 3249.7 3233.0 3223.7 3162.1 1646.9
1635.3 1557.7 1456.0
1376.2 1346.7 1264.8 1110.9 1106.3 1008.0 988.73
971.44 968.73 958.27
918.77 825.40 806.12 803.56 727.25 682.71 647.16
529.16 359.12 350.29
264.55 196.18

ZeroEnergy[kcal/mol] 50.772002961276442
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
Tunneling Eckart
ImaginaryFrequency[1/cm] 461.58810000000000
WellDepth[kcal/mol] 50.88
WellDepth[kcal/mol] 0.88
End
End
Barrier TS4 W2 W3
RRHO ! transition state
Geometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.49079
C 1.14938 0.00000 2.34025
C -1.34498 -0.34749 1.85836
C -2.08569 -0.53547 0.71826
C -1.27951 -0.31810 -0.42010
H 0.88370 0.17443 -0.59242
H -0.10990 1.09019 0.88638
H 2.13557 0.18834 1.94393
H 1.03150 -0.12633 3.40493
H -1.69025 -0.42706 2.87667
H -3.14111 -0.76014 0.69095
H -1.60950 -0.34325 -1.44584
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
275.79 322.18 330.36 551.96 598.79 645.05 692.55
776.79 785.53 849.96
906.67 920.29 961.21 965.79 1082.7 1088.8 1097.7
1151.4 1264.0 1324.6
1331.4 1462.0 1473.9 1501.9 1549.9 2086.1 3177.5
3224.8 3241.2 3249.2
3259.7 3282.7
ZeroEnergy[kcal/mol] 40.36906131589037
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
Tunneling Eckart
ImaginaryFrequency[1/cm] 1224.8017000000000
WellDepth[kcal/mol] 39.01
WellDepth[kcal/mol] 16.99
End
End
!**********************************
Barrier TS5 W2 W4
RRHO ! transition state
Geometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.42206
C 1.12300 0.00000 2.24861
C -1.36992 0.01927 1.82516
C -2.19905 0.04240 0.72890
C -1.40502 0.03817 -0.44433
H 0.84450 -0.13355 -0.65649
H -0.66291 1.08129 -0.41289
H 1.01761 -0.01468 3.32320
H 2.12096 -0.00175 1.83561
H -1.69261 0.06880 2.85450
H -3.27540 0.09448 0.74080
H -1.72544 -0.11709 -1.46158
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
259.02 344.54 475.52 594.64 614.74 672.72 681.81
760.14 790.92 849.22
925.98 951.13 967.07 974.79 1020.3 1081.6 1095.9
1235.7 1257.0 1291.3
1378.9 1423.4 1477.6 1507.1 1519.7 2148.5 3170.1
3224.1 3242.7 3250.5

```
 3261.0    3267.1
ZeroEnergy[kcal/mol] 35.42493306054502
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
   Tunneling   Eckart
  ImaginaryFrequency[1/cm]    1357.7312999999999
  WellDepth[kcal/mol]      34.06
  WellDepth[kcal/mol]      28.65
 End
 End
!************************************
Barrier TS6 W2 Pr1
 Variational
 RRHO     !     1
 Geometry[angstrom]     13
 C   0.61009  0.02637  -0.99170
 C   0.60745  0.00989  0.48531
 C   1.67167  0.00712  1.28422
 C  -0.80128  -0.02468  0.88420
 C  -1.55370  -0.07833  -0.23380
 C  -0.68612  -0.07945  -1.40016
 H   1.49340  -0.08031  -1.59969
 H   0.87728  1.97174  -1.18669
 H   2.67589  0.03528  0.88277
 H   1.56451  -0.01791  2.36050
 H  -1.14634  -0.00657  1.90569
 H  -2.63161  -0.11506  -0.27386
 H  -1.02452  -0.13136  -2.42288
        Core      RigidRotor
     SymmetryFactor  0.50000000000000000
 End
   Frequencies[1/cm]     32
  3258.2   3251.5   3250.7   3238.2   3226.6   3161.1   1742.2
1599.9   1486.9   1438.7
  1386.5   1351.1   1265.3   1108.9   1096.7   1019.1   990.33
971.94   969.96   954.92
  914.52   821.68   811.93   802.77   732.14   681.35   655.61
515.70   442.98   377.89
  345.08   205.95
 ZeroEnergy[kcal/mol]   51.416027998285900
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO     !     2
 Geometry[angstrom]     13
 C   0.60966  0.02455  -0.99162
 C   0.60739  0.00981  0.48506
 C   1.67159  0.00725  1.28411
 C  -0.80148  -0.02472  0.88421
 C  -1.55378  -0.07824  -0.23342
 C  -0.68543  -0.07924  -1.40015
 H   1.49333  -0.07756  -1.59990
 H   0.87902  1.98676  -1.18814
 H   2.67586  0.03502  0.88270
 H   1.56443  -0.01747  2.36043
 H  -1.14638  -0.00664  1.90576
 H  -2.63167  -0.11496  -0.27372
 H  -1.02410  -0.13113  -2.42285
        Core      RigidRotor
     SymmetryFactor  0.50000000000000000
 End
   Frequencies[1/cm]     32
  3258.1   3251.5   3250.6   3238.0   3226.5   3161.0   1742.1
1602.6   1488.7   1441.7
  1386.5   1351.6   1265.4   1109.2   1097.5   1019.2   991.31
972.02   970.25   954.46
  914.73   821.31   811.07   803.21   731.39   681.51   654.97
513.35   424.59   363.96
  343.33   205.45
 ZeroEnergy[kcal/mol]   51.518583088003518
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO     !     3
 Geometry[angstrom]     13
 C   0.60925  0.02273  -0.99153
 C   0.60733  0.00971  0.48482
 C   1.67152  0.00738  1.28401
 C  -0.80167  -0.02475  0.88422
 C  -1.55387  -0.07816  -0.23305
 C  -0.68477  -0.07904  -1.40015
 H   1.49325  -0.07484  -1.60010
 H   0.88074  2.00180  -1.18958
 H   2.67583  0.03476  0.88264
 H   1.56434  -0.01699  2.36035
 H  -1.14642  -0.00672  1.90583
 H  -2.63173  -0.11486  -0.27359
 H  -1.02368  -0.13088  -2.42283
        Core      RigidRotor
     SymmetryFactor  0.50000000000000000
 End
   Frequencies[1/cm]     32
  3258.1   3251.4   3250.6   3237.7   3226.4   3160.9   1742.0
1605.2   1490.8   1444.5
  1386.5   1352.0   1265.6   1109.4   1098.3   1019.2   992.18
972.11   970.51   954.34
  914.92   820.93   810.27   803.61   730.70   681.71   654.39
511.73   406.29   353.70
  338.28   204.86
 ZeroEnergy[kcal/mol]   51.597910538279999
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO     !     4
 Geometry[angstrom]     13
 C   0.60886  0.02092  -0.99145
 C   0.60727  0.00961  0.48458
 C   1.67145  0.00751  1.28391
 C  -0.80186  -0.02479  0.88424
 C  -1.55395  -0.07808  -0.23269
 C  -0.68412  -0.07884  -1.40014
 H   1.49317  -0.07216  -1.60029
 H   0.88246  2.01687  -1.19100
 H   2.67579  0.03447  0.88257
 H   1.56426  -0.01647  2.36027
 H  -1.14646  -0.00680  1.90591
 H  -2.63180  -0.11476  -0.27347
 H  -1.02326  -0.13060  -2.42281
        Core      RigidRotor
     SymmetryFactor  0.50000000000000000
 End
   Frequencies[1/cm]     32
  3258.0   3251.4   3250.5   3237.5   3226.4   3160.8   1741.9
1607.7   1493.2   1447.1
  1386.5   1352.4   1265.7   1109.6   1099.0   1019.1   992.96
972.21   970.73   954.42
  915.09   820.54   809.55   803.99   730.07   681.92   653.84
510.52   388.35   349.46
  327.62   204.16
 ZeroEnergy[kcal/mol]   51.659870867915829
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO     !     5
 Geometry[angstrom]     13
 C   0.60849  0.01912  -0.99136
 C   0.60720  0.00949  0.48435
 C   1.67137  0.00765  1.28380
 C  -0.80205  -0.02482  0.88427
 C  -1.55403  -0.07799  -0.23233
 C  -0.68350  -0.07865  -1.40014
 H   1.49310  -0.06952  -1.60046
 H   0.88417  2.03198  -1.19242
 H   2.67576  0.03416  0.88250
```

```
H   1.56417  -0.01592  2.36019
H  -1.14649  -0.00690  1.90599
H  -2.63187  -0.11465  -0.27334
H  -1.02284  -0.13029  -2.42279
        Core        RigidRotor
    SymmetryFactor  0.50000000000000000
End
  Frequencies[1/cm]      32
 3258.0   3251.4   3250.4   3237.2   3226.3   3160.7   1741.7
1610.1   1495.8   1449.4
 1386.5   1352.8   1265.8   1109.8   1099.8   1019.0   993.65
972.31   970.92   954.63
 915.26   820.12   808.88   804.35   729.50   682.12   653.35
509.55   370.99   347.82
 314.82   203.34
ZeroEnergy[kcal/mol]   51.698160390871729
 ElectronicLevels[1/cm]          1
 0.0000000000000000     2.0000000000000000
End
!**********************************************
RRHO       !       6
Geometry[angstrom]       13
C   0.60814  0.01732  -0.99128
C   0.60713  0.00936  0.48412
C   1.67130  0.00780  1.28370
C  -0.80223  -0.02486  0.88431
C  -1.55412  -0.07790  -0.23199
C  -0.68290  -0.07846  -1.40014
H   1.49302  -0.06694  -1.60063
H   0.88589  2.04713  -1.19382
H   2.67573  0.03384  0.88243
H   1.56409  -0.01533  2.36011
H  -1.14653  -0.00700  1.90608
H  -2.63193  -0.11454  -0.27321
H  -1.02243  -0.12996  -2.42278
        Core        RigidRotor
    SymmetryFactor  0.50000000000000000
End
  Frequencies[1/cm]      32
 3257.9   3251.4   3250.3   3237.0   3226.2   3160.6   1741.6
1612.4   1498.6   1451.4
 1386.4   1353.1   1266.0   1110.0   1100.5   1018.8   994.25
972.42   971.07   954.84
 915.41   819.62   808.24   804.67   728.96   682.28   652.90
508.73   355.21   346.05
 301.93   202.36
ZeroEnergy[kcal/mol]   51.724886129117907
 ElectronicLevels[1/cm]          1
 0.0000000000000000     2.0000000000000000
End
!**********************************************
RRHO       !       7
Geometry[angstrom]       13
C   0.60781  0.01553  -0.99119
C   0.60707  0.00921  0.48390
C   1.67123  0.00795  1.28359
C  -0.80241  -0.02489  0.88434
C  -1.55420  -0.07781  -0.23166
C  -0.68232  -0.07828  -1.40014
H   1.49295  -0.06442  -1.60078
H   0.88762  2.06234  -1.19520
H   2.67570  0.03350  0.88236
H   1.56401  -0.01470  2.36002
H  -1.14656  -0.00711  1.90617
H  -2.63200  -0.11442  -0.27309
H  -1.02203  -0.12961  -2.42277
        Core        RigidRotor
    SymmetryFactor  0.50000000000000000
End
  Frequencies[1/cm]      32
 3257.9   3251.4   3250.2   3236.8   3226.1   3160.5   1741.4
1614.6   1501.5   1453.0
 1386.4   1353.5   1266.1   1110.2   1101.1   1018.6   994.77
972.53   971.19   954.95
 915.54   819.03   807.61   804.95   728.40   682.38   652.48
507.99   348.40   336.49
 289.35   201.19
ZeroEnergy[kcal/mol]   51.739733576871957
 ElectronicLevels[1/cm]          1
 0.0000000000000000     2.0000000000000000
End
!**********************************************
RRHO       !       8
Geometry[angstrom]       13
C   0.60750  0.01376  -0.99111
C   0.60700  0.00906  0.48368
C   1.67115  0.00810  1.28349
C  -0.80258  -0.02492  0.88439
C  -1.55428  -0.07772  -0.23135
C  -0.68177  -0.07810  -1.40015
H   1.49288  -0.06200  -1.60091
H   0.88935  2.07759  -1.19658
H   2.67566  0.03315  0.88228
H   1.56392  -0.01404  2.35994
H  -1.14660  -0.00723  1.90626
H  -2.63207  -0.11430  -0.27298
H  -1.02164  -0.12924  -2.42277
        Core        RigidRotor
    SymmetryFactor  0.50000000000000000
End
  Frequencies[1/cm]      32
 3257.8   3251.3   3250.2   3236.5   3226.0   3160.4   1741.3
1616.7   1504.4   1454.5
 1386.3   1353.7   1266.2   1110.3   1101.7   1018.4   995.23
972.64   971.28   955.00
 915.67   818.37   806.97   805.16   727.78   682.42   652.09
507.30   347.44   321.96
 277.06   199.75
ZeroEnergy[kcal/mol]   51.735941585138492
 ElectronicLevels[1/cm]          1
 0.0000000000000000     2.0000000000000000
End
!**********************************************
RRHO       !       9
Geometry[angstrom]       13
C   0.60722  0.01201  -0.99102
C   0.60693  0.00890  0.48348
C   1.67108  0.00825  1.28338
C  -0.80275  -0.02494  0.88443
C  -1.55436  -0.07763  -0.23105
C  -0.68125  -0.07794  -1.40015
H   1.49281  -0.05967  -1.60102
H   0.89109  2.09290  -1.19793
H   2.67563  0.03278  0.88220
H   1.56384  -0.01336  2.35986
H  -1.14663  -0.00735  1.90635
H  -2.63214  -0.11418  -0.27287
H  -1.02126  -0.12886  -2.42278
        Core        RigidRotor
    SymmetryFactor  0.50000000000000000
End
  Frequencies[1/cm]      32
 3257.7   3251.3   3250.1   3236.3   3225.9   3160.3   1741.1
1618.7   1507.5   1455.7
 1386.2   1354.0   1266.3   1110.5   1102.3   1018.1   995.62
972.74   971.35   955.15
 915.78   817.77   806.40   805.29   727.14   682.48   651.73
506.67   347.02   307.52
 265.10   198.00
ZeroEnergy[kcal/mol]   51.726574988952160
 ElectronicLevels[1/cm]          1
 0.0000000000000000     2.0000000000000000
End
!**********************************************
RRHO       !       10
Geometry[angstrom]       13
C   0.60700  0.01026  -0.99090
C   0.60682  0.00876  0.48327
```

C 1.67101 0.00838 1.28327
C -0.80296 -0.02496 0.88448
C -1.55445 -0.07754 -0.23077
C -0.68073 -0.07780 -1.40017
H 1.49285 -0.05744 -1.60108
H 0.89291 2.10824 -1.19921
H 2.67559 0.03236 0.88211
H 1.56377 -0.01266 2.35973
H -1.14671 -0.00747 1.90647
H -2.63221 -0.11407 -0.27278
H -1.02087 -0.12846 -2.42276
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.6 3251.1 3250.1 3236.2 3225.9 3160.4 1740.9
1620.6 1510.5 1456.7
1386.1 1354.3 1266.4 1110.6 1102.8 1017.7 995.90
972.83 971.39 955.48
915.89 817.29 806.09 805.24 726.55 682.57 651.43
506.10 346.74 293.72
253.75 195.95
ZeroEnergy[kcal/mol] 51.706216436751335
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 11
Geometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.47395
C 1.06417 0.00000 2.27402
C -1.40984 -0.03354 1.87539
C -2.16125 -0.08599 0.76034
C -1.28701 -0.08621 -0.40932
H 0.88598 -0.06385 -0.61035
H 0.28789 2.11516 -0.20972
H 2.06879 0.02343 1.87289
H 0.95693 -0.02040 3.35054
H -1.75344 -0.01617 2.89740
H -3.23902 -0.12248 0.71817
H -1.62729 -0.13656 -1.43195
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.5 3251.1 3250.0 3236.0 3225.8 3160.3 1740.8
1622.4 1513.5 1457.7
1386.0 1354.5 1266.5 1110.7 1103.3 1017.4 996.19
972.94 971.44 955.95
915.99 816.88 806.07 804.96 726.02 682.67 651.13
505.63 346.53 280.93
243.10 193.48
ZeroEnergy[kcal/mol] 51.681884400444248
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 12
Geometry[angstrom] 13
C 0.60651 0.00683 -0.99074
C 0.60669 0.00834 0.48289
C 1.67088 0.00872 1.28306
C -0.80327 -0.02502 0.88459
C -1.55460 -0.07734 -0.23022
C -0.67981 -0.07752 -1.40018
H 1.49272 -0.05318 -1.60126
H 0.89638 2.13910 -1.20182
H 2.67553 0.03159 0.88194
H 1.56363 -0.01105 2.35956
H -1.14675 -0.00777 1.90668
H -2.63235 -0.11379 -0.27255
H -1.02019 -0.12755 -2.42279
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.4 3251.0 3249.9 3235.8 3225.7 3160.2 1740.7
1624.1 1516.6 1458.5
1385.8 1354.7 1266.5 1110.8 1103.9 1017.1 996.43
973.04 971.47 956.58
916.07 816.53 806.20 804.69 725.54 682.74 650.86
505.19 346.37 269.18
232.97 190.39
ZeroEnergy[kcal/mol] 51.646517520970542
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 13
Geometry[angstrom] 13
C 0.60624 0.00515 -0.99069
C 0.60665 0.00805 0.48273
C 1.67083 0.00893 1.28295
C -0.80338 -0.02506 0.88467
C -1.55466 -0.07723 -0.22995
C -0.67942 -0.07738 -1.40018
H 1.49254 -0.05117 -1.60139
H 0.89799 2.15459 -1.20316
H 2.67550 0.03123 0.88186
H 1.56357 -0.01015 2.35951
H -1.14672 -0.00794 1.90678
H -2.63242 -0.11362 -0.27241
H -1.01991 -0.12704 -2.42282
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.5 3251.1 3249.7 3235.6 3225.5 3159.9 1740.6
1625.7 1519.6 1459.2
1385.8 1354.8 1266.6 1110.9 1104.3 1016.8 996.70
973.16 971.51 957.25
916.14 816.23 806.35 804.42 725.04 682.79 650.59
504.81 346.23 258.49
223.23 186.50
ZeroEnergy[kcal/mol] 51.612008384539637
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 14
Geometry[angstrom] 13
C 0.60603 0.00347 -0.99062
C 0.60659 0.00780 0.48256
C 1.67077 0.00911 1.28284
C -0.80351 -0.02510 0.88474
C -1.55473 -0.07712 -0.22969
C -0.67903 -0.07727 -1.40018
H 1.49247 -0.04927 -1.60147
H 0.89968 2.17014 -1.20445
H 2.67548 0.03084 0.88177
H 1.56350 -0.00923 2.35942
H -1.14672 -0.00811 1.90690
H -2.63249 -0.11345 -0.27228
H -1.01963 -0.12652 -2.42283
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.4 3251.1 3249.6 3235.4 3225.4 3159.9 1740.5
1627.2 1522.4 1459.8
1385.7 1355.0 1266.7 1111.0 1104.8 1016.4 996.87
973.26 971.53 957.91
916.21 815.97 806.53 804.16 724.54 682.85 650.36
504.44 346.10 248.88
213.82 181.66
ZeroEnergy[kcal/mol] 51.564934763182394
ElectronicLevels[1/cm] 1

```
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO      !     15
Geometry[angstrom]     13
C   0.60584  0.00182  -0.99054
C   0.60653  0.00753  0.48239
C   1.67071  0.00930  1.28273
C  -0.80365  -0.02513  0.88480
C  -1.55481  -0.07702  -0.22945
C  -0.67866  -0.07716  -1.40019
H   1.49241  -0.04747  -1.60153
H   0.90139  2.18573  -1.20572
H   2.67545  0.03044  0.88168
H   1.56344  -0.00830  2.35934
H  -1.14672  -0.00828  1.90701
H  -2.63256  -0.11327  -0.27217
H  -1.01936  -0.12599  -2.42285
          Core       RigidRotor
     SymmetryFactor  0.50000000000000000
End
   Frequencies[1/cm]      32
 3257.3   3251.0   3249.5   3235.3   3225.3   3159.8   1740.5
1628.7   1525.2   1460.3
 1385.5   1355.2   1266.7   1111.1   1105.2   1016.1   997.01
973.35   971.55   958.46
 916.28   815.72   806.70   803.82   724.01   682.94   650.13
504.11   346.00   240.78
 204.83   175.90
ZeroEnergy[kcal/mol]  51.518690293433176
 ElectronicLevels[1/cm]            1
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO      !     16
Geometry[angstrom]     13
C   0.60567  0.00019  -0.99047
C   0.60647  0.00725  0.48224
C   1.67066  0.00949  1.28263
C  -0.80378  -0.02516  0.88488
C  -1.55488  -0.07691  -0.22922
C  -0.67832  -0.07706  -1.40019
H   1.49235  -0.04576  -1.60159
H   0.90312  2.20135  -1.20696
H   2.67542  0.03003  0.88159
H   1.56339  -0.00733  2.35925
H  -1.14673  -0.00845  1.90713
H  -2.63263  -0.11309  -0.27205
H  -1.01910  -0.12545  -2.42287
          Core       RigidRotor
     SymmetryFactor  0.50000000000000000
End
   Frequencies[1/cm]      32
 3257.3   3251.0   3249.4   3235.1   3225.2   3159.7   1740.4
1630.1   1527.9   1460.8
 1385.4   1355.3   1266.8   1111.1   1105.6   1015.8   997.12
973.42   971.57   958.84
 916.34   815.43   806.83   803.38   723.43   683.04   649.90
503.81   345.92   234.57
 196.27   169.60
ZeroEnergy[kcal/mol]  51.461482459104198
 ElectronicLevels[1/cm]            1
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO      !     17
Geometry[angstrom]     13
C   0.60550  -0.00143  -0.99040
C   0.60640  0.00695  0.48208
C   1.67060  0.00969  1.28252
C  -0.80391  -0.02519  0.88495
C  -1.55495  -0.07680  -0.22899
C  -0.67798  -0.07698  -1.40020
H   1.49229  -0.04412  -1.60163
H   0.90486  2.21701  -1.20817
H   2.67539  0.02961  0.88149
H   1.56333  -0.00631  2.35916
H  -1.14674  -0.00862  1.90724
H  -2.63270  -0.11289  -0.27195
H  -1.01885  -0.12488  -2.42289
          Core       RigidRotor
     SymmetryFactor  0.50000000000000000
End
   Frequencies[1/cm]      32
 3257.2   3250.9   3249.3   3234.9   3225.1   3159.6   1740.3
1631.4   1530.4   1461.1
 1385.3   1355.5   1266.8   1111.2   1105.9   1015.4   997.21
973.48   971.58   959.06
 916.40   815.13   806.94   802.87   722.71   683.10   649.66
503.50   345.85   229.89
 188.01   163.04
ZeroEnergy[kcal/mol]  51.411507532444270
 ElectronicLevels[1/cm]            1
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO      !     18
Geometry[angstrom]     13
C   0.60536  -0.00303  -0.99033
C   0.60634  0.00663  0.48194
C   1.67055  0.00989  1.28241
C  -0.80404  -0.02522  0.88503
C  -1.55502  -0.07668  -0.22878
C  -0.67766  -0.07690  -1.40021
H   1.49224  -0.04258  -1.60166
H   0.90660  2.23270  -1.20935
H   2.67536  0.02919  0.88139
H   1.56328  -0.00525  2.35907
H  -1.14675  -0.00879  1.90736
H  -2.63277  -0.11268  -0.27184
H  -1.01861  -0.12430  -2.42291
          Core       RigidRotor
     SymmetryFactor  0.50000000000000000
End
   Frequencies[1/cm]      32
 3257.1   3250.8   3249.3   3234.8   3225.0   3159.6   1740.2
1632.6   1532.7   1461.5
 1385.2   1355.6   1266.9   1111.3   1106.2   1015.0   997.27
973.52   971.59   959.30
 916.44   814.87   807.04   802.43   721.90   683.10   649.39
503.20   345.78   225.96
 179.69   156.08
ZeroEnergy[kcal/mol]  51.348853755118890
 ElectronicLevels[1/cm]            1
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO      !     19
Geometry[angstrom]     13
C   0.60522  -0.00460  -0.99026
C   0.60627  0.00629  0.48180
C   1.67050  0.01010  1.28231
C  -0.80417  -0.02525  0.88510
C  -1.55509  -0.07656  -0.22858
C  -0.67737  -0.07684  -1.40021
H   1.49220  -0.04116  -1.60167
H   0.90836  2.24844  -1.21052
H   2.67533  0.02877  0.88129
H   1.56324  -0.00415  2.35899
H  -1.14676  -0.00897  1.90748
H  -2.63284  -0.11246  -0.27174
H  -1.01838  -0.12371  -2.42293
          Core       RigidRotor
     SymmetryFactor  0.50000000000000000
End
   Frequencies[1/cm]      32
 3257.0   3250.8   3249.2   3234.7   3224.9   3159.5   1740.2
1633.7   1535.0   1461.8
```

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  1385.1     1355.7     1266.9     1111.3     1106.5     1014.7     997.32
973.59     971.60     959.73
  916.48     814.68     807.17     802.21     721.26     683.12     649.17
502.95     345.72     222.79
  171.29     148.75
 ZeroEnergy[kcal/mol]    51.293690208375340
  ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
 RRHO          !         20
 Geometry[angstrom]          13
 C    0.60510  -0.00615  -0.99020
 C    0.60621   0.00594   0.48168
 C    1.67045   0.01030   1.28220
 C   -0.80429  -0.02527   0.88518
 C   -1.55515  -0.07643  -0.22838
 C   -0.67709  -0.07679  -1.40022
 H    1.49215  -0.03987  -1.60168
 H    0.91012   2.26421  -1.21165
 H    2.67530   0.02835   0.88118
 H    1.56320  -0.00303   2.35890
 H   -1.14678  -0.00914   1.90760
 H   -2.63291  -0.11223  -0.27165
 H   -1.01818  -0.12312  -2.42296
              Core           RigidRotor
          SymmetryFactor   0.50000000000000000
 End
    Frequencies[1/cm]          32
  3256.9     3250.7     3249.1     3234.5     3224.8     3159.4     1740.1
1634.8     1537.0     1462.0
  1385.0     1355.8     1267.0     1111.4     1106.7     1014.3     997.36
973.69     971.62     960.42
  916.52     814.57     807.38     802.24     720.96     683.18     649.06
502.76     345.67     220.56
  163.21     141.53
 ZeroEnergy[kcal/mol]    51.235668243481202
  ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
 RRHO          !         21
 Geometry[angstrom]          13
 C    0.60499  -0.00767  -0.99013
 C    0.60615   0.00556   0.48155
 C    1.67040   0.01052   1.28210
 C   -0.80441  -0.02530   0.88526
 C   -1.55522  -0.07630  -0.22820
 C   -0.67683  -0.07676  -1.40023
 H    1.49211  -0.03868  -1.60168
 H    0.91190   2.28002  -1.21277
 H    2.67526   0.02793   0.88108
 H    1.56316  -0.00188   2.35881
 H   -1.14679  -0.00930   1.90771
 H   -2.63298  -0.11198  -0.27155
 H   -1.01798  -0.12252  -2.42298
              Core           RigidRotor
          SymmetryFactor   0.50000000000000000
 End
    Frequencies[1/cm]          32
  3256.9     3250.7     3249.0     3234.4     3224.7     3159.4     1740.1
1635.8     1539.0     1462.2
  1384.9     1355.9     1267.0     1111.4     1107.0     1014.0     997.38
973.81     971.63     961.15
  916.56     814.49     807.62     802.37     720.80     683.25     649.00
502.60     345.63     219.04
  155.87     134.87
 ZeroEnergy[kcal/mol]    51.174544833241080
  ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    562.93209000000002
      WellDepth[kcal/mol]         50.32
      WellDepth[kcal/mol]          1.68
 End
End
Barrier TS7 W3 W5
 RRHO    ! transition state
 Geometry[angstrom]          13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.49284
 C    1.49168   0.00000   1.37127
 C   -0.55789   1.33896   1.83442
 C   -0.76143   2.03907   0.69711
 C   -0.40731   1.23625  -0.44301
 H    0.24117  -0.86160  -0.59919
 H   -0.41073  -0.86113   2.01327
 H    2.02045   0.93635   1.29592
 H    2.03372  -0.92975   1.29181
 H   -0.70985   1.68673   2.84401
 H   -1.10833   3.06052   0.64376
 H   -0.43220   1.56237  -1.47090
        Core    RigidRotor
              SymmetryFactor   0.50000000000000000
        End
    Frequencies[1/cm]          32
  288.26     428.25     516.16     582.71     609.49     738.86     745.25
792.38     827.43     872.86
  895.97     962.68     973.69     1027.2     1047.3     1089.9     1112.8
1119.7     1198.7     1295.0
  1332.5     1396.3     1427.4     1452.8     1583.7     3123.1     3174.4
3217.7     3235.2     3246.6
  3262.4     3295.0
ZeroEnergy[kcal/mol] 30.27879385419367
  ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
      Tunneling    Eckart
   ImaginaryFrequency[1/cm]      534.84569999999997
   WellDepth[kcal/mol]          6.90
   WellDepth[kcal/mol]         14.42
 End
 End
!************************************
Barrier TS8 W3 Pr1
 Variational
 RRHO          !          3
 Geometry[angstrom]          13
 C    0.58253  -0.20005  -1.00873
 C    0.58549  -0.18603   0.46593
 C    1.66570  -0.20345   1.26105
 C   -0.78933   0.17019   0.86306
 C   -1.49566   0.40060  -0.25526
 C   -0.63996   0.16961  -1.42277
 H    1.44196  -0.43432  -1.61607
 H    0.02337  -2.17356   0.44723
 H    2.65644  -0.36411   0.85737
 H    1.57632  -0.07276   2.33123
 H   -1.12345   0.25820   1.88432
 H   -2.52928   0.70701  -0.30502
 H   -0.95905   0.28303  -2.44749
              Core           RigidRotor
          SymmetryFactor   1.0000000000000000
 End
    Frequencies[1/cm]          32
  3257.8     3252.4     3251.6     3234.2     3224.3     3159.3     1682.8
1649.0     1558.5     1460.7
  1380.7     1347.7     1263.9     1112.9     1108.6     1013.7     974.71
972.30     969.69     960.59
  913.11     811.90     795.21     779.24     696.32     690.90     619.09
507.71     345.25     289.23
  245.62     40.520
 ZeroEnergy[kcal/mol]    53.545142819340950
  ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
```

RRHO ! 4
Geometry[angstrom] 13
C 0.58239 -0.20020 -1.00886
C 0.58505 -0.18787 0.46597
C 1.66610 -0.20311 1.26128
C -0.78952 0.17005 0.86300
C -1.49564 0.40082 -0.25538
C -0.64004 0.16985 -1.42277
H 1.44184 -0.43459 -1.61610
H 0.02805 -2.15848 0.44768
H 2.65677 -0.36368 0.85748
H 1.57661 -0.07232 2.33141
H -1.12355 0.25792 1.88429
H -2.52923 0.70730 -0.30511
H -0.95907 0.28334 -2.44749
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3257.9 3252.6 3251.8 3234.3 3224.4 3159.5 1678.6
1648.9 1558.2 1460.4
1380.4 1347.4 1263.8 1112.9 1108.5 1013.9 974.66
970.53 969.55 959.73
913.05 811.85 794.85 778.13 694.96 691.34 618.28
507.90 345.30 303.32
245.93 62.940
ZeroEnergy[kcal/mol] 53.683370801201531
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 5
Geometry[angstrom] 13
C 0.58225 -0.20034 -1.00899
C 0.58459 -0.18971 0.46599
C 1.66652 -0.20277 1.26153
C -0.78971 0.16992 0.86294
C -1.49562 0.40102 -0.25551
C -0.64012 0.17008 -1.42277
H 1.44174 -0.43484 -1.61611
H 0.03271 -2.14340 0.44811
H 2.65711 -0.36328 0.85760
H 1.57689 -0.07191 2.33159
H -1.12365 0.25766 1.88426
H -2.52919 0.70755 -0.30520
H -0.95910 0.28362 -2.44750
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3258.0 3252.9 3252.0 3234.4 3224.4 3159.6 1674.2
1648.9 1557.9 1460.1
1380.2 1347.2 1263.7 1112.9 1108.5 1014.0 974.60
969.42 968.83 958.50
913.01 811.83 794.50 776.96 693.45 691.80 617.50
508.08 345.37 319.11
246.19 83.480
ZeroEnergy[kcal/mol] 53.807947823614837
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 6
Geometry[angstrom] 13
C 0.58211 -0.20047 -1.00912
C 0.58411 -0.19155 0.46601
C 1.66696 -0.20244 1.26178
C -0.78990 0.16981 0.86288
C -1.49560 0.40122 -0.25564
C -0.64020 0.17031 -1.42277
H 1.44164 -0.43508 -1.61613
H 0.03734 -2.12832 0.44854
H 2.65746 -0.36290 0.85772
H 1.57718 -0.07153 2.33179
H -1.12373 0.25741 1.88424
H -2.52917 0.70777 -0.30529
H -0.95914 0.28386 -2.44750
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3258.1 3253.3 3252.2 3234.4 3224.5 3159.8 1669.6
1648.9 1557.6 1459.8
1379.9 1347.0 1263.6 1112.9 1108.4 1014.2 974.55
969.28 967.38 956.77
912.97 811.83 794.16 775.74 692.19 691.75 616.74
508.26 345.47 336.26
246.10 103.74
ZeroEnergy[kcal/mol] 53.926421300032187
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 7
Geometry[angstrom] 13
C 0.58198 -0.20057 -1.00925
C 0.58361 -0.19340 0.46601
C 1.66741 -0.20212 1.26205
C -0.79008 0.16971 0.86282
C -1.49559 0.40141 -0.25577
C -0.64028 0.17053 -1.42277
H 1.44155 -0.43531 -1.61613
H 0.04196 -2.11324 0.44895
H 2.65780 -0.36256 0.85784
H 1.57747 -0.07117 2.33199
H -1.12380 0.25717 1.88422
H -2.52915 0.70796 -0.30538
H -0.95919 0.28406 -2.44751
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3258.2 3253.7 3252.4 3234.5 3224.6 3159.9 1665.0
1648.9 1557.3 1459.4
1379.6 1346.8 1263.5 1112.8 1108.3 1014.4 974.48
969.14 966.22 954.46
912.95 811.87 793.82 774.50 692.52 689.87 615.96
508.42 354.52 345.62
245.68 123.89
ZeroEnergy[kcal/mol] 54.038776934736253
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 8
Geometry[angstrom] 13
C 0.58185 -0.20067 -1.00938
C 0.58310 -0.19525 0.46600
C 1.66787 -0.20180 1.26232
C -0.79026 0.16962 0.86276
C -1.49557 0.40159 -0.25590
C -0.64037 0.17074 -1.42277
H 1.44147 -0.43552 -1.61614
H 0.04657 -2.09816 0.44935
H 2.65815 -0.36224 0.85797
H 1.57776 -0.07084 2.33220
H -1.12386 0.25695 1.88420
H -2.52914 0.70811 -0.30547
H -0.95924 0.28424 -2.44751
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3258.3 3254.1 3252.5 3234.6 3224.6 3160.2 1660.3
1648.8 1557.0 1459.1
1379.2 1346.6 1263.5 1112.8 1108.2 1014.5 974.42
969.01 965.34 951.59

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 912.94  811.95  793.46  773.22  692.88  687.77  615.16
508.55  373.71  345.83
 245.50  143.99
ZeroEnergy[kcal/mol]  54.139468714708888
 ElectronicLevels[1/cm]  1
 0.0000000000000000  2.0000000000000000
End
!**********************************************
RRHO  !  9
Geometry[angstrom]  13
C  0.58173 -0.20075 -1.00951
C  0.58258 -0.19710  0.46597
C  1.66835 -0.20148  1.26261
C -0.79043  0.16955  0.86271
C -1.49556  0.40177 -0.25603
C -0.64046  0.17095 -1.42276
H  1.44139 -0.43573 -1.61613
H  0.05116 -2.08309  0.44973
H  2.65850 -0.36194  0.85811
H  1.57804 -0.07053  2.33242
H -1.12391  0.25673  1.88418
H -2.52913  0.70824 -0.30555
H -0.95931  0.28439 -2.44752
  Core  RigidRotor
  SymmetryFactor  1.0000000000000000
End
 Frequencies[1/cm]  32
 3258.4  3254.6  3252.7  3234.7  3224.6  3160.4  1655.6
1648.8  1556.7  1458.8
 1378.9  1346.5  1263.4  1112.8  1108.1  1014.7  974.34
968.88  964.67  948.20
 912.95  812.07  793.11  771.92  693.40  685.44  614.35
508.66  393.64  346.14
 245.82  163.84
ZeroEnergy[kcal/mol]  54.222421685388985
 ElectronicLevels[1/cm]  1
 0.0000000000000000  2.0000000000000000
End
!**********************************************
RRHO  !  10
Geometry[angstrom]  13
C  0.58157 -0.20079 -1.00966
C  0.58203 -0.19899  0.46596
C  1.66884 -0.20115  1.26291
C -0.79057  0.16948  0.86267
C -1.49554  0.40194 -0.25617
C -0.64054  0.17115 -1.42278
H  1.44124 -0.43590 -1.61613
H  0.05571 -2.06809  0.45011
H  2.65882 -0.36163  0.85825
H  1.57833 -0.07023  2.33261
H -1.12391  0.25651  1.88414
H -2.52915  0.70836 -0.30564
H -0.95936  0.28452 -2.44756
  Core  RigidRotor
  SymmetryFactor  1.0000000000000000
End
 Frequencies[1/cm]  32
 3258.7  3255.5  3253.1  3234.8  3224.6  3161.0  1651.0
1648.8  1556.3  1458.3
 1378.5  1346.3  1263.3  1112.8  1108.0  1014.8  974.27
968.66  964.10  944.24
 912.96  812.22  792.73  770.47  694.09  682.72  613.46
508.65  414.08  346.47
 246.37  183.10
ZeroEnergy[kcal/mol]  54.286806695168484
 ElectronicLevels[1/cm]  1
 0.0000000000000000  2.0000000000000000
End
!**********************************************
RRHO  !  11
Geometry[angstrom]  13
C  0.00000  0.00000  0.00000
C  0.00000  0.00000  1.47565
C  1.08792  0.00000  2.27299
C -1.37224  0.37030  1.87236
C -2.07702  0.60296  0.75347
C -1.22214  0.37220 -0.41297
H  0.85976 -0.23525 -0.60634
H -0.52120 -1.85221  1.46021
H  2.07777 -0.16055  1.86813
H  0.99718  0.13088  3.34264
H -1.70547  0.45717  2.89392
H -3.11064  0.90928  0.70405
H -1.54094  0.48546 -1.43775
  Core  RigidRotor
  SymmetryFactor  1.0000000000000000
End
 Frequencies[1/cm]  32
 3258.8  3256.1  3253.2  3234.8  3224.7  3161.4  1648.8
1646.4  1555.9  1458.0
 1378.2  1346.2  1263.3  1112.8  1108.0  1015.0  974.19
968.53  963.67  939.97
 912.97  812.45  792.42  769.15  694.96  679.86  612.64
508.64  435.05  347.11
 246.96  201.75
ZeroEnergy[kcal/mol]  54.338327009956591
 ElectronicLevels[1/cm]  1
 0.0000000000000000  2.0000000000000000
End
!**********************************************
RRHO  !  12
Geometry[angstrom]  13
C  0.58134 -0.20090 -1.00992
C  0.58088 -0.20270  0.46586
C  1.66988 -0.20054  1.26356
C -0.79090  0.16939  0.86255
C -1.49552  0.40227 -0.25644
C -0.64073  0.17154 -1.42277
H  1.44112 -0.43628 -1.61609
H  0.06482 -2.03801  0.45082
H  2.65955 -0.36115  0.85853
H  1.57892 -0.06971  2.33309
H -1.12398  0.25612  1.88411
H -2.52918  0.70850 -0.30582
H -0.95952  0.28469 -2.44758
  Core  RigidRotor
  SymmetryFactor  1.0000000000000000
End
 Frequencies[1/cm]  32
 3258.8  3256.8  3253.3  3234.9  3224.7  3161.7  1648.8
1642.1  1555.5  1457.6
 1377.9  1346.1  1263.2  1112.7  1107.9  1015.1  974.10
968.41  963.30  935.33
 912.93  812.73  792.11  767.84  695.94  676.74  611.81
508.58  456.55  348.05
 247.32  220.11
ZeroEnergy[kcal/mol]  54.364818424913655
 ElectronicLevels[1/cm]  1
 0.0000000000000000  2.0000000000000000
End
!**********************************************
RRHO  !  13
Geometry[angstrom]  13
C  0.58126 -0.20097 -1.01003
C  0.58028 -0.20453  0.46576
C  1.67043 -0.20026  1.26390
C -0.79109  0.16938  0.86247
C -1.49551  0.40244 -0.25659
C -0.64084  0.17173 -1.42275
H  1.44114 -0.43649 -1.61605
H  0.06936 -2.02296  0.45115
H  2.65995 -0.36096  0.85867
H  1.57920 -0.06948  2.33337
H -1.12404  0.25594  1.88412
H -2.52919  0.70852 -0.30591
H -0.95961  0.28473 -2.44756
  Core  RigidRotor
```

SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3258.7 3257.1 3253.1 3234.9 3224.8 3161.8 1648.8
1637.8 1555.1 1457.2
1377.6 1346.1 1263.3 1112.8 1107.9 1015.4 974.00
968.40 963.01 930.43
912.83 813.10 791.84 766.69 696.98 673.44 611.09
508.51 478.76 349.66
247.54 238.59
ZeroEnergy[kcal/mol] 54.373571030578146
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 14
Geometry[angstrom] 13
C 0.58115 -0.20100 -1.01015
C 0.57966 -0.20638 0.46567
C 1.67099 -0.19996 1.26425
C -0.79125 0.16937 0.86240
C -1.49551 0.40259 -0.25673
C -0.64094 0.17191 -1.42274
H 1.44109 -0.43666 -1.61601
H 0.07387 -2.00793 0.45147
H 2.66032 -0.36077 0.85882
H 1.57949 -0.06927 2.33363
H -1.12407 0.25577 1.88411
H -2.52923 0.70853 -0.30601
H -0.95971 0.28476 -2.44756
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3258.8 3257.8 3253.3 3234.9 3224.8 3162.2 1648.8
1633.6 1554.6 1456.9
1377.3 1346.1 1263.2 1112.7 1107.8 1015.5 973.91
968.29 962.72 925.21
912.45 813.53 791.46 765.42 698.06 669.69 610.41
508.24 501.51 352.17
257.02 247.51
ZeroEnergy[kcal/mol] 54.352134707762756
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 15
Geometry[angstrom] 13
C 0.58105 -0.20102 -1.01027
C 0.57902 -0.20823 0.46558
C 1.67156 -0.19967 1.26461
C -0.79140 0.16936 0.86235
C -1.49550 0.40275 -0.25687
C -0.64103 0.17209 -1.42274
H 1.44105 -0.43682 -1.61597
H 0.07836 -1.99292 0.45179
H 2.66069 -0.36060 0.85896
H 1.57978 -0.06907 2.33389
H -1.12408 0.25560 1.88410
H -2.52927 0.70852 -0.30610
H -0.95980 0.28476 -2.44757
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3258.9 3258.6 3253.3 3235.0 3224.8 3162.7 1648.9
1629.5 1554.1 1456.5
1376.9 1346.2 1263.2 1112.7 1107.8 1015.7 973.80
968.20 962.44 920.38
911.27 814.04 791.00 764.21 699.22 665.63 609.96
524.46 507.81 356.40
274.53 247.31
ZeroEnergy[kcal/mol] 54.306384270985288
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 16
Geometry[angstrom] 13
C 0.58095 -0.20104 -1.01039
C 0.57837 -0.21009 0.46547
C 1.67214 -0.19939 1.26498
C -0.79155 0.16936 0.86228
C -1.49550 0.40289 -0.25701
C -0.64114 0.17226 -1.42273
H 1.44102 -0.43698 -1.61593
H 0.08284 -1.97792 0.45210
H 2.66106 -0.36044 0.85911
H 1.58006 -0.06889 2.33415
H -1.12408 0.25544 1.88409
H -2.52931 0.70850 -0.30619
H -0.95990 0.28475 -2.44758
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3259.4 3259.0 3253.4 3235.0 3224.8 3163.3 1648.9
1625.7 1553.5 1456.1
1376.6 1346.3 1263.2 1112.7 1107.7 1015.9 973.70
968.11 962.19 917.33
907.99 814.63 790.47 763.05 700.61 661.30 610.10
546.92 507.19 363.46
289.73 247.00
ZeroEnergy[kcal/mol] 54.229672936989443
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 17
Geometry[angstrom] 13
C 0.58085 -0.20104 -1.01051
C 0.57771 -0.21194 0.46534
C 1.67273 -0.19911 1.26536
C -0.79170 0.16937 0.86223
C -1.49549 0.40303 -0.25715
C -0.64124 0.17243 -1.42272
H 1.44098 -0.43713 -1.61589
H 0.08731 -1.96291 0.45240
H 2.66142 -0.36029 0.85926
H 1.58034 -0.06872 2.33441
H -1.12408 0.25528 1.88408
H -2.52936 0.70845 -0.30628
H -0.96000 0.28472 -2.44759
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3260.3 3259.0 3253.5 3235.0 3224.8 3163.8 1649.0
1622.0 1552.9 1455.7
1376.2 1346.5 1263.3 1112.6 1107.6 1016.1 973.59
968.02 961.95 916.25
902.50 815.30 789.88 761.95 702.47 656.73 611.78
567.54 506.33 374.42
301.29 246.62
ZeroEnergy[kcal/mol] 54.115425401105666
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 18
Geometry[angstrom] 13
C 0.58076 -0.20104 -1.01063
C 0.57703 -0.21378 0.46521
C 1.67333 -0.19883 1.26574
C -0.79183 0.16939 0.86217
C -1.49549 0.40316 -0.25729
C -0.64134 0.17259 -1.42271
H 1.44095 -0.43727 -1.61584

```
H   0.09176  -1.94790   0.45270
H   2.66179  -0.36017   0.85941
H   1.58062  -0.06857   2.33468
H  -1.12408   0.25514   1.88408
H  -2.52942   0.70839  -0.30637
H  -0.96011   0.28468  -2.44760
         Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]         32
 3261.2    3259.1    3253.6    3235.1    3224.8    3164.5    1649.1
1618.7    1552.3    1455.4
 1375.9    1346.6    1263.3    1112.6    1107.6    1016.3    973.48
967.94    961.73    916.02
 896.05    816.06    789.23    760.93    705.11    651.97    617.62
583.22    505.18    389.45
 308.89    246.16
ZeroEnergy[kcal/mol]    53.957352273012146
 ElectronicLevels[1/cm]                1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO        !        19
Geometry[angstrom]          13
C   0.58066  -0.20103  -1.01074
C   0.57634  -0.21562   0.46508
C   1.67393  -0.19856   1.26613
C  -0.79197   0.16941   0.86211
C  -1.49549   0.40330  -0.25743
C  -0.64144   0.17275  -1.42271
H   1.44093  -0.43741  -1.61580
H   0.09621  -1.93290   0.45299
H   2.66215  -0.36005   0.85956
H   1.58090  -0.06843   2.33494
H  -1.12407   0.25499   1.88407
H  -2.52947   0.70832  -0.30645
H  -0.96022   0.28462  -2.44761
         Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]         32
 3262.1    3259.1    3253.7    3235.1    3224.8    3165.1    1649.2
1615.8    1551.6    1455.1
 1375.7    1346.9    1263.3    1112.5    1107.5    1016.5    973.36
967.86    961.51    916.12
 889.30    816.90    788.53    759.99    708.97    647.06    630.14
590.84    503.65    407.73
 313.36    245.60
ZeroEnergy[kcal/mol]    53.761628577291622
 ElectronicLevels[1/cm]                1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO        !        20
Geometry[angstrom]          13
C   0.58057  -0.20101  -1.01085
C   0.57564  -0.21746   0.46493
C   1.67454  -0.19829   1.26652
C  -0.79210   0.16944   0.86205
C  -1.49548   0.40342  -0.25757
C  -0.64155   0.17291  -1.42270
H   1.44090  -0.43754  -1.61575
H   0.10064  -1.91790   0.45327
H   2.66251  -0.35995   0.85971
H   1.58117  -0.06830   2.33521
H  -1.12406   0.25485   1.88407
H  -2.52953   0.70823  -0.30654
H  -0.96033   0.28454  -2.44762
         Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]         32
 3263.1    3259.2    3253.7    3235.1    3224.8    3165.8    1649.3
1613.2    1550.9    1454.8
 1375.4    1347.2    1263.4    1112.5    1107.5    1016.7    973.25
967.78    961.32    916.42
 882.61    817.84    787.74    759.13    714.70    645.75    642.10
593.04    501.67    428.25
 315.77    244.87
ZeroEnergy[kcal/mol]    53.521893445035344
 ElectronicLevels[1/cm]                1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO        !        21
Geometry[angstrom]          13
C   0.58049  -0.20099  -1.01096
C   0.57493  -0.21929   0.46477
C   1.67516  -0.19803   1.26692
C  -0.79222   0.16947   0.86199
C  -1.49548   0.40355  -0.25771
C  -0.64166   0.17306  -1.42269
H   1.44088  -0.43767  -1.61570
H   0.10507  -1.90290   0.45354
H   2.66287  -0.35985   0.85986
H   1.58144  -0.06819   2.33549
H  -1.12405   0.25471   1.88407
H  -2.52960   0.70814  -0.30662
H  -0.96045   0.28446  -2.44764
         Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
  Frequencies[1/cm]         32
 3264.1    3259.2    3253.8    3235.0    3224.8    3166.6    1649.4
1610.9    1550.2    1454.5
 1375.2    1347.5    1263.5    1112.4    1107.5    1017.0    973.13
967.70    961.13    916.87
 876.37    818.88    786.82    758.35    723.05    659.86    637.18
593.14    499.16    450.28
 316.90    243.93
ZeroEnergy[kcal/mol]    53.237718004721981
 ElectronicLevels[1/cm]                1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
   Tunneling    Eckart
   ImaginaryFrequency[1/cm]    900.77900000000000
   WellDepth[kcal/mol]        31.17
   WellDepth[kcal/mol]        4.55
End
End
Barrier TS9 W4 Pr1
 Variational
 RRHO        !        1
 Geometry[angstrom]          13
C   0.63490  -0.03026  -0.97458
C   0.63191  -0.03018   0.48202
C   1.69949  -0.02982   1.28661
C  -0.78077  -0.03444   0.89125
C  -1.53843  -0.02239  -0.21289
C  -0.66077   0.01124  -1.39943
H   1.51930  -0.04504  -1.59044
H   1.59199  -0.03583   2.36302
H   2.70396  -0.02517   0.88492
H  -1.11780  -0.03698   1.91583
H  -2.61610  -0.01381  -0.25695
H  -0.99914  -0.11677  -2.41546
H  -0.91938   1.89098  -1.76981
         Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
  Frequencies[1/cm]         32
 3257.8    3251.7    3251.1    3236.2    3229.1    3160.6    1694.1
1626.3    1495.6    1455.0
 1377.3    1352.6    1266.4    1112.3    1093.4    1002.3    982.16
973.16    971.25    961.93
 915.81    824.53    812.39    790.50    693.75    681.08    640.19
554.86    428.98    401.71
```

```
  346.59     207.01
 ZeroEnergy[kcal/mol]    51.561710460163050
  ElectronicLevels[1/cm]                   1
   0.0000000000000000        2.0000000000000000
 End
!***********************************************
 RRHO          !          2
 Geometry[angstrom]          13
 C    0.63449  -0.03019  -0.97496
 C    0.63189  -0.03015   0.48226
 C    1.69936  -0.02983   1.28651
 C   -0.78077  -0.03434   0.89142
 C   -1.53827  -0.02241  -0.21300
 C   -0.66022   0.00957  -1.39900
 H    1.51907  -0.04494  -1.59063
 H    1.59197  -0.03580   2.36297
 H    2.70385  -0.02518   0.88481
 H   -1.11783  -0.03687   1.91596
 H   -2.61596  -0.01393  -0.25703
 H   -0.99893  -0.11379  -2.41551
 H   -0.92108   1.90578  -1.77255
             Core          RigidRotor
        SymmetryFactor    0.50000000000000000
 End
    Frequencies[1/cm]          32
  3257.7     3251.5     3251.0     3236.2     3229.0     3160.4     1697.3
1626.2     1498.4     1455.8
  1377.5     1353.0     1266.6     1112.3     1094.3     1001.9     980.76
974.76     971.49     962.12
  916.02     823.71     812.59     791.51     694.33     681.14     640.44
548.42     413.21     385.74
  346.44     205.65
 ZeroEnergy[kcal/mol]    51.687821990821528
  ElectronicLevels[1/cm]                   1
   0.0000000000000000        2.0000000000000000
 End
!***********************************************
 RRHO          !          3
 Geometry[angstrom]          13
 C    0.63409  -0.03012  -0.97534
 C    0.63186  -0.03011   0.48250
 C    1.69923  -0.02984   1.28642
 C   -0.78076  -0.03424   0.89158
 C   -1.53811  -0.02244  -0.21310
 C   -0.65969   0.00791  -1.39857
 H    1.51885  -0.04483  -1.59081
 H    1.59196  -0.03577   2.36291
 H    2.70374  -0.02520   0.88470
 H   -1.11787  -0.03676   1.91609
 H   -2.61583  -0.01406  -0.25711
 H   -0.99872  -0.11084  -2.41555
 H   -0.92278   1.92062  -1.77528
             Core          RigidRotor
        SymmetryFactor    0.50000000000000000
 End
    Frequencies[1/cm]          32
  3257.6     3251.4     3250.8     3236.1     3228.9     3160.3     1700.4
1626.2     1501.4     1456.6
  1377.6     1353.5     1266.7     1112.2     1095.1     1001.7     979.63
976.52     971.60     962.14
  916.21     823.04     812.78     792.41     694.95     681.20     640.69
542.98     398.34     368.75
  346.10     204.16
 ZeroEnergy[kcal/mol]    51.790162644778428
  ElectronicLevels[1/cm]                   1
   0.0000000000000000        2.0000000000000000
 End
!***********************************************
 RRHO          !          4
 Geometry[angstrom]          13
 C    0.63370  -0.03007  -0.97570
 C    0.63182  -0.03008   0.48274
 C    1.69910  -0.02984   1.28633
 C   -0.78075  -0.03413   0.89174
 C   -1.53794  -0.02247  -0.21321
 C   -0.65918   0.00625  -1.39816
 H    1.51862  -0.04471  -1.59100
 H    1.59195  -0.03573   2.36286
 H    2.70363  -0.02522   0.88459
 H   -1.11790  -0.03663   1.91622
 H   -2.61569  -0.01420  -0.25719
 H   -0.99852  -0.10792  -2.41558
 H   -0.92447   1.93550  -1.77799
             Core          RigidRotor
        SymmetryFactor    0.50000000000000000
 End
    Frequencies[1/cm]          32
  3257.6     3251.3     3250.7     3236.1     3228.7     3160.2     1703.3
1626.3     1504.6     1457.3
  1377.8     1353.9     1266.8     1112.2     1096.0     1001.6     978.75
978.23     971.66     962.10
  916.38     822.47     812.94     793.23     695.57     681.28     640.92
538.40     384.00     352.54
  344.51     202.50
 ZeroEnergy[kcal/mol]    51.862514510298810
  ElectronicLevels[1/cm]                   1
   0.0000000000000000        2.0000000000000000
 End
!***********************************************
 RRHO          !          5
 Geometry[angstrom]          13
 C    0.63333  -0.03002  -0.97605
 C    0.63179  -0.03005   0.48296
 C    1.69898  -0.02985   1.28625
 C   -0.78074  -0.03402   0.89191
 C   -1.53777  -0.02252  -0.21331
 C   -0.65868   0.00460  -1.39776
 H    1.51840  -0.04457  -1.59119
 H    1.59194  -0.03569   2.36281
 H    2.70352  -0.02524   0.88448
 H   -1.11794  -0.03649   1.91635
 H   -2.61555  -0.01435  -0.25727
 H   -0.99831  -0.10505  -2.41560
 H   -0.92615   1.95042  -1.78070
             Core          RigidRotor
        SymmetryFactor    0.50000000000000000
 End
    Frequencies[1/cm]          32
  3257.5     3251.2     3250.5     3236.0     3228.6     3160.1     1706.0
1626.4     1507.9     1458.0
  1378.0     1354.3     1266.9     1112.1     1096.9     1001.5     979.96
977.94     971.70     962.05
  916.54     822.01     813.09     793.96     696.17     681.36     641.13
534.55     370.15     346.98
  332.24     200.69
 ZeroEnergy[kcal/mol]    51.917542142330634
  ElectronicLevels[1/cm]                   1
   0.0000000000000000        2.0000000000000000
 End
!***********************************************
 RRHO          !          6
 Geometry[angstrom]          13
 C    0.63297  -0.02997  -0.97639
 C    0.63175  -0.03003   0.48318
 C    1.69886  -0.02986   1.28617
 C   -0.78073  -0.03391   0.89207
 C   -1.53760  -0.02257  -0.21341
 C   -0.65819   0.00297  -1.39737
 H    1.51819  -0.04442  -1.59137
 H    1.59193  -0.03565   2.36277
 H    2.70341  -0.02527   0.88436
 H   -1.11799  -0.03633   1.91649
 H   -2.61540  -0.01450  -0.25736
 H   -0.99811  -0.10222  -2.41561
 H   -0.92783   1.96539  -1.78339
             Core          RigidRotor
        SymmetryFactor    0.50000000000000000
 End
```

Frequencies[1/cm] 32
3257.4 3251.1 3250.3 3235.9 3228.4 3160.0 1708.5
1626.6 1511.2 1458.6
1378.1 1354.6 1267.0 1112.1 1097.8 1001.6 981.52
977.30 971.71 961.99
916.68 821.64 813.21 794.61 696.76 681.44 641.32
531.32 357.37 345.46
315.59 198.71
ZeroEnergy[kcal/mol] 51.955059696547965
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 7
Geometry[angstrom] 13
C 0.63262 -0.02994 -0.97671
C 0.63171 -0.03000 0.48340
C 1.69875 -0.02987 1.28609
C -0.78073 -0.03379 0.89223
C -1.53743 -0.02262 -0.21351
C -0.65773 0.00134 -1.39700
H 1.51798 -0.04425 -1.59155
H 1.59193 -0.03560 2.36273
H 2.70330 -0.02530 0.88425
H -1.11803 -0.03617 1.91662
H -2.61526 -0.01466 -0.25745
H -0.99790 -0.09944 -2.41562
H -0.92951 1.98040 -1.78608
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.4 3251.0 3250.2 3235.8 3228.3 3159.9 1711.0
1626.9 1514.5 1459.1
1378.3 1354.9 1267.1 1112.0 1098.5 1001.6 982.97
976.75 971.70 961.91
916.77 821.34 813.29 795.18 697.32 681.51 641.46
528.61 349.58 339.65
299.07 196.55
ZeroEnergy[kcal/mol] 51.981013466055602
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 8
Geometry[angstrom] 13
C 0.63230 -0.02991 -0.97703
C 0.63167 -0.02997 0.48360
C 1.69863 -0.02987 1.28603
C -0.78072 -0.03367 0.89239
C -1.53726 -0.02269 -0.21360
C -0.65728 -0.00027 -1.39664
H 1.51778 -0.04407 -1.59173
H 1.59193 -0.03554 2.36269
H 2.70319 -0.02534 0.88414
H -1.11808 -0.03599 1.91675
H -2.61511 -0.01483 -0.25754
H -0.99770 -0.09674 -2.41562
H -0.93120 1.99546 -1.78875
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.3 3250.9 3250.1 3235.7 3228.1 3159.8 1713.2
1627.2 1517.7 1459.6
1378.5 1355.2 1267.2 1112.0 1099.3 1001.8 984.30
976.28 971.68 961.84
916.84 821.08 813.33 795.68 697.84 681.58 641.57
526.35 347.96 328.19
282.91 194.12
ZeroEnergy[kcal/mol] 51.982653121601176
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 9
Geometry[angstrom] 13
C 0.63199 -0.02989 -0.97732
C 0.63162 -0.02995 0.48380
C 1.69853 -0.02988 1.28596
C -0.78072 -0.03354 0.89255
C -1.53709 -0.02277 -0.21370
C -0.65684 -0.00186 -1.39630
H 1.51760 -0.04388 -1.59189
H 1.59193 -0.03548 2.36266
H 2.70308 -0.02538 0.88403
H -1.11814 -0.03579 1.91688
H -2.61497 -0.01501 -0.25764
H -0.99750 -0.09410 -2.41561
H -0.93292 2.01058 -1.79142
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.3 3250.8 3249.9 3235.6 3227.9 3159.7 1715.3
1627.5 1520.9 1460.1
1378.6 1355.4 1267.2 1112.0 1100.0 1001.9 985.51
975.88 971.65 961.79
916.89 820.84 813.34 796.12 698.33 681.66 641.65
524.46 347.47 316.22
267.22 191.36
ZeroEnergy[kcal/mol] 51.979018382758889
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 10
Geometry[angstrom] 13
C 0.63177 -0.02989 -0.97758
C 0.63154 -0.02992 0.48399
C 1.69844 -0.02990 1.28592
C -0.78075 -0.03341 0.89273
C -1.53696 -0.02285 -0.21382
C -0.65642 -0.00344 -1.39600
H 1.51750 -0.04369 -1.59203
H 1.59197 -0.03542 2.36264
H 2.70297 -0.02543 0.88393
H -1.11822 -0.03559 1.91708
H -2.61481 -0.01520 -0.25777
H -0.99732 -0.09154 -2.41561
H -0.93468 2.02575 -1.79408
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.2 3250.7 3249.9 3235.5 3227.8 3159.7 1717.0
1627.8 1523.7 1460.4
1378.8 1355.6 1267.3 1111.9 1100.6 1002.0 986.55
975.46 971.57 961.67
916.92 820.57 813.34 796.47 698.82 681.72 641.74
522.84 347.26 304.81
252.25 188.30
ZeroEnergy[kcal/mol] 51.956915753037615
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 11
Geometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.46203
C 1.06682 0.00000 2.26371
C -1.41220 -0.00337 1.87074
C -2.16824 0.00695 0.76399
C -1.28751 0.02492 -0.41778
H 0.88581 -0.01358 -0.61435
H 0.96045 -0.00545 3.34046
H 2.07136 0.00442 1.86166

H -1.74971 -0.00546 2.89502
H -3.24616 0.01449 0.72003
H -1.62862 -0.05923 -1.43769
H -1.56790 2.07089 -0.81882
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.2 3250.6 3249.8 3235.4 3227.7 3159.6 1718.8
1628.3 1526.7 1460.8
1378.9 1355.8 1267.3 1111.8 1101.2 1002.2 987.53
975.14 971.53 961.60
916.95 820.26 813.34 796.79 699.25 681.80 641.76
521.42 347.09 294.00
238.06 184.64
ZeroEnergy[kcal/mol] 51.930367880536567
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 12
Geometry[angstrom] 13
C 0.63123 -0.02991 -0.97811
C 0.63146 -0.02988 0.48433
C 1.69825 -0.02991 1.28581
C -0.78073 -0.03314 0.89304
C -1.53662 -0.02305 -0.21397
C -0.65567 -0.00653 -1.39538
H 1.51714 -0.04327 -1.59236
H 1.59199 -0.03528 2.36258
H 2.70277 -0.02553 0.88372
H -1.11830 -0.03514 1.91734
H -2.61452 -0.01561 -0.25793
H -0.99698 -0.08673 -2.41554
H -0.93819 2.05628 -1.79939
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.1 3250.6 3249.6 3235.3 3227.5 3159.6 1720.5
1628.8 1529.7 1461.1
1379.1 1356.0 1267.3 1111.8 1101.9 1002.4 988.42
974.89 971.49 961.59
916.97 819.95 813.33 797.07 699.67 681.88 641.78
520.16 346.95 283.78
224.76 180.28
ZeroEnergy[kcal/mol] 51.892427771934360
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 13
Geometry[angstrom] 13
C 0.63092 -0.02993 -0.97838
C 0.63145 -0.02987 0.48449
C 1.69816 -0.02990 1.28574
C -0.78069 -0.03300 0.89318
C -1.53643 -0.02317 -0.21402
C -0.65534 -0.00804 -1.39505
H 1.51689 -0.04304 -1.59257
H 1.59199 -0.03519 2.36253
H 2.70269 -0.02558 0.88360
H -1.11830 -0.03489 1.91740
H -2.61440 -0.01582 -0.25796
H -0.99683 -0.08448 -2.41549
H -0.93993 2.07159 -1.80202
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3257.0 3250.6 3249.4 3235.1 3227.1 3159.4 1722.2
1629.6 1532.7 1461.5
1379.3 1356.2 1267.4 1111.8 1102.5 1002.7 989.27
974.75 971.50 961.69
917.00 819.67 813.32 797.35 700.03 681.98 641.75
519.08 346.80 274.33
212.48 175.01
ZeroEnergy[kcal/mol] 51.850328334899986
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 14
Geometry[angstrom] 13
C 0.63068 -0.02997 -0.97861
C 0.63142 -0.02985 0.48464
C 1.69808 -0.02990 1.28569
C -0.78067 -0.03286 0.89333
C -1.53627 -0.02329 -0.21407
C -0.65502 -0.00953 -1.39477
H 1.51672 -0.04281 -1.59274
H 1.59200 -0.03510 2.36251
H 2.70260 -0.02563 0.88350
H -1.11833 -0.03463 1.91754
H -2.61426 -0.01605 -0.25801
H -0.99670 -0.08231 -2.41543
H -0.94170 2.08698 -1.80467
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3256.9 3250.5 3249.3 3235.0 3226.9 3159.3 1723.6
1630.2 1535.3 1461.7
1379.5 1356.3 1267.4 1111.8 1103.1 1002.9 989.99
974.69 971.52 961.92
917.02 819.43 813.32 797.58 700.40 682.07 641.78
518.17 346.71 265.90
201.34 168.99
ZeroEnergy[kcal/mol] 51.803326192129598
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 15
Geometry[angstrom] 13
C 0.63046 -0.03002 -0.97883
C 0.63138 -0.02984 0.48478
C 1.69801 -0.02990 1.28565
C -0.78066 -0.03272 0.89348
C -1.53611 -0.02343 -0.21413
C -0.65472 -0.01100 -1.39451
H 1.51656 -0.04257 -1.59290
H 1.59202 -0.03500 2.36249
H 2.70252 -0.02569 0.88341
H -1.11836 -0.03436 1.91767
H -2.61412 -0.01629 -0.25807
H -0.99657 -0.08022 -2.41538
H -0.94349 2.10243 -1.80731
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Frequencies[1/cm] 32
3256.9 3250.4 3249.2 3234.9 3226.8 3159.3 1724.9
1630.9 1537.8 1462.0
1379.7 1356.5 1267.4 1111.7 1103.6 1003.1 990.63
974.76 971.58 962.32
917.05 819.29 813.33 797.80 700.75 682.16 641.85
517.39 346.63 258.48
191.20 162.12
ZeroEnergy[kcal/mol] 51.752007468035908
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 16
Geometry[angstrom] 13
C 0.63026 -0.03009 -0.97904
C 0.63135 -0.02983 0.48492

```
C   1.69794  -0.02990   1.28561
C  -0.78065  -0.03256   0.89362
C  -1.53596  -0.02357  -0.21419
C  -0.65443  -0.01245  -1.39426
H   1.51642  -0.04233  -1.59305
H   1.59204  -0.03490   2.36247
H   2.70244  -0.02576   0.88331
H  -1.11839  -0.03407   1.91779
H  -2.61398  -0.01655  -0.25814
H  -0.99645  -0.07822  -2.41532
H  -0.94528   2.11791  -1.80994
            Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
  Frequencies[1/cm]        32
 3256.8    3250.4    3249.1    3234.7    3226.6    3159.2    1726.1
1631.6    1540.2    1462.2
 1379.8    1356.6    1267.4    1111.7    1104.1    1003.4    991.21
974.86    971.66    962.73
 917.08    819.15    813.34    798.01    701.08    682.25    641.91
516.67    346.55    251.98
 181.84    154.48
ZeroEnergy[kcal/mol]   51.689182142101979
 ElectronicLevels[1/cm]              1
 0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO         !         17
Geometry[angstrom]         13
C   0.63007  -0.03017  -0.97923
C   0.63131  -0.02981   0.48505
C   1.69787  -0.02990   1.28558
C  -0.78063  -0.03241   0.89377
C  -1.53580  -0.02373  -0.21424
C  -0.65416  -0.01388  -1.39402
H   1.51628  -0.04208  -1.59320
H   1.59206  -0.03478   2.36245
H   2.70236  -0.02584   0.88322
H  -1.11842  -0.03376   1.91792
H  -2.61385  -0.01682  -0.25820
H  -0.99633  -0.07630  -2.41526
H  -0.94709   2.13344  -1.81256
            Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
  Frequencies[1/cm]        32
 3256.8    3250.3    3249.0    3234.6    3226.4    3159.2    1727.3
1632.3    1542.4    1462.4
 1380.0    1356.7    1267.5    1111.7    1104.6    1003.6    991.73
974.77    971.69    962.89
 917.09    818.84    813.35    798.16    701.39    682.33    641.92
515.95    346.48    246.27
 173.08    146.03
ZeroEnergy[kcal/mol]   51.625570551712068
 ElectronicLevels[1/cm]              1
 0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO         !         18
Geometry[angstrom]         13
C   0.62989  -0.03026  -0.97942
C   0.63128  -0.02980   0.48518
C   1.69781  -0.02990   1.28555
C  -0.78062  -0.03225   0.89391
C  -1.53565  -0.02390  -0.21430
C  -0.65390  -0.01528  -1.39380
H   1.51616  -0.04183  -1.59333
H   1.59208  -0.03466   2.36244
H   2.70228  -0.02592   0.88314
H  -1.11846  -0.03344   1.91804
H  -2.61371  -0.01710  -0.25826
H  -0.99622  -0.07446  -2.41520
H  -0.94889   2.14902  -1.81517
            Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
  Frequencies[1/cm]        32
 3256.7    3250.3    3248.9    3234.5    3226.2    3159.1    1728.3
1633.1    1544.4    1462.5
 1380.1    1356.8    1267.5    1111.7    1105.0    1003.8    992.19
974.41    971.63    962.69
 917.09    818.29    813.34    798.25    701.67    682.42    641.82
515.24    346.41    241.29
 164.84    136.51
ZeroEnergy[kcal/mol]   51.559957560888948
 ElectronicLevels[1/cm]              1
 0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO         !         19
Geometry[angstrom]         13
C   0.62973  -0.03036  -0.97959
C   0.63125  -0.02979   0.48530
C   1.69775  -0.02989   1.28553
C  -0.78061  -0.03209   0.89405
C  -1.53550  -0.02409  -0.21435
C  -0.65365  -0.01666  -1.39359
H   1.51604  -0.04158  -1.59346
H   1.59211  -0.03453   2.36243
H   2.70220  -0.02601   0.88305
H  -1.11849  -0.03310   1.91816
H  -2.61358  -0.01739  -0.25832
H  -0.99611  -0.07272  -2.41513
H  -0.95070   2.16464  -1.81777
            Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
  Frequencies[1/cm]        32
 3256.6    3250.2    3248.9    3234.4    3226.0    3159.1    1729.3
1633.8    1546.3    1462.7
 1380.3    1356.9    1267.5    1111.7    1105.4    1004.0    992.60
974.03    971.54    962.36
 917.07    817.65    813.31    798.30    701.95    682.50    641.68
514.60    346.35    237.05
 157.05    126.01
ZeroEnergy[kcal/mol]   51.487311802440162
 ElectronicLevels[1/cm]              1
 0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO         !         20
Geometry[angstrom]         13
C   0.62958  -0.03048  -0.97975
C   0.63122  -0.02978   0.48542
C   1.69769  -0.02989   1.28550
C  -0.78060  -0.03193   0.89418
C  -1.53535  -0.02428  -0.21439
C  -0.65342  -0.01800  -1.39339
H   1.51593  -0.04133  -1.59358
H   1.59214  -0.03439   2.36243
H   2.70213  -0.02611   0.88297
H  -1.11853  -0.03275   1.91828
H  -2.61345  -0.01770  -0.25838
H  -0.99602  -0.07109  -2.41507
H  -0.95252   2.18030  -1.82037
            Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
  Frequencies[1/cm]        32
 3256.6    3250.2    3248.8    3234.3    3225.8    3159.0    1730.1
1634.6    1548.0    1462.8
 1380.4    1356.9    1267.5    1111.6    1105.7    1004.2    992.97
973.89    971.52    962.35
 917.05    817.22    813.27    798.37    702.22    682.58    641.61
514.06    346.29    233.56
 149.50    115.59
ZeroEnergy[kcal/mol]   51.417153498815560
 ElectronicLevels[1/cm]              1
```

```
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
 RRHO          !          21
 Geometry[angstrom]          13
 C    0.62944  -0.03061  -0.97989
 C    0.63119  -0.02977   0.48553
 C    1.69764  -0.02988   1.28549
 C   -0.78059  -0.03176   0.89431
 C   -1.53521  -0.02449  -0.21444
 C   -0.65321  -0.01932  -1.39320
 H    1.51583  -0.04109  -1.59369
 H    1.59217  -0.03425   2.36242
 H    2.70206  -0.02622   0.88290
 H   -1.11856  -0.03238   1.91839
 H   -2.61332  -0.01802  -0.25844
 H   -0.99592  -0.06958  -2.41500
 H   -0.95436   2.19602  -1.82296
            Core            RigidRotor
      SymmetryFactor   0.50000000000000000
 End
   Frequencies[1/cm]          32
  3256.5     3250.1     3248.7     3234.1     3225.7     3159.0     1730.9
1635.4     1549.6     1463.0
  1380.5     1357.0     1267.4     1111.6     1106.0     1004.4     993.30
974.03     971.63     962.81
  917.04     817.12     813.25     798.49     702.49     682.65     641.66
513.68     346.23     230.66
  141.92     106.07
 ZeroEnergy[kcal/mol]    51.344665718583494
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
     Tunneling    Eckart
     ImaginaryFrequency[1/cm]    630.71830000000000
     WellDepth[kcal/mol]          45.15
     WellDepth[kcal/mol]           1.93
 End
End
Barrier TS10 W5 W6
 RRHO     ! transition state
 Geometry[angstrom]          13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.46140
 C    1.50289   0.00000   1.27316
 C    2.14470   1.10408   0.74504
 C    1.38460   1.91724  -0.16635
 C    0.29557   1.27616  -0.64854
 H   -0.21227  -0.89957  -0.56186
 H   -0.36159  -0.90801   1.92986
 H   -0.39501   0.89561   1.94017
 H    2.05780  -0.85083   1.64393
 H    3.21125   1.23842   0.86351
 H    1.71487   2.88614  -0.50945
 H   -0.32181   1.65155  -1.45321
       Core    RigidRotor
          SymmetryFactor   0.50000000000000000
       End
   Frequencies[1/cm]          32
  353.60     400.61     530.86     601.40     661.05     709.14     742.02
812.86     859.76     920.12
  930.44     973.99     1033.7     1066.4     1103.9     1116.6     1179.7
1191.6     1212.4     1324.5
  1402.2     1418.2     1455.8     1492.6     1587.6     3069.5     3171.6
3190.4     3195.7     3205.3
  3207.8     3230.7
ZeroEnergy[kcal/mol] 33.79867720360777
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
     Tunneling    Eckart
   ImaginaryFrequency[1/cm]     752.16099999999994
   WellDepth[kcal/mol]          17.94
   WellDepth[kcal/mol]          36.75
 End
 End
!************************************
Barrier TS11 W6 Pr2
 Variational
 RRHO          !          1
 Geometry[angstrom]          13
 C   -1.20893   0.03006  -0.70929
 C   -1.21191   0.02900   0.66759
 C    0.00856   0.05047   1.37950
 C    1.21368  -0.10090   0.65732
 C    1.19919  -0.09882  -0.71949
 C   -0.00696  -0.01833  -1.41115
 H   -2.14554   0.05747  -1.24948
 H   -2.14319   0.06361   1.21474
 H    0.00285  -0.14033   2.44411
 H    0.09666   1.66643   1.76732
 H    2.14792  -0.16625   1.19653
 H    2.12879  -0.17128  -1.26754
 H   -0.01149  -0.01750  -2.49209
            Core            RigidRotor
      SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]          32
  3223.2     3215.7     3211.9     3197.6     3193.3     3186.4     1636.9
1615.9     1518.0     1506.5
  1384.6     1334.0     1205.2     1188.8     1174.7     1111.5     1065.3
1051.7     1032.0     1015.3
  1002.0     998.97     915.16     852.24     786.79     694.02     663.66
632.93     618.98     561.76
  404.92     339.92
 ZeroEnergy[kcal/mol]    22.736902307243850
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
 RRHO          !          2
 Geometry[angstrom]          13
 C   -1.20881   0.03011  -0.70944
 C   -1.21148   0.02917   0.66789
 C    0.00844   0.04847   1.37874
 C    1.21327  -0.10068   0.65763
 C    1.19907  -0.09876  -0.71964
 C   -0.00696  -0.01840  -1.41102
 H   -2.14546   0.05766  -1.24954
 H   -2.14288   0.06371   1.21491
 H    0.00303  -0.13689   2.44423
 H    0.09746   1.68121   1.77061
 H    2.14763  -0.16612   1.19670
 H    2.12873  -0.17107  -1.26760
 H   -0.01150  -0.01753  -2.49201
            Core            RigidRotor
      SymmetryFactor    1.0000000000000000
 End
   Frequencies[1/cm]          32
  3223.1     3215.6     3211.9     3197.7     3193.8     3187.0     1638.1
1617.7     1518.7     1507.1
  1384.8     1333.2     1205.3     1189.9     1174.9     1102.8     1065.7
1052.5     1031.4     1016.2
  1002.7     1000.0     914.55     853.38     780.37     695.47     636.64
630.40     619.24     555.92
  404.73     339.14
 ZeroEnergy[kcal/mol]    23.031010369834560
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
 RRHO          !          3
 Geometry[angstrom]          13
 C   -1.20869   0.03015  -0.70958
 C   -1.21105   0.02933   0.66819
 C    0.00834   0.04647   1.37798
 C    1.21286  -0.10047   0.65794
 C    1.19895  -0.09870  -0.71978
```

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C   -0.00696  -0.01848  -1.41090
H   -2.14538   0.05787  -1.24959
H   -2.14258   0.06382   1.21508
H    0.00322  -0.13345   2.44434
H    0.09827   1.69599   1.77389
H    2.14734  -0.16598   1.19688
H    2.12867  -0.17086  -1.26765
H   -0.01150  -0.01757  -2.49193
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
   Frequencies[1/cm]          32
  3223.0     3215.4     3211.8     3197.7     3194.4     3187.4     1639.3
1619.6     1519.3     1507.7
  1385.0     1332.5     1205.5     1190.9     1175.1     1095.4     1066.1
1053.3     1030.8     1017.0
  1003.4     1001.1     914.04     854.82     774.45     696.90     628.15
619.50     609.38     548.79
  404.47     337.52
ZeroEnergy[kcal/mol]    23.274703239828581
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
End
!***********************************************
RRHO          !           4
Geometry[angstrom]          13
C   -1.20857   0.03020  -0.70972
C   -1.21062   0.02950   0.66849
C    0.00822   0.04447   1.37723
C    1.21246  -0.10026   0.65823
C    1.19884  -0.09863  -0.71991
C   -0.00697  -0.01855  -1.41077
H   -2.14530   0.05808  -1.24965
H   -2.14227   0.06393   1.21526
H    0.00340  -0.13002   2.44443
H    0.09907   1.71079   1.77716
H    2.14705  -0.16584   1.19706
H    2.12861  -0.17064  -1.26771
H   -0.01150  -0.01760  -2.49185
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
   Frequencies[1/cm]          32
  3223.0     3215.3     3211.8     3197.7     3194.9     3187.7     1640.6
1621.5     1519.9     1508.3
  1385.2     1331.8     1205.7     1191.9     1175.2     1089.0     1066.5
1054.1     1030.3     1017.7
  1004.1     1002.3     913.58     856.42     769.13     698.32     626.30
619.75     582.29     540.59
  404.11     334.99
ZeroEnergy[kcal/mol]    23.468724294529748
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
End
!***********************************************
RRHO          !           5
Geometry[angstrom]          13
C   -1.20845   0.03025  -0.70985
C   -1.21020   0.02967   0.66878
C    0.00812   0.04246   1.37649
C    1.21206  -0.10005   0.65853
C    1.19873  -0.09857  -0.72005
C   -0.00697  -0.01863  -1.41066
H   -2.14521   0.05830  -1.24970
H   -2.14196   0.06405   1.21543
H    0.00359  -0.12660   2.44452
H    0.09988   1.72560   1.78042
H    2.14676  -0.16569   1.19723
H    2.12855  -0.17041  -1.26776
H   -0.01150  -0.01763  -2.49177
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
   Frequencies[1/cm]          32
  3222.9     3215.2     3211.8     3197.7     3195.3     3187.9     1641.8
1623.4     1520.5     1508.9
  1385.4     1331.3     1205.8     1192.9     1175.2     1083.6     1067.0
1054.8     1030.0     1018.3
  1004.7     1003.5     913.14     858.07     764.43     699.67     624.88
620.00     555.74     531.63
  403.59     331.52
ZeroEnergy[kcal/mol]    23.625866750342508
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
End
!***********************************************
RRHO          !           6
Geometry[angstrom]          13
C   -1.20834   0.03030  -0.70998
C   -1.20978   0.02984   0.66906
C    0.00801   0.04046   1.37577
C    1.21166  -0.09984   0.65881
C    1.19861  -0.09850  -0.72018
C   -0.00698  -0.01871  -1.41054
H   -2.14513   0.05853  -1.24975
H   -2.14165   0.06418   1.21561
H    0.00377  -0.12319   2.44459
H    0.10068   1.74043   1.78366
H    2.14647  -0.16553   1.19741
H    2.12849  -0.17017  -1.26781
H   -0.01150  -0.01767  -2.49170
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
   Frequencies[1/cm]          32
  3222.9     3215.0     3211.8     3197.7     3195.7     3188.0     1643.0
1625.3     1521.0     1509.5
  1385.6     1330.8     1206.0     1193.8     1175.3     1078.7     1067.4
1055.5     1029.8     1018.7
  1005.4     1004.6     912.69     859.72     760.33     700.93     623.82
620.24     530.07     522.25
  402.82     327.10
ZeroEnergy[kcal/mol]    23.733137250819110
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
End
!***********************************************
RRHO          !           7
Geometry[angstrom]          13
C   -1.20822   0.03036  -0.71011
C   -1.20937   0.03000   0.66933
C    0.00790   0.03846   1.37505
C    1.21127  -0.09964   0.65909
C    1.19850  -0.09844  -0.72030
C   -0.00698  -0.01879  -1.41043
H   -2.14505   0.05876  -1.24980
H   -2.14134   0.06431   1.21578
H    0.00395  -0.11981   2.44465
H    0.10149   1.75529   1.78690
H    2.14618  -0.16537   1.19758
H    2.12844  -0.16992  -1.26786
H   -0.01150  -0.01770  -2.49162
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
   Frequencies[1/cm]          32
  3222.8     3214.9     3211.8     3197.7     3196.1     3188.0     1644.2
1627.3     1521.5     1510.1
  1385.8     1330.5     1206.1     1194.7     1175.3     1073.9     1067.8
1056.2     1029.7     1018.9
  1006.0     1005.8     912.19     861.33     756.76     702.06     623.06
620.48     512.71     505.49
  401.63     321.66
ZeroEnergy[kcal/mol]    23.808717772490864
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
End
!***********************************************
```

```
RRHO ! 8
Geometry[angstrom] 13
C -1.20811 0.03041 -0.71023
C -1.20897 0.03016 0.66959
C 0.00779 0.03646 1.37436
C 1.21089 -0.09943 0.65935
C 1.19839 -0.09837 -0.72042
C -0.00698 -0.01887 -1.41033
H -2.14497 0.05901 -1.24985
H -2.14103 0.06446 1.21595
H 0.00413 -0.11647 2.44470
H 0.10230 1.77019 1.79013
H 2.14588 -0.16520 1.19776
H 2.12838 -0.16966 -1.26791
H -0.01150 -0.01774 -2.49155
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.8 3214.8 3211.7 3197.7 3196.3 3188.1 1645.2
1629.1 1522.0 1510.7
1386.0 1330.2 1206.2 1195.5 1175.3 1069.2 1068.2
1056.8 1029.7 1018.8
1006.9 1006.5 911.61 862.87 753.66 703.04 622.51
620.71 503.21 482.28
399.66 315.07
ZeroEnergy[kcal/mol] 23.852279513858049
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 9
Geometry[angstrom] 13
C -1.20799 0.03046 -0.71034
C -1.20856 0.03032 0.66984
C 0.00768 0.03448 1.37367
C 1.21051 -0.09924 0.65961
C 1.19828 -0.09830 -0.72053
C -0.00699 -0.01896 -1.41022
H -2.14488 0.05926 -1.24989
H -2.14072 0.06460 1.21612
H 0.00431 -0.11317 2.44472
H 0.10311 1.78513 1.79335
H 2.14559 -0.16503 1.19793
H 2.12832 -0.16940 -1.26794
H -0.01151 -0.01778 -2.49148
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.7 3214.6 3211.7 3197.7 3196.6 3188.0 1646.3
1631.0 1522.4 1511.3
1386.1 1330.1 1206.3 1196.4 1175.3 1068.6 1065.1
1057.3 1029.8 1018.6
1007.9 1007.1 910.94 864.33 750.97 703.91 622.15
620.93 494.06 461.05
396.16 307.20
ZeroEnergy[kcal/mol] 23.864565852224414
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 10
Geometry[angstrom] 13
C -1.20782 0.03052 -0.71041
C -1.20809 0.03042 0.67005
C 0.00760 0.03257 1.37290
C 1.21004 -0.09911 0.65983
C 1.19812 -0.09819 -0.72058
C -0.00701 -0.01904 -1.41006
H -2.14472 0.05952 -1.24989
H -2.14029 0.06475 1.21624
H 0.00451 -0.10987 2.44460
H 0.10391 1.80009 1.79656
H 2.14518 -0.16486 1.19807
H 2.12820 -0.16912 -1.26792
H -0.01151 -0.01781 -2.49132
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.9 3214.8 3212.0 3197.9 3197.0 3188.2 1647.7
1633.1 1522.9 1512.1
1386.3 1330.4 1206.4 1197.2 1175.4 1069.1 1061.9
1057.8 1030.0 1018.3
1009.1 1007.6 910.13 865.62 748.58 704.60 621.94
621.15 485.50 443.21
389.57 297.96
ZeroEnergy[kcal/mol] 23.849894094238861
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 11
Geometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.38079
C 1.21521 0.00000 2.08277
C 2.41744 -0.12950 1.37055
C 2.40578 -0.12871 -0.01017
C 1.20076 -0.04972 -0.69945
H -0.93691 0.02923 -0.53941
H -0.93227 0.03436 1.92693
H 1.21239 -0.13726 3.15512
H 1.31244 1.78457 2.51031
H 3.35264 -0.19522 1.90872
H 3.33588 -0.19940 -0.55744
H 1.19626 -0.04844 -1.78072
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.9 3214.6 3212.0 3197.8 3197.2 3188.2 1648.7
1634.8 1523.3 1512.7
1386.4 1330.3 1206.5 1197.9 1175.5 1069.4 1060.2
1057.3 1030.2 1018.0
1010.1 1008.1 909.33 866.91 746.55 705.34 621.84
621.35 477.90 430.74
378.39 287.72
ZeroEnergy[kcal/mol] 23.808120557402090
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 12
Geometry[angstrom] 13
C -1.20762 0.03063 -0.71062
C -1.20735 0.03073 0.67051
C 0.00739 0.02858 1.37162
C 1.20934 -0.09872 0.66030
C 1.19793 -0.09806 -0.72079
C -0.00702 -0.01923 -1.40989
H -2.14456 0.06010 -1.24998
H -2.13969 0.06513 1.21658
H 0.00485 -0.10349 2.44462
H 0.10554 1.83011 1.80302
H 2.14462 -0.16442 1.19841
H 2.12810 -0.16853 -1.26800
H -0.01152 -0.01791 -2.49121
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.8 3214.5 3211.9 3197.8 3197.2 3188.1 1649.8
1636.6 1523.7 1513.3
1386.5 1330.4 1206.6 1198.6 1175.5 1069.8 1060.0
1055.8 1030.4 1017.6
```

1011.2 1008.5 908.53 868.12 744.77 706.03 621.84
621.56 471.24 423.59
362.69 276.63
ZeroEnergy[kcal/mol] 23.743376704037031
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 13
Geometry[angstrom] 13
C -1.20758 0.03069 -0.71076
C -1.20707 0.03095 0.67077
C 0.00724 0.02652 1.37111
C 1.20911 -0.09846 0.66055
C 1.19789 -0.09803 -0.72095
C -0.00701 -0.01933 -1.40988
H -2.14458 0.06041 -1.25007
H -2.13951 0.06536 1.21680
H 0.00499 -0.10040 2.44476
H 0.10636 1.84510 1.80625
H 2.14447 -0.16415 1.19863
H 2.12813 -0.16822 -1.26812
H -0.01152 -0.01799 -2.49125
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.6 3214.1 3211.7 3197.5 3197.0 3187.8 1650.5
1637.9 1523.9 1513.9
1386.7 1330.1 1206.7 1199.2 1175.4 1070.0 1060.3
1054.1 1030.6 1017.3
1011.9 1009.0 907.75 869.32 743.29 706.75 621.90
621.75 465.60 419.94
344.79 265.14
ZeroEnergy[kcal/mol] 23.658506656576931
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 14
Geometry[angstrom] 13
C -1.20749 0.03075 -0.71086
C -1.20673 0.03112 0.67099
C 0.00713 0.02450 1.37052
C 1.20878 -0.09825 0.66077
C 1.19781 -0.09796 -0.72105
C -0.00701 -0.01944 -1.40982
H -2.14450 0.06075 -1.25012
H -2.13921 0.06560 1.21698
H 0.00515 -0.09729 2.44476
H 0.10718 1.86014 1.80945
H 2.14421 -0.16387 1.19880
H 2.12810 -0.16789 -1.26817
H -0.01152 -0.01806 -2.49120
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.5 3214.0 3211.7 3197.4 3197.0 3187.7 1651.5
1639.5 1524.2 1514.5
1386.8 1330.2 1206.8 1199.8 1175.5 1070.3 1060.7
1052.5 1030.8 1016.9
1012.9 1009.4 906.84 870.35 741.93 707.25 622.01
621.94 460.59 417.84
326.32 253.31
ZeroEnergy[kcal/mol] 23.566547383947109
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 15
Geometry[angstrom] 13
C -1.20739 0.03082 -0.71096
C -1.20639 0.03128 0.67119
C 0.00702 0.02250 1.36995
C 1.20846 -0.09805 0.66097
C 1.19772 -0.09789 -0.72115
C -0.00702 -0.01956 -1.40976
H -2.14443 0.06110 -1.25016
H -2.13891 0.06587 1.21716
H 0.00532 -0.09418 2.44474
H 0.10800 1.87519 1.81262
H 2.14393 -0.16356 1.19898
H 2.12806 -0.16753 -1.26822
H -0.01152 -0.01814 -2.49116
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.5 3213.9 3211.7 3197.4 3197.0 3187.6 1652.3
1641.1 1524.4 1515.1
1386.8 1330.4 1206.8 1200.3 1175.5 1070.5 1061.2
1050.8 1031.0 1016.4
1013.7 1009.7 905.85 871.30 740.74 707.59 622.15
622.12 456.06 416.60
308.16 241.37
ZeroEnergy[kcal/mol] 23.451174627550257
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 16
Geometry[angstrom] 13
C -1.20730 0.03088 -0.71105
C -1.20604 0.03143 0.67139
C 0.00691 0.02049 1.36938
C 1.20813 -0.09786 0.66117
C 1.19763 -0.09782 -0.72123
C -0.00702 -0.01967 -1.40970
H -2.14435 0.06148 -1.25020
H -2.13860 0.06615 1.21733
H 0.00548 -0.09112 2.44471
H 0.10882 1.89028 1.81578
H 2.14366 -0.16325 1.19916
H 2.12802 -0.16716 -1.26825
H -0.01153 -0.01822 -2.49112
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 32
3222.4 3213.8 3211.7 3197.3 3197.1 3187.5 1653.1
1642.7 1524.7 1515.7
1386.9 1330.7 1206.8 1200.9 1175.6 1070.8 1061.7
1049.1 1031.2 1015.9
1014.4 1010.0 904.77 872.17 739.69 707.76 622.30
622.28 451.85 415.80
290.36 229.20
ZeroEnergy[kcal/mol] 23.336359404131256
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 17
Geometry[angstrom] 13
C -1.20720 0.03096 -0.71113
C -1.20571 0.03158 0.67157
C 0.00680 0.01850 1.36884
C 1.20782 -0.09767 0.66136
C 1.19755 -0.09774 -0.72132
C -0.00703 -0.01980 -1.40965
H -2.14427 0.06188 -1.25023
H -2.13829 0.06645 1.21751
H 0.00564 -0.08811 2.44467
H 0.10965 1.90542 1.81893
H 2.14339 -0.16291 1.19934
H 2.12799 -0.16676 -1.26829
H -0.01153 -0.01830 -2.49108
Core RigidRotor

```
        SymmetryFactor    1.0000000000000000
End
    Frequencies[1/cm]         32
  3222.4      3213.7      3211.7      3197.3      3197.1      3187.5      1653.9
1644.2      1525.0      1516.3
  1387.0      1331.0      1206.8      1201.4      1175.7      1071.1      1062.2
1047.7      1031.3      1016.0
  1014.4      1010.3      903.68      872.97      738.76      707.84      622.46
622.41      448.01      415.27
  272.74      216.63
ZeroEnergy[kcal/mol]    23.203305021311328
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          18
Geometry[angstrom]          13
C   -1.20711   0.03103  -0.71121
C   -1.20539   0.03172   0.67174
C    0.00669   0.01652   1.36831
C    1.20752  -0.09750   0.66153
C    1.19746  -0.09767  -0.72140
C   -0.00704  -0.01992  -1.40960
H   -2.14419   0.06229  -1.25026
H   -2.13799   0.06676   1.21768
H    0.00580  -0.08519   2.44462
H    0.11048   1.92062   1.82207
H    2.14312  -0.16256   1.19951
H    2.12795  -0.16634  -1.26832
H   -0.01154  -0.01839  -2.49105
              Core            RigidRotor
        SymmetryFactor    1.0000000000000000
End
    Frequencies[1/cm]         32
  3222.4      3213.6      3211.7      3197.2      3197.0      3187.4      1654.7
1645.6      1525.2      1516.9
  1387.1      1331.3      1206.9      1201.9      1175.7      1071.3      1062.7
1046.6      1031.5      1016.5
  1014.1      1010.6      902.66      873.70      737.93      707.90      622.61
622.55      444.66      414.91
  255.33      203.78
ZeroEnergy[kcal/mol]    23.065347932755470
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          19
Geometry[angstrom]          13
C   -1.20702   0.03110  -0.71128
C   -1.20508   0.03185   0.67190
C    0.00659   0.01456   1.36781
C    1.20723  -0.09734   0.66170
C    1.19738  -0.09758  -0.72147
C   -0.00704  -0.02005  -1.40956
H   -2.14411   0.06272  -1.25029
H   -2.13769   0.06708   1.21784
H    0.00595  -0.08237   2.44456
H    0.11131   1.93587   1.82522
H    2.14286  -0.16220   1.19968
H    2.12792  -0.16592  -1.26835
H   -0.01154  -0.01848  -2.49102
              Core            RigidRotor
        SymmetryFactor    1.0000000000000000
End
    Frequencies[1/cm]         32
  3222.4      3213.4      3211.7      3197.2      3197.0      3187.3      1655.5
1647.0      1525.5      1517.4
  1387.1      1331.6      1206.9      1202.4      1175.8      1071.5      1063.2
1045.9      1031.6      1017.2
  1013.8      1010.8      901.72      874.36      737.20      707.97      622.77
622.71      441.76      414.67
  238.35      190.89
ZeroEnergy[kcal/mol]    22.916813463989099
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          20
Geometry[angstrom]          13
C   -1.20693   0.03118  -0.71136
C   -1.20479   0.03197   0.67206
C    0.00648   0.01261   1.36733
C    1.20694  -0.09718   0.66185
C    1.19730  -0.09750  -0.72154
C   -0.00705  -0.02018  -1.40952
H   -2.14404   0.06317  -1.25032
H   -2.13740   0.06742   1.21800
H    0.00609  -0.07964   2.44449
H    0.11214   1.95119   1.82837
H    2.14261  -0.16183   1.19984
H    2.12790  -0.16547  -1.26838
H   -0.01155  -0.01857  -2.49099
              Core            RigidRotor
        SymmetryFactor    1.0000000000000000
End
    Frequencies[1/cm]         32
  3222.3      3213.3      3211.7      3197.1      3197.0      3187.2      1656.2
1648.3      1525.7      1518.0
  1387.2      1332.0      1206.9      1202.8      1175.9      1071.8      1063.6
1045.3      1031.7      1017.9
  1013.7      1011.1      900.88      874.97      736.57      708.04      622.91
622.87      439.23      414.50
  221.92      178.05
ZeroEnergy[kcal/mol]    22.770080255612696
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          21
Geometry[angstrom]          13
C   -1.20684   0.03126  -0.71142
C   -1.20450   0.03208   0.67220
C    0.00637   0.01068   1.36687
C    1.20667  -0.09703   0.66199
C    1.19722  -0.09742  -0.72161
C   -0.00706  -0.02031  -1.40949
H   -2.14396   0.06363  -1.25034
H   -2.13712   0.06777   1.21816
H    0.00624  -0.07700   2.44442
H    0.11298   1.96656   1.83152
H    2.14236  -0.16145   1.20000
H    2.12787  -0.16501  -1.26840
H   -0.01155  -0.01866  -2.49098
              Core            RigidRotor
        SymmetryFactor    1.0000000000000000
End
    Frequencies[1/cm]         32
  3222.3      3213.3      3211.7      3197.1      3197.0      3187.2      1657.1
1649.7      1526.1      1518.7
  1388.8      1332.6      1207.0      1203.2      1176.0      1072.1      1064.2
1045.2      1031.9      1018.6
  1013.7      1011.4      901.26      876.57      736.11      708.24      623.56
623.52      437.01      414.43
  206.07      165.22
ZeroEnergy[kcal/mol]    22.622376389105460
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
     Tunneling    Eckart
     ImaginaryFrequency[1/cm]    947.24378999999999
     WellDepth[kcal/mol]         26.76
     WellDepth[kcal/mol]          5.35
End
End
End
```

A.1.2. H-Abstraction from Methylcyclopentadiene Reactions

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                      direct    ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                        diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!test!!!!!!!!!!!!!!!!!!!
!WellCutoff                  10
!ChemicalEigenvalueMin               1.e-6          #only for direct
diagonalization method
!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                1.3
!!
RateOutput                          rate.out                    ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                              ! Default collisional
energy relaxation kernel
    Exponential                                                 ! Currently the only
possible energy relaxation model
       Factor[1/cm]             316                             ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                0.535                          ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff                10                          ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                             ! Collision frequency
model
    LennardJones                                                ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                  90.58  281.367              ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]                 3.54    4.694                 ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                     39.948  79.05478              ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50263
 C    1.24622   0.00000   2.31947
 C   -1.27227   0.00046   1.92591
 C   -2.17585   0.00051   0.77474
 C   -1.45565   0.00011  -0.35294
 H    0.51979   0.87601  -0.40113
 H    1.85947   0.87812   2.10478
 H    1.01835  -0.00094   3.38445
 H    1.86045  -0.87709   2.10340
 H   -1.59049   0.00052   2.95892
 H   -3.25397   0.00095   0.84079
 H   -1.83452  -0.00013  -1.36297
 H    0.51979  -0.87591  -0.40126
        Core    RigidRotor
              SymmetryFactor    1.0000000000000000
        End
 Rotor                        Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.08    0.32    0.65    0.99    1.24    1.34    1.25    1.00    0.65    0.32
0.09
 End
    Frequencies[1/cm]           35
  3245.2      3221.6      3209.3      3128.8      3090.6      3074.8      3042.5
3036.2      1695.3      1615.6
  1495.0      1486.6      1424.0      1421.5      1397.2      1340.1      1274.6
1198.6      1152.9      1130.9
  1060.1      1033.7      1005.4      976.89      961.82      922.95      892.68
863.70      828.81      700.71
  623.69      533.08      369.88      325.94      227.72
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
 End
!************************************
 Fragment REACT2
  Atom
  Name H
  ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]          13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.41507
 C    1.18585   0.00000   2.30525
 C   -1.37924  -0.00034   1.86264
 C   -2.17195  -0.00056   0.76525
 C   -1.30652  -0.00033  -0.41759
 H    0.87955   0.00028  -0.62343
 H    2.11567   0.00259   1.73998
 H    1.17551   0.87449   2.96082
 H    1.17824  -0.87748   2.95691
```

```
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
      Core    RigidRotor
          SymmetryFactor    2.0000000000000000
      End
Rotor                       Hindered
Group    8   9  10
Axis            3          2
Symmetry           3
Potential[kcal/mol]          12
  0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
  Frequencies[1/cm]          32
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
!************************************
Fragment PROD2
RRHO
Geometry[angstrom]              2
H    0.00000   0.00000   0.00000
H    0.00000   0.00000   0.74312
      Core    RigidRotor
          SymmetryFactor    2.0000000000000000
      End
  Frequencies[1/cm]            1
 4433.4
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End

GroundEnergy[kcal/mol]   -23.54
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]              15
C   -0.00101   0.01760   0.01909
C   -0.00408   0.07105   1.52078
C    1.24046   0.09856   2.33962
C   -1.27712   0.08750   1.94115
C   -2.17840   0.04736   0.78868
C   -1.45584   0.00637  -0.33668
H    0.52036   0.87839  -0.41187
H    1.85684   0.96607   2.09300
H    1.01059   0.13861   3.40343
H    1.85256  -0.78790   2.15827
H   -1.59747   0.12470   2.97284
H   -3.25664   0.05090   0.85237
H   -1.83249  -0.02925  -1.34696
H    0.51912  -0.87220  -0.34991
H    0.16507  -5.33187   1.14988
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
  Frequencies[1/cm]          39
  7.2923      10.441      24.028      149.77      232.54      325.13      371.15
533.27      623.60      701.44
  828.95      863.98      892.50      923.19      962.23      977.14      1004.9
1033.5      1059.8      1130.9
  1152.9      1198.7      1274.6      1340.3      1397.5      1421.6      1424.5
1487.1      1495.2      1616.1
  1695.6      3035.5      3044.0      3076.1      3089.5      3128.8      3209.7
3221.9      3245.3
 ZeroEnergy[kcal/mol]            0.04
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]              15
C   -0.00197  -0.00055   0.00465
C   -0.00172  -0.00054   1.45324
C    1.20981   0.00076   2.30735
C   -1.34904  -0.03877   1.89031
C   -2.14857  -0.06264   0.77725
C   -1.29065  -0.03838  -0.41045
H    0.88177   0.02341  -0.61297
H    1.89239   0.80172   2.01569
H    0.96189   0.11657   3.36058
H    1.75782  -0.93816   2.18621
H   -1.66993  -0.04892   2.91938
H   -3.22717  -0.09427   0.76096
H   -1.64374  -0.04908  -1.42949
H   -0.50407  -2.73775   1.05934
H   -0.25479  -3.43579   1.13249
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
  Frequencies[1/cm]          39
  34.556      52.229      56.222      150.41      175.47      208.16      225.75
329.00      525.75      533.02
  605.22      638.07      730.62      741.88      902.14      924.22      931.45
955.24      1012.8      1022.4
  1051.7      1097.9      1179.2      1293.5      1311.4      1406.6      1438.2
1475.1      1484.8      1505.6
  1581.3      3032.0      3088.4      3139.2      3226.3      3234.1      3248.4
3256.4      4404.9
 ZeroEnergy[kcal/mol]            -24.19
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier        B1  REACS WR
  RRHO
    Stoichiometry  H9C6
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]              14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50263
C    1.24622   0.00000   2.31947
C   -1.27227   0.00046   1.92591
C   -2.17585   0.00051   0.77474
C   -1.45565   0.00011  -0.35294
H    0.51979   0.87601  -0.40113
H    1.85947   0.87812   2.10478
H    1.01835  -0.00094   3.38445
H    1.86045  -0.87709   2.10340
H   -1.59049   0.00052   2.95892
H   -3.25397   0.00095   0.84079
H   -1.83452  -0.00013  -1.36297
H    0.51979  -0.87591  -0.40126
      FragmentGeometry[angstrom]              1
H                   0. 0. 0.
                              SymmetryFactor     1.0000000000000000
          PotentialPrefactor[au]             10.
          PotentialPowerExponent            6
                    End
Rotor                       Hindered
Geometry[angstrom]              14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50263
```

```
C   1.24622  0.00000  2.31947
C  -1.27227  0.00046  1.92591
C  -2.17585  0.00051  0.77474
C  -1.45565  0.00011 -0.35294
H   0.51979  0.87601 -0.40113
H   1.85947  0.87812  2.10478
H   1.01835 -0.00094  3.38445
H   1.86045 -0.87709  2.10340
H  -1.59049  0.00052  2.95892
H  -3.25397  0.00095  0.84079
H  -1.83452 -0.00013 -1.36297
H   0.51979 -0.87591 -0.40126
Group   8  9  10
Axis          3         2
Symmetry          3
Potential[kcal/mol]         12
  0.0000    0.80000E-01 0.32000    0.65000    0.99000    1.2400    1.3400
1.2500    1.0000    0.65000
 0.32000    0.90000E-01
End
    Frequencies[1/cm]          35
  3245.2    3221.6    3209.3    3128.8    3090.6    3074.8    3042.5
3036.2    1695.3    1615.6
  1495.0    1486.6    1424.0    1421.5    1397.2    1340.1    1274.6
1198.6    1152.9    1130.9
  1060.1    1033.7    1005.4    976.89    961.82    922.95    892.68
863.70    828.81    700.71
  623.69    533.08    369.88    325.94    227.72
 ZeroEnergy[kcal/mol]          0.
 ElectronicLevels[1/cm]              1
  0.0000000000000000      4.0000000000000000
End
!************************************
Barrier       B3  WP PRODS
  RRHO
    Stoichiometry  H9C6
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]             13
C   0.00000  0.00000  0.00000
C   0.00000  0.00000  1.41507
C   1.18585  0.00000  2.30525
C  -1.37924 -0.00034  1.86264
C  -2.17195 -0.00056  0.76525
C  -1.30652 -0.00033 -0.41759
H   0.87955  0.00028 -0.62343
H   2.11567  0.00259  1.73998
H   1.17551  0.87449  2.96082
H   1.17824 -0.87748  2.95691
H  -1.69366 -0.00045  2.89442
H  -3.25029 -0.00080  0.74358
H  -1.65471 -0.00041 -1.43915
      FragmentGeometry[angstrom]             2
H   0.00000  0.00000  0.00000
H   0.00000  0.00000  0.74312
                        SymmetryFactor     4.0000000000000000
        PotentialPrefactor[au]             10.
        PotentialPowerExponent             6
                  End
Rotor                        Hindered
Geometry[angstrom]            13
C   0.00000  0.00000  0.00000
C   0.00000  0.00000  1.41507
C   1.18585  0.00000  2.30525
C  -1.37924 -0.00034  1.86264
C  -2.17195 -0.00056  0.76525
C  -1.30652 -0.00033 -0.41759
H   0.87955  0.00028 -0.62343
H   2.11567  0.00259  1.73998
H   1.17551  0.87449  2.96082
H   1.17824 -0.87748  2.95691
H  -1.69366 -0.00045  2.89442
H  -3.25029 -0.00080  0.74358
H  -1.65471 -0.00041 -1.43915
Group   8  9  10
```

```
Axis          3         2
Symmetry          3
Potential[kcal/mol]         12
  0.0000    0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01  0.0000    0.20000E-01 0.40000E-01 0.60000E-01
 0.40000E-01 0.10000E-01
End
    Frequencies[1/cm]          33
  3255.2    3247.0    3232.4    3224.7    3138.6    3086.9    3034.1
1584.1    1503.1    1481.1
  1477.9    1438.4    1407.4    1311.3    1292.6    1178.7    1098.1
1049.4    1023.5    1013.2
  953.40    929.99    923.03    899.45    740.46    727.81    638.42
604.77    528.85    520.52
  329.55    215.83
  4433.4
 ZeroEnergy[kcal/mol]          -23.540086481622119
 ElectronicLevels[1/cm]              1
  0.0000000000000000      4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO          !          1
Geometry[angstrom]          15
C   0.52967  0.04842 -0.99633
C   0.53733  0.03848  0.48800
C   1.77923  0.03955  1.30991
C  -0.74309  0.00155  0.89880
C  -1.63195  0.00824 -0.26418
C  -0.89304  0.04714 -1.38624
H   1.20850  0.72799 -1.50557
H   2.37925  0.93231  1.12063
H   1.54671  0.00705  2.37317
H   2.40602 -0.82315  1.07234
H  -1.07318 -0.02799  1.92704
H  -2.71026 -0.01190 -0.21328
H  -1.25359  0.06246 -2.40189
H   1.05779 -1.13202 -1.36587
H   1.46163 -1.91816 -1.60135
                 Core            RigidRotor
          SymmetryFactor    1.5000000000000000
End
 Rotor                        Hindered
 Group   8  9  10
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.31   0.95   1.30   0.98   0.33   0.00   0.30   0.95   1.30   0.98
0.33   0.00   0.28   0.94   1.30   0.96   0.31
 End
    Frequencies[1/cm]          37
  3253.7    3229.4    3216.8    3145.5    3131.8    3090.5    3036.7
1729.5    1665.9    1570.4
  1495.1    1486.5    1424.5    1387.5    1309.3    1269.5    1195.3
1146.9    1128.3    1077.8
  1037.4    1032.4    1001.9    965.07    957.10    916.49    880.04
858.86    795.79    730.74
  629.90    606.79    558.19    356.17    297.53    234.57    186.73
ZeroEnergy[kcal/mol]    3.0723966441278199
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
End
!*********************************************
RRHO          !          2
Geometry[angstrom]          15
C   0.53047  0.04726 -0.99682
C   0.53722  0.03858  0.48819
C   1.77921  0.03954  1.30994
C  -0.74304  0.00161  0.89877
C  -1.63192  0.00831 -0.26426
C  -0.89335  0.04723 -1.38614
H   1.20686  0.73098 -1.50424
H   2.37920  0.93231  1.12059
```

```
H   1.54677   0.00703   2.37321
H   2.40600  -0.82313   1.07230
H  -1.07319  -0.02810   1.92701
H  -2.71024  -0.01206  -0.21327
H  -1.25379   0.06224  -2.40185
H   1.05222  -1.11981  -1.36254
H   1.46389  -1.92278  -1.60271
           Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.95    1.30    0.98    0.33    0.00    0.30    0.95    1.30    0.98
0.33    0.00    0.28    0.94    1.30    0.96    0.31
 End
   Frequencies[1/cm]          37
  3253.5     3229.2     3216.6     3142.7     3131.8     3090.6     3036.8
1669.8     1621.3     1554.5
  1495.1     1486.5     1424.5     1387.4     1312.5     1269.7     1196.0
1169.8     1128.8     1083.7
  1047.2     1032.3     1003.6     966.28     958.77     920.87     884.43
860.25     799.43     731.26
  630.02     607.26     559.07     362.12     301.26     246.04     196.21
 ZeroEnergy[kcal/mol]    3.4827029880957516
  ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           3
Geometry[angstrom]          15
C   0.53122   0.04617  -0.99729
C   0.53711   0.03868   0.48837
C   1.77919   0.03954   1.30996
C  -0.74299   0.00166   0.89875
C  -1.63189   0.00837  -0.26433
C  -0.89365   0.04733  -1.38604
H   1.20527   0.73386  -1.50296
H   2.37915   0.93231   1.12054
H   1.54683   0.00700   2.37325
H   2.40599  -0.82311   1.07226
H  -1.07321  -0.02821   1.92699
H  -2.71022  -0.01221  -0.21325
H  -1.25398   0.06203  -2.40181
H   1.04670  -1.10770  -1.35926
H   1.46645  -1.92798  -1.60424
           Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.95    1.30    0.98    0.33    0.00    0.30    0.95    1.30    0.98
0.33    0.00    0.28    0.94    1.30    0.96    0.31
 End
   Frequencies[1/cm]          37
  3253.4     3229.0     3216.3     3139.8     3131.8     3090.6     3036.8
1670.3     1593.5     1495.2
  1490.9     1486.3     1424.4     1386.5     1315.7     1269.9     1199.2
1188.7     1128.8     1090.0
  1052.1     1032.3     1004.6     967.08     960.40     924.75     887.28
861.49     802.87     730.99
  629.91     606.43     559.51     367.25     304.03     255.19     203.04
 ZeroEnergy[kcal/mol]    3.8679818828837247
  ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           4
Geometry[angstrom]          15
C   0.53193   0.04515  -0.99774
C   0.53700   0.03877   0.48855
C   1.77917   0.03953   1.30998
C  -0.74295   0.00172   0.89873
C  -1.63186   0.00844  -0.26440
C  -0.89394   0.04742  -1.38594
H   1.20372   0.73665  -1.50170
H   2.37910   0.93231   1.12050
H   1.54688   0.00698   2.37329
H   2.40599  -0.82308   1.07223
H  -1.07323  -0.02831   1.92698
H  -2.71021  -0.01236  -0.21324
H  -1.25417   0.06182  -2.40177
H   1.04123  -1.09573  -1.35605
H   1.46927  -1.93371  -1.60593
           Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.95    1.30    0.98    0.33    0.00    0.30    0.95    1.30    0.98
0.33    0.00    0.28    0.94    1.30    0.96    0.31
 End
   Frequencies[1/cm]          37
  3253.3     3228.7     3216.1     3137.0     3131.8     3090.7     3036.8
1671.5     1590.7     1495.1
  1486.5     1431.4     1422.6     1381.9     1318.9     1270.1     1214.2
1194.5     1128.7     1095.6
  1054.3     1032.2     1005.3     967.65     961.96     927.85     889.20
862.57     806.09     729.92
  629.60     603.91     559.39     370.68     305.84     262.05     207.71
 ZeroEnergy[kcal/mol]    4.2128954743935045
  ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           5
Geometry[angstrom]          15
C   0.53261   0.04418  -0.99817
C   0.53689   0.03887   0.48872
C   1.77914   0.03953   1.31000
C  -0.74291   0.00177   0.89871
C  -1.63184   0.00850  -0.26446
C  -0.89421   0.04751  -1.38584
H   1.20219   0.73938  -1.50046
H   2.37905   0.93232   1.12046
H   1.54694   0.00696   2.37333
H   2.40598  -0.82306   1.07221
H  -1.07325  -0.02842   1.92696
H  -2.71020  -0.01251  -0.21321
H  -1.25436   0.06163  -2.40173
H   1.03585  -1.08391  -1.35291
H   1.47234  -1.93992  -1.60776
           Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.95    1.30    0.98    0.33    0.00    0.30    0.95    1.30    0.98
0.33    0.00    0.28    0.94    1.30    0.96    0.31
 End
   Frequencies[1/cm]          37
  3253.1     3228.5     3215.8     3134.2     3131.7     3090.7     3036.8
1672.8     1591.1     1495.2
  1486.5     1425.2     1401.6     1361.8     1322.0     1270.3     1233.1
1195.7     1128.4     1099.9
  1055.1     1032.2     1005.6     968.06     963.42     930.09     890.56
863.49     809.06     728.11
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 629.16    599.30    558.66    371.71    306.72    266.47    210.58
ZeroEnergy[kcal/mol]   4.5197446477978209
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO        !        6
Geometry[angstrom]        15
C   0.53327   0.04327  -0.99858
C   0.53678   0.03897   0.48889
C   1.77912   0.03952   1.31003
C  -0.74287   0.00182   0.89870
C  -1.63182   0.00856  -0.26451
C  -0.89448   0.04761  -1.38575
H   1.20067   0.74209  -1.49923
H   2.37900   0.93232   1.12043
H   1.54700   0.00694   2.37337
H   2.40598  -0.82304   1.07218
H  -1.07327  -0.02853   1.92695
H  -2.71019  -0.01266  -0.21319
H  -1.25455   0.06145  -2.40168
H   1.03057  -1.07228  -1.34986
H   1.47564  -1.94660  -1.60973
          Core         RigidRotor
     SymmetryFactor   1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.31   0.95   1.30   0.98   0.33   0.00   0.30   0.95   1.30   0.98
0.33   0.00   0.28   0.94   1.30   0.96   0.31
 End
   Frequencies[1/cm]        37
 3252.9    3228.2    3215.5    3131.9    3131.1    3090.7    3036.9
1674.2    1592.3    1495.2
 1486.6    1425.0    1396.8    1337.5    1324.4    1270.4    1251.4
1196.5    1128.2    1103.1
 1055.3    1032.1    1005.8    968.35    964.78    931.49    891.63
864.23    811.78    725.75
 628.64    592.31    557.29    369.95    306.60    268.30    211.94
ZeroEnergy[kcal/mol]   4.7730342961073111
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO        !        7
Geometry[angstrom]        15
C   0.53389   0.04240  -0.99897
C   0.53667   0.03907   0.48905
C   1.77910   0.03952   1.31005
C  -0.74283   0.00188   0.89868
C  -1.63180   0.00863  -0.26456
C  -0.89475   0.04771  -1.38565
H   1.19914   0.74478  -1.49799
H   2.37895   0.93232   1.12039
H   1.54706   0.00691   2.37341
H   2.40597  -0.82301   1.07216
H  -1.07329  -0.02864   1.92694
H  -2.71018  -0.01281  -0.21316
H  -1.25475   0.06127  -2.40164
H   1.02541  -1.06085  -1.34692
H   1.47916  -1.95374  -1.61183
          Core         RigidRotor
     SymmetryFactor   1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.31   0.95   1.30   0.98   0.33   0.00   0.30   0.95   1.30   0.98
0.33   0.00   0.28   0.94   1.30   0.96   0.31
 End
   Frequencies[1/cm]        37
 3252.8    3228.0    3215.3    3131.7    3128.5    3090.8    3036.9
1675.6    1593.8    1495.2
 1486.6    1425.0    1395.9    1330.6    1323.4    1270.6    1266.9
1197.2    1128.0    1105.4
 1055.3    1032.1    1005.7    968.56    966.01    932.22    892.61
864.77    814.24    723.07
 628.10    582.87    555.30    365.41    305.28    267.34    211.92
ZeroEnergy[kcal/mol]   4.9777243079275015
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO        !        8
Geometry[angstrom]        15
C   0.53450   0.04159  -0.99935
C   0.53656   0.03918   0.48921
C   1.77907   0.03951   1.31007
C  -0.74280   0.00193   0.89867
C  -1.63178   0.00869  -0.26461
C  -0.89500   0.04781  -1.38556
H   1.19758   0.74749  -1.49674
H   2.37891   0.93232   1.12035
H   1.54712   0.00689   2.37346
H   2.40597  -0.82298   1.07214
H  -1.07332  -0.02876   1.92692
H  -2.71018  -0.01297  -0.21313
H  -1.25495   0.06109  -2.40159
H   1.02040  -1.04967  -1.34410
H   1.48291  -1.96134  -1.61406
          Core         RigidRotor
     SymmetryFactor   1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.31   0.95   1.30   0.98   0.33   0.00   0.30   0.95   1.30   0.98
0.33   0.00   0.28   0.94   1.30   0.96   0.31
 End
   Frequencies[1/cm]        37
 3252.6    3227.7    3215.0    3131.7    3125.8    3090.8    3036.9
1677.0    1595.5    1495.2
 1486.6    1425.0    1395.8    1336.4    1329.8    1276.6    1270.2
1197.9    1128.1    1107.3
 1055.1    1032.0    1005.6    968.72    967.12    932.45    893.61
865.13    816.45    720.35
 627.57    571.39    552.61    358.61    302.40    263.39    210.46
ZeroEnergy[kcal/mol]   5.1225654043309978
 ElectronicLevels[1/cm]              1
 0.0000000000000000     2.0000000000000000
End
!*********************************************
RRHO        !        9
Geometry[angstrom]        15
C   0.53507   0.04083  -0.99971
C   0.53644   0.03928   0.48937
C   1.77904   0.03951   1.31010
C  -0.74277   0.00199   0.89865
C  -1.63177   0.00876  -0.26465
C  -0.89526   0.04792  -1.38546
H   1.19600   0.75024  -1.49546
H   2.37886   0.93233   1.12032
H   1.54719   0.00687   2.37350
H   2.40596  -0.82296   1.07212
H  -1.07334  -0.02887   1.92691
H  -2.71017  -0.01313  -0.21309
H  -1.25516   0.06092  -2.40153
H   1.01556  -1.03877  -1.34143
H   1.48689  -1.96941  -1.61644
          Core         RigidRotor
     SymmetryFactor   1.5000000000000000
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End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.95    1.30    0.98    0.33    0.00    0.30    0.95    1.30    0.98
0.33    0.00    0.28    0.94    1.30    0.96    0.31
 End
   Frequencies[1/cm]          37
  3252.4     3227.5     3214.8     3131.6     3123.1     3090.8     3036.9
1678.5     1597.2     1495.2
  1486.7     1425.1     1396.0     1363.6     1333.6     1281.7     1270.5
1198.5     1128.3     1108.9
  1055.0     1032.0     1005.4     968.89     968.06     932.29     894.67
865.35     818.41     717.78
  627.09     559.54     548.10     350.69     297.36     256.14     207.31
 ZeroEnergy[kcal/mol]    5.2290847597161436
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          10
Geometry[angstrom]          15
C    0.53562   0.04012  -1.00005
C    0.53626   0.03939   0.48956
C    1.77900   0.03951   1.31011
C   -0.74267   0.00204   0.89861
C   -1.63171   0.00883  -0.26473
C   -0.89555   0.04803  -1.38532
H    1.19432   0.75300  -1.49409
H    2.37878   0.93232   1.12028
H    1.54728   0.00685   2.37347
H    2.40589  -0.82287   1.07211
H   -1.07331  -0.02899   1.92679
H   -2.71013  -0.01329  -0.21307
H   -1.25538   0.06074  -2.40138
H    1.01092  -1.02821  -1.33891
H    1.49110  -1.97795  -1.61895
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.95    1.30    0.98    0.33    0.00    0.30    0.95    1.30    0.98
0.33    0.00    0.28    0.94    1.30    0.96    0.31
 End
   Frequencies[1/cm]          37
  3252.6     3227.5     3214.9     3132.3     3121.1     3091.1     3037.3
1680.3     1599.5     1495.2
  1486.7     1425.2     1406.9     1396.2     1336.0     1287.5     1271.0
1198.9     1128.7     1110.3
  1054.7     1031.9     1005.1     969.28     968.56     931.74     895.75
865.24     820.13     715.29
  626.65     552.12     537.51     343.10     289.67     245.13     201.77
 ZeroEnergy[kcal/mol]    5.2948099403017315
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          11
Geometry[angstrom]          15
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.49010
C    1.24283   0.00000   2.31053
C   -1.27880  -0.03740   1.89899
C   -2.16786  -0.03061   0.73563
C   -1.43195   0.00865  -0.38484
H    0.65645   0.71642  -0.49232
H    1.84259   0.89282   2.12063
H    1.01122  -0.03268   3.37391
H    1.86975  -0.86235   2.07249
H   -1.60950  -0.06862   2.92717
H   -3.24628  -0.05296   0.78737
H   -1.79177   0.02107  -1.40094
H    0.47059  -1.05787  -0.33641
H    0.95961  -2.02690  -0.62133
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.95    1.30    0.98    0.33    0.00    0.30    0.95    1.30    0.98
0.33    0.00    0.28    0.94    1.30    0.96    0.31
 End
   Frequencies[1/cm]          37
  3252.3     3227.3     3214.6     3132.2     3118.7     3091.1     3037.3
1681.6     1601.5     1495.2
  1487.1     1463.0     1424.8     1396.5     1337.9     1294.7     1271.5
1199.2     1129.1     1111.9
  1054.7     1031.9     1005.0     969.99     968.70     931.05     896.72
865.26     821.60     713.38
  626.29     548.81     523.08     337.40     280.31     230.82     193.73
 ZeroEnergy[kcal/mol]    5.3327628939702825
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          12
Geometry[angstrom]          15
C    0.53667   0.03889  -1.00072
C    0.53602   0.03963   0.48987
C    1.77894   0.03950   1.31018
C   -0.74264   0.00217   0.89861
C   -1.63172   0.00896  -0.26477
C   -0.89607   0.04828  -1.38512
H    1.19087   0.75886  -1.49132
H    2.37869   0.93232   1.12022
H    1.54744   0.00680   2.37358
H    2.40590  -0.82281   1.07209
H   -1.07340  -0.02923   1.92678
H   -2.71015  -0.01363  -0.21296
H   -1.25588   0.06041  -2.40126
H    1.00256  -1.00851  -1.33467
H    1.50040  -1.99683  -1.62448
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.95    1.30    0.98    0.33    0.00    0.30    0.95    1.30    0.98
0.33    0.00    0.28    0.94    1.30    0.96    0.31
 End
   Frequencies[1/cm]          37
  3252.1     3227.0     3214.4     3132.1     3116.1     3091.0     3037.3
1682.9     1605.2     1536.4
  1495.1     1486.3     1424.9     1396.8     1339.5     1303.0     1271.9
1199.3     1129.6     1113.0
  1054.4     1031.9     1004.8     970.68     968.69     930.04     897.64
865.16     822.90     711.64
  625.98     546.31     507.28     333.24     270.07     210.92     180.67
 ZeroEnergy[kcal/mol]    5.3421573562658429
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          13
Geometry[angstrom]          15
C    0.53717   0.03838  -1.00106
```

C 0.53597 0.03976 0.49001
C 1.77894 0.03950 1.31022
C -0.74272 0.00224 0.89865
C -1.63179 0.00903 -0.26473
C -0.89630 0.04842 -1.38506
H 1.18910 0.76199 -1.48992
H 2.37868 0.93234 1.12020
H 1.54751 0.00677 2.37374
H 2.40597 -0.82284 1.07208
H -1.07353 -0.02933 1.92689
H -2.71023 -0.01381 -0.21286
H -1.25615 0.06024 -2.40128
H 0.99897 -0.99957 -1.33305
H 1.50549 -2.00722 -1.62751
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.31 0.95 1.30 0.98 0.33 0.00 0.30 0.95 1.30 0.98
0.33 0.00 0.28 0.94 1.30 0.96 0.31
End
Frequencies[1/cm] 37
3251.4 3226.5 3213.7 3131.3 3113.2 3090.6 3036.8
1683.8 1634.1 1593.0
1495.2 1486.6 1425.0 1397.2 1340.8 1311.2 1272.2
1199.5 1130.0 1114.1
1054.3 1031.9 1004.7 971.29 968.70 929.00 898.35
865.19 823.98 710.42
625.74 544.47 492.59 330.71 261.57 187.56 163.44
ZeroEnergy[kcal/mol] 5.3407321364809510
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 14
Geometry[angstrom] 15
C 0.53763 0.03794 -1.00136
C 0.53585 0.03989 0.49016
C 1.77892 0.03950 1.31026
C -0.74273 0.00231 0.89866
C -1.63183 0.00910 -0.26473
C -0.89656 0.04857 -1.38496
H 1.18720 0.76515 -1.48841
H 2.37865 0.93234 1.12018
H 1.54761 0.00675 2.37381
H 2.40598 -0.82281 1.07208
H -1.07361 -0.02945 1.92690
H -2.71027 -0.01399 -0.21278
H -1.25643 0.06008 -2.40121
H 0.99576 -0.99123 -1.33170
H 1.51082 -2.01809 -1.63067
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.31 0.95 1.30 0.98 0.33 0.00 0.30 0.95 1.30 0.98
0.33 0.00 0.28 0.94 1.30 0.96 0.31
End
Frequencies[1/cm] 37
3251.1 3226.2 3213.5 3131.2 3111.0 3090.5 3036.7
1723.6 1683.7 1600.5
1495.2 1486.7 1425.0 1397.4 1341.8 1319.1 1272.4
1199.4 1130.4 1115.1
1054.0 1031.9 1004.5 971.84 968.58 927.82 898.91
864.94 824.89 709.20
625.53 542.72 478.69 328.91 254.84 160.28 140.51
ZeroEnergy[kcal/mol] 5.3123059331920492
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 15
Geometry[angstrom] 15
C 0.53806 0.03757 -1.00165
C 0.53572 0.04003 0.49031
C 1.77889 0.03950 1.31031
C -0.74275 0.00238 0.89867
C -1.63187 0.00918 -0.26473
C -0.89683 0.04872 -1.38485
H 1.18524 0.76839 -1.48685
H 2.37862 0.93234 1.12017
H 1.54772 0.00672 2.37389
H 2.40598 -0.82277 1.07208
H -1.07369 -0.02956 1.92691
H -2.71031 -0.01418 -0.21269
H -1.25673 0.05992 -2.40112
H 0.99300 -0.98357 -1.33069
H 1.51639 -2.02945 -1.63397
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.31 0.95 1.30 0.98 0.33 0.00 0.30 0.95 1.30 0.98
0.33 0.00 0.28 0.94 1.30 0.96 0.31
End
Frequencies[1/cm] 37
3250.9 3226.0 3213.2 3131.2 3109.0 3090.4 3036.7
1820.8 1685.1 1602.6
1495.2 1486.7 1425.0 1397.7 1342.6 1326.3 1272.5
1199.4 1130.7 1116.0
1053.8 1031.9 1004.4 972.32 968.44 926.72 899.34
864.66 825.65 708.18
625.36 541.19 466.13 327.67 249.78 129.81 110.89
ZeroEnergy[kcal/mol] 5.2664975882195639
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 16
Geometry[angstrom] 15
C 0.53846 0.03728 -1.00191
C 0.53559 0.04016 0.49046
C 1.77886 0.03951 1.31035
C -0.74277 0.00247 0.89869
C -1.63191 0.00926 -0.26471
C -0.89709 0.04888 -1.38474
H 1.18323 0.77170 -1.48524
H 2.37858 0.93234 1.12015
H 1.54783 0.00670 2.37397
H 2.40598 -0.82274 1.07208
H -1.07377 -0.02966 1.92692
H -2.71036 -0.01436 -0.21259
H -1.25705 0.05977 -2.40102
H 0.99072 -0.97660 -1.33002
H 1.52215 -2.04125 -1.63740
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.31 0.95 1.30 0.98 0.33 0.00 0.30 0.95 1.30 0.98
0.33 0.00 0.28 0.94 1.30 0.96 0.31
End

```
    Frequencies[1/cm]          37
   3250.6      3225.7      3213.0      3131.1      3107.2      3090.4      3036.6
1917.7      1686.0      1604.0
   1495.2      1486.7      1425.0      1397.9      1343.2      1332.9      1272.6
1199.3      1131.0      1117.0
   1053.7      1031.9      1004.2      972.74      968.29      925.76      899.67
864.38      826.27      707.32
   625.23      539.85      455.09      326.79      245.92      95.110      70.360
 ZeroEnergy[kcal/mol]    5.1936424712887677
  ElectronicLevels[1/cm]                    1
   0.0000000000000000        2.0000000000000000
 End
 !**********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1227.0799000000000
      WellDepth[kcal/mol]          5.45
      WellDepth[kcal/mol]         29.68
 End
End
End
```

```
!****************************************************
!             GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct    ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                            10
!ChemicalEigenvalueMin                 1.e-6          #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                  1.3
!!
RateOutput                            rate.out                   ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!             MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                           ! Default collisional
energy relaxation kernel
    Exponential                                              ! Currently the only
possible energy relaxation model
       Factor[1/cm]              316                         ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                  0.535                          ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff            10                          ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                         ! Collision frequency
model
    LennardJones                                             ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]               90.58  281.367              ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]          3.54    4.694               ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]               39.948  79.05478            ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REACT1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50263
 C    1.24622   0.00000   2.31948
 C   -1.27228   0.00030   1.92591
 C   -2.17585   0.00031   0.77474
 C   -1.45565   0.00001  -0.35294
 H    0.51977   0.87599  -0.40120
 H    1.85912   0.87851   2.10535
 H    1.01836  -0.00170   3.38445
 H    1.86080  -0.87670   2.10283
 H   -1.59050   0.00020   2.95892
 H   -3.25397   0.00072   0.84079
 H   -1.83450  -0.00027  -1.36298
 H    0.51981  -0.87594  -0.40119
        Core    RigidRotor
             SymmetryFactor    1.0000000000000000
        End
 Rotor                       Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          3
 Potential[kcal/mol]          12
   0.00    0.08    0.30    0.62    0.95    1.20    1.29    1.21    0.95    0.62    0.30
0.08
 End
    Frequencies[1/cm]          35
   3245.1     3221.6     3209.3     3128.8     3090.6     3074.8     3042.5
3036.2     1695.3     1615.6
   1495.0     1486.6     1424.0     1421.5     1397.2     1340.1     1274.6
1198.6     1152.9     1130.9
   1060.1     1033.7     1005.4     976.88     961.83     922.95     892.68
863.70     828.81     700.71
   623.69     533.07     369.88     325.94     227.71
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                  1
   0.0000000000000000        2.0000000000000000
 End
!************************************
 Fragment REACT2
  Atom
  Name H
  ElectronicLevels[1/cm]                  1
   0.0000000000000000        2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]          13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.51694
 C    1.09843   0.00000   2.30770
 C   -1.35798   0.00031   1.92840
 C   -2.19992   0.00042   0.79313
 C   -1.45663   0.00024  -0.34805
 H    0.51600  -0.87687  -0.39945
 H    0.51620   0.87681  -0.39935
 H    2.09538  -0.00023   1.88922
 H    1.00817   0.00002   3.38527
```

```
H -1.68677 0.00025 2.95662
H -3.27947 0.00064 0.83092
H -1.83825 0.00021 -1.35705
    Core RigidRotor
       SymmetryFactor 1.0000000000000000
    End
  Frequencies[1/cm] 33
 182.10 356.98 395.70 533.46 629.59 643.35 680.57
792.84 824.96 845.75
 867.02 937.43 954.59 969.91 992.63 1039.9 1117.1
1156.6 1270.0 1282.1
 1315.8 1407.1 1426.7 1447.0 1530.6 1581.6 3052.2
3085.2 3159.4 3215.5
 3230.8 3244.8 3250.3
 ZeroEnergy[kcal/mol] 0.
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End

!************************************
Fragment PROD2
RRHO
Geometry[angstrom] 2
H 0.00000 0.00000 0.00000
H 0.00000 0.00000 0.74312
    Core RigidRotor
       SymmetryFactor 2.0000000000000000
    End
  Frequencies[1/cm] 1
 4433.4
 ZeroEnergy[kcal/mol] 0.
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End

GroundEnergy[kcal/mol] -22.18
End
!************************************
Well WR
Species
RRHO ! transition state
Geometry[angstrom] 15
C -0.01763 0.06595 -0.00416
C -0.01812 0.05629 1.49843
C 1.22769 0.03407 2.31547
C -1.29031 0.07099 1.92143
C -2.19349 0.09069 0.76989
C -1.47294 0.08803 -0.35748
H 0.51427 0.93726 -0.39965
H 1.85340 0.90468 2.10601
H 0.99969 0.03000 3.38042
H 1.82969 -0.85025 2.09428
H -1.60886 0.06874 2.95434
H -3.27153 0.10500 0.83561
H -1.85129 0.09963 -1.36769
H 0.49051 -0.81422 -0.41105
H 0.39679 -5.43381 1.42177
    Core RigidRotor
       SymmetryFactor 0.50000000000000000
    End
  Frequencies[1/cm] 38
 9.5990 20.775 151.99 232.67 325.10 370.95 533.29
623.59 701.49 828.91
 863.82 892.51 922.94 962.16 977.15 1004.9 1033.6
1059.8 1130.9 1152.8
 1198.7 1274.5 1340.2 1397.5 1421.4 1424.5 1487.4
1495.3 1616.2 1695.6
 3035.4 3044.1 3076.2 3089.2 3129.0 3209.5 3221.8
3245.3
 ZeroEnergy[kcal/mol] 0.03
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
 End
End
```

```
!************************************
Well WP
Species
RRHO ! transition state
Geometry[angstrom] 15
C -0.00099 0.00021 0.00411
C -0.00073 0.00055 1.52053
C 1.09820 0.00097 2.31118
C -1.35815 -0.00502 1.93262
C -2.20059 -0.00675 0.79731
C -1.45719 -0.00356 -0.34371
H 0.51500 0.87608 -0.39724
H 2.09484 0.00276 1.89212
H 1.00829 -0.00102 3.38873
H -0.80090 -2.73094 0.94961
H -1.68657 -0.00707 2.96099
H -3.28007 -0.01184 0.83522
H -1.83895 -0.00673 -1.35257
H 0.51376 -0.87896 -0.39266
H -0.55934 -3.34362 0.60275
    Core RigidRotor
       SymmetryFactor 0.50000000000000000
    End
  Frequencies[1/cm] 38
 80.027 113.29 180.25 195.00 283.59 356.91 407.46
535.09 628.82 643.59
 682.77 795.08 825.25 846.25 867.70 940.19 955.07
971.06 993.17 1040.2
 1117.5 1157.3 1270.6 1282.4 1316.8 1407.3 1426.7
1453.6 1531.3 1580.3
 3052.9 3086.3 3159.9 3216.1 3231.1 3245.5 3251.1
4414.6
 ZeroEnergy[kcal/mol] -22.55
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
End
!************************************
Barrier B1 REACS WR
 RRHO
  Stoichiometry H9C6
  Core PhaseSpaceTheory
   FragmentGeometry[angstrom] 14
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.50263
C 1.24622 0.00000 2.31948
C -1.27228 0.00030 1.92591
C -2.17585 0.00031 0.77474
C -1.45565 0.00001 -0.35294
H 0.51977 0.87599 -0.40120
H 1.85912 0.87851 2.10535
H 1.01836 -0.00170 3.38445
H 1.86080 -0.87670 2.10283
H -1.59050 0.00020 2.95892
H -3.25397 0.00072 0.84079
H -1.83450 -0.00027 -1.36298
H 0.51981 -0.87594 -0.40119
   FragmentGeometry[angstrom] 1
H 0. 0. 0.
              SymmetryFactor 1.0000000000000000
     PotentialPrefactor[au] 10.
     PotentialPowerExponent 6
        End
Rotor Hindered
Geometry[angstrom] 14
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.50263
C 1.24622 0.00000 2.31948
C -1.27228 0.00030 1.92591
C -2.17585 0.00031 0.77474
C -1.45565 0.00001 -0.35294
H 0.51977 0.87599 -0.40120
H 1.85912 0.87851 2.10535
H 1.01836 -0.00170 3.38445
```

H 1.86080 -0.87670 2.10283
H -1.59050 0.00020 2.95892
H -3.25397 0.00072 0.84079
H -1.83450 -0.00027 -1.36298
H 0.51981 -0.87594 -0.40119
Group 8 9 10
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.0000 0.80000E-01 0.30000 0.62000 0.95000 1.2000 1.2900
1.2100 0.95000 0.62000
0.30000 0.80000E-01
End
Frequencies[1/cm] 35
3245.1 3221.6 3209.3 3128.8 3090.6 3074.8 3042.5
3036.2 1695.3 1615.6
1495.0 1486.6 1424.0 1421.5 1397.2 1340.1 1274.6
1198.6 1152.9 1130.9
1060.1 1033.7 1005.4 976.88 961.83 922.95 892.68
863.70 828.81 700.71
623.69 533.07 369.88 325.94 227.71
ZeroEnergy[kcal/mol] 0.
ElectronicLevels[1/cm] 1
0.0000000000000000 4.0000000000000000
End
!************************************
Barrier B3 WP PRODS
RRHO
Stoichiometry H9C6
Core PhaseSpaceTheory
FragmentGeometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.51694
C 1.09843 0.00000 2.30770
C -1.35798 0.00031 1.92840
C -2.19992 0.00042 0.79313
C -1.45663 0.00024 -0.34805
H 0.51600 -0.87687 -0.39945
H 0.51620 0.87681 -0.39935
H 2.09538 -0.00023 1.88922
H 1.00817 0.00002 3.38527
H -1.68677 0.00025 2.95662
H -3.27947 0.00064 0.83092
H -1.83825 0.00021 -1.35705
FragmentGeometry[angstrom] 2
H 0.00000 0.00000 0.00000
H 0.00000 0.00000 0.74312
SymmetryFactor 2.0000000000000000
PotentialPrefactor[au] 10.
PotentialPowerExponent 6
End
Frequencies[1/cm] 34
182.10 356.98 395.70 533.46 629.59 643.35 680.57
792.84 824.96 845.75
867.02 937.43 954.59 969.91 992.63 1039.9 1117.1
1156.6 1270.0 1282.1
1315.8 1407.1 1426.7 1447.0 1530.6 1581.6 3052.2
3085.2 3159.4 3215.5
3230.8 3244.8 3250.3
4433.4
ZeroEnergy[kcal/mol] -22.178170779922215
ElectronicLevels[1/cm] 1
0.0000000000000000 4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO ! 1
Geometry[angstrom] 15
C 0.52982 0.06516 -1.05631
C 0.53492 0.06488 0.44783
C 1.73936 0.07479 1.25204
C -0.75160 0.00001 0.87064
C -1.64605 -0.02922 -0.27597
C -0.92357 0.00583 -1.40610
H 1.01444 0.95842 -1.46157
H 2.56202 0.66570 0.85849
H 1.58422 0.23968 2.31415
H 2.29823 -1.16086 1.22902
H -1.06791 -0.02162 1.90346
H -2.72328 -0.07114 -0.21263
H -1.30372 -0.00144 -2.41561
H 1.08334 -0.79267 -1.45206
H 2.70994 -1.97668 1.23560
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.3 3226.4 3215.2 3187.7 3107.5 3078.5 3044.1
1817.8 1635.2 1512.6
1472.4 1424.4 1396.2 1350.7 1279.9 1216.6 1191.2
1182.4 1146.0 1130.2
1033.9 1010.0 995.63 978.08 963.76 916.81 895.81
875.08 829.38 705.57
666.01 634.45 543.90 446.47 336.69 303.32 167.13
ZeroEnergy[kcal/mol] 3.6025631516111742
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 2
Geometry[angstrom] 15
C 0.52975 0.06514 -1.05626
C 0.53427 0.06488 0.44765
C 1.74039 0.07355 1.25233
C -0.75130 0.00012 0.87062
C -1.64608 -0.02921 -0.27616
C -0.92365 0.00583 -1.40609
H 1.01440 0.95846 -1.46145
H 2.56060 0.66845 0.85909
H 1.58373 0.24153 2.31387
H 2.29232 -1.14809 1.22914
H -1.06773 -0.02160 1.90344
H -2.72330 -0.07118 -0.21271
H -1.30373 -0.00143 -2.41563
H 1.08333 -0.79264 -1.45205
H 2.71173 -1.98040 1.23554
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.3 3226.3 3215.0 3185.3 3105.6 3078.5 3044.1
1701.5 1631.9 1515.2
1472.3 1424.0 1397.4 1350.7 1280.2 1227.7 1204.6
1201.9 1146.4 1130.4
1035.7 1012.5 1002.9 978.32 964.57 917.32 896.05
877.51 829.40 705.73
666.67 635.51 544.16 449.56 336.82 307.32 178.25
ZeroEnergy[kcal/mol] 4.0666349633215004
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End

```
!*********************************************
RRHO          !           3
Geometry[angstrom]          15
C   0.52967   0.06513  -1.05621
C   0.53364   0.06489   0.44749
C   1.74137   0.07237   1.25260
C  -0.75100   0.00023   0.87061
C  -1.64612  -0.02921  -0.27634
C  -0.92372   0.00581  -1.40608
H   1.01437   0.95850  -1.46133
H   2.55921   0.67111   0.85967
H   1.58324   0.24335   2.31360
H   2.28643  -1.13537   1.22925
H  -1.06757  -0.02157   1.90342
H  -2.72332  -0.07123  -0.21279
H  -1.30374  -0.00141  -2.41565
H   1.08331  -0.79260  -1.45205
H   2.71383  -1.98475   1.23548
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.17    0.70    1.59    2.78    4.07    5.12    2.24    1.61    1.01    0.50
0.13
 End
   Frequencies[1/cm]          37
  3247.4     3226.2     3214.9     3182.8     3103.6     3078.5     3044.2
1652.8     1593.5     1508.0
  1472.2     1423.6     1398.6     1350.8     1280.7     1243.8     1224.0
1205.8     1146.6     1130.6
  1037.5     1016.6     1007.0     978.52     965.08     917.62     896.21
879.49     829.41     705.82
  663.90     636.35     544.17     451.79     337.20     310.37     186.61
ZeroEnergy[kcal/mol]    4.4738291928536951
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !           4
Geometry[angstrom]          15
C   0.52960   0.06512  -1.05616
C   0.53304   0.06489   0.44733
C   1.74231   0.07126   1.25286
C  -0.75072   0.00034   0.87059
C  -1.64615  -0.02921  -0.27651
C  -0.92379   0.00581  -1.40608
H   1.01434   0.95853  -1.46121
H   2.55785   0.67371   0.86024
H   1.58275   0.24513   2.31333
H   2.28058  -1.12275   1.22937
H  -1.06741  -0.02154   1.90340
H  -2.72335  -0.07127  -0.21286
H  -1.30375  -0.00139  -2.41567
H   1.08330  -0.79257  -1.45205
H   2.71621  -1.98967   1.23543
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.17    0.70    1.59    2.78    4.07    5.12    2.24    1.61    1.01    0.50
0.13
 End
   Frequencies[1/cm]          37
  3247.4     3226.1     3214.7     3180.4     3101.6     3078.4     3044.2
1650.0     1561.6     1472.3
  1469.5     1423.2     1399.4     1350.7     1281.5     1260.3     1241.1
1207.6     1146.8     1130.8
  1039.4     1021.5     1008.9     978.67     965.41     917.80     896.29
881.00     829.42     705.82
  657.47     636.84     543.87     452.75     337.68     312.35     192.67
ZeroEnergy[kcal/mol]    4.8379404821543757
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !           5
Geometry[angstrom]          15
C   0.52953   0.06510  -1.05612
C   0.53245   0.06490   0.44717
C   1.74322   0.07020   1.25312
C  -0.75046   0.00045   0.87058
C  -1.64619  -0.02922  -0.27667
C  -0.92386   0.00580  -1.40608
H   1.01431   0.95857  -1.46110
H   2.55650   0.67627   0.86079
H   1.58225   0.24690   2.31305
H   2.27479  -1.11025   1.22948
H  -1.06726  -0.02151   1.90338
H  -2.72337  -0.07132  -0.21294
H  -1.30377  -0.00137  -2.41569
H   1.08328  -0.79253  -1.45205
H   2.71886  -1.99511   1.23538
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.17    0.70    1.59    2.78    4.07    5.12    2.24    1.61    1.01    0.50
0.13
 End
   Frequencies[1/cm]          37
  3247.4     3225.9     3214.5     3177.9     3099.7     3078.4     3044.2
1651.4     1558.7     1472.2
  1423.2     1419.5     1398.3     1350.0     1283.4     1276.2     1255.6
1208.7     1147.0     1130.9
  1041.6     1025.8     1009.8     978.80     965.62     917.94     896.31
882.03     829.42     705.76
  647.53     636.66     543.26     452.05     338.06     313.33     196.87
ZeroEnergy[kcal/mol]    5.1509932715763069
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !           6
Geometry[angstrom]          15
C   0.52947   0.06509  -1.05608
C   0.53187   0.06492   0.44703
C   1.74409   0.06920   1.25337
C  -0.75020   0.00056   0.87056
C  -1.64622  -0.02922  -0.27683
C  -0.92393   0.00579  -1.40608
H   1.01427   0.95861  -1.46098
H   2.55515   0.67880   0.86134
H   1.58175   0.24866   2.31278
H   2.26907  -1.09790   1.22959
H  -1.06711  -0.02147   1.90337
H  -2.72339  -0.07136  -0.21302
H  -1.30378  -0.00135  -2.41571
H   1.08327  -0.79249  -1.45206
H   2.72177  -2.00106   1.23534
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15
 Axis            3          2
```

Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.4 3225.8 3214.3 3175.5 3097.7 3078.4 3044.2
1653.7 1562.3 1472.2
1422.6 1404.6 1375.6 1345.7 1292.8 1286.6 1266.5
1209.5 1147.4 1131.0
1044.2 1029.2 1010.3 978.89 965.76 918.10 896.28
882.58 829.43 705.63
639.19 630.73 542.33 449.40 338.07 313.43 199.48
ZeroEnergy[kcal/mol] 5.4072557037753723
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 7
Geometry[angstrom] 15
C 0.52940 0.06508 -1.05603
C 0.53131 0.06493 0.44688
C 1.74494 0.06825 1.25362
C -0.74996 0.00066 0.87055
C -1.64625 -0.02922 -0.27699
C -0.92400 0.00578 -1.40608
H 1.01424 0.95864 -1.46087
H 2.55379 0.68134 0.86189
H 1.58123 0.25044 2.31250
H 2.26345 -1.08574 1.22971
H -1.06696 -0.02143 1.90335
H -2.72342 -0.07140 -0.21311
H -1.30380 -0.00134 -2.41573
H 1.08325 -0.79245 -1.45207
H 2.72491 -2.00750 1.23530
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.3 3225.7 3214.2 3173.0 3095.7 3078.3 3044.2
1656.4 1567.7 1472.3
1422.3 1405.0 1362.8 1330.3 1308.3 1293.8 1272.2
1210.2 1147.9 1131.1
1047.1 1031.6 1010.7 978.95 965.83 918.30 896.23
882.70 829.43 705.46
638.01 613.75 541.16 444.61 337.47 312.76 200.65
ZeroEnergy[kcal/mol] 5.6068135530559955
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 8
Geometry[angstrom] 15
C 0.52933 0.06507 -1.05599
C 0.53076 0.06495 0.44675
C 1.74576 0.06736 1.25387
C -0.74972 0.00077 0.87053
C -1.64627 -0.02922 -0.27715
C -0.92407 0.00577 -1.40609
H 1.01421 0.95868 -1.46075
H 2.55241 0.68389 0.86243
H 1.58070 0.25225 2.31221
H 2.25796 -1.07380 1.22982
H -1.06682 -0.02139 1.90334
H -2.72344 -0.07145 -0.21319
H -1.30382 -0.00132 -2.41576
H 1.08323 -0.79241 -1.45208
H 2.72831 -2.01444 1.23527
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.3 3225.6 3214.0 3170.5 3093.8 3078.2 3044.2
1659.4 1573.7 1472.4
1422.1 1406.3 1363.3 1325.7 1317.8 1297.7 1274.6
1210.9 1148.5 1131.2
1050.2 1033.4 1010.9 978.98 965.87 918.55 896.17
882.42 829.45 705.25
637.50 592.69 539.77 437.79 336.05 311.28 200.37
ZeroEnergy[kcal/mol] 5.7500528037873364
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 9
Geometry[angstrom] 15
C 0.52925 0.06506 -1.05594
C 0.53021 0.06497 0.44661
C 1.74656 0.06651 1.25412
C -0.74949 0.00088 0.87051
C -1.64630 -0.02922 -0.27731
C -0.92415 0.00576 -1.40609
H 1.01418 0.95871 -1.46063
H 2.55099 0.68648 0.86298
H 1.58014 0.25409 2.31191
H 2.25261 -1.06212 1.22994
H -1.06667 -0.02134 1.90332
H -2.72346 -0.07149 -0.21329
H -1.30384 -0.00130 -2.41578
H 1.08320 -0.79237 -1.45208
H 2.73195 -2.02188 1.23523
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.3 3225.4 3213.8 3168.0 3091.9 3078.1 3044.1
1662.7 1580.0 1472.9
1421.9 1408.8 1370.0 1338.7 1324.0 1294.7 1275.7
1211.5 1149.2 1131.3
1053.1 1034.8 1011.0 978.99 965.87 918.86 896.12
881.81 829.46 705.01
637.07 568.98 537.94 429.36 333.72 308.77 198.51
ZeroEnergy[kcal/mol] 5.8452499510071716
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 10
Geometry[angstrom] 15
C 0.52916 0.06504 -1.05587
C 0.52962 0.06500 0.44649
C 1.74731 0.06571 1.25436
C -0.74918 0.00098 0.87045
C -1.64626 -0.02922 -0.27754

```
C   -0.92427   0.00575  -1.40603
H    1.01409   0.95868  -1.46046
H    2.54949   0.68912   0.86355
H    1.57957   0.25597   2.31154
H    2.24740  -1.05076   1.23006
H   -1.06649  -0.02130   1.90325
H   -2.72342  -0.07154  -0.21341
H   -1.30387  -0.00129  -2.41571
H    1.08311  -0.79227  -1.45203
H    2.73582  -2.02976   1.23519
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                     Hindered
 Group    8   9  10  15
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.17    0.70    1.59    2.78    4.07    5.12    2.24    1.61    1.01    0.50
0.13
 End
   Frequencies[1/cm]          37
 3247.5     3225.3     3213.4     3165.9     3090.3     3078.7     3044.8
1667.0     1587.2     1473.9
 1421.8     1414.7     1384.1     1348.5     1333.2     1296.1     1276.4
1211.9     1149.7     1131.4
 1055.3     1035.7     1010.9     979.03     965.79     919.20     896.10
880.97     829.48     704.66
 636.71     546.41     532.21     419.89     330.39     304.60     194.72
ZeroEnergy[kcal/mol]    5.9038551390118199
 ElectronicLevels[1/cm]                   1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          11
Geometry[angstrom]          15
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50224
C    1.21897   0.00000   2.31050
C   -1.27808  -0.06393   1.92632
C   -2.17539  -0.09426   0.77819
C   -1.45343  -0.05930  -0.35020
H    0.48499   0.89372  -0.40451
H    2.01883   0.62685   1.92002
H    1.04983   0.19294   3.36711
H    1.71355  -1.10512   2.28606
H   -1.59543  -0.08626   2.95908
H   -3.25251  -0.13662   0.84237
H   -1.83298  -0.06631  -1.35990
H    0.55402  -0.85729  -0.39624
H    2.21111  -2.10374   2.29103
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                     Hindered
 Group    8   9  10  15
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.17    0.70    1.59    2.78    4.07    5.12    2.24    1.61    1.01    0.50
0.13
 End
   Frequencies[1/cm]          37
 3247.5     3225.2     3213.3     3163.6     3088.6     3078.6     3044.7
1671.3     1594.5     1477.4
 1433.4     1421.3     1396.6     1355.7     1341.1     1302.9     1276.8
1212.2     1150.1     1131.5
 1056.7     1036.5     1010.8     979.00     965.75     919.56     896.03
879.95     829.50     704.42
 636.43     539.48     510.29     411.00     327.03     298.87     189.27
ZeroEnergy[kcal/mol]    5.9271978695174665
 ElectronicLevels[1/cm]                   1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          12
Geometry[angstrom]          15
C    0.52900   0.06502  -1.05580
C    0.52855   0.06506   0.44623
C    1.74881   0.06435   1.25490
C   -0.74879   0.00122   0.87042
C   -1.64634  -0.02923  -0.27786
C   -0.92444   0.00572  -1.40608
H    1.01402   0.95876  -1.46020
H    2.54640   0.69468   0.86472
H    1.57828   0.25997   2.31091
H    2.23789  -1.02943   1.23032
H   -1.06620  -0.02115   1.90324
H   -2.72349  -0.07163  -0.21362
H   -1.30393  -0.00126  -2.41580
H    1.08306  -0.79218  -1.45208
H    2.74457  -2.04764   1.23513
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                     Hindered
 Group    8   9  10  15
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.17    0.70    1.59    2.78    4.07    5.12    2.24    1.61    1.01    0.50
0.13
 End
   Frequencies[1/cm]          37
 3247.4     3225.0     3213.1     3161.2     3086.8     3078.5     3044.6
1677.4     1604.9     1496.2
 1458.0     1421.4     1402.0     1363.4     1346.8     1313.0     1277.0
1212.2     1150.4     1131.5
 1057.2     1036.9     1010.6     978.93     965.68     919.92     895.94
878.72     829.53     704.18
 636.26     537.84     480.82     402.75     323.59     290.69     180.28
ZeroEnergy[kcal/mol]    5.9203952840209650
 ElectronicLevels[1/cm]                   1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          13
Geometry[angstrom]          15
C    0.52894   0.06502  -1.05581
C    0.52808   0.06509   0.44610
C    1.74956   0.06381   1.25519
C   -0.74870   0.00135   0.87047
C   -1.64647  -0.02924  -0.27796
C   -0.92449   0.00571  -1.40620
H    1.01403   0.95888  -1.46011
H    2.54479   0.69763   0.86533
H    1.57756   0.26210   2.31065
H    2.23374  -1.01975   1.23047
H   -1.06609  -0.02102   1.90329
H   -2.72362  -0.07168  -0.21371
H   -1.30396  -0.00123  -2.41596
H    1.08311  -0.79218  -1.45217
H    2.74951  -2.05773   1.23509
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                     Hindered
 Group    8   9  10  15
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.17    0.70    1.59    2.78    4.07    5.12    2.24    1.61    1.01    0.50
0.13
 End
   Frequencies[1/cm]          37
 3247.2     3224.9     3213.0     3158.6     3085.0     3077.6     3043.9
1688.4     1622.3     1537.5
```

1465.1 1421.5 1404.7 1371.4 1351.1 1322.2 1277.1
1212.1 1150.6 1131.4
1057.0 1037.2 1010.4 978.80 965.66 920.23 895.81
877.42 829.56 704.07
636.12 537.13 451.63 396.51 320.55 281.63 168.52
ZeroEnergy[kcal/mol] 5.8973127777302308
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 14
Geometry[angstrom] 15
C 0.52886 0.06502 -1.05579
C 0.52756 0.06513 0.44598
C 1.75026 0.06334 1.25549
C -0.74855 0.00148 0.87047
C -1.64653 -0.02925 -0.27813
C -0.92459 0.00570 -1.40626
H 1.01399 0.95893 -1.45997
H 2.54308 0.70066 0.86597
H 1.57682 0.26428 2.31031
H 2.22994 -1.01069 1.23064
H -1.06596 -0.02090 1.90329
H -2.72369 -0.07173 -0.21383
H -1.30400 -0.00121 -2.41604
H 1.08309 -0.79212 -1.45221
H 2.75472 -2.06837 1.23505
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.1 3224.8 3212.8 3156.5 3083.6 3077.5 3043.8
1722.9 1648.5 1568.5
1467.0 1421.5 1407.0 1378.7 1355.3 1329.3 1277.1
1211.8 1150.6 1131.4
1056.2 1037.2 1010.0 978.71 965.56 920.52 895.70
876.05 829.60 703.85
636.00 536.50 422.51 391.35 317.16 272.12 152.40
ZeroEnergy[kcal/mol] 5.8571204737116700
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 15
Geometry[angstrom] 15
C 0.52876 0.06501 -1.05577
C 0.52706 0.06517 0.44586
C 1.75093 0.06297 1.25578
C -0.74841 0.00163 0.87047
C -1.64659 -0.02926 -0.27830
C -0.92469 0.00569 -1.40631
H 1.01395 0.95898 -1.45982
H 2.54131 0.70378 0.86661
H 1.57602 0.26652 2.30997
H 2.22662 -1.00241 1.23083
H -1.06582 -0.02077 1.90330
H -2.72375 -0.07178 -0.21397
H -1.30404 -0.00120 -2.41611
H 1.08306 -0.79205 -1.45225
H 2.76023 -2.07963 1.23501
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.1 3224.7 3212.7 3154.5 3082.4 3077.3 3043.7
1795.9 1663.1 1582.3
1467.8 1421.6 1409.2 1383.6 1359.9 1333.8 1277.0
1211.4 1150.5 1131.4
1055.1 1036.9 1009.0 978.63 965.29 920.78 895.43
874.66 829.61 703.64
635.82 535.77 387.45 338.67 265.30 158.40 127.65
ZeroEnergy[kcal/mol] 5.8145715523019375
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 16
Geometry[angstrom] 15
C 0.52866 0.06501 -1.05575
C 0.52657 0.06522 0.44576
C 1.75155 0.06270 1.25609
C -0.74829 0.00177 0.87046
C -1.64666 -0.02927 -0.27847
C -0.92480 0.00567 -1.40638
H 1.01389 0.95904 -1.45966
H 2.53949 0.70696 0.86726
H 1.57519 0.26878 2.30964
H 2.22379 -0.99493 1.23104
H -1.06569 -0.02063 1.90330
H -2.72382 -0.07184 -0.21412
H -1.30410 -0.00119 -2.41620
H 1.08303 -0.79199 -1.45229
H 2.76602 -2.09148 1.23496
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.17 0.70 1.59 2.78 4.07 5.12 2.24 1.61 1.01 0.50
0.13
End
Frequencies[1/cm] 37
3247.0 3224.6 3212.6 3152.6 3081.3 3077.1 3043.7
1886.1 1669.8 1589.4
1468.4 1421.9 1411.9 1388.8 1364.6 1336.9 1277.0
1211.0 1150.5 1131.4
1054.2 1036.9 1008.7 978.55 965.21 921.01 895.37
873.34 829.64 703.45
635.74 535.42 384.43 335.75 257.21 128.06 97.280
ZeroEnergy[kcal/mol] 5.8452610416833535
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 17
Geometry[angstrom] 15
C 0.52855 0.06501 -1.05573
C 0.52611 0.06527 0.44566
C 1.75214 0.06252 1.25639
C -0.74819 0.00193 0.87045
C -1.64673 -0.02928 -0.27865
C -0.92492 0.00566 -1.40645
H 1.01383 0.95909 -1.45950
H 2.53764 0.71017 0.86791
H 1.57432 0.27105 2.30930
H 2.22149 -0.98826 1.23128
H -1.06556 -0.02047 1.90331
H -2.72390 -0.07190 -0.21428
H -1.30416 -0.00118 -2.41629

```
 H    1.08299  -0.79192  -1.45232
 H    2.77206  -2.10382   1.23491
                  Core            RigidRotor
         SymmetryFactor   0.50000000000000000
 End
  Rotor                          Hindered
  Group    8   9  10  15
  Axis           3           2
  Symmetry           3
  Potential[kcal/mol]           12
   0.00    0.17    0.70    1.59    2.78    4.07    5.12    2.24    1.61    1.01    0.50
0.13
  End
     Frequencies[1/cm]           37
   3247.0      3224.5      3212.5      3150.9      3080.4      3076.9      3043.6
1978.7      1673.9      1593.9
   1468.8      1422.5      1414.8      1392.4      1369.1      1338.8      1276.9
1210.6      1150.4      1131.4
   1053.4      1036.8      1008.5      978.47      965.14      921.21      895.31
872.15      829.68      703.27
   635.69      535.13      382.16      333.53      250.86      95.080      53.860
 ZeroEnergy[kcal/mol]    5.6991139577195424
  ElectronicLevels[1/cm]                   1
   0.0000000000000000        2.0000000000000000
 End
 !*********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1235.7600000000000
      WellDepth[kcal/mol]           5.43
      WellDepth[kcal/mol]          28.00
 End
End
End
```

```
!***************************************************
!            GLOBAL SECTION
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                    0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30         ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                      direct     ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                        diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                  10
!ChemicalEigenvalueMin               1.e-6          #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                1.3
!!
RateOutput                           rate.out                ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***************************************************
!            MODEL SECTION
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                    ! Default collisional
energy relaxation kernel
    Exponential                                     ! Currently the only
possible energy relaxation model
       Factor[1/cm]               316                     ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                  0.535                    ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff                10                       ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                  ! Collision frequency
model
    LennardJones                                    ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                    90.58  281.367              ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]               3.54    4.694                ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                   39.948  79.05478             ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!*************************************************
!
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***************************************************
!  REACTANTS
!***************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50112
 C    1.39710   0.00000   2.12644
 C   -0.81569  -1.21840   1.82234
 C   -1.21870  -1.80451   0.68960
 C   -0.70750  -1.04109  -0.45233
 H    0.50817   0.74374  -0.59543
 H    1.95008   0.89431   1.83920
 H    1.33447  -0.02486   3.21435
 H    1.96018  -0.87263   1.79528
 H   -1.02550  -1.54600   2.82960
 H   -1.82229  -2.69676   0.61182
 H   -0.88231  -1.29309  -1.48790
 H   -0.53850   0.88886   1.85441
         Core    RigidRotor
                SymmetryFactor    1.0000000000000000
         End
 Rotor                      Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          3
 Potential[kcal/mol]         12
    0.00    0.25    0.91    1.86    2.83    3.54    3.75    3.41    2.65    1.71    0.83
0.22
 End
     Frequencies[1/cm]          35
   3244.1      3235.6      3219.3      3210.9      3128.0      3124.4      3049.0
3020.3      1670.2      1591.0
   1503.9      1503.7      1422.5      1406.8      1334.3      1293.1      1277.9
1155.2      1119.2      1104.0
   1090.8      1028.3      1004.1      983.75      981.16      957.17      883.24
817.77      792.34      742.25
   721.84      567.90      547.80      294.51      164.97
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                1
   0.0000000000000000        2.0000000000000000
 End
!************************************
 Fragment REACT2
  Atom
  Name H
  ElectronicLevels[1/cm]                1
   0.0000000000000000        2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]          13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.41507
 C    1.18585   0.00000   2.30525
 C   -1.37924  -0.00034   1.86264
 C   -2.17195  -0.00056   0.76525
 C   -1.30652  -0.00033  -0.41759
 H    0.87955   0.00028  -0.62343
 H    2.11567   0.00259   1.73998
 H    1.17551   0.87449   2.96082
 H    1.17824  -0.87748   2.95691
```

```
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
      Core    RigidRotor
           SymmetryFactor    2.0000000000000000
      End
Rotor                    Hindered
Group    8   9  10
Axis          3          2
Symmetry          3
Potential[kcal/mol]          12
  0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
   Frequencies[1/cm]          32
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!************************************
Fragment PROD2
RRHO
Geometry[angstrom]               2
H    0.00000   0.00000   0.00000
H    0.00000   0.00000   0.74312
      Core    RigidRotor
           SymmetryFactor    2.0000000000000000
      End
   Frequencies[1/cm]           1
  4433.4
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End

GroundEnergy[kcal/mol]   -26.53
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]               15
C    0.05829  -0.06945   0.00293
C    0.05354  -0.06023   1.50402
C    1.44835  -0.07282   2.13417
C   -0.77795  -1.26662   1.82994
C   -1.18446  -1.85476   0.69954
C   -0.66047  -1.10456  -0.44538
H    0.57688   0.66478  -0.59528
H    2.01287   0.81305   1.84323
H    1.38175  -0.09001   3.22199
H    2.00223  -0.95410   1.81052
H   -0.99469  -1.58551   2.83853
H   -1.79863  -2.74005   0.62519
H   -0.83529  -1.36069  -1.47993
H   -0.47553   0.83721   1.84979
H   -3.46327   4.53080   0.71649
      Core    RigidRotor
           SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]          38
  2.4499      16.122      164.70      261.41      295.01      547.53      567.90
720.23      739.84      791.47
  818.16      882.95      957.88      979.09      981.72      1003.9      1028.4
1090.6      1104.0      1118.7
  1155.2      1277.6      1293.0      1333.8      1406.9      1422.1      1503.6
1504.2      1590.9      1669.9
  3020.3      3049.1      3124.6      3127.9      3210.4      3218.7      3235.1
3243.6
 ZeroEnergy[kcal/mol]            0.02
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]               15
C    0.00726   0.00235   0.00961
C    0.00728  -0.00325   1.45818
C    1.21848  -0.02016   2.31226
C   -1.33995   0.04323   1.89528
C   -2.13906   0.07675   0.78244
C   -1.28105   0.05078  -0.40546
H    0.89089  -0.02520  -0.60809
H    1.78448   0.90706   2.18409
H    0.96885  -0.12421   3.36629
H    1.88609  -0.83586   2.02624
H   -1.66074   0.05224   2.92445
H   -3.21738   0.11645   0.76606
H   -1.63394   0.06808  -1.42449
H   -0.52905   2.74361   0.98087
H   -0.29137   3.44272   1.07813
      Core    RigidRotor
           SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]          38
  35.618      56.002      114.61      168.05      204.96      224.68      329.03
527.45      532.97      605.52
  637.92      730.90      742.09      902.42      924.16      931.57      955.31
1012.8      1022.3      1052.1
  1097.9      1179.3      1293.6      1311.5      1406.9      1438.1      1475.5
1484.7      1506.0      1581.4
  3032.1      3087.6      3139.2      3226.2      3233.8      3248.0      3256.2
4405.7
 ZeroEnergy[kcal/mol]            -27.98
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier       B1  REACS WR
  RRHO
    Stoichiometry  H9C6
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]             14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50112
C    1.39710   0.00000   2.12644
C   -0.81569  -1.21840   1.82234
C   -1.21870  -1.80451   0.68960
C   -0.70750  -1.04109  -0.45233
H    0.50817   0.74374  -0.59543
H    1.95008   0.89431   1.83920
H    1.33447  -0.02486   3.21435
H    1.96018  -0.87263   1.79528
H   -1.02550  -1.54600   2.82960
H   -1.82229  -2.69676   0.61182
H   -0.88231  -1.29309  -1.48790
H   -0.53850   0.88886   1.85441
      FragmentGeometry[angstrom]             1
H                0. 0. 0.
                         SymmetryFactor     1.0000000000000000
        PotentialPrefactor[au]           10.
        PotentialPowerExponent          6
                End
Rotor                    Hindered
Geometry[angstrom]             14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50112
```

```
C   1.39710   0.00000   2.12644
C  -0.81569  -1.21840   1.82234
C  -1.21870  -1.80451   0.68960
C  -0.70750  -1.04109  -0.45233
H   0.50817   0.74374  -0.59543
H   1.95008   0.89431   1.83920
H   1.33447  -0.02486   3.21435
H   1.96018  -0.87263   1.79528
H  -1.02550  -1.54600   2.82960
H  -1.82229  -2.69676   0.61182
H  -0.88231  -1.29309  -1.48790
H  -0.53850   0.88886   1.85441
Group    8   9  10
Axis           3          2
Symmetry          3
Potential[kcal/mol]          12
  0.0000     0.25000     0.91000      1.8600      2.8300      3.5400      3.7500
3.4100      2.6500      1.7100
 0.83000     0.22000
End
    Frequencies[1/cm]          35
  3244.1      3235.6      3219.3      3210.9      3128.0      3124.4      3049.0
3020.3      1670.2      1591.0
  1503.9      1503.7      1422.5      1406.8      1334.3      1293.1      1277.9
1155.2      1119.2      1104.0
  1090.8      1028.3      1004.1      983.75      981.16      957.17      883.24
817.77      792.34      742.25
  721.84      567.90      547.80      294.51      164.97
 ZeroEnergy[kcal/mol]           0.
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        4.0000000000000000
End
!************************************
Barrier        B3  WP PRODS
  RRHO
    Stoichiometry  H9C6
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]              13
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.41507
C   1.18585   0.00000   2.30525
C  -1.37924  -0.00034   1.86264
C  -2.17195  -0.00056   0.76525
C  -1.30652  -0.00033  -0.41759
H   0.87955   0.00028  -0.62343
H   2.11567   0.00259   1.73998
H   1.17551   0.87449   2.96082
H   1.17824  -0.87748   2.95691
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
      FragmentGeometry[angstrom]              2
H   0.00000   0.00000   0.00000
H   0.00000   0.00000   0.74312
                              SymmetryFactor     4.0000000000000000
        PotentialPrefactor[au]              10.
        PotentialPowerExponent             6
                 End
Rotor                          Hindered
Geometry[angstrom]              13
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.41507
C   1.18585   0.00000   2.30525
C  -1.37924  -0.00034   1.86264
C  -2.17195  -0.00056   0.76525
C  -1.30652  -0.00033  -0.41759
H   0.87955   0.00028  -0.62343
H   2.11567   0.00259   1.73998
H   1.17551   0.87449   2.96082
H   1.17824  -0.87748   2.95691
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
Group    8   9  10
Axis           3          2
Symmetry          3
Potential[kcal/mol]          12
  0.0000     0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01  0.0000     0.20000E-01 0.40000E-01 0.60000E-01
 0.40000E-01 0.10000E-01
End
    Frequencies[1/cm]          33
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
  4433.4
 ZeroEnergy[kcal/mol]          -26.532034490402612
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO          !           1
Geometry[angstrom]          15
C   0.30069   0.54413  -1.01190
C   0.30464   0.53270   0.47273
C   1.63992   0.54481   1.18640
C  -0.67121  -0.52960   0.82434
C  -1.18761  -1.04022  -0.30421
C  -0.57893  -0.36790  -1.45409
H   0.91260   1.20072  -1.61078
H   2.24221   1.39970   0.87972
H   1.50794   0.58744   2.26733
H   2.19167  -0.36556   0.94545
H  -0.91225  -0.81477   1.83666
H  -1.93178  -1.81957  -0.37064
H  -0.81178  -0.58273  -2.48618
H  -0.27561   1.65016   0.81920
H  -0.63088   2.50814   1.13320
            Core            RigidRotor
      SymmetryFactor     3.0000000000000000
End
 Rotor                          Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
    Frequencies[1/cm]          37
  3249.7      3242.6      3226.3      3217.4      3130.9      3117.8      3046.2
1636.3      1575.0      1497.1
  1491.3      1424.3      1408.1      1382.0      1318.4      1243.3      1228.2
1158.1      1112.7      1092.1
  1088.5      1022.5      1005.8      968.70      964.87      964.05      889.74
796.94      787.21      749.03
  693.04      576.64      572.91      387.48      376.43      291.99      185.06
ZeroEnergy[kcal/mol]    1.5225298350167491
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
End
!*********************************************
RRHO          !           2
Geometry[angstrom]          15
C   0.30070   0.54393  -1.01210
C   0.30418   0.53385   0.47316
C   1.64011   0.54455   1.18635
C  -0.67126  -0.52987   0.82426
C  -1.18755  -1.04026  -0.30416
C  -0.57886  -0.36790  -1.45409
H   0.91244   1.20076  -1.61093
H   2.24220   1.39960   0.87976
```

```
H   1.50800  0.58741  2.26725
H   2.19200 -0.36566  0.94556
H  -0.91247 -0.81480  1.83662
H  -1.93189 -1.81947 -0.37067
H  -0.81191 -0.58266 -2.48618
H  -0.27031  1.63867  0.81528
H  -0.63392  2.51509  1.13566
         Core         RigidRotor
     SymmetryFactor   3.0000000000000000
End
 Rotor                 Hindered
 Group   8  9  10
 Axis         3        2
 Symmetry         1
 Potential[kcal/mol]        18
  0.00   0.75   2.35   3.16   2.30   0.74   0.00   0.73   2.33   3.16   2.30
0.74   0.00   0.74   2.35   3.16   2.28   0.73
 End
   Frequencies[1/cm]        37
  3249.6    3242.5    3226.1    3217.2    3130.8    3118.6    3046.6
1638.5    1573.6    1496.8
  1492.3    1419.6    1408.1    1344.4    1319.8    1247.0    1232.3
1161.4    1112.9    1092.0
  1090.2    1024.2    1006.3    969.82    966.31    964.18    890.37
799.11    789.01    749.55
  694.84    576.83    571.94    389.73    380.67    292.39    185.16
ZeroEnergy[kcal/mol]   1.9410305263458496
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO        !         3
Geometry[angstrom]        15
C   0.30072  0.54374 -1.01230
C   0.30375  0.53493  0.47357
C   1.64030  0.54429  1.18630
C  -0.67130 -0.53013  0.82417
C  -1.18751 -1.04029 -0.30412
C  -0.57879 -0.36791 -1.45410
H   0.91229  1.20079 -1.61109
H   2.24220  1.39951  0.87980
H   1.50806  0.58738  2.26717
H   2.19234 -0.36576  0.94568
H  -0.91268 -0.81483  1.83658
H  -1.93200 -1.81937 -0.37071
H  -0.81205 -0.58258 -2.48617
H  -0.26513  1.62739  0.81143
H  -0.63715  2.52250  1.13828
         Core         RigidRotor
     SymmetryFactor   3.0000000000000000
End
 Rotor                 Hindered
 Group   8  9  10
 Axis         3        2
 Symmetry         1
 Potential[kcal/mol]        18
  0.00   0.75   2.35   3.16   2.30   0.74   0.00   0.73   2.33   3.16   2.30
0.74   0.00   0.74   2.35   3.16   2.28   0.73
 End
   Frequencies[1/cm]        37
  3249.4    3242.3    3225.9    3217.0    3130.8    3119.2    3047.1
1640.7    1573.6    1497.0
  1493.2    1418.9    1408.5    1321.3    1318.1    1251.0    1236.3
1163.1    1113.0    1092.0
  1090.1    1025.9    1006.8    970.87    967.67    964.14    890.87
801.21    790.60    749.69
  696.57    576.58    570.68    388.07    381.20    292.30    185.03
ZeroEnergy[kcal/mol]   2.3146484677045094
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO        !         4
Geometry[angstrom]        15
C   0.30074  0.54354 -1.01249
C   0.30334  0.53597  0.47396
C   1.64050  0.54403  1.18625
C  -0.67134 -0.53039  0.82409
C  -1.18746 -1.04033 -0.30408
C  -0.57872 -0.36792 -1.45410
H   0.91214  1.20081 -1.61124
H   2.24221  1.39941  0.87984
H   1.50813  0.58735  2.26709
H   2.19267 -0.36586  0.94580
H  -0.91290 -0.81487  1.83653
H  -1.93212 -1.81928 -0.37074
H  -0.81218 -0.58251 -2.48617
H  -0.26007  1.61637  0.80766
H  -0.64058  2.53036  1.14107
         Core         RigidRotor
     SymmetryFactor   3.0000000000000000
End
 Rotor                 Hindered
 Group   8  9  10
 Axis         3        2
 Symmetry         1
 Potential[kcal/mol]        18
  0.00   0.75   2.35   3.16   2.30   0.74   0.00   0.73   2.33   3.16   2.30
0.74   0.00   0.74   2.35   3.16   2.28   0.73
 End
   Frequencies[1/cm]        37
  3249.3    3242.2    3225.8    3216.8    3130.7    3119.9    3047.5
1642.8    1574.1    1497.2
  1494.2    1419.0    1408.9    1322.7    1305.2    1255.1    1239.9
1163.9    1113.1    1092.1
  1089.1    1027.8    1007.2    971.87    968.96    963.94    891.21
803.23    791.99    749.53
  698.22    575.94    569.17    382.39    377.83    291.82    184.71
ZeroEnergy[kcal/mol]   2.6292466452545766
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO        !         5
Geometry[angstrom]        15
C   0.30077  0.54334 -1.01268
C   0.30295  0.53697  0.47433
C   1.64070  0.54376  1.18620
C  -0.67137 -0.53065  0.82401
C  -1.18742 -1.04037 -0.30405
C  -0.57865 -0.36794 -1.45411
H   0.91198  1.20083 -1.61141
H   2.24223  1.39930  0.87988
H   1.50821  0.58731  2.26702
H   2.19302 -0.36597  0.94592
H  -0.91311 -0.81492  1.83648
H  -1.93224 -1.81918 -0.37078
H  -0.81232 -0.58243 -2.48617
H  -0.25516  1.60565  0.80398
H  -0.64422  2.53869  1.14402
         Core         RigidRotor
     SymmetryFactor   3.0000000000000000
End
 Rotor                 Hindered
 Group   8  9  10
 Axis         3        2
 Symmetry         1
 Potential[kcal/mol]        18
  0.00   0.75   2.35   3.16   2.30   0.74   0.00   0.73   2.33   3.16   2.30
0.74   0.00   0.74   2.35   3.16   2.28   0.73
 End
   Frequencies[1/cm]        37
  3249.1    3242.0    3225.6    3216.6    3130.6    3120.6    3047.9
1644.9    1574.9    1497.6
  1495.1    1419.2    1409.4    1324.1    1306.0    1258.8    1243.2
1164.3    1113.2    1092.6
  1087.8    1029.6    1007.4    972.78    970.17    963.65    891.35
805.11    793.16    749.10
```

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  699.79    574.98    567.49    372.74    370.55    290.91    184.18
 ZeroEnergy[kcal/mol]   2.8907570563833445
  ElectronicLevels[1/cm]          1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        6
Geometry[angstrom]        15
C   0.30079  0.54314  -1.01287
C   0.30257  0.53792  0.47469
C   1.64090  0.54349  1.18615
C   -0.67139  -0.53092  0.82392
C   -1.18737  -1.04042  -0.30402
C   -0.57859  -0.36797  -1.45412
H   0.91183  1.20084  -1.61158
H   2.24226  1.39919  0.87992
H   1.50830  0.58727  2.26695
H   2.19337  -0.36609  0.94604
H   -0.91332  -0.81498  1.83643
H   -1.93236  -1.81908  -0.37082
H   -0.81247  -0.58236  -2.48617
H   -0.25041  1.59527  0.80042
H   -0.64807  2.54751  1.14714
          Core          RigidRotor
       SymmetryFactor   3.0000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis         3        2
 Symmetry         1
 Potential[kcal/mol]        18
  0.00   0.75   2.35   3.16   2.30   0.74   0.00   0.73   2.33   3.16   2.30
0.74   0.00   0.74   2.35   3.16   2.28   0.73
 End
   Frequencies[1/cm]        37
  3248.9    3241.9    3225.3    3216.3    3130.4    3121.2    3048.2
1646.8    1576.0    1498.0
  1496.0    1419.6    1409.8    1325.4    1321.1    1261.7    1246.2
1164.6    1113.2    1093.3
  1086.5    1031.1    1007.5    973.61    971.30    963.31    891.33
806.84    794.16    748.49
  701.30    573.83    565.76    359.79    359.26    289.47    183.43
 ZeroEnergy[kcal/mol]   3.1010095529156074
  ElectronicLevels[1/cm]          1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        7
Geometry[angstrom]        15
C   0.30083  0.54293  -1.01306
C   0.30222  0.53883  0.47503
C   1.64111  0.54322  1.18610
C   -0.67141  -0.53119  0.82384
C   -1.18733  -1.04046  -0.30401
C   -0.57853  -0.36800  -1.45413
H   0.91168  1.20084  -1.61177
H   2.24231  1.39907  0.87997
H   1.50841  0.58722  2.26688
H   2.19373  -0.36621  0.94616
H   -0.91354  -0.81506  1.83638
H   -1.93249  -1.81899  -0.37087
H   -0.81262  -0.58229  -2.48617
H   -0.24586  1.58530  0.79699
H   -0.65215  2.55683  1.15044
          Core          RigidRotor
       SymmetryFactor   3.0000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis         3        2
 Symmetry         1
 Potential[kcal/mol]        18
  0.00   0.75   2.35   3.16   2.30   0.74   0.00   0.73   2.33   3.16   2.30
0.74   0.00   0.74   2.35   3.16   2.28   0.73
 End
   Frequencies[1/cm]        37
  3248.8    3241.7    3225.1    3216.1    3130.3    3121.8    3048.5
1648.7    1577.3    1498.5
  1496.8    1420.0    1410.2    1351.1    1326.7    1264.3    1248.8
1165.0    1113.3    1094.3
  1085.4    1032.1    1007.5    974.37    972.36    962.95    891.15
808.41    795.01    747.79
  702.73    572.61    564.06    346.06    342.59    287.09    182.41
 ZeroEnergy[kcal/mol]   3.2752562146451907
  ElectronicLevels[1/cm]          1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        8
Geometry[angstrom]        15
C   0.30087  0.54271  -1.01324
C   0.30188  0.53970  0.47536
C   1.64132  0.54293  1.18604
C   -0.67142  -0.53146  0.82376
C   -1.18729  -1.04052  -0.30399
C   -0.57847  -0.36804  -1.45414
H   0.91153  1.20083  -1.61196
H   2.24237  1.39894  0.88001
H   1.50852  0.58715  2.26682
H   2.19409  -0.36634  0.94627
H   -0.91376  -0.81515  1.83632
H   -1.93263  -1.81889  -0.37092
H   -0.81279  -0.58222  -2.48617
H   -0.24154  1.57580  0.79371
H   -0.65647  2.56668  1.15392
          Core          RigidRotor
       SymmetryFactor   3.0000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis         3        2
 Symmetry         1
 Potential[kcal/mol]        18
  0.00   0.75   2.35   3.16   2.30   0.74   0.00   0.73   2.33   3.16   2.30
0.74   0.00   0.74   2.35   3.16   2.28   0.73
 End
   Frequencies[1/cm]        37
  3248.6    3241.5    3224.9    3215.9    3130.1    3122.4    3048.8
1650.4    1579.0    1499.2
  1497.6    1420.4    1410.7    1396.0    1327.8    1266.6    1251.1
1165.5    1113.4    1095.2
  1084.5    1032.4    1007.5    975.04    973.34    962.61    890.85
809.81    795.70    747.02
  704.04    571.40    562.47    331.07    323.18    282.86    181.07
 ZeroEnergy[kcal/mol]   3.4100239075741086
  ElectronicLevels[1/cm]          1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        9
Geometry[angstrom]        15
C   0.30092  0.54249  -1.01343
C   0.30156  0.54052  0.47567
C   1.64155  0.54263  1.18599
C   -0.67143  -0.53175  0.82367
C   -1.18724  -1.04058  -0.30398
C   -0.57842  -0.36808  -1.45416
H   0.91138  1.20081  -1.61217
H   2.24245  1.39879  0.88006
H   1.50866  0.58707  2.26675
H   2.19447  -0.36649  0.94639
H   -0.91399  -0.81525  1.83626
H   -1.93277  -1.81879  -0.37098
H   -0.81296  -0.58215  -2.48618
H   -0.23747  1.56683  0.79061
H   -0.66102  2.57706  1.15758
          Core          RigidRotor
       SymmetryFactor   3.0000000000000000
```

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End
 Rotor                     Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
   Frequencies[1/cm]          37
  3248.4      3241.2      3224.6      3215.6      3129.8      3123.0      3049.1
1652.0      1581.9      1501.0
  1498.4      1455.1      1420.5      1410.8      1328.9      1268.7      1253.0
1166.1      1113.4      1096.2
  1083.8      1032.3      1007.5      975.62      974.22      962.29      890.46
811.04      796.23      746.23
  705.22      570.25      561.01      317.45      301.77      274.67      179.26
ZeroEnergy[kcal/mol]    3.5196783770188431
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           10
Geometry[angstrom]           15
C    0.30095   0.54224  -1.01360
C    0.30128   0.54130   0.47595
C    1.64178   0.54232   1.18592
C   -0.67143  -0.53204   0.82356
C   -1.18719  -1.04063  -0.30397
C   -0.57837  -0.36813  -1.45417
H    0.91121   1.20077  -1.61238
H    2.24253   1.39861   0.88012
H    1.50880   0.58698   2.26665
H    2.19484  -0.36661   0.94651
H   -0.91423  -0.81537   1.83618
H   -1.93291  -1.81868  -0.37103
H   -0.81313  -0.58208  -2.48618
H   -0.23366   1.55841   0.78768
H   -0.66580   2.58794   1.16142
                Core            RigidRotor
         SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
   Frequencies[1/cm]          37
  3248.1      3240.9      3224.3      3215.3      3129.9      3123.9      3049.6
1653.6      1590.8      1530.1
  1499.0      1495.3      1420.9      1411.1      1329.8      1270.6      1254.5
1166.8      1113.5      1096.9
  1083.2      1031.7      1007.4      976.16      975.07      961.95      890.01
812.12      796.58      745.53
  706.26      569.17      559.70      308.03      279.11      260.17      176.65
ZeroEnergy[kcal/mol]    3.6106090833227511
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           11
Geometry[angstrom]           15
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.49000
C    1.34101   0.00000   2.19965
C   -0.97243  -1.07433   1.83726
C   -1.48818  -1.58271   0.70980
C   -0.87935  -0.91020  -0.44042
H    0.61004   0.65873  -0.59884
H    1.94163   0.85642   1.89395
H    1.20797   0.04486   3.28036
H    1.89421  -0.90880   1.96039
H   -1.21548  -1.35752   2.84988
H   -2.23409  -2.36057   0.64268
H   -1.11435  -1.12401  -1.47242
H   -0.53145   1.00921   1.79896
H   -0.97198   2.05770   2.17935
                Core            RigidRotor
         SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
   Frequencies[1/cm]          37
  3247.9      3240.7      3224.1      3215.1      3129.6      3124.3      3049.8
1654.9      1635.6      1566.6
  1499.7      1497.9      1421.2      1411.3      1330.6      1272.4      1255.8
1167.5      1113.6      1097.5
  1083.2      1031.0      1007.4      976.59      975.75      961.74      889.53
813.01      796.79      744.86
  707.06      568.28      558.60      303.08      257.57      241.41      173.29
ZeroEnergy[kcal/mol]    3.6837731142248713
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           12
Geometry[angstrom]           15
C    0.30109   0.54175  -1.01397
C    0.30077   0.54268   0.47649
C    1.64228   0.54166   1.18580
C   -0.67139  -0.53264   0.82338
C   -1.18712  -1.04079  -0.30400
C   -0.57828  -0.36828  -1.45423
H    0.91091   1.20066  -1.61286
H    2.24279   1.39823   0.88022
H    1.50918   0.58673   2.26652
H    2.19563  -0.36700   0.94670
H   -0.91469  -0.81567   1.83601
H   -1.93323  -1.81848  -0.37118
H   -0.81352  -0.58195  -2.48622
H   -0.22719   1.54400   0.78267
H   -0.67612   2.61144   1.16971
                Core            RigidRotor
         SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
   Frequencies[1/cm]          37
  3247.7      3240.5      3223.9      3214.9      3129.3      3124.8      3050.0
1724.7      1656.1      1574.3
  1500.2      1498.6      1421.5      1411.5      1331.3      1273.6      1256.7
1168.1      1113.6      1097.9
  1082.7      1030.0      1007.3      976.97      976.39      961.50      889.05
813.80      796.92      744.17
  707.83      567.38      557.58      300.11      235.96      218.13      167.39
ZeroEnergy[kcal/mol]    3.7396851155509068
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           13
Geometry[angstrom]           15
C    0.30119   0.54150  -1.01416
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C   0.30053   0.54329   0.47674
C   1.64254   0.54131   1.18574
C  -0.67135  -0.53295   0.82330
C  -1.18709  -1.04089  -0.30404
C  -0.57824  -0.36836  -1.45427
H   0.91078   1.20059  -1.61313
H   2.24297   1.39803   0.88026
H   1.50942   0.58657   2.26649
H   2.19604  -0.36727   0.94676
H  -0.91492  -0.81584   1.83593
H  -1.93340  -1.81840  -0.37128
H  -0.81372  -0.58190  -2.48625
H  -0.22458   1.53814   0.78064
H  -0.68164   2.62396   1.17412
           Core          RigidRotor
       SymmetryFactor    3.0000000000000000
End
 Rotor                  Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
   Frequencies[1/cm]          37
  3247.6     3240.3     3223.7     3214.7     3128.8     3124.8     3049.8
1814.2     1657.0     1576.6
  1500.8     1499.1     1421.7     1411.7     1331.8     1274.8     1257.5
1168.7     1113.6     1098.2
  1082.8     1029.3     1007.2     977.27     976.88     961.38     888.59
814.44     796.97     743.56
  708.39     566.69     556.74     298.46     219.20     195.03     158.23
 ZeroEnergy[kcal/mol]    3.7796731383661579
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           14
Geometry[angstrom]          15
C   0.30128   0.54123  -1.01434
C   0.30032   0.54387   0.47697
C   1.64281   0.54095   1.18568
C  -0.67131  -0.53326   0.82321
C  -1.18705  -1.04099  -0.30408
C  -0.57820  -0.36846  -1.45432
H   0.91065   1.20049  -1.61339
H   2.24316   1.39778   0.88030
H   1.50967   0.58638   2.26643
H   2.19642  -0.36752   0.94682
H  -0.91515  -0.81604   1.83582
H  -1.93357  -1.81831  -0.37138
H  -0.81392  -0.58185  -2.48627
H  -0.22220   1.53282   0.77880
H  -0.68727   2.63673   1.17861
           Core          RigidRotor
       SymmetryFactor    3.0000000000000000
End
 Rotor                  Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
   Frequencies[1/cm]          37
  3247.4     3240.1     3223.5     3214.5     3128.5     3125.2     3049.9
1904.2     1658.0     1578.0
  1501.2     1499.4     1421.9     1411.8     1332.3     1275.8     1258.2
1169.3     1113.6     1098.4
  1083.0     1028.5     1007.1     977.58     977.32     961.23     888.13
814.99     796.90     743.06
  708.81     566.05     556.00     297.28     207.32     170.92     143.37
 ZeroEnergy[kcal/mol]    3.8029509182147421
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           15
Geometry[angstrom]          15
C   0.30138   0.54096  -1.01451
C   0.30013   0.54441   0.47719
C   1.64308   0.54058   1.18561
C  -0.67126  -0.53358   0.82312
C  -1.18702  -1.04110  -0.30412
C  -0.57816  -0.36856  -1.45436
H   0.91052   1.20037  -1.61366
H   2.24338   1.39750   0.88035
H   1.50995   0.58617   2.26637
H   2.19679  -0.36779   0.94686
H  -0.91537  -0.81625   1.83572
H  -1.93373  -1.81823  -0.37148
H  -0.81412  -0.58181  -2.48631
H  -0.22012   1.52817   0.77718
H  -0.69302   2.64976   1.18319
           Core          RigidRotor
       SymmetryFactor    3.0000000000000000
End
 Rotor                  Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
   Frequencies[1/cm]          37
  3247.2     3239.9     3223.3     3214.3     3128.2     3125.5     3050.0
1989.1     1658.8     1579.0
  1501.6     1499.7     1422.0     1411.8     1332.6     1276.8     1258.7
1169.8     1113.6     1098.5
  1083.3     1027.6     1007.1     977.89     977.64     961.10     887.69
815.45     796.67     742.60
  708.97     565.49     555.34     296.41     199.95     146.31     123.11
 ZeroEnergy[kcal/mol]    3.8026136236017947
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           16
Geometry[angstrom]          15
C   0.30147   0.54069  -1.01467
C   0.29995   0.54491   0.47739
C   1.64335   0.54021   1.18553
C  -0.67120  -0.53389   0.82302
C  -1.18698  -1.04121  -0.30417
C  -0.57812  -0.36868  -1.45441
H   0.91039   1.20024  -1.61394
H   2.24362   1.39721   0.88038
H   1.51024   0.58594   2.26631
H   2.19714  -0.36809   0.94687
H  -0.91558  -0.81649   1.83560
H  -1.93389  -1.81817  -0.37158
H  -0.81431  -0.58178  -2.48634
H  -0.21829   1.52410   0.77577
H  -0.69886   2.66299   1.18783
           Core          RigidRotor
       SymmetryFactor    3.0000000000000000
End
 Rotor                  Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
 End
```

```
    Frequencies[1/cm]          37
  3247.1     3239.7     3223.1     3214.1     3127.9     3125.8     3050.0
2067.7     1659.6     1579.8
  1502.0     1499.9     1422.2     1411.9     1333.0     1277.7     1259.1
1170.3     1113.7     1098.5
  1083.6     1026.8     1007.1     978.22     977.87     960.98     887.27
815.85     796.36     742.20
  708.96     565.01     554.74     295.75     195.31     120.35     97.980
 ZeroEnergy[kcal/mol]    3.7805189724614165
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
 !**********************************************
 RRHO          !          17
 Geometry[angstrom]          15
 C    0.30157   0.54042  -1.01482
 C    0.29978   0.54539   0.47758
 C    1.64363   0.53983   1.18546
 C   -0.67113  -0.53419   0.82292
 C   -1.18694  -1.04133  -0.30423
 C   -0.57809  -0.36880  -1.45446
 H    0.91028   1.20009  -1.61421
 H    2.24388   1.39690   0.88042
 H    1.51055   0.58568   2.26625
 H    2.19747  -0.36840   0.94686
 H   -0.91578  -0.81673   1.83548
 H   -1.93405  -1.81811  -0.37168
 H   -0.81449  -0.58176  -2.48638
 H   -0.21667   1.52052   0.77454
 H   -0.70477   2.67637   1.19253
               Core           RigidRotor
        SymmetryFactor    3.0000000000000000
 End
  Rotor                       Hindered
  Group    8   9  10
  Axis           3          2
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.75    2.35    3.16    2.30    0.74    0.00    0.73    2.33    3.16    2.30
0.74    0.00    0.74    2.35    3.16    2.28    0.73
  End
    Frequencies[1/cm]          37
  3246.9     3239.4     3222.9     3214.0     3127.7     3126.1     3050.1
2140.7     1660.3     1580.4
  1502.3     1500.1     1422.3     1411.9     1333.2     1278.5     1259.5
1170.7     1113.7     1098.5
  1084.0     1026.2     1007.0     978.53     978.04     960.87     886.90
816.19     796.15     741.85
  709.03     564.59     554.22     295.21     192.78     91.640     66.000
 ZeroEnergy[kcal/mol]    3.7269180108655262
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
 !**********************************************
     Tunneling    Eckart
     ImaginaryFrequency[1/cm]    970.65998999999999
     WellDepth[kcal/mol]          4.08
     WellDepth[kcal/mol]         32.08
 End
End
End
```

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                      direct    ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                        diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                    10
!ChemicalEigenvalueMin               1.e-6         #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                  1.3
!!
RateOutput                             rate.out                 ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                            ! Default collisional
energy relaxation kernel
    Exponential                                               ! Currently the only
possible energy relaxation model
       Factor[1/cm]                    316                    ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                    0.535                         ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff                  10                     ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                          ! Collision frequency
model
    LennardJones                                              ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                     90.58  281.367         ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]                3.54    4.694          ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                     39.948  79.05478       ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!****************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]           14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.34058
 C    1.17550   0.00000   2.25991
 C   -1.39560  -0.00008   1.80105
 C   -2.21870  -0.00003   0.74716
 C   -1.40657  -0.00007  -0.51024
 H    0.87312   0.00029  -0.63540
 H    2.11196   0.00080   1.70444
 H    1.16259   0.87759   2.90932
 H    1.16343  -0.87842   2.90820
 H   -1.69080  -0.00015   2.84114
 H   -3.29750  -0.00010   0.77029
 H   -1.62068  -0.87614  -1.13069
 H   -1.62069   0.87579  -1.13094
        Core    RigidRotor
              SymmetryFactor    1.0000000000000000
        End
 Rotor                        Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry          3
 Potential[kcal/mol]          12
   0.00    0.09    0.33    0.68    1.06    1.36    1.47    1.36    1.06    0.68    0.33
0.09
 End
    Frequencies[1/cm]          35
  3241.0     3225.5     3207.9     3133.2     3100.2     3075.2     3043.9
3042.9     1708.1     1610.0
  1497.4     1487.3     1428.4     1422.7     1402.8     1311.9     1272.8
1227.8     1137.4     1111.0
  1073.3     1028.7     984.40     980.54     951.47     936.30     920.52
826.70     765.47     719.11
  624.46     583.63     368.96     327.69     231.38
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
 End
!************************************
 Fragment REACT2
  Atom
  Name H
  ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]           13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.41507
 C    1.18585   0.00000   2.30525
 C   -1.37924  -0.00034   1.86264
 C   -2.17195  -0.00056   0.76525
 C   -1.30652  -0.00033  -0.41759
 H    0.87955   0.00028  -0.62343
 H    2.11567   0.00259   1.73998
 H    1.17551   0.87449   2.96082
 H    1.17824  -0.87748   2.95691
```

```
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
      Core    RigidRotor
           SymmetryFactor    2.0000000000000000
      End
Rotor                          Hindered
Group    8   9  10
Axis            3           2
Symmetry            3
Potential[kcal/mol]          12
  0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
   Frequencies[1/cm]           32
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                     1
  0.0000000000000000       2.0000000000000000
End
!************************************
Fragment PROD2
RRHO
Geometry[angstrom]               2
H    0.00000   0.00000   0.00000
H    0.00000   0.00000   0.74312
      Core    RigidRotor
           SymmetryFactor    2.0000000000000000
      End
   Frequencies[1/cm]            1
  4433.4
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                     1
  0.0000000000000000       2.0000000000000000
End

GroundEnergy[kcal/mol]   -23.32
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]              15
C    0.00931  -0.07379   0.02173
C    0.01022  -0.04119   1.36182
C    1.18583   0.00299   2.27972
C   -1.38509  -0.05631   1.82377
C   -2.20858  -0.09746   0.77112
C   -1.39728  -0.11289  -0.48675
H    0.88187  -0.07280  -0.61452
H    2.12193   0.00766   1.72366
H    1.15688   0.89565   2.90779
H    1.19027  -0.85947   2.94926
H   -1.67959  -0.03658   2.86388
H   -3.28722  -0.11729   0.79522
H   -1.59508  -1.00781  -1.08537
H   -1.62839   0.74308  -1.12871
H   -2.66853   5.30700  -1.82485
      Core    RigidRotor
           SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]           38
  8.7211      18.630      156.72      234.80      327.31      368.19      583.61
624.59      719.14      766.53
  826.89      920.82      936.34      951.66      980.45      984.76      1029.1
1073.9      1110.9      1138.1
  1227.9      1273.5      1312.6      1402.9      1423.5      1429.0      1488.2
1498.0      1610.1      1709.1
  3041.6      3042.9      3074.3      3098.2      3133.7      3207.9      3224.8
3240.8
 ZeroEnergy[kcal/mol]             0.03
 ElectronicLevels[1/cm]                     1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]              15
C   -0.00234   0.00109   0.00448
C   -0.00153   0.00118   1.42136
C    1.18495  -0.00041   2.30992
C   -1.37880   0.03918   1.86883
C   -2.17166   0.06197   0.77078
C   -1.30734   0.03804  -0.41241
H    0.87694  -0.02129  -0.61873
H    2.10831  -0.14134   1.75166
H    1.25305   0.94803   2.85056
H    1.10605  -0.78587   3.06458
H   -1.69300   0.04830   2.90047
H   -3.24958   0.09153   0.74958
H   -1.65599   0.04839  -1.43366
H   -0.61218   2.74193   1.11442
H   -0.36891   3.43886   1.21364
      Core    RigidRotor
           SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]           39
  6.3107      38.664      62.874      110.59      181.04      217.33      226.10
329.58      527.51      533.43
  605.59      637.98      730.58      742.39      902.50      923.96      931.36
955.69      1013.1      1023.0
  1052.0      1097.8      1179.4      1293.5      1311.7      1407.2      1438.2
1475.2      1484.9      1506.0
  1581.9      3031.9      3087.4      3139.1      3226.3      3234.1      3248.4
3256.5      4405.4
 ZeroEnergy[kcal/mol]             -24.06
 ElectronicLevels[1/cm]                     1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier       B1  REACS WR
  RRHO
    Stoichiometry  H9C6
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]              14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34058
C    1.17550   0.00000   2.25991
C   -1.39560  -0.00008   1.80105
C   -2.21870  -0.00003   0.74716
C   -1.40657  -0.00007  -0.51024
H    0.87312   0.00029  -0.63540
H    2.11196   0.00080   1.70444
H    1.16259   0.87759   2.90932
H    1.16343  -0.87842   2.90820
H   -1.69080  -0.00015   2.84114
H   -3.29750  -0.00010   0.77029
H   -1.62068  -0.87614  -1.13069
H   -1.62069   0.87579  -1.13094
      FragmentGeometry[angstrom]              1
H                  0. 0. 0.
                         SymmetryFactor     1.0000000000000000
         PotentialPrefactor[au]              10.
         PotentialPowerExponent           6
                 End
Rotor                          Hindered
Geometry[angstrom]             14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34058
```

```
C   1.17550   0.00000   2.25991
C  -1.39560  -0.00008   1.80105
C  -2.21870  -0.00003   0.74716
C  -1.40657  -0.00007  -0.51024
H   0.87312   0.00029  -0.63540
H   2.11196   0.00080   1.70444
H   1.16259   0.87759   2.90932
H   1.16343  -0.87842   2.90820
H  -1.69080  -0.00015   2.84114
H  -3.29750  -0.00010   0.77029
H  -1.62068  -0.87614  -1.13069
H  -1.62069   0.87579  -1.13094
Group    8   9  10
Axis            3          2
Symmetry           3
Potential[kcal/mol]          12
  0.0000     0.90000E-01 0.33000     0.68000      1.0600      1.3600      1.4700
1.3600      1.0600     0.68000
 0.33000     0.90000E-01
End
   Frequencies[1/cm]          35
  3241.0      3225.5      3207.9      3133.2      3100.2      3075.2      3043.9
3042.9      1708.1      1610.0
  1497.4      1487.3      1428.4      1422.7      1402.8      1311.9      1272.8
1227.8      1137.4      1111.0
  1073.3      1028.7      984.40      980.54      951.47      936.30      920.52
826.70      765.47      719.11
  624.46      583.63      368.96      327.69      231.38
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       4.0000000000000000
End
!************************************
Barrier        B3  WP PRODS
  RRHO
    Stoichiometry  H9C6
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]              13
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.41507
C   1.18585   0.00000   2.30525
C  -1.37924  -0.00034   1.86264
C  -2.17195  -0.00056   0.76525
C  -1.30652  -0.00033  -0.41759
H   0.87955   0.00028  -0.62343
H   2.11567   0.00259   1.73998
H   1.17551   0.87449   2.96082
H   1.17824  -0.87748   2.95691
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
      FragmentGeometry[angstrom]              2
H   0.00000   0.00000   0.00000
H   0.00000   0.00000   0.74312
                                        SymmetryFactor     4.0000000000000000
        PotentialPrefactor[au]                 10.
        PotentialPowerExponent            6
                End
Rotor                               Hindered
Geometry[angstrom]              13
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.41507
C   1.18585   0.00000   2.30525
C  -1.37924  -0.00034   1.86264
C  -2.17195  -0.00056   0.76525
C  -1.30652  -0.00033  -0.41759
H   0.87955   0.00028  -0.62343
H   2.11567   0.00259   1.73998
H   1.17551   0.87449   2.96082
H   1.17824  -0.87748   2.95691
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
Group    8   9  10
Axis            3          2
Symmetry           3
Potential[kcal/mol]          12
  0.0000     0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01  0.0000     0.20000E-01 0.40000E-01 0.60000E-01
 0.40000E-01 0.10000E-01
End
   Frequencies[1/cm]          33
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
  4433.4
 ZeroEnergy[kcal/mol]          -23.324282260871254
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO           !           6
Geometry[angstrom]           15
C   0.62775  -0.03577  -0.92097
C   0.62708  -0.03551   0.42168
C   1.80186  -0.03502   1.34003
C  -0.76953  -0.03646   0.88226
C  -1.59241  -0.03844  -0.17377
C  -0.77194  -0.00347  -1.41328
H   1.49691  -0.03089  -1.56080
H   2.73832  -0.04271   0.78487
H   1.79269   0.84747   1.98295
H   1.78435  -0.90830   1.99511
H  -1.06509  -0.03420   1.92201
H  -2.67082  -0.03348  -0.15904
H  -1.03564  -0.72130  -2.19014
H  -0.95421   1.02036  -1.92022
H  -1.16744   2.10190  -2.47365
              Core            RigidRotor
         SymmetryFactor    1.5000000000000000
End
 Rotor                         Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]          37
  3246.4      3231.9      3211.6      3135.3      3107.7      3098.4      3041.8
1920.2      1696.9      1599.6
  1496.9      1487.6      1425.5      1404.1      1337.1      1319.2      1270.9
1230.2      1112.7      1096.9
  1072.1      1027.4      986.24      975.60      965.98      937.99      919.45
829.81      773.84      723.83
  623.99      587.19      442.68      328.25      254.79      105.24      58.780
ZeroEnergy[kcal/mol]    5.2195259538240908
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO           !           7
Geometry[angstrom]           15
C   0.62760  -0.03562  -0.92119
C   0.62706  -0.03542   0.42168
C   1.80184  -0.03504   1.33999
C  -0.76955  -0.03637   0.88225
C  -1.59242  -0.03830  -0.17399
C  -0.77174  -0.00376  -1.41284
H   1.49671  -0.03101  -1.56106
H   2.73830  -0.04270   0.78485
```

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H   1.79261   0.84746   1.98290
H   1.78429  -0.90830   1.99509
H  -1.06517  -0.03430   1.92196
H  -2.67081  -0.03356  -0.15937
H  -1.03639  -0.71787  -2.19256
H  -0.95513   1.02736  -1.92217
H  -1.16515   2.08996  -2.46762
            Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.31   0.99   1.37   0.98   0.31   0.00   0.28   0.96   1.37   0.96
0.28   0.00   0.31   0.98   1.37   0.99   0.30
 End
   Frequencies[1/cm]          37
  3246.7     3232.3     3211.9     3135.4     3109.7     3098.4     3041.8
1822.7     1695.2     1598.3
  1496.7     1487.5     1425.5     1403.8     1330.5     1319.2     1270.8
1229.8     1112.5     1096.3
  1071.9     1027.1     986.55     975.25     966.45     939.16     919.51
829.49     775.10     724.51
  623.71     587.89     453.10     328.62     259.59     142.32     99.790
ZeroEnergy[kcal/mol]    5.3020156589437892
 ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !          8
Geometry[angstrom]          15
C   0.62745  -0.03548  -0.92142
C   0.62705  -0.03533   0.42168
C   1.80182  -0.03506   1.33995
C  -0.76956  -0.03630   0.88224
C  -1.59243  -0.03816  -0.17422
C  -0.77152  -0.00413  -1.41236
H   1.49651  -0.03115  -1.56129
H   2.73829  -0.04270   0.78483
H   1.79254   0.84746   1.98286
H   1.78425  -0.90829   1.99508
H  -1.06525  -0.03440   1.92192
H  -2.67079  -0.03365  -0.15968
H  -1.03713  -0.71452  -2.19491
H  -0.95625   1.03507  -1.92466
H  -1.16294   2.07847  -2.46181
            Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.31   0.99   1.37   0.98   0.31   0.00   0.28   0.96   1.37   0.96
0.28   0.00   0.31   0.98   1.37   0.99   0.30
 End
   Frequencies[1/cm]          37
  3247.0     3232.6     3212.1     3135.5     3112.0     3098.3     3041.8
1726.5     1691.4     1596.1
  1496.6     1487.5     1425.4     1403.5     1323.3     1319.2     1270.7
1229.2     1112.3     1095.6
  1071.7     1026.7     986.90     974.88     966.87     940.43     919.56
829.11     776.53     725.29
  623.41     588.67     464.96     329.13     265.66     174.46     129.18
ZeroEnergy[kcal/mol]    5.3480098482422154
 ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !          9
Geometry[angstrom]          15
C   0.62729  -0.03535  -0.92164
C   0.62703  -0.03525   0.42169
C   1.80179  -0.03507   1.33990
C  -0.76956  -0.03623   0.88223
C  -1.59243  -0.03803  -0.17444
C  -0.77130  -0.00456  -1.41186
H   1.49632  -0.03129  -1.56151
H   2.73827  -0.04270   0.78482
H   1.79246   0.84745   1.98282
H   1.78420  -0.90828   1.99507
H  -1.06531  -0.03451   1.92188
H  -2.67077  -0.03374  -0.15996
H  -1.03783  -0.71125  -2.19717
H  -0.95754   1.04348  -1.92768
H  -1.16083   2.06748  -2.45625
            Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.31   0.99   1.37   0.98   0.31   0.00   0.28   0.96   1.37   0.96
0.28   0.00   0.31   0.98   1.37   0.99   0.30
 End
   Frequencies[1/cm]          37
  3247.3     3232.9     3212.4     3135.6     3114.4     3098.3     3041.7
1694.3     1633.2     1588.1
  1496.4     1487.4     1425.3     1403.1     1318.9     1315.4     1270.4
1228.4     1112.1     1094.9
  1071.4     1026.3     987.30     974.49     967.21     941.76     919.59
828.68     778.15     726.20
  623.08     589.54     478.18     329.90     273.43     202.92     152.27
ZeroEnergy[kcal/mol]    5.3694318753402275
 ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !          10
Geometry[angstrom]          15
C   0.62712  -0.03522  -0.92179
C   0.62697  -0.03517   0.42165
C   1.80175  -0.03508   1.33985
C  -0.76958  -0.03615   0.88216
C  -1.59236  -0.03791  -0.17461
C  -0.77104  -0.00507  -1.41129
H   1.49609  -0.03144  -1.56162
H   2.73820  -0.04269   0.78481
H   1.79237   0.84742   1.98275
H   1.78414  -0.90826   1.99504
H  -1.06535  -0.03462   1.92172
H  -2.67068  -0.03382  -0.16020
H  -1.03848  -0.70803  -2.19930
H  -0.95898   1.05246  -1.93111
H  -1.15881   2.05695  -2.45092
            Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.31   0.99   1.37   0.98   0.31   0.00   0.28   0.96   1.37   0.96
0.28   0.00   0.31   0.98   1.37   0.99   0.30
 End
   Frequencies[1/cm]          37
  3247.6     3233.6     3213.0     3136.0     3117.3     3098.5     3042.0
1692.1     1603.0     1533.2
  1496.0     1487.3     1425.1     1402.7     1318.5     1307.3     1270.0
1227.2     1111.9     1094.0
  1071.1     1025.7     987.68     974.11     967.43     943.01     919.59
828.25     779.80     727.21
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 622.73     590.33     492.31     331.08     283.13     227.14     169.97
ZeroEnergy[kcal/mol]   5.3776611312726619
 ElectronicLevels[1/cm]              1
 0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO         !         11
Geometry[angstrom]         15
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34370
C    1.17478   0.00000   2.26183
C   -1.39654  -0.00099   1.80419
C   -2.21933  -0.00269   0.74718
C   -1.39776   0.02942  -0.48872
H    0.86896   0.00350  -0.63980
H    2.11124  -0.00759   1.70681
H    1.16535   0.88252   2.90474
H    1.15716  -0.87315   2.91706
H   -1.69236   0.00037   2.84372
H   -3.29762   0.00116   0.76157
H   -1.66609  -0.66990  -1.27935
H   -1.58762   1.09751  -1.01327
H   -1.78393   2.08251  -1.52407
           Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                       Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]         37
 3247.8     3233.9     3213.3     3136.1     3120.2     3098.4     3041.9
1689.8     1599.1     1496.3
 1487.2     1460.5     1425.0     1402.3     1317.9     1299.2     1269.4
1225.7     1111.7     1093.2
 1070.7     1025.2     988.23     973.78     967.46     944.12     919.53
827.76     781.90     728.44
 622.36     591.44     507.80     333.53     295.26     247.53     183.93
ZeroEnergy[kcal/mol]   5.3689957505635437
 ElectronicLevels[1/cm]              1
 0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO         !         12
Geometry[angstrom]         15
C    0.62680  -0.03498  -0.92223
C    0.62695  -0.03502   0.42173
C    1.80173  -0.03511   1.33979
C   -0.76957  -0.03603   0.88220
C   -1.59237  -0.03767  -0.17505
C   -0.77055  -0.00630  -1.41016
H    1.49576  -0.03175  -1.56200
H    2.73819  -0.04269   0.78479
H    1.79225   0.84742   1.98270
H    1.78409  -0.90824   1.99506
H   -1.06545  -0.03484   1.92169
H   -2.67064  -0.03405  -0.16068
H   -1.03978  -0.70197  -2.20342
H   -0.96234   1.07236  -1.93945
H   -1.15513   2.03787  -2.44123
           Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                       Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]         37
 3248.1     3234.1     3213.6     3136.1     3122.9     3098.3     3041.9
1687.6     1597.3     1496.0
 1487.1     1424.8     1406.2     1400.4     1317.0     1292.5     1268.6
1223.7     1111.5     1091.9
 1070.4     1024.5     988.69     973.52     967.28     944.85     919.40
827.33     784.10     729.72
 622.00     592.59     522.75     338.20     306.47     261.82     192.80
ZeroEnergy[kcal/mol]   5.3327725786980427
 ElectronicLevels[1/cm]              1
 0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO         !         13
Geometry[angstrom]         15
C    0.62665  -0.03487  -0.92251
C    0.62697  -0.03495   0.42183
C    1.80174  -0.03513   1.33979
C   -0.76955  -0.03597   0.88230
C   -1.59243  -0.03755  -0.17531
C   -0.77031  -0.00701  -1.40959
H    1.49566  -0.03190  -1.56224
H    2.73823  -0.04269   0.78477
H    1.79221   0.84745   1.98272
H    1.78409  -0.90826   1.99510
H   -1.06552  -0.03494   1.92179
H   -2.67067  -0.03419  -0.16091
H   -1.04041  -0.69912  -2.20541
H   -0.96422   1.08305  -1.94420
H   -1.15347   2.02927  -2.43684
           Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                       Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]         37
 3248.4     3234.0     3213.5     3135.9     3125.4     3097.9     3041.5
1684.7     1595.4     1495.7
 1487.0     1424.7     1401.6     1360.8     1315.9     1287.6     1267.7
1221.5     1111.3     1090.7
 1070.0     1023.9     989.30     973.40     966.88     945.28     919.21
826.94     786.80     731.19
 621.66     594.03     537.57     346.71     314.53     272.56     198.96
ZeroEnergy[kcal/mol]   5.2627879996586149
 ElectronicLevels[1/cm]              1
 0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO         !         14
Geometry[angstrom]         15
C    0.62649  -0.03477  -0.92274
C    0.62697  -0.03488   0.42189
C    1.80174  -0.03515   1.33977
C   -0.76953  -0.03592   0.88235
C   -1.59244  -0.03745  -0.17553
C   -0.77006  -0.00778  -1.40897
H    1.49552  -0.03205  -1.56241
H    2.73823  -0.04269   0.78476
H    1.79216   0.84745   1.98271
H    1.78408  -0.90825   1.99512
H   -1.06556  -0.03504   1.92180
H   -2.67066  -0.03432  -0.16112
H   -1.04101  -0.69629  -2.20730
H   -0.96617   1.09406  -1.94916
H   -1.15189   2.02111  -2.43269
           Core          RigidRotor
      SymmetryFactor    1.5000000000000000
```

```
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]          37
  3248.6     3234.2     3213.8     3135.9     3128.4     3097.8     3041.4
1682.1     1594.2     1495.5
  1486.9     1424.5     1401.2     1332.0     1314.0     1284.0     1267.0
1219.6     1111.0     1089.5
  1069.6     1023.0     989.84     973.40     966.22     945.21     918.94
826.71     789.59     732.73
  621.36     595.43     550.85     357.16     318.52     279.63     202.28
 ZeroEnergy[kcal/mol]    5.1580984960981358
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
RRHO          !          15
Geometry[angstrom]          15
C    0.62633  -0.03467  -0.92297
C    0.62696  -0.03481   0.42195
C    1.80174  -0.03517   1.33975
C   -0.76952  -0.03586   0.88239
C   -1.59244  -0.03735  -0.17575
C   -0.76979  -0.00859  -1.40833
H    1.49539  -0.03221  -1.56257
H    2.73823  -0.04268   0.78476
H    1.79211   0.84745   1.98270
H    1.78407  -0.90824   1.99514
H   -1.06559  -0.03513   1.92180
H   -2.67064  -0.03445  -0.16132
H   -1.04159  -0.69350  -2.20915
H   -0.96818   1.10534  -1.95432
H   -1.15040   2.01342  -2.42877
             Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]          37
  3248.8     3234.4     3214.1     3136.0     3131.4     3097.7     3041.3
1679.4     1593.1     1495.2
  1486.8     1424.3     1400.9     1322.7     1311.3     1275.7     1266.5
1218.4     1110.9     1088.1
  1069.1     1022.1     990.30     973.53     965.34     944.60     918.59
826.64     792.50     734.24
  621.12     596.88     562.01     366.49     320.33     283.72     203.35
 ZeroEnergy[kcal/mol]    5.0086406083062531
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
RRHO          !          16
Geometry[angstrom]          15
C    0.62617  -0.03457  -0.92319
C    0.62696  -0.03475   0.42202
C    1.80174  -0.03518   1.33973
C   -0.76950  -0.03581   0.88244
C   -1.59244  -0.03725  -0.17597
C   -0.76951  -0.00945  -1.40767
H    1.49526  -0.03238  -1.56272
H    2.73823  -0.04268   0.78475
H    1.79207   0.84745   1.98269
H    1.78406  -0.90824   1.99516
H   -1.06563  -0.03523   1.92181
H   -2.67062  -0.03458  -0.16151
H   -1.04216  -0.69073  -2.21097
H   -0.97025   1.11687  -1.95967
H   -1.14901   2.00618  -2.42508
             Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]          37
  3249.0     3234.6     3214.3     3136.0     3134.5     3097.5     3041.2
1676.6     1592.3     1495.0
  1486.7     1424.1     1400.9     1332.0     1310.9     1267.2     1258.6
1217.9     1110.7     1086.3
  1068.5     1021.1     990.59     973.78     964.28     943.40     918.17
826.77     795.34     735.61
  620.95     598.31     570.64     372.88     321.12     285.17     202.48
 ZeroEnergy[kcal/mol]    4.7993481008150685
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          17
Geometry[angstrom]          15
C    0.62600  -0.03448  -0.92342
C    0.62695  -0.03468   0.42209
C    1.80173  -0.03520   1.33971
C   -0.76948  -0.03576   0.88249
C   -1.59244  -0.03715  -0.17619
C   -0.76922  -0.01035  -1.40698
H    1.49513  -0.03255  -1.56286
H    2.73823  -0.04268   0.78474
H    1.79202   0.84745   1.98268
H    1.78406  -0.90823   1.99518
H   -1.06566  -0.03533   1.92181
H   -2.67060  -0.03472  -0.16169
H   -1.04272  -0.68795  -2.21278
H   -0.97237   1.12861  -1.96516
H   -1.14770   1.99939  -2.42162
             Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]          37
  3249.1     3234.8     3214.6     3137.6     3136.0     3097.3     3041.1
1673.7     1591.9     1494.8
  1486.6     1423.9     1402.4     1357.0     1310.2     1266.8     1240.6
1217.4     1110.6     1083.9
  1067.9     1020.0     990.59     974.08     963.04     941.43     917.66
827.06     797.86     736.70
  620.80     599.55     576.71     375.67     321.31     284.19     199.74
 ZeroEnergy[kcal/mol]    4.5351951579475287
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          18
Geometry[angstrom]          15
C    0.62582  -0.03438  -0.92365
```

```
C   0.62694  -0.03462   0.42217
C   1.80173  -0.03521   1.33969
C  -0.76945  -0.03570   0.88254
C  -1.59244  -0.03706  -0.17641
C  -0.76892  -0.01131  -1.40626
H   1.49500  -0.03273  -1.56300
H   2.73822  -0.04268   0.78474
H   1.79198   0.84746   1.98267
H   1.78405  -0.90822   1.99520
H  -1.06568  -0.03542   1.92182
H  -2.67058  -0.03486  -0.16187
H  -1.04329  -0.68516  -2.21459
H  -0.97452   1.14052  -1.97077
H  -1.14647   1.99305  -2.41839
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]          37
  3249.3      3234.9      3214.9      3140.7      3136.1      3097.2      3041.0
1670.7      1592.5      1494.7
  1486.4      1423.7      1416.3      1386.5      1309.1      1266.5      1224.4
1214.3      1110.4      1080.2
  1067.2      1018.8      990.18      974.37      961.67      938.43      917.05
827.43      799.83      737.42
  620.58      600.42      580.56      374.77      321.02      280.95      195.02
ZeroEnergy[kcal/mol]    4.2169394527246613
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!********************************************
RRHO          !          19
Geometry[angstrom]          15
C   0.62565  -0.03429  -0.92389
C   0.62693  -0.03455   0.42226
C   1.80173  -0.03522   1.33968
C  -0.76943  -0.03565   0.88260
C  -1.59243  -0.03697  -0.17664
C  -0.76861  -0.01233  -1.40551
H   1.49487  -0.03291  -1.56314
H   2.73822  -0.04268   0.78473
H   1.79193   0.84746   1.98266
H   1.78405  -0.90821   1.99522
H  -1.06571  -0.03552   1.92184
H  -2.67056  -0.03501  -0.16204
H  -1.04386  -0.68231  -2.21642
H  -0.97670   1.15259  -1.97648
H  -1.14534   1.98718  -2.41540
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]          37
  3249.4      3235.0      3215.1      3143.7      3136.1      3097.0      3040.8
1667.8      1596.0      1495.6
  1486.3      1469.1      1423.4      1393.5      1307.9      1266.2      1219.4
1199.1      1110.2      1074.8
  1066.3      1017.5      989.25      974.59      960.20      934.23      916.32
827.74      801.10      737.70
  620.16      600.78      582.70      370.57      320.23      275.60      188.02
ZeroEnergy[kcal/mol]    3.8471113271228621
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!********************************************
RRHO          !          20
Geometry[angstrom]          15
C   0.62546  -0.03420  -0.92413
C   0.62692  -0.03449   0.42235
C   1.80172  -0.03524   1.33966
C  -0.76939  -0.03559   0.88266
C  -1.59242  -0.03687  -0.17688
C  -0.76828  -0.01340  -1.40472
H   1.49474  -0.03311  -1.56329
H   2.73822  -0.04268   0.78472
H   1.79189   0.84746   1.98266
H   1.78404  -0.90821   1.99525
H  -1.06573  -0.03561   1.92186
H  -2.67054  -0.03517  -0.16222
H  -1.04444  -0.67937  -2.21829
H  -0.97891   1.16478  -1.98228
H  -1.14431   1.98180  -2.41267
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
   Frequencies[1/cm]          37
  3249.5      3235.1      3215.4      3146.8      3136.1      3096.8      3040.7
1665.3      1616.1      1538.9
  1492.7      1486.2      1423.2      1394.4      1306.8      1265.9      1218.2
1178.8      1110.0      1068.5
  1063.0      1016.3      987.69      974.63      958.65      928.76      915.42
827.84      801.66      737.56
  619.46      600.64      583.62      363.86      318.75      268.24      178.35
ZeroEnergy[kcal/mol]    3.4355455093743377
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!********************************************
RRHO          !          21
Geometry[angstrom]          15
C   0.62526  -0.03411  -0.92439
C   0.62690  -0.03442   0.42245
C   1.80171  -0.03525   1.33964
C  -0.76936  -0.03554   0.88273
C  -1.59242  -0.03678  -0.17713
C  -0.76793  -0.01455  -1.40389
H   1.49461  -0.03332  -1.56343
H   2.73822  -0.04267   0.78471
H   1.79185   0.84746   1.98266
H   1.78404  -0.90820   1.99527
H  -1.06576  -0.03571   1.92188
H  -2.67052  -0.03533  -0.16240
H  -1.04504  -0.67634  -2.22022
H  -0.98114   1.17709  -1.98813
H  -1.14339   1.97698  -2.41023
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.31    0.99    1.37    0.98    0.31    0.00    0.28    0.96    1.37    0.96
0.28    0.00    0.31    0.98    1.37    0.99    0.30
 End
```

```
    Frequencies[1/cm]       37
  3249.6    3235.2    3215.7    3149.9    3136.1    3096.5    3040.5
1706.1    1659.2    1567.8
  1492.9    1486.0    1423.0    1394.3    1305.8    1265.7    1217.1
1156.1    1109.9    1066.5
  1051.7    1015.1    985.34    974.36    957.04    922.14    914.10
827.57    801.49    737.04
  618.46    600.08    583.67    355.86    316.22    258.84    165.66
 ZeroEnergy[kcal/mol]    2.9982660480116028
  ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
 !*********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1243.4800000000000
      WellDepth[kcal/mol]         5.46
      WellDepth[kcal/mol]        29.56
 End
End
End
```

```
!****************************************************
!             GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                  0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature          .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature        30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]         400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                  direct    ! direct or low-eigenvalue
!
WellCutoff                         20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax              0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                    diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!
!WellCutoff                        10
!ChemicalEigenvalueMin             1.e-6        #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]              1.3
!!
RateOutput                         rate.out              ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!             MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                   ! Default collisional
energy relaxation kernel
    Exponential                                      ! Currently the only
possible energy relaxation model
       Factor[1/cm]           316                    ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                  0.535                  ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff         10                     ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                 ! Collision frequency
model
    LennardJones                                     ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]            90.58  281.367         ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]       3.54   4.694           ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]            39.948  79.05478       ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.34058
 C    1.17550   0.00000   2.25991
 C   -1.39560  -0.00008   1.80105
 C   -2.21870  -0.00003   0.74716
 C   -1.40657  -0.00007  -0.51024
 H    0.87312   0.00029  -0.63540
 H    2.11196   0.00080   1.70444
 H    1.16259   0.87759   2.90932
 H    1.16343  -0.87842   2.90820
 H   -1.69080  -0.00015   2.84114
 H   -3.29750  -0.00010   0.77029
 H   -1.62068  -0.87614  -1.13069
 H   -1.62069   0.87579  -1.13094
        Core    RigidRotor
            SymmetryFactor    1.0000000000000000
        End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]         12
   0.00    0.08    0.32    0.66    1.03    1.33    1.44    1.32    1.03    0.66    0.32
0.08
 End
    Frequencies[1/cm]          35
   3241.0      3225.5      3207.9      3133.2      3100.2      3075.2      3043.9
3042.9      1708.1      1610.0
   1497.4      1487.3      1428.4      1422.7      1402.8      1311.9      1272.8
1227.8      1137.4      1111.0
   1073.3      1028.7      984.40      980.54      951.47      936.30      920.52
826.70      765.47      719.11
   624.46      583.63      368.96      327.69      231.38
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                  1
   0.0000000000000000       2.0000000000000000
 End
!************************************
 Fragment REACT2
  Atom
  Name H
  ElectronicLevels[1/cm]                  1
   0.0000000000000000       2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]          13
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.39409
 C    1.09038   0.00000   2.23479
 C   -1.41361  -0.00005   1.81740
 C   -2.21408  -0.00003   0.75182
 C   -1.40220  -0.00009  -0.51215
 H    0.87980   0.00015  -0.62484
 H    0.96884   0.00014   3.30847
 H    2.09635   0.00011   1.83997
```

```
H  -1.72745  -0.00007   2.85132
H  -3.29354  -0.00010   0.76608
H  -1.61710  -0.87505  -1.13573
H  -1.61723   0.87450  -1.13618
    Core    RigidRotor
        SymmetryFactor    1.0000000000000000
    End
  Frequencies[1/cm]          33
  219.96     352.42     358.87     544.30     592.50     660.67     666.69
754.46     795.14     796.70
  925.16     926.06     951.77     962.74     984.98     1025.4     1111.8
1138.0     1259.1     1288.2
  1330.6     1389.7     1438.7     1448.7     1521.5     1659.2     3024.6
3049.1     3164.7     3213.4
  3231.7     3238.8     3260.5
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End

!************************************
Fragment PROD2
RRHO
Geometry[angstrom]              2
H    0.00000   0.00000   0.00000
H    0.00000   0.00000   0.74312
    Core    RigidRotor
        SymmetryFactor    2.0000000000000000
    End
  Frequencies[1/cm]           1
  4433.4
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End

GroundEnergy[kcal/mol]   -16.57
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]             15
C    0.00011  -0.03461  -0.00904
C    0.00314  -0.07208   1.33092
C    1.18043  -0.09643   2.24739
C   -1.39170  -0.08645   1.79434
C   -2.21699  -0.05786   0.74269
C   -1.40753  -0.02178  -0.51594
H    0.87182  -0.01603  -0.64619
H    2.11580  -0.08102   1.69029
H    1.16890   0.76366   2.91986
H    1.16956  -0.99161   2.87243
H   -1.68461  -0.11584   2.83466
H   -3.29578  -0.05966   0.76797
H   -1.62217  -0.88009  -1.16057
H   -1.62386   0.87096  -1.11136
H   -0.71217   5.29072   2.98853
    Core    RigidRotor
        SymmetryFactor   0.50000000000000000
    End
  Frequencies[1/cm]          39
  1.9701     9.3266     19.247     156.29     235.01     327.39     368.31
583.67     624.59     719.14
  766.42     826.89     920.85     936.36     951.69     980.48     984.79
1029.2     1074.0     1111.0
  1138.2     1227.9     1273.5     1312.6     1402.9     1423.6     1429.0
1488.2     1498.0     1610.1
  1709.1     3041.7     3042.6     3073.9     3098.3     3133.7     3208.0
3224.9     3240.7
 ZeroEnergy[kcal/mol]             0.03
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]             15
C   -0.00157   0.00062   0.00430
C   -0.00141   0.00015   1.39830
C    1.08930  -0.00053   2.23918
C   -1.41477   0.00691   1.82167
C   -2.21502   0.01208   0.75560
C   -1.40324   0.00896  -0.50771
H    0.87825  -0.00066  -0.62043
H    2.09514  -0.00289   1.84415
H   -0.79938   2.72401   0.58489
H    0.96776   0.00065   3.31282
H   -1.72886   0.00923   2.85546
H   -3.29439   0.01958   0.76977
H   -1.62368  -0.86192  -1.13475
H   -1.61169   0.88882  -1.12702
H   -0.99028   3.35857   0.24540
    Core    RigidRotor
        SymmetryFactor   0.50000000000000000
    End
  Frequencies[1/cm]          38
  73.478     102.66     157.57     223.93     239.73     352.31     356.64
545.49     593.60     660.98
  670.51     754.95     795.09     797.37     924.83     925.52     952.46
963.35     985.88     1026.0
  1111.9     1138.9     1259.3     1288.4     1331.2     1390.0     1435.5
1448.0     1521.1     1658.2
  3024.5     3049.7     3165.1     3214.1     3232.4     3239.6     3261.2
4409.5
 ZeroEnergy[kcal/mol]            -16.86
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier        B1  REACS WR
  RRHO
    Stoichiometry  H9C6
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]             14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34058
C    1.17550   0.00000   2.25991
C   -1.39560  -0.00008   1.80105
C   -2.21870  -0.00003   0.74716
C   -1.40657  -0.00007  -0.51024
H    0.87312   0.00029  -0.63540
H    2.11196   0.00080   1.70444
H    1.16259   0.87759   2.90932
H    1.16343  -0.87842   2.90820
H   -1.69080  -0.00015   2.84114
H   -3.29750  -0.00010   0.77029
H   -1.62068  -0.87614  -1.13069
H   -1.62069   0.87579  -1.13094
      FragmentGeometry[angstrom]             1
H                  0. 0. 0.
                          SymmetryFactor     1.0000000000000000
      PotentialPrefactor[au]            10.
      PotentialPowerExponent            6
              End
Rotor                     Hindered
Geometry[angstrom]             14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34058
C    1.17550   0.00000   2.25991
C   -1.39560  -0.00008   1.80105
C   -2.21870  -0.00003   0.74716
C   -1.40657  -0.00007  -0.51024
H    0.87312   0.00029  -0.63540
H    2.11196   0.00080   1.70444
```

```
H   1.16259   0.87759   2.90932
H   1.16343  -0.87842   2.90820
H  -1.69080  -0.00015   2.84114
H  -3.29750  -0.00010   0.77029
H  -1.62068  -0.87614  -1.13069
H  -1.62069   0.87579  -1.13094
Group    8   9  10
Axis            3           2
Symmetry           3
Potential[kcal/mol]          12
  0.0000     0.80000E-01 0.32000     0.66000      1.0300      1.3300      1.4400
1.3200      1.0300     0.66000
 0.32000     0.80000E-01
End
  Frequencies[1/cm]          35
  3241.0      3225.5      3207.9      3133.2      3100.2      3075.2      3043.9
3042.9      1708.1      1610.0
  1497.4      1487.3      1428.4      1422.7      1402.8      1311.9      1272.8
1227.8      1137.4      1111.0
  1073.3      1028.7      984.40      980.54      951.47      936.30      920.52
826.70      765.47      719.11
  624.46      583.63      368.96      327.69      231.38
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       4.0000000000000000
End
!************************************
Barrier        B3  WP PRODS
 RRHO
  Stoichiometry  H9C6
  Core PhaseSpaceTheory
    FragmentGeometry[angstrom]              13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.39409
C    1.09038   0.00000   2.23479
C   -1.41361  -0.00005   1.81740
C   -2.21408  -0.00003   0.75182
C   -1.40220  -0.00009  -0.51215
H    0.87980   0.00015  -0.62484
H    0.96884   0.00014   3.30847
H    2.09635   0.00011   1.83997
H   -1.72745  -0.00007   2.85132
H   -3.29354  -0.00010   0.76608
H   -1.61710  -0.87505  -1.13573
H   -1.61723   0.87450  -1.13618
    FragmentGeometry[angstrom]              2
H    0.00000   0.00000   0.00000
H    0.00000   0.00000   0.74312
                        SymmetryFactor     2.0000000000000000
       PotentialPrefactor[au]               10.
       PotentialPowerExponent              6
               End
  Frequencies[1/cm]          34
  219.96      352.42      358.87      544.30      592.50      660.67      666.69
754.46      795.14      796.70
  925.16      926.06      951.77      962.74      984.98      1025.4      1111.8
1138.0      1259.1      1288.2
  1330.6      1389.7      1438.7      1448.7      1521.5      1659.2      3024.6
3049.1      3164.7      3213.4
  3231.7      3238.8      3260.5
  4433.4
 ZeroEnergy[kcal/mol]          -16.568221582375752
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO          !           5
Geometry[angstrom]          15
C    0.58706  -0.05656  -0.97497
C    0.58580  -0.05651   0.36893
C    1.75223  -0.05183   1.26726
C   -0.80812  -0.00941   0.83063
C   -1.62887   0.01156  -0.22410
C   -0.81821  -0.01673  -1.48245
H    1.45991  -0.08501  -1.60993
H    2.68698  -0.30589   0.77304
H    1.91222   1.02950   1.66827
H    1.61678  -0.64426   2.17087
H   -1.10214   0.00378   1.87066
H   -2.70714   0.04341  -0.20158
H   -1.05825  -0.88593  -2.10298
H   -1.00502   0.86442  -2.10477
H    2.12720   2.11702   2.09293
          Core           RigidRotor
     SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15
 Axis            3           2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.13    0.53    1.16    2.00    2.94    3.89    2.13    1.53    0.95    0.46
0.12
 End
   Frequencies[1/cm]          37
  3242.9      3227.6      3211.6      3160.1      3087.3      3073.8      3042.6
1821.0      1681.2      1605.7
  1469.2      1429.4      1416.9      1381.8      1355.8      1312.5      1274.1
1236.6      1138.0      1111.9
  1064.9      1034.5      984.34      980.45      952.70      935.49      924.38
826.26      765.53      721.72
  636.42      595.41      373.07      363.16      310.28      258.85      76.430
ZeroEnergy[kcal/mol]    6.5834749479909025
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !           6
Geometry[angstrom]          15
C    0.58712  -0.05646  -0.97503
C    0.58605  -0.05641   0.36931
C    1.75178  -0.05230   1.26677
C   -0.80812  -0.00941   0.83069
C   -1.62879   0.01155  -0.22406
C   -0.81818  -0.01673  -1.48245
H    1.45994  -0.08492  -1.61001
H    2.68774  -0.30348   0.77363
H    1.91366   1.03837   1.67111
H    1.61691  -0.64103   2.17270
H   -1.10220   0.00383   1.87069
H   -2.70705   0.04342  -0.20155
H   -1.05814  -0.88594  -2.10302
H   -1.00494   0.86440  -2.10483
H    2.12510   2.10577   2.08856
          Core           RigidRotor
     SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15
 Axis            3           2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.13    0.53    1.16    2.00    2.94    3.89    2.13    1.53    0.95    0.46
0.12
 End
   Frequencies[1/cm]          37
  3242.9      3227.8      3211.8      3162.3      3088.6      3073.7      3042.5
1737.2      1658.1      1602.1
  1468.6      1428.7      1415.6      1374.8      1349.2      1311.9      1274.1
1236.5      1138.0      1112.0
  1066.0      1034.9      984.50      980.49      952.74      935.54      924.53
826.08      765.59      722.23
  636.50      597.21      392.82      369.85      318.47      266.91      116.50
 ZeroEnergy[kcal/mol]    6.7608695688462692
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       2.0000000000000000
```

```
End
!*********************************************
RRHO ! 7
Geometry[angstrom] 15
C 0.58716 -0.05636 -0.97511
C 0.58630 -0.05632 0.36969
C 1.75131 -0.05287 1.26626
C -0.80812 -0.00942 0.83074
C -1.62872 0.01155 -0.22402
C -0.81815 -0.01674 -1.48245
H 1.45998 -0.08483 -1.61010
H 2.68847 -0.30115 0.77417
H 1.91529 1.04811 1.67437
H 1.61702 -0.63792 2.17445
H -1.10225 0.00387 1.87071
H -2.70698 0.04344 -0.20151
H -1.05805 -0.88594 -2.10306
H -1.00486 0.86437 -2.10489
H 2.12315 2.09527 2.08448
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.13 0.53 1.16 2.00 2.94 3.89 2.13 1.53 0.95 0.46
0.12
End
Frequencies[1/cm] 37
3243.0 3227.9 3211.9 3164.5 3090.1 3073.6 3042.4
1704.6 1616.8 1573.7
1467.3 1428.0 1414.4 1366.3 1342.0 1311.0 1274.1
1236.2 1138.0 1112.0
1066.4 1035.1 984.63 980.53 952.78 935.58 924.68
825.88 765.62 722.79
636.62 599.15 421.96 371.62 323.18 276.68 144.60
ZeroEnergy[kcal/mol] 6.7467451892811798
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!*********************************************
RRHO ! 8
Geometry[angstrom] 15
C 0.58721 -0.05627 -0.97521
C 0.58655 -0.05624 0.37008
C 1.75085 -0.05354 1.26572
C -0.80813 -0.00943 0.83079
C -1.62865 0.01154 -0.22398
C -0.81812 -0.01675 -1.48245
H 1.46001 -0.08476 -1.61018
H 2.68916 -0.29890 0.77467
H 1.91709 1.05859 1.67800
H 1.61711 -0.63495 2.17611
H -1.10230 0.00391 1.87073
H -2.70691 0.04345 -0.20148
H -1.05797 -0.88594 -2.10311
H -1.00479 0.86434 -2.10495
H 2.12133 2.08553 2.08069
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.13 0.53 1.16 2.00 2.94 3.89 2.13 1.53 0.95 0.46
0.12
End
Frequencies[1/cm] 37
3243.1 3228.1 3212.1 3166.9 3091.6 3073.4 3042.3
1695.0 1609.1 1508.0
1462.3 1427.2 1413.2 1356.5 1334.8 1309.6 1274.0
1235.8 1138.0 1112.1
1065.8 1035.3 984.72 980.57 952.82 935.58 924.82
825.66 765.59 723.38
636.85 601.21 452.73 373.50 326.85 287.67 164.94
ZeroEnergy[kcal/mol] 6.8662164646130837
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!*********************************************
RRHO ! 9
Geometry[angstrom] 15
C 0.58724 -0.05618 -0.97530
C 0.58681 -0.05616 0.37047
C 1.75037 -0.05428 1.26516
C -0.80814 -0.00943 0.83083
C -1.62858 0.01154 -0.22394
C -0.81810 -0.01676 -1.48246
H 1.46004 -0.08470 -1.61026
H 2.68982 -0.29675 0.77513
H 1.91903 1.06969 1.68193
H 1.61719 -0.63210 2.17770
H -1.10234 0.00395 1.87074
H -2.70684 0.04347 -0.20145
H -1.05789 -0.88594 -2.10315
H -1.00473 0.86432 -2.10501
H 2.11965 2.07652 2.07719
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.13 0.53 1.16 2.00 2.94 3.89 2.13 1.53 0.95 0.46
0.12
End
Frequencies[1/cm] 37
3243.1 3228.3 3212.3 3169.3 3093.3 3073.2 3042.2
1689.7 1606.7 1477.7
1436.6 1422.9 1410.4 1345.5 1328.7 1307.5 1273.8
1235.1 1138.0 1112.1
1063.8 1035.2 984.77 980.61 952.85 935.54 924.95
825.42 765.52 724.02
637.27 603.33 483.32 376.06 330.73 298.44 179.20
ZeroEnergy[kcal/mol] 6.9562836252699274
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!*********************************************
RRHO ! 10
Geometry[angstrom] 15
C 0.58729 -0.05610 -0.97537
C 0.58705 -0.05608 0.37082
C 1.74986 -0.05510 1.26456
C -0.80819 -0.00944 0.83079
C -1.62845 0.01153 -0.22384
C -0.81806 -0.01676 -1.48242
H 1.46000 -0.08463 -1.61030
H 2.69037 -0.29465 0.77558
H 1.92106 1.08121 1.68605
H 1.61723 -0.62931 2.17914
H -1.10239 0.00398 1.87061
H -2.70664 0.04349 -0.20139
H -1.05779 -0.88589 -2.10313
H -1.00465 0.86423 -2.10499
H 2.11808 2.06811 2.07393
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15
Axis 3 2
```

```
 Symmetry 3
 Potential[kcal/mol] 12
  0.00 0.13 0.53 1.16 2.00 2.94 3.89 2.13 1.53 0.95 0.46
0.12
 End
   Frequencies[1/cm] 37
  3243.8 3229.0 3213.1 3172.4 3095.6 3073.6 3042.6
1686.1 1605.5 1473.7
  1429.0 1414.0 1384.6 1333.9 1325.2 1305.9 1273.4
1234.1 1137.9 1112.0
  1060.2 1034.7 984.67 980.47 952.87 935.33 924.96
825.16 765.14 724.39
  637.94 605.26 512.23 379.33 335.11 306.86 188.41
 ZeroEnergy[kcal/mol] 7.0212225413996467
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!**********************************************
RRHO ! 11
Geometry[angstrom] 15
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.34665
C 1.16209 0.00000 2.23941
C -1.39549 0.04658 1.80626
C -2.21570 0.06755 0.75160
C -1.40535 0.03925 -0.50704
H 0.87277 -0.02857 -0.63486
H 2.10370 -0.23665 1.75142
H 1.33594 1.14948 2.66597
H 1.03000 -0.57068 3.15605
H -1.68972 0.06003 2.84609
H -3.29393 0.09952 0.77404
H -1.64503 -0.82988 -1.12778
H -1.59192 0.92026 -1.12969
H 1.52944 2.11686 3.04655
          Core RigidRotor
      SymmetryFactor 0.50000000000000000
End
 Rotor Hindered
 Group 8 9 10 15
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
  0.00 0.13 0.53 1.16 2.00 2.94 3.89 2.13 1.53 0.95 0.46
0.12
 End
   Frequencies[1/cm] 37
  3243.9 3229.3 3213.3 3175.1 3097.6 3073.3 3042.4
1682.4 1603.8 1472.7
  1428.2 1412.8 1354.8 1326.3 1321.8 1305.1 1272.7
1232.8 1137.9 1112.0
  1055.5 1033.8 984.63 980.49 952.89 935.22 925.07
824.87 764.96 725.09
  638.89 607.35 539.96 384.26 340.09 312.68 194.68
 ZeroEnergy[kcal/mol] 7.0560161415270475
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!**********************************************
RRHO ! 12
Geometry[angstrom] 15
C 0.58734 -0.05595 -0.97561
C 0.58758 -0.05597 0.37161
C 1.74891 -0.05695 1.26335
C -0.80822 -0.00945 0.83087
C -1.62835 0.01153 -0.22378
C -0.81804 -0.01677 -1.48246
H 1.46005 -0.08455 -1.61047
H 2.69157 -0.29069 0.77636
H 1.92539 1.10563 1.69496
H 1.61736 -0.62407 2.18202
H -1.10245 0.00403 1.87064
H -2.70654 0.04351 -0.20135
H -1.05768 -0.88589 -2.10323
H -1.00459 0.86419 -2.10513
H 2.11537 2.05349 2.06823
          Core RigidRotor
      SymmetryFactor 0.50000000000000000
End
 Rotor Hindered
 Group 8 9 10 15
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
  0.00 0.13 0.53 1.16 2.00 2.94 3.89 2.13 1.53 0.95 0.46
0.12
 End
   Frequencies[1/cm] 37
  3243.9 3229.4 3213.5 3177.5 3099.3 3073.1 3042.2
1679.1 1602.0 1472.4
  1428.0 1412.4 1342.4 1329.3 1312.6 1299.8 1271.1
1231.5 1137.9 1111.9
  1050.4 1032.2 984.50 980.50 952.91 935.05 925.14
824.56 764.71 725.76
  640.04 609.20 564.11 389.67 343.93 316.01 197.78
 ZeroEnergy[kcal/mol] 7.0477418224659036
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!**********************************************
RRHO ! 13
Geometry[angstrom] 15
C 0.58735 -0.05587 -0.97578
C 0.58785 -0.05593 0.37204
C 1.74845 -0.05797 1.26275
C -0.80818 -0.00946 0.83097
C -1.62835 0.01153 -0.22380
C -0.81804 -0.01678 -1.48251
H 1.46014 -0.08452 -1.61059
H 2.69222 -0.28880 0.77670
H 1.92765 1.11833 1.69966
H 1.61742 -0.62159 2.18346
H -1.10249 0.00404 1.87078
H -2.70662 0.04352 -0.20135
H -1.05767 -0.88594 -2.10333
H -1.00461 0.86423 -2.10528
H 2.11421 2.04719 2.06578
          Core RigidRotor
      SymmetryFactor 0.50000000000000000
End
 Rotor Hindered
 Group 8 9 10 15
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
  0.00 0.13 0.53 1.16 2.00 2.94 3.89 2.13 1.53 0.95 0.46
0.12
 End
   Frequencies[1/cm] 37
  3243.3 3229.1 3213.0 3179.5 3100.7 3072.2 3041.4
1675.7 1599.8 1472.3
  1428.0 1412.3 1363.8 1322.6 1299.8 1290.2 1267.3
1230.0 1138.0 1111.9
  1046.0 1029.4 984.43 980.66 952.94 934.98 925.29
824.21 764.62 726.70
  641.41 611.10 585.64 395.09 346.73 318.28 199.33
 ZeroEnergy[kcal/mol] 6.9983580974972259
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!**********************************************
RRHO ! 14
Geometry[angstrom] 15
C 0.58736 -0.05579 -0.97593
C 0.58813 -0.05588 0.37245
C 1.74796 -0.05903 1.26210
C -0.80819 -0.00948 0.83102
C -1.62831 0.01153 -0.22377
```

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C   -0.81803  -0.01678  -1.48255
H    1.46016  -0.08449  -1.61068
H    2.69278  -0.28691   0.77706
H    1.92993   1.13119   1.70442
H    1.61747  -0.61907   2.18483
H   -1.10251   0.00405   1.87081
H   -2.70659   0.04353  -0.20134
H   -1.05763  -0.88594  -2.10339
H   -1.00460   0.86421  -2.10537
H    2.11315   2.04137   2.06351
            Core            RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.13    0.53    1.16    2.00    2.94    3.89    2.13    1.53    0.95    0.46
0.12
 End
   Frequencies[1/cm]          37
  3243.3     3229.3     3213.1     3182.1     3102.6     3071.9     3041.2
1673.0     1598.2     1472.3
  1428.5     1414.0     1399.0     1320.1     1284.3     1282.4     1258.2
1228.2     1138.0     1111.7
  1042.7     1025.0     984.20     980.64     952.95     934.72     925.33
823.84     764.19     727.30
  642.82     613.24     602.41     398.98     347.91     319.54     198.88
 ZeroEnergy[kcal/mol]    6.9065783520568349
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           15
Geometry[angstrom]          15
C    0.58737  -0.05572  -0.97607
C    0.58841  -0.05584   0.37287
C    1.74746  -0.06016   1.26144
C   -0.80820  -0.00949   0.83106
C   -1.62826   0.01153  -0.22374
C   -0.81803  -0.01678  -1.48258
H    1.46019  -0.08446  -1.61077
H    2.69334  -0.28503   0.77741
H    1.93225   1.14421   1.70925
H    1.61751  -0.61655   2.18619
H   -1.10254   0.00407   1.87083
H   -2.70655   0.04355  -0.20132
H   -1.05760  -0.88594  -2.10345
H   -1.00460   0.86419  -2.10546
H    2.11219   2.03609   2.06146
            Core            RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.13    0.53    1.16    2.00    2.94    3.89    2.13    1.53    0.95    0.46
0.12
 End
   Frequencies[1/cm]          37
  3243.2     3229.6     3213.2     3184.6     3104.6     3071.5     3040.9
1671.0     1597.5     1472.5
  1455.9     1426.8     1410.3     1319.0     1280.3     1266.7     1243.6
1225.6     1138.0     1111.5
  1040.5     1019.0     983.90     980.58     952.97     934.42     925.32
823.44     763.62     727.82
  644.16     619.84     610.28     401.06     348.04     320.25     196.74
 ZeroEnergy[kcal/mol]    6.7515473104631898
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           16
Geometry[angstrom]          15
C    0.58739  -0.05564  -0.97623
C    0.58870  -0.05580   0.37330
C    1.74693  -0.06135   1.26074
C   -0.80822  -0.00950   0.83109
C   -1.62822   0.01153  -0.22370
C   -0.81802  -0.01678  -1.48261
H    1.46021  -0.08444  -1.61087
H    2.69389  -0.28314   0.77775
H    1.93460   1.15737   1.71414
H    1.61754  -0.61401   2.18756
H   -1.10257   0.00408   1.87085
H   -2.70651   0.04356  -0.20131
H   -1.05757  -0.88595  -2.10351
H   -1.00461   0.86417  -2.10555
H    2.11135   2.03140   2.05964
            Core            RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.13    0.53    1.16    2.00    2.94    3.89    2.13    1.53    0.95    0.46
0.12
 End
   Frequencies[1/cm]          37
  3243.2     3229.8     3213.3     3187.2     3106.5     3071.1     3040.6
1670.9     1601.4     1517.9
  1472.2     1427.3     1410.6     1318.3     1279.0     1251.4     1225.9
1220.8     1138.0     1111.3
  1038.9     1011.8     983.48     980.48     952.97     934.05     925.27
823.02     762.86     728.24
  645.35     628.26     611.71     401.29     347.33     320.50     192.88
 ZeroEnergy[kcal/mol]    6.5579364796128718
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           17
Geometry[angstrom]          15
C    0.58740  -0.05556  -0.97639
C    0.58900  -0.05577   0.37374
C    1.74639  -0.06260   1.26002
C   -0.80823  -0.00951   0.83113
C   -1.62817   0.01152  -0.22367
C   -0.81802  -0.01678  -1.48264
H    1.46023  -0.08442  -1.61096
H    2.69444  -0.28123   0.77809
H    1.93695   1.17064   1.71907
H    1.61757  -0.61141   2.18894
H   -1.10261   0.00409   1.87086
H   -2.70647   0.04357  -0.20129
H   -1.05754  -0.88595  -2.10356
H   -1.00462   0.86415  -2.10563
H    2.11063   2.02733   2.05807
            Core            RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.13    0.53    1.16    2.00    2.94    3.89    2.13    1.53    0.95    0.46
0.12
 End
   Frequencies[1/cm]          37
  3243.2     3230.0     3213.4     3189.7     3108.4     3070.7     3040.2
1682.0     1629.6     1563.7
```

```
 1472.3    1427.5    1410.5    1317.9    1278.3    1240.1    1211.3
1205.3    1138.0    1111.1
 1037.4    1003.7    982.89    980.31    952.98    933.62    925.17
822.57    761.89    728.52
 646.24    633.32    612.06    399.93    345.98    320.25    187.15
 ZeroEnergy[kcal/mol]   6.3051336110198211
 ElectronicLevels[1/cm]         1
 0.0000000000000000    2.0000000000000000
 End
!**********************************************
 RRHO    !    18
 Geometry[angstrom]    15
 C   0.58742  -0.05548  -0.97656
 C   0.58931  -0.05574  0.37419
 C   1.74582  -0.06392  1.25926
 C  -0.80824  -0.00952  0.83117
 C  -1.62812  0.01152  -0.22364
 C  -0.81801  -0.01678  -1.48268
 H   1.46026  -0.08441  -1.61107
 H   2.69499  -0.27928  0.77843
 H   1.93931  1.18397  1.72402
 H   1.61759  -0.60875  2.19035
 H  -1.10265  0.00410  1.87088
 H  -2.70643  0.04359  -0.20127
 H  -1.05751  -0.88596  -2.10362
 H  -1.00465  0.86413  -2.10573
 H   2.11006  2.02394  2.05677
           Core        RigidRotor
      SymmetryFactor  0.50000000000000000
 End
 Rotor           Hindered
 Group   8  9  10  15
 Axis     3     2
 Symmetry     3
 Potential[kcal/mol]     12
  0.00   0.13   0.53   1.16   2.00   2.94   3.89   2.13   1.53   0.95   0.46
0.12
 End
  Frequencies[1/cm]     37
 3243.1    3230.2    3213.5    3192.2    3110.3    3070.3    3039.9
1757.3    1651.7    1571.9
 1472.5    1427.6    1410.5    1317.6    1278.0    1234.1    1194.5
1182.9    1138.0    1110.9
 1035.9    994.66    981.93    979.93    952.97    933.08    925.01
822.10    760.69    728.67
 646.35    635.02    611.98    397.45    344.17    319.36    179.31
 ZeroEnergy[kcal/mol]   6.0021285349398088
 ElectronicLevels[1/cm]         1
 0.0000000000000000    2.0000000000000000
 End
!**********************************************
 RRHO    !    19
 Geometry[angstrom]    15
 C   0.58743  -0.05540  -0.97674
 C   0.58963  -0.05571  0.37467
 C   1.74523  -0.06532  1.25846
 C  -0.80826  -0.00953  0.83120
 C  -1.62806  0.01152  -0.22360
 C  -0.81800  -0.01678  -1.48272
 H   1.46028  -0.08439  -1.61118
 H   2.69555  -0.27729  0.77877
 H   1.94167  1.19733  1.72897
 H   1.61761  -0.60600  2.19179
 H  -1.10270  0.00410  1.87090
 H  -2.70639  0.04360  -0.20124
 H  -1.05748  -0.88596  -2.10367
 H  -1.00468  0.86411  -2.10582
 H   2.10963  2.02129  2.05576
           Core        RigidRotor
      SymmetryFactor  0.50000000000000000
 End
 Rotor           Hindered
 Group   8  9  10  15
 Axis     3     2
 Symmetry     3
 Potential[kcal/mol]     12
  0.00   0.13   0.53   1.16   2.00   2.94   3.89   2.13   1.53   0.95   0.46
0.12
 End
  Frequencies[1/cm]     37
 3243.1    3230.4    3213.6    3194.7    3112.3    3069.8    3039.5
1881.7    1653.9    1571.0
 1472.6    1427.8    1410.4    1317.3    1277.8    1231.1    1173.2
1158.3    1138.0    1110.6
 1034.1    986.43    980.42    977.68    952.93    932.38    924.77
821.61    759.25    728.66
 645.34    633.98    611.59    394.38    342.20    317.65    169.00
 ZeroEnergy[kcal/mol]   5.7394838956524783
 ElectronicLevels[1/cm]         1
 0.0000000000000000    2.0000000000000000
 End
!**********************************************
 RRHO    !    20
 Geometry[angstrom]    15
 C   0.58744  -0.05531  -0.97692
 C   0.58997  -0.05568  0.37516
 C   1.74460  -0.06680  1.25762
 C  -0.80827  -0.00955  0.83124
 C  -1.62801  0.01152  -0.22356
 C  -0.81800  -0.01677  -1.48276
 H   1.46030  -0.08439  -1.61129
 H   2.69612  -0.27524  0.77912
 H   1.94401  1.21066  1.73390
 H   1.61762  -0.60314  2.19329
 H  -1.10275  0.00411  1.87092
 H  -2.70634  0.04362  -0.20122
 H  -1.05746  -0.88597  -2.10373
 H  -1.00472  0.86409  -2.10593
 H   2.10938  2.01948  2.05509
           Core        RigidRotor
      SymmetryFactor  0.50000000000000000
 End
 Rotor           Hindered
 Group   8  9  10  15
 Axis     3     2
 Symmetry     3
 Potential[kcal/mol]     12
  0.00   0.13   0.53   1.16   2.00   2.94   3.89   2.13   1.53   0.95   0.46
0.12
 End
  Frequencies[1/cm]     37
 3243.0    3230.6    3213.6    3197.1    3114.2    3069.3    3039.1
2027.9    1653.6    1568.0
 1472.8    1427.9    1410.3    1317.2    1277.6    1229.1    1149.0
1138.1    1131.8    1110.4
 1031.6    983.19    979.36    968.31    952.77    931.36    924.45
821.10    757.60    728.50
 643.67    630.29    610.91    391.16    340.38    314.93    155.69
 ZeroEnergy[kcal/mol]   5.4900378301348898
 ElectronicLevels[1/cm]         1
 0.0000000000000000    2.0000000000000000
 End
!**********************************************
 RRHO    !    21
 Geometry[angstrom]    15
 C   0.58745  -0.05522  -0.97712
 C   0.59032  -0.05566  0.37568
 C   1.74395  -0.06837  1.25675
 C  -0.80828  -0.00956  0.83128
 C  -1.62795  0.01152  -0.22352
 C  -0.81799  -0.01677  -1.48280
 H   1.46033  -0.08438  -1.61142
 H   2.69670  -0.27311  0.77947
 H   1.94631  1.22389  1.73879
 H   1.61763  -0.60015  2.19484
 H  -1.10280  0.00411  1.87094
 H  -2.70630  0.04364  -0.20119
 H  -1.05743  -0.88597  -2.10379
```

```
 H   -1.00477   0.86406  -2.10604
 H    2.10931   2.01858   2.05478
                  Core            RigidRotor
         SymmetryFactor   0.50000000000000000
 End
  Rotor                          Hindered
  Group    8   9  10  15
  Axis            3          2
  Symmetry           3
  Potential[kcal/mol]          12
    0.00    0.13    0.53    1.16    2.00    2.94    3.89    2.13    1.53    0.95    0.46
0.12
  End
     Frequencies[1/cm]          37
   3242.9      3230.8      3213.6      3199.6      3116.1      3068.8      3038.8
2187.1      1652.8      1564.3
   1473.1      1428.1      1410.2      1317.1      1277.6      1227.8      1138.1
1122.8      1110.2      1104.7
   1027.7      982.17      977.91      956.62      951.47      929.44      923.95
820.58      755.74      728.19
   641.99      624.09      609.74      388.15      339.00      311.22      138.80
 ZeroEnergy[kcal/mol]    5.2043685927518855
  ElectronicLevels[1/cm]                    1
   0.0000000000000000        2.0000000000000000
 End
 !*********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1355.8800000000001
      WellDepth[kcal/mol]          6.42
      WellDepth[kcal/mol]          23.32
 End
End
End
```

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                      direct    ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                        diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                            10
!ChemicalEigenvalueMin                 1.e-6         #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                  1.3
!!
RateOutput                             rate.out                 ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                     ! Default collisional
energy relaxation kernel
    Exponential                                        ! Currently the only
possible energy relaxation model
       Factor[1/cm]              316                   ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                 0.535                     ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff            10                    ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                   ! Collision frequency
model
    LennardJones                                       ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]               90.58  281.367        ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]          3.54    4.694         ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]               39.948  79.05478      ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50263
 C    1.24622   0.00000   2.31947
 C   -1.27227   0.00046   1.92591
 C   -2.17585   0.00051   0.77474
 C   -1.45565   0.00011  -0.35294
 H    0.51979   0.87601  -0.40113
 H    1.85947   0.87812   2.10478
 H    1.01835  -0.00094   3.38445
 H    1.86045  -0.87709   2.10340
 H   -1.59049   0.00052   2.95892
 H   -3.25397   0.00095   0.84079
 H   -1.83452  -0.00013  -1.36297
 H    0.51979  -0.87591  -0.40126
        Core    RigidRotor
             SymmetryFactor    1.0000000000000000
        End
 Rotor                        Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.08    0.30    0.62    0.95    1.20    1.29    1.21    0.96    0.62    0.30
0.08
 End
    Frequencies[1/cm]          35
  3245.2      3221.6      3209.3      3128.8      3090.6      3074.8      3042.5
3036.2      1695.3      1615.6
  1495.0      1486.6      1424.0      1421.5      1397.2      1340.1      1274.6
1198.6      1152.9      1130.9
  1060.1      1033.7      1005.4      976.89      961.82      922.95      892.68
863.70      828.81      700.71
  623.69      533.08      369.88      325.94      227.72
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]           4
 C    0.00000   0.00000   0.00000
 H    0.00000   0.00000   1.07813
 H    0.93365   0.00000  -0.53917
 H   -0.93365  -0.00105  -0.53917
        Core    RigidRotor
             SymmetryFactor    6.0000000000000000
        End
    Frequencies[1/cm]           6
  526.68      1409.6      1409.7      3123.2      3304.4      3304.6
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]            13
```

```
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.41507
C    1.18585   0.00000   2.30525
C   -1.37924  -0.00034   1.86264
C   -2.17195  -0.00056   0.76525
C   -1.30652  -0.00033  -0.41759
H    0.87955   0.00028  -0.62343
H    2.11567   0.00259   1.73998
H    1.17551   0.87449   2.96082
H    1.17824  -0.87748   2.95691
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
      Core    RigidRotor
          SymmetryFactor    2.0000000000000000
      End
Rotor                         Hindered
Group    8   9  10
Axis            3            2
Symmetry           3
Potential[kcal/mol]           12
   0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
   Frequencies[1/cm]           32
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
 ZeroEnergy[kcal/mol]              0.
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!*************************************
Fragment PROD2
RRHO
Geometry[angstrom]              5
C    0.00000   0.00000   0.00000
H    0.00000   0.00000   1.08780
H    1.02552   0.00000  -0.36267
H   -0.51271  -0.88842  -0.36222
H   -0.51307   0.88794  -0.36267
      Core    RigidRotor
          SymmetryFactor    12.000000000000000
      End
   Frequencies[1/cm]           9
  1341.0      1341.5      1341.7      1562.7      1563.0      3043.7      3161.5
3162.0      3162.4
 ZeroEnergy[kcal/mol]              0.
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End

GroundEnergy[kcal/mol]    -23.22
End
!*************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]              18
C   -0.01380   0.05482  -0.01020
C    0.00910  -0.05090   1.48751
C    1.26846  -0.10248   2.28101
C   -1.25578  -0.10765   1.92900
C   -2.17671  -0.04743   0.79364
C   -1.47374   0.04619  -0.34185
H    0.48321   0.96531  -0.35963
H    1.87798   0.78895   2.11704
H    1.06005  -0.17914   3.34724
H    1.87804  -0.96168   1.99050
H   -1.55755  -0.19284   2.96334
H   -3.25352  -0.07509   0.87432
H   -1.86858   0.11091  -1.34370
H    0.51507  -0.78556  -0.47249
C   -0.19353  -3.41659   0.58251
H   -0.99261  -2.72906   0.35055
H    0.37997  -3.28162   1.48595
H    0.02243  -4.24520  -0.07346
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]           48
  45.271      52.386      66.373      96.035      130.78      152.08      230.40
268.78      324.72      376.22
  534.83      569.61      624.11      703.77      829.32      864.04      893.05
922.60      962.08      978.74
  1005.5      1034.1      1059.5      1130.7      1154.7      1199.4      1275.3
1341.3      1397.1      1404.0
  1415.5      1420.5      1423.7      1486.0      1495.0      1613.5      1694.7
3034.6      3041.4      3075.2
  3088.8      3116.6      3128.5      3210.5      3222.4      3245.3      3297.8
3298.6
 ZeroEnergy[kcal/mol]              -1.48
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
End
!*************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]              18
C   -0.00187  -0.00129   0.00422
C   -0.00135  -0.00162   1.45162
C    1.20915  -0.00013   2.30675
C   -1.34923  -0.05187   1.88934
C   -2.14827  -0.08545   0.77796
C   -1.29067  -0.05303  -0.41030
H    0.88136   0.03143  -0.61378
H    1.91054   0.77545   1.99301
H    0.96242   0.15148   3.35588
H    1.73405  -0.95578   2.21574
H   -1.66919  -0.06641   2.91873
H   -3.22646  -0.12873   0.76179
H   -1.64417  -0.06586  -1.42925
H   -0.34281  -2.82220   0.71020
C    0.11171  -3.47968   1.44818
H   -0.07762  -3.08170   2.44298
H    1.18488  -3.53446   1.27477
H   -0.31719  -4.47635   1.36855
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]           47
  33.706      44.399      48.560      58.469      97.562      103.31      224.23
329.42      527.22      540.24
  605.15      637.77      730.54      740.22      902.78      924.57      930.74
956.43      1011.7      1022.8
  1053.9      1097.3      1180.0      1294.0      1310.9      1333.5      1341.7
1345.7      1406.3      1438.2
  1474.6      1485.9      1509.6      1559.0      1561.8      1579.6      3031.2
3040.2      3088.9      3137.7
  3153.8      3158.3      3163.8      3225.7      3233.4      3247.4      3255.7
 ZeroEnergy[kcal/mol]              -26.66
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
End
!*************************************
Barrier        B1  REACS WR
  RRHO
    Stoichiometry  H11C7
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]              14
C    0.00000   0.00000   0.00000
```

C 0.00000 0.00000 1.50263
C 1.24622 0.00000 2.31947
C -1.27227 0.00046 1.92591
C -2.17585 0.00051 0.77474
C -1.45565 0.00011 -0.35294
H 0.51979 0.87601 -0.40113
H 1.85947 0.87812 2.10478
H 1.01835 -0.00094 3.38445
H 1.86045 -0.87709 2.10340
H -1.59049 0.00052 2.95892
H -3.25397 0.00095 0.84079
H -1.83452 -0.00013 -1.36297
H 0.51979 -0.87591 -0.40126
FragmentGeometry[angstrom] 4
C 0.00000 0.00000 0.00000
H 0.00000 0.00000 1.07813
H 0.93365 0.00000 -0.53917
H -0.93365 -0.00105 -0.53917
SymmetryFactor 6.0000000000000000
PotentialPrefactor[au] 10.
PotentialPowerExponent 6
End
Rotor Hindered
Geometry[angstrom] 14
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.50263
C 1.24622 0.00000 2.31947
C -1.27227 0.00046 1.92591
C -2.17585 0.00051 0.77474
C -1.45565 0.00011 -0.35294
H 0.51979 0.87601 -0.40113
H 1.85947 0.87812 2.10478
H 1.01835 -0.00094 3.38445
H 1.86045 -0.87709 2.10340
H -1.59049 0.00052 2.95892
H -3.25397 0.00095 0.84079
H -1.83452 -0.00013 -1.36297
H 0.51979 -0.87591 -0.40126
Group 8 9 10
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.0000 0.80000E-01 0.30000 0.62000 0.95000 1.2000 1.2900
1.2100 0.96000 0.62000
0.30000 0.80000E-01
End
Frequencies[1/cm] 41
3245.2 3221.6 3209.3 3128.8 3090.6 3074.8 3042.5
3036.2 1695.3 1615.6
1495.0 1486.6 1424.0 1421.5 1397.2 1340.1 1274.6
1198.6 1152.9 1130.9
1060.1 1033.7 1005.4 976.89 961.82 922.95 892.68
863.70 828.81 700.71
623.69 533.08 369.88 325.94 227.72
526.68 1409.6 1409.7 3123.2 3304.4 3304.6
ZeroEnergy[kcal/mol] 0.
ElectronicLevels[1/cm] 1
0.0000000000000000 4.0000000000000000
End
!***********************************
Barrier B3 WP PRODS
RRHO
Stoichiometry H11C7
Core PhaseSpaceTheory
FragmentGeometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.41507
C 1.18585 0.00000 2.30525
C -1.37924 -0.00034 1.86264
C -2.17195 -0.00056 0.76525
C -1.30652 -0.00033 -0.41759
H 0.87955 0.00028 -0.62343
H 2.11567 0.00259 1.73998
H 1.17551 0.87449 2.96082
H 1.17824 -0.87748 2.95691
H -1.69366 -0.00045 2.89442
H -3.25029 -0.00080 0.74358
H -1.65471 -0.00041 -1.43915
FragmentGeometry[angstrom] 5
C 0.00000 0.00000 0.00000
H 0.00000 0.00000 1.08780
H 1.02552 0.00000 -0.36267
H -0.51271 -0.88842 -0.36222
H -0.51307 0.88794 -0.36267
SymmetryFactor 24.000000000000000
PotentialPrefactor[au] 10.
PotentialPowerExponent 6
End
Rotor Hindered
Geometry[angstrom] 13
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.41507
C 1.18585 0.00000 2.30525
C -1.37924 -0.00034 1.86264
C -2.17195 -0.00056 0.76525
C -1.30652 -0.00033 -0.41759
H 0.87955 0.00028 -0.62343
H 2.11567 0.00259 1.73998
H 1.17551 0.87449 2.96082
H 1.17824 -0.87748 2.95691
H -1.69366 -0.00045 2.89442
H -3.25029 -0.00080 0.74358
H -1.65471 -0.00041 -1.43915
Group 8 9 10
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.0000 0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01 0.0000 0.20000E-01 0.40000E-01 0.60000E-01
0.40000E-01 0.10000E-01
End
Frequencies[1/cm] 41
3255.2 3247.0 3232.4 3224.7 3138.6 3086.9 3034.1
1584.1 1503.1 1481.1
1477.9 1438.4 1407.4 1311.3 1292.6 1178.7 1098.1
1049.4 1023.5 1013.2
953.40 929.99 923.03 899.45 740.46 727.81 638.42
604.77 528.85 520.52
329.55 215.83
1341.0 1341.5 1341.7 1562.7 1563.0 3043.7 3161.5
3162.0 3162.4
ZeroEnergy[kcal/mol] -23.215482033529419
ElectronicLevels[1/cm] 1
0.0000000000000000 4.0000000000000000
End
!***********************************
Barrier B2 WR WP
Variational
RRHO ! 1
Geometry[angstrom] 18
C 0.31962 0.42719 -0.76000
C 0.32584 0.41912 0.71838
C 1.56608 0.42046 1.54408
C -0.95668 0.35888 1.13113
C -1.84162 0.37585 -0.02921
C -1.09653 0.44454 -1.15057
H 1.03435 1.05056 -1.28972
H 2.16308 1.31727 1.36394
H 1.33165 0.37864 2.60675
H 2.19896 -0.43735 1.30357
H -1.28523 0.30559 2.15896
H -2.91973 0.34054 0.01756
H -1.45683 0.47457 -2.16633
H 0.79722 -0.85308 -1.09806
C 1.20532 -2.07863 -1.34671
H 0.50694 -2.66030 -0.75479
H 2.23184 -2.10740 -0.99731
H 1.08892 -2.18375 -2.41976

```
          Core          RigidRotor
        SymmetryFactor   1.5000000000000000
 End
  Rotor                  Hindered
  Group   8  9  10
  Axis        3       2
  Symmetry       1
  Potential[kcal/mol]       18
   0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
 0.32   0.00   0.27   0.89   1.24   0.93   0.31
  End
  Rotor                  Hindered
  Group   16  17  18
  Axis        15      14
  Symmetry       3
  Potential[kcal/mol]       6
   0.00   0.04   0.12   0.15   0.10   0.03
  End
    Frequencies[1/cm]       45
   3249.9    3227.8    3220.4    3217.6    3215.4    3155.2    3129.0
 3086.8    3075.6    3034.4
   1657.0    1564.7    1494.6    1486.5    1455.2    1449.7    1423.4
 1395.2    1349.8    1327.3
   1308.1    1268.2    1206.4    1180.8    1129.9    1070.6    1034.4
 1006.0    973.37    972.16
   947.00    909.38    854.25    799.15    739.37    658.17    630.21
 577.32    480.10    441.25
   401.75    327.43    245.47    116.39    105.47
  ZeroEnergy[kcal/mol]   4.7050412628036504
  ElectronicLevels[1/cm]              1
   0.0000000000000000      2.0000000000000000
 End
!**********************************************
 RRHO        !        2
 Geometry[angstrom]       18
 C   0.32021   0.42634  -0.76034
 C   0.32575   0.41924   0.71851
 C   1.56606   0.42045   1.54409
 C  -0.95666   0.35891   1.13111
 C  -1.84159   0.37590  -0.02926
 C  -1.09679   0.44465  -1.15047
 H   1.03317   1.05313  -1.28874
 H   2.16305   1.31726   1.36391
 H   1.33170   0.37861   2.60678
 H   2.19896  -0.43735   1.30353
 H  -1.28525   0.30543   2.15895
 H  -2.91972   0.34034   0.01757
 H  -1.45699   0.47440  -2.16630
 H   0.79203  -0.83853  -1.09487
 C   1.20570  -2.07981  -1.34695
 H   0.50615  -2.65888  -0.75424
 H   2.23187  -2.10605  -0.99691
 H   1.08847  -2.18240  -2.41996
          Core          RigidRotor
        SymmetryFactor   1.5000000000000000
 End
  Rotor                  Hindered
  Group   8  9  10
  Axis        3       2
  Symmetry       1
  Potential[kcal/mol]       18
   0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
 0.32   0.00   0.27   0.89   1.24   0.93   0.31
  End
  Rotor                  Hindered
  Group   16  17  18
  Axis        15      14
  Symmetry       3
  Potential[kcal/mol]       6
   0.00   0.04   0.12   0.15   0.10   0.03
  End
    Frequencies[1/cm]       45
   3249.6    3227.4    3223.1    3220.4    3215.0    3152.9    3128.9
 3086.8    3077.1    3034.3
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   1658.0    1566.6    1494.7    1486.5    1450.5    1446.0    1423.3
 1395.6    1344.6    1322.0
   1307.4    1266.8    1203.4    1171.0    1130.0    1070.2    1034.1
 1007.1    974.25    964.92
   948.16    910.47    855.54    803.66    741.57    660.67    631.31
 580.17    485.99    445.66
   399.45    327.28    245.00    117.04    106.20
  ZeroEnergy[kcal/mol]   5.4090648185075487
  ElectronicLevels[1/cm]              1
   0.0000000000000000      2.0000000000000000
 End
!**********************************************
 RRHO        !        3
 Geometry[angstrom]       18
 C   0.32077   0.42551  -0.76067
 C   0.32565   0.41936   0.71864
 C   1.56604   0.42045   1.54410
 C  -0.95664   0.35895   1.13108
 C  -1.84157   0.37595  -0.02931
 C  -1.09705   0.44475  -1.15037
 H   1.03199   1.05568  -1.28776
 H   2.16303   1.31725   1.36387
 H   1.33175   0.37857   2.60682
 H   2.19896  -0.43734   1.30348
 H  -1.28527   0.30527   2.15894
 H  -2.91971   0.34014   0.01758
 H  -1.45715   0.47424  -2.16628
 H   0.78687  -0.82396  -1.09170
 C   1.20610  -2.08103  -1.34720
 H   0.50537  -2.65748  -0.75369
 H   2.23190  -2.10472  -0.99653
 H   1.08802  -2.18108  -2.42015
          Core          RigidRotor
        SymmetryFactor   1.5000000000000000
 End
  Rotor                  Hindered
  Group   8  9  10
  Axis        3       2
  Symmetry       1
  Potential[kcal/mol]       18
   0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
 0.32   0.00   0.27   0.89   1.24   0.93   0.31
  End
  Rotor                  Hindered
  Group   16  17  18
  Axis        15      14
  Symmetry       3
  Potential[kcal/mol]       6
   0.00   0.04   0.12   0.15   0.10   0.03
  End
    Frequencies[1/cm]       45
   3249.3    3227.1    3225.9    3223.1    3214.6    3150.6    3128.9
 3086.7    3078.5    3034.2
   1659.0    1568.5    1494.7    1486.4    1446.5    1442.7    1423.2
 1396.1    1340.1    1322.1
   1301.7    1264.7    1201.9    1160.8    1130.2    1069.9    1033.9
 1008.3    975.10    959.74
   949.07    911.48    856.86    807.87    743.44    662.76    632.30
 582.74    490.53    449.77
   398.17    327.01    244.47    117.04    106.25
  ZeroEnergy[kcal/mol]   6.0319981987439384
  ElectronicLevels[1/cm]              1
   0.0000000000000000      2.0000000000000000
 End
!**********************************************
 RRHO        !        4
 Geometry[angstrom]       18
 C   0.32132   0.42473  -0.76100
 C   0.32556   0.41948   0.71878
 C   1.56602   0.42045   1.54412
 C  -0.95662   0.35899   1.13106
 C  -1.84154   0.37599  -0.02935
 C  -1.09730   0.44486  -1.15028
 H   1.03081   1.05824  -1.28678
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H   2.16300   1.31724   1.36383
H   1.33180   0.37854   2.60685
H   2.19895  -0.43734   1.30343
H  -1.28529   0.30511   2.15892
H  -2.91970   0.33995   0.01760
H  -1.45731   0.47408  -2.16625
H   0.78174  -0.80937  -1.08857
C   1.20651  -2.08227  -1.34746
H   0.50460  -2.65609  -0.75314
H   2.23194  -2.10340  -0.99614
H   1.08758  -2.17978  -2.42035
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                        Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.29    0.91    1.24    0.94    0.32    0.00    0.28    0.90    1.24    0.94
0.32    0.00    0.27    0.89    1.24    0.93    0.31
 End
 Rotor                        Hindered
 Group   16  17  18
 Axis            15          14
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.04    0.12    0.15    0.10    0.03
 End
   Frequencies[1/cm]          45
  3249.1      3228.6      3226.8      3225.8      3214.2      3148.2      3128.8
3086.6      3079.9      3034.2
  1660.1      1570.4      1494.8      1486.4      1442.9      1439.8      1423.2
1396.7      1336.6      1324.8
  1294.6      1261.3      1200.8      1150.9      1130.3      1069.6      1033.7
1009.4      975.88      956.28
  949.17      912.37      858.18      811.73      744.87      664.39      633.14
584.91      493.89      453.62
  397.70      326.67      243.89      116.32      105.56
 ZeroEnergy[kcal/mol]    6.5842043479627144
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
!********************************************
RRHO           !            5
Geometry[angstrom]          18
C   0.32186   0.42397  -0.76132
C   0.32547   0.41960   0.71892
C   1.56600   0.42044   1.54413
C  -0.95660   0.35902   1.13104
C  -1.84152   0.37604  -0.02940
C  -1.09755   0.44497  -1.15018
H   1.02962   1.06080  -1.28579
H   2.16297   1.31724   1.36380
H   1.33185   0.37850   2.60688
H   2.19895  -0.43733   1.30339
H  -1.28531   0.30495   2.15891
H  -2.91969   0.33975   0.01761
H  -1.45747   0.47391  -2.16622
H   0.77665  -0.79478  -1.08547
C   1.20693  -2.08356  -1.34772
H   0.50383  -2.65469  -0.75260
H   2.23198  -2.10209  -0.99576
H   1.08715  -2.17848  -2.42055
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                        Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.29    0.91    1.24    0.94    0.32    0.00    0.28    0.90    1.24    0.94
0.32    0.00    0.27    0.89    1.24    0.93    0.31
 End
 Rotor                        Hindered
 Group   16  17  18
 Axis            15          14
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.04    0.12    0.15    0.10    0.03
 End
   Frequencies[1/cm]          45
  3248.8      3231.2      3228.5      3226.4      3213.9      3145.7      3128.7
3086.5      3081.4      3034.1
  1661.2      1572.3      1494.8      1486.4      1439.8      1437.3      1423.1
1397.3      1334.2      1328.2
  1288.7      1256.1      1199.9      1141.8      1130.2      1069.3      1033.6
1010.6      976.59      955.14
  947.32      913.07      859.46      815.21      745.73      665.58      633.82
586.54      496.17      457.36
  397.80      326.28      243.27      114.84      104.10
 ZeroEnergy[kcal/mol]    7.0460002393074213
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
!********************************************
RRHO           !            6
Geometry[angstrom]          18
C   0.32238   0.42326  -0.76163
C   0.32537   0.41972   0.71906
C   1.56598   0.42044   1.54415
C  -0.95657   0.35906   1.13102
C  -1.84150   0.37608  -0.02945
C  -1.09780   0.44509  -1.15009
H   1.02841   1.06340  -1.28478
H   2.16294   1.31723   1.36376
H   1.33191   0.37847   2.60692
H   2.19894  -0.43732   1.30334
H  -1.28533   0.30479   2.15890
H  -2.91969   0.33955   0.01763
H  -1.45764   0.47375  -2.16619
H   0.77160  -0.78021  -1.08243
C   1.20737  -2.08489  -1.34799
H   0.50305  -2.65329  -0.75206
H   2.23203  -2.10078  -0.99538
H   1.08671  -2.17719  -2.42075
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                        Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.29    0.91    1.24    0.94    0.32    0.00    0.28    0.90    1.24    0.94
0.32    0.00    0.27    0.89    1.24    0.93    0.31
 End
 Rotor                        Hindered
 Group   16  17  18
 Axis            15          14
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.04    0.12    0.15    0.10    0.03
 End
   Frequencies[1/cm]          45
  3248.5      3233.8      3231.1      3226.0      3213.5      3143.2      3128.6
3086.4      3082.8      3034.0
  1662.4      1574.2      1494.8      1486.3      1437.1      1435.0      1423.0
1398.0      1333.2      1331.8
  1284.8      1249.4      1198.8      1134.8      1129.0      1069.0      1033.4
1011.7      977.22      955.61
  943.95      913.53      860.66      818.30      745.93      666.37      634.29
587.56      497.46      461.38
  398.19      325.87      242.62      112.59      101.84
 ZeroEnergy[kcal/mol]    7.4176574914084092
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
```

```
End
!*********************************************
RRHO        !        7
Geometry[angstrom]        18
C   0.32290   0.42258  -0.76194
C   0.32527   0.41985   0.71921
C   1.56597   0.42043   1.54417
C  -0.95655   0.35909   1.13100
C  -1.84148   0.37613  -0.02950
C  -1.09805   0.44520  -1.14999
H   1.02716   1.06605  -1.28376
H   2.16291   1.31722   1.36372
H   1.33196   0.37843   2.60696
H   2.19893  -0.43732   1.30329
H  -1.28535   0.30463   2.15889
H  -2.91968   0.33935   0.01764
H  -1.45781   0.47358  -2.16616
H   0.76660  -0.76566  -1.07944
C   1.20782  -2.08627  -1.34827
H   0.50227  -2.65187  -0.75150
H   2.23208  -2.09946  -0.99499
H   1.08627  -2.17589  -2.42096
          Core          RigidRotor
     SymmetryFactor    1.5000000000000000
End
 Rotor                   Hindered
 Group   8  9  10
 Axis          3         2
 Symmetry         1
 Potential[kcal/mol]         18
  0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
0.32   0.00   0.27   0.89   1.24   0.93   0.31
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        14
 Symmetry         3
 Potential[kcal/mol]         6
  0.00   0.04   0.12   0.15   0.10   0.03
 End
   Frequencies[1/cm]        45
  3248.2     3236.4     3233.7     3225.7     3213.1     3140.6     3128.6
3086.4     3084.3     3034.0
  1663.6     1576.0     1494.9     1486.3     1434.7     1433.0     1423.0
1398.7     1335.4     1333.5
  1282.5     1242.1     1197.5     1132.4     1124.6     1068.6     1033.3
1012.8     977.75     956.59
  940.12     913.68     861.73     821.01     745.38     666.90     634.55
587.89     497.82     466.21
  398.57     325.45     241.94     109.57     98.800
ZeroEnergy[kcal/mol]    7.7063375333476678
 ElectronicLevels[1/cm]              1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO        !        8
Geometry[angstrom]        18
C   0.32340   0.42194  -0.76224
C   0.32517   0.41998   0.71936
C   1.56594   0.42043   1.54418
C  -0.95652   0.35913   1.13099
C  -1.84147   0.37618  -0.02955
C  -1.09831   0.44533  -1.14990
H   1.02588   1.06878  -1.28270
H   2.16288   1.31721   1.36367
H   1.33202   0.37840   2.60699
H   2.19893  -0.43731   1.30324
H  -1.28538   0.30446   2.15889
H  -2.91968   0.33915   0.01767
H  -1.45799   0.47341  -2.16613
H   0.76168  -0.75115  -1.07654
C   1.20830  -2.08772  -1.34857
H   0.50147  -2.65043  -0.75094
H   2.23213  -2.09813  -0.99460
H   1.08583  -2.17457  -2.42117
          Core          RigidRotor
     SymmetryFactor    1.5000000000000000
End
 Rotor                   Hindered
 Group   8  9  10
 Axis          3         2
 Symmetry         1
 Potential[kcal/mol]         18
  0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
0.32   0.00   0.27   0.89   1.24   0.93   0.31
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        14
 Symmetry         3
 Potential[kcal/mol]         6
  0.00   0.04   0.12   0.15   0.10   0.03
 End
   Frequencies[1/cm]        45
  3248.0     3239.0     3236.2     3225.4     3212.8     3137.9     3128.5
3086.4     3085.7     3033.9
  1664.8     1577.8     1494.9     1486.3     1432.6     1431.2     1422.9
1399.3     1338.8     1335.2
  1281.2     1235.0     1195.9     1132.3     1120.2     1068.1     1033.2
1013.6     978.18     957.70
  936.26     913.41     862.64     823.37     744.08     667.34     634.60
587.53     497.49     472.19
  398.52     325.01     241.22     105.76     94.930
ZeroEnergy[kcal/mol]    7.9128552210159349
 ElectronicLevels[1/cm]              1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO        !        9
Geometry[angstrom]        18
C   0.32389   0.42136  -0.76254
C   0.32506   0.42012   0.71952
C   1.56592   0.42043   1.54420
C  -0.95649   0.35917   1.13098
C  -1.84146   0.37622  -0.02960
C  -1.09857   0.44546  -1.14980
H   1.02455   1.07161  -1.28160
H   2.16285   1.31720   1.36363
H   1.33209   0.37836   2.60704
H   2.19891  -0.43729   1.30318
H  -1.28540   0.30429   2.15888
H  -2.91968   0.33894   0.01769
H  -1.45818   0.47324  -2.16610
H   0.75686  -0.73671  -1.07372
C   1.20880  -2.08924  -1.34888
H   0.50065  -2.64895  -0.75036
H   2.23219  -2.09677  -0.99420
H   1.08538  -2.17323  -2.42140
          Core          RigidRotor
     SymmetryFactor    1.5000000000000000
End
 Rotor                   Hindered
 Group   8  9  10
 Axis          3         2
 Symmetry         1
 Potential[kcal/mol]         18
  0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
0.32   0.00   0.27   0.89   1.24   0.93   0.31
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        14
 Symmetry         3
 Potential[kcal/mol]         6
  0.00   0.04   0.12   0.15   0.10   0.03
 End
   Frequencies[1/cm]        45
```

3247.7 3241.5 3238.8 3225.1 3212.4 3135.2 3128.4
3087.1 3086.3 3033.9
1666.0 1579.7 1494.9 1486.4 1430.7 1429.5 1422.8
1400.0 1341.9 1338.1
1280.4 1228.9 1193.8 1132.8 1118.2 1067.5 1033.2
1014.3 978.50 958.83
932.62 912.67 863.34 825.40 742.05 668.03 634.46
586.49 497.33 478.91
397.61 324.55 240.43 101.16 90.220
ZeroEnergy[kcal/mol] 8.0448866293210166
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 10
Geometry[angstrom] 18
C 0.32437 0.42083 -0.76284
C 0.32495 0.42025 0.71969
C 1.56591 0.42042 1.54423
C -0.95648 0.35921 1.13099
C -1.84147 0.37627 -0.02964
C -1.09883 0.44560 -1.14971
H 1.02315 1.07455 -1.28046
H 2.16282 1.31719 1.36358
H 1.33215 0.37832 2.60711
H 2.19889 -0.43726 1.30313
H -1.28545 0.30412 2.15890
H -2.91965 0.33872 0.01772
H -1.45840 0.47306 -2.16611
H 0.75213 -0.72234 -1.07102
C 1.20932 -2.09084 -1.34920
H 0.49983 -2.64742 -0.74978
H 2.23224 -2.09537 -0.99379
H 1.08492 -2.17188 -2.42168
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.29 0.91 1.24 0.94 0.32 0.00 0.28 0.90 1.24 0.94
0.32 0.00 0.27 0.89 1.24 0.93 0.31
End
Rotor Hindered
Group 16 17 18
Axis 15 14
Symmetry 3
Potential[kcal/mol] 6
0.00 0.04 0.12 0.15 0.10 0.03
End
Frequencies[1/cm] 45
3247.3 3244.0 3241.4 3224.8 3212.2 3132.7 3128.2
3088.7 3086.4 3033.9
1667.2 1581.4 1495.0 1486.4 1429.1 1427.9 1422.7
1400.6 1344.8 1341.9
1279.8 1223.9 1191.0 1134.2 1119.9 1067.0 1033.1
1014.8 978.72 959.86
929.42 911.39 863.83 827.13 739.45 669.69 634.15
584.85 501.02 483.05
395.49 324.06 239.51 95.830 84.570
ZeroEnergy[kcal/mol] 8.1103222689313306
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 11
Geometry[angstrom] 18
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.48300
C 1.24105 0.00000 2.30737
C -1.28127 -0.06116 1.89411
C -2.16629 -0.04409 0.73343
C -1.42396 0.02533 -0.38649
H 0.69676 0.65740 -0.51606
H 1.83795 0.89676 2.12666
H 1.00741 -0.04215 3.37028
H 1.87403 -0.85767 2.06618
H -1.61031 -0.11649 2.92201
H -3.24449 -0.08193 0.78087
H -1.78346 0.05244 -1.40294
H 0.42286 -1.12868 -0.30547
C 0.88508 -2.51305 -0.58645
H 0.17407 -3.06619 0.01399
H 1.90750 -2.51433 -0.23023
H 0.75960 -2.59085 -1.65884
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.29 0.91 1.24 0.94 0.32 0.00 0.28 0.90 1.24 0.94
0.32 0.00 0.27 0.89 1.24 0.93 0.31
End
Rotor Hindered
Group 16 17 18
Axis 15 14
Symmetry 3
Potential[kcal/mol] 6
0.00 0.04 0.12 0.15 0.10 0.03
End
Frequencies[1/cm] 45
3247.1 3246.6 3244.0 3224.5 3211.8 3130.1 3128.1
3090.1 3086.4 3033.9
1668.5 1583.3 1495.0 1486.4 1427.7 1426.5 1422.5
1401.3 1347.4 1346.2
1279.5 1220.7 1187.7 1139.7 1124.7 1066.4 1033.1
1015.1 978.85 960.92
926.84 909.75 864.01 828.57 736.49 673.59 633.69
582.71 511.39 481.76
392.21 323.47 238.46 89.730 78.070
ZeroEnergy[kcal/mol] 8.1246436764444816
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 12
Geometry[angstrom] 18
C 0.32528 0.42001 -0.76340
C 0.32470 0.42059 0.72007
C 1.56585 0.42042 1.54428
C -0.95641 0.35931 1.13099
C -1.84146 0.37638 -0.02974
C -1.09942 0.44591 -1.14950
H 1.02003 1.08109 -1.27789
H 2.16274 1.31717 1.36348
H 1.33231 0.37823 2.60721
H 2.19883 -0.43724 1.30299
H -1.28552 0.30375 2.15888
H -2.91966 0.33825 0.01779
H -1.45887 0.47267 -2.16601
H 0.74325 -0.69418 -1.06617
C 1.21050 -2.09443 -1.34994
H 0.49798 -2.64412 -0.74848
H 2.23243 -2.09245 -0.99291
H 1.08394 -2.16897 -2.42223
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18

```
 0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
0.32   0.00   0.27   0.89   1.24   0.93   0.31
 End
 Rotor                 Hindered
 Group  16 17 18
 Axis        15       14
 Symmetry        3
 Potential[kcal/mol]        6
  0.00   0.04   0.12   0.15   0.10   0.03
 End
   Frequencies[1/cm]        45
  3249.1    3246.9    3246.4    3224.2    3211.6    3128.2    3127.1
3091.5    3086.4    3033.9
  1669.7    1585.3    1495.0    1486.4    1426.6    1425.2    1422.2
1402.0    1352.1    1349.1
  1279.2    1220.4    1184.6    1157.8    1128.1    1065.8    1033.1
1015.2    978.89    961.94
  924.71    907.97    863.92    829.78    733.65    682.42    633.04
580.18    525.76    477.37
  387.74    322.82    237.22    82.820    70.570
 ZeroEnergy[kcal/mol]    8.1106653661484422
  ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
!***********************************************
RRHO        !       13
Geometry[angstrom]        18
C    0.32570   0.41978  -0.76364
C    0.32456   0.42079   0.72027
C    1.56581   0.42041   1.54430
C   -0.95636   0.35936   1.13099
C   -1.84146   0.37644  -0.02981
C   -1.09975   0.44610  -1.14937
H    1.01824   1.08481  -1.27642
H    2.16269   1.31716   1.36343
H    1.33241   0.37818   2.60724
H    2.19880  -0.43725   1.30289
H   -1.28556   0.30354   2.15885
H   -2.91971   0.33799   0.01783
H   -1.45914   0.47245  -2.16589
H    0.73925  -0.68057  -1.06414
C    1.21118  -2.09649  -1.35037
H    0.49693  -2.64233  -0.74774
H    2.23260  -2.09086  -0.99241
H    1.08342  -2.16741  -2.42251
          Core          RigidRotor
     SymmetryFactor    1.5000000000000000
End
 Rotor                 Hindered
 Group   8  9 10
 Axis        3       2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
0.32   0.00   0.27   0.89   1.24   0.93   0.31
 End
 Rotor                 Hindered
 Group  16 17 18
 Axis        15       14
 Symmetry        3
 Potential[kcal/mol]        6
  0.00   0.04   0.12   0.15   0.10   0.03
 End
   Frequencies[1/cm]        45
  3251.6    3248.9    3246.7    3223.9    3211.2    3128.2    3124.6
3092.9    3086.3    3033.8
  1671.1    1587.8    1495.0    1486.4    1425.8    1424.1    1421.7
1403.0    1359.1    1350.8
  1279.5    1233.7    1193.3    1174.1    1129.3    1065.2    1033.0
1015.1    978.86    962.98
  922.96    906.36    863.56    830.74    732.39    697.65    632.20
577.39    539.24    471.68
  382.41    322.11    235.88    75.220    62.190
 ZeroEnergy[kcal/mol]    8.1018800278892975
  ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
!***********************************************
RRHO        !       14
Geometry[angstrom]        18
C    0.32610   0.41968  -0.76388
C    0.32440   0.42100   0.72051
C    1.56578   0.42040   1.54433
C   -0.95632   0.35942   1.13100
C   -1.84147   0.37651  -0.02986
C   -1.10010   0.44631  -1.14925
H    1.01628   1.08887  -1.27482
H    2.16264   1.31714   1.36337
H    1.33251   0.37812   2.60731
H    2.19874  -0.43724   1.30278
H   -1.28561   0.30333   2.15884
H   -2.91972   0.33771   0.01788
H   -1.45946   0.47223  -2.16581
H    0.73564  -0.66743  -1.06246
C    1.21193  -2.09875  -1.35084
H    0.49584  -2.64040  -0.74697
H    2.23275  -2.08921  -0.99190
H    1.08288  -2.16579  -2.42286
          Core          RigidRotor
     SymmetryFactor    1.5000000000000000
End
 Rotor                 Hindered
 Group   8  9 10
 Axis        3       2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.29   0.91   1.24   0.94   0.32   0.00   0.28   0.90   1.24   0.94
0.32   0.00   0.27   0.89   1.24   0.93   0.31
 End
 Rotor                 Hindered
 Group  16 17 18
 Axis        15       14
 Symmetry        3
 Potential[kcal/mol]        6
  0.00   0.04   0.12   0.15   0.10   0.03
 End
   Frequencies[1/cm]        45
  3254.1    3251.4    3246.6    3223.6    3211.0    3128.2    3122.1
3094.3    3086.2    3033.8
  1672.4    1591.0    1495.0    1486.4    1425.6    1422.9    1421.0
1405.6    1374.1    1352.1
  1295.8    1273.6    1202.6    1171.2    1129.9    1064.5    1033.0
1014.9    978.74    963.87
  921.36    905.02    863.03    831.50    739.46    712.60    631.26
574.44    548.25    465.22
  376.21    321.40    234.33    67.060    52.530
 ZeroEnergy[kcal/mol]    8.1115826788306187
  ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
!***********************************************
RRHO        !       15
Geometry[angstrom]        18
C    0.32646   0.41978  -0.76409
C    0.32424   0.42124   0.72076
C    1.56574   0.42040   1.54437
C   -0.95629   0.35948   1.13103
C   -1.84150   0.37658  -0.02992
C   -1.10048   0.44654  -1.14912
H    1.01411   1.09335  -1.27305
H    2.16259   1.31712   1.36332
H    1.33264   0.37806   2.60738
H    2.19867  -0.43722   1.30265
H   -1.28567   0.30309   2.15884
H   -2.91975   0.33740   0.01795
H   -1.45982   0.47199  -2.16573
H    0.73258  -0.65498  -1.06126
C    1.21276  -2.10126  -1.35135
```

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H    0.49467  -2.63834  -0.74614
H    2.23294  -2.08749  -0.99137
H    1.08231  -2.16412  -2.42326
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.29    0.91    1.24    0.94    0.32    0.00    0.28    0.90    1.24    0.94
0.32    0.00    0.27    0.89    1.24    0.93    0.31
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          14
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.04    0.12    0.15    0.10    0.03
 End
   Frequencies[1/cm]           45
  3256.7      3254.0      3246.4      3223.4      3210.7      3128.1      3119.8
3095.8      3086.2      3033.7
  1673.7      1596.8      1495.0      1486.6      1451.7      1423.5      1421.8
1419.8      1398.3      1353.1
  1338.9      1276.3      1203.8      1166.5      1130.2      1063.7      1033.0
1014.6      978.56      964.68
  919.93      904.02      862.34      832.05      759.63      715.56      630.39
571.33      551.31      458.53
  369.62      320.70      232.65      58.370      41.220
 ZeroEnergy[kcal/mol]    8.1796561944874533
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!********************************************
RRHO           !           16
Geometry[angstrom]           18
C    0.32677   0.42010  -0.76428
C    0.32406   0.42150   0.72103
C    1.56569   0.42039   1.54442
C   -0.95626   0.35956   1.13107
C   -1.84155   0.37666  -0.02996
C   -1.10089   0.44681  -1.14898
H    1.01171   1.09829  -1.27110
H    2.16254   1.31710   1.36326
H    1.33278   0.37799   2.60747
H    2.19857  -0.43721   1.30250
H   -1.28575   0.30284   2.15885
H   -2.91979   0.33707   0.01803
H   -1.46023   0.47175  -2.16562
H    0.73022  -0.64349  -1.06063
C    1.21367  -2.10403  -1.35193
H    0.49343  -2.63617  -0.74525
H    2.23318  -2.08576  -0.99081
H    1.08174  -2.16244  -2.42370
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.29    0.91    1.24    0.94    0.32    0.00    0.28    0.90    1.24    0.94
0.32    0.00    0.27    0.89    1.24    0.93    0.31
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          14
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.04    0.12    0.15    0.10    0.03
 End
   Frequencies[1/cm]           45
  3259.2      3256.5      3246.2      3223.2      3210.5      3128.1      3117.6
3097.1      3086.2      3033.7
  1675.4      1621.7      1548.3      1495.0      1486.2      1424.1      1420.8
1419.1      1401.1      1354.3
  1350.3      1276.3      1203.6      1161.9      1130.4      1062.9      1033.0
1014.2      978.33      965.40
  918.71      903.36      861.55      832.42      777.29      714.32      629.67
568.18      549.67      452.10
  363.09      320.08      230.92      49.210      26.890
 ZeroEnergy[kcal/mol]    8.1754663094371303
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
 End
!********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1383.9400000000001
      WellDepth[kcal/mol]          7.07
      WellDepth[kcal/mol]          32.25
 End
End
End
```

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                   0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature             .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature           30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]            400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                   direct    ! direct or low-eigenvalue
!
WellCutoff                          20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax               0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                     diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                         10
!ChemicalEigenvalueMin              1.e-6         #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]               1.3
!!
RateOutput                          rate.out                ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                          ! Default collisional
energy relaxation kernel
    Exponential                                             ! Currently the only
possible energy relaxation model
       Factor[1/cm]              316                        ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                0.535                        ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff            10                         ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                        ! Collision frequency
model
    LennardJones                                            ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]               90.58  281.367             ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]          3.54    4.694              ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]               39.948  79.05478           ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!*************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50263
 C    1.24622   0.00000   2.31947
 C   -1.27227   0.00046   1.92591
 C   -2.17585   0.00051   0.77474
 C   -1.45565   0.00011  -0.35294
 H    0.51979   0.87601  -0.40113
 H    1.85947   0.87812   2.10478
 H    1.01835  -0.00094   3.38445
 H    1.86045  -0.87709   2.10340
 H   -1.59049   0.00052   2.95892
 H   -3.25397   0.00095   0.84079
 H   -1.83452  -0.00013  -1.36297
 H    0.51979  -0.87591  -0.40126
      Core    RigidRotor
          SymmetryFactor    1.0000000000000000
      End
 Rotor                     Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          3
 Potential[kcal/mol]         12
   0.00    0.08    0.30    0.62    0.95    1.20    1.29    1.21    0.96    0.62    0.30
0.08
 End
   Frequencies[1/cm]          35
  3245.2      3221.6      3209.3      3128.8      3090.6      3074.8      3042.5
3036.2      1695.3      1615.6
  1495.0      1486.6      1424.0      1421.5      1397.2      1340.1      1274.6
1198.6      1152.9      1130.9
  1060.1      1033.7      1005.4      976.89      961.82      922.95      892.68
863.70      828.81      700.71
  623.69      533.08      369.88      325.94      227.72
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]           4
 C    0.00000   0.00000   0.00000
 H    0.00000   0.00000   1.07813
 H    0.93365   0.00000  -0.53917
 H   -0.93365  -0.00105  -0.53917
      Core    RigidRotor
          SymmetryFactor    6.0000000000000000
      End
   Frequencies[1/cm]           6
  526.68      1409.6      1409.7      3123.2      3304.4      3304.6
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]           13
```

```
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.51694
C    1.09843   0.00000   2.30770
C   -1.35798   0.00031   1.92840
C   -2.19992   0.00042   0.79313
C   -1.45663   0.00024  -0.34805
H    0.51600  -0.87687  -0.39945
H    0.51620   0.87681  -0.39935
H    2.09538  -0.00023   1.88922
H    1.00817   0.00002   3.38527
H   -1.68677   0.00025   2.95662
H   -3.27947   0.00064   0.83092
H   -1.83825   0.00021  -1.35705
      Core    RigidRotor
          SymmetryFactor    1.0000000000000000
      End
   Frequencies[1/cm]          33
  182.10      356.98      395.70      533.46      629.59      643.35      680.57
792.84      824.96      845.75
  867.02      937.43      954.59      969.91      992.63      1039.9      1117.1
1156.6      1270.0      1282.1
  1315.8      1407.1      1426.7      1447.0      1530.6      1581.6      3052.2
3085.2      3159.4      3215.5
  3230.8      3244.8      3250.3
 ZeroEnergy[kcal/mol]           0.
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End

!************************************
Fragment PROD2
RRHO
Geometry[angstrom]              5
C    0.00000   0.00000   0.00000
H    0.00000   0.00000   1.08780
H    1.02552   0.00000  -0.36267
H   -0.51271  -0.88842  -0.36222
H   -0.51307   0.88794  -0.36267
      Core    RigidRotor
          SymmetryFactor    12.000000000000000
      End
   Frequencies[1/cm]          9
  1341.0      1341.5      1341.7      1562.7      1563.0      3043.7      3161.5
3162.0      3162.4
 ZeroEnergy[kcal/mol]           0.
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End

GroundEnergy[kcal/mol]   -21.85
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]             18
C   -0.00090  -0.00142   0.00397
C   -0.00150  -0.00114   1.50572
C    1.24480   0.00017   2.32156
C   -1.27421  -0.01869   1.92936
C   -2.17708  -0.03247   0.77784
C   -1.45551  -0.02369  -0.34936
H    0.50895   0.87903  -0.39970
H    1.86412   0.87147   2.09749
H    1.01848   0.01017   3.38680
H    1.85035  -0.88436   2.11083
H   -1.59244  -0.02527   2.96236
H   -3.25508  -0.04902   0.84314
H   -1.83396  -0.03025  -1.35951
H    0.52746  -0.87598  -0.39085
C   -0.29291  -3.50487   0.44121
H   -0.73123  -2.69399   1.00277
H    0.45681  -4.13638   0.89156
H   -0.61984  -3.69854  -0.56825
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]          46
  48.179      69.269      92.281      154.40      203.13      241.46      325.28
368.50      535.36      554.79
  624.15      702.91      829.58      864.26      893.16      922.16      962.95
978.00      1005.5      1033.6
  1059.8      1130.9      1154.8      1199.6      1275.1      1341.6      1397.1
1405.5      1408.4      1416.3
  1423.9      1486.9      1494.9      1614.5      1693.4      3035.5      3041.1
3075.3      3090.6      3116.0
  3129.4      3209.6      3222.1      3245.8      3296.9      3299.2
 ZeroEnergy[kcal/mol]              -1.75
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]             18
C   -0.00071  -0.00103   0.00445
C   -0.00057   0.00004   1.52054
C    1.09817   0.00134   2.31105
C   -1.35779  -0.00801   1.93292
C   -2.20023  -0.01326   0.79815
C   -1.45699  -0.01010  -0.34320
H    0.51141   0.87698  -0.39727
H    2.09487   0.00486   1.89194
H    1.00827  -0.00045   3.38864
H    0.38645  -2.99089   1.35854
H   -1.68595  -0.01237   2.96131
H   -3.27975  -0.02070   0.83620
H   -1.83887  -0.01400  -1.35208
H    0.51735  -0.87828  -0.39179
C   -0.27352  -3.49320   0.65432
H   -0.64678  -4.41395   1.09762
H    0.27316  -3.72811  -0.25702
H   -1.10929  -2.83655   0.42013
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]          48
  35.421      50.200      66.867      75.354      93.128      120.97      182.26
356.92      388.78      533.38
  629.65      643.84      682.06      794.68      825.22      844.94      867.71
934.54      954.85      971.00
  993.07      1040.4      1117.2      1158.0      1270.8      1282.8      1316.7
1335.4      1343.3      1347.8
  1407.1      1426.0      1437.4      1530.7      1562.0      1564.1      1581.3
3039.2      3052.6      3086.3
  3154.9      3159.1      3159.3      3160.0      3215.6      3231.1      3244.9
3250.3
 ZeroEnergy[kcal/mol]             -25.22
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
End
!************************************
Barrier       B1  REACS WR
  RRHO
    Stoichiometry  H11C7
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]             14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50263
C    1.24622   0.00000   2.31947
C   -1.27227   0.00046   1.92591
C   -2.17585   0.00051   0.77474
C   -1.45565   0.00011  -0.35294
H    0.51979   0.87601  -0.40113
H    1.85947   0.87812   2.10478
```

```
H   1.01835  -0.00094   3.38445
H   1.86045  -0.87709   2.10340
H  -1.59049   0.00052   2.95892
H  -3.25397   0.00095   0.84079
H  -1.83452  -0.00013  -1.36297
H   0.51979  -0.87591  -0.40126
    FragmentGeometry[angstrom]          4
C   0.00000   0.00000   0.00000
H   0.00000   0.00000   1.07813
H   0.93365   0.00000  -0.53917
H  -0.93365  -0.00105  -0.53917
                          SymmetryFactor     6.0000000000000000
      PotentialPrefactor[au]           10.
      PotentialPowerExponent          6
             End
Rotor                    Hindered
Geometry[angstrom]           14
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.50263
C   1.24622   0.00000   2.31947
C  -1.27227   0.00046   1.92591
C  -2.17585   0.00051   0.77474
C  -1.45565   0.00011  -0.35294
H   0.51979   0.87601  -0.40113
H   1.85947   0.87812   2.10478
H   1.01835  -0.00094   3.38445
H   1.86045  -0.87709   2.10340
H  -1.59049   0.00052   2.95892
H  -3.25397   0.00095   0.84079
H  -1.83452  -0.00013  -1.36297
H   0.51979  -0.87591  -0.40126
Group   8   9  10
Axis         3        2
Symmetry         3
Potential[kcal/mol]         12
  0.0000    0.80000E-01 0.30000    0.62000    0.95000    1.2000    1.2900
1.2100    0.96000    0.62000
 0.30000    0.80000E-01
End
    Frequencies[1/cm]         41
  3245.2    3221.6    3209.3    3128.8    3090.6    3074.8    3042.5
3036.2    1695.3    1615.6
  1495.0    1486.6    1424.0    1421.5    1397.2    1340.1    1274.6
1198.6    1152.9    1130.9
  1060.1    1033.7    1005.4    976.89    961.82    922.95    892.68
863.70    828.81    700.71
  623.69    533.08    369.88    325.94    227.72
  526.68    1409.6    1409.7    3123.2    3304.4    3304.6
 ZeroEnergy[kcal/mol]         0.
 ElectronicLevels[1/cm]              1
  0.0000000000000000       4.0000000000000000
End
!************************************
Barrier       B3  WP PRODS
  RRHO
    Stoichiometry  H11C7
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]          13
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.51694
C   1.09843   0.00000   2.30770
C  -1.35798   0.00031   1.92840
C  -2.19992   0.00042   0.79313
C  -1.45663   0.00024  -0.34805
H   0.51600  -0.87687  -0.39945
H   0.51620   0.87681  -0.39935
H   2.09538  -0.00023   1.88922
H   1.00817   0.00002   3.38527
H  -1.68677   0.00025   2.95662
H  -3.27947   0.00064   0.83092
H  -1.83825   0.00021  -1.35705
      FragmentGeometry[angstrom]          5
C   0.00000   0.00000   0.00000
H   0.00000   0.00000   1.08780
H   1.02552   0.00000  -0.36267
H  -0.51271  -0.88842  -0.36222
H  -0.51307   0.88794  -0.36267
                          SymmetryFactor     12.000000000000000
      PotentialPrefactor[au]           10.
      PotentialPowerExponent          6
             End
    Frequencies[1/cm]         42
  182.10    356.98    395.70    533.46    629.59    643.35    680.57
792.84    824.96    845.75
  867.02    937.43    954.59    969.91    992.63    1039.9    1117.1
1156.6    1270.0    1282.1
  1315.8    1407.1    1426.7    1447.0    1530.6    1581.6    3052.2
3085.2    3159.4    3215.5
  3230.8    3244.8    3250.3
  1341.0    1341.5    1341.7    1562.7    1563.0    3043.7    3161.5
3162.0    3162.4
 ZeroEnergy[kcal/mol]         -21.853599497897033
 ElectronicLevels[1/cm]              1
  0.0000000000000000       4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO        !         1
Geometry[angstrom]         18
C   0.12057   0.45378  -1.23458
C   0.12515   0.45337   0.27099
C   1.33131   0.46146   1.06797
C  -1.16233   0.36435   0.69109
C  -2.05313   0.31821  -0.45769
C  -1.33122   0.36755  -1.58784
H   0.59008   1.35586  -1.63817
H   2.16218   1.02884   0.65760
H   1.18511   0.64894   2.12761
H   1.87406  -0.84924   1.05895
H  -1.48084   0.33706   1.72308
H  -3.12980   0.25706  -0.39641
H  -1.71043   0.35644  -2.59767
H   0.69089  -0.39369  -1.62852
C   2.34139  -2.06428   1.04593
H   1.44361  -2.67156   0.98190
H   2.88452  -2.17555   1.97912
H   2.97121  -2.11430   0.16297
            Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                    Hindered
 Group   8   9  10  15  16  17  18
 Axis         3        2
 Symmetry         1
 Potential[kcal/mol]         18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis         15       10
 Symmetry         3
 Potential[kcal/mol]         6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
    Frequencies[1/cm]         45
  3246.1    3224.9    3213.4    3203.3    3201.2    3187.1    3107.9
3077.0    3066.4    3043.0
  1635.7    1515.3    1475.4    1472.3    1450.0    1426.3    1396.1
1384.2    1350.9    1282.0
  1256.9    1224.5    1175.4    1147.3    1129.2    1073.2    1033.5
1007.8    976.49    964.35
  921.60    894.38    866.10    829.28    703.40    646.42    614.46
572.06    522.32    448.45
  378.91    343.27    239.10    88.350    83.610
 ZeroEnergy[kcal/mol]   6.4169856028922680
 ElectronicLevels[1/cm]              1
```

```
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           2
Geometry[angstrom]          18
C   0.12052   0.45377  -1.23453
C   0.12461   0.45339   0.27086
C   1.33207   0.46054   1.06820
C  -1.16207   0.36442   0.69108
C  -2.05316   0.31820  -0.45784
C  -1.33128   0.36754  -1.58783
H   0.59008   1.35587  -1.63808
H   2.16113   1.03101   0.65800
H   1.18472   0.65052   2.12737
H   1.86827  -0.83493   1.05905
H  -1.48071   0.33711   1.72306
H  -3.12981   0.25703  -0.39648
H  -1.71044   0.35645  -2.59768
H   0.69090  -0.39368  -1.62849
C   2.34177  -2.06529   1.04591
H   1.44271  -2.67031   0.98190
H   2.88425  -2.17425   1.97952
H   2.97098  -2.11298   0.16264
            Core           RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                        Hindered
 Group   8   9  10  15  16  17  18
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.66    2.59    4.81    5.65    4.36    2.05    0.38    0.03    0.74    2.00
3.25    4.20    4.54    4.06    3.02    1.73    0.52
 End
 Rotor                        Hindered
 Group   16  17  18
 Axis           15         10
 Symmetry          3
 Potential[kcal/mol]           6
  0.00    0.01    0.05    0.06    0.05    0.02
 End
   Frequencies[1/cm]          45
  3246.1      3224.8      3213.2      3206.1      3204.0      3184.9      3106.0
3076.9      3067.9      3042.9
  1637.7      1520.7      1473.2      1468.3      1447.9      1425.9      1396.8
1382.4      1350.5      1282.8
  1261.9      1221.1      1167.1      1146.7      1129.3      1069.5      1034.5
1008.2      976.59      964.58
  921.40      894.56      867.97      829.30      703.59      646.01      619.13
574.54      522.39      449.13
  378.64      342.50      239.00      90.300      85.000
ZeroEnergy[kcal/mol]    7.1819023867071223
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           3
Geometry[angstrom]          18
C   0.12047   0.45376  -1.23449
C   0.12407   0.45342   0.27073
C   1.33281   0.45965   1.06842
C  -1.16182   0.36450   0.69107
C  -2.05318   0.31820  -0.45799
C  -1.33134   0.36754  -1.58783
H   0.59007   1.35589  -1.63799
H   2.16010   1.03314   0.65840
H   1.18433   0.65209   2.12713
H   1.86248  -0.82059   1.05915
H  -1.48059   0.33716   1.72305
H  -3.12983   0.25700  -0.39654
H  -1.71044   0.35647  -2.59770
H   0.69091  -0.39368  -1.62846
C   2.34215  -2.06632   1.04590
H   1.44182  -2.66907   0.98189
H   2.88400  -2.17296   1.97992
H   2.97076  -2.11167   0.16231
            Core           RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                        Hindered
 Group   8   9  10  15  16  17  18
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.66    2.59    4.81    5.65    4.36    2.05    0.38    0.03    0.74    2.00
3.25    4.20    4.54    4.06    3.02    1.73    0.52
 End
 Rotor                        Hindered
 Group   16  17  18
 Axis           15         10
 Symmetry          3
 Potential[kcal/mol]           6
  0.00    0.01    0.05    0.06    0.05    0.02
 End
   Frequencies[1/cm]          45
  3246.0      3224.6      3212.9      3208.9      3206.8      3182.6      3104.1
3076.8      3069.5      3042.8
  1639.8      1526.7      1472.9      1462.8      1445.8      1425.4      1397.8
1380.5      1350.2      1284.5
  1267.2      1219.3      1159.0      1145.7      1129.5      1067.8      1035.5
1008.6      976.67      964.82
  921.20      894.74      869.86      829.31      703.75      646.58      622.08
576.75      522.84      449.87
  378.23      341.51      238.76      91.490      85.640
ZeroEnergy[kcal/mol]    7.8803377675663739
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           4
Geometry[angstrom]          18
C   0.12041   0.45376  -1.23444
C   0.12355   0.45345   0.27060
C   1.33353   0.45879   1.06864
C  -1.16157   0.36457   0.69105
C  -2.05320   0.31819  -0.45813
C  -1.33140   0.36753  -1.58782
H   0.59007   1.35591  -1.63790
H   2.15908   1.03526   0.65879
H   1.18394   0.65365   2.12688
H   1.85670  -0.80622   1.05925
H  -1.48047   0.33721   1.72303
H  -3.12985   0.25697  -0.39661
H  -1.71045   0.35648  -2.59771
H   0.69093  -0.39367  -1.62843
C   2.34255  -2.06738   1.04588
H   1.44093  -2.66784   0.98189
H   2.88374  -2.17168   1.98031
H   2.97054  -2.11037   0.16198
            Core           RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                        Hindered
 Group   8   9  10  15  16  17  18
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.66    2.59    4.81    5.65    4.36    2.05    0.38    0.03    0.74    2.00
3.25    4.20    4.54    4.06    3.02    1.73    0.52
 End
 Rotor                        Hindered
 Group   16  17  18
 Axis           15         10
 Symmetry          3
 Potential[kcal/mol]           6
  0.00    0.01    0.05    0.06    0.05    0.02
 End
   Frequencies[1/cm]          45
```

```
 3246.0    3224.3    3212.7    3211.7    3209.6    3180.3    3102.2
3076.8    3071.0    3042.7
 1642.0    1533.0    1472.7    1457.8    1443.8    1425.0    1398.9
1379.0    1350.0    1288.0
 1271.7    1218.4    1152.3    1143.5    1129.6    1067.3    1036.5
1009.0    976.75    965.05
 920.98    894.89    871.68    829.32    703.87    647.65    623.14
578.55    523.44    450.92
 377.73    340.31    238.35    91.890    85.530
ZeroEnergy[kcal/mol]    8.4965107241328468
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
End
!**********************************************
RRHO    !    5
Geometry[angstrom]    18
C   0.12036   0.45375  -1.23440
C   0.12304   0.45348   0.27048
C   1.33424   0.45796   1.06886
C  -1.16133   0.36464   0.69104
C  -2.05322   0.31818  -0.45826
C  -1.33145   0.36752  -1.58781
H   0.59006   1.35593  -1.63781
H   2.15806   1.03736   0.65917
H   1.18354   0.65522   2.12664
H   1.85094  -0.79183   1.05937
H  -1.48035   0.33726   1.72302
H  -3.12987   0.25694  -0.39667
H  -1.71046   0.35649  -2.59773
H   0.69094  -0.39366  -1.62840
C   2.34296  -2.06847   1.04586
H   1.44005  -2.66661   0.98188
H   2.88348  -2.17040   1.98070
H   2.97032  -2.10907   0.16166
        Core        RigidRotor
     SymmetryFactor    1.0000000000000000
End
 Rotor        Hindered
 Group   8  9  10  15  16  17  18
 Axis     3     2
 Symmetry     1
 Potential[kcal/mol]     18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor        Hindered
 Group   16  17  18
 Axis     15     10
 Symmetry     3
 Potential[kcal/mol]     6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]     45
 3245.9    3224.2    3214.5    3212.6    3212.3    3177.8    3100.2
3076.7    3072.6    3042.6
 1644.3    1539.7    1472.6    1453.3    1441.9    1424.6    1400.1
1378.0    1349.7    1294.3
 1274.6    1217.9    1149.2    1138.4    1129.7    1067.4    1037.6
1009.5    976.81    965.27
 920.73    895.03    873.40    829.34    703.96    648.89    622.24
579.88    524.09    452.43
 377.20    338.95    237.79    91.440    84.640
ZeroEnergy[kcal/mol]    9.0352381878384023
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
End
!**********************************************
RRHO    !    6
Geometry[angstrom]    18
C   0.12031   0.45374  -1.23436
C   0.12253   0.45350   0.27036
C   1.33493   0.45716   1.06908
C  -1.16110   0.36471   0.69103
C  -2.05324   0.31818  -0.45840
C  -1.33151   0.36751  -1.58781
H   0.59006   1.35595  -1.63772
H   2.15702   1.03947   0.65956
H   1.18313   0.65680   2.12640
H   1.84519  -0.77745   1.05949
H  -1.48024   0.33731   1.72301
H  -3.12989   0.25691  -0.39673
H  -1.71046   0.35651  -2.59774
H   0.69095  -0.39365  -1.62838
C   2.34338  -2.06959   1.04584
H   1.43917  -2.66538   0.98187
H   2.88322  -2.16912   1.98109
H   2.97010  -2.10777   0.16133
        Core        RigidRotor
     SymmetryFactor    1.0000000000000000
End
 Rotor        Hindered
 Group   8  9  10  15  16  17  18
 Axis     3     2
 Symmetry     1
 Potential[kcal/mol]     18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor        Hindered
 Group   16  17  18
 Axis     15     10
 Symmetry     3
 Potential[kcal/mol]     6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]     45
 3245.9    3224.0    3217.3    3215.3    3212.2    3175.4    3098.2
3076.6    3074.2    3042.5
 1646.7    1546.5    1472.5    1449.3    1440.0    1424.2    1401.3
1377.9    1349.6    1302.7
 1276.2    1217.7    1148.2    1132.2    1129.5    1067.4    1038.5
1010.0    976.86    965.46
 920.44    895.14    874.91    829.35    703.98    650.01    619.30
580.75    524.73    454.55
 376.64    337.44    237.04    90.070    82.960
ZeroEnergy[kcal/mol]    9.4759222059142587
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
End
!**********************************************
RRHO    !    7
Geometry[angstrom]    18
C   0.12026   0.45373  -1.23432
C   0.12203   0.45354   0.27024
C   1.33561   0.45639   1.06930
C  -1.16087   0.36478   0.69102
C  -2.05327   0.31817  -0.45854
C  -1.33156   0.36750  -1.58780
H   0.59005   1.35597  -1.63763
H   2.15598   1.04159   0.65994
H   1.18272   0.65839   2.12615
H   1.83947  -0.76308   1.05962
H  -1.48012   0.33736   1.72299
H  -3.12991   0.25688  -0.39680
H  -1.71047   0.35652  -2.59776
H   0.69096  -0.39363  -1.62835
C   2.34381  -2.07075   1.04582
H   1.43827  -2.66413   0.98187
H   2.88297  -2.16782   1.98149
H   2.96987  -2.10646   0.16100
        Core        RigidRotor
     SymmetryFactor    1.0000000000000000
End
 Rotor        Hindered
 Group   8  9  10  15  16  17  18
 Axis     3     2
 Symmetry     1
 Potential[kcal/mol]     18
```

```
 0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
 0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]          45
 3245.8     3223.8     3220.2     3218.1     3212.0     3172.9     3096.1
3076.6     3075.8     3042.4
 1649.2     1553.3     1472.4     1445.9     1438.2     1423.8     1402.5
1378.7     1349.8     1312.4
 1277.0     1217.5     1148.0     1130.2     1125.5     1067.2     1039.5
1010.5     976.89     965.63
 920.14     895.22     876.21     829.37     703.94     650.82     614.32
581.21     525.39     457.43
 376.07     335.80     236.14     87.740     80.440
 ZeroEnergy[kcal/mol]    9.8244375928783825
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          8
Geometry[angstrom]          18
C    0.12021   0.45372  -1.23428
C    0.12153   0.45357   0.27011
C    1.33628   0.45565   1.06951
C   -1.16065   0.36485   0.69100
C   -2.05329   0.31817  -0.45867
C   -1.33162   0.36750  -1.58780
H    0.59005   1.35599  -1.63754
H    2.15492   1.04374   0.66032
H    1.18229   0.66001   2.12590
H    1.83378  -0.74872   1.05976
H   -1.48001   0.33742   1.72298
H   -3.12993   0.25685  -0.39686
H   -1.71048   0.35653  -2.59778
H    0.69097  -0.39362  -1.62833
C    2.34426  -2.07195   1.04580
H    1.43737  -2.66287   0.98186
H    2.88271  -2.16651   1.98189
H    2.96965  -2.10513   0.16066
             Core           RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                   Hindered
 Group    8   9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]          18
 0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
 0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]          45
 3245.8     3223.6     3223.0     3220.9     3211.7     3170.3     3094.0
3077.5     3076.4     3042.4
 1651.9     1560.0     1472.3     1442.9     1436.5     1423.4     1403.8
1380.4     1350.7     1322.4
 1277.5     1217.5     1148.0     1130.2     1120.8     1066.5     1040.3
1010.9     976.92     965.76
 919.82     895.28     877.24     829.39     703.83     651.19     607.38
581.36     526.10     461.26
 375.46     334.06     235.07     84.370     77.070
 ZeroEnergy[kcal/mol]    10.073665806800804
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          9
Geometry[angstrom]          18
C    0.12016   0.45372  -1.23424
C    0.12103   0.45361   0.26999
C    1.33693   0.45495   1.06973
C   -1.16043   0.36493   0.69099
C   -2.05331   0.31816  -0.45880
C   -1.33168   0.36749  -1.58780
H    0.59005   1.35601  -1.63745
H    2.15384   1.04594   0.66071
H    1.18183   0.66167   2.12564
H    1.82813  -0.73440   1.05991
H   -1.47989   0.33748   1.72297
H   -3.12995   0.25682  -0.39693
H   -1.71049   0.35654  -2.59780
H    0.69098  -0.39361  -1.62831
C    2.34473  -2.07321   1.04577
H    1.43644  -2.66159   0.98185
H    2.88244  -2.16518   1.98231
H    2.96942  -2.10378   0.16031
             Core           RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                   Hindered
 Group    8   9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]          18
 0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
 0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]          45
 3245.7     3225.8     3223.7     3223.4     3211.5     3167.8     3091.8
3079.2     3076.3     3042.3
 1654.6     1566.6     1472.2     1440.3     1434.9     1423.0     1405.3
1382.9     1353.3     1331.4
 1277.8     1217.4     1148.4     1130.3     1117.7     1065.3     1041.0
1011.3     976.93     965.86
 919.50     895.32     877.97     829.42     703.70     651.07     598.63
581.42     527.02     466.12
 374.78     332.26     233.82     79.910     72.810
 ZeroEnergy[kcal/mol]    10.236314289781632
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          10
Geometry[angstrom]          18
C    0.12011   0.45370  -1.23419
C    0.12055   0.45366   0.26987
C    1.33757   0.45428   1.06995
C   -1.16022   0.36500   0.69098
C   -2.05335   0.31815  -0.45892
C   -1.33173   0.36748  -1.58782
H    0.59007   1.35606  -1.63736
H    2.15274   1.04820   0.66109
H    1.18135   0.66339   2.12541
H    1.82252  -0.72012   1.06007
H   -1.47978   0.33754   1.72297
H   -3.13002   0.25679  -0.39699
H   -1.71053   0.35655  -2.59787
H    0.69102  -0.39362  -1.62829
C    2.34523  -2.07451   1.04575
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H   1.43547  -2.66030   0.98184
H   2.88218  -2.16381   1.98273
H   2.96918  -2.10240   0.15998
          Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                  Hindered
 Group   8  9  10  15  16  17  18
 Axis          3        2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                  Hindered
 Group   16  17  18
 Axis          15       10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]         45
  3245.3     3228.5     3226.6     3223.0     3211.1     3164.8     3089.3
3080.8     3075.8     3041.8
  1657.4     1572.8     1472.1     1438.1     1433.4     1422.8     1407.2
1386.1     1359.0     1337.6
  1278.1     1217.4     1149.0     1130.4     1117.0     1063.9     1041.6
1011.8     977.05     965.96
  919.26     895.37     878.39     829.46     703.73     650.52     588.37
581.81     528.48     471.89
  374.20     330.45     232.51     74.390     67.720
 ZeroEnergy[kcal/mol]    10.312726139038034
  ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !          11
Geometry[angstrom]          18
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.50393
C   1.21819   0.00000   2.30439
C  -1.28003  -0.08862   1.92514
C  -2.17338  -0.13555   0.77511
C  -1.45182  -0.08623  -0.35361
H   0.46998   0.90235  -0.40311
H   2.03150   0.59688   1.89571
H   1.06082   0.21152   3.35930
H   1.69702  -1.15964   2.29446
H  -1.59966  -0.11609   2.95712
H  -3.25001  -0.19694   0.83710
H  -1.83055  -0.09714  -1.36364
H   0.57094  -0.84727  -0.39412
C   2.22572  -2.52957   2.27993
H   1.31445  -3.11250   2.21604
H   2.76185  -2.61599   3.21740
H   2.84892  -2.55456   1.39377
          Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                  Hindered
 Group   8  9  10  15  16  17  18
 Axis          3        2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                  Hindered
 Group   16  17  18
 Axis          15       10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]         45
  3245.2     3231.3     3229.5     3222.9     3210.9     3162.2     3087.3
3082.5     3075.7     3041.7
  1660.5     1578.8     1472.0     1436.3     1432.1     1422.5     1409.5
1389.7     1367.6     1340.6
  1278.2     1217.5     1150.1     1130.5     1119.1     1062.4     1042.0
1012.0     977.05     966.01
  919.00     895.37     878.46     829.49     703.53     649.58     584.56
575.99     530.77     477.78
  373.32     328.57     230.94     67.480     61.580
 ZeroEnergy[kcal/mol]    10.295653425858134
  ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !          12
Geometry[angstrom]          18
C   0.11999   0.45369  -1.23412
C   0.11954   0.45374   0.26962
C   1.33883   0.45311   1.07041
C  -1.15981   0.36516   0.69095
C  -2.05340   0.31814  -0.45920
C  -1.33186   0.36746  -1.58783
H   0.59006   1.35610  -1.63716
H   2.15034   1.05300   0.66190
H   1.18031   0.66706   2.12486
H   1.81158  -0.69186   1.06043
H  -1.47953   0.33768   1.72294
H  -3.13007   0.25672  -0.39714
H  -1.71055   0.35657  -2.59791
H   0.69103  -0.39358  -1.62824
C   2.34630  -2.07736   1.04570
H   1.43343  -2.65748   0.98182
H   2.88161  -2.16091   1.98365
H   2.96869  -2.09945   0.15921
          Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                  Hindered
 Group   8  9  10  15  16  17  18
 Axis          3        2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                  Hindered
 Group   16  17  18
 Axis          15       10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]         45
  3245.2     3234.1     3232.2     3222.7     3210.7     3159.6     3085.2
3084.2     3075.6     3041.6
  1663.7     1584.6     1472.0     1434.9     1430.9     1422.4     1412.8
1393.3     1377.2     1342.0
  1278.3     1217.7     1152.5     1130.9     1125.4     1061.3     1042.3
1012.2     977.03     966.03
  918.80     895.35     878.22     829.53     703.33     648.40     590.62
563.29     534.24     482.88
  372.32     326.68     229.20     59.080     54.320
 ZeroEnergy[kcal/mol]    10.282147599561256
  ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !          13
Geometry[angstrom]          18
C   0.11993   0.45369  -1.23409
C   0.11901   0.45377   0.26949
C   1.33945   0.45265   1.07067
C  -1.15960   0.36524   0.69093
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C   -2.05342   0.31813  -0.45935
C   -1.33192   0.36745  -1.58782
H    0.59003   1.35609  -1.63705
H    2.14900   1.05558   0.66235
H    1.17974   0.66906   2.12453
H    1.80631  -0.67797   1.06065
H   -1.47939   0.33776   1.72292
H   -3.13005   0.25669  -0.39723
H   -1.71054   0.35658  -2.59789
H    0.69101  -0.39353  -1.62822
C    2.34689  -2.07895   1.04567
H    1.43236  -2.65594   0.98182
H    2.88131  -2.15934   1.98415
H    2.96846  -2.09786   0.15876
          Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                   Hindered
 Group   8  9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]         45
  3245.5     3237.2     3235.0     3222.8     3210.6     3157.4     3085.9
3083.5     3075.8     3041.8
  1667.3     1590.2     1472.2     1434.3     1429.8     1422.3     1416.9
1397.0     1385.9     1342.7
  1278.5     1218.7     1160.4     1136.6     1129.9     1060.5     1042.5
1012.3     976.89     965.99
  918.59     895.29     877.64     829.57     702.93     647.16     605.28
549.95     537.85     485.64
  370.97     324.75     227.18     48.660     45.490
 ZeroEnergy[kcal/mol]    10.165789889316216
 ElectronicLevels[1/cm]                1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          14
Geometry[angstrom]          18
C    0.11986   0.45369  -1.23405
C    0.11847   0.45382   0.26936
C    1.34005   0.45226   1.07093
C   -1.15940   0.36533   0.69092
C   -2.05345   0.31812  -0.45949
C   -1.33199   0.36745  -1.58783
H    0.59001   1.35612  -1.63693
H    2.14759   1.05837   0.66281
H    1.17910   0.67121   2.12422
H    1.80120  -0.66431   1.06088
H   -1.47924   0.33785   1.72291
H   -3.13008   0.25665  -0.39733
H   -1.71056   0.35658  -2.59791
H    0.69101  -0.39350  -1.62820
C    2.34753  -2.08066   1.04564
H    1.43118  -2.65432   0.98181
H    2.88099  -2.15768   1.98470
H    2.96820  -2.09617   0.15830
          Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                   Hindered
 Group   8  9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]         45
  3245.5     3240.1     3237.9     3222.6     3210.5     3154.9     3087.7
3081.6     3075.6     3041.7
  1671.3     1595.9     1473.0     1436.5     1429.0     1423.0     1420.7
1402.0     1392.1     1343.1
  1278.9     1223.8     1185.2     1142.9     1130.2     1060.0     1042.6
1012.3     976.87     965.95
  918.50     895.25     876.78     829.63     702.79     646.85     632.73
541.05     535.24     485.69
  369.68     322.88     225.07     35.940     33.970
 ZeroEnergy[kcal/mol]    10.081616916173289
 ElectronicLevels[1/cm]                1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          15
Geometry[angstrom]          18
C    0.11978   0.45368  -1.23402
C    0.11792   0.45388   0.26922
C    1.34063   0.45200   1.07122
C   -1.15921   0.36542   0.69090
C   -2.05348   0.31810  -0.45965
C   -1.33206   0.36744  -1.58785
H    0.59000   1.35614  -1.63680
H    2.14604   1.06139   0.66329
H    1.17839   0.67354   2.12389
H    1.79635  -0.65100   1.06115
H   -1.47908   0.33795   1.72290
H   -3.13011   0.25660  -0.39743
H   -1.71059   0.35659  -2.59795
H    0.69101  -0.39348  -1.62817
C    2.34824  -2.08255   1.04560
H    1.42989  -2.65259   0.98179
H    2.88067  -2.15590   1.98528
H    2.96792  -2.09436   0.15780
          Core          RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                   Hindered
 Group   8  9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.59   4.81   5.65   4.36   2.05   0.38   0.03   0.74   2.00
3.25   4.20   4.54   4.06   3.02   1.73   0.52
 End
 Rotor                   Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.01   0.05   0.06   0.05   0.02
 End
   Frequencies[1/cm]         45
  3245.4     3243.0     3240.8     3222.5     3210.3     3152.5     3089.4
3079.9     3075.4     3041.6
  1676.4     1602.5     1476.4     1446.4     1428.3     1424.5     1421.9
1408.6     1395.4     1343.4
  1282.3     1257.7     1207.0     1145.3     1130.3     1059.5     1042.6
1012.1     976.85     965.89
  918.45     895.19     875.63     829.69     702.95     676.92     643.42
541.41     521.60     483.25
  368.27     321.03     222.75     20.320     9.4100
```

```
ZeroEnergy[kcal/mol]    10.002293817849960
 ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
 End
!********************************************
     Tunneling    Eckart
     ImaginaryFrequency[1/cm]    1624.0599000000000
     WellDepth[kcal/mol]          9.17
     WellDepth[kcal/mol]         32.64
 End
End
End
```

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                  0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature            .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature          30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]           400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                  direct     ! direct or low-eigenvalue
!
WellCutoff                         20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax              0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                    diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                        10
!ChemicalEigenvalueMin             1.e-6        #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]              1.3
!!
RateOutput                         rate.out                ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                       ! Default collisional
energy relaxation kernel
    Exponential                                          ! Currently the only
possible energy relaxation model
       Factor[1/cm]             316                      ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                 0.535                       ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff           10                       ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                     ! Collision frequency
model
    LennardJones                                         ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]              90.58  281.367           ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]         3.54    4.694            ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]              39.948  79.05478         ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50112
 C    1.39710   0.00000   2.12644
 C   -0.81569  -1.21840   1.82234
 C   -1.21870  -1.80451   0.68960
 C   -0.70750  -1.04109  -0.45233
 H    0.50817   0.74374  -0.59543
 H    1.95008   0.89431   1.83920
 H    1.33447  -0.02486   3.21435
 H    1.96018  -0.87263   1.79528
 H   -1.02550  -1.54600   2.82960
 H   -1.82229  -2.69676   0.61182
 H   -0.88231  -1.29309  -1.48790
 H   -0.53850   0.88886   1.85441
      Core    RigidRotor
          SymmetryFactor    1.0000000000000000
      End
 Rotor                       Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          3
 Potential[kcal/mol]          12
   0.00    0.23    0.90    1.84    2.83    3.55    3.78    3.44    2.69    1.75    0.87
0.23
 End
    Frequencies[1/cm]          35
  3244.1     3235.6     3219.3     3210.9     3128.0     3124.4     3049.0
3020.3     1670.2     1591.0
  1503.9     1503.7     1422.5     1406.8     1334.3     1293.1     1277.9
1155.2     1119.2     1104.0
  1090.8     1028.3     1004.1     983.75     981.16     957.17     883.24
817.77     792.34     742.25
  721.84     567.90     547.80     294.51     164.97
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]            4
 C    0.00000   0.00000   0.00000
 H    0.00000   0.00000   1.07813
 H    0.93365   0.00000  -0.53917
 H   -0.93365  -0.00105  -0.53917
      Core    RigidRotor
          SymmetryFactor    6.0000000000000000
      End
    Frequencies[1/cm]           6
  526.68     1409.6     1409.7     3123.2     3304.4     3304.6
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]            13
```

```
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.41507
C   1.18585   0.00000   2.30525
C  -1.37924  -0.00034   1.86264
C  -2.17195  -0.00056   0.76525
C  -1.30652  -0.00033  -0.41759
H   0.87955   0.00028  -0.62343
H   2.11567   0.00259   1.73998
H   1.17551   0.87449   2.96082
H   1.17824  -0.87748   2.95691
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
      Core    RigidRotor
          SymmetryFactor    2.0000000000000000
      End
Rotor                       Hindered
Group    8   9  10
Axis            3           2
Symmetry           3
Potential[kcal/mol]          12
   0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
   Frequencies[1/cm]          32
  3255.2     3247.0     3232.4     3224.7     3138.6     3086.9     3034.1
1584.1     1503.1     1481.1
  1477.9     1438.4     1407.4     1311.3     1292.6     1178.7     1098.1
1049.4     1023.5     1013.2
  953.40     929.99     923.03     899.45     740.46     727.81     638.42
604.77     528.85     520.52
  329.55     215.83
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!************************************
Fragment PROD2
RRHO
Geometry[angstrom]              5
C   0.00000   0.00000   0.00000
H   0.00000   0.00000   1.08780
H   1.02552   0.00000  -0.36267
H  -0.51271  -0.88842  -0.36222
H  -0.51307   0.88794  -0.36267
      Core    RigidRotor
          SymmetryFactor    12.000000000000000
      End
   Frequencies[1/cm]           9
  1341.0     1341.5     1341.7     1562.7     1563.0     3043.7     3161.5
3162.0     3162.4
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End

GroundEnergy[kcal/mol]   -26.21
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]             18
C  -0.00273  -0.00576   0.00407
C   0.00151  -0.00587   1.50431
C   1.39675  -0.00202   2.13232
C  -0.81908  -1.21954   1.82762
C  -1.23142  -1.80198   0.69549
C  -0.72001  -1.04091  -0.44743
H   0.50546   0.73702  -0.59249
H   1.94818   0.89266   1.84352
H   1.33122  -0.02290   3.22008
H   1.96313  -0.87431   1.80594
H  -1.02697  -1.54696   2.83531
H  -1.84184  -2.68979   0.61957
H  -0.90395  -1.28820  -1.48248
H  -0.54184   0.88355   1.85158
C  -3.13793   1.64091   0.88169
H  -2.68366   2.23543   0.10498
H  -3.82162   2.09867   1.57923
H  -2.91230   0.58775   0.95104
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]          48
  32.448     49.299     74.290     78.197     118.91     164.08     195.31
259.60     295.41     547.86
  551.47     568.67     719.60     742.72     793.08     818.81     883.65
958.54     980.25     982.50
  1004.9     1028.7     1091.4     1106.0     1119.7     1156.9     1278.7
1293.5     1334.5     1404.8
  1407.1     1415.7     1422.5     1503.9     1504.2     1588.7     1668.1
3011.5     3049.4     3117.7
  3125.3     3127.9     3210.7     3219.0     3235.2     3243.6     3298.7
3299.7
 ZeroEnergy[kcal/mol]             -1.35
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]             18
C  -0.00185   0.00120   0.00452
C  -0.00104   0.00169   1.42147
C   1.18538   0.00079   2.30982
C  -1.37805   0.03619   1.86882
C  -2.17099   0.05870   0.77134
C  -1.30668   0.03673  -0.41214
H   0.87760  -0.01881  -0.61861
H   2.11122  -0.10538   1.74789
H   1.23374   0.93401   2.87800
H   1.12371  -0.80852   3.04085
H  -1.69206   0.04655   2.90056
H  -3.24897   0.08758   0.75033
H  -1.65555   0.04614  -1.43337
H  -0.62148   2.85636   0.79439
C  -0.06419   3.44160   1.52230
H   0.99962   3.24656   1.40097
H  -0.37583   3.15301   2.52417
H  -0.25717   4.50199   1.37383
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]          47
  10.588     40.203     56.231     69.418     77.979     149.30     225.81
329.63     527.67     536.03
  605.36     637.60     729.65     741.27     902.39     924.09     930.80
955.69     1013.1     1022.5
  1052.4     1097.7     1179.7     1293.4     1311.6     1332.7     1342.4
1348.3     1406.0     1438.1
  1476.6     1483.5     1506.7     1557.7     1563.7     1583.6     3032.6
3041.3     3087.4     3137.6
  3154.8     3156.6     3167.5     3225.5     3233.2     3247.6     3255.8
 ZeroEnergy[kcal/mol]            -30.29
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier        B1  REACS WR
  RRHO
   Stoichiometry  H11C7
   Core PhaseSpaceTheory
     FragmentGeometry[angstrom]            14
C    0.00000   0.00000   0.00000
```

```
C    0.00000   0.00000   1.50112
C    1.39710   0.00000   2.12644
C   -0.81569  -1.21840   1.82234
C   -1.21870  -1.80451   0.68960
C   -0.70750  -1.04109  -0.45233
H    0.50817   0.74374  -0.59543
H    1.95008   0.89431   1.83920
H    1.33447  -0.02486   3.21435
H    1.96018  -0.87263   1.79528
H   -1.02550  -1.54600   2.82960
H   -1.82229  -2.69676   0.61182
H   -0.88231  -1.29309  -1.48790
H   -0.53850   0.88886   1.85441
   FragmentGeometry[angstrom]          4
C    0.00000   0.00000   0.00000
H    0.00000   0.00000   1.07813
H    0.93365   0.00000  -0.53917
H   -0.93365  -0.00105  -0.53917
                    SymmetryFactor    6.0000000000000000
     PotentialPrefactor[au]          10.
     PotentialPowerExponent          6
          End
Rotor                     Hindered
Geometry[angstrom]          14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50112
C    1.39710   0.00000   2.12644
C   -0.81569  -1.21840   1.82234
C   -1.21870  -1.80451   0.68960
C   -0.70750  -1.04109  -0.45233
H    0.50817   0.74374  -0.59543
H    1.95008   0.89431   1.83920
H    1.33447  -0.02486   3.21435
H    1.96018  -0.87263   1.79528
H   -1.02550  -1.54600   2.82960
H   -1.82229  -2.69676   0.61182
H   -0.88231  -1.29309  -1.48790
H   -0.53850   0.88886   1.85441
Group    8   9  10
Axis        3       2
Symmetry        3
Potential[kcal/mol]       12
  0.0000    0.23000    0.90000    1.8400    2.8300    3.5500    3.7800
3.4400    2.6900    1.7500
 0.87000    0.23000
End
   Frequencies[1/cm]        41
  3244.1    3235.6    3219.3    3210.9    3128.0    3124.4    3049.0
3020.3    1670.2    1591.0
  1503.9    1503.7    1422.5    1406.8    1334.3    1293.1    1277.9
1155.2    1119.2    1104.0
  1090.8    1028.3    1004.1    983.75    981.16    957.17    883.24
817.77    792.34    742.25
  721.84    567.90    547.80    294.51    164.97
  526.68    1409.6    1409.7    3123.2    3304.4    3304.6
 ZeroEnergy[kcal/mol]        0.
 ElectronicLevels[1/cm]              1
  0.0000000000000000      4.0000000000000000
End
!************************************
Barrier      B3  WP PRODS
  RRHO
   Stoichiometry  H11C7
   Core PhaseSpaceTheory
   FragmentGeometry[angstrom]          13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.41507
C    1.18585   0.00000   2.30525
C   -1.37924  -0.00034   1.86264
C   -2.17195  -0.00056   0.76525
C   -1.30652  -0.00033  -0.41759
H    0.87955   0.00028  -0.62343
H    2.11567   0.00259   1.73998
H    1.17551   0.87449   2.96082
H    1.17824  -0.87748   2.95691
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
   FragmentGeometry[angstrom]          5
C    0.00000   0.00000   0.00000
H    0.00000   0.00000   1.08780
H    1.02552   0.00000  -0.36267
H   -0.51271  -0.88842  -0.36222
H   -0.51307   0.88794  -0.36267
                    SymmetryFactor    24.000000000000000
     PotentialPrefactor[au]          10.
     PotentialPowerExponent          6
          End
Rotor                     Hindered
Geometry[angstrom]          13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.41507
C    1.18585   0.00000   2.30525
C   -1.37924  -0.00034   1.86264
C   -2.17195  -0.00056   0.76525
C   -1.30652  -0.00033  -0.41759
H    0.87955   0.00028  -0.62343
H    2.11567   0.00259   1.73998
H    1.17551   0.87449   2.96082
H    1.17824  -0.87748   2.95691
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
Group    8   9  10
Axis        3       2
Symmetry        3
Potential[kcal/mol]       12
  0.0000    0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01  0.0000    0.20000E-01 0.40000E-01 0.60000E-01
 0.40000E-01 0.10000E-01
End
   Frequencies[1/cm]        41
  3255.2    3247.0    3232.4    3224.7    3138.6    3086.9    3034.1
1584.1    1503.1    1481.1
  1477.9    1438.4    1407.4    1311.3    1292.6    1178.7    1098.1
1049.4    1023.5    1013.2
  953.40    929.99    923.03    899.45    740.46    727.81    638.42
604.77    528.85    520.52
  329.55    215.83
  1341.0    1341.5    1341.7    1562.7    1563.0    3043.7    3161.5
3162.0    3162.4
 ZeroEnergy[kcal/mol]        -26.207430042327744
 ElectronicLevels[1/cm]              1
  0.0000000000000000      4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO        !         7
Geometry[angstrom]        18
C    0.47568   0.04723  -1.18603
C    0.47559   0.04985   0.29710
C    1.79262   0.04685   1.04398
C   -0.56784  -0.94342   0.64985
C   -1.15274  -1.38621  -0.47563
C   -0.49944  -0.76603  -1.62500
H    1.13658   0.65261  -1.78797
H    2.41619   0.88443   0.72956
H    1.62698   0.13417   2.11831
H    2.34435  -0.87537   0.85931
H   -0.82535  -1.20996   1.66387
H   -1.97681  -2.08147  -0.53642
H   -0.77218  -0.93806  -2.65563
H   -0.02827   1.07724   0.56510
C   -0.66498   2.48228   0.96211
H    0.07645   3.16785   0.57559
H   -0.73164   2.38867   2.03726
H   -1.58598   2.38939   0.40337
```

```
            Core            RigidRotor
       SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.66    2.09    2.81    2.03    0.65    0.00    0.65    2.08    2.81    2.04
0.66    0.00    0.66    2.10    2.81    2.02    0.65
 End
 Rotor                     Hindered
 Group   16  17  18
 Axis           15         14
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.04    0.10    0.13    0.10    0.03
 End
   Frequencies[1/cm]          45
  3263.3      3261.7      3244.0      3235.6      3220.0      3211.5      3119.9
3119.4      3099.7      3045.3
  1644.6      1615.1      1506.0      1503.8      1490.0      1426.3      1419.3
1419.0      1414.7      1337.0
  1306.8      1268.0      1208.0      1138.9      1111.0      1097.8      1044.5
1012.8      969.65      969.25
  967.21      891.88      821.67      800.65      743.56      738.26      671.88
581.35      565.02      455.44
  451.03      293.60      194.21      80.000      15.470
 ZeroEnergy[kcal/mol]    6.7498565229787593
  ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO           !            8
Geometry[angstrom]           18
C    0.47550   0.04778  -1.18562
C    0.47531   0.04996   0.29700
C    1.79210   0.04752   1.04404
C   -0.56788  -0.94273   0.64999
C   -1.15275  -1.38605  -0.47563
C   -0.49950  -0.76592  -1.62490
H    1.13688   0.65265  -1.78751
H    2.41610   0.88472   0.72954
H    1.62680   0.13439   2.11844
H    2.34333  -0.87502   0.85892
H   -0.82487  -1.20974   1.66400
H   -1.97641  -2.08179  -0.53630
H   -0.77173  -0.93834  -2.65559
H   -0.03248   1.08637   0.56764
C   -0.66336   2.47877   0.96114
H    0.07502   3.16890   0.57629
H   -0.73243   2.39036   2.03679
H   -1.58636   2.39167   0.40437
            Core            RigidRotor
       SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.66    2.09    2.81    2.03    0.65    0.00    0.65    2.08    2.81    2.04
0.66    0.00    0.66    2.10    2.81    2.02    0.65
 End
 Rotor                     Hindered
 Group   16  17  18
 Axis           15         14
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.04    0.10    0.13    0.10    0.03
 End
   Frequencies[1/cm]          45
  3260.6      3259.0      3244.1      3235.7      3220.1      3211.7      3120.1
3118.9      3098.3      3045.2
  1643.2      1581.7      1503.4      1498.0      1427.3      1420.4      1420.1
1414.5      1397.9      1336.5
  1306.8      1268.9      1209.4      1144.5      1110.9      1097.5      1046.5
1012.9      970.00      968.77
  966.36      892.28      821.26      800.34      744.28      729.06      652.02
582.98      562.70      462.86
  458.68      294.52      193.08      87.260      34.290
 ZeroEnergy[kcal/mol]    6.6577705540759089
  ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO           !            9
Geometry[angstrom]           18
C    0.47536   0.04826  -1.18525
C    0.47516   0.04985   0.29685
C    1.79165   0.04810   1.04410
C   -0.56788  -0.94211   0.65012
C   -1.15277  -1.38592  -0.47564
C   -0.49957  -0.76584  -1.62483
H    1.13718   0.65265  -1.78710
H    2.41606   0.88494   0.72951
H    1.62668   0.13452   2.11856
H    2.34240  -0.87474   0.85854
H   -0.82442  -1.20959   1.66412
H   -1.97607  -2.08209  -0.53621
H   -0.77134  -0.93860  -2.65557
H   -0.03743   1.09720   0.57067
C   -0.66191   2.47563   0.96027
H    0.07357   3.17009   0.57702
H   -0.73327   2.39215   2.03639
H   -1.58678   2.39400   0.40537
            Core            RigidRotor
       SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.66    2.09    2.81    2.03    0.65    0.00    0.65    2.08    2.81    2.04
0.66    0.00    0.66    2.10    2.81    2.02    0.65
 End
 Rotor                     Hindered
 Group   16  17  18
 Axis           15         14
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.04    0.10    0.13    0.10    0.03
 End
   Frequencies[1/cm]          45
  3257.9      3256.2      3244.2      3235.8      3220.3      3211.9      3120.3
3118.3      3096.8      3045.0
  1641.5      1571.4      1502.9      1497.3      1426.4      1421.5      1421.3
1414.3      1335.7      1319.5
  1272.5      1269.7      1210.8      1151.1      1110.8      1097.2      1048.4
1013.1      970.36      968.16
  965.37      892.67      820.64      799.75      745.05      720.67      620.07
584.80      553.86      470.20
  467.03      295.60      192.34      94.970      47.370
 ZeroEnergy[kcal/mol]    6.5379373230631321
  ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO           !            10
Geometry[angstrom]           18
C    0.47527   0.04868  -1.18488
C    0.47511   0.04957   0.29665
C    1.79126   0.04861   1.04415
C   -0.56788  -0.94158   0.65026
C   -1.15281  -1.38583  -0.47566
C   -0.49965  -0.76579  -1.62480
H    1.13751   0.65265  -1.78674
```

```
H   2.41604   0.88507   0.72949
H   1.62659   0.13461   2.11863
H   2.34158  -0.87452   0.85819
H  -0.82400  -1.20950   1.66426
H  -1.97575  -2.08234  -0.53612
H  -0.77101  -0.93883  -2.65554
H  -0.04290   1.10928   0.57405
C  -0.66062   2.47284   0.95949
H   0.07211   3.17130   0.57774
H  -0.73411   2.39395   2.03608
H  -1.58724   2.39627   0.40631
          Core          RigidRotor
     SymmetryFactor    3.0000000000000000
End
 Rotor                    Hindered
 Group   8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.09   2.81   2.03   0.65   0.00   0.65   2.08   2.81   2.04
0.66   0.00   0.66   2.10   2.81   2.02   0.65
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15         14
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.04   0.10   0.13   0.10   0.03
 End
   Frequencies[1/cm]          45
  3255.0     3253.3     3244.4     3235.8     3220.4     3212.2     3121.1
3117.7     3095.2     3045.1
  1639.6     1566.6     1502.3     1496.8     1426.0     1422.7     1422.6
1414.0     1334.7     1316.3
  1270.3     1215.3     1188.2     1158.2     1110.7     1096.7     1050.3
1013.1     970.59     967.38
  964.28     893.03     819.79     799.02     745.99     715.62     597.40
586.65     530.14     475.79
  475.08     296.76     191.97     102.71     58.490
 ZeroEnergy[kcal/mol]    6.4450958571156880
  ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
 End
!*********************************************
RRHO          !          11
Geometry[angstrom]          18
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.48104
C    1.31576   0.00000   2.22883
C   -1.04303  -0.99015   1.83500
C   -1.62803  -1.43476   0.70893
C   -0.97492  -0.81477  -0.44011
H    0.66250   0.60354  -0.60189
H    1.94090   0.83618   1.91409
H    1.15134   0.08562   3.30341
H    1.86571  -0.92341   2.04252
H   -1.29882  -1.25843   2.84891
H   -2.45073  -2.13159   0.64856
H   -1.24595  -0.98805  -1.47092
H   -0.52419   1.07368   1.76248
C   -1.13479   2.42158   2.14350
H   -0.40432   3.12350   1.76301
H   -1.21008   2.34660   3.22043
H   -2.06286   2.34933   1.59182
          Core          RigidRotor
     SymmetryFactor    3.0000000000000000
End
 Rotor                    Hindered
 Group   8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.09   2.81   2.03   0.65   0.00   0.65   2.08   2.81   2.04
0.66   0.00   0.66   2.10   2.81   2.02   0.65
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15         14
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.04   0.10   0.13   0.10   0.03
 End
   Frequencies[1/cm]          45
  3252.4     3250.6     3244.6     3236.0     3220.7     3212.5     3121.4
3117.0     3093.7     3044.8
  1637.7     1563.6     1501.5     1496.3     1425.6     1424.0     1424.0
1413.6     1333.3     1317.2
  1270.8     1216.9     1166.1     1137.7     1110.6     1095.8     1052.1
1013.2     970.82     966.55
  963.05     893.33     818.64     798.15     746.74     712.63     590.43
588.52     507.97     483.76
  469.10     298.09     191.99     110.32     68.420
 ZeroEnergy[kcal/mol]    6.3875105315306646
  ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
 End
!*********************************************
RRHO          !          12
Geometry[angstrom]          18
C    0.47514   0.04936  -1.18431
C    0.47529   0.04847   0.29616
C    1.79064   0.04943   1.04424
C   -0.56781  -0.94071   0.65048
C   -1.15288  -1.38569  -0.47574
C   -0.49980  -0.76573  -1.62473
H    1.13799   0.65255  -1.78620
H    2.41610   0.88527   0.72943
H    1.62650   0.13467   2.11882
H    2.34023  -0.87425   0.85757
H   -0.82330  -1.20939   1.66440
H   -1.97528  -2.08279  -0.53601
H   -0.77048  -0.93923  -2.65553
H   -0.05506   1.13612   0.58164
C   -0.65853   2.46832   0.95823
H    0.06960   3.17363   0.57902
H   -0.73564   2.39723   2.03557
H   -1.58810   2.40038   0.40803
          Core          RigidRotor
     SymmetryFactor    3.0000000000000000
End
 Rotor                    Hindered
 Group   8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]         18
  0.00   0.66   2.09   2.81   2.03   0.65   0.00   0.65   2.08   2.81   2.04
0.66   0.00   0.66   2.10   2.81   2.02   0.65
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15         14
 Symmetry          3
 Potential[kcal/mol]          6
  0.00   0.04   0.10   0.13   0.10   0.03
 End
   Frequencies[1/cm]          45
  3249.6     3247.7     3244.8     3236.2     3220.9     3212.7     3121.7
3116.3     3092.1     3044.6
  1635.6     1561.4     1500.6     1495.9     1425.6     1425.4     1425.2
1413.2     1331.7     1317.9
  1270.9     1219.8     1174.0     1114.7     1110.5     1094.7     1053.5
1013.3     970.99     965.67
  961.78     893.64     817.25     797.26     747.37     711.02     590.20
589.39     506.80     490.86
  448.81     299.48     192.38     117.25     77.080
 ZeroEnergy[kcal/mol]    6.3402089040208116
  ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
```

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End
!*********************************************
RRHO          !          13
Geometry[angstrom]          18
C    0.47508   0.04964  -1.18408
C    0.47547   0.04776   0.29589
C    1.79039   0.04976   1.04428
C   -0.56776  -0.94035   0.65058
C   -1.15291  -1.38563  -0.47579
C   -0.49987  -0.76570  -1.62470
H    1.13815   0.65246  -1.78599
H    2.41616   0.88537   0.72938
H    1.62647   0.13468   2.11895
H    2.33967  -0.87417   0.85730
H   -0.82300  -1.20935   1.66440
H   -1.97511  -2.08300  -0.53598
H   -0.77026  -0.93940  -2.65556
H   -0.06146   1.15030   0.58566
C   -0.65767   2.46643   0.95771
H    0.06851   3.17473   0.57958
H   -0.73634   2.39873   2.03533
H   -1.58848   2.40220   0.40879
            Core          RigidRotor
      SymmetryFactor    3.0000000000000000
End
 Rotor                    Hindered
 Group   8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.66   2.09   2.81   2.03   0.65   0.00   0.65   2.08   2.81   2.04
0.66   0.00   0.66   2.10   2.81   2.02   0.65
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15         14
 Symmetry          3
 Potential[kcal/mol]           6
  0.00   0.04   0.10   0.13   0.10   0.03
 End
   Frequencies[1/cm]          45
  3247.0     3245.0     3245.0     3236.5     3221.2     3212.9     3121.6
3115.5     3090.6     3044.1
  1633.6     1559.7     1499.7     1495.6     1427.3     1426.8     1424.7
1412.8     1329.9     1318.8
  1271.0     1223.3     1182.3     1110.4     1105.6     1093.7     1054.8
1013.5     971.11     964.77
  960.42     893.89     815.53     796.33     747.75     710.00     591.64
590.01     511.18     496.90
  428.56     300.99     193.03     123.70     84.770
ZeroEnergy[kcal/mol]    6.2703258456540842
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !          14
Geometry[angstrom]          18
C    0.47505   0.04991  -1.18385
C    0.47568   0.04699   0.29561
C    1.79016   0.05008   1.04432
C   -0.56772  -0.94002   0.65068
C   -1.15294  -1.38559  -0.47583
C   -0.49993  -0.76569  -1.62468
H    1.13834   0.65240  -1.78581
H    2.41620   0.88542   0.72935
H    1.62645   0.13467   2.11903
H    2.33915  -0.87409   0.85704
H   -0.82273  -1.20933   1.66444
H   -1.97493  -2.08318  -0.53594
H   -0.77005  -0.93956  -2.65556
H   -0.06794   1.16468   0.58975
C   -0.65686   2.46468   0.95722
H    0.06743   3.17579   0.58012
H   -0.73701   2.40019   2.03515
H   -1.58886   2.40395   0.40950
            Core          RigidRotor
      SymmetryFactor    3.0000000000000000
End
 Rotor                    Hindered
 Group   8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.66   2.09   2.81   2.03   0.65   0.00   0.65   2.08   2.81   2.04
0.66   0.00   0.66   2.10   2.81   2.02   0.65
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15         14
 Symmetry          3
 Potential[kcal/mol]           6
  0.00   0.04   0.10   0.13   0.10   0.03
 End
   Frequencies[1/cm]          45
  3245.3     3244.3     3242.3     3236.8     3221.5     3213.2     3121.9
3114.8     3089.1     3043.8
  1631.5     1558.3     1498.7     1495.2     1429.2     1428.3     1424.2
1412.3     1328.0     1319.8
  1271.3     1227.1     1190.6     1110.3     1103.5     1093.9     1056.0
1013.6     971.05     963.74
  958.99     894.10     813.50     795.35     748.05     709.43     592.68
591.22     515.89     501.49
  412.67     302.49     193.79     129.50     91.490
ZeroEnergy[kcal/mol]    6.1458268297575094
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !          15
Geometry[angstrom]          18
C    0.47502   0.05015  -1.18364
C    0.47592   0.04618   0.29530
C    1.78995   0.05037   1.04436
C   -0.56768  -0.93971   0.65077
C   -1.15298  -1.38555  -0.47587
C   -0.50000  -0.76567  -1.62467
H    1.13851   0.65233  -1.78563
H    2.41625   0.88547   0.72931
H    1.62644   0.13466   2.11910
H    2.33865  -0.87403   0.85679
H   -0.82247  -1.20932   1.66448
H   -1.97476  -2.08335  -0.53591
H   -0.76986  -0.93971  -2.65556
H   -0.07447   1.17922   0.59388
C   -0.65611   2.46305   0.95677
H    0.06640   3.17682   0.58065
H   -0.73767   2.40159   2.03498
H   -1.58924   2.40563   0.41019
            Core          RigidRotor
      SymmetryFactor    3.0000000000000000
End
 Rotor                    Hindered
 Group   8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.66   2.09   2.81   2.03   0.65   0.00   0.65   2.08   2.81   2.04
0.66   0.00   0.66   2.10   2.81   2.02   0.65
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15         14
 Symmetry          3
 Potential[kcal/mol]           6
  0.00   0.04   0.10   0.13   0.10   0.03
 End
   Frequencies[1/cm]          45
```

3245.5 3241.7 3239.5 3237.0 3221.8 3213.5 3122.3
3114.2 3087.5 3043.6
1629.2 1557.0 1497.6 1494.8 1431.3 1430.0 1423.6
1411.7 1325.9 1321.3
1272.2 1231.0 1198.6 1110.1 1105.6 1094.8 1057.2
1013.8 970.85 962.65
957.50 894.28 811.17 794.35 748.14 709.16 593.22
592.48 519.75 504.55
400.38 303.99 194.59 134.55 97.200
ZeroEnergy[kcal/mol] 5.9448980422594522
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 16
Geometry[angstrom] 18
C 0.47501 0.05038 -1.18343
C 0.47619 0.04532 0.29499
C 1.78974 0.05065 1.04439
C -0.56763 -0.93941 0.65086
C -1.15302 -1.38552 -0.47591
C -0.50006 -0.76566 -1.62467
H 1.13868 0.65227 -1.78547
H 2.41630 0.88551 0.72928
H 1.62644 0.13465 2.11917
H 2.33818 -0.87397 0.85655
H -0.82223 -1.20932 1.66452
H -1.97460 -2.08352 -0.53589
H -0.76968 -0.93986 -2.65557
H -0.08105 1.19388 0.59806
C -0.65540 2.46151 0.95634
H 0.06539 3.17783 0.58117
H -0.73831 2.40296 2.03483
H -1.58961 2.40727 0.41086
Core RigidRotor
SymmetryFactor 3.0000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.66 2.09 2.81 2.03 0.65 0.00 0.65 2.08 2.81 2.04
0.66 0.00 0.66 2.10 2.81 2.02 0.65
End
Rotor Hindered
Group 16 17 18
Axis 15 14
Symmetry 3
Potential[kcal/mol] 6
0.00 0.04 0.10 0.13 0.10 0.03
End
Frequencies[1/cm] 45
3245.8 3239.0 3237.4 3236.5 3222.1 3213.8 3122.6
3113.6 3085.9 3043.3
1626.9 1555.9 1496.5 1494.4 1433.6 1431.9 1422.9
1411.1 1323.8 1323.5
1274.3 1234.9 1205.5 1111.1 1110.0 1095.2 1058.1
1014.0 970.53 961.51
955.96 894.45 808.54 793.37 747.98 709.16 593.48
593.14 522.40 506.06
390.99 305.48 195.35 138.82 101.86
ZeroEnergy[kcal/mol] 5.6565753932546832
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 17
Geometry[angstrom] 18
C 0.47499 0.05061 -1.18323
C 0.47648 0.04442 0.29467
C 1.78955 0.05093 1.04443
C -0.56758 -0.93913 0.65095
C -1.15306 -1.38549 -0.47594
C -0.50013 -0.76565 -1.62467
H 1.13884 0.65220 -1.78532
H 2.41636 0.88555 0.72925
H 1.62644 0.13463 2.11924
H 2.33772 -0.87392 0.85632
H -0.82200 -1.20932 1.66455
H -1.97445 -2.08369 -0.53586
H -0.76951 -0.94001 -2.65558
H -0.08766 1.20863 0.60227
C -0.65473 2.46005 0.95593
H 0.06441 3.17883 0.58167
H -0.73894 2.40431 2.03469
H -1.58997 2.40888 0.41152
Core RigidRotor
SymmetryFactor 3.0000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.66 2.09 2.81 2.03 0.65 0.00 0.65 2.08 2.81 2.04
0.66 0.00 0.66 2.10 2.81 2.02 0.65
End
Rotor Hindered
Group 16 17 18
Axis 15 14
Symmetry 3
Potential[kcal/mol] 6
0.00 0.04 0.10 0.13 0.10 0.03
End
Frequencies[1/cm] 45
3246.0 3237.5 3236.2 3233.9 3222.3 3214.1 3122.9
3113.0 3084.4 3043.1
1624.5 1554.9 1495.3 1494.0 1436.3 1434.0 1422.3
1410.5 1326.6 1321.8
1278.6 1238.4 1210.9 1119.1 1109.8 1095.2 1058.8
1014.2 970.08 960.34
954.41 894.61 805.62 792.48 747.56 709.45 594.08
592.45 523.77 506.10
384.06 306.93 196.06 142.33 105.56
ZeroEnergy[kcal/mol] 5.2731399206832483
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 18
Geometry[angstrom] 18
C 0.47498 0.05082 -1.18304
C 0.47678 0.04349 0.29434
C 1.78936 0.05119 1.04446
C -0.56753 -0.93886 0.65104
C -1.15310 -1.38546 -0.47598
C -0.50019 -0.76564 -1.62467
H 1.13899 0.65213 -1.78518
H 2.41641 0.88558 0.72922
H 1.62643 0.13461 2.11931
H 2.33728 -0.87388 0.85610
H -0.82178 -1.20932 1.66458
H -1.97430 -2.08385 -0.53584
H -0.76934 -0.94015 -2.65558
H -0.09428 1.22344 0.60650
C -0.65409 2.45865 0.95554
H 0.06345 3.17982 0.58217
H -0.73956 2.40564 2.03455
H -1.59033 2.41047 0.41216
Core RigidRotor
SymmetryFactor 3.0000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18

```
  0.00    0.66    2.09    2.81    2.03    0.65    0.00    0.65    2.08    2.81    2.04
0.66    0.00    0.66    2.10    2.81    2.02    0.65
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          14
 Symmetry          3
 Potential[kcal/mol]           6
  0.00    0.04    0.10    0.13    0.10    0.03
 End
   Frequencies[1/cm]          45
  3246.3      3237.8      3233.4      3231.0      3222.6      3214.4      3123.2
3112.4      3082.8      3042.8
  1622.2      1554.0      1494.1      1493.7      1439.3      1436.3      1421.7
1409.8      1330.9      1319.8
  1285.3      1241.4      1214.0      1128.7      1109.5      1095.1      1059.3
1014.5      969.51      959.14
  952.84      894.78      802.44      791.76      746.89      710.06      594.22
591.12      523.81      504.68
  379.24      308.30      196.67      145.05      108.30
 ZeroEnergy[kcal/mol]    4.7873301254414420
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!***********************************************
 RRHO          !          19
 Geometry[angstrom]          18
 C    0.47497   0.05103  -1.18285
 C    0.47711   0.04252   0.29400
 C    1.78918   0.05145   1.04450
 C   -0.56748  -0.93860   0.65113
 C   -1.15315  -1.38543  -0.47602
 C   -0.50025  -0.76563  -1.62467
 H    1.13914   0.65207  -1.78504
 H    2.41647   0.88561   0.72919
 H    1.62644   0.13459   2.11938
 H    2.33685  -0.87383   0.85587
 H   -0.82157  -1.20933   1.66461
 H   -1.97415  -2.08401  -0.53582
 H   -0.76918  -0.94030  -2.65559
 H   -0.10090   1.23830   0.61076
 C   -0.65347   2.45731   0.95517
 H    0.06249   3.18081   0.58266
 H   -0.74017   2.40696   2.03442
 H   -1.59069   2.41205   0.41280
               Core            RigidRotor
         SymmetryFactor    3.0000000000000000
 End
 Rotor                      Hindered
 Group   8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.66    2.09    2.81    2.03    0.65    0.00    0.65    2.08    2.81    2.04
0.66    0.00    0.66    2.10    2.81    2.02    0.65
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          14
 Symmetry          3
 Potential[kcal/mol]           6
  0.00    0.04    0.10    0.13    0.10    0.03
 End
   Frequencies[1/cm]          45
  3246.5      3238.0      3230.6      3228.2      3222.9      3214.8      3123.5
3111.9      3081.2      3042.5
  1619.8      1553.3      1493.4      1492.9      1442.8      1438.9      1421.1
1409.1      1336.2      1318.0
  1294.1      1243.8      1215.0      1139.4      1109.3      1095.0      1059.7
1014.7      968.85      957.94
  951.29      895.00      799.05      791.37      745.93      711.08      593.99
589.25      522.47      501.80
  376.32      309.56      197.10      147.00      110.13
 ZeroEnergy[kcal/mol]    4.1984026302255435
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!***********************************************
 RRHO          !          20
 Geometry[angstrom]          18
 C    0.47496   0.05124  -1.18266
 C    0.47744   0.04152   0.29366
 C    1.78900   0.05170   1.04454
 C   -0.56743  -0.93834   0.65122
 C   -1.15319  -1.38541  -0.47605
 C   -0.50031  -0.76563  -1.62468
 H    1.13929   0.65200  -1.78491
 H    2.41653   0.88564   0.72916
 H    1.62644   0.13456   2.11944
 H    2.33643  -0.87379   0.85565
 H   -0.82136  -1.20934   1.66463
 H   -1.97401  -2.08417  -0.53580
 H   -0.76902  -0.94044  -2.65560
 H   -0.10753   1.25318   0.61503
 C   -0.65287   2.45601   0.95481
 H    0.06153   3.18180   0.58315
 H   -0.74079   2.40829   2.03429
 H   -1.59106   2.41363   0.41344
               Core            RigidRotor
         SymmetryFactor    3.0000000000000000
 End
 Rotor                      Hindered
 Group   8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.66    2.09    2.81    2.03    0.65    0.00    0.65    2.08    2.81    2.04
0.66    0.00    0.66    2.10    2.81    2.02    0.65
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          14
 Symmetry          3
 Potential[kcal/mol]           6
  0.00    0.04    0.10    0.13    0.10    0.03
 End
   Frequencies[1/cm]          45
  3246.8      3238.2      3227.8      3225.3      3223.2      3215.1      3123.8
3111.3      3079.6      3042.2
  1617.4      1552.6      1493.1      1491.7      1446.9      1441.9      1420.5
1408.5      1342.4      1316.5
  1304.2      1245.6      1214.3      1150.9      1109.0      1094.9      1060.1
1015.0      968.12      956.74
  949.77      895.28      795.51      791.50      744.74      712.58      593.50
586.96      519.67      497.42
  375.22      310.71      197.31      148.19      111.10
 ZeroEnergy[kcal/mol]    3.5131042883134560
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!***********************************************
 RRHO          !          21
 Geometry[angstrom]          18
 C    0.47496   0.05144  -1.18247
 C    0.47779   0.04049   0.29330
 C    1.78882   0.05196   1.04457
 C   -0.56738  -0.93808   0.65130
 C   -1.15324  -1.38539  -0.47608
 C   -0.50037  -0.76562  -1.62469
 H    1.13944   0.65193  -1.78478
 H    2.41659   0.88567   0.72913
 H    1.62644   0.13454   2.11951
 H    2.33601  -0.87375   0.85544
 H   -0.82115  -1.20936   1.66466
 H   -1.97386  -2.08433  -0.53578
 H   -0.76886  -0.94058  -2.65562
 H   -0.11414   1.26808   0.61930
 C   -0.65229   2.45474   0.95445
```

```
 H    0.06056   3.18280   0.58365
 H   -0.74141   2.40963   2.03416
 H   -1.59142   2.41522   0.41409
                  Core            RigidRotor
         SymmetryFactor    3.0000000000000000
 End
  Rotor                          Hindered
  Group    8   9  10
  Axis            3           2
  Symmetry           1
  Potential[kcal/mol]          18
    0.00    0.66    2.09    2.81    2.03    0.65    0.00    0.65    2.08    2.81    2.04
0.66    0.00    0.66    2.10    2.81    2.02    0.65
  End
  Rotor                          Hindered
  Group   16  17  18
  Axis           15          14
  Symmetry           3
  Potential[kcal/mol]           6
    0.00    0.04    0.10    0.13    0.10    0.03
  End
     Frequencies[1/cm]           45
   3247.1      3238.5      3224.8      3223.5      3222.3      3215.4      3124.1
3110.8      3078.0      3041.9
   1615.0      1552.0      1492.8      1490.5      1451.5      1445.3      1420.0
1407.8      1348.8      1318.0
   1312.2      1246.9      1212.5      1163.2      1108.6      1094.9      1060.8
1015.2      967.35      955.56
   948.29      895.68      792.45      791.89      743.23      714.65      592.92
584.40      515.26      491.52
   376.09      311.73      197.29      148.63      111.29
 ZeroEnergy[kcal/mol]    2.7384392758961544
  ElectronicLevels[1/cm]                    1
   0.0000000000000000        2.0000000000000000
 End
 !*********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1176.5998999999999
      WellDepth[kcal/mol]           5.05
      WellDepth[kcal/mol]          33.99
 End
End
End
```

```
!****************************************************
!           GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                   0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature             .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]            400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                   direct     ! direct or low-eigenvalue
!
WellCutoff                          20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax               0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                     diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                         10
!ChemicalEigenvalueMin              1.e-6         #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]               1.3
!!
RateOutput                          rate.out                    ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!           MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                        ! Default collisional
energy relaxation kernel
    Exponential                                           ! Currently the only
possible energy relaxation model
      Factor[1/cm]                316                     ! (Delta_E_down)^(0)
@ standard T (300 K)
      Power                 0.535                    ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
      ExponentCutoff              10                      ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                      ! Collision frequency
model
    LennardJones                                          ! Currently the only
possible collisional frequency model  based on LJ potential
      Epsilons[K]                 90.58  281.367          ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
      Sigmas[angstrom]            3.54    4.694           ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
      Masses[amu]                 39.948  79.05478        ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.34058
 C    1.17550   0.00000   2.25991
 C   -1.39560  -0.00008   1.80105
 C   -2.21870  -0.00003   0.74716
 C   -1.40657  -0.00007  -0.51024
 H    0.87312   0.00029  -0.63540
 H    2.11196   0.00080   1.70444
 H    1.16259   0.87759   2.90932
 H    1.16343  -0.87842   2.90820
 H   -1.69080  -0.00015   2.84114
 H   -3.29750  -0.00010   0.77029
 H   -1.62068  -0.87614  -1.13069
 H   -1.62069   0.87579  -1.13094
       Core    RigidRotor
           SymmetryFactor    1.0000000000000000
       End
 Rotor                        Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.08    0.32    0.66    1.03    1.33    1.44    1.32    1.03    0.66    0.32
0.08
 End
    Frequencies[1/cm]          35
  3241.0     3225.5     3207.9     3133.2     3100.2     3075.2     3043.9
3042.9     1708.1     1610.0
  1497.4     1487.3     1428.4     1422.7     1402.8     1311.9     1272.8
1227.8     1137.4     1111.0
  1073.3     1028.7     984.40     980.54     951.47     936.30     920.52
826.70     765.47     719.11
  624.46     583.63     368.96     327.69     231.38
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]            4
 C    0.00000   0.00000   0.00000
 H    0.00000   0.00000   1.07813
 H    0.93365   0.00000  -0.53917
 H   -0.93365  -0.00105  -0.53917
       Core    RigidRotor
           SymmetryFactor    6.0000000000000000
       End
    Frequencies[1/cm]           6
  526.68     1409.6     1409.7     3123.2     3304.4     3304.6
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]            13
```

```
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.41507
C   1.18585   0.00000   2.30525
C  -1.37924  -0.00034   1.86264
C  -2.17195  -0.00056   0.76525
C  -1.30652  -0.00033  -0.41759
H   0.87955   0.00028  -0.62343
H   2.11567   0.00259   1.73998
H   1.17551   0.87449   2.96082
H   1.17824  -0.87748   2.95691
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
     Core    RigidRotor
          SymmetryFactor    2.0000000000000000
     End
Rotor                       Hindered
Group    8   9  10
Axis            3           2
Symmetry            3
Potential[kcal/mol]           12
   0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
   Frequencies[1/cm]          32
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
!*************************************
Fragment PROD2
RRHO
Geometry[angstrom]              5
C   0.00000   0.00000   0.00000
H   0.00000   0.00000   1.08780
H   1.02552   0.00000  -0.36267
H  -0.51271  -0.88842  -0.36222
H  -0.51307   0.88794  -0.36267
     Core    RigidRotor
          SymmetryFactor    12.000000000000000
     End
   Frequencies[1/cm]          9
  1341.0      1341.5      1341.7      1562.7      1563.0      3043.7      3161.5
3162.0      3162.4
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End

GroundEnergy[kcal/mol]   -23.00
End
!*************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]             18
C  -0.00242   0.00006   0.00470
C  -0.00271   0.00044   1.34594
C   1.17226   0.00279   2.26574
C  -1.39806   0.00498   1.80580
C  -2.22018   0.00778   0.75100
C  -1.40838   0.00725  -0.50577
H   0.87101  -0.00248  -0.63025
H   2.10911  -0.00370   1.71104
H   1.16128   0.88552   2.90829
H   1.15634  -0.87045   2.92077
H  -1.69354   0.00878   2.84569
H  -3.29897   0.01404   0.77346
H  -1.62721  -0.86214  -1.13344
H  -1.61678   0.89240  -1.11631
C  -1.29656   3.51483   0.37094
H  -2.32079   3.43430   0.69860
H  -0.94894   4.42644  -0.08915
H  -0.62145   2.68509   0.51615
     Core    RigidRotor
          SymmetryFactor   0.50000000000000000
     End
   Frequencies[1/cm]          48
  36.386      45.522      65.808      68.556      101.60      155.72      179.51
245.62      327.61      371.69
  552.67      584.94      624.81      720.33      767.94      827.25      921.80
936.36      952.17      981.27
  985.46      1029.1      1074.0      1110.9      1140.0      1228.2      1273.8
1313.7      1402.8      1404.1
  1407.8      1422.9      1428.8      1488.0      1498.0      1608.8      1707.2
3040.0      3041.9      3073.5
  3098.9      3114.7      3134.3      3209.0      3225.4      3241.2      3294.5
3299.7
 ZeroEnergy[kcal/mol]              -1.50
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
End
!*************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]             18
C  -0.00335  -0.03210   0.00743
C   0.02820   0.03178   1.42320
C   1.23291   0.01624   2.28609
C  -1.33457   0.16320   1.89454
C  -2.14844   0.18095   0.81198
C  -1.31222   0.05813  -0.38557
H   0.86016  -0.12882  -0.63077
H   2.13110  -0.22856   1.72240
H   1.37674   0.99818   2.74665
H   1.12166  -0.70057   3.10218
H  -1.62535   0.23613   2.93054
H  -3.22355   0.26774   0.81018
H  -1.68188   0.04290  -1.39936
H  -0.59906   2.87483   1.01598
C   0.25250   3.49590   1.28482
H   0.11938   4.49944   0.88620
H   1.15836   3.05830   0.87016
H   0.33535   3.54689   2.36897
     Core    RigidRotor
          SymmetryFactor   0.50000000000000000
     End
   Frequencies[1/cm]          47
  30.474      48.740      66.714      76.786      88.889      143.52      227.48
329.96      527.71      541.20
  605.74      638.16      729.89      739.88      902.13      924.95      930.64
956.71      1012.1      1023.8
  1053.8      1097.8      1180.7      1294.0      1311.7      1333.1      1342.5
1346.3      1407.7      1438.9
  1475.3      1486.6      1508.7      1557.9      1563.4      1582.2      3032.7
3040.9      3089.4      3138.1
  3153.7      3157.1      3167.2      3225.7      3233.7      3247.7      3255.9
 ZeroEnergy[kcal/mol]             -26.34
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
End
!*************************************
Barrier        B1  REACS WR
  RRHO
    Stoichiometry  H11C7
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]             14
C    0.00000   0.00000   0.00000
```

```
C    0.00000   0.00000   1.34058
C    1.17550   0.00000   2.25991
C   -1.39560  -0.00008   1.80105
C   -2.21870  -0.00003   0.74716
C   -1.40657  -0.00007  -0.51024
H    0.87312   0.00029  -0.63540
H    2.11196   0.00080   1.70444
H    1.16259   0.87759   2.90932
H    1.16343  -0.87842   2.90820
H   -1.69080  -0.00015   2.84114
H   -3.29750  -0.00010   0.77029
H   -1.62068  -0.87614  -1.13069
H   -1.62069   0.87579  -1.13094
    FragmentGeometry[angstrom]          4
C    0.00000   0.00000   0.00000
H    0.00000   0.00000   1.07813
H    0.93365   0.00000  -0.53917
H   -0.93365  -0.00105  -0.53917
                      SymmetryFactor     6.0000000000000000
      PotentialPrefactor[au]         10.
      PotentialPowerExponent         6
              End
Rotor                   Hindered
Geometry[angstrom]          14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34058
C    1.17550   0.00000   2.25991
C   -1.39560  -0.00008   1.80105
C   -2.21870  -0.00003   0.74716
C   -1.40657  -0.00007  -0.51024
H    0.87312   0.00029  -0.63540
H    2.11196   0.00080   1.70444
H    1.16259   0.87759   2.90932
H    1.16343  -0.87842   2.90820
H   -1.69080  -0.00015   2.84114
H   -3.29750  -0.00010   0.77029
H   -1.62068  -0.87614  -1.13069
H   -1.62069   0.87579  -1.13094
Group    8   9  10
Axis         3        2
Symmetry         3
Potential[kcal/mol]        12
 0.0000    0.80000E-01 0.32000    0.66000    1.0300    1.3300    1.4400
1.3200    1.0300    0.66000
 0.32000    0.80000E-01
End
   Frequencies[1/cm]        41
 3241.0    3225.5    3207.9    3133.2    3100.2    3075.2    3043.9
3042.9    1708.1    1610.0
 1497.4    1487.3    1428.4    1422.7    1402.8    1311.9    1272.8
1227.8    1137.4    1111.0
 1073.3    1028.7    984.40    980.54    951.47    936.30    920.52
826.70    765.47    719.11
 624.46    583.63    368.96    327.69    231.38
 526.68    1409.6    1409.7    3123.2    3304.4    3304.6
 ZeroEnergy[kcal/mol]         0.
 ElectronicLevels[1/cm]              1
 0.0000000000000000      4.0000000000000000
End
!************************************
Barrier      B3  WP PRODS
 RRHO
   Stoichiometry  H11C7
   Core PhaseSpaceTheory
    FragmentGeometry[angstrom]          13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.41507
C    1.18585   0.00000   2.30525
C   -1.37924  -0.00034   1.86264
C   -2.17195  -0.00056   0.76525
C   -1.30652  -0.00033  -0.41759
H    0.87955   0.00028  -0.62343
H    2.11567   0.00259   1.73998
H    1.17551   0.87449   2.96082
H    1.17824  -0.87748   2.95691
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
    FragmentGeometry[angstrom]          5
C    0.00000   0.00000   0.00000
H    0.00000   0.00000   1.08780
H    1.02552   0.00000  -0.36267
H   -0.51271  -0.88842  -0.36222
H   -0.51307   0.88794  -0.36267
                      SymmetryFactor     24.000000000000000
      PotentialPrefactor[au]         10.
      PotentialPowerExponent         6
              End
Rotor                   Hindered
Geometry[angstrom]          13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.41507
C    1.18585   0.00000   2.30525
C   -1.37924  -0.00034   1.86264
C   -2.17195  -0.00056   0.76525
C   -1.30652  -0.00033  -0.41759
H    0.87955   0.00028  -0.62343
H    2.11567   0.00259   1.73998
H    1.17551   0.87449   2.96082
H    1.17824  -0.87748   2.95691
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
Group    8   9  10
Axis         3        2
Symmetry         3
Potential[kcal/mol]        12
 0.0000    0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01  0.0000    0.20000E-01 0.40000E-01 0.60000E-01
 0.40000E-01 0.10000E-01
End
   Frequencies[1/cm]        41
 3255.2    3247.0    3232.4    3224.7    3138.6    3086.9    3034.1
1584.1    1503.1    1481.1
 1477.9    1438.4    1407.4    1311.3    1292.6    1178.7    1098.1
1049.4    1023.5    1013.2
 953.40    929.99    923.03    899.45    740.46    727.81    638.42
604.77    528.85    520.52
 329.55    215.83
 1341.0    1341.5    1341.7    1562.7    1563.0    3043.7    3161.5
3162.0    3162.4
 ZeroEnergy[kcal/mol]         -22.999677812778550
 ElectronicLevels[1/cm]              1
 0.0000000000000000      4.0000000000000000
End
!************************************
Barrier B2 WR WP
RRHO     ! transition state
Geometry[angstrom]          18
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34739
C    1.17719   0.00000   2.26398
C   -1.39292   0.00016   1.80357
C   -2.21339  -0.00107   0.73935
C   -1.39145   0.05622  -0.48682
H    0.87141   0.00297  -0.63729
H    2.11237  -0.01458   1.70633
H    1.17581   0.88533   2.90339
H    1.15907  -0.87022   2.92331
H   -1.69320   0.00298   2.84196
H   -3.29209   0.00272   0.75269
H   -1.67530  -0.57030  -1.32962
H   -1.55608   1.20044  -0.94261
C   -1.72720   2.60319  -1.41813
H   -2.77956   2.65155  -1.66740
H   -1.04056   2.66029  -2.25310
H   -1.42852   3.13454  -0.52342
     Core    RigidRotor
```

```
            SymmetryFactor    1.5000000000000000
        End
 Rotor                  Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.29    0.93    1.30    0.93    0.29    0.00    0.27    0.91    1.30    0.92
0.27    0.00    0.29    0.93    1.30    0.94    0.29
 End
 Rotor                  Hindered
 Group   16  17  18
 Axis          15         14
 Symmetry          3
 Potential[kcal/mol]          6
   0.00    0.04    0.12    0.16    0.12    0.04
 End
    Frequencies[1/cm]          45
  3245.9      3245.3      3242.5      3227.5      3210.4      3131.7      3131.6
3096.5      3090.3      3040.6
  1676.0      1580.5      1497.1      1487.2      1426.9      1426.2      1423.8
1404.9      1351.8      1328.5
  1276.3      1234.9      1189.7      1134.9      1107.8      1069.9      1029.7
1001.6      979.82      960.64
  936.28      923.89      839.91      798.57      736.49      668.41      627.92
606.58      494.51      494.48
  382.91      327.66      243.91      100.75      62.400
  ZeroEnergy[kcal/mol]              8.32
  ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
      Tunneling    Eckart
   ImaginaryFrequency[1/cm]      1406.1500000000001
   WellDepth[kcal/mol]          7.32
   WellDepth[kcal/mol]         32.16
 End
 End
!************************************
End
End
```

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                    0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30         ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]            400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct     ! direct or low-eigenvalue
!
WellCutoff                            20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                 0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                           10
!ChemicalEigenvalueMin                1.e-6         #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                 1.3
!!
RateOutput                            rate.out                    ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                          ! Default collisional
energy relaxation kernel
    Exponential                                             ! Currently the only
possible energy relaxation model
       Factor[1/cm]               316                        ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                0.535                      ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff                 10                          ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                        ! Collision frequency
model
    LennardJones                                            ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                 90.58  281.367               ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]                 3.54    4.694                ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                     39.948  79.05478               ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]            14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.34058
 C    1.17550   0.00000   2.25991
 C   -1.39560  -0.00008   1.80105
 C   -2.21870  -0.00003   0.74716
 C   -1.40657  -0.00007  -0.51024
 H    0.87312   0.00029  -0.63540
 H    2.11196   0.00080   1.70444
 H    1.16259   0.87759   2.90932
 H    1.16343  -0.87842   2.90820
 H   -1.69080  -0.00015   2.84114
 H   -3.29750  -0.00010   0.77029
 H   -1.62068  -0.87614  -1.13069
 H   -1.62069   0.87579  -1.13094
       Core    RigidRotor
            SymmetryFactor    1.0000000000000000
       End
 Rotor                          Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.08    0.32    0.66    1.03    1.33    1.44    1.32    1.03    0.66    0.32
0.08
 End
    Frequencies[1/cm]           35
  3241.0     3225.5     3207.9     3133.2     3100.2     3075.2     3043.9
3042.9     1708.1     1610.0
  1497.4     1487.3     1428.4     1422.7     1402.8     1311.9     1272.8
1227.8     1137.4     1111.0
  1073.3     1028.7     984.40     980.54     951.47     936.30     920.52
826.70     765.47     719.11
  624.46     583.63     368.96     327.69     231.38
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
 End
 !************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]            4
 C    0.00000   0.00000   0.00000
 H    0.00000   0.00000   1.07813
 H    0.93365   0.00000  -0.53917
 H   -0.93365  -0.00105  -0.53917
       Core    RigidRotor
            SymmetryFactor    6.0000000000000000
       End
    Frequencies[1/cm]           6
  526.68     1409.6     1409.7     3123.2     3304.4     3304.6
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
 End
 GroundEnergy[kcal/mol] 0.0
 End
 !************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]            13
```

```
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.39409
C    1.09038   0.00000   2.23479
C   -1.41361  -0.00005   1.81740
C   -2.21408  -0.00003   0.75182
C   -1.40220  -0.00009  -0.51215
H    0.87980   0.00015  -0.62484
H    0.96884   0.00014   3.30847
H    2.09635   0.00011   1.83997
H   -1.72745  -0.00007   2.85132
H   -3.29354  -0.00010   0.76608
H   -1.61710  -0.87505  -1.13573
H   -1.61723   0.87450  -1.13618
      Core    RigidRotor
          SymmetryFactor    1.0000000000000000
      End
   Frequencies[1/cm]          33
  219.96     352.42     358.87     544.30     592.50     660.67     666.69
754.46     795.14     796.70
  925.16     926.06     951.77     962.74     984.98     1025.4     1111.8
1138.0     1259.1     1288.2
  1330.6     1389.7     1438.7     1448.7     1521.5     1659.2     3024.6
3049.1     3164.7     3213.4
  3231.7     3238.8     3260.5
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End

!************************************
Fragment PROD2
RRHO
Geometry[angstrom]              5
C    0.00000   0.00000   0.00000
H    0.00000   0.00000   1.08780
H    1.02552   0.00000  -0.36267
H   -0.51271  -0.88842  -0.36222
H   -0.51307   0.88794  -0.36267
      Core    RigidRotor
          SymmetryFactor    12.000000000000000
      End
   Frequencies[1/cm]          9
  1341.0     1341.5     1341.7     1562.7     1563.0     3043.7     3161.5
3162.0     3162.4
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End

GroundEnergy[kcal/mol]   -16.24
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]             18
C    0.00058   0.00704   0.01324
C   -0.00301   0.00814   1.35381
C    1.16919   0.01606   2.27664
C   -1.39990  -0.01217   1.80958
C   -2.21946  -0.02819   0.75235
C   -1.40303  -0.02107  -0.50176
H    0.87569   0.01527  -0.61946
H    2.10711   0.03514   1.72399
H    1.14260   0.88623   2.93551
H    1.16690  -0.86999   2.91475
H   -1.69881  -0.01459   2.84862
H   -3.29824  -0.04478   0.77167
H   -1.59461  -0.91244  -1.10900
H   -1.63369   0.84132  -1.13475
C   -0.75383  -3.49896   0.23419
H    0.21574  -3.31473  -0.20051
H   -1.25015  -2.71387   0.78402
H   -1.21824  -4.46643   0.12527
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]          48
  34.927     58.563     72.234     83.124     130.67     153.38     160.31
241.42     327.46     368.40
  549.05     584.23     624.97     721.50     767.68     827.34     921.18
936.65     952.01     982.15
  985.68     1029.5     1074.1     1110.7     1140.1     1228.6     1273.7
1313.6     1402.7     1403.5
  1414.6     1422.3     1428.2     1488.1     1497.8     1608.4     1708.9
3039.6     3041.5     3073.5
  3098.5     3117.1     3133.7     3207.9     3224.5     3240.9     3298.5
3299.5
 ZeroEnergy[kcal/mol]             -1.46
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]             18
C   -0.00134  -0.00179   0.00471
C   -0.00122  -0.00086   1.39897
C    1.08978   0.00064   2.23871
C   -1.41427  -0.00965   1.82241
C   -2.21444  -0.01768   0.75678
C   -1.40308  -0.01346  -0.50686
H    0.87852   0.00245  -0.62007
H    2.09533   0.00473   1.84279
H    0.96951  -0.00089   3.31250
H   -0.47733  -2.80707   0.58000
H   -1.72806  -0.01299   2.85630
H   -3.29381  -0.02889   0.77099
H   -1.60977  -0.89353  -1.12589
H   -1.62526   0.85698  -1.13404
C   -1.26804  -3.54485   0.45937
H   -1.76646  -3.38989  -0.49566
H   -1.98978  -3.42888   1.26448
H   -0.84472  -4.54664   0.48695
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]          47
  42.578     60.775     82.252     87.517     172.82     225.02     352.46
356.63     546.77     593.12
  660.96     668.38     754.65     795.56     796.92     924.40     925.64
952.30     963.09     985.99
  1025.7     1112.0     1138.5     1259.5     1288.7     1331.0     1336.3
1342.4     1351.2     1389.7
  1435.5     1447.7     1522.0     1560.5     1567.0     1659.6     3025.3
3041.1     3050.0     3154.5
  3161.2     3163.1     3164.8     3213.6     3231.5     3239.0     3260.7
 ZeroEnergy[kcal/mol]            -18.97
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
End
!************************************
Barrier        B1  REACS WR
  RRHO
    Stoichiometry  H11C7
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]             14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34058
C    1.17550   0.00000   2.25991
C   -1.39560  -0.00008   1.80105
C   -2.21870  -0.00003   0.74716
C   -1.40657  -0.00007  -0.51024
H    0.87312   0.00029  -0.63540
H    2.11196   0.00080   1.70444
```

```
H   1.16259  0.87759  2.90932
H   1.16343  -0.87842  2.90820
H  -1.69080  -0.00015  2.84114
H  -3.29750  -0.00010  0.77029
H  -1.62068  -0.87614  -1.13069
H  -1.62069  0.87579  -1.13094
    FragmentGeometry[angstrom]          4
C   0.00000  0.00000  0.00000
H   0.00000  0.00000  1.07813
H   0.93365  0.00000  -0.53917
H  -0.93365  -0.00105  -0.53917
                    SymmetryFactor    6.0000000000000000
      PotentialPrefactor[au]          10.
      PotentialPowerExponent          6
             End
Rotor                 Hindered
Geometry[angstrom]          14
C   0.00000  0.00000  0.00000
C   0.00000  0.00000  1.34058
C   1.17550  0.00000  2.25991
C  -1.39560  -0.00008  1.80105
C  -2.21870  -0.00003  0.74716
C  -1.40657  -0.00007  -0.51024
H   0.87312  0.00029  -0.63540
H   2.11196  0.00080  1.70444
H   1.16259  0.87759  2.90932
H   1.16343  -0.87842  2.90820
H  -1.69080  -0.00015  2.84114
H  -3.29750  -0.00010  0.77029
H  -1.62068  -0.87614  -1.13069
H  -1.62069  0.87579  -1.13094
Group   8  9  10
Axis        3       2
Symmetry        3
Potential[kcal/mol]       12
 0.0000    0.80000E-01 0.32000    0.66000    1.0300    1.3300    1.4400
1.3200    1.0300    0.66000
 0.32000    0.80000E-01
End
   Frequencies[1/cm]       41
 3241.0    3225.5    3207.9    3133.2    3100.2    3075.2    3043.9
3042.9    1708.1    1610.0
 1497.4    1487.3    1428.4    1422.7    1402.8    1311.9    1272.8
1227.8    1137.4    1111.0
 1073.3    1028.7    984.40    980.54    951.47    936.30    920.52
826.70    765.47    719.11
 624.46    583.63    368.96    327.69    231.38
 526.68    1409.6    1409.7    3123.2    3304.4    3304.6
 ZeroEnergy[kcal/mol]        0.
 ElectronicLevels[1/cm]           1
 0.0000000000000000    4.0000000000000000
End
!************************************
Barrier     B3  WP PRODS
 RRHO
   Stoichiometry  H11C7
   Core PhaseSpaceTheory
    FragmentGeometry[angstrom]          13
C   0.00000  0.00000  0.00000
C   0.00000  0.00000  1.39409
C   1.09038  0.00000  2.23479
C  -1.41361  -0.00005  1.81740
C  -2.21408  -0.00003  0.75182
C  -1.40220  -0.00009  -0.51215
H   0.87980  0.00015  -0.62484
H   0.96884  0.00014  3.30847
H   2.09635  0.00011  1.83997
H  -1.72745  -0.00007  2.85132
H  -3.29354  -0.00010  0.76608
H  -1.61710  -0.87505  -1.13573
H  -1.61723  0.87450  -1.13618
    FragmentGeometry[angstrom]          5
C   0.00000  0.00000  0.00000
H   0.00000  0.00000  1.08780
H   1.02552  0.00000  -0.36267
H  -0.51271  -0.88842  -0.36222
H  -0.51307  0.88794  -0.36267
                    SymmetryFactor    12.000000000000000
      PotentialPrefactor[au]          10.
      PotentialPowerExponent          6
             End
   Frequencies[1/cm]       42
 219.96    352.42    358.87    544.30    592.50    660.67    666.69
754.46    795.14    796.70
 925.16    926.06    951.77    962.74    984.98    1025.4    1111.8
1138.0    1259.1    1288.2
 1330.6    1389.7    1438.7    1448.7    1521.5    1659.2    3024.6
3049.1    3164.7    3213.4
 3231.7    3238.8    3260.5
 1341.0    1341.5    1341.7    1562.7    1563.0    3043.7    3161.5
3162.0    3162.4
 ZeroEnergy[kcal/mol]        -16.243617134283049
 ElectronicLevels[1/cm]           1
 0.0000000000000000    4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO       !       1
Geometry[angstrom]       18
C   0.27296  0.44975  -1.28448
C   0.27516  0.44960  0.06838
C   1.42159  0.45863  0.96096
C  -1.12415  0.37802  0.52004
C  -1.94265  0.34215  -0.53533
C  -1.13122  0.38553  -1.79335
H   1.14555  0.49609  -1.91825
H   2.37066  0.70727  0.49653
H   1.27262  0.96842  1.90831
H   1.63884  -0.88775  1.40126
H  -1.42032  0.36085  1.55948
H  -3.02044  0.29200  -0.51420
H  -1.30341  -0.49798  -2.41724
H  -1.38729  1.25098  -2.41320
C   1.81999  -2.09481  1.76078
H   2.16448  -2.59403  0.86022
H   0.84008  -2.42624  2.09130
H   2.56094  -2.06152  2.55375
         Core        RigidRotor
     SymmetryFactor    1.0000000000000000
End
 Rotor                 Hindered
 Group   8  9  10  15  16  17  18
 Axis        3       2
 Symmetry        1
 Potential[kcal/mol]       18
  0.00   0.47   1.57   2.68   3.43   3.69   3.39   2.58   1.43   0.35   0.01
0.68   2.21   4.06   4.95   3.85   1.97   0.53
 End
 Rotor                 Hindered
 Group   16  17  18
 Axis        15       10
 Symmetry        3
 Potential[kcal/mol]       6
  0.00   0.00   0.01   0.02   0.01   0.01
 End
   Frequencies[1/cm]       45
 3241.1    3229.3    3210.2    3200.8    3198.8    3193.7    3112.5
3066.5    3066.1    3036.7
 1655.2    1571.0    1480.1    1471.9    1451.2    1429.7    1410.1
1384.0    1317.1    1277.9
 1247.6    1241.2    1196.0    1137.2    1109.0    1090.5    1037.8
982.96    979.61    952.73
 932.43    924.05    819.95    760.48    724.69    658.27    626.06
610.45    533.34    444.32
 367.45    341.40    244.42    83.400    81.570
ZeroEnergy[kcal/mol]   7.6436902749710463
 ElectronicLevels[1/cm]           1
```

```
  0.0000000000000000       2.0000000000000000
End
!***********************************************
RRHO          !          2
Geometry[angstrom]          18
C    0.27295   0.44980  -1.28432
C    0.27491   0.44965   0.06799
C    1.42204   0.45762   0.96151
C   -1.12413   0.37801   0.52002
C   -1.94269   0.34214  -0.53536
C   -1.13122   0.38552  -1.79333
H    1.14552   0.49614  -1.91817
H    2.37019   0.70890   0.49630
H    1.27256   0.97055   1.90729
H    1.63647  -0.87328   1.39674
H   -1.42029   0.36087   1.55947
H   -3.02048   0.29201  -0.51422
H   -1.30344  -0.49800  -2.41717
H   -1.38731   1.25098  -2.41315
C    1.82012  -2.09577   1.76106
H    2.16441  -2.59272   0.85940
H    0.83946  -2.42489   2.09101
H    2.56105  -2.06007   2.55368
            Core            RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15  16  17  18
 Axis           3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          10
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
  3241.1      3229.0      3210.1      3203.6      3201.5      3191.5      3110.7
3067.9      3066.5      3036.9
  1656.5      1574.2      1475.2      1470.4      1449.0      1429.5      1410.2
1381.9      1316.8      1278.3
  1248.8      1239.7      1187.2      1137.1      1108.9      1081.8      1038.2
983.24      979.75      952.73
  932.66      924.18      820.37      761.74      725.20      657.95      626.89
616.92      528.89      447.83
  367.68      341.21      244.14      85.480      83.570
ZeroEnergy[kcal/mol]    8.3235991314307363
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!***********************************************
RRHO          !          3
Geometry[angstrom]          18
C    0.27293   0.44984  -1.28418
C    0.27467   0.44971   0.06761
C    1.42248   0.45665   0.96205
C   -1.12411   0.37800   0.51999
C   -1.94272   0.34214  -0.53539
C   -1.13123   0.38552  -1.79330
H    1.14550   0.49619  -1.91810
H    2.36972   0.71050   0.49607
H    1.27249   0.97263   1.90630
H    1.63411  -0.85875   1.39221
H   -1.42027   0.36089   1.55947
H   -3.02051   0.29202  -0.51423
H   -1.30346  -0.49801  -2.41711
H   -1.38733   1.25098  -2.41309
C    1.82026  -2.09676   1.76134
H    2.16435  -2.59143   0.85860
H    0.83885  -2.42356   2.09073
H    2.56117  -2.05866   2.55361
            Core            RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15  16  17  18
 Axis           3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          10
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
  3241.1      3228.7      3209.9      3206.3      3204.3      3189.2      3108.9
3069.3      3066.8      3037.2
  1657.9      1577.6      1473.3      1466.2      1446.8      1429.4      1410.3
1379.8      1316.7      1279.2
  1254.5      1237.7      1177.7      1137.1      1109.0      1077.0      1038.7
983.55      979.84      952.73
  932.90      924.29      820.82      763.08      725.65      658.70      627.83
621.41      527.19      450.03
  367.82      340.80      243.74      87.020      84.580
ZeroEnergy[kcal/mol]    8.9614414942439105
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!***********************************************
RRHO          !          4
Geometry[angstrom]          18
C    0.27292   0.44988  -1.28404
C    0.27443   0.44977   0.06724
C    1.42290   0.45572   0.96257
C   -1.12409   0.37799   0.51997
C   -1.94276   0.34214  -0.53542
C   -1.13123   0.38551  -1.79328
H    1.14547   0.49624  -1.91802
H    2.36926   0.71208   0.49584
H    1.27243   0.97468   1.90532
H    1.63175  -0.84419   1.38769
H   -1.42025   0.36091   1.55946
H   -3.02054   0.29203  -0.51424
H   -1.30349  -0.49802  -2.41704
H   -1.38735   1.25099  -2.41304
C    1.82040  -2.09778   1.76164
H    2.16429  -2.59017   0.85781
H    0.83825  -2.42226   2.09045
H    2.56129  -2.05727   2.55355
            Core            RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15  16  17  18
 Axis           3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          10
 Symmetry           3
 Potential[kcal/mol]           6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
```

```
 3241.0    3228.4    3209.8    3209.1    3207.0    3186.9    3107.1
3070.8    3067.2    3037.5
 1659.7    1581.0    1472.9    1461.3    1444.7    1429.3    1410.4
1377.8    1316.7    1280.8
 1260.7    1237.0    1168.3    1137.0    1109.2    1074.7    1039.1
983.87    979.89    952.72
 933.14    924.39    821.28    764.39    726.04    659.94    628.89
623.78    527.16    451.60
 367.91    340.15    243.22    87.870    84.720
ZeroEnergy[kcal/mol]    9.5333313956444918
 ElectronicLevels[1/cm]                1
 0.0000000000000000      2.0000000000000000
End
!*********************************************
RRHO          !          5
Geometry[angstrom]          18
C   0.27291   0.44993  -1.28390
C   0.27420   0.44982   0.06688
C   1.42332   0.45483   0.96308
C  -1.12407   0.37799   0.51995
C  -1.94280   0.34214  -0.53545
C  -1.13123   0.38550  -1.79326
H   1.14545   0.49629  -1.91795
H   2.36880   0.71366   0.49560
H   1.27236   0.97671   1.90435
H   1.62940  -0.82961   1.38317
H  -1.42023   0.36094   1.55945
H  -3.02057   0.29204  -0.51426
H  -1.30351  -0.49803  -2.41698
H  -1.38737   1.25099  -2.41298
C   1.82055  -2.09883   1.76195
H   2.16423  -2.58891   0.85702
H   0.83766  -2.42097   2.09018
H   2.56140  -2.05589   2.55348
           Core           RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15  16  17  18
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
 3241.0    3228.1    3211.9    3210.0    3209.5    3184.6    3105.3
3072.3    3067.5    3037.8
 1661.8    1584.4    1472.7    1456.7    1442.6    1429.2    1410.6
1376.2    1316.7    1284.2
 1266.2    1237.1    1159.4    1137.0    1109.3    1073.9    1039.6
984.19    979.92    952.72
 933.38    924.47    821.74    765.59    726.37    661.25    629.46
624.57    527.99    453.05
 367.99    339.33    242.58    87.920    84.010
ZeroEnergy[kcal/mol]    10.035780680591596
 ElectronicLevels[1/cm]                1
 0.0000000000000000      2.0000000000000000
End
!*********************************************
RRHO          !          6
Geometry[angstrom]          18
C   0.27289   0.44997  -1.28377
C   0.27397   0.44988   0.06653
C   1.42372   0.45396   0.96357
C  -1.12406   0.37798   0.51992
C  -1.94283   0.34213  -0.53548
C  -1.13124   0.38550  -1.79324
H   1.14543   0.49634  -1.91788
H   2.36834   0.71523   0.49536
H   1.27228   0.97872   1.90338
H   1.62706  -0.81501   1.37867
H  -1.42021   0.36096   1.55945
H  -3.02061   0.29205  -0.51427
H  -1.30354  -0.49804  -2.41692
H  -1.38739   1.25099  -2.41293
C   1.82070  -2.09991   1.76226
H   2.16417  -2.58767   0.85625
H   0.83707  -2.41968   2.08991
H   2.56152  -2.05452   2.55342
           Core           RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15  16  17  18
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                      Hindered
 Group   16  17  18
 Axis           15          10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
 3241.0    3227.9    3214.7    3212.7    3209.4    3182.2    3103.4
3073.8    3067.9    3038.0
 1664.0    1587.6    1472.5    1452.5    1440.6    1429.1    1410.9
1375.2    1316.9    1290.3
 1269.8    1237.5    1151.1    1136.9    1109.4    1074.0    1040.0
984.52    979.93    952.72
 933.61    924.54    822.20    766.61    726.63    662.36    629.17
624.12    529.12    454.69
 368.07    338.34    241.81    87.090    82.490
ZeroEnergy[kcal/mol]    10.459955321069653
 ElectronicLevels[1/cm]                1
 0.0000000000000000      2.0000000000000000
End
!*********************************************
RRHO          !          7
Geometry[angstrom]          18
C   0.27288   0.45001  -1.28364
C   0.27375   0.44994   0.06618
C   1.42412   0.45313   0.96405
C  -1.12404   0.37797   0.51990
C  -1.94287   0.34213  -0.53551
C  -1.13124   0.38549  -1.79322
H   1.14540   0.49639  -1.91782
H   2.36787   0.71680   0.49511
H   1.27221   0.98074   1.90241
H   1.62473  -0.80041   1.37418
H  -1.42020   0.36098   1.55944
H  -3.02064   0.29205  -0.51428
H  -1.30357  -0.49806  -2.41686
H  -1.38742   1.25099  -2.41288
C   1.82086  -2.10102   1.76259
H   2.16411  -2.58642   0.85547
H   0.83647  -2.41839   2.08963
H   2.56164  -2.05315   2.55336
           Core           RigidRotor
      SymmetryFactor    1.0000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15  16  17  18
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
```

0.00 0.47 1.57 2.68 3.43 3.69 3.39 2.58 1.43 0.35 0.01
0.68 2.21 4.06 4.95 3.85 1.97 0.53
End
Rotor Hindered
Group 16 17 18
Axis 15 10
Symmetry 3
Potential[kcal/mol] 6
0.00 0.00 0.01 0.02 0.01 0.01
End
Frequencies[1/cm] 45
3241.0 3227.6 3217.4 3215.4 3209.3 3179.8 3101.4
3075.3 3068.2 3038.3
1666.6 1590.6 1472.4 1448.8 1438.6 1429.1 1411.2
1374.8 1317.5 1298.8
1271.7 1238.0 1143.6 1136.8 1109.5 1074.2 1040.4
984.84 979.92 952.71
933.82 924.59 822.64 767.40 726.80 663.07 628.66
621.75 530.32 456.74
368.12 337.21 240.91 85.310 80.110
ZeroEnergy[kcal/mol] 10.791989921870648
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 8
Geometry[angstrom] 18
C 0.27287 0.45005 -1.28351
C 0.27352 0.45000 0.06583
C 1.42451 0.45234 0.96453
C -1.12402 0.37796 0.51988
C -1.94291 0.34213 -0.53553
C -1.13124 0.38548 -1.79320
H 1.14538 0.49645 -1.91775
H 2.36740 0.71840 0.49486
H 1.27213 0.98277 1.90143
H 1.62241 -0.78582 1.36970
H -1.42018 0.36100 1.55944
H -3.02067 0.29206 -0.51430
H -1.30360 -0.49807 -2.41680
H -1.38744 1.25100 -2.41283
C 1.82102 -2.10217 1.76292
H 2.16405 -2.58516 0.85468
H 0.83588 -2.41710 2.08936
H 2.56175 -2.05177 2.55330
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17 18
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.47 1.57 2.68 3.43 3.69 3.39 2.58 1.43 0.35 0.01
0.68 2.21 4.06 4.95 3.85 1.97 0.53
End
Rotor Hindered
Group 16 17 18
Axis 15 10
Symmetry 3
Potential[kcal/mol] 6
0.00 0.00 0.01 0.02 0.01 0.01
End
Frequencies[1/cm] 45
3240.9 3227.3 3220.2 3218.2 3209.1 3177.3 3099.5
3076.9 3068.5 3038.5
1669.3 1593.4 1472.3 1445.5 1436.8 1429.1 1411.5
1375.5 1319.5 1307.4
1272.7 1238.6 1137.4 1136.8 1109.6 1074.3 1040.8
985.15 979.90 952.70
934.00 924.64 823.07 767.95 726.89 663.25 628.53
616.98 531.60 459.45
368.23 335.97 239.91 82.520 76.890
ZeroEnergy[kcal/mol] 11.044634812246994
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 9
Geometry[angstrom] 18
C 0.27285 0.45009 -1.28339
C 0.27329 0.45006 0.06549
C 1.42490 0.45157 0.96499
C -1.12400 0.37796 0.51985
C -1.94294 0.34212 -0.53556
C -1.13124 0.38548 -1.79318
H 1.14536 0.49650 -1.91769
H 2.36691 0.72002 0.49459
H 1.27204 0.98483 1.90043
H 1.62012 -0.77125 1.36526
H -1.42016 0.36102 1.55943
H -3.02070 0.29207 -0.51431
H -1.30363 -0.49808 -2.41674
H -1.38746 1.25100 -2.41277
C 1.82119 -2.10337 1.76327
H 2.16399 -2.58389 0.85389
H 0.83527 -2.41579 2.08908
H 2.56188 -2.05038 2.55324
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17 18
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.47 1.57 2.68 3.43 3.69 3.39 2.58 1.43 0.35 0.01
0.68 2.21 4.06 4.95 3.85 1.97 0.53
End
Rotor Hindered
Group 16 17 18
Axis 15 10
Symmetry 3
Potential[kcal/mol] 6
0.00 0.00 0.01 0.02 0.01 0.01
End
Frequencies[1/cm] 45
3240.9 3227.0 3222.9 3221.0 3208.9 3174.8 3097.5
3078.4 3068.8 3038.8
1672.3 1595.9 1472.3 1442.7 1435.1 1429.1 1412.0
1377.2 1326.3 1312.3
1273.3 1239.1 1136.8 1132.8 1109.6 1073.9 1041.1
985.43 979.87 952.69
934.16 924.65 823.48 768.25 726.82 662.83 628.71
610.04 533.36 462.92
368.20 334.61 238.74 78.630 72.790
ZeroEnergy[kcal/mol] 11.204939522902972
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 10
Geometry[angstrom] 18
C 0.27284 0.45014 -1.28329
C 0.27304 0.45011 0.06517
C 1.42528 0.45085 0.96544
C -1.12399 0.37795 0.51982
C -1.94297 0.34212 -0.53558
C -1.13124 0.38547 -1.79315
H 1.14538 0.49656 -1.91767
H 2.36641 0.72167 0.49432
H 1.27195 0.98691 1.89939
H 1.61784 -0.75671 1.36084
H -1.42014 0.36105 1.55941
H -3.02070 0.29208 -0.51432
H -1.30366 -0.49812 -2.41670
H -1.38746 1.25098 -2.41270
C 1.82136 -2.10461 1.76363

```
H   2.16392  -2.58259   0.85310
H   0.83466  -2.41447   2.08880
H   2.56202  -2.04898   2.55320
              Core           RigidRotor
       SymmetryFactor    1.0000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
  3241.1      3226.4      3225.7      3223.8      3208.8      3172.4      3095.8
3080.1      3069.1      3038.9
  1675.3      1598.1      1472.2      1440.2      1433.5      1429.2      1412.6
1379.8      1337.0      1313.6
  1273.6      1239.7      1136.7      1130.5      1109.6      1073.1      1041.3
985.70      979.83      952.70
  934.32      924.65      823.88      768.42      726.66      661.79      629.15
601.08      535.99      467.01
  368.22      333.14      237.45      73.600      67.730
 ZeroEnergy[kcal/mol]    11.279379288486393
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          11
Geometry[angstrom]          18
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34795
C    1.15284   0.00000   2.24901
C   -1.39683  -0.07224   1.80293
C   -2.21589  -0.10807   0.74751
C   -1.40412  -0.06472  -0.51004
H    0.87252   0.04644  -0.63436
H    2.09308   0.27323   1.77714
H    0.99902   0.53895   3.18148
H    1.34279  -1.19245   2.63963
H   -1.69297  -0.08911   2.84255
H   -3.29364  -0.15810   0.76878
H   -1.57656  -0.94829  -1.13352
H   -1.66036   0.80082  -1.12957
C    1.54873  -2.55610   3.04714
H    1.89105  -3.03140   2.13534
H    0.56118  -2.86322   3.37163
H    2.28931  -2.49763   3.83625
              Core           RigidRotor
       SymmetryFactor    1.0000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
```

```
   Frequencies[1/cm]          45
  3241.0      3228.5      3226.6      3226.1      3208.6      3169.9      3093.8
3081.7      3069.4      3039.1
  1678.5      1600.1      1472.1      1438.1      1432.0      1429.2      1413.3
1383.2      1348.7      1314.0
  1273.8      1240.2      1136.7      1130.9      1109.7      1072.1      1041.5
985.94      979.80      952.67
  934.42      924.64      824.24      768.34      726.37      660.15      629.88
590.65      540.41      471.05
  368.20      331.64      236.04      67.320      61.700
 ZeroEnergy[kcal/mol]    11.281433519836025
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          12
Geometry[angstrom]          18
C    0.27280   0.45023  -1.28306
C    0.27260   0.45026   0.06448
C    1.42605   0.44953   0.96632
C   -1.12396   0.37794   0.51977
C   -1.94304   0.34211  -0.53563
C   -1.13125   0.38545  -1.79312
H    1.14533   0.49669  -1.91753
H    2.36538   0.72516   0.49372
H    1.27174   0.99132   1.89724
H    1.61338  -0.72783   1.35217
H   -1.42009   0.36110   1.55940
H   -3.02077   0.29209  -0.51435
H   -1.30374  -0.49815  -2.41658
H   -1.38751   1.25099  -2.41260
C    1.82174  -2.10730   1.76442
H    2.16380  -2.57989   0.85140
H    0.83336  -2.41168   2.08822
H    2.56229  -2.04600   2.55309
              Core           RigidRotor
       SymmetryFactor    1.0000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                    Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
  3241.0      3231.2      3229.3      3225.9      3208.4      3167.3      3091.8
3083.3      3069.7      3039.3
  1681.7      1601.9      1472.1      1436.4      1430.8      1429.3      1414.4
1387.2      1360.3      1314.1
  1274.0      1240.7      1136.7      1135.4      1109.9      1071.0      1041.6
986.14      979.77      952.64
  934.50      924.62      824.57      768.14      725.98      658.01      631.28
578.88      548.21      474.38
  368.13      330.11      234.46      59.510      54.450
 ZeroEnergy[kcal/mol]    11.209658349496404
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          13
Geometry[angstrom]          18
C    0.27277   0.45027  -1.28293
C    0.27239   0.45034   0.06412
C    1.42643   0.44895   0.96674
C   -1.12394   0.37794   0.51975
```

```
C   -1.94310   0.34211  -0.53567
C   -1.13127   0.38544  -1.79311
H    1.14527   0.49675  -1.91741
H    2.36483   0.72703   0.49338
H    1.27160   0.99370   1.89612
H    1.61122  -0.71355   1.34795
H   -1.42006   0.36113   1.55940
H   -3.02085   0.29209  -0.51437
H   -1.30379  -0.49813  -2.41651
H   -1.38756   1.25101  -2.41257
C    1.82195  -2.10877   1.76485
H    2.16375  -2.57846   0.85046
H    0.83265  -2.41020   2.08791
H    2.56243  -2.04443   2.55302
          Core           RigidRotor
       SymmetryFactor    1.0000000000000000
End
 Rotor                  Hindered
 Group    8   9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                  Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
  3240.8     3233.9     3232.1     3226.1     3208.2     3164.7     3089.7
3084.8     3069.9     3039.6
  1685.0     1603.5     1472.2     1435.1     1430.2     1428.8     1415.7
1391.9     1371.2     1314.1
  1274.0     1241.4     1146.5     1136.7     1110.0     1070.4     1041.6
986.28     979.75     952.59
  934.53     924.58     824.88     767.80     725.53     655.54     634.34
566.68     560.62     476.02
  367.99     328.58     232.75     49.850     45.690
ZeroEnergy[kcal/mol]    11.109083836564889
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          14
Geometry[angstrom]          18
C    0.27274   0.45032  -1.28282
C    0.27217   0.45043   0.06377
C    1.42681   0.44844   0.96715
C   -1.12393   0.37793   0.51972
C   -1.94315   0.34210  -0.53570
C   -1.13129   0.38543  -1.79310
H    1.14524   0.49682  -1.91732
H    2.36424   0.72901   0.49301
H    1.27146   0.99619   1.89490
H    1.60911  -0.69942   1.34382
H   -1.42003   0.36116   1.55939
H   -3.02089   0.29210  -0.51439
H   -1.30384  -0.49815  -2.41646
H   -1.38759   1.25101  -2.41252
C    1.82217  -2.11035   1.76531
H    2.16368  -2.57695   0.84949
H    0.83191  -2.40864   2.08759
H    2.56259  -2.04278   2.55297
          Core           RigidRotor
       SymmetryFactor    1.0000000000000000
End
 Rotor                  Hindered
 Group    8   9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                  Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
  3240.8     3236.7     3234.9     3225.8     3208.1     3162.2     3087.8
3086.5     3070.2     3039.8
  1688.4     1604.9     1472.4     1434.8     1430.1     1428.0     1417.4
1397.6     1380.6     1314.1
  1274.2     1242.9     1168.8     1136.6     1110.2     1070.1     1041.5
986.36     979.72     952.55
  934.56     924.52     825.17     767.61     725.02     653.12     642.32
579.08     552.50     475.62
  367.79     326.97     230.84     37.650     34.090
ZeroEnergy[kcal/mol]    10.953605275779264
 ElectronicLevels[1/cm]                 1
 0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          15
Geometry[angstrom]          18
C    0.27271   0.45038  -1.28271
C    0.27193   0.45053   0.06340
C    1.42720   0.44803   0.96755
C   -1.12391   0.37792   0.51968
C   -1.94320   0.34210  -0.53573
C   -1.13130   0.38542  -1.79309
H    1.14522   0.49690  -1.91723
H    2.36361   0.73113   0.49261
H    1.27130   0.99887   1.89359
H    1.60709  -0.68552   1.33985
H   -1.41999   0.36120   1.55938
H   -3.02094   0.29210  -0.51441
H   -1.30389  -0.49816  -2.41640
H   -1.38762   1.25102  -2.41247
C    1.82241  -2.11206   1.76582
H    2.16362  -2.57534   0.84846
H    0.83111  -2.40699   2.08725
H    2.56277  -2.04104   2.55293
          Core           RigidRotor
       SymmetryFactor    1.0000000000000000
End
 Rotor                  Hindered
 Group    8   9  10  15  16  17  18
 Axis          3         2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.47    1.57    2.68    3.43    3.69    3.39    2.58    1.43    0.35    0.01
0.68    2.21    4.06    4.95    3.85    1.97    0.53
 End
 Rotor                  Hindered
 Group   16  17  18
 Axis          15        10
 Symmetry          3
 Potential[kcal/mol]          6
  0.00    0.00    0.01    0.02    0.01    0.01
 End
   Frequencies[1/cm]          45
  3240.7     3239.5     3237.7     3225.7     3207.9     3159.7     3088.2
3086.0     3070.4     3040.0
  1692.1     1606.3     1473.2     1436.7     1429.8     1427.2     1419.5
1404.8     1388.1     1314.0
  1274.5     1248.8     1207.1     1136.6     1110.3     1070.1     1041.2
986.37     979.70     952.52
  934.56     924.44     825.44     767.66     724.54     665.04     649.71
595.23     538.74     473.21
  367.51     325.33     228.73     21.380     11.490
```

```
ZeroEnergy[kcal/mol]    10.822161442537844
 ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
 End
!*********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1661.6700000000001
      WellDepth[kcal/mol]         10.03
      WellDepth[kcal/mol]         27.55
 End
End
End
```

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                      direct    ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                        diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                            10
!ChemicalEigenvalueMin                 1.e-6          #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                  1.3
!!
RateOutput                             rate.out                   ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                          ! Default collisional
energy relaxation kernel
    Exponential                                             ! Currently the only
possible energy relaxation model
      Factor[1/cm]              316                         ! (Delta_E_down)^(0)
@ standard T (300 K)
      Power                     0.535                       ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
      ExponentCutoff            10                          ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                        ! Collision frequency
model
    LennardJones                                            ! Currently the only
possible collisional frequency model  based on LJ potential
      Epsilons[K]               90.58  281.367              ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
      Sigmas[angstrom]          3.54    4.694               ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
      Masses[amu]               39.948  79.05478            ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50263
 C    1.24622   0.00000   2.31947
 C   -1.27227   0.00046   1.92591
 C   -2.17585   0.00051   0.77474
 C   -1.45565   0.00011  -0.35294
 H    0.51979   0.87601  -0.40113
 H    1.85947   0.87812   2.10478
 H    1.01835  -0.00094   3.38445
 H    1.86045  -0.87709   2.10340
 H   -1.59049   0.00052   2.95892
 H   -3.25397   0.00095   0.84079
 H   -1.83452  -0.00013  -1.36297
 H    0.51979  -0.87591  -0.40126
       Core    RigidRotor
            SymmetryFactor    1.0000000000000000
       End
 Rotor                         Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]         12
   0.00    0.08    0.30    0.62    0.95    1.20    1.29    1.21    0.96    0.62    0.30
0.08
 End
    Frequencies[1/cm]          35
  3245.2     3221.6     3209.3     3128.8     3090.6     3074.8     3042.5
3036.2     1695.3     1615.6
  1495.0     1486.6     1424.0     1421.5     1397.2     1340.1     1274.6
1198.6     1152.9     1130.9
  1060.1     1033.7     1005.4     976.89     961.82     922.95     892.68
863.70     828.81     700.71
  623.69     533.08     369.88     325.94     227.72
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]            2
 O    0.00000   0.00000   0.00000
 H    0.00000   0.00000   0.97032
       Core    RigidRotor
            SymmetryFactor    1.0000000000000000
       End
    Frequencies[1/cm]           1
  3774.5
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Well WR
 Species
 RRHO     ! transition state
 Geometry[angstrom]            16
 C   -0.00100   0.00118   0.00312
```

```
C  -0.00088 -0.00026  1.56136
C   1.40190  0.00288  2.14767
C  -0.78115  1.24364  1.90002
C  -1.21415  1.88274  0.75743
C  -0.79268  1.21287 -0.37649
H   1.01423  0.03970 -0.39993
H   1.96724  0.85672  1.77582
H   1.35583  0.05704  3.23477
H   1.92257 -0.91355  1.86839
H  -0.96181  1.55198  2.91924
H  -1.80214  2.78962  0.74670
H  -0.99419  1.51211 -1.39368
H  -0.44572 -0.92413 -0.37005
O  -0.63512 -1.16506  2.09689
H  -1.56995 -1.11709  1.88989
            Core          RigidRotor
                          SymmetryFactor    1.0000000000000000
            End
   Frequencies[1/cm]        42
  51.219    262.65    284.74    321.13    367.80    394.21    437.98
521.79    620.18    630.47
  712.17    798.52    814.46    900.21    949.63    958.72    970.19
1000.3    1068.9    1073.1
  1101.0    1134.2    1217.5    1223.8    1294.4    1318.7    1378.4
1407.6    1417.3    1477.2
  1491.0    1494.4    1505.2    3045.4    3052.4    3080.6    3131.1
3138.8    3207.6    3224.8
  3237.6    3879.3
 ZeroEnergy[kcal/mol]          -40.28
 ElectronicLevels[1/cm]               1
  0.0000000000000000      2.0000000000000000
End
End
!************************************
Barrier TS REACS WR
Variational
RRHO          !          1
Geometry[angstrom]          16
C   0.29829  0.45830 -0.76989
C   0.29659  0.43862  0.72868
C   1.54349  0.43677  1.54253
C  -0.97929  0.40138  1.14101
C  -1.87349  0.40131 -0.02091
C  -1.14388  0.43668 -1.14344
H   0.86690  1.28547 -1.20263
H   2.13445  1.33684  1.35932
H   1.31962  0.38879  2.60713
H   2.17315 -0.41664  1.28242
H  -1.30754  0.37356  2.17029
H  -2.95193  0.37953  0.03553
H  -1.50902  0.44549 -2.15795
H   0.82707 -0.45365 -1.16427
O   1.26612 -1.99501 -1.24455
H   0.47934 -2.31414 -0.77603
            Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                    Hindered
 Group   16
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3778.7    3250.5    3224.8    3212.3    3132.1    3096.3    3080.4
3039.7    2426.0    1689.2
  1607.7    1496.6    1485.7    1424.5    1397.3    1379.5    1336.1
1268.8    1195.6    1131.1
  1103.5    1044.6    1031.7    996.76    976.60    956.99    911.66
889.22    857.18    822.56
  715.56    644.73    623.17    530.26    335.94    324.74    215.48
76.440    43.880
 ZeroEnergy[kcal/mol]    1.0894435787996863
  ElectronicLevels[1/cm]               1
  0.0000000000000000      2.0000000000000000
End
!*********************************************
RRHO          !          2
Geometry[angstrom]          16
C   0.29831  0.45582 -0.76966
C   0.29671  0.43834  0.72879
C   1.54363  0.43666  1.54255
C  -0.97923  0.40168  1.14097
C  -1.87328  0.40148 -0.02114
C  -1.14347  0.43601 -1.14365
H   0.87158  1.27767 -1.20606
H   2.13448  1.33677  1.35918
H   1.31980  0.38882  2.60716
H   2.17328 -0.41674  1.28246
H  -1.30765  0.37444  2.17020
H  -2.95173  0.38034  0.03514
H  -1.50834  0.44449 -2.15823
H   0.82397 -0.46169 -1.16061
O   1.26516 -1.99163 -1.24439
H   0.48031 -2.31608 -0.77646
            Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                    Hindered
 Group   16
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3779.4    3250.6    3224.9    3212.4    3132.2    3096.4    3081.8
3039.7    2381.8    1689.0
  1607.2    1496.6    1485.7    1424.4    1396.9    1377.0    1335.9
1268.8    1195.7    1131.1
  1102.2    1043.9    1031.7    996.45    976.45    956.79    911.54
889.12    857.17    822.17
  717.44    650.09    623.31    530.35    336.14    324.93    215.31
69.390    45.060
 ZeroEnergy[kcal/mol]    1.0526420503091865
  ElectronicLevels[1/cm]               1
  0.0000000000000000      2.0000000000000000
End
!*********************************************
RRHO          !          3
Geometry[angstrom]          16
C   0.29832  0.45339 -0.76944
C   0.29684  0.43807  0.72889
C   1.54377  0.43656  1.54256
C  -0.97916  0.40195  1.14094
C  -1.87305  0.40164 -0.02137
C  -1.14305  0.43537 -1.14386
H   0.87626  1.26984 -1.20950
H   2.13452  1.33670  1.35904
```

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H   1.31997   0.38885   2.60717
H   2.17342  -0.41684   1.28248
H  -1.30775   0.37525   2.17011
H  -2.95152   0.38112   0.03476
H  -1.50767   0.44355  -2.15851
H   0.82095  -0.46995  -1.15688
O   1.26418  -1.98826  -1.24422
H   0.48128  -2.31805  -0.77691
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                    Hindered
 Group   16
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3780.2      3250.8      3225.1      3212.5      3132.3      3096.5      3083.3
3039.8      2328.9      1688.8
  1606.6      1496.5      1485.7      1424.4      1396.5      1373.9      1335.6
1268.8      1195.8      1131.0
  1100.9      1043.2      1031.6      996.13      976.29      956.52      911.44
889.02      857.22      821.71
  719.73      655.33      623.37      530.50      336.64      325.16      215.39
65.740      46.710
ZeroEnergy[kcal/mol]    1.0018171483940088
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !           4
Geometry[angstrom]          16
C   0.29834   0.45101  -0.76923
C   0.29698   0.43781   0.72898
C   1.54391   0.43646   1.54258
C  -0.97908   0.40220   1.14090
C  -1.87283   0.40178  -0.02161
C  -1.14263   0.43473  -1.14407
H   0.88092   1.26198  -1.21294
H   2.13455   1.33665   1.35891
H   1.32013   0.38888   2.60719
H   2.17355  -0.41693   1.28251
H  -1.30784   0.37601   2.17002
H  -2.95131   0.38188   0.03438
H  -1.50700   0.44266  -2.15880
H   0.81803  -0.47843  -1.15311
O   1.26319  -1.98489  -1.24403
H   0.48226  -2.32001  -0.77738
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                    Hindered
 Group   16
 Axis           15         14
 Symmetry          1
```

```
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3781.1      3251.0      3225.2      3212.6      3132.3      3096.6      3084.8
3039.8      2273.8      1688.5
  1606.0      1496.5      1485.6      1424.4      1396.2      1371.0      1335.3
1268.8      1195.8      1131.0
  1099.7      1042.5      1031.5      995.84      976.11      956.33      911.38
888.94      857.36      821.21
  722.53      660.44      623.41      530.73      337.78      325.41      215.93
65.250      49.050
ZeroEnergy[kcal/mol]    0.96147028199312756
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !           5
Geometry[angstrom]          16
C   0.29833   0.44868  -0.76901
C   0.29712   0.43754   0.72906
C   1.54404   0.43637   1.54258
C  -0.97900   0.40242   1.14086
C  -1.87260   0.40190  -0.02184
C  -1.14220   0.43411  -1.14430
H   0.88559   1.25408  -1.21638
H   2.13458   1.33660   1.35878
H   1.32028   0.38890   2.60719
H   2.17368  -0.41702   1.28252
H  -1.30791   0.37674   2.16993
H  -2.95110   0.38263   0.03399
H  -1.50632   0.44182  -2.15909
H   0.81518  -0.48706  -1.14933
O   1.26217  -1.98153  -1.24382
H   0.48324  -2.32197  -0.77787
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                    Hindered
 Group   16
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3782.0      3251.2      3225.3      3212.8      3132.4      3096.7      3086.4
3039.9      2222.5      1688.2
  1605.3      1496.5      1485.6      1424.4      1396.0      1369.1      1334.9
1268.8      1195.9      1131.0
  1098.5      1041.9      1031.5      995.62      975.93      956.31      911.35
888.91      857.60      820.65
  725.89      665.27      623.46      531.03      339.52      325.67      216.83
66.300      51.810
ZeroEnergy[kcal/mol]    0.91986684311393474
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !           6
Geometry[angstrom]          16
C   0.29831   0.44640  -0.76879
C   0.29726   0.43728   0.72914
C   1.54418   0.43629   1.54258
```

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C  -0.97891  0.40262  1.14081
C  -1.87236  0.40201  -0.02208
C  -1.14175  0.43349  -1.14453
H   0.89027  1.24610  -1.21984
H   2.13462  1.33655  1.35865
H   1.32042  0.38893  2.60720
H   2.17381  -0.41710  1.28254
H  -1.30798  0.37742  2.16984
H  -2.95088  0.38337  0.03360
H  -1.50564  0.44100  -2.15939
H   0.81239  -0.49575  -1.14555
O   1.26115  -1.97818  -1.24360
H   0.48422  -2.32392  -0.77839
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.32   1.04   1.45   1.08   0.38   0.00   0.32   1.05   1.45   1.08
0.39   0.00   0.29   1.03   1.45   1.05   0.35
 End
 Rotor                    Hindered
 Group   16
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.07   0.29   0.64   0.95   1.15   1.22   1.21   1.21   1.25   1.30
1.34   1.38   1.37   1.16   0.74   0.31   0.06
 End
   Frequencies[1/cm]          39
  3783.1     3251.4     3225.4     3212.9     3132.5     3096.8     3088.0
3039.9     2174.4     1687.9
  1604.5     1496.5     1485.6     1424.3     1395.7     1367.9     1334.5
1268.8     1196.0     1131.0
  1097.3     1041.2     1031.4     995.44     975.74     956.43     911.33
888.90     857.90     820.04
  729.82     669.70     623.53     531.36     341.53     325.93     217.85
67.890     54.620
ZeroEnergy[kcal/mol]   0.89170065324675618
 ElectronicLevels[1/cm]                1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO          !          7
Geometry[angstrom]          16
C   0.29828  0.44416  -0.76857
C   0.29741  0.43701  0.72921
C   1.54432  0.43620  1.54258
C  -0.97882  0.40279  1.14077
C  -1.87212  0.40210  -0.02232
C  -1.14130  0.43288  -1.14476
H   0.89497  1.23803  -1.22332
H   2.13464  1.33652  1.35853
H   1.32055  0.38895  2.60719
H   2.17394  -0.41718  1.28255
H  -1.30803  0.37807  2.16974
H  -2.95065  0.38409  0.03320
H  -1.50494  0.44023  -2.15969
H   0.80965  -0.50451  -1.14177
O   1.26011  -1.97483  -1.24335
H   0.48521  -2.32586  -0.77893
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.32   1.04   1.45   1.08   0.38   0.00   0.32   1.05   1.45   1.08
0.39   0.00   0.29   1.03   1.45   1.05   0.35
 End
 Rotor                    Hindered
 Group   16
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.07   0.29   0.64   0.95   1.15   1.22   1.21   1.21   1.25   1.30
1.34   1.38   1.37   1.16   0.74   0.31   0.06
 End
   Frequencies[1/cm]          39
  3784.2     3251.6     3225.6     3213.0     3132.6     3097.0     3089.6
3040.0     2122.0     1687.6
  1603.6     1496.4     1485.5     1424.3     1395.5     1366.6     1334.1
1268.8     1196.0     1131.0
  1096.0     1040.5     1031.3     995.23     975.53     956.56     911.28
888.91     858.25     819.37
  734.25     673.62     623.58     531.69     343.58     326.17     218.85
69.510     57.330
ZeroEnergy[kcal/mol]   0.84896785269442687
 ElectronicLevels[1/cm]                1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO          !          8
Geometry[angstrom]          16
C   0.29823  0.44197  -0.76835
C   0.29757  0.43675  0.72928
C   1.54446  0.43613  1.54258
C  -0.97872  0.40294  1.14072
C  -1.87187  0.40218  -0.02256
C  -1.14084  0.43229  -1.14501
H   0.89968  1.22990  -1.22682
H   2.13466  1.33649  1.35842
H   1.32067  0.38897  2.60718
H   2.17408  -0.41725  1.28255
H  -1.30807  0.37866  2.16965
H  -2.95042  0.38481  0.03281
H  -1.50424  0.43953  -2.15999
H   0.80701  -0.51346  -1.13797
O   1.25905  -1.97150  -1.24309
H   0.48621  -2.32781  -0.77949
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.32   1.04   1.45   1.08   0.38   0.00   0.32   1.05   1.45   1.08
0.39   0.00   0.29   1.03   1.45   1.05   0.35
 End
 Rotor                    Hindered
 Group   16
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.07   0.29   0.64   0.95   1.15   1.22   1.21   1.21   1.25   1.30
1.34   1.38   1.37   1.16   0.74   0.31   0.06
 End
   Frequencies[1/cm]          39
  3785.4     3251.9     3225.8     3213.2     3132.7     3097.1     3091.3
3040.1     2056.8     1687.3
  1602.6     1496.4     1485.5     1424.3     1395.3     1364.5     1333.6
1268.8     1196.1     1131.0
  1094.7     1039.7     1031.3     994.96     975.31     956.58     911.19
888.93     858.65     818.63
  739.18     677.04     623.58     532.05     345.67     326.41     219.82
71.160     60.060
ZeroEnergy[kcal/mol]   0.77286957310167081
 ElectronicLevels[1/cm]                1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
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RRHO        !        9
Geometry[angstrom]        16
C   0.29817   0.43987  -0.76814
C   0.29773   0.43649   0.72932
C   1.54459   0.43606   1.54257
C  -0.97861   0.40306   1.14068
C  -1.87163   0.40224  -0.02279
C  -1.14037   0.43171  -1.14525
H   0.90439   1.22174  -1.23033
H   2.13467   1.33648   1.35832
H   1.32076   0.38900   2.60716
H   2.17420  -0.41730   1.28256
H  -1.30809   0.37920   2.16956
H  -2.95019   0.38552   0.03241
H  -1.50355   0.43890  -2.16029
H   0.80458  -0.52276  -1.13417
O   1.25798  -1.96818  -1.24281
H   0.48721  -2.32974  -0.78008
        Core        RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor              Hindered
 Group    8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.32   1.04   1.45   1.08   0.38   0.00   0.32   1.05   1.45   1.08
0.39   0.00   0.29   1.03   1.45   1.05   0.35
 End
 Rotor              Hindered
 Group   16
 Axis        15        14
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.07   0.29   0.64   0.95   1.15   1.22   1.21   1.21   1.25   1.30
1.34   1.38   1.37   1.16   0.74   0.31   0.06
 End
   Frequencies[1/cm]        39
  3786.8     3252.1     3225.9     3213.4     3132.8     3097.3     3093.0
3040.1     1975.8     1686.9
  1601.4     1496.4     1485.4     1424.3     1395.0     1361.8     1332.9
1268.8     1196.1     1130.9
  1093.2     1038.8     1031.2     994.65     975.06     956.51     911.06
888.98     859.13     817.76
  744.56     680.00     623.54     532.49     348.04     326.67     220.86
73.250     63.130
ZeroEnergy[kcal/mol]   0.70216077896131224
 ElectronicLevels[1/cm]              1
  0.0000000000000000       2.0000000000000000
End
!********************************************
RRHO        !        10
Geometry[angstrom]        16
C   0.29807   0.43782  -0.76789
C   0.29778   0.43621   0.72937
C   1.54461   0.43601   1.54254
C  -0.97838   0.40312   1.14058
C  -1.87126   0.40229  -0.02306
C  -1.13989   0.43116  -1.14542
H   0.90895   1.21362  -1.23371
H   2.13453   1.33653   1.35821
H   1.32079   0.38901   2.60705
H   2.17421  -0.41725   1.28251
H  -1.30796   0.37966   2.16934
H  -2.94984   0.38625   0.03201
H  -1.50288   0.43838  -2.16047
H   0.80245  -0.53243  -1.13048
O   1.25691  -1.96491  -1.24251
H   0.48810  -2.33121  -0.78072
        Core        RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor              Hindered
 Group    8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.32   1.04   1.45   1.08   0.38   0.00   0.32   1.05   1.45   1.08
0.39   0.00   0.29   1.03   1.45   1.05   0.35
 End
 Rotor              Hindered
 Group   16
 Axis        15        14
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.07   0.29   0.64   0.95   1.15   1.22   1.21   1.21   1.25   1.30
1.34   1.38   1.37   1.16   0.74   0.31   0.06
 End
   Frequencies[1/cm]        39
  3789.5     3252.5     3226.3     3213.9     3133.5     3098.0     3095.1
3040.5     1884.5     1687.3
  1600.7     1496.3     1485.3     1424.2     1394.7     1359.1     1332.2
1268.7     1196.2     1131.0
  1091.6     1038.0     1031.1     994.34     974.88     956.53     910.80
889.14     859.58     816.80
  750.04     682.37     623.50     532.82     350.54     326.83     221.93
75.480     66.160
ZeroEnergy[kcal/mol]   0.59511372189090905
 ElectronicLevels[1/cm]              1
  0.0000000000000000       2.0000000000000000
End
!********************************************
RRHO        !        11
Geometry[angstrom]        16
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.49707
C   1.24674   0.00000   2.31016
C  -1.27624  -0.03277   1.90824
C  -2.16902  -0.03364   0.74442
C  -1.43740  -0.00534  -0.37798
H   0.61564   0.76948  -0.46955
H   1.83655   0.90053   2.12576
H   1.02285  -0.04691   3.37469
H   1.87633  -0.85331   2.05014
H  -1.60594  -0.05584   2.93699
H  -3.24756  -0.04902   0.79933
H  -1.80021   0.00197  -1.39304
H   0.50289  -0.97898  -0.35915
O   0.95789  -2.39764  -0.47452
H   0.19122  -2.76919  -0.01361
        Core        RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor              Hindered
 Group    8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.32   1.04   1.45   1.08   0.38   0.00   0.32   1.05   1.45   1.08
0.39   0.00   0.29   1.03   1.45   1.05   0.35
 End
 Rotor              Hindered
 Group   16
 Axis        15        14
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.07   0.29   0.64   0.95   1.15   1.22   1.21   1.21   1.25   1.30
1.34   1.38   1.37   1.16   0.74   0.31   0.06
 End
   Frequencies[1/cm]        39
  3791.4     3252.8     3226.5     3214.1     3133.7     3098.9     3096.7
3040.6     1782.1     1686.8
  1598.3     1496.3     1485.2     1424.2     1394.3     1356.9     1331.1
1268.7     1196.2     1130.9
  1090.0     1037.4     1031.0     994.19     974.59     956.84     910.44
889.38     860.21     815.54
  756.17     684.74     623.44     533.58     354.10     327.21     223.47
78.990     70.420
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ZeroEnergy[kcal/mol]   0.48613674297412307
 ElectronicLevels[1/cm]                  1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO          !          12
Geometry[angstrom]          16
C    0.29782   0.43409  -0.76751
C    0.29812   0.43571   0.72942
C    1.54485   0.43590   1.54249
C   -0.97813   0.40326   1.14053
C   -1.87079   0.40233  -0.02346
C   -1.13892   0.43008  -1.14592
H    0.91823   1.19725  -1.24079
H    2.13458   1.33650   1.35800
H    1.32090   0.38909   2.60698
H    2.17438  -0.41739   1.28249
H   -1.30791   0.38057   2.16920
H   -2.94940   0.38762   0.03130
H   -1.50156   0.43748  -2.16103
H    0.79922  -0.55360  -1.12322
O    1.25475  -1.95845  -1.24192
H    0.49030  -2.33522  -0.78192
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                      Hindered
 Group   16
 Axis          15          14
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3792.8     3253.1     3226.8     3214.4     3133.8     3100.1     3097.3
3040.7     1686.5     1684.2
  1593.7     1496.2     1485.1     1424.2     1394.0     1355.0     1329.7
1268.5     1196.2     1130.8
  1088.2     1036.6     1031.0     994.01     974.27     957.26     909.80
889.75     860.80     814.16
  762.14     686.77     623.36     534.31     357.69     327.59     224.98
82.660     74.640
ZeroEnergy[kcal/mol]   0.36698266393355344
 ElectronicLevels[1/cm]                  1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO          !          13
Geometry[angstrom]          16
C    0.29766   0.43245  -0.76737
C    0.29841   0.43547   0.72942
C    1.54506   0.43583   1.54249
C   -0.97812   0.40333   1.14059
C   -1.87070   0.40232  -0.02360
C   -1.13843   0.42956  -1.14627
H    0.92286   1.18915  -1.24441
H    2.13474   1.33644   1.35789
H    1.32096   0.38916   2.60700
H    2.17455  -0.41757   1.28252
H   -1.30798   0.38103   2.16929
H   -2.94930   0.38828   0.03098
H   -1.50093   0.43711  -2.16141
H    0.79824  -0.56502  -1.11976
O    1.25368  -1.95530  -1.24161
H    0.49153  -2.33758  -0.78249
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                      Hindered
 Group   16
 Axis          15          14
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3793.4     3253.4     3226.8     3214.3     3133.4     3101.6     3097.3
3040.4     1684.7     1607.3
  1548.4     1496.2     1484.6     1424.1     1393.5     1352.2     1327.3
1268.2     1196.2     1130.5
  1085.8     1035.8     1030.9     993.87     973.83     957.84     908.44
890.22     861.27     812.42
  768.19     688.74     623.19     535.41     361.96     328.16     226.77
87.260     79.740
ZeroEnergy[kcal/mol]   0.21576401613408597
 ElectronicLevels[1/cm]                  1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO          !          14
Geometry[angstrom]          16
C    0.29741   0.43097  -0.76718
C    0.29858   0.43522   0.72942
C    1.54517   0.43578   1.54246
C   -0.97799   0.40336   1.14059
C   -1.87050   0.40231  -0.02376
C   -1.13793   0.42906  -1.14653
H    0.92733   1.18113  -1.24790
H    2.13477   1.33642   1.35778
H    1.32098   0.38921   2.60694
H    2.17459  -0.41765   1.28250
H   -1.30792   0.38144   2.16925
H   -2.94911   0.38896   0.03067
H   -1.50031   0.43685  -2.16167
H    0.79797  -0.57752  -1.11666
O    1.25263  -1.95224  -1.24130
H    0.49267  -2.33947  -0.78311
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                      Hindered
 Group   16
 Axis          15          14
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3795.5     3253.7     3227.1     3214.7     3133.6     3103.8     3097.6
3040.6     1684.0     1597.7
```

1496.1 1486.1 1429.1 1418.2 1392.9 1344.9 1319.3
1266.5 1196.0 1130.2
1082.0 1035.0 1030.8 993.67 973.41 958.60 905.31
890.66 860.89 810.31
773.48 690.38 622.95 536.44 366.23 328.67 228.55
92.060 84.800
ZeroEnergy[kcal/mol] 3.74068990366016596E-004
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 15
Geometry[angstrom] 16
C 0.29711 0.42974 -0.76699
C 0.29875 0.43496 0.72940
C 1.54527 0.43574 1.54243
C -0.97787 0.40338 1.14060
C -1.87033 0.40228 -0.02390
C -1.13743 0.42860 -1.14679
H 0.93161 1.17344 -1.25126
H 2.13479 1.33641 1.35769
H 1.32097 0.38927 2.60688
H 2.17461 -0.41772 1.28247
H -1.30785 0.38181 2.16922
H -2.94894 0.38961 0.03037
H -1.49972 0.43668 -2.16192
H 0.79868 -0.59135 -1.11410
O 1.25162 -1.94932 -1.24098
H 0.49379 -2.34125 -0.78372
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.32 1.04 1.45 1.08 0.38 0.00 0.32 1.05 1.45 1.08
0.39 0.00 0.29 1.03 1.45 1.05 0.35
End
Rotor Hindered
Group 16
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18
0.00 0.07 0.29 0.64 0.95 1.15 1.22 1.21 1.21 1.25 1.30
1.34 1.38 1.37 1.16 0.74 0.31 0.06
End
Frequencies[1/cm] 39
3798.0 3254.2 3227.5 3215.1 3133.8 3106.2 3097.9
3040.7 1683.1 1593.8
1496.0 1485.5 1424.7 1392.6 1365.3 1331.9 1277.0
1234.4 1194.8 1129.4
1074.4 1033.6 1030.7 993.46 972.94 959.63 899.57
889.36 858.36 807.65
777.74 691.94 622.62 537.64 370.67 329.28 230.49
97.590 90.370
ZeroEnergy[kcal/mol] -0.24775089497804198
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 16
Geometry[angstrom] 16
C 0.29674 0.42882 -0.76678
C 0.29891 0.43471 0.72938
C 1.54535 0.43571 1.54240
C -0.97775 0.40337 1.14063
C -1.87018 0.40224 -0.02402
C -1.13694 0.42818 -1.14704
H 0.93561 1.16623 -1.25443
H 2.13479 1.33642 1.35762
H 1.32094 0.38932 2.60682
H 2.17461 -0.41778 1.28243
H -1.30777 0.38215 2.16919
H -2.94879 0.39023 0.03011
H -1.49918 0.43661 -2.16213
H 0.80052 -0.60657 -1.11222
O 1.25066 -1.94660 -1.24068
H 0.49489 -2.34288 -0.78432
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.32 1.04 1.45 1.08 0.38 0.00 0.32 1.05 1.45 1.08
0.39 0.00 0.29 1.03 1.45 1.05 0.35
End
Rotor Hindered
Group 16
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18
0.00 0.07 0.29 0.64 0.95 1.15 1.22 1.21 1.21 1.25 1.30
1.34 1.38 1.37 1.16 0.74 0.31 0.06
End
Frequencies[1/cm] 39
3800.8 3254.7 3227.9 3215.5 3134.1 3108.8 3098.2
3040.8 1682.1 1590.2
1495.9 1485.4 1424.6 1391.9 1360.5 1326.9 1271.5
1197.0 1147.5 1124.1
1055.6 1031.1 1028.1 992.95 972.45 960.68 896.70
879.15 845.83 804.32
779.60 693.33 622.13 538.91 374.86 329.99 232.52
103.65 96.210
ZeroEnergy[kcal/mol] -0.50832452748268708
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 17
Geometry[angstrom] 16
C 0.29629 0.42821 -0.76657
C 0.29906 0.43447 0.72935
C 1.54542 0.43569 1.54238
C -0.97765 0.40336 1.14066
C -1.87006 0.40219 -0.02410
C -1.13646 0.42781 -1.14728
H 0.93926 1.15964 -1.25736
H 2.13479 1.33643 1.35756
H 1.32090 0.38938 2.60675
H 2.17459 -0.41784 1.28239
H -1.30770 0.38245 2.16918
H -2.94867 0.39081 0.02989
H -1.49870 0.43661 -2.16232
H 0.80346 -0.62301 -1.11113
O 1.24978 -1.94413 -1.24040
H 0.49594 -2.34436 -0.78489
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.32 1.04 1.45 1.08 0.38 0.00 0.32 1.05 1.45 1.08
0.39 0.00 0.29 1.03 1.45 1.05 0.35
End
Rotor Hindered
Group 16
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18

```
 0.00  0.07  0.29  0.64  0.95  1.15  1.22  1.21  1.21  1.25  1.30
1.34  1.38  1.37  1.16  0.74  0.31  0.06
 End
  Frequencies[1/cm]      39
 3803.9   3255.2   3228.3   3216.0   3134.3   3111.6   3098.5
3041.0   1681.0   1586.2
 1495.8   1485.3   1424.6   1391.2   1362.2   1323.1   1270.7
1196.1   1133.5   1104.8
 1041.4   1031.0   1008.4   990.38   972.00   960.97   897.15
870.78   811.88   798.19
 772.76   694.28   621.40   540.14   378.37   330.76   234.57
109.96   102.02
ZeroEnergy[kcal/mol]  -0.77987146833133836
 ElectronicLevels[1/cm]          1
 0.0000000000000000     2.0000000000000000
End
!**********************************************
RRHO      !     18
Geometry[angstrom]      16
C   0.29579  0.42792  -0.76633
C   0.29920  0.43425  0.72932
C   1.54548  0.43567  1.54235
C  -0.97756  0.40333  1.14071
C  -1.86997  0.40213  -0.02415
C  -1.13600  0.42748  -1.14751
H   0.94251  1.15376  -1.25998
H   2.13479  1.33644  1.35750
H   1.32085  0.38943  2.60669
H   2.17456  -0.41789  1.28235
H  -1.30763  0.38272  2.16917
H  -2.94858  0.39134  0.02970
H  -1.49829  0.43666  -2.16247
H   0.80743  -0.64046  -1.11083
O   1.24900  -1.94194  -1.24015
H   0.49693  -2.34565  -0.78543
      Core      RigidRotor
    SymmetryFactor   1.5000000000000000
End
 Rotor             Hindered
 Group   8  9  10
 Axis        3      2
 Symmetry       1
 Potential[kcal/mol]      18
 0.00  0.32  1.04  1.45  1.08  0.38  0.00  0.32  1.05  1.45  1.08
0.39  0.00  0.29  1.03  1.45  1.05  0.35
 End
 Rotor             Hindered
 Group   16
 Axis        15      14
 Symmetry       1
 Potential[kcal/mol]      18
 0.00  0.07  0.29  0.64  0.95  1.15  1.22  1.21  1.21  1.25  1.30
1.34  1.38  1.37  1.16  0.74  0.31  0.06
 End
  Frequencies[1/cm]      39
 3807.2   3255.7   3228.8   3216.5   3134.6   3114.6   3098.8
3041.1   1679.8   1581.8
 1495.6   1485.2   1424.6   1390.3   1367.6   1319.2   1270.3
1195.4   1132.4   1096.2
 1039.0   1031.1   999.50   984.06   971.54   960.00   897.87
867.28   801.92   785.96
 736.36   693.57   620.36   541.20   380.89   331.56   236.55
116.15   107.50
ZeroEnergy[kcal/mol]  -1.0561294679857005
 ElectronicLevels[1/cm]          1
 0.0000000000000000     2.0000000000000000
End
!**********************************************
RRHO      !     19
Geometry[angstrom]      16
C   0.29523  0.42789  -0.76609
C   0.29932  0.43405  0.72928
C   1.54552  0.43565  1.54233
C  -0.97748  0.40331  1.14076
C  -1.86991  0.40207  -0.02417
C  -1.13557  0.42721  -1.14772
H   0.94539  1.14856  -1.26232
H   2.13478  1.33645  1.35746
H   1.32079  0.38948  2.60664
H   2.17451  -0.41793  1.28230
H  -1.30757  0.38296  2.16917
H  -2.94850  0.39181  0.02955
H  -1.49792  0.43676  -2.16260
H   0.81222  -0.65858  -1.11123
O   1.24829  -1.93999  -1.23992
H   0.49786  -2.34679  -0.78592
      Core      RigidRotor
    SymmetryFactor   1.5000000000000000
End
 Rotor             Hindered
 Group   8  9  10
 Axis        3      2
 Symmetry       1
 Potential[kcal/mol]      18
 0.00  0.32  1.04  1.45  1.08  0.38  0.00  0.32  1.05  1.45  1.08
0.39  0.00  0.29  1.03  1.45  1.05  0.35
 End
 Rotor             Hindered
 Group   16
 Axis        15      14
 Symmetry       1
 Potential[kcal/mol]      18
 0.00  0.07  0.29  0.64  0.95  1.15  1.22  1.21  1.21  1.25  1.30
1.34  1.38  1.37  1.16  0.74  0.31  0.06
 End
  Frequencies[1/cm]      39
 3810.6   3256.2   3229.4   3217.1   3134.8   3117.6   3099.0
3041.3   1678.7   1576.9
 1495.4   1485.1   1424.7   1389.4   1377.0   1314.8   1270.0
1194.5   1132.0   1091.8
 1038.3   1031.3   998.11   980.20   970.72   958.41   898.26
864.80   799.69   777.76
 707.90   681.79   618.94   542.00   382.35   332.31   238.39
121.74   112.24
ZeroEnergy[kcal/mol]  -1.3901312859742794
 ElectronicLevels[1/cm]          1
 0.0000000000000000     2.0000000000000000
End
!**********************************************
RRHO      !     20
Geometry[angstrom]      16
C   0.29464  0.42807  -0.76583
C   0.29943  0.43386  0.72924
C   1.54556  0.43564  1.54232
C  -0.97742  0.40328  1.14081
C  -1.86987  0.40202  -0.02418
C  -1.13516  0.42697  -1.14792
H   0.94795  1.14393  -1.26442
H   2.13477  1.33647  1.35743
H   1.32074  0.38953  2.60659
H   2.17447  -0.41797  1.28226
H  -1.30751  0.38317  2.16917
H  -2.94845  0.39223  0.02943
H  -1.49761  0.43688  -2.16271
H   0.81761  -0.67712  -1.11219
O   1.24766  -1.93826  -1.23971
H   0.49873  -2.34780  -0.78639
      Core      RigidRotor
    SymmetryFactor   1.5000000000000000
End
 Rotor             Hindered
 Group   8  9  10
 Axis        3      2
 Symmetry       1
 Potential[kcal/mol]      18
 0.00  0.32  1.04  1.45  1.08  0.38  0.00  0.32  1.05  1.45  1.08
0.39  0.00  0.29  1.03  1.45  1.05  0.35
 End
```

```
 Rotor                      Hindered
 Group   16
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3814.1      3256.7      3229.9      3217.6      3135.1      3120.5      3099.3
3041.4      1677.6      1571.5
  1495.1      1485.0      1424.7      1391.3      1387.9      1310.2      1269.7
1193.4      1131.8      1088.7
  1037.9      1031.5      997.59      977.87      969.61      956.80      898.19
862.49      797.74      768.36
  703.57      656.89      617.04      542.44      382.98      332.95      240.04
126.40      115.95
 ZeroEnergy[kcal/mol]   -1.8113103537321840
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!*********************************************
 RRHO          !          21
 Geometry[angstrom]          16
 C    0.29402   0.42840  -0.76557
 C    0.29953   0.43369   0.72919
 C    1.54559   0.43564   1.54230
 C   -0.97736   0.40325   1.14086
 C   -1.86984   0.40196  -0.02416
 C   -1.13476   0.42675  -1.14810
 H    0.95025   1.13975  -1.26632
 H    2.13476   1.33648   1.35740
 H    1.32069   0.38957   2.60654
 H    2.17442  -0.41801   1.28222
 H   -1.30747   0.38337   2.16917
 H   -2.94841   0.39262   0.02933
 H   -1.49734   0.43701  -2.16280
 H    0.82344  -0.69592  -1.11358
 O    1.24709  -1.93670  -1.23952
 H    0.49955  -2.34872  -0.78683
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
 End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.32    1.04    1.45    1.08    0.38    0.00    0.32    1.05    1.45    1.08
0.39    0.00    0.29    1.03    1.45    1.05    0.35
 End
 Rotor                      Hindered
 Group   16
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.07    0.29    0.64    0.95    1.15    1.22    1.21    1.21    1.25    1.30
1.34    1.38    1.37    1.16    0.74    0.31    0.06
 End
   Frequencies[1/cm]          39
  3817.6      3257.2      3230.4      3218.2      3135.3      3123.5      3099.5
3041.5      1676.6      1565.9
  1494.8      1484.9      1424.8      1409.0      1387.3      1305.3      1269.4
1192.1      1131.5      1086.3
  1037.5      1031.7      996.88      975.15      968.44      955.12      897.66
860.22      795.25      757.49
  703.15      636.06      614.53      542.48      383.05      333.40      241.46
129.87      118.44
 ZeroEnergy[kcal/mol]   -2.3636652627289312
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!*********************************************
     Tunneling    Eckart
     ImaginaryFrequency[1/cm]    463.25000000000000
     WellDepth[kcal/mol]          0.01
     WellDepth[kcal/mol]          0.01
 End
End
End
```

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                   0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature             .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]            400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                    direct     ! direct or low-eigenvalue
!
WellCutoff                           20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                      diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                          10
!ChemicalEigenvalueMin               1.e-6         #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                1.3
!!
RateOutput                           rate.out                    ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                          ! Default collisional
energy relaxation kernel
    Exponential                                             ! Currently the only
possible energy relaxation model
       Factor[1/cm]               316                       ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                 0.535                      ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff             10                        ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                        ! Collision frequency
model
    LennardJones                                            ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                90.58  281.367            ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]           3.54    4.694             ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                39.948  79.05478          ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50263
 C    1.24622   0.00000   2.31947
 C   -1.27227   0.00046   1.92591
 C   -2.17585   0.00051   0.77474
 C   -1.45565   0.00011  -0.35294
 H    0.51979   0.87601  -0.40113
 H    1.85947   0.87812   2.10478
 H    1.01835  -0.00094   3.38445
 H    1.86045  -0.87709   2.10340
 H   -1.59049   0.00052   2.95892
 H   -3.25397   0.00095   0.84079
 H   -1.83452  -0.00013  -1.36297
 H    0.51979  -0.87591  -0.40126
        Core    RigidRotor
            SymmetryFactor    1.0000000000000000
        End
 Rotor                       Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          3
 Potential[kcal/mol]         12
   0.00    0.08    0.30    0.62    0.95    1.20    1.29    1.21    0.96    0.62    0.30
0.08
 End
    Frequencies[1/cm]          35
  3245.2      3221.6      3209.3      3128.8      3090.6      3074.8      3042.5
3036.2      1695.3      1615.6
  1495.0      1486.6      1424.0      1421.5      1397.2      1340.1      1274.6
1198.6      1152.9      1130.9
  1060.1      1033.7      1005.4      976.89      961.82      922.95      892.68
863.70      828.81      700.71
  623.69      533.08      369.88      325.94      227.72
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                 1
   0.0000000000000000        2.0000000000000000
 End
 !***********************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]           2
 O    0.00000   0.00000   0.00000
 H    0.00000   0.00000   0.97032
        Core    RigidRotor
            SymmetryFactor    1.0000000000000000
        End
    Frequencies[1/cm]           1
  3774.5
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                 1
   0.0000000000000000        2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
 !***********************************
 Well WR
 Species
 RRHO     ! transition state
 Geometry[angstrom]           16
 C   -0.00047   0.00198   0.00303
```

C -0.00047 0.00035 1.56103
C 1.40206 0.00214 2.14765
C -0.77888 1.24560 1.89970
C -1.21030 1.88577 0.75699
C -0.78904 1.21565 -0.37695
H 1.01471 0.03653 -0.40064
H 1.96807 0.85549 1.77551
H 1.35535 0.05681 3.23474
H 1.92210 -0.91490 1.86905
H -0.95944 1.55393 2.91898
H -1.79691 2.79364 0.74618
H -0.98965 1.51525 -1.39427
H -0.44870 -0.92251 -0.36841
O -0.63539 -1.16338 2.09695
H -1.56997 -1.11586 1.88881
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 42
51.983 263.65 284.89 321.49 367.91 394.42 438.17
521.94 620.31 630.75
712.38 798.49 814.73 900.60 949.63 959.46 970.41
1000.5 1068.9 1073.2
1101.1 1134.4 1217.9 1224.0 1294.7 1318.7 1378.3
1407.5 1417.4 1477.2
1491.0 1494.3 1505.3 3044.6 3051.9 3079.6 3130.7
3138.3 3207.0 3224.3
3237.1 3879.6
ZeroEnergy[kcal/mol] -40.27
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
End
!************************************
Barrier TS REACS WR
Variational
RRHO ! 1
Geometry[angstrom] 16
C 0.11260 0.47958 -1.20084
C 0.11239 0.47981 0.30059
C 1.34549 0.48305 1.11232
C -1.16291 0.42957 0.72550
C -2.06351 0.40128 -0.42355
C -1.34098 0.42653 -1.55133
H 0.59795 1.37523 -1.60136
H 2.07545 1.21699 0.76803
H 1.14813 0.62791 2.17256
H 1.88002 -0.50522 1.01019
H -1.47982 0.41723 1.75893
H -3.14091 0.36712 -0.35845
H -1.72043 0.41798 -2.56115
H 0.67031 -0.37406 -1.59886
O 2.16897 -2.10209 0.75188
H 1.22989 -2.32781 0.82824
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.18 0.64 1.41 2.43 3.53 4.38 1.61 1.19 0.74 0.34
0.07
End
Rotor Hindered
Group 16
Axis 15 10
Symmetry 1
Potential[kcal/mol] 18
0.00 0.10 0.42 0.80 1.04 1.09 1.01 0.88 0.74 0.64 8.71
0.62 0.62 0.61 0.54 0.43 0.28 0.11
End
Frequencies[1/cm] 39
3787.5 3247.0 3224.0 3211.1 3145.1 3080.0 3073.8
3046.2 2346.0 1672.8
1590.7 1470.6 1434.5 1421.3 1397.3 1383.7 1343.5
1275.3 1206.9 1147.9
1131.8 1037.5 1029.3 998.05 979.55 962.90 923.39
895.06 865.47 829.60
706.11 643.06 590.97 530.06 368.33 330.24 212.27
59.660 42.270
ZeroEnergy[kcal/mol] 0.67271073022298833
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 2
Geometry[angstrom] 16
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.50144
C 1.23267 0.00000 2.31256
C -1.27547 -0.05016 1.92651
C -2.17604 -0.07801 0.77769
C -1.45357 -0.05281 -0.35017
H 0.48539 0.89553 -0.40061
H 1.96721 0.72831 1.96639
H 1.03721 0.14614 3.37292
H 1.76281 -0.99345 2.21083
H -1.59222 -0.06309 2.95993
H -3.25342 -0.11192 0.84286
H -1.83318 -0.06106 -1.35991
H 0.55752 -0.85379 -0.39797
O 2.05601 -2.57809 1.95358
H 1.11868 -2.81017 2.03110
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.18 0.64 1.41 2.43 3.53 4.38 1.61 1.19 0.74 0.34
0.07
End
Rotor Hindered
Group 16
Axis 15 10
Symmetry 1
Potential[kcal/mol] 18
0.00 0.10 0.42 0.80 1.04 1.09 1.01 0.88 0.74 0.64 8.71
0.62 0.62 0.61 0.54 0.43 0.28 0.11
End
Frequencies[1/cm] 39
3789.2 3247.0 3224.1 3211.2 3146.1 3080.2 3074.5
3046.3 2307.8 1671.4
1588.7 1470.0 1433.6 1421.3 1397.2 1381.0 1343.6
1275.3 1207.2 1147.8
1131.8 1037.3 1029.1 997.87 979.62 962.97 923.31
895.18 865.95 829.59
706.40 646.60 595.30 530.21 368.54 330.68 213.08
61.140 44.030
ZeroEnergy[kcal/mol] 0.64330443957135242
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 3
Geometry[angstrom] 16
C 0.11266 0.47966 -1.20112
C 0.11286 0.47943 0.30025
C 1.34511 0.47620 1.11076
C -1.16284 0.42936 0.72549
C -2.06338 0.40194 -0.42310
C -1.34091 0.42709 -1.55112
H 0.59817 1.37513 -1.60180
H 2.08425 1.19888 0.76270

```
 H    1.15155   0.62363   2.17128
 H    1.87083  -0.52237   1.00943
 H   -1.47945   0.41583   1.75899
 H   -3.14078   0.36827  -0.35788
 H   -1.72069   0.41915  -2.56084
 H    0.67002  -0.37426  -1.59898
 O    2.16827  -2.09470   0.75325
 H    1.23277  -2.33311   0.83192
              Core           RigidRotor
       SymmetryFactor   0.50000000000000000
 End
  Rotor                      Hindered
  Group    8   9  10  15  16
  Axis            3          2
  Symmetry           3
  Potential[kcal/mol]          12
   0.00    0.18    0.64    1.41    2.43    3.53    4.38    1.61    1.19    0.74    0.34
0.07
  End
  Rotor                      Hindered
  Group   16
  Axis           15         10
  Symmetry           1
  Potential[kcal/mol]          18
   0.00    0.10    0.42    0.80    1.04    1.09    1.01    0.88    0.74    0.64    8.71
0.62    0.62    0.61    0.54    0.43    0.28    0.11
  End
    Frequencies[1/cm]          39
   3790.4      3247.1      3224.2      3211.3      3146.8      3080.4      3074.9
3046.5      2268.5      1670.0
   1586.4      1469.4      1432.7      1421.2      1397.2      1378.2      1343.8
1275.3      1207.6      1147.7
   1131.8      1037.2      1028.8      997.65      979.71      963.03      923.22
895.30      866.50      829.58
   706.75      650.78      599.28      530.33      368.76      331.14      213.89
62.590      45.830
 ZeroEnergy[kcal/mol]   0.61356934742001112
  ElectronicLevels[1/cm]                    1
   0.0000000000000000        2.0000000000000000
 End
 !*********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    203.09000000000000
      WellDepth[kcal/mol]          0.01
      WellDepth[kcal/mol]          0.01
 End
End
End
```

```
!***************************************************
!             GLOBAL SECTION
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature             .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature           30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]            400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct    ! direct or low-eigenvalue
!
WellCutoff                            20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                 0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!
!WellCutoff                           10
!ChemicalEigenvalueMin                1.e-6          #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                 1.3
!!
RateOutput                            rate.out                    ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***************************************************
!             MODEL SECTION
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                          ! Default collisional
energy relaxation kernel
    Exponential                                             ! Currently the only
possible energy relaxation model
       Factor[1/cm]                 316                     ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                        0.535                   ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff               10                      ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                        ! Collision frequency
model
    LennardJones                                            ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                  90.58  281.367          ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]             3.54   4.694            ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                  39.948  79.05478        ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***************************************************
!  REACTANTS
!***************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50112
 C    1.39710   0.00000   2.12644
 C   -0.81569  -1.21840   1.82234
 C   -1.21870  -1.80451   0.68960
 C   -0.70750  -1.04109  -0.45233
 H    0.50817   0.74374  -0.59543
 H    1.95008   0.89431   1.83920
 H    1.33447  -0.02486   3.21435
 H    1.96018  -0.87263   1.79528
 H   -1.02550  -1.54600   2.82960
 H   -1.82229  -2.69676   0.61182
 H   -0.88231  -1.29309  -1.48790
 H   -0.53850   0.88886   1.85441
       Core    RigidRotor
          SymmetryFactor    1.0000000000000000
       End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          3
 Potential[kcal/mol]         12
   0.00    0.23    0.90    1.84    2.83    3.55    3.78    3.44    2.69    1.75    0.87
0.23
 End
    Frequencies[1/cm]          35
  3244.1      3235.6      3219.3      3210.9      3128.0      3124.4      3049.0
3020.3      1670.2      1591.0
  1503.9      1503.7      1422.5      1406.8      1334.3      1293.1      1277.9
1155.2      1119.2      1104.0
  1090.8      1028.3      1004.1      983.75      981.16      957.17      883.24
817.77      792.34      742.25
  721.84      567.90      547.80      294.51      164.97
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]           2
 O    0.00000   0.00000   0.00000
 H    0.00000   0.00000   0.97032
       Core    RigidRotor
          SymmetryFactor    1.0000000000000000
       End
    Frequencies[1/cm]          1
  3774.5
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Well WR
 Species
 RRHO     ! transition state
 Geometry[angstrom]           16
 C   -0.00014  -0.01005   0.00158
```

```
C   0.00063  -0.01069  1.55874
C   1.40126   0.01214  2.16736
C  -0.78026  -1.24173  1.91371
C  -1.19513  -1.90310  0.77439
C  -0.76903  -1.24571  -0.36279
H   1.02474  -0.05099  -0.37528
H   1.93499   0.91472  1.86791
H   1.35793  -0.01169  3.25659
H   1.97762  -0.85306  1.83540
H  -0.97243  -1.55604  2.92911
H  -1.77294  -2.81676  0.77416
H  -0.94935  -1.54591  -1.38392
H  -0.53167   0.88660  1.89036
O  -0.53433   1.17335  -0.57686
H  -1.48223   1.17116  -0.43126
              Core          RigidRotor
                            SymmetryFactor    1.0000000000000000
              End
   Frequencies[1/cm]          42
  29.615     250.04     253.57     289.96     304.73     389.11     513.33
542.51     624.76     703.13
  720.87     799.73     850.98     917.73     969.93     1013.4     1049.8
1057.3     1079.8     1097.4
  1125.2     1137.1     1241.5     1294.1     1296.8     1326.9     1353.0
1407.3     1414.2     1424.2
  1495.8     1504.6     1505.2     3032.0     3042.0     3057.0     3117.0
3122.0     3205.8     3222.6
  3236.7     3872.6
 ZeroEnergy[kcal/mol]            -41.24
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier TS REACS WR
Variational
RRHO          !           1
Geometry[angstrom]          16
C   0.44372   0.08523  -1.12821
C   0.44277   0.08666   0.36956
C   1.80166   0.08931   1.05281
C  -0.48518  -1.03151   0.70905
C  -0.96635  -1.56816  -0.41972
C  -0.38559  -0.86768  -1.57041
H   1.02851   0.76969  -1.72367
H   2.37977   0.96399   0.75779
H   1.69079   0.10206   2.13636
H   2.36142  -0.80480   0.77456
H  -0.72180  -1.32399   1.72042
H  -1.66840  -2.38577  -0.48917
H  -0.60183  -1.09849  -2.60294
H  -0.08353   1.04977   0.69542
O  -0.83386   2.43488   0.67110
H  -1.28411   2.25903  -0.16884
              Core          RigidRotor
       SymmetryFactor    4.5000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.80    2.49    3.34    2.40    0.77   -0.00    0.78    2.47    3.34    2.42
0.78   -0.00    0.79    2.48    3.34    2.40    0.77
 End
 Rotor                     Hindered
 Group   16
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.04    0.01    0.06    0.33    0.67    0.97    1.16    1.25    1.26    1.25
1.25    1.26    1.23    1.07    0.80    0.46    0.14
 End
   Frequencies[1/cm]          39
  3785.0     3248.0     3240.7     3223.8     3214.5     3136.3     3124.5
3050.3     2066.1     1658.0
  1582.2     1500.3     1496.7     1419.3     1407.4     1327.8     1268.4
1247.1     1177.4     1113.3
  1094.6     1052.5     1028.8     1002.5     981.31     978.68     950.27
884.99     809.26     800.24
  746.31     713.38     618.54     561.10     538.64     294.37     190.43
91.300     61.410
 ZeroEnergy[kcal/mol]  -0.15389396255997723
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           2
Geometry[angstrom]          16
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.49796
C   1.36021   0.00000   2.17923
C  -0.92760  -1.11922   1.83621
C  -1.40944  -1.65445   0.70713
C  -0.82925  -0.95269  -0.44290
H   0.58460   0.68485  -0.59523
H   1.93847   0.87478   1.88468
H   1.25066   0.01168   3.26295
H   1.91911  -0.89402   1.89930
H  -1.16410  -1.41276   2.84729
H  -2.11175  -2.47176   0.63707
H  -1.04572  -1.18252  -1.47564
H  -0.52361   0.95949   1.82677
O  -1.28161   2.35610   1.79700
H  -1.72879   2.17487   0.95649
              Core          RigidRotor
       SymmetryFactor    4.5000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.80    2.49    3.34    2.40    0.77   -0.00    0.78    2.47    3.34    2.42
0.78   -0.00    0.79    2.48    3.34    2.40    0.77
 End
 Rotor                     Hindered
 Group   16
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.04    0.01    0.06    0.33    0.67    0.97    1.16    1.25    1.26    1.25
1.25    1.26    1.23    1.07    0.80    0.46    0.14
 End
   Frequencies[1/cm]          39
  3783.9     3247.8     3240.4     3223.6     3214.3     3136.0     3124.8
3050.5     2141.5     1658.5
  1582.5     1500.5     1497.1     1419.5     1407.5     1328.2     1270.9
1248.0     1177.3     1113.3
  1094.7     1056.1     1028.3     1002.7     981.46     978.81     951.21
884.95     809.87     800.35
  745.88     713.85     612.92     560.99     539.24     294.13     191.67
88.550     59.020
 ZeroEnergy[kcal/mol]  -4.88347355309747128E-002
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !           3
Geometry[angstrom]          16
C   0.44353   0.08570  -1.12614
C   0.44447   0.08427   0.37209
C   1.80603   0.08162   1.05140
C  -0.48281  -1.03603   0.70911
C  -0.96530  -1.56983  -0.42029
C  -0.38564  -0.86674  -1.56972
H   1.02795   0.77096  -1.72114
H   2.38444   0.95647   0.75733
```

```
 H    1.69782   0.09224   2.13528
 H    2.36412  -0.81235   0.76979
 H   -0.71918  -1.33064   1.71996
 H   -1.66790  -2.38687  -0.49095
 H   -0.60234  -1.09557  -2.60263
 H   -0.07650   1.04023   0.70388
 O   -0.84213   2.44828   0.66865
 H   -1.28628   2.26166  -0.17249
             Core           RigidRotor
       SymmetryFactor    4.5000000000000000
 End
  Rotor                         Hindered
  Group    8   9  10
  Axis            3           2
  Symmetry           1
  Potential[kcal/mol]           18
   0.00    0.80    2.49    3.34    2.40    0.77   -0.00    0.78    2.47    3.34    2.42
0.78   -0.00    0.79    2.48    3.34    2.40    0.77
  End
  Rotor                         Hindered
  Group   16
  Axis           15          14
  Symmetry           1
  Potential[kcal/mol]           18
   0.00    0.04    0.01    0.06    0.33    0.67    0.97    1.16    1.25    1.26    1.25
1.25    1.26    1.23    1.07    0.80    0.46    0.14
  End
    Frequencies[1/cm]           39
   3782.3      3247.6      3240.2      3223.4      3214.1      3135.6      3125.0
3050.6      2218.1      1659.0
   1582.7      1500.8      1497.5      1419.8      1407.6      1328.5      1273.4
1248.7      1177.4      1113.3
   1094.8      1059.6      1027.7      1002.9      981.61      978.93      952.06
884.92      810.43      800.56
   745.50      714.41      607.64      560.88      540.10      293.99      194.06
86.470      57.600
 ZeroEnergy[kcal/mol]   6.47733304915613234E-002
  ElectronicLevels[1/cm]                    1
   0.0000000000000000        2.0000000000000000
 End
 !*********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    185.21000000000001
      WellDepth[kcal/mol]           0.01
      WellDepth[kcal/mol]           0.01
 End
End
End
```

```
!****************************************************
!             GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct     ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!test!!!!!!!!!!!!!!!!!!!
!WellCutoff                           10
!ChemicalEigenvalueMin                 1.e-6          #only for direct
diagonalization method
!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                  1.3
!!
RateOutput                            rate.out                  ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!             MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                            ! Default collisional
energy relaxation kernel
    Exponential                                             ! Currently the only
possible energy relaxation model
       Factor[1/cm]               316                         ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                   0.535                       ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff             10                          ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                          ! Collision frequency
model
    LennardJones                                              ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                90.58  281.367               ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]             3.54    4.694               ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                39.948  79.05478              ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]             14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.34058
 C    1.17550   0.00000   2.25991
 C   -1.39560  -0.00008   1.80105
 C   -2.21870  -0.00003   0.74716
 C   -1.40657  -0.00007  -0.51024
 H    0.87312   0.00029  -0.63540
 H    2.11196   0.00080   1.70444
 H    1.16259   0.87759   2.90932
 H    1.16343  -0.87842   2.90820
 H   -1.69080  -0.00015   2.84114
 H   -3.29750  -0.00010   0.77029
 H   -1.62068  -0.87614  -1.13069
 H   -1.62069   0.87579  -1.13094
       Core    RigidRotor
            SymmetryFactor    1.0000000000000000
       End
 Rotor                          Hindered
 Group    8   9  10
 Axis           3           2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.08    0.32    0.66    1.03    1.33    1.44    1.32    1.03    0.66    0.32
0.08
 End
    Frequencies[1/cm]          35
  3241.0      3225.5      3207.9      3133.2      3100.2      3075.2      3043.9
3042.9      1708.1      1610.0
  1497.4      1487.3      1428.4      1422.7      1402.8      1311.9      1272.8
1227.8      1137.4      1111.0
  1073.3      1028.7      984.40      980.54      951.47      936.30      920.52
826.70      765.47      719.11
  624.46      583.63      368.96      327.69      231.38
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]              2
 O    0.00000   0.00000   0.00000
 H    0.00000   0.00000   0.97032
       Core    RigidRotor
            SymmetryFactor    1.0000000000000000
       End
    Frequencies[1/cm]           1
  3774.5
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Well WR
 Species
 RRHO     ! transition state
 Geometry[angstrom]             16
 C   -0.00295  -0.00182   0.00458
```

```
C   -0.00389  -0.00155   1.38897
C    1.22199   0.00068   2.25022
C   -1.30730  -0.02587   1.85885
C   -2.29424   0.00620   0.73141
C   -1.39782  -0.04375  -0.53318
H    0.88477   0.01277  -0.61132
H    2.10283   0.29597   1.68224
H    1.11041   0.68441   3.09125
H    1.40556  -0.99386   2.65900
H   -1.60544  -0.02817   2.89747
H   -2.98084  -0.84082   0.76138
H   -1.57462  -0.94955  -1.11889
H   -1.62861   0.79871  -1.18881
O   -3.14827   1.14543   0.78117
H   -2.60030   1.91426   0.95021
          Core          RigidRotor
                    SymmetryFactor    1.0000000000000000
          End
   Frequencies[1/cm]          42
   29.651     69.554     206.36     299.92     310.79     430.91     446.09
527.34     620.03     669.79
   694.23     762.64     851.15     938.26     951.00     997.09     1021.3
1060.3     1061.3     1075.3
   1160.0     1199.6     1256.5     1278.3     1304.7     1332.7     1349.2
1419.6     1423.7     1478.4
   1493.8     1499.4     1575.4     3044.6     3054.7     3073.6     3084.9
3119.4     3137.2     3213.6
   3219.3     3872.1
 ZeroEnergy[kcal/mol]             -39.78
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier TS REACS WR
Variational
RRHO          !          1
Geometry[angstrom]          16
C    0.86475  -0.41798  -0.55286
C    0.86774  -0.42218   0.79476
C    2.04138  -0.42460   1.71250
C   -0.53169  -0.42908   1.25851
C   -1.35309  -0.43419   0.20224
C   -0.52774  -0.40313  -1.03714
H    1.73371  -0.41346  -1.19173
H    2.97862  -0.42351   1.15941
H    2.02403   0.45414   2.36103
H    2.02528  -1.30101   2.36344
H   -0.82515  -0.43216   2.29839
H   -2.43115  -0.43794   0.21236
H   -0.79615  -1.09871  -1.83107
H   -0.77379   0.73132  -1.60814
O   -1.18717   1.93934  -1.95452
H   -1.30342   2.28058  -1.05850
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                    Hindered
 Group   16
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3821.9     3252.8     3241.3     3217.8     3140.5     3128.9     3098.0
3041.6     1648.9     1589.6
  1489.7     1484.7     1422.5     1409.7     1390.8     1306.1     1265.5
1214.8     1111.0     1089.2
  1062.0     1010.5     988.66     972.20     966.48     946.44     909.92
846.92     807.60     760.97
  711.23     620.14     601.92     589.23     364.32     332.59     261.00
147.18     107.00
 ZeroEnergy[kcal/mol]   -2.2392612339614564
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          2
Geometry[angstrom]          16
C    0.86502  -0.41825  -0.55243
C    0.86773  -0.42228   0.79471
C    2.04141  -0.42455   1.71258
C   -0.53159  -0.42911   1.25847
C   -1.35306  -0.43432   0.20235
C   -0.52811  -0.40273  -1.03777
H    1.73391  -0.41330  -1.19147
H    2.97864  -0.42352   1.15943
H    2.02426   0.45414   2.36112
H    2.02540  -1.30103   2.36342
H   -0.82510  -0.43200   2.29839
H   -2.43116  -0.43796   0.21255
H   -0.79529  -1.10316  -1.82817
H   -0.76758   0.71196  -1.60338
O   -1.18772   1.94094  -1.95503
H   -1.30316   2.27975  -1.05761
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                    Hindered
 Group   16
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3818.1     3252.3     3240.8     3217.1     3140.2     3125.4     3098.1
3041.7     1653.9     1592.4
  1490.6     1485.0     1422.7     1391.8     1390.5     1307.5     1265.7
1218.0     1110.9     1098.1
  1063.6     1012.0     991.12     973.21     966.99     945.85     912.71
847.92     808.26     762.48
  712.68     632.58     606.28     589.10     365.43     331.93     260.21
143.01     105.15
 ZeroEnergy[kcal/mol]   -1.6402087442124715
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          3
Geometry[angstrom]          16
C    0.86531  -0.41856  -0.55197
C    0.86773  -0.42239   0.79468
C    2.04145  -0.42450   1.71267
C   -0.53148  -0.42914   1.25843
C   -1.35302  -0.43445   0.20247
C   -0.52845  -0.40250  -1.03838
H    1.73413  -0.41317  -1.19117
H    2.97866  -0.42351   1.15945
```

```
 H   2.02452  0.45415  2.36124
 H   2.02555 -1.30105  2.36341
 H  -0.82503 -0.43182  2.29839
 H  -2.43117 -0.43801  0.21278
 H  -0.79434 -1.10808 -1.82495
 H  -0.76144  0.69290 -1.59924
 O  -1.18833  1.94271 -1.95559
 H  -1.30287  2.27883 -1.05668
           Core           RigidRotor
      SymmetryFactor   1.5000000000000000
 End
  Rotor                    Hindered
  Group   8  9  10
  Axis          3          2
  Symmetry          1
  Potential[kcal/mol]          18
   0.00   0.30   0.99   1.39   1.00   0.32   0.00   0.27   0.96   1.39   0.98
0.29   0.00   0.31   0.99   1.39   1.01   0.32
  End
  Rotor                    Hindered
  Group   16
  Axis          15         14
  Symmetry          1
  Potential[kcal/mol]          18
   0.00   0.01   0.05   0.12   0.37   0.68   0.93   1.08   1.16   1.18   1.18
1.18   1.17   1.11   0.96   0.73   0.44   0.15
  End
    Frequencies[1/cm]          39
   3814.4     3251.6     3240.2     3216.4     3139.9     3121.9     3098.1
3041.7     1659.1     1594.9
   1491.4     1485.3     1423.0     1392.9     1376.3     1308.9     1266.2
1220.8     1111.1     1108.7
   1064.9     1013.8     993.12     974.01     967.19     944.92     915.15
847.80     808.44     763.16
   716.90     650.90     609.68     588.65     366.40     331.18     258.77
137.39     101.85
 ZeroEnergy[kcal/mol]   -1.1894418934301560
  ElectronicLevels[1/cm]                  1
   0.0000000000000000      2.0000000000000000
 End
 !********************************************
 RRHO          !          4
 Geometry[angstrom]          16
 C   0.86562 -0.41894 -0.55147
 C   0.86774 -0.42251  0.79468
 C   2.04149 -0.42443  1.71279
 C  -0.53135 -0.42917  1.25840
 C  -1.35297 -0.43458  0.20258
 C  -0.52876 -0.40249 -1.03896
 H   1.73440 -0.41307 -1.19082
 H   2.97869 -0.42351  1.15949
 H   2.02480  0.45416  2.36137
 H   2.02571 -1.30106  2.36342
 H  -0.82495 -0.43163  2.29840
 H  -2.43117 -0.43809  0.21304
 H  -0.79325 -1.11361 -1.82134
 H  -0.75544  0.67434 -1.59595
 O  -1.18902  1.94473 -1.95622
 H  -1.30254  2.27779 -1.05567
           Core           RigidRotor
      SymmetryFactor   1.5000000000000000
 End
  Rotor                    Hindered
  Group   8  9  10
  Axis          3          2
  Symmetry          1
  Potential[kcal/mol]          18
   0.00   0.30   0.99   1.39   1.00   0.32   0.00   0.27   0.96   1.39   0.98
0.29   0.00   0.31   0.99   1.39   1.01   0.32
  End
  Rotor                    Hindered
  Group   16
  Axis          15         14
  Symmetry          1
  Potential[kcal/mol]          18
   0.00   0.01   0.05   0.12   0.37   0.68   0.93   1.08   1.16   1.18   1.18
1.18   1.17   1.11   0.96   0.73   0.44   0.15
  End
    Frequencies[1/cm]          39
   3810.7     3250.9     3239.6     3215.7     3139.5     3118.3     3098.1
3041.7     1664.2     1597.1
   1492.1     1485.6     1423.3     1394.0     1366.8     1310.2     1267.0
1223.1     1124.6     1110.5
   1066.2     1015.6     995.11     974.74     967.12     943.88     917.34
847.52     807.79     763.35
   731.35     671.87     612.32     587.96     366.77     330.43     256.74
130.64     97.350
 ZeroEnergy[kcal/mol]  -0.84833655455460555
  ElectronicLevels[1/cm]                  1
   0.0000000000000000      2.0000000000000000
 End
 !********************************************
 RRHO          !          5
 Geometry[angstrom]          16
 C   0.86595 -0.41939 -0.55094
 C   0.86777 -0.42265  0.79472
 C   2.04155 -0.42436  1.71293
 C  -0.53121 -0.42920  1.25837
 C  -1.35289 -0.43473  0.20269
 C  -0.52903 -0.40278 -1.03951
 H   1.73471 -0.41302 -1.19040
 H   2.97872 -0.42349  1.15953
 H   2.02510  0.45419  2.36153
 H   2.02591 -1.30107  2.36345
 H  -0.82486 -0.43142  2.29841
 H  -2.43115 -0.43821  0.21333
 H  -0.79201 -1.11987 -1.81727
 H  -0.74972  0.65657 -1.59379
 O  -1.18982  1.94704 -1.95693
 H  -1.30214  2.27659 -1.05459
           Core           RigidRotor
      SymmetryFactor   1.5000000000000000
 End
  Rotor                    Hindered
  Group   8  9  10
  Axis          3          2
  Symmetry          1
  Potential[kcal/mol]          18
   0.00   0.30   0.99   1.39   1.00   0.32   0.00   0.27   0.96   1.39   0.98
0.29   0.00   0.31   0.99   1.39   1.01   0.32
  End
  Rotor                    Hindered
  Group   16
  Axis          15         14
  Symmetry          1
  Potential[kcal/mol]          18
   0.00   0.01   0.05   0.12   0.37   0.68   0.93   1.08   1.16   1.18   1.18
1.18   1.17   1.11   0.96   0.73   0.44   0.15
  End
    Frequencies[1/cm]          39
   3807.1     3250.2     3239.0     3215.1     3139.2     3114.8     3098.1
3041.8     1669.1     1599.0
   1492.8     1485.9     1423.6     1395.0     1362.0     1311.8     1268.5
1224.9     1151.2     1110.4
   1067.3     1017.7     998.27     975.55     966.83     943.62     919.59
850.23     806.23     772.63
   758.43     683.92     614.39     587.10     366.14     329.73     254.20
123.21     92.030
 ZeroEnergy[kcal/mol]  -0.55851336975723509
  ElectronicLevels[1/cm]                  1
   0.0000000000000000      2.0000000000000000
 End
 !********************************************
 RRHO          !          6
 Geometry[angstrom]          16
 C   0.86630 -0.41992 -0.55037
 C   0.86781 -0.42280  0.79482
 C   2.04163 -0.42428  1.71310
```

```
C   -0.53105  -0.42922   1.25836
C   -1.35280  -0.43487   0.20280
C   -0.52923  -0.40341  -1.04001
H    1.73507  -0.41308  -1.18990
H    2.97876  -0.42346   1.15959
H    2.02543   0.45422   2.36173
H    2.02615  -1.30107   2.36350
H   -0.82477  -0.43119   2.29843
H   -2.43111  -0.43837   0.21365
H   -0.79060  -1.12687  -1.81274
H   -0.74446   0.63997  -1.59299
O   -1.19073   1.94966  -1.95772
H   -1.30166   2.27524  -1.05345
            Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis             3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                     Hindered
 Group   16
 Axis            15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3803.8      3249.6      3238.4      3214.5      3138.9      3111.5      3098.1
3041.8      1673.6      1600.8
  1493.5      1486.1      1423.9      1396.0      1362.3      1314.6      1273.2
1227.0      1200.0      1110.3
  1068.2      1020.3      1004.3      976.53      966.42      945.84      922.16
866.63      812.79      799.09
  759.42      687.13      615.98      586.14      364.41      329.12      251.30
115.67      86.360
ZeroEnergy[kcal/mol]  -0.27970420447931499
 ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
End
!********************************************
RRHO          !           7
Geometry[angstrom]          16
C    0.86668  -0.42055  -0.54978
C    0.86786  -0.42297   0.79496
C    2.04172  -0.42418   1.71330
C   -0.53088  -0.42922   1.25836
C   -1.35269  -0.43502   0.20289
C   -0.52936  -0.40442  -1.04046
H    1.73548  -0.41325  -1.18933
H    2.97881  -0.42342   1.15968
H    2.02577   0.45427   2.36196
H    2.02642  -1.30105   2.36360
H   -0.82468  -0.43094   2.29846
H   -2.43104  -0.43859   0.21398
H   -0.78904  -1.13452  -1.80781
H   -0.73985   0.62483  -1.59361
O   -1.19174   1.95258  -1.95859
H   -1.30111   2.27374  -1.05226
            Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis             3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                     Hindered
 Group   16
 Axis            15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3800.8      3249.0      3237.8      3213.9      3138.6      3108.4      3098.2
3041.8      1677.8      1602.7
  1494.2      1486.3      1424.1      1396.8      1380.9      1327.7      1296.0
1251.8      1225.5      1110.3
  1069.1      1025.5      1012.2      977.65      966.04      952.25      924.35
891.50      823.37      796.04
  757.86      686.95      617.19      585.17      361.78      328.61      248.23
108.50      80.780
ZeroEnergy[kcal/mol]  -5.40668328942128795E-003
 ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
End
!********************************************
RRHO          !           8
Geometry[angstrom]          16
C    0.86706  -0.42126  -0.54919
C    0.86794  -0.42314   0.79516
C    2.04183  -0.42407   1.71354
C   -0.53071  -0.42920   1.25838
C   -1.35254  -0.43515   0.20297
C   -0.52940  -0.40576  -1.04087
H    1.73594  -0.41358  -1.18871
H    2.97886  -0.42335   1.15978
H    2.02611   0.45434   2.36222
H    2.02672  -1.30102   2.36375
H   -0.82461  -0.43067   2.29848
H   -2.43094  -0.43885   0.21430
H   -0.78735  -1.14263  -1.80260
H   -0.73605   0.61132  -1.59554
O   -1.19284   1.95573  -1.95951
H   -1.30048   2.27215  -1.05106
            Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis             3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                     Hindered
 Group   16
 Axis            15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3798.4      3248.4      3237.3      3213.4      3138.3      3105.7      3098.2
3041.8      1682.1      1605.5
  1497.5      1486.8      1474.9      1424.3      1397.5      1346.1      1307.3
1260.7      1226.7      1110.3
  1069.8      1034.9      1016.7      978.71      965.93      959.05      925.11
903.30      826.02      791.28
  755.92      685.42      618.11      584.31      358.76      328.22      245.25
102.13      75.670
ZeroEnergy[kcal/mol]  0.25884384988414499
 ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
End
!********************************************
```

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RRHO        !        9
Geometry[angstrom]        16
C   0.86745  -0.42203  -0.54859
C   0.86804  -0.42332   0.79541
C   2.04195  -0.42396   1.71380
C  -0.53054  -0.42917   1.25840
C  -1.35238  -0.43528   0.20303
C  -0.52938  -0.40736  -1.04123
H   1.73643  -0.41404  -1.18804
H   2.97892  -0.42327   1.15991
H   2.02644   0.45443   2.36250
H   2.02705  -1.30096   2.36393
H  -0.82454  -0.43037   2.29851
H  -2.43081  -0.43915   0.21460
H  -0.78560  -1.15097  -1.79726
H  -0.73297   0.59917  -1.59842
O  -1.19400   1.95904  -1.96046
H  -1.29978   2.27051  -1.04987
          Core        RigidRotor
     SymmetryFactor   1.5000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis        3       2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.30   0.99   1.39   1.00   0.32   0.00   0.27   0.96   1.39   0.98
0.29   0.00   0.31   0.99   1.39   1.01   0.32
 End
 Rotor                  Hindered
 Group   16
 Axis        15      14
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.01   0.05   0.12   0.37   0.68   0.93   1.08   1.16   1.18   1.18
1.18   1.17   1.11   0.96   0.73   0.44   0.15
 End
   Frequencies[1/cm]        39
  3796.3    3247.9    3236.9    3213.0    3138.1    3103.2    3098.2
3041.8    1689.5    1624.7
  1583.4    1493.8    1486.5    1424.5    1398.2    1350.8    1309.3
1262.8    1227.3    1110.2
  1070.5    1043.6    1018.5    979.53    966.55    961.94    924.95
907.83    826.69    786.62
  753.66    683.18    618.78    583.54    355.71    327.90    242.43
96.580    71.090
ZeroEnergy[kcal/mol]   0.47606364885261687
 ElectronicLevels[1/cm]            1
  0.0000000000000000      2.0000000000000000
End
!*********************************************
RRHO        !        10
Geometry[angstrom]        16
C   0.86788  -0.42283  -0.54799
C   0.86814  -0.42352   0.79567
C   2.04205  -0.42382   1.71407
C  -0.53039  -0.42912   1.25843
C  -1.35220  -0.43541   0.20308
C  -0.52930  -0.40915  -1.04154
H   1.73698  -0.41461  -1.18735
H   2.97899  -0.42315   1.16003
H   2.02671   0.45452   2.36274
H   2.02738  -1.30087   2.36415
H  -0.82452  -0.43005   2.29852
H  -2.43070  -0.43950   0.21486
H  -0.78380  -1.15936  -1.79191
H  -0.73044   0.58799  -1.60185
O  -1.19519   1.96244  -1.96142
H  -1.29902   2.26899  -1.04874
          Core        RigidRotor
     SymmetryFactor   1.5000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis        3       2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.30   0.99   1.39   1.00   0.32   0.00   0.27   0.96   1.39   0.98
0.29   0.00   0.31   0.99   1.39   1.01   0.32
 End
 Rotor                  Hindered
 Group   16
 Axis        15      14
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.01   0.05   0.12   0.37   0.68   0.93   1.08   1.16   1.18   1.18
1.18   1.17   1.11   0.96   0.73   0.44   0.15
 End
   Frequencies[1/cm]        39
  3794.3    3247.3    3236.4    3212.8    3137.8    3100.7    3098.3
3041.9    1739.0    1675.1
  1599.7    1494.4    1486.7    1424.7    1398.8    1353.1    1310.1
1263.7    1227.7    1110.2
  1071.1    1049.8    1019.6    980.12    967.56    962.39    924.51
909.95    826.78    782.49
  751.20    680.47    619.28    582.84    352.72    327.65    239.73
91.640    66.840
ZeroEnergy[kcal/mol]   0.63698908875336802
 ElectronicLevels[1/cm]            1
  0.0000000000000000      2.0000000000000000
End
!*********************************************
RRHO        !        11
Geometry[angstrom]        16
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.34342
C   1.17395   0.00000   2.26185
C  -1.39847  -0.00533   1.80592
C  -2.22025  -0.01183   0.75053
C  -1.39741   0.01255  -0.49443
H   0.86922   0.00831  -0.63921
H   2.11080   0.00066   1.70769
H   1.15875   0.87835   2.91054
H   1.15948  -0.87709   2.91186
H  -1.69275  -0.00596   2.84600
H  -3.29874  -0.01614   0.76251
H  -1.65023  -0.74399  -1.23914
H  -1.59684   1.00147  -1.05847
O  -2.06467   2.38962  -1.41494
H  -2.16652   2.69108  -0.50022
          Core        RigidRotor
     SymmetryFactor   1.5000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis        3       2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.30   0.99   1.39   1.00   0.32   0.00   0.27   0.96   1.39   0.98
0.29   0.00   0.31   0.99   1.39   1.01   0.32
 End
 Rotor                  Hindered
 Group   16
 Axis        15      14
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.01   0.05   0.12   0.37   0.68   0.93   1.08   1.16   1.18   1.18
1.18   1.17   1.11   0.96   0.73   0.44   0.15
 End
   Frequencies[1/cm]        39
  3793.0    3246.9    3236.0    3212.5    3137.6    3099.0    3098.3
3041.9    1830.6    1682.7
  1602.0    1494.8    1486.8    1424.8    1399.3    1355.3    1310.5
1264.2    1228.1    1110.2
  1071.7    1054.7    1020.4    980.53    968.55    962.33    924.01
911.15    826.85    779.20
  748.52    677.32    619.64    582.28    350.02    327.43    237.32
87.370    63.050
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ZeroEnergy[kcal/mol]   0.76729382735072793
 ElectronicLevels[1/cm]              1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          12
Geometry[angstrom]          16
C   0.86865  -0.42456  -0.54688
C   0.86839  -0.42387   0.79626
C   2.04234  -0.42357   1.71469
C  -0.53007  -0.42892   1.25852
C  -1.35180  -0.43564   0.20312
C  -0.52903  -0.41313  -1.04217
H   1.73801  -0.41616  -1.18598
H   2.97915  -0.42291   1.16040
H   2.02729   0.45474   2.36337
H   2.02808  -1.30071   2.36465
H  -0.82449  -0.42926   2.29857
H  -2.43036  -0.44016   0.21529
H  -0.78018  -1.17606  -1.78126
H  -0.72676   0.56756  -1.60994
O  -1.19765   1.96940  -1.96330
H  -1.29752   2.26577  -1.04651
            Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                    Hindered
 Group   16
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3791.3      3246.6      3235.7      3212.2      3137.4      3098.4      3096.6
3041.9      1934.3      1685.9
  1603.2      1495.0      1486.9      1424.9      1399.8      1358.0      1310.7
1264.6      1228.3      1110.2
  1072.4      1059.1      1021.2      980.93      969.57      962.11      923.55
912.11      827.02      776.41
  745.67      673.71      619.98      581.72      347.45      327.26      234.84
83.340      59.310
ZeroEnergy[kcal/mol]   0.89514115320967935
 ElectronicLevels[1/cm]              1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          13
Geometry[angstrom]          16
C   0.86899  -0.42549  -0.54638
C   0.86854  -0.42401   0.79658
C   2.04252  -0.42347   1.71504
C  -0.52989  -0.42875   1.25857
C  -1.35159  -0.43573   0.20311
C  -0.52885  -0.41530  -1.04249
H   1.73849  -0.41717  -1.18531
H   2.97926  -0.42281   1.16064
H   2.02760   0.45485   2.36375
H   2.02844  -1.30065   2.36494
H  -0.82447  -0.42877   2.29861
H  -2.43013  -0.44048   0.21547
H  -0.77836  -1.18437  -1.77595
H  -0.72565   0.55830  -1.61449
O  -1.19892   1.97294  -1.96420
H  -1.29669   2.26414  -1.04541
            Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                    Hindered
 Group   16
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3790.2      3246.5      3235.5      3211.9      3137.4      3098.2      3095.1
3041.8      2018.7      1687.8
  1603.7      1495.2      1487.0      1425.0      1400.2      1360.7      1310.9
1264.9      1228.5      1110.2
  1073.2      1062.5      1021.7      981.21      970.50      961.77      923.19
912.77      827.11      774.40
  742.89      669.87      620.18      581.33      345.49      327.14      232.88
80.230      56.340
ZeroEnergy[kcal/mol]   0.99532626593750795
 ElectronicLevels[1/cm]              1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          14
Geometry[angstrom]          16
C   0.86937  -0.42644  -0.54587
C   0.86869  -0.42417   0.79690
C   2.04268  -0.42333   1.71539
C  -0.52973  -0.42856   1.25862
C  -1.35135  -0.43584   0.20309
C  -0.52864  -0.41753  -1.04280
H   1.73904  -0.41828  -1.18463
H   2.97937  -0.42267   1.16089
H   2.02785   0.45498   2.36409
H   2.02880  -1.30054   2.36526
H  -0.82449  -0.42821   2.29862
H  -2.42992  -0.44083   0.21561
H  -0.77651  -1.19264  -1.77066
H  -0.72485   0.54941  -1.61909
O  -1.20020   1.97649  -1.96509
H  -1.29581   2.26268  -1.04437
            Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group   8  9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                    Hindered
 Group   16
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3789.0      3246.2      3235.2      3211.6      3137.3      3098.2      3093.3
3041.9      2087.3      1689.4
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 1604.2     1495.4     1487.0     1425.1     1400.6     1362.7     1311.0
1265.1     1228.7     1110.2
 1074.2     1065.0     1022.2     981.43     971.10     961.36     922.92
913.26     827.02     772.75
 740.31     665.74     620.28     580.96     343.69     327.03     231.06
77.530     53.670
ZeroEnergy[kcal/mol]   1.0575148125190603
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
End
!********************************************
RRHO          !          15
Geometry[angstrom]          16
C   0.86975  -0.42741  -0.54538
C   0.86884  -0.42433   0.79723
C   2.04284  -0.42319   1.71575
C  -0.52957  -0.42834   1.25866
C  -1.35111  -0.43595   0.20306
C  -0.52841  -0.41983  -1.04311
H   1.73958  -0.41948  -1.18395
H   2.97949  -0.42252   1.16115
H   2.02808   0.45512   2.36443
H   2.02915  -1.30042   2.36561
H  -0.82452  -0.42759   2.29863
H  -2.42970  -0.44117   0.21572
H  -0.77467  -1.20081  -1.76544
H  -0.72422   0.54074  -1.62373
O  -1.20148   1.98007  -1.96595
H  -1.29488   2.26130  -1.04337
           Core          RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                      Hindered
 Group   16
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
 3787.9     3245.9     3234.9     3211.4     3137.2     3098.2     3091.7
3041.9     2142.5     1690.7
 1604.6     1495.6     1487.1     1425.2     1400.9     1364.0     1311.0
1265.3     1228.8     1110.2
 1075.3     1066.7     1022.6     981.57     971.42     960.91     922.72
913.63     826.81     771.31
 737.88     661.25     620.27     580.57     341.86     326.90     229.24
74.920     51.040
ZeroEnergy[kcal/mol]   1.1029480530052362
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
End
!********************************************
RRHO          !          16
Geometry[angstrom]          16
C   0.87013  -0.42840  -0.54490
C   0.86899  -0.42448   0.79755
C   2.04300  -0.42305   1.71611
C  -0.52943  -0.42810   1.25869
C  -1.35086  -0.43608   0.20301
C  -0.52817  -0.42218  -1.04340
H   1.74013  -0.42074  -1.18328
H   2.97960  -0.42236   1.16144
H   2.02829   0.45527   2.36477
H   2.02949  -1.30028   2.36596
H  -0.82456  -0.42693   2.29862
H  -2.42947  -0.44152   0.21579
H  -0.77283  -1.20888  -1.76027
H  -0.72366   0.53216  -1.62841
O  -1.20278   1.98366  -1.96679
H  -1.29391   2.25996  -1.04239
           Core          RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                      Hindered
 Group   16
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
 3786.9     3245.7     3234.6     3211.2     3137.1     3098.2     3090.1
3041.9     2193.6     1692.0
 1604.9     1495.7     1487.2     1425.3     1401.2     1365.2     1311.0
1265.5     1229.0     1110.2
 1076.5     1067.9     1022.9     981.70     971.71     960.49     922.54
913.94     826.63     770.09
 735.64     656.40     620.18     580.17     340.05     326.75     227.40
72.450     48.330
ZeroEnergy[kcal/mol]   1.1284974012662170
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
End
!********************************************
RRHO          !          17
Geometry[angstrom]          16
C   0.87050  -0.42940  -0.54444
C   0.86915  -0.42463   0.79787
C   2.04315  -0.42289   1.71648
C  -0.52928  -0.42784   1.25872
C  -1.35062  -0.43620   0.20294
C  -0.52791  -0.42457  -1.04368
H   1.74068  -0.42204  -1.18263
H   2.97972  -0.42219   1.16173
H   2.02848   0.45543   2.36511
H   2.02982  -1.30014   2.36632
H  -0.82461  -0.42622   2.29861
H  -2.42924  -0.44186   0.21584
H  -0.77100  -1.21686  -1.75513
H  -0.72317   0.52368  -1.63312
O  -1.20407   1.98725  -1.96761
H  -1.29291   2.25862  -1.04143
           Core          RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                      Hindered
 Group   16
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
```

```
 0.00 0.01 0.05 0.12 0.37 0.68 0.93 1.08 1.16 1.18 1.18
1.18 1.17 1.11 0.96 0.73 0.44 0.15
 End
  Frequencies[1/cm] 39
 3785.8 3245.4 3234.4 3211.1 3137.0 3098.2 3088.5
3041.9 2247.8 1693.1
 1605.2 1495.8 1487.2 1425.3 1401.6 1367.1 1311.0
1265.6 1229.1 1110.2
 1078.1 1069.0 1023.3 981.86 972.16 960.12 922.41
914.25 826.58 769.16
 733.63 651.37 620.00 579.79 338.51 326.65 225.68
70.500 45.690
 ZeroEnergy[kcal/mol] 1.1616663668909704
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 18
Geometry[angstrom] 16
C 0.87088 -0.43042 -0.54399
C 0.86930 -0.42477 0.79818
C 2.04329 -0.42273 1.71685
C -0.52914 -0.42756 1.25874
C -1.35037 -0.43633 0.20287
C -0.52763 -0.42702 -1.04396
H 1.74123 -0.42340 -1.18198
H 2.97984 -0.42201 1.16203
H 2.02866 0.45561 2.36546
H 2.03013 -1.29998 2.36669
H -0.82467 -0.42547 2.29859
H -2.42901 -0.44220 0.21587
H -0.76916 -1.22478 -1.75000
H -0.72283 0.51538 -1.63788
O -1.20537 1.99084 -1.96841
H -1.29188 2.25729 -1.04048
     Core RigidRotor
   SymmetryFactor 1.5000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.30 0.99 1.39 1.00 0.32 0.00 0.27 0.96 1.39 0.98
0.29 0.00 0.31 0.99 1.39 1.01 0.32
 End
 Rotor Hindered
 Group 16
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.01 0.05 0.12 0.37 0.68 0.93 1.08 1.16 1.18 1.18
1.18 1.17 1.11 0.96 0.73 0.44 0.15
 End
  Frequencies[1/cm] 39
 3784.8 3245.2 3234.1 3210.9 3136.9 3098.3 3086.9
3041.9 2305.2 1694.1
 1605.4 1496.0 1487.3 1425.4 1402.0 1369.8 1311.0
1265.8 1229.2 1110.2
 1080.2 1069.8 1023.6 982.04 972.80 959.79 922.37
914.59 826.67 768.51
 731.92 646.40 619.67 579.43 337.52 326.64 224.30
69.850 43.490
 ZeroEnergy[kcal/mol] 1.2051997276166739
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 19
Geometry[angstrom] 16
C 0.87126 -0.43146 -0.54355
C 0.86946 -0.42490 0.79850
C 2.04344 -0.42256 1.71723
C -0.52900 -0.42725 1.25876
C -1.35011 -0.43646 0.20277
C -0.52734 -0.42951 -1.04424
H 1.74179 -0.42485 -1.18133
H 2.97996 -0.42183 1.16236
H 2.02882 0.45579 2.36580
H 2.03044 -1.29982 2.36708
H -0.82475 -0.42467 2.29856
H -2.42877 -0.44255 0.21586
H -0.76732 -1.23266 -1.74489
H -0.72267 0.50733 -1.64266
O -1.20667 1.99445 -1.96917
H -1.29080 2.25600 -1.03954
     Core RigidRotor
   SymmetryFactor 1.5000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.30 0.99 1.39 1.00 0.32 0.00 0.27 0.96 1.39 0.98
0.29 0.00 0.31 0.99 1.39 1.01 0.32
 End
 Rotor Hindered
 Group 16
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.01 0.05 0.12 0.37 0.68 0.93 1.08 1.16 1.18 1.18
1.18 1.17 1.11 0.96 0.73 0.44 0.15
 End
  Frequencies[1/cm] 39
 3783.8 3245.0 3233.9 3210.7 3136.8 3098.3 3085.3
3041.9 2359.3 1694.9
 1605.6 1496.1 1487.3 1425.5 1402.4 1372.8 1311.0
1266.0 1229.3 1110.2
 1082.5 1070.4 1024.0 982.21 973.46 959.48 922.42
914.91 826.79 768.07
 730.47 641.67 619.07 579.11 337.08 326.73 223.38
71.550 42.080
 ZeroEnergy[kcal/mol] 1.2444593941710176
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 20
Geometry[angstrom] 16
C 0.87164 -0.43253 -0.54313
C 0.86962 -0.42503 0.79882
C 2.04358 -0.42239 1.71762
C -0.52887 -0.42691 1.25877
C -1.34985 -0.43661 0.20267
C -0.52704 -0.43205 -1.04453
H 1.74236 -0.42639 -1.18069
H 2.98008 -0.42163 1.16270
H 2.02897 0.45599 2.36615
H 2.03075 -1.29963 2.36748
H -0.82483 -0.42378 2.29852
H -2.42852 -0.44289 0.21583
H -0.76548 -1.24049 -1.73982
H -0.72271 0.49950 -1.64741
O -1.20798 1.99806 -1.96992
H -1.28969 2.25476 -1.03863
     Core RigidRotor
   SymmetryFactor 1.5000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.30 0.99 1.39 1.00 0.32 0.00 0.27 0.96 1.39 0.98
0.29 0.00 0.31 0.99 1.39 1.01 0.32
 End
```

```
 Rotor                      Hindered
 Group   16
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3782.8      3244.8      3233.7      3210.6      3136.7      3098.3      3083.7
3041.9      2404.3      1695.7
  1605.8      1496.2      1487.4      1425.5      1402.8      1375.2      1311.0
1266.2      1229.3      1110.2
  1084.7      1070.8      1024.3      982.35      973.96      959.16      922.55
915.20      826.83      767.73
  729.23      637.27      617.99      578.76      336.86      326.82      222.77
75.630      41.300
 ZeroEnergy[kcal/mol]    1.2732260041681380
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
 RRHO          !          21
 Geometry[angstrom]          16
 C    0.87203  -0.43364  -0.54272
 C    0.86979  -0.42515   0.79913
 C    2.04372  -0.42219   1.71802
 C   -0.52874  -0.42653   1.25877
 C   -1.34957  -0.43677   0.20254
 C   -0.52673  -0.43463  -1.04483
 H    1.74294  -0.42804  -1.18005
 H    2.98021  -0.42142   1.16307
 H    2.02910   0.45621   2.36650
 H    2.03104  -1.29942   2.36791
 H   -0.82492  -0.42280   2.29846
 H   -2.42826  -0.44325   0.21577
 H   -0.76364  -1.24823  -1.73480
 H   -0.72287   0.49184  -1.65211
 O   -1.20930   2.00168  -1.97062
 H   -1.28853   2.25361  -1.03775
                 Core            RigidRotor
         SymmetryFactor    1.5000000000000000
 End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.30    0.99    1.39    1.00    0.32    0.00    0.27    0.96    1.39    0.98
0.29    0.00    0.31    0.99    1.39    1.01    0.32
 End
 Rotor                      Hindered
 Group   16
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.01    0.05    0.12    0.37    0.68    0.93    1.08    1.16    1.18    1.18
1.18    1.17    1.11    0.96    0.73    0.44    0.15
 End
   Frequencies[1/cm]          39
  3781.8      3244.6      3233.4      3210.4      3136.6      3098.3      3082.2
3041.9      2438.9      1696.4
  1605.9      1496.3      1487.4      1425.5      1403.1      1376.6      1311.0
1266.3      1229.4      1110.2
  1086.4      1071.1      1024.5      982.43      974.26      958.81      922.73
915.41      826.75      767.40
  728.14      633.38      616.13      578.32      336.38      326.82      222.07
77.950      40.280
 ZeroEnergy[kcal/mol]    1.2729866036003168
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
     Tunneling    Eckart
       ImaginaryFrequency[1/cm]    426.67000000000002
       WellDepth[kcal/mol]          0.01
       WellDepth[kcal/mol]          0.01
 End
End
End
```

```
!****************************************************
!              GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                      direct     ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                        diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                            10
!ChemicalEigenvalueMin                 1.e-6          #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                  1.3
!!
RateOutput                             rate.out                ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!              MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                        ! Default collisional
energy relaxation kernel
    Exponential                                           ! Currently the only
possible energy relaxation model
       Factor[1/cm]                 316                   ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                        0.535                 ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff               10                    ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                      ! Collision frequency
model
    LennardJones                                          ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                  90.58  281.367        ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]             3.54    4.694         ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                  39.948  79.05478      ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.34058
 C    1.17550   0.00000   2.25991
 C   -1.39560  -0.00008   1.80105
 C   -2.21870  -0.00003   0.74716
 C   -1.40657  -0.00007  -0.51024
 H    0.87312   0.00029  -0.63540
 H    2.11196   0.00080   1.70444
 H    1.16259   0.87759   2.90932
 H    1.16343  -0.87842   2.90820
 H   -1.69080  -0.00015   2.84114
 H   -3.29750  -0.00010   0.77029
 H   -1.62068  -0.87614  -1.13069
 H   -1.62069   0.87579  -1.13094
       Core    RigidRotor
            SymmetryFactor    1.0000000000000000
       End
 Rotor                        Hindered
 Group    8   9  10
 Axis           3           2
 Symmetry           3
 Potential[kcal/mol]         12
   0.00    0.08    0.32    0.66    1.03    1.33    1.44    1.32    1.03    0.66    0.32
0.08
 End
    Frequencies[1/cm]          35
  3241.0      3225.5      3207.9      3133.2      3100.2      3075.2      3043.9
3042.9      1708.1      1610.0
  1497.4      1487.3      1428.4      1422.7      1402.8      1311.9      1272.8
1227.8      1137.4      1111.0
  1073.3      1028.7      984.40      980.54      951.47      936.30      920.52
826.70      765.47      719.11
  624.46      583.63      368.96      327.69      231.38
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]           2
 O    0.00000   0.00000   0.00000
 H    0.00000   0.00000   0.97032
       Core    RigidRotor
            SymmetryFactor    1.0000000000000000
       End
    Frequencies[1/cm]           1
  3774.5
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Well WR
 Species
 RRHO     ! transition state
 Geometry[angstrom]           16
 C   -0.00233  -0.00377   0.00359
```

```
C   -0.00323  0.00161   1.51179
C   1.25093   0.00998   2.30613
C   -1.30754  0.01850   1.97289
C   -2.21939  -0.03129  0.93711
C   -1.50038  -0.10304  -0.37564
H   0.56734   -0.84586  -0.39394
H   1.80953   -0.92073  2.16516
H   1.91256   0.81829   1.98617
H   1.05159   0.12608   3.37059
H   -1.57560  0.05974   3.02044
H   -3.29316  -0.03442  1.04309
H   -1.72150  -1.03397  -0.90379
H   -1.76941  0.70828   -1.05604
O   0.65132   1.13893   -0.54191
H   0.25639   1.91909   -0.14722
            Core            RigidRotor
                            SymmetryFactor    1.0000000000000000
            End
    Frequencies[1/cm]           42
  62.200    123.36    206.67    280.11    321.60    384.45    429.88
572.24    613.67    633.81
  769.92    826.75    899.97    945.25    961.48    975.48    1021.7
1037.7    1069.6    1084.1
  1159.3    1222.9    1269.2    1294.2    1304.8    1323.2    1414.5
1424.1    1441.6    1474.6
  1477.2    1481.2    1524.5    3022.7    3044.7    3067.1    3076.8
3082.3    3127.2    3199.1
  3234.6    3868.7
 ZeroEnergy[kcal/mol]          -40.88
 ElectronicLevels[1/cm]                 1
  0.0000000000000000      2.0000000000000000
End
End
!************************************
Barrier TS REACS WR
Variational
RRHO          !           1
Geometry[angstrom]          16
C   0.32284   -0.44436  -1.35146
C   0.32371   -0.44386  -0.00065
C   1.48198   -0.43229  0.89388
C   -1.07404  -0.41141  0.45642
C   -1.89328  -0.39535  -0.59915
C   -1.08294  -0.42157  -1.85803
H   1.19658   -0.46210  -1.98516
H   2.43855   -0.54944  0.39230
H   1.53814   0.73356   1.45585
H   1.38823   -1.08556  1.75914
H   -1.36562  -0.39831  1.49659
H   -2.97173  -0.37138  -0.57747
H   -1.31261  -1.29678  -2.47386
H   -1.27490  0.45275   -2.48841
O   1.41627   1.95776   1.91753
H   0.76782   2.25459   1.26729
            Core            RigidRotor
       SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15  16
 Axis            3          2
 Symmetry            3
 Potential[kcal/mol]          12
  0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
 End
 Rotor                      Hindered
 Group   16
 Axis            15          9
 Symmetry            1
 Potential[kcal/mol]          18
  0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
 End
    Frequencies[1/cm]           39
  3829.0    3245.6    3232.1    3218.6    3182.1    3100.1    3074.2
3043.1    1658.8    1582.5
  1475.0    1458.1    1425.3    1408.4    1318.8    1279.0    1236.4
1207.4    1139.9    1113.0
  1100.5    1033.8    986.42    981.58    952.52    939.93    925.71
823.08    812.93    757.51
  729.66    630.23    620.49    544.27    515.45    363.79    328.04
248.66    111.30
 ZeroEnergy[kcal/mol]   -1.6777517001788596
 ElectronicLevels[1/cm]                 1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO          !           2
Geometry[angstrom]          16
C   0.32279   -0.44446  -1.35129
C   0.32342   -0.44401  -0.00126
C   1.48250   -0.43200  0.89448
C   -1.07401  -0.41135  0.45636
C   -1.89337  -0.39533  -0.59920
C   -1.08298  -0.42153  -1.85802
H   1.19650   -0.46232  -1.98510
H   2.43806   -0.55217  0.39141
H   1.54066   0.71272   1.44833
H   1.38851   -1.08975  1.75657
H   -1.36562  -0.39842  1.49656
H   -2.97183  -0.37143  -0.57748
H   -1.31276  -1.29679  -2.47375
H   -1.27512  0.45278   -2.48834
O   1.41612   1.95950   1.91823
H   0.76741   2.25336   1.26634
            Core            RigidRotor
       SymmetryFactor   0.50000000000000000
End
 Rotor                      Hindered
 Group    8   9  10  15  16
 Axis            3          2
 Symmetry            3
 Potential[kcal/mol]          12
  0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
 End
 Rotor                      Hindered
 Group   16
 Axis            15          9
 Symmetry            1
 Potential[kcal/mol]          18
  0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
 End
    Frequencies[1/cm]           39
  3825.1    3245.4    3231.6    3218.1    3179.2    3098.0    3074.4
3043.2    1662.3    1588.2
  1472.3    1443.3    1424.9    1407.8    1318.8    1279.7    1240.3
1222.5    1139.7    1113.2
  1106.3    1034.1    986.16    982.04    952.55    940.07    925.75
824.38    814.64    760.27
  729.09    629.99    627.81    541.25    513.41    364.09    326.98
246.53    108.36
 ZeroEnergy[kcal/mol]   -1.0850050724457247
 ElectronicLevels[1/cm]                 1
  0.0000000000000000      2.0000000000000000
End
!**********************************************
RRHO          !           3
Geometry[angstrom]          16
C   0.32274   -0.44458  -1.35113
C   0.32312   -0.44417  -0.00189
C   1.48307   -0.43194  0.89502
C   -1.07397  -0.41130  0.45628
C   -1.89347  -0.39530  -0.59925
C   -1.08303  -0.42148  -1.85801
H   1.19641   -0.46259  -1.98505
H   2.43754   -0.55525  0.39035
```

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H   1.54349  0.69228  1.44129
H   1.38879  -1.09440  1.75373
H  -1.36562  -0.39855  1.49653
H  -2.97193  -0.37149  -0.57748
H  -1.31294  -1.29680  -2.47363
H  -1.27538  0.45281  -2.48827
O   1.41595  1.96145  1.91900
H   0.76698  2.25203  1.26534
          Core          RigidRotor
      SymmetryFactor  0.50000000000000000
End
 Rotor                   Hindered
 Group   8  9  10  15  16
 Axis        3       2
 Symmetry        3
 Potential[kcal/mol]        12
  0.00   0.15   0.52   1.10   1.85   2.69   3.48   1.57   1.17   0.73   0.33
0.07
 End
 Rotor                   Hindered
 Group   16
 Axis        15       9
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.09   0.30   0.57   0.77   0.88   0.90   0.88   0.84   0.83   0.83
0.82   0.79   0.73   0.61   0.43   0.22   0.05
 End
   Frequencies[1/cm]        39
  3821.1     3245.2     3231.2     3217.5     3176.4     3095.9     3074.5
3043.3     1666.5     1593.3
  1471.7     1432.9     1423.4     1406.5     1318.7     1281.4     1247.9
1233.2     1139.6     1114.2
  1110.8     1034.1     985.90     982.44     952.57     940.09     925.75
825.75     815.12     764.26
  729.35     645.26     627.95     549.92     496.24     364.36     325.85
243.99     104.04
 ZeroEnergy[kcal/mol]  -0.65229371271493619
  ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        4
Geometry[angstrom]        16
C   0.32266  -0.44470  -1.35100
C   0.32283  -0.44434  -0.00254
C   1.48370  -0.43220  0.89550
C  -1.07393  -0.41123  0.45620
C  -1.89359  -0.39526  -0.59931
C  -1.08309  -0.42143  -1.85801
H   1.19631  -0.46292  -1.98501
H   2.43697  -0.55878  0.38907
H   1.54668  0.67251  1.43492
H   1.38910  -1.09964  1.75055
H  -1.36561  -0.39869  1.49649
H  -2.97205  -0.37154  -0.57748
H  -1.31315  -1.29681  -2.47350
H  -1.27567  0.45284  -2.48820
O   1.41574  1.96368  1.91987
H   0.76652  2.25058  1.26428
          Core          RigidRotor
      SymmetryFactor  0.50000000000000000
End
 Rotor                   Hindered
 Group   8  9  10  15  16
 Axis        3       2
 Symmetry        3
 Potential[kcal/mol]        12
  0.00   0.15   0.52   1.10   1.85   2.69   3.48   1.57   1.17   0.73   0.33
0.07
 End
 Rotor                   Hindered
 Group   16
 Axis        15       9
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.09   0.30   0.57   0.77   0.88   0.90   0.88   0.84   0.83   0.83
0.82   0.79   0.73   0.61   0.43   0.22   0.05
 End
   Frequencies[1/cm]        39
  3817.1     3244.9     3230.7     3217.0     3173.5     3093.9     3074.6
3043.4     1671.2     1597.6
  1471.5     1429.3     1420.2     1404.2     1318.6     1285.3     1258.6
1238.0     1139.4     1119.6
  1112.3     1034.0     985.63     982.81     952.58     940.05     925.79
828.58     816.01     772.72
  731.87     672.50     627.23     558.83     473.10     364.55     324.61
241.13     98.660
 ZeroEnergy[kcal/mol]  -0.31978082531057339
  ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        5
Geometry[angstrom]        16
C   0.32257  -0.44485  -1.35089
C   0.32255  -0.44454  -0.00321
C   1.48441  -0.43287  0.89586
C  -1.07389  -0.41116  0.45609
C  -1.89372  -0.39521  -0.59937
C  -1.08318  -0.42137  -1.85802
H   1.19618  -0.46332  -1.98499
H   2.43635  -0.56282  0.38753
H   1.55029  0.65382  1.42953
H   1.38942  -1.10559  1.74698
H  -1.36559  -0.39884  1.49643
H  -2.97219  -0.37157  -0.57748
H  -1.31339  -1.29681  -2.47336
H  -1.27601  0.45288  -2.48814
O   1.41549  1.96624  1.92087
H   0.76603  2.24898  1.26316
          Core          RigidRotor
      SymmetryFactor  0.50000000000000000
End
 Rotor                   Hindered
 Group   8  9  10  15  16
 Axis        3       2
 Symmetry        3
 Potential[kcal/mol]        12
  0.00   0.15   0.52   1.10   1.85   2.69   3.48   1.57   1.17   0.73   0.33
0.07
 End
 Rotor                   Hindered
 Group   16
 Axis        15       9
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.09   0.30   0.57   0.77   0.88   0.90   0.88   0.84   0.83   0.83
0.82   0.79   0.73   0.61   0.43   0.22   0.05
 End
   Frequencies[1/cm]        39
  3813.1     3244.7     3230.3     3216.4     3170.7     3091.9     3074.7
3043.5     1676.5     1601.2
  1471.9     1428.7     1418.1     1401.7     1318.8     1292.9     1266.8
1241.8     1139.3     1133.9
  1112.4     1033.7     985.37     983.33     952.57     940.14     926.18
848.50     820.65     787.52
  737.98     697.33     626.60     564.04     447.58     364.64     323.17
238.11     92.630
 ZeroEnergy[kcal/mol]  -4.44956597635695061E-002
  ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        6
Geometry[angstrom]        16
C   0.32246  -0.44501  -1.35083
C   0.32230  -0.44475  -0.00386
C   1.48520  -0.43405  0.89609
```

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C  -1.07384  -0.41107   0.45598
C  -1.89387  -0.39515  -0.59943
C  -1.08329  -0.42129  -1.85804
H   1.19603  -0.46380  -1.98501
H   2.43571  -0.56736   0.38571
H   1.55429   0.63665   1.42536
H   1.38976  -1.11223   1.74303
H  -1.36554  -0.39901   1.49636
H  -2.97234  -0.37160  -0.57747
H  -1.31367  -1.29681  -2.47322
H  -1.27639   0.45293  -2.48810
O   1.41519   1.96916   1.92199
H   0.76552   2.24724   1.26199
         Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                       Hindered
 Group    8   9  10  15  16
 Axis             3           2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
 End
 Rotor                       Hindered
 Group   16
 Axis            15           9
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
 End
   Frequencies[1/cm]          39
  3809.4     3244.5     3230.0     3215.9     3168.0     3090.2     3074.7
3043.5     1682.4     1604.3
  1473.1     1428.8     1417.3     1399.9     1320.2     1303.7     1272.8
1249.0     1168.3     1139.1
  1112.4     1033.3     985.46     984.63     952.64     942.84     930.66
908.84     823.22     791.35
  742.63     706.06     625.97     566.18     421.97     364.51     321.38
235.09     86.530
ZeroEnergy[kcal/mol]   0.22605130619398039
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO           !            7
Geometry[angstrom]          16
C   0.32232  -0.44518  -1.35082
C   0.32209  -0.44498  -0.00449
C   1.48606  -0.43573   0.89616
C  -1.07379  -0.41098   0.45585
C  -1.89402  -0.39506  -0.59949
C  -1.08343  -0.42119  -1.85807
H   1.19585  -0.46437  -1.98507
H   2.43507  -0.57227   0.38365
H   1.55857   0.62135   1.42253
H   1.39010  -1.11941   1.73882
H  -1.36548  -0.39918   1.49628
H  -2.97249  -0.37158  -0.57744
H  -1.31399  -1.29679  -2.47309
H  -1.27679   0.45298  -2.48808
O   1.41484   1.97240   1.92321
H   0.76499   2.24542   1.26083
         Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                       Hindered
 Group    8   9  10  15  16
 Axis             3           2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
 End
 Rotor                       Hindered
 Group   16
 Axis            15           9
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
 End
   Frequencies[1/cm]          39
  3806.1     3244.3     3229.7     3215.4     3165.7     3088.7     3074.7
3043.5     1689.5     1607.2
  1476.8     1429.3     1417.2     1399.2     1338.4     1314.5     1293.4
1263.8     1212.5     1139.0
  1112.3     1033.2     996.71     984.81     972.63     952.36     937.64
922.35     824.19     788.80
  743.90     707.63     625.35     566.71     398.63     364.05     319.01
232.28     80.860
ZeroEnergy[kcal/mol]   0.49718947384273804
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO           !            8
Geometry[angstrom]          16
C   0.32217  -0.44537  -1.35087
C   0.32192  -0.44522  -0.00509
C   1.48696  -0.43787   0.89610
C  -1.07373  -0.41087   0.45571
C  -1.89417  -0.39495  -0.59955
C  -1.08360  -0.42108  -1.85811
H   1.19565  -0.46503  -1.98519
H   2.43446  -0.57740   0.38140
H   1.56294   0.60802   1.42097
H   1.39045  -1.12695   1.73445
H  -1.36539  -0.39935   1.49619
H  -2.97265  -0.37153  -0.57740
H  -1.31433  -1.29676  -2.47296
H  -1.27721   0.45305  -2.48809
O   1.41444   1.97587   1.92450
H   0.76445   2.24357   1.25970
         Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                       Hindered
 Group    8   9  10  15  16
 Axis             3           2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
 End
 Rotor                       Hindered
 Group   16
 Axis            15           9
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
 End
   Frequencies[1/cm]          39
  3803.3     3244.1     3229.5     3215.0     3163.6     3087.3     3074.7
3043.5     1700.7     1611.5
  1497.2     1433.9     1420.5     1415.8     1398.3     1320.7     1309.7
1268.5     1226.2     1139.0
  1112.2     1034.0     1016.8     984.65     978.66     952.37     937.93
923.07     824.72     785.27
  743.37     707.02     624.72     566.50     380.34     362.68     315.74
229.86     75.980
ZeroEnergy[kcal/mol]   0.75147589200216203
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
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RRHO ! 9
Geometry[angstrom] 16
C 0.32201 -0.44556 -1.35096
C 0.32181 -0.44547 -0.00563
C 1.48788 -0.44033 0.89592
C -1.07367 -0.41076 0.45556
C -1.89432 -0.39482 -0.59959
C -1.08378 -0.42096 -1.85816
H 1.19542 -0.46574 -1.98535
H 2.43388 -0.58258 0.37905
H 1.56728 0.59617 1.42031
H 1.39080 -1.13463 1.73005
H -1.36527 -0.39949 1.49609
H -2.97280 -0.37144 -0.57734
H -1.31470 -1.29672 -2.47285
H -1.27763 0.45312 -2.48812
O 1.41399 1.97949 1.92583
H 0.76392 2.24176 1.25862
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.15 0.52 1.10 1.85 2.69 3.48 1.57 1.17 0.73 0.33
0.07
End
Rotor Hindered
Group 16
Axis 15 9
Symmetry 1
Potential[kcal/mol] 18
0.00 0.09 0.30 0.57 0.77 0.88 0.90 0.88 0.84 0.83 0.83
0.82 0.79 0.73 0.61 0.43 0.22 0.05
End
Frequencies[1/cm] 39
3800.8 3244.0 3229.3 3214.7 3161.8 3086.2 3074.7
3043.5 1724.5 1623.1
1563.4 1457.0 1428.4 1417.6 1399.3 1327.5 1312.7
1269.8 1229.6 1138.9
1112.2 1036.2 1024.4 984.52 979.57 952.35 937.85
923.14 825.07 781.96
741.88 705.35 624.05 565.95 370.09 357.54 311.02
227.70 71.800
ZeroEnergy[kcal/mol] 0.94415066955390614
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 10
Geometry[angstrom] 16
C 0.32187 -0.44578 -1.35105
C 0.32171 -0.44568 -0.00613
C 1.48878 -0.44303 0.89564
C -1.07361 -0.41063 0.45543
C -1.89445 -0.39467 -0.59963
C -1.08395 -0.42084 -1.85822
H 1.19524 -0.46653 -1.98550
H 2.43334 -0.58776 0.37661
H 1.57159 0.58535 1.42024
H 1.39109 -1.14230 1.72569
H -1.36517 -0.39960 1.49597
H -2.97296 -0.37132 -0.57727
H -1.31505 -1.29667 -2.47275
H -1.27799 0.45319 -2.48815
O 1.41352 1.98319 1.92717
H 0.76336 2.24001 1.25765
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.15 0.52 1.10 1.85 2.69 3.48 1.57 1.17 0.73 0.33
0.07
End
Rotor Hindered
Group 16
Axis 15 9
Symmetry 1
Potential[kcal/mol] 18
0.00 0.09 0.30 0.57 0.77 0.88 0.90 0.88 0.84 0.83 0.83
0.82 0.79 0.73 0.61 0.43 0.22 0.05
End
Frequencies[1/cm] 39
3798.5 3243.7 3229.2 3214.5 3159.9 3085.0 3074.8
3043.6 1778.4 1649.4
1594.2 1462.4 1429.1 1417.9 1399.7 1334.1 1313.5
1270.5 1231.0 1138.8
1112.1 1038.6 1026.3 984.39 979.83 952.29 937.69
923.09 825.33 779.15
739.94 702.97 623.34 565.17 367.37 348.99 304.38
225.68 68.060
ZeroEnergy[kcal/mol] 1.0863773111209980
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 11
Geometry[angstrom] 16
C 0.00000 0.00000 0.00000
C 0.00000 0.00000 1.34464
C 1.16805 0.00000 2.24655
C -1.39518 0.03544 1.80653
C -2.21627 0.05147 0.75156
C -1.40587 0.02529 -0.50706
H 0.87327 -0.02134 -0.63458
H 2.11120 -0.14677 1.72548
H 1.25396 1.02150 2.77208
H 1.06979 -0.70399 3.07261
H -1.68668 0.04623 2.84714
H -3.29475 0.07485 0.77406
H -1.63715 -0.85061 -1.12142
H -1.60011 0.89928 -1.13699
O 1.09133 2.43288 3.27973
H 0.44118 2.68431 2.60793
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.15 0.52 1.10 1.85 2.69 3.48 1.57 1.17 0.73 0.33
0.07
End
Rotor Hindered
Group 16
Axis 15 9
Symmetry 1
Potential[kcal/mol] 18
0.00 0.09 0.30 0.57 0.77 0.88 0.90 0.88 0.84 0.83 0.83
0.82 0.79 0.73 0.61 0.43 0.22 0.05
End
Frequencies[1/cm] 39
3796.8 3243.6 3229.0 3214.3 3158.6 3084.2 3074.8
3043.6 1856.9 1666.2
1600.7 1464.4 1429.5 1418.3 1400.3 1339.9 1313.7
1270.8 1231.7 1138.8
1112.0 1040.1 1026.8 984.29 979.87 952.26 937.55
922.98 825.53 776.89
737.68 698.72 622.54 563.67 365.72 332.65 225.53
65.180 54.970
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ZeroEnergy[kcal/mol]    1.2045163942275678
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          12
Geometry[angstrom]          16
C    0.32151  -0.44615  -1.35135
C    0.32167  -0.44625  -0.00707
C    1.49065  -0.44890   0.89495
C   -1.07340  -0.41042   0.45517
C   -1.89470  -0.39432  -0.59965
C   -1.08439  -0.42051  -1.85833
H    1.19471  -0.46808  -1.98603
H    2.43244  -0.59773   0.37180
H    1.57966   0.56579   1.42144
H    1.39181  -1.15763   1.71704
H   -1.36483  -0.39987   1.49580
H   -2.97321  -0.37092  -0.57701
H   -1.31585  -1.29650  -2.47254
H   -1.27884   0.45341  -2.48825
O    1.41247   1.99072   1.92982
H    0.76235   2.23677   1.25574
          Core            RigidRotor
     SymmetryFactor   0.50000000000000000
End
 Rotor                         Hindered
 Group    8   9  10  15  16
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
 End
 Rotor                         Hindered
 Group   16
 Axis           15          9
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
 End
   Frequencies[1/cm]          39
  3794.6     3243.4     3228.9     3214.0     3157.1     3083.2     3074.8
3043.6     1955.5     1675.3
  1603.4     1465.7     1429.9     1418.8     1401.3     1345.8     1313.8
1271.2     1232.1     1138.8
  1111.9     1041.5     1026.8     984.19     979.92     952.23     937.41
922.88     825.70     775.10
  735.59     695.32     621.81     562.85     365.72     332.08     224.35
62.620     51.590
ZeroEnergy[kcal/mol]    1.3200551074219931
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          13
Geometry[angstrom]          16
C    0.32129  -0.44629  -1.35158
C    0.32174  -0.44664  -0.00751
C    1.49163  -0.45205   0.89456
C   -1.07323  -0.41036   0.45506
C   -1.89480  -0.39409  -0.59963
C   -1.08468  -0.42029  -1.85838
H    1.19434  -0.46884  -1.98645
H    2.43212  -0.60238   0.36947
H    1.58326   0.55706   1.42271
H    1.39230  -1.16531   1.71274
H   -1.36456  -0.40004   1.49577
H   -2.97328  -0.37059  -0.57678
H   -1.31631  -1.29636  -2.47241
H   -1.27933   0.45358  -2.48832
O    1.41187   1.99454   1.93112
H    0.76192   2.23535   1.25479
          Core            RigidRotor
     SymmetryFactor   0.50000000000000000
End
 Rotor                         Hindered
 Group    8   9  10  15  16
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
 End
 Rotor                         Hindered
 Group   16
 Axis           15          9
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
 End
   Frequencies[1/cm]          39
  3792.9     3243.5     3228.8     3213.7     3156.2     3082.7     3074.8
3043.6     2034.1     1679.6
  1604.4     1466.5     1430.4     1419.3     1402.3     1350.8     1314.0
1271.5     1232.3     1138.7
  1111.8     1042.3     1026.6     984.13     979.97     952.25     937.31
922.78     825.83     773.77
  733.69     691.56     621.03     562.09     365.78     331.67     223.64
60.940     49.000
ZeroEnergy[kcal/mol]    1.4038859194665463
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          14
Geometry[angstrom]          16
C    0.32110  -0.44648  -1.35180
C    0.32182  -0.44701  -0.00793
C    1.49257  -0.45529   0.89413
C   -1.07306  -0.41028   0.45495
C   -1.89488  -0.39383  -0.59959
C   -1.08494  -0.42007  -1.85843
H    1.19402  -0.46968  -1.98683
H    2.43183  -0.60693   0.36712
H    1.58671   0.54865   1.42417
H    1.39274  -1.17300   1.70845
H   -1.36428  -0.40018   1.49571
H   -2.97336  -0.37021  -0.57654
H   -1.31678  -1.29620  -2.47230
H   -1.27975   0.45375  -2.48837
O    1.41125   1.99837   1.93241
H    0.76144   2.23401   1.25393
          Core            RigidRotor
     SymmetryFactor   0.50000000000000000
End
 Rotor                         Hindered
 Group    8   9  10  15  16
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
 End
 Rotor                         Hindered
 Group   16
 Axis           15          9
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
 End
   Frequencies[1/cm]          39
  3791.3     3243.4     3228.7     3213.5     3155.1     3082.0     3074.8
3043.6     2096.0     1682.5
```

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  1605.1     1467.1     1430.7     1419.7     1402.9     1355.3     1314.0
1271.7     1232.3     1138.7
  1111.8     1043.0     1026.5     984.06     980.01     952.23     937.20
922.68     825.94     772.72
  732.02     687.31     620.19     561.21     365.80     331.24     222.85
59.150     46.550
 ZeroEnergy[kcal/mol]    1.4533648479713719
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
 RRHO          !          15
 Geometry[angstrom]          16
 C    0.32092  -0.44668  -1.35202
 C    0.32191  -0.44741  -0.00835
 C    1.49349  -0.45858   0.89367
 C   -1.07287  -0.41020   0.45485
 C   -1.89495  -0.39355  -0.59953
 C   -1.08520  -0.41983  -1.85848
 H    1.19370  -0.47054  -1.98722
 H    2.43158  -0.61135   0.36480
 H    1.59002   0.54041   1.42575
 H    1.39319  -1.18063   1.70418
 H   -1.36399  -0.40030   1.49565
 H   -2.97343  -0.36978  -0.57629
 H   -1.31726  -1.29602  -2.47219
 H   -1.28016   0.45394  -2.48842
 O    1.41060   2.00221   1.93368
 H    0.76097   2.23273   1.25309
           Core            RigidRotor
      SymmetryFactor   0.50000000000000000
 End
  Rotor                        Hindered
  Group    8   9  10  15  16
  Axis           3          2
  Symmetry           3
  Potential[kcal/mol]          12
   0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
  End
  Rotor                        Hindered
  Group   16
  Axis           15          9
  Symmetry           1
  Potential[kcal/mol]          18
   0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
  End
    Frequencies[1/cm]          39
  3789.8     3243.3     3228.6     3213.3     3154.0     3081.3     3074.8
3043.6     2147.6     1684.7
  1605.6     1467.7     1431.0     1420.0     1403.4     1359.6     1314.0
1271.8     1232.3     1138.7
  1111.7     1043.4     1026.3     984.00     980.02     952.22     937.11
922.57     826.03     771.87
  730.57     682.67     619.28     560.17     365.82     330.71     221.94
57.070     44.160
 ZeroEnergy[kcal/mol]    1.4782844593420918
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
 RRHO          !          16
 Geometry[angstrom]          16
 C    0.32074  -0.44688  -1.35225
 C    0.32202  -0.44782  -0.00875
 C    1.49440  -0.46192   0.89320
 C   -1.07267  -0.41012   0.45476
 C   -1.89501  -0.39326  -0.59947
 C   -1.08545  -0.41958  -1.85852
 H    1.19339  -0.47140  -1.98762
 H    2.43134  -0.61566   0.36251
 H    1.59326   0.53225   1.42743
 H    1.39364  -1.18821   1.69994
 H   -1.36368  -0.40042   1.49561
 H   -2.97348  -0.36931  -0.57601
 H   -1.31775  -1.29583  -2.47208
 H   -1.28055   0.45415  -2.48846
 O    1.40992   2.00605   1.93492
 H    0.76051   2.23148   1.25226
           Core            RigidRotor
      SymmetryFactor   0.50000000000000000
 End
  Rotor                        Hindered
  Group    8   9  10  15  16
  Axis           3          2
  Symmetry           3
  Potential[kcal/mol]          12
   0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
  End
  Rotor                        Hindered
  Group   16
  Axis           15          9
  Symmetry           1
  Potential[kcal/mol]          18
   0.00    0.09    0.30    0.57    0.77    0.88    0.90    0.88    0.84    0.83    0.83
0.82    0.79    0.73    0.61    0.43    0.22    0.05
  End
    Frequencies[1/cm]          39
  3788.3     3243.3     3228.5     3213.1     3153.1     3080.7     3074.8
3043.6     2200.4     1686.6
  1606.0     1468.2     1431.4     1420.3     1404.0     1363.5     1314.0
1272.0     1232.3     1138.6
  1111.7     1043.9     1026.1     983.95     980.03     952.20     937.02
922.47     826.11     771.18
  729.32     677.84     618.32     559.00     365.83     330.27     221.16
55.320     41.780
 ZeroEnergy[kcal/mol]    1.5047908953420546
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
 RRHO          !          17
 Geometry[angstrom]          16
 C    0.32056  -0.44708  -1.35248
 C    0.32214  -0.44824  -0.00915
 C    1.49529  -0.46531   0.89270
 C   -1.07246  -0.41004   0.45467
 C   -1.89506  -0.39294  -0.59939
 C   -1.08570  -0.41932  -1.85856
 H    1.19307  -0.47227  -1.98803
 H    2.43114  -0.61987   0.36023
 H    1.59640   0.52425   1.42922
 H    1.39409  -1.19575   1.69571
 H   -1.36336  -0.40054   1.49558
 H   -2.97352  -0.36880  -0.57572
 H   -1.31823  -1.29562  -2.47196
 H   -1.28093   0.45437  -2.48850
 O    1.40923   2.00989   1.93616
 H    0.76008   2.23025   1.25143
           Core            RigidRotor
      SymmetryFactor   0.50000000000000000
 End
  Rotor                        Hindered
  Group    8   9  10  15  16
  Axis           3          2
  Symmetry           3
  Potential[kcal/mol]          12
   0.00    0.15    0.52    1.10    1.85    2.69    3.48    1.57    1.17    0.73    0.33
0.07
  End
  Rotor                        Hindered
  Group   16
  Axis           15          9
  Symmetry           1
  Potential[kcal/mol]          18
```

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  0.00   0.09   0.30   0.57   0.77   0.88   0.90   0.88   0.84   0.83   0.83
0.82   0.79   0.73   0.61   0.43   0.22   0.05
 End
   Frequencies[1/cm]        39
  3787.0     3243.2     3228.4     3213.0     3152.1     3080.2     3074.8
3043.6     2259.3     1688.3
  1606.3     1468.7     1431.9     1420.8     1405.1     1367.2     1314.0
1272.1     1232.2     1138.6
  1111.6     1044.4     1025.9     983.90     980.04     952.19     936.95
922.38     826.19     770.65
  728.28     673.12     617.33     557.83     365.88     330.07     220.91
55.130     39.600
 ZeroEnergy[kcal/mol]   1.5386603511184802
  ElectronicLevels[1/cm]             1
   0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        18
Geometry[angstrom]        16
C   0.32039  -0.44728  -1.35272
C   0.32228  -0.44869  -0.00953
C   1.49618  -0.46875   0.89219
C  -1.07224  -0.40997   0.45460
C  -1.89510  -0.39261  -0.59931
C  -1.08595  -0.41904  -1.85859
H   1.19275  -0.47315  -1.98846
H   2.43096  -0.62397   0.35798
H   1.59937   0.51651   1.43116
H   1.39456  -1.20330   1.69147
H  -1.36301  -0.40066   1.49555
H  -2.97356  -0.36825  -0.57542
H  -1.31873  -1.29539  -2.47185
H  -1.28130   0.45461  -2.48854
O   1.40851   2.01375   1.93736
H   0.75965   2.22906   1.25061
           Core          RigidRotor
       SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group   8   9  10  15  16
 Axis         3        2
 Symmetry        3
 Potential[kcal/mol]        12
  0.00   0.15   0.52   1.10   1.85   2.69   3.48   1.57   1.17   0.73   0.33
0.07
 End
 Rotor                    Hindered
 Group   16
 Axis         15        9
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.09   0.30   0.57   0.77   0.88   0.90   0.88   0.84   0.83   0.83
0.82   0.79   0.73   0.61   0.43   0.22   0.05
 End
   Frequencies[1/cm]        39
  3785.7     3243.1     3228.3     3212.8     3151.3     3079.6     3074.8
3043.6     2318.6     1689.7
  1606.5     1469.3     1432.5     1421.4     1406.3     1370.6     1314.0
1272.2     1232.2     1138.6
  1111.6     1044.9     1025.8     983.85     980.09     952.18     936.89
922.29     826.25     770.24
  727.42     668.64     616.26     556.68     365.95     330.14     221.41
58.440     37.850
 ZeroEnergy[kcal/mol]   1.5821651204093570
  ElectronicLevels[1/cm]             1
   0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        19
Geometry[angstrom]        16
C   0.32023  -0.44749  -1.35297
C   0.32245  -0.44918  -0.00991
C   1.49707  -0.47224   0.89167
C  -1.07199  -0.40990   0.45453
C  -1.89512  -0.39224  -0.59920
C  -1.08621  -0.41874  -1.85862
H   1.19243  -0.47406  -1.98891
H   2.43084  -0.62792   0.35576
H   1.60211   0.50903   1.43326
H   1.39506  -1.21086   1.68723
H  -1.36264  -0.40077   1.49553
H  -2.97357  -0.36763  -0.57508
H  -1.31924  -1.29513  -2.47173
H  -1.28166   0.45487  -2.48857
O   1.40775   2.01760   1.93855
H   0.75923   2.22795   1.24981
           Core          RigidRotor
       SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group   8   9  10  15  16
 Axis         3        2
 Symmetry        3
 Potential[kcal/mol]        12
  0.00   0.15   0.52   1.10   1.85   2.69   3.48   1.57   1.17   0.73   0.33
0.07
 End
 Rotor                    Hindered
 Group   16
 Axis         15        9
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.09   0.30   0.57   0.77   0.88   0.90   0.88   0.84   0.83   0.83
0.82   0.79   0.73   0.61   0.43   0.22   0.05
 End
   Frequencies[1/cm]        39
  3784.4     3243.1     3228.2     3212.7     3150.4     3079.1     3074.7
3043.6     2369.3     1690.9
  1606.7     1469.8     1433.2     1421.9     1407.3     1373.8     1314.0
1272.3     1232.0     1138.5
  1111.5     1045.5     1025.8     983.81     980.16     952.17     936.85
922.21     826.30     769.92
  726.72     664.36     615.11     555.49     366.04     330.28     222.36
66.910     36.570
 ZeroEnergy[kcal/mol]   1.6220673689203124
  ElectronicLevels[1/cm]             1
   0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        20
Geometry[angstrom]        16
C   0.32006  -0.44772  -1.35324
C   0.32264  -0.44971  -0.01029
C   1.49795  -0.47578   0.89116
C  -1.07172  -0.40984   0.45447
C  -1.89513  -0.39184  -0.59908
C  -1.08647  -0.41841  -1.85864
H   1.19209  -0.47498  -1.98938
H   2.43076  -0.63169   0.35359
H   1.60461   0.50173   1.43549
H   1.39560  -1.21844   1.68297
H  -1.36222  -0.40089   1.49552
H  -2.97357  -0.36693  -0.57471
H  -1.31978  -1.29485  -2.47160
H  -1.28201   0.45516  -2.48860
O   1.40696   2.02145   1.93970
H   0.75880   2.22695   1.24903
           Core          RigidRotor
       SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group   8   9  10  15  16
 Axis         3        2
 Symmetry        3
 Potential[kcal/mol]        12
  0.00   0.15   0.52   1.10   1.85   2.69   3.48   1.57   1.17   0.73   0.33
0.07
 End
```

```
 Rotor                  Hindered
 Group   16
 Axis        15        9
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.09   0.30   0.57   0.77   0.88   0.90   0.88   0.84   0.83   0.83
0.82   0.79   0.73   0.61   0.43   0.22   0.05
 End
   Frequencies[1/cm]        39
  3783.3     3243.0     3228.2     3212.5     3149.7     3078.7     3074.7
3043.6     2407.7     1691.8
  1606.8     1470.3     1433.6     1422.2     1408.2     1376.6     1314.0
1272.4     1231.9     1138.5
  1111.5     1046.0     1025.7     983.78     980.23     952.16     936.81
922.12     826.35     769.64
  726.11     660.21     613.84     554.07     366.11     330.23     222.76
73.320     35.640
 ZeroEnergy[kcal/mol]    1.6403116055999192
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
!*********************************************
 RRHO        !        21
 Geometry[angstrom]        16
 C    0.31990  -0.44795  -1.35351
 C    0.32286  -0.45029  -0.01066
 C    1.49881  -0.47935   0.89064
 C   -1.07142  -0.40979   0.45442
 C   -1.89512  -0.39140  -0.59894
 C   -1.08673  -0.41806  -1.85865
 H    1.19175  -0.47592  -1.98989
 H    2.43074  -0.63526   0.35147
 H    1.60692   0.49449   1.43781
 H    1.39618  -1.22601   1.67871
 H   -1.36177  -0.40101   1.49553
 H   -2.97355  -0.36616  -0.57430
 H   -1.32036  -1.29452  -2.47147
 H   -1.28234   0.45550  -2.48861
 O    1.40613   2.02530   1.94082
 H    0.75837   2.22604   1.24825
            Core          RigidRotor
       SymmetryFactor   0.50000000000000000
 End
 Rotor                  Hindered
 Group    8   9  10  15  16
 Axis         3        2
 Symmetry        3
 Potential[kcal/mol]        12
  0.00   0.15   0.52   1.10   1.85   2.69   3.48   1.57   1.17   0.73   0.33
0.07
 End
 Rotor                  Hindered
 Group   16
 Axis        15        9
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.09   0.30   0.57   0.77   0.88   0.90   0.88   0.84   0.83   0.83
0.82   0.79   0.73   0.61   0.43   0.22   0.05
 End
   Frequencies[1/cm]        39
  3782.2     3242.9     3228.1     3212.4     3149.0     3078.3     3074.7
3043.6     2436.0     1692.7
  1606.9     1470.8     1433.9     1422.3     1408.7     1379.2     1314.0
1272.5     1231.8     1138.5
  1111.5     1046.5     1025.7     983.75     980.29     952.15     936.78
922.03     826.38     769.40
  725.59     656.16     612.44     552.29     366.15     329.90     222.12
69.190     34.730
 ZeroEnergy[kcal/mol]    1.6218594610893717
 ElectronicLevels[1/cm]              1
  0.0000000000000000      2.0000000000000000
 End
!*********************************************
     Tunneling    Eckart
       ImaginaryFrequency[1/cm]    383.81999000000002
       WellDepth[kcal/mol]       0.01
       WellDepth[kcal/mol]       0.01
   End
 End
 End
```

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!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                      direct     ! direct or low-eigenvalue
!
WellCutoff                             20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                  0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                        diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!
!WellCutoff                            10
!ChemicalEigenvalueMin                 1.e-6         #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                  1.3
!!
RateOutput                             rate.out                  ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                       ! Default collisional
energy relaxation kernel
    Exponential                                          ! Currently the only
possible energy relaxation model
       Factor[1/cm]            316                       ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                   0.535                     ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff          10                        ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                     ! Collision frequency
model
    LennardJones                                         ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]             90.58  281.367            ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]        3.54    4.694             ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]             39.948  79.05478          ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50263
 C    1.24622   0.00000   2.31947
 C   -1.27227   0.00046   1.92591
 C   -2.17585   0.00051   0.77474
 C   -1.45565   0.00011  -0.35294
 H    0.51979   0.87601  -0.40113
 H    1.85947   0.87812   2.10478
 H    1.01835  -0.00094   3.38445
 H    1.86045  -0.87709   2.10340
 H   -1.59049   0.00052   2.95892
 H   -3.25397   0.00095   0.84079
 H   -1.83452  -0.00013  -1.36297
 H    0.51979  -0.87591  -0.40126
      Core    RigidRotor
          SymmetryFactor    1.0000000000000000
      End
 Rotor                       Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          3
 Potential[kcal/mol]          12
   0.00    0.08    0.30    0.62    0.95    1.20    1.29    1.21    0.96    0.62    0.30
0.08
 End
    Frequencies[1/cm]          35
   3245.2      3221.6      3209.3      3128.8      3090.6      3074.8      3042.5
3036.2      1695.3      1615.6
   1495.0      1486.6      1424.0      1421.5      1397.2      1340.1      1274.6
1198.6      1152.9      1130.9
   1060.1      1033.7      1005.4      976.89      961.82      922.95      892.68
863.70      828.81      700.71
   623.69      533.08      369.88      325.94      227.72
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                   1
   0.0000000000000000       2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]           3
 O    0.00000   0.00000   0.00000
 O    0.00000   0.00000   1.31234
 H    0.93494   0.00000   1.57303
      Core    RigidRotor
          SymmetryFactor    1.0000000000000000
      End
    Frequencies[1/cm]           3
   1234.9      1462.2      3683.2
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                   1
   0.0000000000000000       2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]            13
```

```
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.41507
C    1.18585   0.00000   2.30525
C   -1.37924  -0.00034   1.86264
C   -2.17195  -0.00056   0.76525
C   -1.30652  -0.00033  -0.41759
H    0.87955   0.00028  -0.62343
H    2.11567   0.00259   1.73998
H    1.17551   0.87449   2.96082
H    1.17824  -0.87748   2.95691
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
        Core    RigidRotor
            SymmetryFactor    2.0000000000000000
        End
Rotor                           Hindered
Group    8   9  10
Axis            3           2
Symmetry           3
Potential[kcal/mol]           12
   0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
    Frequencies[1/cm]           32
   3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
   1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
   953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
   329.55      215.83
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!************************************
Fragment PROD2
RRHO
Geometry[angstrom]               4
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.42622
H    0.94322   0.00000   1.61480
H   -0.34861  -0.87643  -0.18855
        Core    RigidRotor
            SymmetryFactor    2.0000000000000000
        End
Rotor                           Hindered
Group    4
Axis            1           2
Symmetry           1
Potential[kcal/mol]           18
   0.00    0.07    0.48    0.80    0.77    0.40    0.02    0.06    0.91    2.62    4.92
7.15    8.51    8.38    6.81    4.51    2.28    0.70
End
    Frequencies[1/cm]            5
   3840.9      3839.6      1465.2      1361.0      1016.3
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
GroundEnergy[kcal/mol]    -6.19
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]              17
C    0.00080   0.00719   0.00268
C   -0.00098   0.00265   1.50390
C    1.24549   0.00161   2.31846
C   -1.27279  -0.01377   1.93172
C   -2.17580  -0.02367   0.78032
C   -1.45365  -0.01693  -0.35221
H    0.49850   0.89661  -0.39598
H    1.85934   0.87750   2.09842
H    1.02076   0.00202   3.38370
H    1.85396  -0.87791   2.09842
H   -1.59190  -0.02561   2.96366
H   -3.25454  -0.02468   0.84451
H   -1.83310  -0.00529  -1.36205
H    0.53485  -0.85645  -0.40585
O   -0.54001  -3.28492  -0.72956
O   -1.53476  -3.13852   0.11080
H   -1.71460  -2.17284   0.13958
        Core    RigidRotor
            SymmetryFactor    0.50000000000000000
        End
    Frequencies[1/cm]           45
   18.379      41.224      74.922      110.69      152.09      168.28      245.11
326.53      381.29      472.31
   541.43      624.24      722.09      831.58      864.65      893.69      923.43
961.54      987.50      1007.0
   1035.5      1061.0      1130.9      1157.3      1200.0      1259.5      1276.2
1344.1      1398.4      1420.3
   1426.2      1487.5      1493.9      1515.2      1601.9      1687.6      3041.2
3050.1      3085.1      3098.0
   3135.0      3212.4      3226.0      3245.8      3465.6
 ZeroEnergy[kcal/mol]             -6.01
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]              17
C    0.01539   0.01534   0.01367
C    0.01643  -0.00267   1.43840
C    1.20718   0.02425   2.31767
C   -1.35329  -0.11430   1.87869
C   -2.14581  -0.16382   0.77777
C   -1.28601  -0.07663  -0.40471
H    0.89157   0.11238  -0.60746
H    2.06801   0.46423   1.81695
H    1.00970   0.57160   3.23949
H    1.47120  -1.00091   2.59541
H   -1.66823  -0.14455   2.90999
H   -3.22087  -0.24625   0.75484
H   -1.63558  -0.07968  -1.42560
H   -0.18948  -2.31738  -0.08654
O   -0.35077  -3.23080   0.19153
O   -0.05192  -3.16573   1.58210
H   -0.91329  -2.95283   1.95719
        Core    RigidRotor
            SymmetryFactor    0.50000000000000000
        End
    Frequencies[1/cm]           45
   27.366      42.673      72.634      80.143      99.481      138.82      209.87
229.84      331.47      519.93
   535.53      605.32      614.33      646.18      740.01      750.83      908.47
926.89      934.71      963.91
   1009.5      1017.7      1025.7      1060.6      1097.1      1189.7      1295.8
1310.9      1404.8      1417.2
   1436.0      1460.2      1475.0      1489.6      1516.6      1570.5      3034.8
3102.1      3139.6      3227.4
   3233.6      3247.1      3256.4      3718.7      3810.9
 ZeroEnergy[kcal/mol]             -8.82
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier       B1  REACS WR
  RRHO
    Stoichiometry  H9C6O2
    Core PhaseSpaceTheory
```

```
   FragmentGeometry[angstrom]        14
C  0.00000  0.00000  0.00000
C  0.00000  0.00000  1.50263
C  1.24622  0.00000  2.31947
C  -1.27227  0.00046  1.92591
C  -2.17585  0.00051  0.77474
C  -1.45565  0.00011  -0.35294
H  0.51979  0.87601  -0.40113
H  1.85947  0.87812  2.10478
H  1.01835  -0.00094  3.38445
H  1.86045  -0.87709  2.10340
H  -1.59049  0.00052  2.95892
H  -3.25397  0.00095  0.84079
H  -1.83452  -0.00013  -1.36297
H  0.51979  -0.87591  -0.40126
   FragmentGeometry[angstrom]        3
O  0.00000  0.00000  0.00000
O  0.00000  0.00000  1.31234
H  0.93494  0.00000  1.57303
                    SymmetryFactor    1.0000000000000000
     PotentialPrefactor[au]        10.
     PotentialPowerExponent        6
            End
Rotor                 Hindered
Geometry[angstrom]           14
C  0.00000  0.00000  0.00000
C  0.00000  0.00000  1.50263
C  1.24622  0.00000  2.31947
C  -1.27227  0.00046  1.92591
C  -2.17585  0.00051  0.77474
C  -1.45565  0.00011  -0.35294
H  0.51979  0.87601  -0.40113
H  1.85947  0.87812  2.10478
H  1.01835  -0.00094  3.38445
H  1.86045  -0.87709  2.10340
H  -1.59049  0.00052  2.95892
H  -3.25397  0.00095  0.84079
H  -1.83452  -0.00013  -1.36297
H  0.51979  -0.87591  -0.40126
Group   8  9  10
Axis        3        2
Symmetry        3
Potential[kcal/mol]        12
  0.0000    0.80000E-01 0.30000    0.62000    0.95000    1.2000    1.2900
1.2100    0.96000    0.62000
 0.30000    0.80000E-01
End
   Frequencies[1/cm]        38
  3245.2    3221.6    3209.3    3128.8    3090.6    3074.8    3042.5
3036.2    1695.3    1615.6
  1495.0    1486.6    1424.0    1421.5    1397.2    1340.1    1274.6
1198.6    1152.9    1130.9
  1060.1    1033.7    1005.4    976.89    961.82    922.95    892.68
863.70    828.81    700.71
  623.69    533.08    369.88    325.94    227.72
  1234.9    1462.2    3683.2
 ZeroEnergy[kcal/mol]        0.
 ElectronicLevels[1/cm]           1
  0.0000000000000000     4.0000000000000000
End
!************************************
Barrier      B3  WP PRODS
  RRHO
   Stoichiometry  H9C6O2
   Core PhaseSpaceTheory
   FragmentGeometry[angstrom]        13
C  0.00000  0.00000  0.00000
C  0.00000  0.00000  1.41507
C  1.18585  0.00000  2.30525
C  -1.37924  -0.00034  1.86264
C  -2.17195  -0.00056  0.76525
C  -1.30652  -0.00033  -0.41759
H  0.87955  0.00028  -0.62343
H  2.11567  0.00259  1.73998
H  1.17551  0.87449  2.96082
H  1.17824  -0.87748  2.95691
H  -1.69366  -0.00045  2.89442
H  -3.25029  -0.00080  0.74358
H  -1.65471  -0.00041  -1.43915
   FragmentGeometry[angstrom]        4
O  0.00000  0.00000  0.00000
O  0.00000  0.00000  1.42622
H  0.94322  0.00000  1.61480
H  -0.34861  -0.87643  -0.18855
                    SymmetryFactor    4.0000000000000000
     PotentialPrefactor[au]        10.
     PotentialPowerExponent        6
            End
Rotor                 Hindered
Geometry[angstrom]           13
C  0.00000  0.00000  0.00000
C  0.00000  0.00000  1.41507
C  1.18585  0.00000  2.30525
C  -1.37924  -0.00034  1.86264
C  -2.17195  -0.00056  0.76525
C  -1.30652  -0.00033  -0.41759
H  0.87955  0.00028  -0.62343
H  2.11567  0.00259  1.73998
H  1.17551  0.87449  2.96082
H  1.17824  -0.87748  2.95691
H  -1.69366  -0.00045  2.89442
H  -3.25029  -0.00080  0.74358
H  -1.65471  -0.00041  -1.43915
Group   8  9  10
Axis        3        2
Symmetry        3
Potential[kcal/mol]        12
  0.0000    0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01  0.0000    0.20000E-01 0.40000E-01 0.60000E-01
 0.40000E-01 0.10000E-01
End
Rotor                 Hindered
Geometry[angstrom]           4
O  0.00000  0.00000  0.00000
O  0.00000  0.00000  1.42622
H  0.94322  0.00000  1.61480
H  -0.34861  -0.87643  -0.18855
Group   4
Axis        1        2
Symmetry        1
Potential[kcal/mol]        18
  0.0000    0.70000E-01 0.48000    0.80000    0.77000    0.40000
0.20000E-01 0.60000E-01 0.91000    2.6200
  4.9200    7.1500    8.5100    8.3800    6.8100    4.5100    2.2800
0.70000
End
   Frequencies[1/cm]        37
  3255.2    3247.0    3232.4    3224.7    3138.6    3086.9    3034.1
1584.1    1503.1    1481.1
  1477.9    1438.4    1407.4    1311.3    1292.6    1178.7    1098.1
1049.4    1023.5    1013.2
  953.40    929.99    923.03    899.45    740.46    727.81    638.42
604.77    528.85    520.52
  329.55    215.83
  3840.9    3839.6    1465.2    1361.0    1016.3
 ZeroEnergy[kcal/mol]        -6.1911681736890189
 ElectronicLevels[1/cm]           1
  0.0000000000000000     4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO        !        1
Geometry[angstrom]        17
C  0.39490  0.84168  -0.73553
C  0.40106  0.83099  0.72861
C  1.63463  0.83246  1.56379
C  -0.88472  0.73039  1.13154
```

```
C  -1.76358  0.72395  -0.04282
C  -1.00560  0.82343  -1.15579
H   1.17267  1.32875  -1.31402
H   2.24810  1.71394   1.36812
H   1.38893  0.81765   2.62419
H   2.24608 -0.04544   1.34577
H  -1.22205  0.65972   2.15467
H  -2.84089  0.66616  -0.00610
H  -1.34784  0.85322  -2.17712
H   0.74104 -0.56253  -0.97584
O   0.83376 -1.63150  -1.10648
O  -0.01108 -2.16464  -0.16435
H  -0.87666 -2.13310  -0.58946
        Core        RigidRotor
    SymmetryFactor   1.5000000000000000
End
 Rotor              Hindered
 Group   8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.26   0.77   1.01   0.76   0.26  -0.00   0.25   0.77   1.01   0.76
0.25  -0.00   0.25   0.76   1.01   0.75   0.24
 End
 Rotor              Hindered
 Group   16  17
 Axis        15        14
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.26   0.87   1.81   2.48   2.72   2.76   2.80   2.83   2.83   2.80
2.75   2.60   2.19   1.71   1.28   0.80   0.21
 End
 Rotor              Hindered
 Group   17
 Axis        16        15
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.50   2.22   5.02   8.55  12.04   8.05   5.02   3.02   2.37  -0.11
1.16   3.44   7.64   7.24   4.62   2.37   0.71
 End
   Frequencies[1/cm]        41
  3778.1    3257.5    3235.7    3223.9    3177.2    3135.7    3100.0
3042.3    1633.0    1555.6
  1496.4    1493.3    1488.0    1455.3    1433.7    1424.5    1354.1
1273.6    1244.7    1193.8
  1124.2    1090.6    1064.2    1033.8    992.06    955.45    941.40
900.15    846.28    822.33
  737.94    652.74    606.44    544.69    508.58    411.12    325.52
265.04    198.82    100.08
  53.470
 ZeroEnergy[kcal/mol]   8.1109645399262984
 ElectronicLevels[1/cm]            1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        2
Geometry[angstrom]        17
C   0.39553  0.84052  -0.73587
C   0.40097  0.83114   0.72875
C   1.63460  0.83245   1.56380
C  -0.88476  0.73040   1.13147
C  -1.76352  0.72398  -0.04282
C  -1.00588  0.82355  -1.15568
H   1.17173  1.33156  -1.31327
H   2.24808  1.71393   1.36808
H   1.38898  0.81762   2.62422
H   2.24608 -0.04542   1.34569
H  -1.22206  0.65953   2.15464
H  -2.84085  0.66594  -0.00609
H  -1.34799  0.85309  -2.17710
H   0.73935 -0.54743  -0.97458
O   0.83344 -1.63213  -1.10616
O  -0.01078 -2.16447  -0.16468
H  -0.87675 -2.13291  -0.58944
        Core        RigidRotor
    SymmetryFactor   1.5000000000000000
End
 Rotor              Hindered
 Group   8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.26   0.77   1.01   0.76   0.26  -0.00   0.25   0.77   1.01   0.76
0.25  -0.00   0.25   0.76   1.01   0.75   0.24
 End
 Rotor              Hindered
 Group   16  17
 Axis        15        14
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.26   0.87   1.81   2.48   2.72   2.76   2.80   2.83   2.83   2.80
2.75   2.60   2.19   1.71   1.28   0.80   0.21
 End
 Rotor              Hindered
 Group   17
 Axis        16        15
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.50   2.22   5.02   8.55  12.04   8.05   5.02   3.02   2.37  -0.11
1.16   3.44   7.64   7.24   4.62   2.37   0.71
 End
   Frequencies[1/cm]        41
  3775.4    3257.2    3235.3    3223.4    3175.9    3135.6    3099.9
3042.2    1632.8    1553.0
  1495.5    1490.8    1487.9    1454.3    1425.8    1392.7    1279.0
1271.0    1246.8    1191.5
  1124.9    1083.4    1055.5    1031.8    992.65    956.57    942.77
902.13    851.78    843.44
  736.74    654.18    608.44    545.37    496.04    449.14    328.21
267.49    214.90    103.48
  70.140
 ZeroEnergy[kcal/mol]   8.7163820397439604
 ElectronicLevels[1/cm]            1
  0.0000000000000000      2.0000000000000000
 End
!**********************************************
RRHO        !        3
Geometry[angstrom]        17
C   0.39612  0.83943  -0.73620
C   0.40087  0.83128   0.72889
C   1.63458  0.83245   1.56381
C  -0.88480  0.73042   1.13140
C  -1.76345  0.72401  -0.04281
C  -1.00615  0.82367  -1.15558
H   1.17082  1.33422  -1.31257
H   2.24807  1.71391   1.36805
H   1.38902  0.81759   2.62426
H   2.24609 -0.04540   1.34562
H  -1.22207  0.65934   2.15462
H  -2.84082  0.66573  -0.00607
H  -1.34812  0.85297  -2.17708
H   0.73768 -0.53220  -0.97326
O   0.83315 -1.63280  -1.10586
O  -0.01048 -2.16432  -0.16500
H  -0.87684 -2.13272  -0.58943
        Core        RigidRotor
    SymmetryFactor   1.5000000000000000
End
 Rotor              Hindered
 Group   8  9  10
 Axis        3        2
 Symmetry        1
 Potential[kcal/mol]        18
  0.00   0.26   0.77   1.01   0.76   0.26  -0.00   0.25   0.77   1.01   0.76
0.25  -0.00   0.25   0.76   1.01   0.75   0.24
 End
 Rotor              Hindered
 Group   16  17
```

```
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.26 0.87 1.81 2.48 2.72 2.76 2.80 2.83 2.83 2.80
2.75 2.60 2.19 1.71 1.28 0.80 0.21
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.50 2.22 5.02 8.55 12.04 8.05 5.02 3.02 2.37 -0.11
1.16 3.44 7.64 7.24 4.62 2.37 0.71
 End
  Frequencies[1/cm] 41
  3772.6 3256.9 3234.8 3222.9 3174.5 3135.4 3099.8
3042.2 1632.8 1553.7
  1495.2 1488.3 1485.4 1453.9 1425.5 1387.7 1274.2
1250.1 1220.3 1178.1
  1125.6 1079.2 1043.2 1024.2 993.08 957.83 944.22
904.60 868.21 846.85
  736.23 656.59 612.54 546.97 511.91 467.21 329.63
268.64 217.26 105.61
  81.330
ZeroEnergy[kcal/mol] 9.3478771040402631
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
End
!*********************************************
RRHO ! 4
Geometry[angstrom] 17
C 0.39667 0.83841 -0.73651
C 0.40077 0.83142 0.72902
C 1.63455 0.83245 1.56381
C -0.88483 0.73044 1.13134
C -1.76340 0.72404 -0.04281
C -1.00640 0.82379 -1.15548
H 1.16996 1.33675 -1.31189
H 2.24805 1.71390 1.36801
H 1.38905 0.81756 2.62429
H 2.24611 -0.04538 1.34555
H -1.22208 0.65915 2.15459
H -2.84078 0.66552 -0.00605
H -1.34824 0.85286 -2.17707
H 0.73603 -0.51687 -0.97191
O 0.83288 -1.63350 -1.10558
O -0.01020 -2.16418 -0.16531
H -0.87694 -2.13252 -0.58943
  Core RigidRotor
  SymmetryFactor 1.5000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.26 0.77 1.01 0.76 0.26 -0.00 0.25 0.77 1.01 0.76
0.25 -0.00 0.25 0.76 1.01 0.75 0.24
 End
 Rotor Hindered
 Group 16 17
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.26 0.87 1.81 2.48 2.72 2.76 2.80 2.83 2.83 2.80
2.75 2.60 2.19 1.71 1.28 0.80 0.21
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.50 2.22 5.02 8.55 12.04 8.05 5.02 3.02 2.37 -0.11
1.16 3.44 7.64 7.24 4.62 2.37 0.71
 End
  Frequencies[1/cm] 41
  3769.9 3256.5 3234.3 3222.4 3173.1 3135.3 3099.7
3042.1 1633.1 1555.2
  1495.1 1488.2 1478.1 1453.4 1425.4 1386.7 1274.5
1254.1 1209.1 1155.2
  1126.3 1077.2 1038.1 1008.4 992.24 959.19 945.75
907.95 881.58 848.19
  736.26 660.84 617.47 550.26 544.11 468.44 330.50
270.98 219.78 108.52
  90.290
ZeroEnergy[kcal/mol] 10.006251743639380
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
End
!*********************************************
RRHO ! 5
Geometry[angstrom] 17
C 0.39720 0.83744 -0.73682
C 0.40067 0.83156 0.72915
C 1.63453 0.83244 1.56382
C -0.88486 0.73046 1.13128
C -1.76334 0.72407 -0.04279
C -1.00663 0.82390 -1.15539
H 1.16911 1.33920 -1.31123
H 2.24804 1.71388 1.36797
H 1.38909 0.81754 2.62432
H 2.24612 -0.04536 1.34548
H -1.22209 0.65897 2.15457
H -2.84075 0.66532 -0.00603
H -1.34836 0.85276 -2.17706
H 0.73440 -0.50149 -0.97054
O 0.83262 -1.63424 -1.10531
O -0.00992 -2.16404 -0.16561
H -0.87704 -2.13233 -0.58944
  Core RigidRotor
  SymmetryFactor 1.5000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.26 0.77 1.01 0.76 0.26 -0.00 0.25 0.77 1.01 0.76
0.25 -0.00 0.25 0.76 1.01 0.75 0.24
 End
 Rotor Hindered
 Group 16 17
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.26 0.87 1.81 2.48 2.72 2.76 2.80 2.83 2.83 2.80
2.75 2.60 2.19 1.71 1.28 0.80 0.21
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.50 2.22 5.02 8.55 12.04 8.05 5.02 3.02 2.37 -0.11
1.16 3.44 7.64 7.24 4.62 2.37 0.71
 End
  Frequencies[1/cm] 41
  3767.1 3256.1 3233.8 3221.9 3171.7 3135.1 3099.6
3042.0 1633.5 1556.9
  1495.1 1488.2 1469.5 1452.8 1425.2 1386.9 1275.2
1258.8 1207.5 1140.4
  1126.9 1076.4 1036.4 1000.4 985.05 960.40 947.35
912.62 892.44 849.47
  736.78 668.65 622.85 576.96 550.05 468.91 331.10
273.19 221.49 111.52
  97.020
ZeroEnergy[kcal/mol] 10.641187934664371
 ElectronicLevels[1/cm] 1
```

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  0.0000000000000000       2.0000000000000000
 End
!*********************************************
RRHO          !            6
Geometry[angstrom]          17
C    0.39771   0.83652  -0.73712
C    0.40057   0.83169   0.72929
C    1.63451   0.83244   1.56383
C   -0.88489   0.73048   1.13122
C   -1.76328   0.72410  -0.04278
C   -1.00686   0.82401  -1.15531
H    1.16827   1.34160  -1.31059
H    2.24803   1.71386   1.36793
H    1.38913   0.81751   2.62435
H    2.24614  -0.04534   1.34542
H   -1.22210   0.65878   2.15455
H   -2.84073   0.66512  -0.00602
H   -1.34848   0.85266  -2.17705
H    0.73279  -0.48607  -0.96916
O    0.83237  -1.63500  -1.10505
O   -0.00965  -2.16391  -0.16590
H   -0.87715  -2.13213  -0.58945
            Core           RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                      Hindered
 Group   16  17
 Axis            15          14
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                      Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3764.3     3255.8     3233.2     3221.3     3170.2     3135.0     3099.4
3041.9     1634.2     1558.9
  1495.2     1488.1     1460.0     1451.9     1425.1     1387.6     1277.1
1263.6     1207.7     1133.2
  1127.5     1076.3     1035.6     1000.5     977.69     960.85     949.01
918.71     899.54     850.70
  737.70     681.76     628.45     598.88     551.97     472.01     331.49
276.68     225.71     114.37
  101.88
 ZeroEnergy[kcal/mol]    11.352099546429924
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
 End
!*********************************************
RRHO          !            7
Geometry[angstrom]          17
C    0.39820   0.83563  -0.73742
C    0.40047   0.83182   0.72943
C    1.63449   0.83243   1.56384
C   -0.88491   0.73050   1.13117
C   -1.76323   0.72412  -0.04276
C   -1.00707   0.82412  -1.15522
H    1.16744   1.34397  -1.30995
H    2.24801   1.71385   1.36790
H    1.38916   0.81748   2.62439
H    2.24616  -0.04532   1.34535
H   -1.22211   0.65860   2.15454
H   -2.84070   0.66493  -0.00600
H   -1.34859   0.85257  -2.17704
H    0.73119  -0.47062  -0.96778
O    0.83212  -1.63579  -1.10481
O   -0.00938  -2.16378  -0.16619
H   -0.87726  -2.13192  -0.58946
            Core           RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                      Hindered
 Group   16  17
 Axis            15          14
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                      Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3761.4     3255.3     3232.7     3220.7     3168.6     3134.8     3099.2
3041.7     1634.9     1561.0
  1495.3     1488.1     1452.9     1447.8     1424.9     1388.4     1281.0
1267.3     1208.0     1128.2
  1128.0     1076.5     1035.0     1001.9     974.96     959.41     950.46
921.66     902.46     851.91
  739.19     698.97     633.86     611.87     553.64     476.23     331.69
278.20     228.74     117.20
  104.71
 ZeroEnergy[kcal/mol]    11.832944586580750
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
 End
!*********************************************
RRHO          !            8
Geometry[angstrom]          17
C    0.39868   0.83478  -0.73771
C    0.40036   0.83196   0.72957
C    1.63446   0.83243   1.56384
C   -0.88494   0.73052   1.13111
C   -1.76317   0.72415  -0.04274
C   -1.00728   0.82423  -1.15514
H    1.16661   1.34632  -1.30931
H    2.24800   1.71383   1.36786
H    1.38920   0.81745   2.62442
H    2.24619  -0.04530   1.34529
H   -1.22212   0.65841   2.15452
H   -2.84068   0.66474  -0.00598
H   -1.34871   0.85248  -2.17703
H    0.72962  -0.45514  -0.96642
O    0.83189  -1.63660  -1.10456
O   -0.00911  -2.16365  -0.16647
H   -0.87737  -2.13171  -0.58948
            Core           RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
```

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 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                        Hindered
 Group   16  17
 Axis           15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                        Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3758.7     3254.9     3232.1     3220.1     3167.0     3134.6     3099.0
3041.6     1636.0     1563.0
  1495.3     1488.1     1451.7     1437.9     1424.7     1389.3     1287.5
1269.2     1208.2     1128.6
  1124.0     1076.7     1034.4     1003.5     974.69     957.45     951.15
922.32     903.60     853.11
  742.30     716.41     638.91     619.24     555.21     480.57     331.69
279.13     230.71     120.02
  106.44
 ZeroEnergy[kcal/mol]    12.214258701168744
 ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
 RRHO           !           9
 Geometry[angstrom]          17
 C    0.39915   0.83396  -0.73801
 C    0.40026   0.83210   0.72971
 C    1.63444   0.83242   1.56385
 C   -0.88497   0.73054   1.13106
 C   -1.76312   0.72418  -0.04272
 C   -1.00748   0.82434  -1.15506
 H    1.16577   1.34869  -1.30867
 H    2.24799   1.71382   1.36782
 H    1.38923   0.81742   2.62445
 H    2.24621  -0.04529   1.34523
 H   -1.22214   0.65822   2.15450
 H   -2.84066   0.66455  -0.00596
 H   -1.34882   0.85239  -2.17702
 H    0.72811  -0.43967  -0.96504
 O    0.83165  -1.63743  -1.10433
 O   -0.00884  -2.16352  -0.16676
 H   -0.87749  -2.13148  -0.58949
               Core            RigidRotor
         SymmetryFactor     1.5000000000000000
 End
 Rotor                        Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                        Hindered
 Group   16  17
 Axis           15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                        Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3755.6     3254.5     3231.5     3219.4     3165.3     3134.5     3098.8
3041.5     1637.3     1565.0
  1495.3     1488.0     1450.9     1428.9     1424.1     1390.4     1295.4
1270.1     1208.3     1129.0
  1122.3     1077.0     1033.9     1005.6     975.93     957.38     950.30
925.74     907.12     854.38
  750.79     728.03     643.87     623.59     556.71     486.10     331.49
281.68     231.99     122.21
  107.45
 ZeroEnergy[kcal/mol]    12.491182796935844
 ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
 RRHO           !           10
 Geometry[angstrom]          17
 C    0.39959   0.83315  -0.73830
 C    0.40017   0.83226   0.72986
 C    1.63441   0.83240   1.56386
 C   -0.88499   0.73057   1.13100
 C   -1.76306   0.72421  -0.04269
 C   -1.00768   0.82445  -1.15498
 H    1.16491   1.35106  -1.30803
 H    2.24798   1.71381   1.36777
 H    1.38926   0.81739   2.62448
 H    2.24622  -0.04525   1.34517
 H   -1.22216   0.65802   2.15451
 H   -2.84063   0.66435  -0.00594
 H   -1.34893   0.85230  -2.17702
 H    0.72662  -0.42418  -0.96370
 O    0.83142  -1.63829  -1.10409
 O   -0.00857  -2.16341  -0.16705
 H   -0.87756  -2.13126  -0.58949
               Core            RigidRotor
         SymmetryFactor     1.5000000000000000
 End
 Rotor                        Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                        Hindered
 Group   16  17
 Axis           15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                        Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
```

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  3753.3     3254.0     3230.8     3218.7     3163.4     3134.3     3098.7
3041.4     1638.8     1567.0
  1495.4     1488.0     1450.0     1425.1     1419.0     1391.4     1304.0
1270.7     1208.4     1129.3
  1120.8     1077.3     1033.5     1007.7     977.00     958.36     947.89
925.66     908.47     855.60
  763.75     732.35     649.46     626.20     557.83     490.53     331.07
282.43     232.14     123.60
  107.22
 ZeroEnergy[kcal/mol]    12.681099015565435
  ElectronicLevels[1/cm]              1
  0.0000000000000000        2.0000000000000000
 End
!***********************************************
 RRHO          !          11
 Geometry[angstrom]          17
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.46861
 C    1.23437   0.00000   2.30249
 C   -1.28505  -0.10181   1.86955
 C   -2.16306  -0.10815   0.69592
 C   -1.40792  -0.00783  -0.41633
 H    0.76399   0.52113  -0.56876
 H    1.84794   0.88138   2.10636
 H    0.98929  -0.01504   3.36314
 H    1.84625  -0.87766   2.08372
 H   -1.62221  -0.17457   2.89306
 H   -3.24067  -0.16824   0.73267
 H   -1.74910   0.01982  -1.43843
 H    0.32520  -1.24108  -0.22379
 O    0.43113  -2.47154  -0.36525
 O   -0.40834  -2.99561   0.57124
 H   -1.27777  -2.96333   0.14908
             Core           RigidRotor
       SymmetryFactor    1.5000000000000000
 End
  Rotor                    Hindered
  Group    8   9  10
  Axis           3          2
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
  End
  Rotor                    Hindered
  Group   16  17
  Axis           15          14
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
  End
  Rotor                    Hindered
  Group   17
  Axis           16          15
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
  End
    Frequencies[1/cm]          41
  3750.3     3253.6     3230.2     3218.0     3161.7     3134.1     3098.4
3041.2     1640.5     1568.8
  1495.4     1488.0     1449.4     1424.8     1411.4     1392.5     1312.6
1271.0     1208.5     1129.6
  1122.1     1078.0     1033.1     1009.9     978.53     959.86     946.41
926.12     910.32     856.81
  776.94     733.94     656.25     627.73     558.83     496.73     330.56
284.19     233.15     124.46
  105.97
 ZeroEnergy[kcal/mol]    12.811699612274635
  ElectronicLevels[1/cm]              1
  0.0000000000000000        2.0000000000000000
 End
!***********************************************
 RRHO          !          12
 Geometry[angstrom]          17
 C    0.40050   0.83165  -0.73889
 C    0.39993   0.83254   0.73016
 C    1.63436   0.83240   1.56387
 C   -0.88504   0.73062   1.13090
 C   -1.76296   0.72428  -0.04263
 C   -1.00808   0.82468  -1.15483
 H    1.16314   1.35600  -1.30669
 H    2.24796   1.71378   1.36768
 H    1.38935   0.81733   2.62454
 H    2.24628  -0.04521   1.34503
 H   -1.22219   0.65763   2.15448
 H   -2.84059   0.66397  -0.00590
 H   -1.34918   0.85213  -2.17700
 H    0.72389  -0.39327  -0.96108
 O    0.83095  -1.64011  -1.10361
 O   -0.00801  -2.16315  -0.16765
 H   -0.87780  -2.13072  -0.58951
             Core           RigidRotor
       SymmetryFactor    1.5000000000000000
 End
  Rotor                    Hindered
  Group    8   9  10
  Axis           3          2
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
  End
  Rotor                    Hindered
  Group   16  17
  Axis           15          14
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
  End
  Rotor                    Hindered
  Group   17
  Axis           16          15
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
  End
    Frequencies[1/cm]          41
  3747.0     3253.1     3229.6     3217.4     3159.7     3133.9     3098.2
3041.0     1642.2     1570.6
  1495.5     1488.0     1448.8     1424.7     1405.2     1393.8     1321.0
1271.2     1208.7     1130.3
  1125.7     1079.0     1032.9     1012.5     980.61     961.48     946.57
925.66     912.40     857.96
  788.54     734.79     664.88     628.58     559.49     504.60     329.95
285.39     234.03     124.72
  103.77
 ZeroEnergy[kcal/mol]    12.838795073989344
  ElectronicLevels[1/cm]              1
  0.0000000000000000        2.0000000000000000
 End
!***********************************************
 RRHO          !          13
 Geometry[angstrom]          17
 C    0.40098   0.83094  -0.73919
 C    0.39978   0.83267   0.73033
 C    1.63434   0.83241   1.56388
 C   -0.88506   0.73065   1.13085
 C   -1.76291   0.72431  -0.04260
 C   -1.00828   0.82480  -1.15476
 H    1.16221   1.35862  -1.30598
 H    2.24793   1.71376   1.36764
 H    1.38939   0.81731   2.62459
 H    2.24633  -0.04521   1.34496
```

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H   -1.22220   0.65743   2.15443
H   -2.84058   0.66376  -0.00587
H   -1.34932   0.85203  -2.17699
H    0.72264  -0.37790  -0.95985
O    0.83071  -1.64108  -1.10337
O   -0.00771  -2.16302  -0.16797
H   -0.87795  -2.13042  -0.58953
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                   Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                   Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                   Hindered
 Group   17
 Axis           16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3743.2      3252.7      3229.1      3216.8      3157.9      3133.7      3097.9
3040.8      1644.3      1572.4
  1495.5      1487.9      1448.6      1424.6      1401.5      1395.0      1328.7
1271.4      1209.0      1134.0
  1128.6      1080.1      1032.7      1014.7      982.25      962.80      946.95
924.24      913.65      858.93
  798.14      735.88      676.28      628.97      559.47      511.16      329.29
286.58      234.06      124.88
  100.58
 ZeroEnergy[kcal/mol]    12.773721179266685
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
RRHO          !          14
Geometry[angstrom]          17
C    0.40144   0.83025  -0.73949
C    0.39964   0.83283   0.73051
C    1.63431   0.83241   1.56389
C   -0.88509   0.73068   1.13080
C   -1.76286   0.72435  -0.04256
C   -1.00848   0.82493  -1.15468
H    1.16123   1.36136  -1.30523
H    2.24792   1.71375   1.36759
H    1.38945   0.81727   2.62463
H    2.24636  -0.04518   1.34489
H   -1.22222   0.65721   2.15442
H   -2.84057   0.66355  -0.00585
H   -1.34946   0.85194  -2.17698
H    0.72147  -0.36258  -0.95875
O    0.83047  -1.64210  -1.10312
O   -0.00741  -2.16288  -0.16829
H   -0.87807  -2.13010  -0.58952
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                   Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                   Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                   Hindered
 Group   17
 Axis           16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3739.9      3252.2      3228.6      3216.2      3155.9      3133.5      3097.7
3040.6      1646.3      1574.1
  1495.5      1487.9      1448.2      1424.6      1398.6      1396.3      1335.8
1271.6      1209.3      1143.1
  1129.1      1081.2      1032.6      1016.8      983.46      964.24      946.94
923.59      914.73      859.97
  805.96      738.80      690.34      629.08      559.12      515.51      328.50
285.74      232.40      124.36
  96.170
 ZeroEnergy[kcal/mol]    12.614961856738843
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
RRHO          !          15
Geometry[angstrom]          17
C    0.40190   0.82960  -0.73980
C    0.39950   0.83299   0.73069
C    1.63428   0.83241   1.56390
C   -0.88511   0.73072   1.13076
C   -1.76281   0.72438  -0.04253
C   -1.00869   0.82507  -1.15460
H    1.16019   1.36425  -1.30444
H    2.24790   1.71373   1.36753
H    1.38950   0.81724   2.62467
H    2.24639  -0.04516   1.34482
H   -1.22224   0.65699   2.15440
H   -2.84055   0.66334  -0.00581
H   -1.34961   0.85184  -2.17697
H    0.72041  -0.34733  -0.95776
O    0.83022  -1.64316  -1.10286
O   -0.00710  -2.16274  -0.16862
H   -0.87818  -2.12975  -0.58950
            Core           RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                   Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                   Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
```

```
 Rotor                    Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3736.3      3251.8      3228.0      3215.6      3153.9      3133.3      3097.4
3040.4      1648.4      1575.6
  1495.6      1487.8      1447.8      1424.6      1397.8      1396.4      1342.1
1271.7      1209.7      1155.1
  1129.1      1081.4      1032.5      1018.2      983.58      965.76      945.07
925.02      914.27      861.02
  812.18      748.36      704.04      628.98      558.27      513.88      327.51
283.47      229.70      123.05
  90.410
ZeroEnergy[kcal/mol]    12.375809947593067
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !          16
Geometry[angstrom]          17
C    0.40236   0.82900  -0.74011
C    0.39935   0.83317   0.73089
C    1.63425   0.83241   1.56392
C   -0.88514   0.73076   1.13071
C   -1.76275   0.72442  -0.04249
C   -1.00890   0.82521  -1.15452
H    1.15908   1.36730  -1.30361
H    2.24788   1.71372   1.36748
H    1.38956   0.81721   2.62472
H    2.24642  -0.04513   1.34473
H   -1.22227   0.65676   2.15437
H   -2.84052   0.66311  -0.00578
H   -1.34978   0.85174  -2.17695
H    0.71954  -0.33216  -0.95686
O    0.82996  -1.64429  -1.10259
O   -0.00678  -2.16260  -0.16897
H   -0.87830  -2.12937  -0.58946
            Core            RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                    Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3733.0      3251.3      3227.4      3214.9      3151.9      3133.2      3097.2
3040.3      1650.4      1577.5
  1495.6      1487.8      1447.8      1424.8      1400.0      1396.0      1347.7
1271.9      1217.2      1184.1
  1129.3      1083.1      1032.7      1020.1      985.25      967.63      946.85
933.90      916.15      862.66
  817.49      773.01      711.79      628.78      557.21      518.87      326.83
285.24      229.66      121.71
  83.400
ZeroEnergy[kcal/mol]    12.180751833452915
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !          17
Geometry[angstrom]          17
C    0.40282   0.82845  -0.74042
C    0.39919   0.83336   0.73109
C    1.63422   0.83241   1.56393
C   -0.88516   0.73080   1.13067
C   -1.76270   0.72447  -0.04245
C   -1.00913   0.82536  -1.15444
H    1.15788   1.37061  -1.30270
H    2.24786   1.71370   1.36742
H    1.38963   0.81717   2.62477
H    2.24644  -0.04510   1.34464
H   -1.22230   0.65651   2.15435
H   -2.84050   0.66287  -0.00574
H   -1.34996   0.85164  -2.17693
H    0.71888  -0.31714  -0.95612
O    0.82970  -1.64548  -1.10232
O   -0.00643  -2.16245  -0.16934
H   -0.87840  -2.12894  -0.58941
            Core            RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                    Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
   Frequencies[1/cm]          41
  3729.3      3250.8      3226.8      3214.3      3149.8      3133.0      3097.0
3040.1      1652.4      1579.5
  1495.7      1487.8      1448.2      1425.3      1405.1      1396.7      1352.5
1272.2      1255.0      1199.9
  1129.4      1083.5      1032.9      1021.1      985.33      970.88      948.84
944.33      915.74      865.03
  821.93      803.59      713.32      628.51      555.47      517.29      325.88
283.37      227.43      121.37
  74.900
ZeroEnergy[kcal/mol]    11.935677356151727
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!**********************************************
RRHO          !          18
Geometry[angstrom]          17
C    0.40329   0.82797  -0.74074
```

```
C   0.39902   0.83357   0.73132
C   1.63418   0.83240   1.56394
C  -0.88519   0.73085   1.13062
C  -1.76265   0.72451  -0.04241
C  -1.00937   0.82553  -1.15435
H   1.15656   1.37421  -1.30171
H   2.24783   1.71368   1.36736
H   1.38971   0.81712   2.62482
H   2.24647  -0.04507   1.34454
H  -1.22233   0.65625   2.15432
H  -2.84047   0.66262  -0.00570
H  -1.35016   0.85152  -2.17690
H   0.71853  -0.30232  -0.95556
O   0.82942  -1.64677  -1.10203
O  -0.00607  -2.16229  -0.16974
H  -0.87851  -2.12847  -0.58933
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.26   0.77   1.01   0.76   0.26  -0.00   0.25   0.77   1.01   0.76
0.25  -0.00   0.25   0.76   1.01   0.75   0.24
 End
 Rotor                     Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.26   0.87   1.81   2.48   2.72   2.76   2.80   2.83   2.83   2.80
2.75   2.60   2.19   1.71   1.28   0.80   0.21
 End
 Rotor                     Hindered
 Group   17
 Axis           16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.50   2.22   5.02   8.55  12.04   8.05   5.02   3.02   2.37  -0.11
1.16   3.44   7.64   7.24   4.62   2.37   0.71
 End
   Frequencies[1/cm]          41
  3726.0     3250.4     3226.3     3213.7     3147.7     3132.8     3096.7
3039.9     1654.5     1583.4
  1496.0     1487.9     1455.3     1436.3     1421.4     1397.9     1358.0
1334.3     1271.8     1202.6
  1129.4     1085.3     1033.7     1022.3     988.23     981.43     963.28
946.92     917.44     869.43
  830.36     822.20     712.55     628.19     552.93     516.36     325.36
283.70     225.68     120.10
  65.130
ZeroEnergy[kcal/mol]    11.803912910784545
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          19
Geometry[angstrom]           17
C   0.40377   0.82757  -0.74107
C   0.39884   0.83380   0.73156
C   1.63414   0.83240   1.56396
C  -0.88522   0.73090   1.13058
C  -1.76259   0.72456  -0.04236
C  -1.00963   0.82571  -1.15425
H   1.15509   1.37821  -1.30061
H   2.24780   1.71366   1.36729
H   1.38980   0.81708   2.62488
H   2.24648  -0.04504   1.34442
H  -1.22238   0.65596   2.15429
H  -2.84044   0.66235  -0.00564
H  -1.35039   0.85140  -2.17686
H   0.71857  -0.28782  -0.95527
O   0.82913  -1.64818  -1.10172
O  -0.00568  -2.16213  -0.17016
H  -0.87862  -2.12792  -0.58922
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.26   0.77   1.01   0.76   0.26  -0.00   0.25   0.77   1.01   0.76
0.25  -0.00   0.25   0.76   1.01   0.75   0.24
 End
 Rotor                     Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.26   0.87   1.81   2.48   2.72   2.76   2.80   2.83   2.83   2.80
2.75   2.60   2.19   1.71   1.28   0.80   0.21
 End
 Rotor                     Hindered
 Group   17
 Axis           16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.50   2.22   5.02   8.55  12.04   8.05   5.02   3.02   2.37  -0.11
1.16   3.44   7.64   7.24   4.62   2.37   0.71
 End
   Frequencies[1/cm]          41
  3722.7     3249.9     3225.8     3213.2     3145.7     3132.6     3096.5
3039.8     1657.3     1608.3
  1548.3     1495.1     1487.5     1446.4     1423.7     1398.8     1371.8
1356.8     1271.9     1203.2
  1129.4     1086.4     1035.7     1023.0     1006.6     985.64     967.30
946.34     917.90     873.96
  839.65     825.94     710.76     627.86     549.80     511.31     324.67
282.34     223.27     118.89
  53.070
ZeroEnergy[kcal/mol]    11.724357150616425
 ElectronicLevels[1/cm]                 1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          20
Geometry[angstrom]           17
C   0.40426   0.82728  -0.74140
C   0.39863   0.83407   0.73184
C   1.63409   0.83240   1.56398
C  -0.88525   0.73096   1.13054
C  -1.76254   0.72462  -0.04231
C  -1.00991   0.82591  -1.15414
H   1.15342   1.38269  -1.29937
H   2.24777   1.71364   1.36722
H   1.38990   0.81702   2.62495
H   2.24649  -0.04500   1.34429
H  -1.22243   0.65565   2.15426
H  -2.84041   0.66206  -0.00558
H  -1.35066   0.85127  -2.17681
H   0.71910  -0.27380  -0.95534
O   0.82881  -1.64973  -1.10139
O  -0.00526  -2.16195  -0.17062
H  -0.87872  -2.12730  -0.58907
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.26   0.77   1.01   0.76   0.26  -0.00   0.25   0.77   1.01   0.76
0.25  -0.00   0.25   0.76   1.01   0.75   0.24
```

```
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                    Hindered
 Group   17
 Axis           16         15
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
    Frequencies[1/cm]          41
  3719.2      3249.5      3225.2      3212.6      3143.6      3132.4      3096.3
3039.6      1764.0      1656.9
  1574.9      1495.4      1487.6      1447.7      1424.1      1399.5      1377.8
1360.0      1271.9      1203.3
  1129.5      1086.6      1042.1      1025.3      1019.8      986.01      968.65
945.22      917.76      877.41
  843.17      828.04      708.76      627.60      547.07      501.54      323.91
280.77      220.62      117.79
  37.690
 ZeroEnergy[kcal/mol]    11.639625615430999
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
 RRHO           !           21
 Geometry[angstrom]          17
 C    0.40475   0.82713  -0.74175
 C    0.39841   0.83436   0.73213
 C    1.63403   0.83240   1.56401
 C   -0.88528   0.73103   1.13050
 C   -1.76248   0.72468  -0.04226
 C   -1.01021   0.82614  -1.15403
 H    1.15153   1.38776  -1.29796
 H    2.24773   1.71361   1.36713
 H    1.39003   0.81696   2.62503
 H    2.24648  -0.04496   1.34413
 H   -1.22249   0.65530   2.15422
 H   -2.84037   0.66174  -0.00550
 H   -1.35097   0.85113  -2.17674
 H    0.72032  -0.26048  -0.95584
 O    0.82848  -1.65145  -1.10104
 O   -0.00481  -2.16177  -0.17112
 H   -0.87882  -2.12658  -0.58887
                Core            RigidRotor
        SymmetryFactor    1.5000000000000000
 End
 Rotor                    Hindered
 Group    8   9  10
 Axis            3          2
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.26    0.77    1.01    0.76    0.26   -0.00    0.25    0.77    1.01    0.76
0.25   -0.00    0.25    0.76    1.01    0.75    0.24
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.26    0.87    1.81    2.48    2.72    2.76    2.80    2.83    2.83    2.80
2.75    2.60    2.19    1.71    1.28    0.80    0.21
 End
 Rotor                    Hindered
 Group   17
 Axis           16         15
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.50    2.22    5.02    8.55   12.04    8.05    5.02    3.02    2.37   -0.11
1.16    3.44    7.64    7.24    4.62    2.37    0.71
 End
    Frequencies[1/cm]          41
  3715.8      3249.1      3224.8      3212.1      3141.6      3132.3      3096.0
3039.4      1931.1      1659.1
  1578.7      1495.5      1487.6      1448.7      1424.2      1399.9      1379.1
1361.9      1271.8      1203.0
  1129.5      1087.0      1053.3      1028.2      1021.7      985.39      969.56
942.90      917.39      879.59
  844.00      829.49      706.50      627.27      543.41      489.96      323.26
277.25      217.38      116.75
  6.2300
 ZeroEnergy[kcal/mol]    11.522383442945850
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1933.7400000000000
      WellDepth[kcal/mol]         18.04
      WellDepth[kcal/mol]         20.85
 End
End
End
```

```
!****************************************************
!             GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30         ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct     ! direct or low-eigenvalue
!
WellCutoff                            20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                 0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                           10
!ChemicalEigenvalueMin                1.e-6          #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                 1.3
!!
RateOutput                            rate.out                   ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!             MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                          ! Default collisional
energy relaxation kernel
    Exponential                                             ! Currently the only
possible energy relaxation model
       Factor[1/cm]                 316                     ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                  0.535                      ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff                 10                        ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                        ! Collision frequency
model
    LennardJones                                            ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]                  90.58  281.367           ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]               3.54    4.694              ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                  39.948  79.05478            ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!*************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]            14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50263
 C    1.24622   0.00000   2.31947
 C   -1.27227   0.00046   1.92591
 C   -2.17585   0.00051   0.77474
 C   -1.45565   0.00011  -0.35294
 H    0.51979   0.87601  -0.40113
 H    1.85947   0.87812   2.10478
 H    1.01835  -0.00094   3.38445
 H    1.86045  -0.87709   2.10340
 H   -1.59049   0.00052   2.95892
 H   -3.25397   0.00095   0.84079
 H   -1.83452  -0.00013  -1.36297
 H    0.51979  -0.87591  -0.40126
      Core    RigidRotor
           SymmetryFactor    1.0000000000000000
      End
 Rotor                         Hindered
 Group    8   9  10
 Axis           3           2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.08    0.30    0.62    0.95    1.20    1.29    1.21    0.96    0.62    0.30
0.08
 End
    Frequencies[1/cm]          35
  3245.2      3221.6      3209.3      3128.8      3090.6      3074.8      3042.5
3036.2      1695.3      1615.6
  1495.0      1486.6      1424.0      1421.5      1397.2      1340.1      1274.6
1198.6      1152.9      1130.9
  1060.1      1033.7      1005.4      976.89      961.82      922.95      892.68
863.70      828.81      700.71
  623.69      533.08      369.88      325.94      227.72
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]             3
 O    0.00000   0.00000   0.00000
 O    0.00000   0.00000   1.31234
 H    0.93494   0.00000   1.57303
      Core    RigidRotor
           SymmetryFactor    1.0000000000000000
      End
    Frequencies[1/cm]           3
  1234.9      1462.2      3683.2
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]             13
```

```
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.51694
C    1.09843   0.00000   2.30770
C   -1.35798   0.00031   1.92840
C   -2.19992   0.00042   0.79313
C   -1.45663   0.00024  -0.34805
H    0.51600  -0.87687  -0.39945
H    0.51620   0.87681  -0.39935
H    2.09538  -0.00023   1.88922
H    1.00817   0.00002   3.38527
H   -1.68677   0.00025   2.95662
H   -3.27947   0.00064   0.83092
H   -1.83825   0.00021  -1.35705
      Core    RigidRotor
           SymmetryFactor    1.0000000000000000
      End
Rotor                        Hindered
Group    8   9  10
Axis            3           2
Symmetry           3
Potential[kcal/mol]           12
  0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
   Frequencies[1/cm]           33
  182.10      356.98      395.70      533.46      629.59      643.35      680.57
792.84      824.96      845.75
  867.02      937.43      954.59      969.91      992.63      1039.9      1117.1
1156.6      1270.0      1282.1
  1315.8      1407.1      1426.7      1447.0      1530.6      1581.6      3052.2
3085.2      3159.4      3215.5
  3230.8      3244.8      3250.3
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End

!************************************
Fragment PROD2
RRHO
Geometry[angstrom]               4
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.42622
H    0.94322   0.00000   1.61480
H   -0.34861  -0.87643  -0.18855
      Core    RigidRotor
           SymmetryFactor    2.0000000000000000
      End
Rotor                        Hindered
Group    4
Axis            1           2
Symmetry           1
Potential[kcal/mol]           18
  0.00    0.07    0.48    0.80    0.77    0.40    0.02    0.06    0.91    2.62    4.92
7.15    8.51    8.38    6.81    4.51    2.28    0.70
End
   Frequencies[1/cm]            5
  3840.9      3839.6      1465.2      1361.0      1016.3
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
GroundEnergy[kcal/mol]    -4.83
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]              17
C    0.00475   0.00199   0.00555
C    0.00067   0.00339   1.50685
C    1.24570   0.00947   2.32361
C   -1.27182  -0.01464   1.93258
C   -2.17302  -0.03122   0.77961
C   -1.44895  -0.02666  -0.35167
H    0.50176   0.89034  -0.39630
H    1.85598   0.88778   2.10327
H    1.01896   0.01072   3.38844
H    1.85866  -0.86764   2.10636
H   -1.59261  -0.02311   2.96405
H   -3.25186  -0.03485   0.84197
H   -1.82635  -0.02064  -1.36228
H    0.54049  -0.86248  -0.39897
O   -0.56771  -3.27803  -0.76776
O   -1.52004  -3.14387   0.12229
H   -1.71000  -2.18037   0.15966
      Core    RigidRotor
           SymmetryFactor    0.50000000000000000
      End
   Frequencies[1/cm]           45
  21.795      41.555      74.811      109.46      151.96      168.14      244.89
326.53      380.96      476.05
  541.66      624.24      721.79      831.59      864.75      893.63      923.48
961.56      987.48      1006.8
  1035.3      1060.9      1130.9      1156.9      1199.9      1259.3      1276.0
1344.1      1398.3      1420.1
  1426.2      1487.5      1493.9      1514.4      1602.1      1687.5      3041.1
3050.2      3085.1      3097.8
  3134.9      3212.4      3226.0      3246.2      3464.3
 ZeroEnergy[kcal/mol]              -6.01
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]              17
C   -0.00152   0.00064   0.00473
C   -0.00117   0.00178   1.52119
C    1.09899   0.00087   2.31309
C   -1.35735  -0.02988   1.93691
C   -2.20036  -0.08059   0.80159
C   -1.45643  -0.07696  -0.34036
H    0.45704   0.91043  -0.39185
H    2.09544   0.02061   1.89367
H    1.00880   0.00195   3.39077
H    0.50805  -2.55601   1.65259
H   -1.68504  -0.03700   2.96512
H   -3.27935  -0.11609   0.84104
H   -1.83860  -0.10131  -1.34886
H    0.56250  -0.84370  -0.39710
O    0.21883  -3.16356   0.95999
O   -1.16226  -3.32375   1.26791
H   -1.56653  -2.62650   0.73716
      Core    RigidRotor
           SymmetryFactor    0.50000000000000000
      End
   Frequencies[1/cm]           45
  34.397      48.917      83.538      107.71      124.44      191.75      228.14
357.05      400.90      509.43
  538.15      636.77      644.93      693.72      801.08      825.76      852.00
867.45      939.76      955.25
  976.07      994.18      1017.8      1041.6      1117.7      1165.9      1276.4
1283.3      1317.4      1407.6
  1424.5      1426.2      1442.3      1451.6      1530.3      1577.7      3056.0
3095.8      3159.0      3217.4
  3234.8      3246.3      3251.5      3768.8      3783.3
 ZeroEnergy[kcal/mol]              -6.92
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
End
!************************************
Barrier         B1  REACS WR
  RRHO
    Stoichiometry  H9C6O2
```

```
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]       14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50263
C    1.24622   0.00000   2.31947
C   -1.27227   0.00046   1.92591
C   -2.17585   0.00051   0.77474
C   -1.45565   0.00011  -0.35294
H    0.51979   0.87601  -0.40113
H    1.85947   0.87812   2.10478
H    1.01835  -0.00094   3.38445
H    1.86045  -0.87709   2.10340
H   -1.59049   0.00052   2.95892
H   -3.25397   0.00095   0.84079
H   -1.83452  -0.00013  -1.36297
H    0.51979  -0.87591  -0.40126
      FragmentGeometry[angstrom]       3
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.31234
H    0.93494   0.00000   1.57303
                    SymmetryFactor     1.0000000000000000
        PotentialPrefactor[au]        10.
        PotentialPowerExponent        6
                End
Rotor                   Hindered
Geometry[angstrom]          14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50263
C    1.24622   0.00000   2.31947
C   -1.27227   0.00046   1.92591
C   -2.17585   0.00051   0.77474
C   -1.45565   0.00011  -0.35294
H    0.51979   0.87601  -0.40113
H    1.85947   0.87812   2.10478
H    1.01835  -0.00094   3.38445
H    1.86045  -0.87709   2.10340
H   -1.59049   0.00052   2.95892
H   -3.25397   0.00095   0.84079
H   -1.83452  -0.00013  -1.36297
H    0.51979  -0.87591  -0.40126
Group    8   9  10
Axis          3        2
Symmetry         3
Potential[kcal/mol]        12
  0.0000     0.80000E-01 0.30000     0.62000     0.95000      1.2000      1.2900
1.2100     0.96000     0.62000
 0.30000     0.80000E-01
End
    Frequencies[1/cm]        38
  3245.2     3221.6     3209.3     3128.8     3090.6     3074.8     3042.5
3036.2     1695.3     1615.6
  1495.0     1486.6     1424.0     1421.5     1397.2     1340.1     1274.6
1198.6     1152.9     1130.9
  1060.1     1033.7     1005.4     976.89     961.82     922.95     892.68
863.70     828.81     700.71
  623.69     533.08     369.88     325.94     227.72
  1234.9     1462.2     3683.2
 ZeroEnergy[kcal/mol]          0.
 ElectronicLevels[1/cm]              1
  0.0000000000000000        4.0000000000000000
End
!************************************
Barrier       B3  WP PRODS
  RRHO
    Stoichiometry  H9C6O2
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]       13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.51694
C    1.09843   0.00000   2.30770
C   -1.35798   0.00031   1.92840
C   -2.19992   0.00042   0.79313
C   -1.45663   0.00024  -0.34805
H    0.51600  -0.87687  -0.39945
H    0.51620   0.87681  -0.39935
H    2.09538  -0.00023   1.88922
H    1.00817   0.00002   3.38527
H   -1.68677   0.00025   2.95662
H   -3.27947   0.00064   0.83092
H   -1.83825   0.00021  -1.35705
      FragmentGeometry[angstrom]       4
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.42622
H    0.94322   0.00000   1.61480
H   -0.34861  -0.87643  -0.18855
                    SymmetryFactor     2.0000000000000000
        PotentialPrefactor[au]        10.
        PotentialPowerExponent        6
                End
Rotor                   Hindered
Geometry[angstrom]          4
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.42622
H    0.94322   0.00000   1.61480
H   -0.34861  -0.87643  -0.18855
Group    4
Axis          1        2
Symmetry         1
Potential[kcal/mol]        18
  0.0000     0.70000E-01 0.48000     0.80000     0.77000     0.40000
0.20000E-01 0.60000E-01 0.91000     2.6200
  4.9200      7.1500      8.5100      8.3800      6.8100      4.5100      2.2800
0.70000
End
    Frequencies[1/cm]        38
  182.10     356.98     395.70     533.46     629.59     643.35     680.57
792.84     824.96     845.75
  867.02     937.43     954.59     969.91     992.63     1039.9     1117.1
1156.6     1270.0     1282.1
  1315.8     1407.1     1426.7     1447.0     1530.6     1581.6     3052.2
3085.2     3159.4     3215.5
  3230.8     3244.8     3250.3
  3840.9     3839.6     1465.2     1361.0     1016.3
 ZeroEnergy[kcal/mol]          -4.8292856380566329
 ElectronicLevels[1/cm]              1
  0.0000000000000000        4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO          !          1
Geometry[angstrom]          17
C    0.15289   0.84623  -1.49467
C    0.15875   0.84549   0.01210
C    1.33486   0.85496   0.81013
C   -1.14263   0.71533   0.43089
C   -2.02040   0.64185  -0.71298
C   -1.29412   0.71157  -1.84537
H    0.58687   1.76704  -1.89439
H    2.23427   1.26205   0.35859
H    1.20941   1.10468   1.85870
H    1.64529  -0.54444   0.92012
H   -1.45498   0.66944   1.46295
H   -3.09457   0.54813  -0.65654
H   -1.67368   0.69171  -2.85492
H    0.75681   0.02479  -1.89108
O    1.70257  -1.65646   0.99204
O    0.39254  -2.02016   1.25456
H    0.00551  -2.12780   0.37945
              Core          RigidRotor
        SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15  16  17
 Axis          3        2
 Symmetry         3
 Potential[kcal/mol]        12
```

```
 0.00 0.27 1.09 2.47 4.41 6.78 9.24 5.07 3.37 1.96 0.89
0.22
 End
 Rotor Hindered
 Group 16 17
 Axis 15 10
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.28 0.87 1.45 1.75 1.72 1.79 2.00 2.09 2.15 2.24
2.38 2.53 2.61 2.53 2.22 1.49 0.39
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.54 2.14 4.26 5.80 5.70 3.98 1.64 -0.16 -0.77 -0.03
1.95 4.82 7.51 7.80 5.38 2.67 0.75
 End
 Frequencies[1/cm] 41
 3801.9 3249.5 3237.0 3222.3 3205.8 3118.6 3084.9
3050.6 1603.6 1556.6
 1500.0 1462.7 1430.3 1427.0 1400.2 1362.8 1293.8
1266.8 1183.3 1154.4
 1128.8 1093.6 1050.6 1022.1 1007.5 981.65 964.37
923.37 894.06 867.95
 829.71 707.99 668.58 636.87 573.05 531.80 411.59
347.76 258.79 178.84
 78.110
 ZeroEnergy[kcal/mol] 8.5739447035577712
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
 End
!**********************************************
 RRHO ! 2
 Geometry[angstrom] 17
 C 0.15281 0.84623 -1.49460
 C 0.15805 0.84556 0.01193
 C 1.33556 0.85391 0.81049
 C -1.14226 0.71536 0.43089
 C -2.02043 0.64184 -0.71321
 C -1.29421 0.71156 -1.84535
 H 0.58687 1.76706 -1.89431
 H 2.23355 1.26421 0.35878
 H 1.20917 1.10671 1.85831
 H 1.64459 -0.52909 0.91908
 H -1.45482 0.66961 1.46293
 H -3.09459 0.54813 -0.65664
 H -1.67369 0.69174 -2.85493
 H 0.75684 0.02480 -1.89098
 O 1.70217 -1.65708 0.99216
 O 0.39292 -2.02008 1.25448
 H 0.00538 -2.12748 0.37942
 Core RigidRotor
 SymmetryFactor 0.50000000000000000
 End
 Rotor Hindered
 Group 8 9 10 15 16 17
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
 0.00 0.27 1.09 2.47 4.41 6.78 9.24 5.07 3.37 1.96 0.89
0.22
 End
 Rotor Hindered
 Group 16 17
 Axis 15 10
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.28 0.87 1.45 1.75 1.72 1.79 2.00 2.09 2.15 2.24
2.38 2.53 2.61 2.53 2.22 1.49 0.39
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.54 2.14 4.26 5.80 5.70 3.98 1.64 -0.16 -0.77 -0.03
1.95 4.82 7.51 7.80 5.38 2.67 0.75
 End
 Frequencies[1/cm] 41
 3800.0 3249.4 3236.7 3222.2 3204.2 3117.3 3084.7
3050.4 1605.2 1550.8
 1497.3 1461.0 1429.7 1426.5 1395.2 1362.4 1289.0
1254.9 1164.1 1154.9
 1129.1 1097.5 1048.2 1024.0 1008.9 981.82 964.70
922.26 894.31 869.66
 829.75 708.22 664.61 636.05 566.23 530.06 411.32
346.83 262.15 180.85
 83.480
 ZeroEnergy[kcal/mol] 9.2391682316399795
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
 End
!**********************************************
 RRHO ! 3
 Geometry[angstrom] 17
 C 0.15273 0.84623 -1.49454
 C 0.15737 0.84563 0.01177
 C 1.33623 0.85291 0.81084
 C -1.14190 0.71540 0.43089
 C -2.02046 0.64183 -0.71343
 C -1.29429 0.71155 -1.84533
 H 0.58686 1.76707 -1.89424
 H 2.23286 1.26630 0.35896
 H 1.20895 1.10868 1.85794
 H 1.64390 -0.51366 0.91805
 H -1.45467 0.66977 1.46292
 H -3.09462 0.54813 -0.65673
 H -1.67370 0.69176 -2.85494
 H 0.75687 0.02481 -1.89090
 O 1.70177 -1.65773 0.99228
 O 0.39330 -2.02001 1.25440
 H 0.00525 -2.12716 0.37939
 Core RigidRotor
 SymmetryFactor 0.50000000000000000
 End
 Rotor Hindered
 Group 8 9 10 15 16 17
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
 0.00 0.27 1.09 2.47 4.41 6.78 9.24 5.07 3.37 1.96 0.89
0.22
 End
 Rotor Hindered
 Group 16 17
 Axis 15 10
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.28 0.87 1.45 1.75 1.72 1.79 2.00 2.09 2.15 2.24
2.38 2.53 2.61 2.53 2.22 1.49 0.39
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.54 2.14 4.26 5.80 5.70 3.98 1.64 -0.16 -0.77 -0.03
1.95 4.82 7.51 7.80 5.38 2.67 0.75
 End
 Frequencies[1/cm] 41
 3797.9 3249.4 3236.4 3222.1 3202.5 3116.0 3084.5
3050.3 1607.0 1543.5
 1497.0 1461.8 1429.3 1426.0 1394.3 1361.9 1287.8
1249.1 1159.5 1154.3
 1129.3 1098.4 1043.0 1024.5 1009.6 981.95 964.95
921.17 894.60 871.46
```

829.79 708.38 663.53 634.32 562.88 529.04 411.14
345.78 265.02 182.84
88.510
ZeroEnergy[kcal/mol] 9.9049107575011277
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 4
Geometry[angstrom] 17
C 0.15266 0.84623 -1.49448
C 0.15670 0.84571 0.01161
C 1.33688 0.85197 0.81117
C -1.14154 0.71543 0.43089
C -2.02049 0.64182 -0.71364
C -1.29437 0.71154 -1.84531
H 0.58686 1.76708 -1.89417
H 2.23218 1.26835 0.35914
H 1.20873 1.11060 1.85758
H 1.64323 -0.49818 0.91702
H -1.45453 0.66992 1.46291
H -3.09464 0.54814 -0.65682
H -1.67371 0.69179 -2.85495
H 0.75690 0.02482 -1.89082
O 1.70137 -1.65841 0.99240
O 0.39368 -2.01994 1.25432
H 0.00512 -2.12684 0.37934
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.27 1.09 2.47 4.41 6.78 9.24 5.07 3.37 1.96 0.89
0.22
End
Rotor Hindered
Group 16 17
Axis 15 10
Symmetry 1
Potential[kcal/mol] 18
0.00 0.28 0.87 1.45 1.75 1.72 1.79 2.00 2.09 2.15 2.24
2.38 2.53 2.61 2.53 2.22 1.49 0.39
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.54 2.14 4.26 5.80 5.70 3.98 1.64 -0.16 -0.77 -0.03
1.95 4.82 7.51 7.80 5.38 2.67 0.75
End
Frequencies[1/cm] 41
3795.8 3249.3 3236.0 3222.0 3200.8 3114.6 3084.3
3050.1 1609.1 1535.3
1497.7 1463.5 1429.0 1425.5 1395.3 1361.6 1287.4
1246.4 1165.5 1152.5
1129.5 1097.3 1040.1 1024.6 1010.1 982.05 965.20
920.26 894.99 873.30
829.82 708.48 663.24 632.34 561.75 528.88 410.96
344.63 267.57 184.85
93.290
ZeroEnergy[kcal/mol] 10.547085448006101
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 5
Geometry[angstrom] 17
C 0.15258 0.84623 -1.49442
C 0.15604 0.84578 0.01145
C 1.33751 0.85106 0.81150
C -1.14118 0.71547 0.43089
C -2.02052 0.64181 -0.71386
C -1.29445 0.71152 -1.84529
H 0.58686 1.76709 -1.89410
H 2.23151 1.27036 0.35932
H 1.20851 1.11248 1.85722
H 1.64258 -0.48267 0.91602
H -1.45440 0.67008 1.46290
H -3.09467 0.54814 -0.65692
H -1.67372 0.69181 -2.85496
H 0.75693 0.02483 -1.89076
O 1.70098 -1.65912 0.99252
O 0.39406 -2.01988 1.25424
H 0.00499 -2.12652 0.37928
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.27 1.09 2.47 4.41 6.78 9.24 5.07 3.37 1.96 0.89
0.22
End
Rotor Hindered
Group 16 17
Axis 15 10
Symmetry 1
Potential[kcal/mol] 18
0.00 0.28 0.87 1.45 1.75 1.72 1.79 2.00 2.09 2.15 2.24
2.38 2.53 2.61 2.53 2.22 1.49 0.39
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.54 2.14 4.26 5.80 5.70 3.98 1.64 -0.16 -0.77 -0.03
1.95 4.82 7.51 7.80 5.38 2.67 0.75
End
Frequencies[1/cm] 41
3793.6 3249.2 3235.7 3221.8 3199.0 3113.2 3084.1
3049.8 1611.3 1526.9
1499.1 1465.5 1428.6 1425.0 1397.0 1361.3 1287.4
1245.3 1174.6 1151.7
1129.6 1096.6 1040.0 1025.4 1010.7 982.12 965.51
919.55 895.49 875.17
829.85 708.53 662.97 630.36 562.11 529.45 411.09
343.41 270.97 187.47
97.720
ZeroEnergy[kcal/mol] 11.144107945887029
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 6
Geometry[angstrom] 17
C 0.15251 0.84623 -1.49435
C 0.15539 0.84585 0.01130
C 1.33814 0.85018 0.81182
C -1.14084 0.71551 0.43089
C -2.02054 0.64180 -0.71406
C -1.29452 0.71151 -1.84527
H 0.58686 1.76711 -1.89404
H 2.23084 1.27237 0.35950
H 1.20829 1.11435 1.85685
H 1.64196 -0.46713 0.91504
H -1.45427 0.67024 1.46289
H -3.09470 0.54815 -0.65701
H -1.67374 0.69184 -2.85498
H 0.75696 0.02484 -1.89069
O 1.70059 -1.65985 0.99264
O 0.39444 -2.01981 1.25417

```
H 0.00486 -2.12618 0.37922
  Core RigidRotor
  SymmetryFactor 0.50000000000000000
End
 Rotor Hindered
 Group 8 9 10 15 16 17
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
 0.00 0.27 1.09 2.47 4.41 6.78 9.24 5.07 3.37 1.96 0.89
0.22
 End
 Rotor Hindered
 Group 16 17
 Axis 15 10
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.28 0.87 1.45 1.75 1.72 1.79 2.00 2.09 2.15 2.24
2.38 2.53 2.61 2.53 2.22 1.49 0.39
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.54 2.14 4.26 5.80 5.70 3.98 1.64 -0.16 -0.77 -0.03
1.95 4.82 7.51 7.80 5.38 2.67 0.75
 End
 Frequencies[1/cm] 41
 3791.3 3249.1 3235.2 3221.6 3197.1 3111.7 3083.9
3049.6 1613.7 1519.5
 1500.3 1467.5 1428.3 1424.5 1399.0 1361.1 1287.5
1245.0 1185.5 1151.2
 1129.8 1096.7 1041.3 1027.4 1011.6 982.16 965.86
918.98 896.02 877.01
 829.89 708.53 662.47 628.26 563.75 530.43 411.22
342.10 274.60 189.98
 101.72
ZeroEnergy[kcal/mol] 11.684141397152871
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!***********************************************
RRHO ! 7
Geometry[angstrom] 17
C 0.15244 0.84623 -1.49429
C 0.15474 0.84592 0.01115
C 1.33875 0.84933 0.81214
C -1.14049 0.71554 0.43089
C -2.02057 0.64179 -0.71427
C -1.29461 0.71150 -1.84526
H 0.58686 1.76712 -1.89397
H 2.23017 1.27437 0.35967
H 1.20808 1.11621 1.85649
H 1.64137 -0.45158 0.91406
H -1.45415 0.67039 1.46288
H -3.09472 0.54815 -0.65710
H -1.67375 0.69186 -2.85499
H 0.75699 0.02485 -1.89064
O 1.70019 -1.66061 0.99277
O 0.39483 -2.01974 1.25410
H 0.00472 -2.12584 0.37914
  Core RigidRotor
  SymmetryFactor 0.50000000000000000
End
 Rotor Hindered
 Group 8 9 10 15 16 17
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
 0.00 0.27 1.09 2.47 4.41 6.78 9.24 5.07 3.37 1.96 0.89
0.22
 End
 Rotor Hindered
 Group 16 17
 Axis 15 10
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.28 0.87 1.45 1.75 1.72 1.79 2.00 2.09 2.15 2.24
2.38 2.53 2.61 2.53 2.22 1.49 0.39
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.54 2.14 4.26 5.80 5.70 3.98 1.64 -0.16 -0.77 -0.03
1.95 4.82 7.51 7.80 5.38 2.67 0.75
 End
 Frequencies[1/cm] 41
 3789.0 3248.9 3234.8 3221.3 3195.2 3110.2 3083.7
3049.3 1616.2 1515.8
 1499.1 1468.9 1427.9 1424.0 1401.0 1360.9 1287.8
1245.1 1196.3 1150.6
 1130.0 1095.8 1042.5 1028.5 1012.1 982.16 966.11
918.38 896.44 878.73
 829.93 708.46 661.51 624.17 566.60 531.47 410.65
340.63 276.82 192.04
 105.17
ZeroEnergy[kcal/mol] 12.211518997377112
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!***********************************************
RRHO ! 8
Geometry[angstrom] 17
C 0.15237 0.84623 -1.49423
C 0.15409 0.84600 0.01100
C 1.33936 0.84852 0.81245
C -1.14015 0.71558 0.43089
C -2.02060 0.64178 -0.71448
C -1.29469 0.71149 -1.84524
H 0.58686 1.76714 -1.89391
H 2.22950 1.27638 0.35985
H 1.20786 1.11807 1.85613
H 1.64082 -0.43604 0.91311
H -1.45403 0.67055 1.46288
H -3.09475 0.54816 -0.65719
H -1.67376 0.69188 -2.85501
H 0.75702 0.02486 -1.89058
O 1.69979 -1.66139 0.99290
O 0.39523 -2.01968 1.25402
H 0.00459 -2.12549 0.37906
  Core RigidRotor
  SymmetryFactor 0.50000000000000000
End
 Rotor Hindered
 Group 8 9 10 15 16 17
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
 0.00 0.27 1.09 2.47 4.41 6.78 9.24 5.07 3.37 1.96 0.89
0.22
 End
 Rotor Hindered
 Group 16 17
 Axis 15 10
 Symmetry 1
 Potential[kcal/mol] 18
 0.00 0.28 0.87 1.45 1.75 1.72 1.79 2.00 2.09 2.15 2.24
2.38 2.53 2.61 2.53 2.22 1.49 0.39
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
```

```
  0.00  0.54  2.14  4.26  5.80  5.70  3.98  1.64  -0.16  -0.77  -0.03
1.95  4.82  7.51  7.80  5.38  2.67  0.75
 End
   Frequencies[1/cm]     41
  3786.7   3248.8   3234.3   3221.0   3193.2   3108.6   3083.4
3049.0   1618.8   1517.4
  1494.3   1469.5   1427.6   1423.5   1402.7   1360.6   1288.3
1246.0   1206.8   1150.1
  1130.2   1094.9   1044.0   1029.0   1012.4   982.11   966.28
917.76   896.80   880.16
  829.97   708.35   660.29   617.87   570.75   532.47   409.59
339.09   277.68   193.88
  108.24
 ZeroEnergy[kcal/mol]   12.533420835857541
 ElectronicLevels[1/cm]          1
  0.0000000000000000    2.0000000000000000
 End
!**********************************************
 RRHO     !     9
 Geometry[angstrom]     17
 C   0.15230   0.84624  -1.49418
 C   0.15345   0.84607   0.01085
 C   1.33997   0.84773   0.81276
 C  -1.13980   0.71562   0.43088
 C  -2.02062   0.64176  -0.71468
 C  -1.29477   0.71147  -1.84523
 H   0.58686   1.76715  -1.89384
 H   2.22882   1.27842   0.36002
 H   1.20764   1.11995   1.85576
 H   1.64031  -0.42051   0.91217
 H  -1.45391   0.67070   1.46287
 H  -3.09478   0.54817  -0.65728
 H  -1.67378   0.69191  -2.85502
 H   0.75705   0.02488  -1.89053
 O   1.69938  -1.66219   0.99303
 O   0.39564  -2.01961   1.25395
 H   0.00445  -2.12512   0.37897
          Core        RigidRotor
      SymmetryFactor   0.50000000000000000
 End
  Rotor            Hindered
  Group   8  9  10  15  16  17
  Axis      3      2
  Symmetry      3
  Potential[kcal/mol]     12
  0.00  0.27  1.09  2.47  4.41  6.78  9.24  5.07  3.37  1.96  0.89
0.22
  End
  Rotor            Hindered
  Group   16  17
  Axis      15      10
  Symmetry      1
  Potential[kcal/mol]     18
  0.00  0.28  0.87  1.45  1.75  1.72  1.79  2.00  2.09  2.15  2.24
2.38  2.53  2.61  2.53  2.22  1.49  0.39
  End
  Rotor            Hindered
  Group   17
  Axis      16      15
  Symmetry      1
  Potential[kcal/mol]     18
  0.00  0.54  2.14  4.26  5.80  5.70  3.98  1.64  -0.16  -0.77  -0.03
1.95  4.82  7.51  7.80  5.38  2.67  0.75
  End
   Frequencies[1/cm]     41
  3784.2   3248.6   3233.8   3220.7   3191.1   3107.0   3083.1
3048.7   1621.6   1522.7
  1489.3   1469.1   1427.3   1423.1   1404.5   1360.5   1289.0
1247.9   1218.3   1149.8
  1130.3   1097.4   1046.6   1031.8   1013.5   982.04   966.63
917.42   897.18   881.68
  830.03   708.21   659.16   612.72   577.05   533.05   408.71
337.56   279.77   196.11
  110.70
 ZeroEnergy[kcal/mol]   12.774590617130499
 ElectronicLevels[1/cm]          1
  0.0000000000000000    2.0000000000000000
 End
!**********************************************
 RRHO     !     10
 Geometry[angstrom]     17
 C   0.15221   0.84624  -1.49411
 C   0.15280   0.84616   0.01070
 C   1.34057   0.84695   0.81307
 C  -1.13946   0.71566   0.43088
 C  -2.02064   0.64175  -0.71488
 C  -1.29484   0.71146  -1.84523
 H   0.58685   1.76717  -1.89377
 H   2.22815   1.28050   0.36019
 H   1.20741   1.12186   1.85543
 H   1.63986  -0.40501   0.91125
 H  -1.45379   0.67086   1.46288
 H  -3.09483   0.54817  -0.65737
 H  -1.67381   0.69193  -2.85508
 H   0.75707   0.02488  -1.89048
 O   1.69895  -1.66302   0.99316
 O   0.39606  -2.01954   1.25388
 H   0.00430  -2.12474   0.37886
          Core        RigidRotor
      SymmetryFactor   0.50000000000000000
 End
  Rotor            Hindered
  Group   8  9  10  15  16  17
  Axis      3      2
  Symmetry      3
  Potential[kcal/mol]     12
  0.00  0.27  1.09  2.47  4.41  6.78  9.24  5.07  3.37  1.96  0.89
0.22
  End
  Rotor            Hindered
  Group   16  17
  Axis      15      10
  Symmetry      1
  Potential[kcal/mol]     18
  0.00  0.28  0.87  1.45  1.75  1.72  1.79  2.00  2.09  2.15  2.24
2.38  2.53  2.61  2.53  2.22  1.49  0.39
  End
  Rotor            Hindered
  Group   17
  Axis      16      15
  Symmetry      1
  Potential[kcal/mol]     18
  0.00  0.54  2.14  4.26  5.80  5.70  3.98  1.64  -0.16  -0.77  -0.03
1.95  4.82  7.51  7.80  5.38  2.67  0.75
  End
   Frequencies[1/cm]     41
  3781.4   3248.2   3233.1   3220.1   3188.6   3105.0   3082.7
3048.3   1624.4   1529.0
  1485.7   1467.0   1427.2   1422.8   1406.0   1360.3   1290.3
1251.6   1225.7   1149.5
  1130.5   1099.6   1048.3   1032.4   1013.8   981.99   966.79
916.95   897.41   882.83
  830.09   708.16   658.02   603.62   584.41   532.99   406.99
335.93   280.04   197.80
  112.38
 ZeroEnergy[kcal/mol]   12.962692004978308
 ElectronicLevels[1/cm]          1
  0.0000000000000000    2.0000000000000000
 End
!**********************************************
 RRHO     !     11
 Geometry[angstrom]     17
 C   0.00000   0.00000   0.00000
 C   0.00000   0.00000   1.50460
 C   1.18904   0.00000   2.30744
 C  -1.29125  -0.13054   1.92492
 C  -2.17281  -0.20450   0.77896
 C  -1.44706  -0.13479  -0.35117
```

```
H   0.43472   0.92094  -0.39965
H   2.07528   0.43644   1.85442
H   1.05504   0.27761   3.34908
H   1.48739  -1.23580   2.40438
H  -1.60581  -0.17522   2.95693
H  -3.24700  -0.29806   0.83657
H  -1.82596  -0.15429  -1.36105
H   0.60497  -0.82134  -0.39638
O   1.54637  -2.51015   2.48735
O   0.24436  -2.86572   2.74785
H  -0.14800  -2.97058   1.87281
          Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15          10
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.28    0.87    1.45    1.75    1.72    1.79    2.00    2.09    2.15    2.24
2.38    2.53    2.61    2.53    2.22    1.49    0.39
 End
 Rotor                    Hindered
 Group   17
 Axis           16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.54    2.14    4.26    5.80    5.70    3.98    1.64   -0.16   -0.77   -0.03
1.95    4.82    7.51    7.80    5.38    2.67    0.75
 End
   Frequencies[1/cm]          41
  3778.8      3248.0      3232.5      3219.8      3186.4      3103.3      3082.3
3048.0      1627.5      1536.6
  1483.9      1463.8      1427.2      1422.5      1407.3      1360.1      1292.1
1257.2      1230.7      1149.5
  1130.7      1104.3      1050.3      1033.4      1014.2      981.85      966.95
916.57      897.54      883.72
  830.14      707.95      657.14      599.98      587.29      531.90      405.15
334.19      279.73      199.36
  113.35
ZeroEnergy[kcal/mol]    13.056595495171848
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO           !           12
Geometry[angstrom]          17
C   0.15207   0.84625  -1.49399
C   0.15148   0.84632   0.01040
C   1.34179   0.84553   0.81370
C  -1.13877   0.71574   0.43087
C  -2.02069   0.64173  -0.71530
C  -1.29501   0.71144  -1.84521
H   0.58686   1.76720  -1.89363
H   2.22669   1.28487   0.36054
H   1.20694   1.12583   1.85464
H   1.63920  -0.37412   0.90942
H  -1.45355   0.67119   1.46287
H  -3.09490   0.54819  -0.65758
H  -1.67384   0.69198  -2.85512
H   0.75714   0.02491  -1.89039
O   1.69807  -1.66478   0.99344
O   0.39695  -2.01942   1.25373
H   0.00399  -2.12393   0.37866
          Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15          10
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.28    0.87    1.45    1.75    1.72    1.79    2.00    2.09    2.15    2.24
2.38    2.53    2.61    2.53    2.22    1.49    0.39
 End
 Rotor                    Hindered
 Group   17
 Axis           16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.54    2.14    4.26    5.80    5.70    3.98    1.64   -0.16   -0.77   -0.03
1.95    4.82    7.51    7.80    5.38    2.67    0.75
 End
   Frequencies[1/cm]          41
  3776.2      3247.9      3232.0      3219.4      3184.2      3101.6      3082.0
3047.6      1631.0      1545.6
  1483.3      1460.8      1427.2      1422.3      1408.6      1360.2      1295.3
1264.2      1235.0      1150.8
  1131.1      1114.7      1052.3      1035.3      1015.2      981.69      967.15
916.46      897.56      884.63
  830.21      707.72      656.94      611.49      580.78      529.77      403.18
332.46      280.77      201.48
  113.74
ZeroEnergy[kcal/mol]    13.086378551754024
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO           !           13
Geometry[angstrom]          17
C   0.15200   0.84626  -1.49394
C   0.15080   0.84640   0.01026
C   1.34241   0.84488   0.81402
C  -1.13841   0.71579   0.43088
C  -2.02072   0.64172  -0.71553
C  -1.29512   0.71142  -1.84520
H   0.58687   1.76721  -1.89357
H   2.22585   1.28723   0.36074
H   1.20668   1.12795   1.85417
H   1.63908  -0.35882   0.90862
H  -1.45342   0.67136   1.46285
H  -3.09492   0.54821  -0.65770
H  -1.67385   0.69200  -2.85511
H   0.75717   0.02494  -1.89036
O   1.69759  -1.66574   0.99359
O   0.39743  -2.01934   1.25364
H   0.00383  -2.12347   0.37857
          Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15          10
 Symmetry           1
```

```
 Potential[kcal/mol]    18
  0.00  0.28  0.87  1.45  1.75  1.72  1.79  2.00  2.09  2.15  2.24
2.38  2.53  2.61  2.53  2.22  1.49  0.39
 End
 Rotor    Hindered
 Group  17
 Axis   16   15
 Symmetry   1
 Potential[kcal/mol]    18
  0.00  0.54  2.14  4.26  5.80  5.70  3.98  1.64  -0.16  -0.77  -0.03
1.95  4.82  7.51  7.80  5.38  2.67  0.75
 End
   Frequencies[1/cm]    41
  3773.7   3248.0   3231.6   3219.1   3182.3   3100.2   3081.7
3047.3   1634.8   1554.7
  1483.2   1458.4   1427.3   1422.0   1409.6   1360.2   1300.5
1270.2   1237.2   1152.9
  1132.1   1123.7   1053.5   1035.8   1015.3   981.44   967.16
916.35   897.42   885.26
  830.26   707.36   658.72   626.96   568.63   524.96   400.35
330.49   279.07   202.66
  113.40
 ZeroEnergy[kcal/mol]   13.012154672582341
 ElectronicLevels[1/cm]    1
  0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO   !   14
 Geometry[angstrom]    17
 C   0.15193  0.84626  -1.49388
 C   0.15010  0.84648  0.01010
 C   1.34304  0.84427  0.81434
 C  -1.13806  0.71584  0.43088
 C  -2.02075  0.64170  -0.71576
 C  -1.29522  0.71140  -1.84520
 H   0.58687  1.76723  -1.89349
 H   2.22500  1.28973  0.36093
 H   1.20641  1.13017  1.85372
 H   1.63911  -0.34364  0.90784
 H  -1.45329  0.67154  1.46285
 H  -3.09496  0.54822  -0.65782
 H  -1.67387  0.69203  -2.85513
 H   0.75721  0.02497  -1.89031
 O   1.69709  -1.66674  0.99375
 O   0.39793  -2.01926  1.25356
 H   0.00365  -2.12297  0.37846
          Core     RigidRotor
       SymmetryFactor   0.50000000000000000
 End
 Rotor    Hindered
 Group   8  9  10  15  16  17
 Axis   3   2
 Symmetry   3
 Potential[kcal/mol]    12
  0.00  0.27  1.09  2.47  4.41  6.78  9.24  5.07  3.37  1.96  0.89
0.22
 End
 Rotor    Hindered
 Group  16  17
 Axis   15   10
 Symmetry   1
 Potential[kcal/mol]    18
  0.00  0.28  0.87  1.45  1.75  1.72  1.79  2.00  2.09  2.15  2.24
2.38  2.53  2.61  2.53  2.22  1.49  0.39
 End
 Rotor    Hindered
 Group  17
 Axis   16   15
 Symmetry   1
 Potential[kcal/mol]    18
  0.00  0.54  2.14  4.26  5.80  5.70  3.98  1.64  -0.16  -0.77  -0.03
1.95  4.82  7.51  7.80  5.38  2.67  0.75
 End
   Frequencies[1/cm]    41
  3770.8   3247.8   3231.1   3218.7   3180.0   3098.5   3081.3
3046.9   1639.2   1564.6
  1483.6   1457.0   1427.8   1421.9   1410.6   1360.6   1308.0
1274.5   1239.8   1160.4
  1137.0   1129.1   1054.4   1036.3   1015.5   981.24   967.19
916.48   897.25   886.08
  830.35   707.28   668.40   640.04   558.79   516.23   396.96
328.62   275.91   203.55
  112.43
 ZeroEnergy[kcal/mol]   12.877153381689823
 ElectronicLevels[1/cm]    1
  0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO   !   15
 Geometry[angstrom]    17
 C   0.15184  0.84627  -1.49382
 C   0.14939  0.84658  0.00995
 C   1.34369  0.84370  0.81467
 C  -1.13769  0.71589  0.43087
 C  -2.02078  0.64169  -0.71599
 C  -1.29532  0.71139  -1.84520
 H   0.58687  1.76725  -1.89341
 H   2.22410  1.29239  0.36112
 H   1.20611  1.13251  1.85325
 H   1.63932  -0.32860  0.90710
 H  -1.45315  0.67173  1.46284
 H  -3.09500  0.54823  -0.65795
 H  -1.67389  0.69206  -2.85516
 H   0.75724  0.02499  -1.89027
 O   1.69656  -1.66780  0.99391
 O   0.39847  -2.01918  1.25347
 H   0.00346  -2.12242  0.37836
          Core     RigidRotor
       SymmetryFactor   0.50000000000000000
 End
 Rotor    Hindered
 Group   8  9  10  15  16  17
 Axis   3   2
 Symmetry   3
 Potential[kcal/mol]    12
  0.00  0.27  1.09  2.47  4.41  6.78  9.24  5.07  3.37  1.96  0.89
0.22
 End
 Rotor    Hindered
 Group  16  17
 Axis   15   10
 Symmetry   1
 Potential[kcal/mol]    18
  0.00  0.28  0.87  1.45  1.75  1.72  1.79  2.00  2.09  2.15  2.24
2.38  2.53  2.61  2.53  2.22  1.49  0.39
 End
 Rotor    Hindered
 Group  17
 Axis   16   15
 Symmetry   1
 Potential[kcal/mol]    18
  0.00  0.54  2.14  4.26  5.80  5.70  3.98  1.64  -0.16  -0.77  -0.03
1.95  4.82  7.51  7.80  5.38  2.67  0.75
 End
   Frequencies[1/cm]    41
  3767.7   3247.6   3230.5   3218.3   3177.7   3096.8   3080.9
3046.5   1644.9   1576.2
  1484.4   1456.6   1428.8   1421.8   1411.8   1361.8   1317.3
1277.2   1245.5   1180.4
  1141.6   1130.0   1055.3   1036.7   1015.6   981.03   967.22
916.81   897.06   887.35
  830.45   708.36   692.36   644.57   552.41   502.94   393.20
326.74   271.59   204.07
  110.92
 ZeroEnergy[kcal/mol]   12.700258596410421
 ElectronicLevels[1/cm]    1
  0.0000000000000000    2.0000000000000000
 End
```

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!*********************************************
RRHO          !          16
Geometry[angstrom]          17
C   0.15175   0.84628  -1.49375
C   0.14866   0.84668   0.00979
C   1.34434   0.84320   0.81501
C  -1.13732   0.71595   0.43087
C  -2.02081   0.64167  -0.71624
C  -1.29543   0.71137  -1.84521
H   0.58687   1.76726  -1.89332
H   2.22312   1.29525   0.36131
H   1.20579   1.13499   1.85275
H   1.63978  -0.31376   0.90641
H  -1.45300   0.67192   1.46283
H  -3.09505   0.54825  -0.65808
H  -1.67392   0.69208  -2.85520
H   0.75727   0.02502  -1.89021
O   1.69600  -1.66894   0.99409
O   0.39905  -2.01910   1.25337
H   0.00326  -2.12183   0.37827
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                     Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
 End
 Rotor                     Hindered
 Group   16  17
 Axis           15         10
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.28    0.87    1.45    1.75    1.72    1.79    2.00    2.09    2.15    2.24
2.38    2.53    2.61    2.53    2.22    1.49    0.39
 End
 Rotor                     Hindered
 Group   17
 Axis           16         15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.54    2.14    4.26    5.80    5.70    3.98    1.64   -0.16   -0.77   -0.03
1.95    4.82    7.51    7.80    5.38    2.67    0.75
 End
   Frequencies[1/cm]          41
  3764.6     3247.5     3230.0     3217.8     3175.3     3095.1     3080.5
3046.1     1654.1     1590.6
  1486.2     1457.2     1430.5     1421.9     1413.7     1365.4     1327.7
1279.9     1263.1     1205.7
  1143.3     1130.3     1055.9     1037.2     1015.7     980.83     967.24
917.47     896.86     889.73
  830.58     731.80     704.81     645.25     548.72     487.29     389.01
324.83     265.67     203.93
  108.85
ZeroEnergy[kcal/mol]    12.507642873965736
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!*********************************************
RRHO          !          17
Geometry[angstrom]          17
C   0.15166   0.84629  -1.49369
C   0.14790   0.84678   0.00962
C   1.34502   0.84278   0.81536
C  -1.13695   0.71601   0.43087
C  -2.02085   0.64165  -0.71649
C  -1.29555   0.71135  -1.84522
H   0.58687   1.76728  -1.89322
H   2.22205   1.29838   0.36151
H   1.20544   1.13767   1.85221
H   1.64056  -0.29921   0.90580
H  -1.45284   0.67214   1.46282
H  -3.09510   0.54826  -0.65823
H  -1.67396   0.69211  -2.85525
H   0.75731   0.02506  -1.89015
O   1.69540  -1.67016   0.99428
O   0.39966  -2.01902   1.25327
H   0.00304  -2.12116   0.37818
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                     Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
 End
 Rotor                     Hindered
 Group   16  17
 Axis           15         10
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.28    0.87    1.45    1.75    1.72    1.79    2.00    2.09    2.15    2.24
2.38    2.53    2.61    2.53    2.22    1.49    0.39
 End
 Rotor                     Hindered
 Group   17
 Axis           16         15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.54    2.14    4.26    5.80    5.70    3.98    1.64   -0.16   -0.77   -0.03
1.95    4.82    7.51    7.80    5.38    2.67    0.75
 End
   Frequencies[1/cm]          41
  3761.2     3247.3     3229.5     3217.4     3173.0     3093.4     3080.1
3045.7     1675.6     1609.0
  1491.5     1459.2     1435.2     1422.6     1417.2     1377.1     1338.0
1303.8     1277.8     1218.7
  1144.0     1130.4     1056.6     1037.5     1015.7     980.63     967.24
918.71     896.77     894.32
  830.75     771.64     705.21     644.92     546.30     470.15     384.04
322.87     257.73     202.94
  106.20
ZeroEnergy[kcal/mol]    12.424020602131762
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
End
!*********************************************
RRHO          !          18
Geometry[angstrom]          17
C   0.15155   0.84630  -1.49362
C   0.14711   0.84690   0.00944
C   1.34571   0.84246   0.81573
C  -1.13656   0.71608   0.43086
C  -2.02089   0.64163  -0.71676
C  -1.29568   0.71133  -1.84525
H   0.58687   1.76729  -1.89311
H   2.22085   1.30184   0.36170
H   1.20504   1.14058   1.85162
H   1.64176  -0.28508   0.90531
H  -1.45266   0.67236   1.46281
H  -3.09516   0.54828  -0.65840
H  -1.67400   0.69214  -2.85530
H   0.75734   0.02510  -1.89008
O   1.69475  -1.67149   0.99448
O   0.40034  -2.01892   1.25316
H   0.00280  -2.12041   0.37811
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                     Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
```

```
 Symmetry          3
 Potential[kcal/mol]          12
  0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
 End
 Rotor                         Hindered
 Group   16  17
 Axis           15          10
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.28    0.87    1.45    1.75    1.72    1.79    2.00    2.09    2.15    2.24
2.38    2.53    2.61    2.53    2.22    1.49    0.39
 End
 Rotor                         Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    2.14    4.26    5.80    5.70    3.98    1.64   -0.16   -0.77   -0.03
1.95    4.82    7.51    7.80    5.38    2.67    0.75
 End
   Frequencies[1/cm]          41
  3757.7      3247.2      3229.0      3217.0      3170.7      3091.8      3079.6
3045.3      1734.7      1625.4
  1507.7      1464.2      1445.3      1425.2      1420.0      1393.4      1345.0
1326.7      1278.8      1222.7
  1144.4      1130.5      1057.1      1037.5      1015.2      980.45      967.15
921.68      902.50      896.30
  831.07      805.94      705.08      644.25      544.33      450.67      377.86
320.87      246.71      200.47
  102.93
 ZeroEnergy[kcal/mol]    12.331108289977024
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
RRHO          !          19
Geometry[angstrom]          17
C    0.15142   0.84632  -1.49355
C    0.14628   0.84702   0.00925
C    1.34643   0.84228   0.81611
C   -1.13616   0.71615   0.43086
C   -2.02093   0.64161  -0.71705
C   -1.29581   0.71130  -1.84528
H    0.58686   1.76731  -1.89299
H    2.21952   1.30570   0.36191
H    1.20459   1.14376   1.85098
H    1.64349  -0.27152   0.90494
H   -1.45245   0.67260   1.46280
H   -3.09522   0.54830  -0.65858
H   -1.67405   0.69218  -2.85536
H    0.75738   0.02515  -1.89000
O    1.69404  -1.67295   0.99471
O    0.40107  -2.01883   1.25303
H    0.00252  -2.11955   0.37805
              Core            RigidRotor
         SymmetryFactor   0.50000000000000000
End
 Rotor                         Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
 Symmetry          3
 Potential[kcal/mol]          12
  0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
 End
 Rotor                         Hindered
 Group   16  17
 Axis           15          10
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.28    0.87    1.45    1.75    1.72    1.79    2.00    2.09    2.15    2.24
2.38    2.53    2.61    2.53    2.22    1.49    0.39
 End
 Rotor                         Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    2.14    4.26    5.80    5.70    3.98    1.64   -0.16   -0.77   -0.03
1.95    4.82    7.51    7.80    5.38    2.67    0.75
 End
   Frequencies[1/cm]          41
  3754.1      3247.1      3228.6      3216.6      3168.5      3090.3      3079.2
3044.9      1847.3      1635.4
  1531.8      1469.2      1451.0      1427.9      1420.7      1400.1      1347.8
1338.0      1279.2      1224.0
  1144.6      1130.6      1057.7      1037.3      1014.6      980.30      967.05
930.27      910.10      896.16
  832.50      825.80      704.84      643.44      542.74      432.76      370.51
318.79      232.72      194.48
  98.860
 ZeroEnergy[kcal/mol]    12.245814869860666
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
RRHO          !          20
Geometry[angstrom]          17
C    0.15129   0.84633  -1.49347
C    0.14543   0.84716   0.00906
C    1.34717   0.84227   0.81650
C   -1.13576   0.71624   0.43086
C   -2.02099   0.64159  -0.71735
C   -1.29596   0.71128  -1.84533
H    0.58684   1.76733  -1.89285
H    2.21801   1.31002   0.36211
H    1.20409   1.14725   1.85028
H    1.64585  -0.25877   0.90475
H   -1.45222   0.67287   1.46279
H   -3.09529   0.54832  -0.65878
H   -1.67411   0.69221  -2.85543
H    0.75741   0.02521  -1.88990
O    1.69327  -1.67456   0.99495
O    0.40187  -2.01873   1.25290
H    0.00221  -2.11856   0.37803
              Core            RigidRotor
         SymmetryFactor   0.50000000000000000
End
 Rotor                         Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
 Symmetry          3
 Potential[kcal/mol]          12
  0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
 End
 Rotor                         Hindered
 Group   16  17
 Axis           15          10
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.28    0.87    1.45    1.75    1.72    1.79    2.00    2.09    2.15    2.24
2.38    2.53    2.61    2.53    2.22    1.49    0.39
 End
 Rotor                         Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    2.14    4.26    5.80    5.70    3.98    1.64   -0.16   -0.77   -0.03
1.95    4.82    7.51    7.80    5.38    2.67    0.75
 End
   Frequencies[1/cm]          41
  3750.5      3246.9      3228.2      3216.3      3166.3      3088.9      3078.8
3044.5      1986.9      1641.8
  1549.7      1471.3      1453.0      1430.2      1420.9      1402.2      1349.0
1345.4      1279.2      1224.2
```

```
  1144.8     1130.6     1058.7     1037.4     1013.9     980.19     966.98
944.40     913.44     896.03
  838.25     829.90     704.60     642.56     541.40     418.77     362.49
316.64     220.03     179.65
  93.190
 ZeroEnergy[kcal/mol]    12.137348091870521
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
 !**********************************************
 RRHO          !          21
 Geometry[angstrom]          17
 C    0.15113   0.84635  -1.49340
 C    0.14455   0.84730   0.00886
 C    1.34793   0.84247   0.81690
 C   -1.13536   0.71633   0.43085
 C   -2.02105   0.64156  -0.71767
 C   -1.29612   0.71125  -1.84539
 H    0.58682   1.76734  -1.89270
 H    2.21632   1.31485   0.36230
 H    1.20351   1.15105   1.84953
 H    1.64894  -0.24705   0.90474
 H   -1.45197   0.67315   1.46278
 H   -3.09536   0.54835  -0.65901
 H   -1.67418   0.69224  -2.85552
 H    0.75743   0.02528  -1.88978
 O    1.69244  -1.67634   0.99521
 O    0.40273  -2.01862   1.25275
 H    0.00186  -2.11744   0.37804
           Core           RigidRotor
      SymmetryFactor   0.50000000000000000
 End
  Rotor                       Hindered
  Group    8   9  10  15  16  17
  Axis           3          2
  Symmetry           3
  Potential[kcal/mol]          12
   0.00    0.27    1.09    2.47    4.41    6.78    9.24    5.07    3.37    1.96    0.89
0.22
  End
  Rotor                       Hindered
  Group   16  17
  Axis           15          10
  Symmetry           1
  Potential[kcal/mol]          18
   0.00    0.28    0.87    1.45    1.75    1.72    1.79    2.00    2.09    2.15    2.24
2.38    2.53    2.61    2.53    2.22    1.49    0.39
  End
  Rotor                       Hindered
  Group   17
  Axis           16          15
  Symmetry           1
  Potential[kcal/mol]          18
   0.00    0.54    2.14    4.26    5.80    5.70    3.98    1.64   -0.16   -0.77   -0.03
1.95    4.82    7.51    7.80    5.38    2.67    0.75
  End
    Frequencies[1/cm]          41
  3746.8     3246.9     3227.9     3215.9     3164.3     3087.7     3078.4
3044.1     2129.8     1646.8
  1561.5     1472.2     1454.3     1432.3     1421.0     1402.9     1352.0
1348.5     1279.1     1223.8
  1144.9     1130.6     1060.3     1037.7     1013.2     980.16     967.14
957.78     914.90     895.92
  841.57     830.40     704.37     641.68     540.24     408.81     354.89
314.45     212.80     152.36
  82.540
 ZeroEnergy[kcal/mol]    11.909266870581476
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
 !**********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1901.6198999999999
      WellDepth[kcal/mol]          16.95
      WellDepth[kcal/mol]          17.86
    End
  End
  End
```

```
!****************************************************
!             GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30         ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400        ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct     ! direct or low-eigenvalue
!
WellCutoff                            20         ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                 0.2        ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!
!WellCutoff                           10
!ChemicalEigenvalueMin                1.e-6          #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                 1.3
!!
RateOutput                            rate.out                 ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!             MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                          ! Default collisional
energy relaxation kernel
    Exponential                                            ! Currently the only
possible energy relaxation model
       Factor[1/cm]             316                        ! (Delta_E_down)^(0)
@ standard T (300 K)
       Power                  0.535                      ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
       ExponentCutoff              10                          ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                        ! Collision frequency
model
    LennardJones                                           ! Currently the only
possible collisional frequency model  based on LJ potential
       Epsilons[K]               90.58  281.367             ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
       Sigmas[angstrom]              3.54    4.694               ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
       Masses[amu]                 39.948  79.05478              ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]            14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.50112
 C    1.39710   0.00000   2.12644
 C   -0.81569  -1.21840   1.82234
 C   -1.21870  -1.80451   0.68960
 C   -0.70750  -1.04109  -0.45233
 H    0.50817   0.74374  -0.59543
 H    1.95008   0.89431   1.83920
 H    1.33447  -0.02486   3.21435
 H    1.96018  -0.87263   1.79528
 H   -1.02550  -1.54600   2.82960
 H   -1.82229  -2.69676   0.61182
 H   -0.88231  -1.29309  -1.48790
 H   -0.53850   0.88886   1.85441
        Core    RigidRotor
             SymmetryFactor    1.0000000000000000
        End
 Rotor                          Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.23    0.90    1.84    2.83    3.55    3.78    3.44    2.69    1.75    0.87
0.23
 End
    Frequencies[1/cm]           35
  3244.1      3235.6      3219.3      3210.9      3128.0      3124.4      3049.0
3020.3      1670.2      1591.0
  1503.9      1503.7      1422.5      1406.8      1334.3      1293.1      1277.9
1155.2      1119.2      1104.0
  1090.8      1028.3      1004.1      983.75      981.16      957.17      883.24
817.77      792.34      742.25
  721.84      567.90      547.80      294.51      164.97
  ZeroEnergy[kcal/mol]             0.
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!***********************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]             3
 O    0.00000   0.00000   0.00000
 O    0.00000   0.00000   1.31234
 H    0.93494   0.00000   1.57303
        Core    RigidRotor
             SymmetryFactor    1.0000000000000000
        End
    Frequencies[1/cm]            3
  1234.9      1462.2      3683.2
  ZeroEnergy[kcal/mol]             0.
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
!***********************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]             13
```

```
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.41507
C   1.18585   0.00000   2.30525
C  -1.37924  -0.00034   1.86264
C  -2.17195  -0.00056   0.76525
C  -1.30652  -0.00033  -0.41759
H   0.87955   0.00028  -0.62343
H   2.11567   0.00259   1.73998
H   1.17551   0.87449   2.96082
H   1.17824  -0.87748   2.95691
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
      Core    RigidRotor
          SymmetryFactor    2.0000000000000000
      End
Rotor                         Hindered
Group    8   9  10
Axis            3           2
Symmetry           3
Potential[kcal/mol]           12
   0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
   Frequencies[1/cm]           32
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!************************************
Fragment PROD2
RRHO
Geometry[angstrom]              4
O   0.00000   0.00000   0.00000
O   0.00000   0.00000   1.42622
H   0.94322   0.00000   1.61480
H  -0.34861  -0.87643  -0.18855
      Core    RigidRotor
          SymmetryFactor    2.0000000000000000
      End
Rotor                         Hindered
Group    4
Axis            1           2
Symmetry           1
Potential[kcal/mol]           18
   0.00    0.07    0.48    0.80    0.77    0.40    0.02    0.06    0.91    2.62    4.92
7.15    8.51    8.38    6.81    4.51    2.28    0.70
End
   Frequencies[1/cm]            5
  3840.9      3839.6      1465.2      1361.0      1016.3
 ZeroEnergy[kcal/mol]            0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
GroundEnergy[kcal/mol]    -9.18
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]             17
C  -0.00250  -0.00249   0.00375
C  -0.00078  -0.00204   1.50323
C   1.39713  -0.00191   2.12929
C  -0.80708  -1.22577   1.82565
C  -1.20149  -1.81940   0.68808
C  -0.69684  -1.05045  -0.45414
H   0.49253   0.75055  -0.59057
H   1.94661   0.89307   1.83959
H   1.33101  -0.02218   3.21650
H   1.96250  -0.87394   1.80103
H  -1.00475  -1.56129   2.83260
H  -1.78259  -2.72722   0.61135
H  -0.87048  -1.30307  -1.48911
H  -0.54159   0.88170   1.86436
O  -3.14999   1.04370   2.49898
O  -3.53415   0.30466   1.48722
H  -2.81415  -0.35138   1.35823
      Core    RigidRotor
          SymmetryFactor    0.50000000000000000
      End
   Frequencies[1/cm]           45
  27.491      48.486      58.438      99.607      168.69      176.16      259.40
297.36      475.58      551.93
  574.40      726.66      756.77      801.71      821.20      884.88      957.67
982.93      988.89      1005.7
  1034.4      1089.0      1104.8      1121.9      1157.4      1257.2      1281.4
1297.4      1336.0      1407.4
  1423.3      1504.2      1505.1      1513.4      1581.5      1660.9      3031.1
3053.3      3131.7      3132.8
  3212.0      3223.5      3238.3      3247.0      3471.4
 ZeroEnergy[kcal/mol]             -5.54
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]             17
C   0.01421   0.05996   0.02066
C   0.01200   0.00453   1.46281
C   1.21276  -0.02422   2.32829
C  -1.34416   0.04383   1.89757
C  -2.13858   0.11619   0.78350
C  -1.27463   0.13172  -0.39901
H   0.89968   0.03984  -0.59515
H   2.00971  -0.62116   1.88448
H   1.59401   0.99482   2.44677
H   0.98536  -0.41085   3.32029
H  -1.66933  -0.00393   2.92465
H  -3.21688   0.15097   0.76249
H  -1.62353   0.18500  -1.41808
H   0.30893   2.89659   0.29973
O   0.22541   3.15491   1.22403
O  -1.18685   3.26736   1.36582
H  -1.42804   2.37159   1.64349
      Core    RigidRotor
          SymmetryFactor    0.50000000000000000
      End
   Frequencies[1/cm]           45
  14.622      59.335      73.711      77.580      103.28      137.63      223.52
235.09      330.57      523.15
  535.93      604.63      614.21      646.25      740.70      752.24      909.19
926.66      935.29      963.44
  1010.0      1017.6      1026.4      1060.2      1097.0      1189.4      1296.0
1310.7      1406.4      1418.3
  1436.2      1461.1      1475.2      1488.8      1516.2      1570.0      3036.0
3102.2      3139.7      3227.5
  3233.6      3247.3      3256.5      3717.2      3812.4
 ZeroEnergy[kcal/mol]             -12.43
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier        B1  REACS WR
  RRHO
    Stoichiometry  H9C6O2
    Core PhaseSpaceTheory
```

```
    FragmentGeometry[angstrom]             14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50112
C    1.39710   0.00000   2.12644
C   -0.81569  -1.21840   1.82234
C   -1.21870  -1.80451   0.68960
C   -0.70750  -1.04109  -0.45233
H    0.50817   0.74374  -0.59543
H    1.95008   0.89431   1.83920
H    1.33447  -0.02486   3.21435
H    1.96018  -0.87263   1.79528
H   -1.02550  -1.54600   2.82960
H   -1.82229  -2.69676   0.61182
H   -0.88231  -1.29309  -1.48790
H   -0.53850   0.88886   1.85441
    FragmentGeometry[angstrom]             3
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.31234
H    0.93494   0.00000   1.57303
                         SymmetryFactor     1.0000000000000000
      PotentialPrefactor[au]             10.
      PotentialPowerExponent             6
              End
Rotor                     Hindered
Geometry[angstrom]            14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.50112
C    1.39710   0.00000   2.12644
C   -0.81569  -1.21840   1.82234
C   -1.21870  -1.80451   0.68960
C   -0.70750  -1.04109  -0.45233
H    0.50817   0.74374  -0.59543
H    1.95008   0.89431   1.83920
H    1.33447  -0.02486   3.21435
H    1.96018  -0.87263   1.79528
H   -1.02550  -1.54600   2.82960
H   -1.82229  -2.69676   0.61182
H   -0.88231  -1.29309  -1.48790
H   -0.53850   0.88886   1.85441
Group    8   9  10
Axis           3          2
Symmetry           3
Potential[kcal/mol]          12
  0.0000     0.23000     0.90000     1.8400      2.8300      3.5500      3.7800
3.4400     2.6900     1.7500
 0.87000    0.23000
End
   Frequencies[1/cm]          38
  3244.1      3235.6      3219.3      3210.9      3128.0      3124.4      3049.0
3020.3      1670.2      1591.0
  1503.9      1503.7      1422.5      1406.8      1334.3      1293.1      1277.9
1155.2      1119.2      1104.0
  1090.8      1028.3      1004.1      983.75      981.16      957.17      883.24
817.77      792.34      742.25
  721.84      567.90      547.80      294.51      164.97
  1234.9      1462.2      3683.2
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        4.0000000000000000
End
!************************************
Barrier       B3  WP PRODS
  RRHO
    Stoichiometry  H9C6O2
    Core PhaseSpaceTheory
    FragmentGeometry[angstrom]             13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.41507
C    1.18585   0.00000   2.30525
C   -1.37924  -0.00034   1.86264
C   -2.17195  -0.00056   0.76525
C   -1.30652  -0.00033  -0.41759
H    0.87955   0.00028  -0.62343
H    2.11567   0.00259   1.73998
H    1.17551   0.87449   2.96082
H    1.17824  -0.87748   2.95691
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
    FragmentGeometry[angstrom]             4
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.42622
H    0.94322   0.00000   1.61480
H   -0.34861  -0.87643  -0.18855
                         SymmetryFactor     4.0000000000000000
      PotentialPrefactor[au]             10.
      PotentialPowerExponent             6
              End
Rotor                     Hindered
Geometry[angstrom]            13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.41507
C    1.18585   0.00000   2.30525
C   -1.37924  -0.00034   1.86264
C   -2.17195  -0.00056   0.76525
C   -1.30652  -0.00033  -0.41759
H    0.87955   0.00028  -0.62343
H    2.11567   0.00259   1.73998
H    1.17551   0.87449   2.96082
H    1.17824  -0.87748   2.95691
H   -1.69366  -0.00045   2.89442
H   -3.25029  -0.00080   0.74358
H   -1.65471  -0.00041  -1.43915
Group    8   9  10
Axis           3          2
Symmetry           3
Potential[kcal/mol]          12
  0.0000     0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01  0.0000     0.20000E-01 0.40000E-01 0.60000E-01
 0.40000E-01 0.10000E-01
End
Rotor                     Hindered
Geometry[angstrom]            4
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.42622
H    0.94322   0.00000   1.61480
H   -0.34861  -0.87643  -0.18855
Group    4
Axis           1          2
Symmetry           1
Potential[kcal/mol]          18
  0.0000     0.70000E-01 0.48000     0.80000     0.77000     0.40000
0.20000E-01 0.60000E-01 0.91000     2.6200
  4.9200      7.1500      8.5100      8.3800      6.8100      4.5100      2.2800
0.70000
End
   Frequencies[1/cm]          37
  3255.2      3247.0      3232.4      3224.7      3138.6      3086.9      3034.1
1584.1      1503.1      1481.1
  1477.9      1438.4      1407.4      1311.3      1292.6      1178.7      1098.1
1049.4      1023.5      1013.2
  953.40      929.99      923.03      899.45      740.46      727.81      638.42
604.77      528.85      520.52
  329.55      215.83
  3840.9      3839.6      1465.2      1361.0      1016.3
 ZeroEnergy[kcal/mol]             -9.1831161824873444
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO           !           1
Geometry[angstrom]          17
C    0.80541  -0.35571  -1.12508
C    0.80502  -0.34548   0.34748
C    2.07608  -0.35615   1.15714
C   -0.37231  -1.16111   0.72265
```

C -1.03918 -1.49418 -0.39745
C -0.30103 -0.98897 -1.55470
H 1.54444 0.14750 -1.72899
H 2.76308 0.41194 0.80277
H 1.86357 -0.16252 2.20857
H 2.57903 -1.32099 1.08540
H -0.65342 -1.37830 1.74190
H -1.96575 -2.04707 -0.44954
H -0.61255 -1.10349 -2.58199
H 0.38122 0.69468 0.52574
O -0.38541 1.89273 0.73472
O -1.33907 1.85265 -0.20914
H -2.03483 1.29751 0.17524
Core RigidRotor
SymmetryFactor 3.0000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.54 1.72 2.33 1.70 0.57 0.00 0.51 1.70 2.33 1.69
0.55 0.00 0.52 1.70 2.33 1.68 0.54
End
Rotor Hindered
Group 16 17
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18
0.00 0.37 1.24 2.06 2.42 2.36 2.12 1.90 1.89 2.02 2.04
1.81 1.47 1.17 0.97 0.84 0.68 0.27
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.52 2.26 5.14 8.93 11.01 7.36 4.30 2.39 1.88 0.14
1.31 3.41 6.16 8.04 4.96 2.45 0.69
End
Frequencies[1/cm] 41
3710.0 3248.2 3239.4 3224.8 3212.9 3128.8 3119.8
3049.1 2116.7 1631.4
1554.6 1507.1 1497.5 1451.9 1426.7 1422.0 1340.3
1306.1 1255.2 1242.3
1109.3 1099.3 1080.3 1017.5 1006.6 990.86 974.28
966.36 931.94 893.35
820.85 802.48 733.67 689.20 571.56 557.61 320.27
290.13 223.58 98.510
56.900
ZeroEnergy[kcal/mol] 10.908732085532112
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 2
Geometry[angstrom] 17
C 0.80535 -0.35500 -1.12456
C 0.80473 -0.34556 0.34716
C 2.07549 -0.35531 1.15711
C -0.37230 -1.16057 0.72275
C -1.03927 -1.49413 -0.39736
C -0.30107 -0.98882 -1.55465
H 1.54483 0.14748 -1.72848
H 2.76318 0.41207 0.80269
H 1.86348 -0.16245 2.20874
H 2.57758 -1.32070 1.08467
H -0.65294 -1.37813 1.74202
H -1.96553 -2.04748 -0.44942
H -0.61207 -1.10395 -2.58202
H 0.37303 0.70155 0.52589
O -0.38348 1.89074 0.73505
O -1.33965 1.85250 -0.20983
H -2.03541 1.29859 0.17576
Core RigidRotor
SymmetryFactor 3.0000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.54 1.72 2.33 1.70 0.57 0.00 0.51 1.70 2.33 1.69
0.55 0.00 0.52 1.70 2.33 1.68 0.54
End
Rotor Hindered
Group 16 17
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18
0.00 0.37 1.24 2.06 2.42 2.36 2.12 1.90 1.89 2.02 2.04
1.81 1.47 1.17 0.97 0.84 0.68 0.27
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.52 2.26 5.14 8.93 11.01 7.36 4.30 2.39 1.88 0.14
1.31 3.41 6.16 8.04 4.96 2.45 0.69
End
Frequencies[1/cm] 41
3713.5 3248.5 3239.8 3225.1 3213.3 3129.4 3119.2
3048.9 1974.4 1629.4
1552.2 1506.5 1497.1 1449.6 1426.3 1421.8 1339.9
1309.7 1255.4 1242.8
1109.1 1099.1 1071.0 1015.7 1005.9 984.89 973.88
965.74 931.43 893.44
820.36 801.92 734.89 689.26 571.44 559.37 310.63
290.92 222.73 101.24
69.380
ZeroEnergy[kcal/mol] 10.880075278527674
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 3
Geometry[angstrom] 17
C 0.80533 -0.35439 -1.12409
C 0.80456 -0.34584 0.34682
C 2.07501 -0.35461 1.15710
C -0.37229 -1.16009 0.72285
C -1.03936 -1.49409 -0.39728
C -0.30112 -0.98870 -1.55462
H 1.54516 0.14743 -1.72806
H 2.76330 0.41215 0.80261
H 1.86343 -0.16244 2.20890
H 2.57635 -1.32049 1.08403
H -0.65254 -1.37802 1.74211
H -1.96533 -2.04786 -0.44932
H -0.61166 -1.10436 -2.58205
H 0.36445 0.71044 0.52644
O -0.38177 1.88902 0.73539
O -1.34021 1.85237 -0.21048
H -2.03590 1.29949 0.17616
Core RigidRotor
SymmetryFactor 3.0000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.54 1.72 2.33 1.70 0.57 0.00 0.51 1.70 2.33 1.69
0.55 0.00 0.52 1.70 2.33 1.68 0.54
End
Rotor Hindered
Group 16 17

```
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.37 1.24 2.06 2.42 2.36 2.12 1.90 1.89 2.02 2.04
1.81 1.47 1.17 0.97 0.84 0.68 0.27
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.52 2.26 5.14 8.93 11.01 7.36 4.30 2.39 1.88 0.14
1.31 3.41 6.16 8.04 4.96 2.45 0.69
 End
   Frequencies[1/cm] 41
  3717.0 3248.8 3240.2 3225.5 3213.7 3129.9 3118.5
3048.6 1785.5 1627.3
  1547.2 1505.7 1496.4 1447.7 1425.5 1421.5 1339.1
1311.7 1255.3 1242.4
  1109.0 1098.8 1063.5 1010.9 1004.0 974.18 969.13
964.71 926.29 892.64
  819.47 799.81 736.13 687.81 569.16 560.81 299.99
288.93 215.23 105.58
  80.010
 ZeroEnergy[kcal/mol] 10.756620668271243
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!**********************************************
RRHO ! 4
Geometry[angstrom] 17
C 0.80532 -0.35386 -1.12366
C 0.80449 -0.34629 0.34649
C 2.07460 -0.35402 1.15708
C -0.37227 -1.15967 0.72294
C -1.03945 -1.49407 -0.39721
C -0.30117 -0.98860 -1.55461
H 1.54544 0.14736 -1.72772
H 2.76343 0.41218 0.80254
H 1.86340 -0.16246 2.20903
H 2.57531 -1.32035 1.08349
H -0.65219 -1.37794 1.74218
H -1.96515 -2.04819 -0.44924
H -0.61131 -1.10472 -2.58208
H 0.35572 0.72075 0.52736
O -0.38026 1.88756 0.73572
O -1.34072 1.85226 -0.21107
H -2.03628 1.30025 0.17645
      Core RigidRotor
    SymmetryFactor 3.0000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.54 1.72 2.33 1.70 0.57 0.00 0.51 1.70 2.33 1.69
0.55 0.00 0.52 1.70 2.33 1.68 0.54
 End
 Rotor Hindered
 Group 16 17
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.37 1.24 2.06 2.42 2.36 2.12 1.90 1.89 2.02 2.04
1.81 1.47 1.17 0.97 0.84 0.68 0.27
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.52 2.26 5.14 8.93 11.01 7.36 4.30 2.39 1.88 0.14
1.31 3.41 6.16 8.04 4.96 2.45 0.69
 End
   Frequencies[1/cm] 41
  3720.6 3249.2 3240.6 3225.9 3214.2 3130.5 3117.8
3048.3 1632.8 1621.5
  1529.6 1504.8 1494.3 1445.8 1423.8 1421.2 1338.1
1310.7 1254.9 1241.6
  1108.8 1098.8 1060.0 1009.8 1002.7 973.07 964.41
948.94 908.93 886.01
  817.97 798.35 737.01 686.99 568.03 561.80 296.36
280.13 214.82 111.74
  88.150
 ZeroEnergy[kcal/mol] 10.655222173956279
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!**********************************************
RRHO ! 5
Geometry[angstrom] 17
C 0.80533 -0.35340 -1.12329
C 0.80451 -0.34685 0.34616
C 2.07427 -0.35352 1.15708
C -0.37224 -1.15931 0.72302
C -1.03952 -1.49405 -0.39715
C -0.30121 -0.98852 -1.55461
H 1.54567 0.14729 -1.72743
H 2.76355 0.41219 0.80248
H 1.86338 -0.16250 2.20915
H 2.57443 -1.32026 1.08302
H -0.65190 -1.37790 1.74223
H -1.96499 -2.04848 -0.44917
H -0.61102 -1.10504 -2.58211
H 0.34700 0.73206 0.52854
O -0.37892 1.88629 0.73602
O -1.34119 1.85217 -0.21160
H -2.03659 1.30089 0.17665
      Core RigidRotor
    SymmetryFactor 3.0000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.54 1.72 2.33 1.70 0.57 0.00 0.51 1.70 2.33 1.69
0.55 0.00 0.52 1.70 2.33 1.68 0.54
 End
 Rotor Hindered
 Group 16 17
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.37 1.24 2.06 2.42 2.36 2.12 1.90 1.89 2.02 2.04
1.81 1.47 1.17 0.97 0.84 0.68 0.27
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.52 2.26 5.14 8.93 11.01 7.36 4.30 2.39 1.88 0.14
1.31 3.41 6.16 8.04 4.96 2.45 0.69
 End
   Frequencies[1/cm] 41
  3724.2 3249.6 3241.0 3226.4 3214.8 3131.0 3117.2
3048.0 1623.1 1570.7
  1504.3 1499.1 1457.8 1440.6 1420.9 1413.9 1336.6
1299.7 1254.1 1237.8
  1108.7 1098.8 1059.0 1009.7 1002.4 972.38 963.50
943.48 898.12 835.74
  813.76 793.35 736.33 684.38 567.93 560.28 297.31
270.10 214.05 119.25
  94.190
 ZeroEnergy[kcal/mol] 10.558854321508196
 ElectronicLevels[1/cm] 1
```

```
  0.0000000000000000      2.0000000000000000
 End
!***********************************************
 RRHO          !          6
 Geometry[angstrom]         17
 C    0.80535  -0.35300  -1.12296
 C    0.80459  -0.34749   0.34583
 C    2.07398  -0.35308   1.15707
 C   -0.37222  -1.15899   0.72310
 C   -1.03959  -1.49404  -0.39709
 C   -0.30126  -0.98845  -1.55462
 H    1.54588   0.14721  -1.72720
 H    2.76366   0.41219   0.80242
 H    1.86337  -0.16254   2.20926
 H    2.57367  -1.32020   1.08261
 H   -0.65165  -1.37787   1.74226
 H   -1.96484  -2.04874  -0.44912
 H   -0.61076  -1.10533  -2.58214
 H    0.33834   0.74404   0.52992
 O   -0.37773   1.88518   0.73631
 O   -1.34163   1.85208  -0.21207
 H   -2.03683   1.30144   0.17680
              Core          RigidRotor
        SymmetryFactor    3.0000000000000000
 End
  Rotor                     Hindered
  Group    8   9  10
  Axis           3          2
  Symmetry          1
  Potential[kcal/mol]         18
   0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
  End
  Rotor                     Hindered
  Group   16  17
  Axis           15         14
  Symmetry          1
  Potential[kcal/mol]         18
   0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
  End
  Rotor                     Hindered
  Group   17
  Axis           16         15
  Symmetry          1
  Potential[kcal/mol]         18
   0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
  End
    Frequencies[1/cm]         41
  3727.8     3249.9     3241.4     3226.9     3215.3     3131.6     3116.6
3047.6     1620.5     1561.2
  1503.0     1497.2     1446.8     1430.0     1420.5     1382.3     1334.4
1276.0     1253.1     1220.7
  1108.5     1098.6     1059.1     1009.1     1001.8     971.55     962.55
941.88     896.85     816.88
  801.56     757.94     724.27     672.88     568.31     554.05     298.85
263.43     212.65     127.17
  98.300
 ZeroEnergy[kcal/mol]    10.495924152012950
  ElectronicLevels[1/cm]                 1
  0.0000000000000000      2.0000000000000000
 End
!***********************************************
 RRHO          !          7
 Geometry[angstrom]         17
 C    0.80537  -0.35264  -1.12266
 C    0.80471  -0.34820   0.34552
 C    2.07373  -0.35270   1.15707
 C   -0.37220  -1.15871   0.72317
 C   -1.03966  -1.49403  -0.39703
 C   -0.30130  -0.98840  -1.55463
 H    1.54605   0.14713  -1.72700
 H    2.76377   0.41218   0.80237
 H    1.86337  -0.16259   2.20935
 H    2.57301  -1.32016   1.08224
 H   -0.65144  -1.37785   1.74229
 H   -1.96470  -2.04898  -0.44907
 H   -0.61053  -1.10559  -2.58216
 H    0.32978   0.75648   0.53142
 O   -0.37666   1.88418   0.73657
 O   -1.34203   1.85201  -0.21251
 H   -2.03702   1.30192   0.17690
              Core          RigidRotor
        SymmetryFactor    3.0000000000000000
 End
  Rotor                     Hindered
  Group    8   9  10
  Axis           3          2
  Symmetry          1
  Potential[kcal/mol]         18
   0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
  End
  Rotor                     Hindered
  Group   16  17
  Axis           15         14
  Symmetry          1
  Potential[kcal/mol]         18
   0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
  End
  Rotor                     Hindered
  Group   17
  Axis           16         15
  Symmetry          1
  Potential[kcal/mol]         18
   0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
  End
    Frequencies[1/cm]         41
  3731.3     3250.4     3241.9     3227.4     3215.9     3132.0     3116.0
3047.2     1617.9     1557.5
  1501.8     1496.5     1445.8     1427.6     1420.0     1372.4     1331.8
1264.6     1252.0     1187.2
  1108.4     1098.3     1059.7     1008.3     1000.2     970.59     961.56
939.75     896.40     813.51
  798.61     748.11     705.67     640.14     568.45     540.47     300.49
258.91     207.99     134.79
  101.35
 ZeroEnergy[kcal/mol]    10.530577274682276
  ElectronicLevels[1/cm]                 1
  0.0000000000000000      2.0000000000000000
 End
!***********************************************
 RRHO          !          8
 Geometry[angstrom]         17
 C    0.80540  -0.35232  -1.12238
 C    0.80487  -0.34895   0.34520
 C    2.07351  -0.35235   1.15707
 C   -0.37217  -1.15845   0.72323
 C   -1.03972  -1.49402  -0.39698
 C   -0.30134  -0.98834  -1.55464
 H    1.54621   0.14706  -1.72682
 H    2.76387   0.41217   0.80232
 H    1.86338  -0.16264   2.20944
 H    2.57241  -1.32013   1.08191
 H   -0.65124  -1.37784   1.74230
 H   -1.96457  -2.04920  -0.44903
 H   -0.61032  -1.10583  -2.58218
 H    0.32131   0.76925   0.53302
 O   -0.37566   1.88328   0.73682
 O   -1.34240   1.85195  -0.21291
 H   -2.03717   1.30234   0.17697
              Core          RigidRotor
        SymmetryFactor    3.0000000000000000
 End
  Rotor                     Hindered
```

```
 Group    8   9  10
 Axis            3           2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
 End
 Rotor                          Hindered
 Group   16  17
 Axis            15          14
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
 End
 Rotor                          Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
 End
   Frequencies[1/cm]          41
  3735.3      3250.8      3242.3      3227.9      3216.5      3132.5      3115.4
3046.8      1615.3      1555.2
  1500.5      1496.0      1445.9      1426.5      1419.5      1373.4      1329.1
1262.5      1250.2      1161.6
  1108.2      1097.8      1060.4      1007.8      998.23      969.57      960.51
937.75      896.17      810.20
  796.62      747.34      700.83      616.51      568.50      522.14      302.31
255.99      204.17      141.71
  103.69
 ZeroEnergy[kcal/mol]    10.690650352558041
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
RRHO           !            9
Geometry[angstrom]          17
C    0.80543  -0.35201  -1.12211
C    0.80506  -0.34974   0.34489
C    2.07330  -0.35203   1.15707
C   -0.37215  -1.15821   0.72329
C   -1.03977  -1.49402  -0.39693
C   -0.30138  -0.98830  -1.55466
H    1.54635   0.14699  -1.72666
H    2.76397   0.41215   0.80227
H    1.86338  -0.16268   2.20952
H    2.57186  -1.32011   1.08160
H   -0.65107  -1.37784   1.74232
H   -1.96445  -2.04940  -0.44899
H   -0.61013  -1.10605  -2.58220
H    0.31291   0.78220   0.53468
O   -0.37472   1.88243   0.73706
O   -1.34276   1.85190  -0.21329
H   -2.03729   1.30273   0.17702
              Core            RigidRotor
       SymmetryFactor     3.0000000000000000
End
 Rotor                          Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
 End
 Rotor                          Hindered
 Group   16  17
 Axis            15          14
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
 End
 Rotor                          Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
 End
   Frequencies[1/cm]          41
  3738.8      3251.2      3242.8      3228.4      3217.1      3133.0      3114.9
3046.4      1612.5      1553.5
  1499.1      1495.6      1446.1      1425.8      1418.9      1378.2      1326.2
1262.9      1247.6      1148.1
  1108.1      1097.7      1061.7      1007.6      997.13      968.59      959.42
937.77      896.15      806.47
  795.27      747.59      699.43      606.14      568.62      509.55      304.43
254.65      204.58      147.91
  105.37
 ZeroEnergy[kcal/mol]    10.846683545019406
 ElectronicLevels[1/cm]                    1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
RRHO           !            10
Geometry[angstrom]          17
C    0.80545  -0.35171  -1.12187
C    0.80525  -0.35060   0.34457
C    2.07312  -0.35172   1.15708
C   -0.37214  -1.15798   0.72335
C   -1.03983  -1.49402  -0.39686
C   -0.30140  -0.98824  -1.55468
H    1.54644   0.14689  -1.72650
H    2.76408   0.41215   0.80222
H    1.86339  -0.16273   2.20960
H    2.57135  -1.32011   1.08132
H   -0.65090  -1.37784   1.74230
H   -1.96433  -2.04960  -0.44895
H   -0.60994  -1.10626  -2.58222
H    0.30460   0.79527   0.53636
O   -0.37382   1.88163   0.73730
O   -1.34312   1.85185  -0.21365
H   -2.03736   1.30308   0.17702
              Core            RigidRotor
       SymmetryFactor     3.0000000000000000
End
 Rotor                          Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
 End
 Rotor                          Hindered
 Group   16  17
 Axis            15          14
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
 End
 Rotor                          Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
 End
   Frequencies[1/cm]          41
```

```
 3743.0   3251.9   3243.5   3229.1   3217.8   3133.4   3114.3
3045.9   1609.8   1552.1
 1497.7   1495.2   1446.5   1425.1   1418.4   1384.9   1323.2
1264.0   1244.3   1140.0
 1107.8   1097.6   1063.0   1007.5   995.72   967.54   958.22
937.85   896.17   802.31
 794.09   747.78   699.14   600.94   568.35   501.50   306.57
255.34   205.89   153.07
 106.78
 ZeroEnergy[kcal/mol]   10.970357035935553
  ElectronicLevels[1/cm]            1
  0.0000000000000000     2.0000000000000000
 End
!**********************************************
 RRHO      !      11
 Geometry[angstrom]      17
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.46586
 C    1.26742   0.00000   2.27866
 C   -1.17760  -0.80634   1.84500
 C   -1.84539  -1.14260   0.72476
 C   -1.10697  -0.63679  -0.43308
 H    0.74111   0.49829  -0.60476
 H    1.95864   0.76356   1.92376
 H    1.05788   0.18866   3.33126
 H    1.76534  -0.96865   2.20262
 H   -1.45625  -1.02641   2.86392
 H   -2.76972  -1.69836   0.67265
 H   -1.41530  -0.75505  -1.46063
 H   -0.50914   1.16007   1.65968
 O   -1.17850   2.23238   1.85912
 O   -2.14892   2.20328   0.90764
 H   -2.84294   1.65484   1.29867
          Core        RigidRotor
      SymmetryFactor   3.0000000000000000
 End
  Rotor               Hindered
  Group   8  9  10
  Axis       3       2
  Symmetry       1
  Potential[kcal/mol]      18
   0.00   0.54   1.72   2.33   1.70   0.57   0.00   0.51   1.70   2.33   1.69
0.55   0.00   0.52   1.70   2.33   1.68   0.54
  End
  Rotor               Hindered
  Group   16  17
  Axis       15      14
  Symmetry       1
  Potential[kcal/mol]      18
   0.00   0.37   1.24   2.06   2.42   2.36   2.12   1.90   1.89   2.02   2.04
1.81   1.47   1.17   0.97   0.84   0.68   0.27
  End
  Rotor               Hindered
  Group   17
  Axis       16      15
  Symmetry       1
  Potential[kcal/mol]      18
   0.00   0.52   2.26   5.14   8.93   11.01   7.36   4.30   2.39   1.88   0.14
1.31   3.41   6.16   8.04   4.96   2.45   0.69
  End
    Frequencies[1/cm]      41
 3746.4   3252.3   3243.9   3229.6   3218.4   3133.8   3113.9
3045.5   1607.0   1550.5
 1496.2   1494.7   1447.2   1424.4   1417.9   1393.2   1320.2
1265.3   1240.1   1132.2
 1107.6   1097.2   1063.6   1007.4   992.23   966.20   956.99
934.96   895.96   797.52
 791.84   747.85   699.13   598.03   567.64   487.81   308.48
252.76   203.25   156.55
 107.60
 ZeroEnergy[kcal/mol]   10.967979594897219
  ElectronicLevels[1/cm]            1
  0.0000000000000000     2.0000000000000000
 End
!**********************************************
 RRHO      !      12
 Geometry[angstrom]      17
 C    0.80552  -0.35118  -1.12140
 C    0.80571  -0.35229   0.34396
 C    2.07277  -0.35118   1.15709
 C   -0.37209  -1.15758   0.72346
 C   -1.03993  -1.49403  -0.39677
 C   -0.30148  -0.98817  -1.55472
 H    1.54668   0.14674  -1.72624
 H    2.76426   0.41210   0.80215
 H    1.86341  -0.16283   2.20975
 H    2.57040  -1.32011   1.08078
 H   -0.65061  -1.37785   1.74231
 H   -1.96410  -2.04997  -0.44890
 H   -0.60960  -1.10667  -2.58225
 H    0.28811   0.82194   0.53980
 O   -0.37218   1.88018   0.73774
 O   -1.34377   1.85176  -0.21432
 H   -2.03751   1.30370   0.17705
          Core        RigidRotor
      SymmetryFactor   3.0000000000000000
 End
  Rotor               Hindered
  Group   8  9  10
  Axis       3       2
  Symmetry       1
  Potential[kcal/mol]      18
   0.00   0.54   1.72   2.33   1.70   0.57   0.00   0.51   1.70   2.33   1.69
0.55   0.00   0.52   1.70   2.33   1.68   0.54
  End
  Rotor               Hindered
  Group   16  17
  Axis       15      14
  Symmetry       1
  Potential[kcal/mol]      18
   0.00   0.37   1.24   2.06   2.42   2.36   2.12   1.90   1.89   2.02   2.04
1.81   1.47   1.17   0.97   0.84   0.68   0.27
  End
  Rotor               Hindered
  Group   17
  Axis       16      15
  Symmetry       1
  Potential[kcal/mol]      18
   0.00   0.52   2.26   5.14   8.93   11.01   7.36   4.30   2.39   1.88   0.14
1.31   3.41   6.16   8.04   4.96   2.45   0.69
  End
    Frequencies[1/cm]      41
 3749.7   3252.8   3244.3   3230.1   3219.0   3134.3   3113.4
3045.0   1604.2   1549.0
 1495.0   1493.9   1447.9   1423.8   1417.7   1402.3   1317.2
1266.3   1235.5   1128.1
 1107.2   1096.7   1063.0   1007.4   990.43   964.90   955.73
934.01   895.80   792.57
 789.32   747.41   699.93   596.52   567.02   472.92   310.54
247.09   199.96   160.04
 107.71
 ZeroEnergy[kcal/mol]   10.872961038748063
  ElectronicLevels[1/cm]            1
  0.0000000000000000     2.0000000000000000
 End
!**********************************************
 RRHO      !      13
 Geometry[angstrom]      17
 C    0.80557  -0.35096  -1.12117
 C    0.80597  -0.35313   0.34365
 C    2.07261  -0.35095   1.15709
 C   -0.37206  -1.15738   0.72351
 C   -1.03999  -1.49403  -0.39674
 C   -0.30152  -0.98815  -1.55474
 H    1.54682   0.14669  -1.72615
 H    2.76434   0.41206   0.80212
 H    1.86341  -0.16289   2.20983
 H    2.56996  -1.32011   1.08053
```

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H   -0.65049  -1.37786   1.74233
H   -1.96399  -2.05014  -0.44888
H   -0.60946  -1.10687  -2.58228
H    0.27982   0.83538   0.54175
O   -0.37143   1.87952   0.73795
O   -1.34406   1.85172  -0.21463
H   -2.03758   1.30398   0.17708
          Core          RigidRotor
     SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
 End
 Rotor                     Hindered
 Group   16  17
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
 End
 Rotor                     Hindered
 Group   17
 Axis          16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
 End
   Frequencies[1/cm]          41
  3752.4      3252.9      3244.6      3230.4      3219.5      3134.6      3113.1
3044.6      1601.6      1547.5
  1494.4      1492.5      1449.0      1424.9      1418.7      1410.4      1314.4
1267.2      1230.0      1126.3
  1106.8      1096.9      1064.3      1007.6      986.37      963.59      954.48
930.40      895.68      790.63
  783.82      746.43      700.29      595.80      565.45      468.73      312.17
246.73      199.80      160.33
  107.85
ZeroEnergy[kcal/mol]    10.693464947437764
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
!********************************************
RRHO          !          14
Geometry[angstrom]          17
C    0.80562  -0.35072  -1.12095
C    0.80623  -0.35401   0.34334
C    2.07245  -0.35071   1.15709
C   -0.37204  -1.15719   0.72356
C   -1.04004  -1.49403  -0.39670
C   -0.30156  -0.98813  -1.55477
H    1.54693   0.14662  -1.72604
H    2.76443   0.41203   0.80208
H    1.86342  -0.16294   2.20990
H    2.56953  -1.32013   1.08029
H   -0.65037  -1.37787   1.74233
H   -1.96389  -2.05031  -0.44887
H   -0.60931  -1.10707  -2.58230
H    0.27162   0.84888   0.54360
O   -0.37069   1.87888   0.73816
O   -1.34436   1.85167  -0.21494
H   -2.03762   1.30424   0.17708
          Core          RigidRotor
     SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
 End
 Rotor                     Hindered
 Group   16  17
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
 End
 Rotor                     Hindered
 Group   17
 Axis          16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
 End
   Frequencies[1/cm]          41
  3755.3      3253.3      3245.0      3230.9      3220.1      3135.0      3112.7
3044.2      1599.0      1546.0
  1494.1      1490.9      1450.0      1432.0      1420.0      1412.8      1311.8
1267.8      1224.2      1127.2
  1106.3      1096.9      1064.5      1007.7      985.15      962.31      953.14
932.08      895.63      789.72
  777.93      744.18      701.89      595.51      564.32      462.92      313.91
246.34      200.36      161.92
  108.54
ZeroEnergy[kcal/mol]    10.423402796013310
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
End
!********************************************
RRHO          !          15
Geometry[angstrom]          17
C    0.80567  -0.35050  -1.12073
C    0.80650  -0.35491   0.34303
C    2.07230  -0.35047   1.15709
C   -0.37201  -1.15701   0.72361
C   -1.04009  -1.49404  -0.39666
C   -0.30160  -0.98810  -1.55479
H    1.54703   0.14655  -1.72593
H    2.76452   0.41201   0.80204
H    1.86343  -0.16299   2.20997
H    2.56912  -1.32014   1.08005
H   -0.65025  -1.37788   1.74233
H   -1.96378  -2.05048  -0.44885
H   -0.60917  -1.10726  -2.58231
H    0.26346   0.86241   0.54545
O   -0.36996   1.87827   0.73838
O   -1.34466   1.85163  -0.21525
H   -2.03765   1.30448   0.17707
          Core          RigidRotor
     SymmetryFactor    3.0000000000000000
End
 Rotor                     Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
 End
 Rotor                     Hindered
 Group   16  17
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
 End
```

Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.52 2.26 5.14 8.93 11.01 7.36 4.30 2.39 1.88 0.14
1.31 3.41 6.16 8.04 4.96 2.45 0.69
End
Frequencies[1/cm] 41
3758.2 3253.7 3245.4 3231.3 3220.7 3135.3 3112.3
3043.7 1596.4 1544.5
1493.9 1489.2 1451.1 1443.6 1419.8 1412.7 1309.4
1268.0 1217.9 1127.8
1105.6 1097.2 1065.2 1007.9 982.03 960.96 951.77
930.33 895.60 789.19
772.24 740.32 703.20 595.52 562.61 457.13 315.21
241.16 197.83 161.40
108.41
ZeroEnergy[kcal/mol] 10.087477584108218
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 16
Geometry[angstrom] 17
C 0.80572 -0.35027 -1.12051
C 0.80678 -0.35585 0.34271
C 2.07215 -0.35024 1.15709
C -0.37198 -1.15682 0.72366
C -1.04014 -1.49404 -0.39662
C -0.30164 -0.98808 -1.55482
H 1.54714 0.14647 -1.72583
H 2.76461 0.41198 0.80201
H 1.86343 -0.16304 2.21004
H 2.56872 -1.32014 1.07983
H -0.65013 -1.37790 1.74233
H -1.96368 -2.05065 -0.44883
H -0.60903 -1.10745 -2.58233
H 0.25532 0.87596 0.54731
O -0.36925 1.87767 0.73859
O -1.34496 1.85160 -0.21555
H -2.03768 1.30472 0.17706
Core RigidRotor
SymmetryFactor 3.0000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.54 1.72 2.33 1.70 0.57 0.00 0.51 1.70 2.33 1.69
0.55 0.00 0.52 1.70 2.33 1.68 0.54
End
Rotor Hindered
Group 16 17
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18
0.00 0.37 1.24 2.06 2.42 2.36 2.12 1.90 1.89 2.02 2.04
1.81 1.47 1.17 0.97 0.84 0.68 0.27
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.52 2.26 5.14 8.93 11.01 7.36 4.30 2.39 1.88 0.14
1.31 3.41 6.16 8.04 4.96 2.45 0.69
End
Frequencies[1/cm] 41
3761.1 3254.1 3245.8 3231.8 3221.2 3135.7 3111.9
3043.1 1594.3 1543.3
1493.8 1487.5 1457.8 1451.8 1419.1 1412.0 1307.3
1268.1 1211.5 1129.8
1104.8 1097.3 1065.7 1008.3 979.20 959.55 950.39
928.28 895.61 789.17
767.82 734.05 705.23 595.75 560.98 451.06 316.33
238.23 197.12 160.56
108.19
ZeroEnergy[kcal/mol] 9.6429015042771660
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 17
Geometry[angstrom] 17
C 0.80577 -0.35004 -1.12029
C 0.80707 -0.35681 0.34239
C 2.07200 -0.35001 1.15710
C -0.37195 -1.15664 0.72372
C -1.04019 -1.49404 -0.39658
C -0.30167 -0.98806 -1.55484
H 1.54724 0.14639 -1.72574
H 2.76470 0.41196 0.80197
H 1.86344 -0.16309 2.21011
H 2.56832 -1.32015 1.07960
H -0.65001 -1.37792 1.74233
H -1.96358 -2.05082 -0.44881
H -0.60889 -1.10763 -2.58235
H 0.24721 0.88953 0.54916
O -0.36855 1.87710 0.73881
O -1.34525 1.85156 -0.21585
H -2.03770 1.30494 0.17705
Core RigidRotor
SymmetryFactor 3.0000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.54 1.72 2.33 1.70 0.57 0.00 0.51 1.70 2.33 1.69
0.55 0.00 0.52 1.70 2.33 1.68 0.54
End
Rotor Hindered
Group 16 17
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18
0.00 0.37 1.24 2.06 2.42 2.36 2.12 1.90 1.89 2.02 2.04
1.81 1.47 1.17 0.97 0.84 0.68 0.27
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.52 2.26 5.14 8.93 11.01 7.36 4.30 2.39 1.88 0.14
1.31 3.41 6.16 8.04 4.96 2.45 0.69
End
Frequencies[1/cm] 41
3763.9 3254.5 3246.2 3232.2 3221.8 3135.9 3111.5
3042.6 1592.4 1542.1
1493.9 1486.0 1469.8 1452.9 1418.4 1411.3 1305.5
1268.0 1205.0 1131.3
1103.9 1097.3 1066.2 1008.6 975.67 958.18 948.97
924.42 895.63 789.00
764.67 725.94 706.54 596.11 559.03 444.45 317.11
228.86 192.12 158.01
107.23
ZeroEnergy[kcal/mol] 9.0680308404061272
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 18
Geometry[angstrom] 17
C 0.80582 -0.34982 -1.12007

```
C   0.80738  -0.35780   0.34206
C   2.07185  -0.34978   1.15710
C  -0.37193  -1.15646   0.72377
C  -1.04025  -1.49405  -0.39654
C  -0.30171  -0.98803  -1.55487
H   1.54735   0.14632  -1.72564
H   2.76479   0.41193   0.80193
H   1.86345  -0.16314   2.21018
H   2.56793  -1.32015   1.07938
H  -0.64990  -1.37794   1.74233
H  -1.96348  -2.05099  -0.44879
H  -0.60875  -1.10782  -2.58237
H   0.23911   0.90311   0.55102
O  -0.36787   1.87655   0.73903
O  -1.34555   1.85153  -0.21615
H  -2.03772   1.30515   0.17704
          Core          RigidRotor
      SymmetryFactor    3.0000000000000000
End
 Rotor                   Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
 End
 Rotor                   Hindered
 Group   16  17
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
 End
 Rotor                   Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
 End
    Frequencies[1/cm]          41
  3766.6     3254.9     3246.5     3232.7     3222.3     3136.2     3111.1
3042.1     1590.6     1541.0
  1494.8     1484.7     1481.5     1453.9     1417.8     1410.5     1304.0
1267.7     1198.8     1136.6
  1103.0     1097.8     1068.2     1008.8     972.56     956.81     947.52
920.50     895.99     791.65
  762.55     719.57     705.50     596.66     557.10     442.30     317.71
225.74     191.75     155.42
  106.55
 ZeroEnergy[kcal/mol]    8.4387036478730018
 ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          19
Geometry[angstrom]          17
C   0.80587  -0.34960  -1.11985
C   0.80770  -0.35882   0.34172
C   2.07171  -0.34955   1.15710
C  -0.37189  -1.15627   0.72382
C  -1.04030  -1.49406  -0.39651
C  -0.30175  -0.98801  -1.55490
H   1.54746   0.14624  -1.72554
H   2.76488   0.41191   0.80189
H   1.86346  -0.16318   2.21026
H   2.56754  -1.32015   1.07917
H  -0.64978  -1.37797   1.74233
H  -1.96338  -2.05117  -0.44877
H  -0.60861  -1.10801  -2.58240
H   0.23105   0.91669   0.55286
O  -0.36720   1.87603   0.73926
O  -1.34584   1.85149  -0.21645
H  -2.03774   1.30535   0.17704
          Core          RigidRotor
      SymmetryFactor    3.0000000000000000
End
 Rotor                   Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
 End
 Rotor                   Hindered
 Group   16  17
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.37    1.24    2.06    2.42    2.36    2.12    1.90    1.89    2.02    2.04
1.81    1.47    1.17    0.97    0.84    0.68    0.27
 End
 Rotor                   Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.52    2.26    5.14    8.93   11.01    7.36    4.30    2.39    1.88    0.14
1.31    3.41    6.16    8.04    4.96    2.45    0.69
 End
    Frequencies[1/cm]          41
  3769.3     3255.2     3246.8     3233.0     3222.8     3136.5     3110.7
3041.5     1589.1     1540.0
  1499.3     1489.2     1482.8     1454.8     1417.2     1409.7     1302.7
1267.3     1192.9     1144.7
  1102.2     1098.5     1071.5     1009.1     969.45     955.47     946.11
915.07     896.69     796.91
  761.09     720.34     696.82     597.43     555.17     441.79     318.09
220.77     190.18     152.31
  105.26
 ZeroEnergy[kcal/mol]    7.5883883895872266
 ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          20
Geometry[angstrom]          17
C   0.80593  -0.34937  -1.11963
C   0.80803  -0.35989   0.34138
C   2.07155  -0.34931   1.15710
C  -0.37186  -1.15608   0.72388
C  -1.04035  -1.49406  -0.39647
C  -0.30179  -0.98800  -1.55493
H   1.54757   0.14616  -1.72544
H   2.76497   0.41189   0.80185
H   1.86346  -0.16323   2.21033
H   2.56715  -1.32014   1.07895
H  -0.64966  -1.37800   1.74234
H  -1.96328  -2.05134  -0.44876
H  -0.60847  -1.10820  -2.58242
H   0.22301   0.93026   0.55469
O  -0.36653   1.87553   0.73950
O  -1.34614   1.85146  -0.21675
H  -2.03776   1.30554   0.17704
          Core          RigidRotor
      SymmetryFactor    3.0000000000000000
End
 Rotor                   Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.54    1.72    2.33    1.70    0.57    0.00    0.51    1.70    2.33    1.69
0.55    0.00    0.52    1.70    2.33    1.68    0.54
```

```
 End
 Rotor                    Hindered
 Group   16  17
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
   0.00   0.37   1.24   2.06   2.42   2.36   2.12   1.90   1.89   2.02   2.04
1.81   1.47   1.17   0.97   0.84   0.68   0.27
 End
 Rotor                    Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]          18
   0.00   0.52   2.26   5.14   8.93   11.01   7.36   4.30   2.39   1.88   0.14
1.31   3.41   6.16   8.04   4.96   2.45   0.69
 End
    Frequencies[1/cm]          41
  3772.0     3255.5     3247.2     3233.4     3223.2     3136.7     3110.3
3040.9     1587.8     1539.4
  1507.8     1491.0     1481.5     1455.6     1416.8     1408.9     1301.6
1267.0     1187.5     1159.0
  1102.3     1098.9     1076.1     1009.4     966.34     954.21     944.70
907.37     896.88     805.85
  760.01     724.64     684.18     598.41     553.25     443.79     318.29
214.17     188.16     147.65
  103.65
 ZeroEnergy[kcal/mol]    6.8203943999079577
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
RRHO          !          21
Geometry[angstrom]          17
C    0.80598  -0.34914  -1.11940
C    0.80838  -0.36101   0.34102
C    2.07140  -0.34907   1.15710
C   -0.37182  -1.15588   0.72393
C   -1.04041  -1.49407  -0.39643
C   -0.30182  -0.98798  -1.55496
H    1.54769   0.14607  -1.72534
H    2.76507   0.41187   0.80180
H    1.86346  -0.16328   2.21041
H    2.56676  -1.32013   1.07874
H   -0.64953  -1.37804   1.74234
H   -1.96317  -2.05153  -0.44874
H   -0.60833  -1.10840  -2.58244
H    0.21502   0.94380   0.55647
O   -0.36588   1.87506   0.73976
O   -1.34645   1.85143  -0.21707
H   -2.03778   1.30571   0.17704
              Core           RigidRotor
      SymmetryFactor    3.0000000000000000
 End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
   0.00   0.54   1.72   2.33   1.70   0.57   0.00   0.51   1.70   2.33   1.69
0.55   0.00   0.52   1.70   2.33   1.68   0.54
 End
 Rotor                    Hindered
 Group   16  17
 Axis          15         14
 Symmetry          1
 Potential[kcal/mol]          18
   0.00   0.37   1.24   2.06   2.42   2.36   2.12   1.90   1.89   2.02   2.04
1.81   1.47   1.17   0.97   0.84   0.68   0.27
 End
 Rotor                    Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]          18
   0.00   0.52   2.26   5.14   8.93   11.01   7.36   4.30   2.39   1.88   0.14
1.31   3.41   6.16   8.04   4.96   2.45   0.69
 End
    Frequencies[1/cm]          41
  3774.8     3255.8     3247.4     3233.8     3223.6     3136.9     3109.8
3040.3     1586.8     1539.1
  1516.2     1491.5     1480.3     1456.3     1417.2     1408.2     1300.8
1266.8     1193.4     1182.8
  1104.9     1098.3     1081.5     1009.7     963.94     953.03     943.35
908.53     892.50     822.25
  759.16     730.10     670.71     599.76     551.42     450.39     318.39
210.21     187.23     144.16
  101.91
 ZeroEnergy[kcal/mol]    6.0763937012717584
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1843.3099000000000
      WellDepth[kcal/mol]         15.10
      WellDepth[kcal/mol]         21.99
 End
End
End
```

```
!****************************************************
!            GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature             .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature           30        ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]            400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct     ! direct or low-eigenvalue
!
WellCutoff                            20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                 0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!
!WellCutoff                           10
!ChemicalEigenvalueMin                1.e-6         #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                 1.3
!!
RateOutput                            rate.out                  ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!            MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                         ! Default collisional
energy relaxation kernel
    Exponential                                            ! Currently the only
possible energy relaxation model
      Factor[1/cm]                316                      ! (Delta_E_down)^(0)
@ standard T (300 K)
      Power                   0.535                        ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
      ExponentCutoff              10                       ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                       ! Collision frequency
model
    LennardJones                                           ! Currently the only
possible collisional frequency model  based on LJ potential
      Epsilons[K]                 90.58  281.367           ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
      Sigmas[angstrom]            3.54    4.694            ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
      Masses[amu]                 39.948  79.05478         ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]          14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.34058
 C    1.17550   0.00000   2.25991
 C   -1.39560  -0.00008   1.80105
 C   -2.21870  -0.00003   0.74716
 C   -1.40657  -0.00007  -0.51024
 H    0.87312   0.00029  -0.63540
 H    2.11196   0.00080   1.70444
 H    1.16259   0.87759   2.90932
 H    1.16343  -0.87842   2.90820
 H   -1.69080  -0.00015   2.84114
 H   -3.29750  -0.00010   0.77029
 H   -1.62068  -0.87614  -1.13069
 H   -1.62069   0.87579  -1.13094
      Core    RigidRotor
           SymmetryFactor    1.0000000000000000
      End
 Rotor                       Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.08    0.32    0.66    1.03    1.33    1.44    1.32    1.03    0.66    0.32
0.08
 End
    Frequencies[1/cm]          35
   3241.0     3225.5     3207.9     3133.2     3100.2     3075.2     3043.9
3042.9     1708.1     1610.0
   1497.4     1487.3     1428.4     1422.7     1402.8     1311.9     1272.8
1227.8     1137.4     1111.0
   1073.3     1028.7     984.40     980.54     951.47     936.30     920.52
826.70     765.47     719.11
   624.46     583.63     368.96     327.69     231.38
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                  1
   0.0000000000000000       2.0000000000000000
 End
 !************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]            3
 O    0.00000   0.00000   0.00000
 O    0.00000   0.00000   1.31234
 H    0.93494   0.00000   1.57303
      Core    RigidRotor
           SymmetryFactor    1.0000000000000000
      End
    Frequencies[1/cm]           3
   1234.9     1462.2     3683.2
  ZeroEnergy[kcal/mol]           0.
  ElectronicLevels[1/cm]                  1
   0.0000000000000000       2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
 !************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]            13
```

```
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.41507
C   1.18585   0.00000   2.30525
C  -1.37924  -0.00034   1.86264
C  -2.17195  -0.00056   0.76525
C  -1.30652  -0.00033  -0.41759
H   0.87955   0.00028  -0.62343
H   2.11567   0.00259   1.73998
H   1.17551   0.87449   2.96082
H   1.17824  -0.87748   2.95691
H  -1.69366  -0.00045   2.89442
H  -3.25029  -0.00080   0.74358
H  -1.65471  -0.00041  -1.43915
      Core    RigidRotor
          SymmetryFactor    2.0000000000000000
      End
Rotor                         Hindered
Group    8   9  10
Axis           3           2
Symmetry           3
Potential[kcal/mol]           12
  0.00    0.01    0.04    0.06    0.04    0.01    0.00    0.02    0.04    0.06    0.04
0.01
End
   Frequencies[1/cm]           32
  3255.2     3247.0     3232.4     3224.7     3138.6     3086.9     3034.1
1584.1     1503.1     1481.1
  1477.9     1438.4     1407.4     1311.3     1292.6     1178.7     1098.1
1049.4     1023.5     1013.2
  953.40     929.99     923.03     899.45     740.46     727.81     638.42
604.77     528.85     520.52
  329.55     215.83
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
!************************************
Fragment PROD2
RRHO
Geometry[angstrom]              4
O   0.00000   0.00000   0.00000
O   0.00000   0.00000   1.42622
H   0.94322   0.00000   1.61480
H  -0.34861  -0.87643  -0.18855
      Core    RigidRotor
          SymmetryFactor    2.0000000000000000
      End
Rotor                         Hindered
Group    4
Axis           1           2
Symmetry           1
Potential[kcal/mol]           18
  0.00    0.07    0.48    0.80    0.77    0.40    0.02    0.06    0.91    2.62    4.92
7.15    8.51    8.38    6.81    4.51    2.28    0.70
End
   Frequencies[1/cm]           5
  3840.9     3839.6     1465.2     1361.0     1016.3
 ZeroEnergy[kcal/mol]             0.
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
GroundEnergy[kcal/mol]    -5.98
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]             17
C  -0.00548  -0.00857  -0.00100
C  -0.00144  -0.00187   1.34498
C   1.17804   0.00858   2.25922
C  -1.39599  -0.01721   1.81008
C  -2.21884  -0.04000   0.75587
C  -1.41449  -0.04058  -0.50438
H   0.86534  -0.01980  -0.63971
H   2.11284   0.03426   1.70213
H   1.14944   0.87326   2.92502
H   1.17971  -0.88078   2.89177
H  -1.68708  -0.00658   2.85059
H  -3.29738  -0.04801   0.78183
H  -1.60929  -0.93085  -1.11013
H  -1.64446   0.82054  -1.13994
O  -0.31462   3.22344  -0.99439
O  -0.06172   3.07812   0.28340
H   0.00044   2.10676   0.42704
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]           45
  25.995     51.540     61.031     105.38     156.74     166.97     256.66
328.57     377.03     497.32
  592.80     624.91     726.41     783.30     827.55     924.25     939.21
952.54     984.61     986.75
  1028.3     1074.2     1113.2     1141.8     1228.7     1258.1     1275.1
1317.0     1402.9     1424.9
  1430.9     1487.7     1497.1     1519.2     1604.5     1695.4     3045.6
3047.1     3080.5     3104.7
  3139.0     3215.8     3226.7     3245.6     3436.2
 ZeroEnergy[kcal/mol]              -5.97
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]             17
C   0.01082   0.03983   0.02101
C   0.01820   0.00201   1.45573
C   1.21771  -0.02508   2.32310
C  -1.34234   0.06045   1.90227
C  -2.14164   0.12701   0.79750
C  -1.28375   0.11918  -0.39078
H   0.89033   0.00227  -0.60227
H   2.06327  -0.49805   1.82538
H   1.50661   1.00238   2.56602
H   1.02070  -0.53964   3.26302
H  -1.65849   0.03065   2.93291
H  -3.21961   0.17062   0.78198
H  -1.63833   0.16379  -1.40845
H  -1.46394   2.38974   1.57502
O  -1.19531   3.27901   1.30164
O   0.22209   3.15146   1.25872
H   0.36643   2.88214   0.34517
      Core    RigidRotor
          SymmetryFactor   0.50000000000000000
      End
   Frequencies[1/cm]           45
  16.512     52.771     73.091     82.698     98.112     136.21     219.98
225.66     331.59     524.88
  536.67     607.86     617.67     639.15     742.55     749.30     912.07
927.34     933.58     965.39
  1007.7     1017.7     1025.6     1065.2     1095.5     1190.1     1297.6
1309.3     1403.2     1416.0
  1435.4     1461.2     1475.9     1489.0     1535.4     1553.3     3031.2
3101.6     3138.7     3227.6
  3233.9     3247.2     3256.2     3716.5     3811.9
 ZeroEnergy[kcal/mol]              -8.60
 ElectronicLevels[1/cm]                    1
 0.0000000000000000       2.0000000000000000
End
End
!************************************
Barrier        B1  REACS WR
  RRHO
    Stoichiometry  H9C6O2
    Core PhaseSpaceTheory
```

```
    FragmentGeometry[angstrom]          14
C   0.00000  0.00000  0.00000
C   0.00000  0.00000  1.34058
C   1.17550  0.00000  2.25991
C  -1.39560 -0.00008  1.80105
C  -2.21870 -0.00003  0.74716
C  -1.40657 -0.00007 -0.51024
H   0.87312  0.00029 -0.63540
H   2.11196  0.00080  1.70444
H   1.16259  0.87759  2.90932
H   1.16343 -0.87842  2.90820
H  -1.69080 -0.00015  2.84114
H  -3.29750 -0.00010  0.77029
H  -1.62068 -0.87614 -1.13069
H  -1.62069  0.87579 -1.13094
    FragmentGeometry[angstrom]          3
O   0.00000  0.00000  0.00000
O   0.00000  0.00000  1.31234
H   0.93494  0.00000  1.57303
                    SymmetryFactor    1.0000000000000000
      PotentialPrefactor[au]          10.
      PotentialPowerExponent          6
             End
Rotor                    Hindered
Geometry[angstrom]          14
C   0.00000  0.00000  0.00000
C   0.00000  0.00000  1.34058
C   1.17550  0.00000  2.25991
C  -1.39560 -0.00008  1.80105
C  -2.21870 -0.00003  0.74716
C  -1.40657 -0.00007 -0.51024
H   0.87312  0.00029 -0.63540
H   2.11196  0.00080  1.70444
H   1.16259  0.87759  2.90932
H   1.16343 -0.87842  2.90820
H  -1.69080 -0.00015  2.84114
H  -3.29750 -0.00010  0.77029
H  -1.62068 -0.87614 -1.13069
H  -1.62069  0.87579 -1.13094
Group   8  9  10
Axis        3       2
Symmetry        3
Potential[kcal/mol]        12
  0.0000    0.80000E-01 0.32000    0.66000    1.0300    1.3300    1.4400
1.3200    1.0300    0.66000
 0.32000    0.80000E-01
End
   Frequencies[1/cm]        38
  3241.0    3225.5    3207.9    3133.2    3100.2    3075.2    3043.9
3042.9    1708.1    1610.0
  1497.4    1487.3    1428.4    1422.7    1402.8    1311.9    1272.8
1227.8    1137.4    1111.0
  1073.3    1028.7    984.40    980.54    951.47    936.30    920.52
826.70    765.47    719.11
  624.46    583.63    368.96    327.69    231.38
  1234.9    1462.2    3683.2
 ZeroEnergy[kcal/mol]          0.
 ElectronicLevels[1/cm]              1
  0.0000000000000000      4.0000000000000000
End
!************************************
Barrier      B3  WP PRODS
  RRHO
   Stoichiometry  H9C6O2
   Core PhaseSpaceTheory
    FragmentGeometry[angstrom]          13
C   0.00000  0.00000  0.00000
C   0.00000  0.00000  1.41507
C   1.18585  0.00000  2.30525
C  -1.37924 -0.00034  1.86264
C  -2.17195 -0.00056  0.76525
C  -1.30652 -0.00033 -0.41759
H   0.87955  0.00028 -0.62343
H   2.11567  0.00259  1.73998
H   1.17551  0.87449  2.96082
H   1.17824 -0.87748  2.95691
H  -1.69366 -0.00045  2.89442
H  -3.25029 -0.00080  0.74358
H  -1.65471 -0.00041 -1.43915
    FragmentGeometry[angstrom]          4
O   0.00000  0.00000  0.00000
O   0.00000  0.00000  1.42622
H   0.94322  0.00000  1.61480
H  -0.34861 -0.87643 -0.18855
                    SymmetryFactor    4.0000000000000000
      PotentialPrefactor[au]          10.
      PotentialPowerExponent          6
             End
Rotor                    Hindered
Geometry[angstrom]          13
C   0.00000  0.00000  0.00000
C   0.00000  0.00000  1.41507
C   1.18585  0.00000  2.30525
C  -1.37924 -0.00034  1.86264
C  -2.17195 -0.00056  0.76525
C  -1.30652 -0.00033 -0.41759
H   0.87955  0.00028 -0.62343
H   2.11567  0.00259  1.73998
H   1.17551  0.87449  2.96082
H   1.17824 -0.87748  2.95691
H  -1.69366 -0.00045  2.89442
H  -3.25029 -0.00080  0.74358
H  -1.65471 -0.00041 -1.43915
Group   8  9  10
Axis        3       2
Symmetry        3
Potential[kcal/mol]        12
  0.0000    0.10000E-01 0.40000E-01 0.60000E-01 0.40000E-01 0.10000E-
01  0.0000    0.20000E-01 0.40000E-01 0.60000E-01
 0.40000E-01 0.10000E-01
End
Rotor                    Hindered
Geometry[angstrom]          4
O   0.00000  0.00000  0.00000
O   0.00000  0.00000  1.42622
H   0.94322  0.00000  1.61480
H  -0.34861 -0.87643 -0.18855
Group   4
Axis        1       2
Symmetry        1
Potential[kcal/mol]        18
  0.0000    0.70000E-01 0.48000    0.80000    0.77000    0.40000
0.20000E-01 0.60000E-01 0.91000    2.6200
  4.9200    7.1500    8.5100    8.3800    6.8100    4.5100    2.2800
0.70000
End
   Frequencies[1/cm]        37
  3255.2    3247.0    3232.4    3224.7    3138.6    3086.9    3034.1
1584.1    1503.1    1481.1
  1477.9    1438.4    1407.4    1311.3    1292.6    1178.7    1098.1
1049.4    1023.5    1013.2
  953.40    929.99    923.03    899.45    740.46    727.81    638.42
604.77    528.85    520.52
  329.55    215.83
  3840.9    3839.6    1465.2    1361.0    1016.3
 ZeroEnergy[kcal/mol]          -5.9753639529381513
 ElectronicLevels[1/cm]              1
  0.0000000000000000      4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO        !        1
Geometry[angstrom]        17
C   0.79731 -0.81964 -0.60601
C   0.79471 -0.81852  0.74383
C   1.96873 -0.81760  1.66265
C  -0.60220 -0.84099  1.20098
```

```
C  -1.41812 -0.85650  0.13499
C  -0.59080 -0.76440 -1.08129
H   1.66543 -0.81181 -1.24774
H   2.90706 -0.80175  1.11030
H   1.94574  0.04819  2.32788
H   1.96162 -1.70478  2.29903
H  -0.90302 -0.83463  2.23882
H  -2.49628 -0.84901  0.13843
H  -0.88658 -1.27094 -1.99605
H  -0.72207  0.33760 -1.36953
O  -0.69314  1.75026 -1.47671
O  -0.28114  2.17822 -0.26691
H   0.68346  2.09303 -0.29916
          Core          RigidRotor
      SymmetryFactor   1.5000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.29   0.98   1.39   1.02   0.33   0.00   0.26   0.94   1.39   1.00
0.29  -0.00   0.29   0.97   1.39   1.03   0.32
 End
 Rotor                  Hindered
 Group   16  17
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.35   1.21   1.95   2.25   2.32   2.37   2.45   2.49   2.46   2.36
2.15   1.84   1.51   1.28   1.16   0.86   0.26
 End
 Rotor                  Hindered
 Group   17
 Axis          16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.51   2.20   4.96  15.41   8.69   7.22   8.73   2.91   2.38  -0.23
1.02   4.49  12.18   7.36   4.41   2.15   0.62
 End
   Frequencies[1/cm]          41
  3721.4     3250.4     3228.3     3215.5     3142.8     3132.3     3095.9
3040.1     2000.3     1667.5
  1577.0     1497.7     1486.7     1449.3     1424.5     1405.2     1386.7
1344.7     1269.9     1238.7
  1109.5     1071.3     1059.0     1040.8     1013.3     983.82     973.47
946.24     915.91     888.73
  837.64     759.12     720.28     627.28     587.49     468.86     325.76
277.89     217.57     85.790
  26.690
 ZeroEnergy[kcal/mol]   11.861948157653188
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          2
Geometry[angstrom]          17
C   0.79703 -0.81939 -0.60639
C   0.79475 -0.81842  0.74390
C   1.96871 -0.81764  1.66260
C  -0.60228 -0.84092  1.20104
C  -1.41812 -0.85618  0.13470
C  -0.59044 -0.76448 -1.08076
H   1.66515 -0.81194 -1.24805
H   2.90704 -0.80174  1.11029
H   1.94552  0.04819  2.32778
H   1.96152 -1.70476  2.29907
H  -0.90313 -0.83495  2.23883
H  -2.49625 -0.84914  0.13809
H  -0.88728 -1.26525 -1.99816
H  -0.72057  0.35022 -1.36733
O  -0.69340  1.74848 -1.47727
O  -0.28090  2.17835 -0.26623
H   0.68352  2.09395 -0.29943
          Core          RigidRotor
      SymmetryFactor   1.5000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.29   0.98   1.39   1.02   0.33   0.00   0.26   0.94   1.39   1.00
0.29  -0.00   0.29   0.97   1.39   1.03   0.32
 End
 Rotor                  Hindered
 Group   16  17
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.35   1.21   1.95   2.25   2.32   2.37   2.45   2.49   2.46   2.36
2.15   1.84   1.51   1.28   1.16   0.86   0.26
 End
 Rotor                  Hindered
 Group   17
 Axis          16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.51   2.20   4.96  15.41   8.69   7.22   8.73   2.91   2.38  -0.23
1.02   4.49  12.18   7.36   4.41   2.15   0.62
 End
   Frequencies[1/cm]          41
  3724.6     3250.9     3228.8     3216.0     3145.0     3132.4     3095.8
3040.1     1843.9     1663.2
  1572.4     1497.2     1486.6     1447.8     1424.3     1404.7     1386.4
1344.9     1270.1     1238.4
  1109.3     1070.6     1046.4     1040.6     1013.3     984.63     972.68
945.14     916.81     885.76
  837.97     762.17     722.28     627.12     589.31     480.39     326.04
280.68     220.57     87.470
  51.280
 ZeroEnergy[kcal/mol]   12.054717506361456
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!**********************************************
RRHO          !          3
Geometry[angstrom]          17
C   0.79678 -0.81916 -0.60675
C   0.79479 -0.81834  0.74398
C   1.96869 -0.81767  1.66255
C  -0.60235 -0.84086  1.20110
C  -1.41813 -0.85589  0.13443
C  -0.59010 -0.76472 -1.08025
H   1.66491 -0.81206 -1.24832
H   2.90702 -0.80173  1.11028
H   1.94531  0.04819  2.32770
H   1.96143 -1.70475  2.29910
H  -0.90323 -0.83523  2.23884
H  -2.49622 -0.84927  0.13780
H  -0.88789 -1.26020 -2.00003
H  -0.71943  0.36375 -1.36589
O  -0.69364  1.74687 -1.47779
O  -0.28068  2.17847 -0.26560
H   0.68355  2.09474 -0.29965
          Core          RigidRotor
      SymmetryFactor   1.5000000000000000
End
 Rotor                  Hindered
 Group   8  9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00   0.29   0.98   1.39   1.02   0.33   0.00   0.26   0.94   1.39   1.00
0.29  -0.00   0.29   0.97   1.39   1.03   0.32
 End
 Rotor                  Hindered
 Group   16  17
```

```
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.35 1.21 1.95 2.25 2.32 2.37 2.45 2.49 2.46 2.36
2.15 1.84 1.51 1.28 1.16 0.86 0.26
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.51 2.20 4.96 15.41 8.69 7.22 8.73 2.91 2.38 -0.23
1.02 4.49 12.18 7.36 4.41 2.15 0.62
 End
   Frequencies[1/cm] 41
  3727.8 3251.3 3229.2 3216.5 3147.3 3132.7 3095.8
3040.1 1685.1 1642.8
  1554.5 1495.8 1486.4 1446.2 1424.2 1403.9 1382.3
1344.7 1270.2 1238.0
  1109.2 1070.1 1039.8 1029.1 1012.5 985.26 971.26
941.67 916.98 879.11
  838.16 764.39 724.36 626.86 590.71 485.87 326.22
281.26 223.21 89.400
  67.060
 ZeroEnergy[kcal/mol] 12.088416231800736
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!*********************************************
RRHO ! 4
Geometry[angstrom] 17
C 0.79653 -0.81895 -0.60709
C 0.79484 -0.81826 0.74405
C 1.96868 -0.81770 1.66250
C -0.60243 -0.84080 1.20115
C -1.41814 -0.85564 0.13418
C -0.58977 -0.76509 -1.07975
H 1.66469 -0.81219 -1.24855
H 2.90700 -0.80172 1.11027
H 1.94511 0.04819 2.32762
H 1.96135 -1.70473 2.29914
H -0.90331 -0.83549 2.23885
H -2.49619 -0.84939 0.13755
H -0.88843 -1.25570 -2.00168
H -0.71854 0.37791 -1.36505
O -0.69386 1.74542 -1.47828
O -0.28047 2.17858 -0.26502
H 0.68356 2.09544 -0.29984
   Core RigidRotor
   SymmetryFactor 1.5000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.29 0.98 1.39 1.02 0.33 0.00 0.26 0.94 1.39 1.00
0.29 -0.00 0.29 0.97 1.39 1.03 0.32
 End
 Rotor Hindered
 Group 16 17
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.35 1.21 1.95 2.25 2.32 2.37 2.45 2.49 2.46 2.36
2.15 1.84 1.51 1.28 1.16 0.86 0.26
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.51 2.20 4.96 15.41 8.69 7.22 8.73 2.91 2.38 -0.23
1.02 4.49 12.18 7.36 4.41 2.15 0.62
 End
   Frequencies[1/cm] 41
  3731.0 3251.8 3229.7 3217.1 3149.6 3132.9 3095.7
3040.0 1663.4 1593.8
  1501.4 1486.4 1466.5 1440.4 1424.0 1403.3 1367.1
1343.4 1270.2 1237.1
  1109.1 1069.5 1038.8 1013.6 1009.8 985.65 969.47
936.84 917.22 865.17
  838.31 765.43 726.26 626.51 592.11 492.29 326.51
283.49 225.82 91.790
  79.510
 ZeroEnergy[kcal/mol] 12.159482511821437
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!*********************************************
RRHO ! 5
Geometry[angstrom] 17
C 0.79631 -0.81876 -0.60740
C 0.79489 -0.81819 0.74413
C 1.96866 -0.81773 1.66246
C -0.60250 -0.84076 1.20121
C -1.41814 -0.85540 0.13396
C -0.58945 -0.76556 -1.07926
H 1.66450 -0.81230 -1.24875
H 2.90698 -0.80171 1.11027
H 1.94491 0.04820 2.32755
H 1.96127 -1.70472 2.29918
H -0.90338 -0.83573 2.23886
H -2.49615 -0.84951 0.13733
H -0.88891 -1.25164 -2.00315
H -0.71785 0.39249 -1.36470
O -0.69407 1.74409 -1.47874
O -0.28028 2.17870 -0.26448
H 0.68354 2.09607 -0.29999
   Core RigidRotor
   SymmetryFactor 1.5000000000000000
End
 Rotor Hindered
 Group 8 9 10
 Axis 3 2
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.29 0.98 1.39 1.02 0.33 0.00 0.26 0.94 1.39 1.00
0.29 -0.00 0.29 0.97 1.39 1.03 0.32
 End
 Rotor Hindered
 Group 16 17
 Axis 15 14
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.35 1.21 1.95 2.25 2.32 2.37 2.45 2.49 2.46 2.36
2.15 1.84 1.51 1.28 1.16 0.86 0.26
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.51 2.20 4.96 15.41 8.69 7.22 8.73 2.91 2.38 -0.23
1.02 4.49 12.18 7.36 4.41 2.15 0.62
 End
   Frequencies[1/cm] 41
  3734.1 3252.2 3230.2 3217.7 3151.9 3133.1 3095.6
3040.0 1658.3 1584.8
  1498.0 1486.2 1447.7 1423.9 1410.7 1402.5 1344.3
1306.0 1269.8 1235.3
  1109.0 1068.9 1037.6 1011.8 999.05 985.60 967.51
931.93 917.47 843.17
  837.07 762.66 727.64 626.03 593.48 498.48 326.92
286.41 228.34 96.560
  87.580
 ZeroEnergy[kcal/mol] 12.273479556461268
 ElectronicLevels[1/cm] 1
```

```
 0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !           6
Geometry[angstrom]          17
C    0.79609  -0.81859  -0.60771
C    0.79494  -0.81812   0.74421
C    1.96865  -0.81776   1.66242
C   -0.60256  -0.84071   1.20126
C   -1.41815  -0.85520   0.13376
C   -0.58913  -0.76610  -1.07879
H    1.66433  -0.81241  -1.24892
H    2.90696  -0.80170   1.11026
H    1.94473   0.04820   2.32748
H    1.96120  -1.70471   2.29922
H   -0.90343  -0.83595   2.23887
H   -2.49612  -0.84962   0.13714
H   -0.88934  -1.24795  -2.00448
H   -0.71735   0.40737  -1.36471
O   -0.69427   1.74286  -1.47917
O   -0.28010   2.17881  -0.26398
H    0.68350   2.09663  -0.30011
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                      Hindered
 Group   16  17
 Axis           15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                      Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]          41
  3737.3     3252.7     3230.7     3218.3     3154.2     3133.4     3095.6
3039.9     1653.9     1581.1
  1497.1     1486.0     1446.3     1423.7     1403.4     1401.3     1342.3
1271.3     1246.2     1222.7
  1109.0     1068.2     1035.7     1011.2     991.08     983.09     965.89
930.08     917.35     839.35
  818.03     752.12     727.14     625.39     594.58     501.32     327.38
288.21     230.64     104.22
  91.160
 ZeroEnergy[kcal/mol]    12.393497274094841
 ElectronicLevels[1/cm]                  1
 0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !           7
Geometry[angstrom]          17
C    0.79589  -0.81842  -0.60799
C    0.79499  -0.81807   0.74429
C    1.96863  -0.81778   1.66238
C   -0.60263  -0.84067   1.20131
C   -1.41816  -0.85500   0.13357
C   -0.58883  -0.76670  -1.07833
H    1.66418  -0.81252  -1.24908
H    2.90694  -0.80169   1.11025
H    1.94456   0.04821   2.32742
H    1.96113  -1.70470   2.29926
H   -0.90349  -0.83615   2.23887
H   -2.49609  -0.84972   0.13697
H   -0.88973  -1.24457  -2.00570
H   -0.71701   0.42248  -1.36501
O   -0.69446   1.74172  -1.47958
O   -0.27993   2.17891  -0.26350
H    0.68344   2.09714  -0.30022
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                      Hindered
 Group   16  17
 Axis           15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                      Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]          41
  3740.4     3253.2     3231.3     3218.9     3156.4     3133.7     3095.5
3039.9     1649.6     1578.7
  1496.4     1485.8     1445.8     1423.6     1402.9     1400.0     1340.3
1270.8     1237.6     1181.2
  1108.9     1067.4     1032.8     1010.4     988.91     974.50     964.33
929.06     917.08     839.28
  806.60     740.32     717.13     624.55     595.32     498.84     327.81
287.56     231.98     112.00
  93.180
 ZeroEnergy[kcal/mol]    12.577605594047114
 ElectronicLevels[1/cm]                  1
 0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !           8
Geometry[angstrom]          17
C    0.79570  -0.81828  -0.60827
C    0.79504  -0.81801   0.74437
C    1.96862  -0.81781   1.66234
C   -0.60269  -0.84064   1.20137
C   -1.41816  -0.85482   0.13339
C   -0.58854  -0.76735  -1.07787
H    1.66403  -0.81262  -1.24922
H    2.90692  -0.80168   1.11024
H    1.94439   0.04822   2.32737
H    1.96106  -1.70468   2.29930
H   -0.90353  -0.83635   2.23888
H   -2.49606  -0.84982   0.13683
H   -0.89010  -1.24142  -2.00683
H   -0.71678   0.43773  -1.36552
O   -0.69464   1.74065  -1.47997
O   -0.27976   2.17901  -0.26306
H    0.68338   2.09761  -0.30031
              Core           RigidRotor
        SymmetryFactor    1.5000000000000000
End
 Rotor                      Hindered
```

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 Group    8   9  10
 Axis            3           2
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                         Hindered
 Group   16  17
 Axis            15          14
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                         Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]           41
  3743.4      3253.6      3231.8      3219.5      3158.7      3133.9      3095.4
3039.9      1645.1      1576.9
  1495.7      1485.5      1445.6      1423.4      1404.1      1399.2      1338.0
1270.7      1235.5      1154.8
  1108.9      1066.6      1029.5      1009.6      988.70      966.42      962.65
929.45      916.86      839.32
  803.53      738.17      696.79      623.45      595.91      494.48      328.31
287.23      232.87      118.90
  94.340
 ZeroEnergy[kcal/mol]    12.749138759983296
 ElectronicLevels[1/cm]                     1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
RRHO           !            9
Geometry[angstrom]           17
C    0.79551  -0.81814  -0.60855
C    0.79509  -0.81796   0.74445
C    1.96861  -0.81783   1.66230
C   -0.60275  -0.84061   1.20142
C   -1.41817  -0.85466   0.13323
C   -0.58825  -0.76804  -1.07742
H    1.66390  -0.81272  -1.24934
H    2.90689  -0.80168   1.11023
H    1.94422   0.04822   2.32731
H    1.96100  -1.70467   2.29934
H   -0.90357  -0.83653   2.23889
H   -2.49604  -0.84992   0.13669
H   -0.89043  -1.23845  -2.00789
H   -0.71660   0.45309  -1.36620
O   -0.69481   1.73963  -1.48035
O   -0.27960   2.17911  -0.26263
H    0.68331   2.09806  -0.30040
              Core            RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                         Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                         Hindered
 Group   16  17
 Axis            15          14
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                         Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]           41
  3746.5      3254.1      3232.3      3220.2      3160.8      3134.2      3095.4
3039.8      1640.5      1575.4
  1495.0      1485.3      1445.6      1423.2      1406.6      1398.4      1335.3
1270.6      1233.6      1141.4
  1108.9      1065.8      1025.9      1008.7      988.82      962.38      960.40
930.42      916.59      839.33
  803.58      738.37      678.97      622.04      596.34      491.32      328.81
287.76      234.58      124.65
  95.360
 ZeroEnergy[kcal/mol]    12.903666550166491
 ElectronicLevels[1/cm]                     1
  0.0000000000000000        2.0000000000000000
 End
!**********************************************
RRHO           !            10
Geometry[angstrom]           17
C    0.79536  -0.81800  -0.60881
C    0.79513  -0.81791   0.74453
C    1.96860  -0.81785   1.66227
C   -0.60282  -0.84058   1.20148
C   -1.41819  -0.85450   0.13306
C   -0.58796  -0.76877  -1.07698
H    1.66376  -0.81281  -1.24944
H    2.90685  -0.80168   1.11024
H    1.94406   0.04821   2.32725
H    1.96094  -1.70467   2.29939
H   -0.90361  -0.83670   2.23890
H   -2.49601  -0.85003   0.13656
H   -0.89077  -1.23561  -2.00892
H   -0.71639   0.46851  -1.36705
O   -0.69499   1.73866  -1.48072
O   -0.27945   2.17920  -0.26221
H    0.68326   2.09851  -0.30046
              Core            RigidRotor
       SymmetryFactor    1.5000000000000000
End
 Rotor                         Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                         Hindered
 Group   16  17
 Axis            15          14
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                         Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]           18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]           41
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  3749.2     3254.6     3233.3     3220.9     3162.9     3134.7     3095.4
3039.9     1635.7     1574.1
  1494.3     1485.0     1445.9     1423.0     1410.6     1397.7     1332.4
1270.6     1231.4     1133.9
  1108.8     1064.8     1022.1     1007.4     988.91     961.16     958.40
930.43     915.92     839.18
  804.23     738.67     665.12     620.25     596.63     486.72     329.29
288.23     235.05     129.26
  95.800
 ZeroEnergy[kcal/mol]    12.989297686482232
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!*********************************************
 RRHO          !          11
 Geometry[angstrom]          17
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.35370
 C    1.17340   0.00000   2.27130
 C   -1.39801  -0.02268   1.81059
 C   -2.21331  -0.03648   0.74200
 C   -1.38278   0.04834  -0.46745
 H    0.86850   0.00496  -0.64049
 H    2.11167   0.01620   1.71929
 H    1.14872   0.86611   2.93628
 H    1.16569  -0.88678   2.90849
 H   -1.69877  -0.01900   2.84797
 H   -3.29110  -0.03224   0.74553
 H   -1.68617  -0.41506  -1.40077
 H   -1.51144   1.30192  -0.75894
 O   -1.49027   2.55561  -0.87200
 O   -1.07442   2.99716   0.34726
 H   -0.11198   2.91675   0.30856
                Core           RigidRotor
        SymmetryFactor    1.5000000000000000
 End
  Rotor                         Hindered
  Group    8   9  10
  Axis           3          2
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
  End
  Rotor                         Hindered
  Group   16  17
  Axis           15          14
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
  End
  Rotor                         Hindered
  Group   17
  Axis           16          15
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
  End
     Frequencies[1/cm]          41
  3752.2     3255.1     3233.8     3221.6     3165.0     3135.0     3095.3
3039.8     1630.9     1572.7
  1493.5     1484.8     1446.3     1422.9     1416.2     1396.9     1329.4
1270.6     1229.0     1128.8
  1108.8     1063.8     1018.5     1006.0     988.84     960.78     954.64
932.34     914.75     838.76
  805.00     738.95     654.93     618.11     596.59     480.95     329.80
287.26     234.90     132.88
  96.170
 ZeroEnergy[kcal/mol]    12.991136756745604
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!*********************************************
 RRHO          !          12
 Geometry[angstrom]          17
 C    0.79499  -0.81774  -0.60934
 C    0.79522  -0.81783   0.74471
 C    1.96857  -0.81789   1.66220
 C   -0.60294  -0.84052   1.20158
 C   -1.41820  -0.85420   0.13276
 C   -0.58738  -0.77030  -1.07610
 H    1.66352  -0.81301  -1.24966
 H    2.90681  -0.80166   1.11022
 H    1.94375   0.04823   2.32715
 H    1.96082  -1.70465   2.29946
 H   -0.90367  -0.83705   2.23891
 H   -2.49595  -0.85020   0.13634
 H   -0.89136  -1.23026  -2.01080
 H   -0.71626   0.49952  -1.36900
 O   -0.69531   1.73683  -1.48143
 O   -0.27915   2.17939  -0.26142
 H    0.68308   2.09925  -0.30058
                Core           RigidRotor
        SymmetryFactor    1.5000000000000000
 End
  Rotor                         Hindered
  Group    8   9  10
  Axis           3          2
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
  End
  Rotor                         Hindered
  Group   16  17
  Axis           15          14
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
  End
  Rotor                         Hindered
  Group   17
  Axis           16          15
  Symmetry          1
  Potential[kcal/mol]          18
   0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
  End
     Frequencies[1/cm]          41
  3755.2     3255.5     3234.3     3222.2     3166.9     3135.3     3095.3
3039.8     1626.1     1571.6
  1492.8     1484.5     1446.8     1424.4     1421.8     1396.2     1326.4
1270.6     1226.3     1127.2
  1108.9     1062.8     1015.3     1003.5     988.63     961.26     951.45
933.36     912.82     838.04
  805.73     738.94     647.26     615.62     596.26     476.92     330.28
288.19     236.31     135.80
  97.520
 ZeroEnergy[kcal/mol]    12.918019239623277
  ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
 End
!*********************************************
 RRHO          !          13
 Geometry[angstrom]          17
 C    0.79478  -0.81761  -0.60960
 C    0.79529  -0.81779   0.74480
 C    1.96856  -0.81791   1.66216
 C   -0.60299  -0.84049   1.20163
 C   -1.41819  -0.85406   0.13262
 C   -0.58709  -0.77111  -1.07565
 H    1.66342  -0.81310  -1.24978
 H    2.90680  -0.80165   1.11020
 H    1.94359   0.04826   2.32712
 H    1.96076  -1.70463   2.29949
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H   -0.90370  -0.83721   2.23892
H   -2.49592  -0.85026   0.13624
H   -0.89163  -1.22768  -2.01170
H   -0.71631   0.51506  -1.37006
O   -0.69546   1.73597  -1.48178
O   -0.27901   2.17949  -0.26103
H    0.68297   2.09956  -0.30064
          Core          RigidRotor
     SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                    Hindered
 Group   17
 Axis           16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]          41
  3758.5     3255.9     3234.3     3222.8     3169.0     3135.4     3095.1
3039.6     1621.5     1570.2
  1492.0     1484.3     1447.5     1432.0     1422.1     1395.6     1323.4
1270.6     1223.2     1125.2
  1109.0     1061.7     1013.0     999.32     987.99     961.80     949.03
930.30     909.57     836.69
  806.38     738.55     641.04     612.86     595.50     469.25     330.63
285.69     234.29     137.23
  97.570
ZeroEnergy[kcal/mol]    12.694236466519342
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !          14
Geometry[angstrom]          17
C    0.79458  -0.81748  -0.60987
C    0.79534  -0.81775   0.74489
C    1.96855  -0.81793   1.66213
C   -0.60305  -0.84047   1.20168
C   -1.41819  -0.85393   0.13249
C   -0.58680  -0.77194  -1.07520
H    1.66330  -0.81320  -1.24989
H    2.90678  -0.80164   1.11019
H    1.94344   0.04827   2.32707
H    1.96070  -1.70462   2.29953
H   -0.90373  -0.83737   2.23893
H   -2.49589  -0.85034   0.13615
H   -0.89191  -1.22514  -2.01259
H   -0.71633   0.53061  -1.37116
O   -0.69562   1.73513  -1.48214
O   -0.27887   2.17958  -0.26065
H    0.68287   2.09988  -0.30070
          Core          RigidRotor
     SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                    Hindered
 Group   17
 Axis           16         15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]          41
  3761.4     3256.3     3234.8     3223.4     3170.9     3135.7     3095.1
3039.6     1617.1     1568.8
  1491.1     1484.0     1448.8     1440.7     1421.9     1395.0     1320.6
1270.6     1219.8     1124.9
  1109.1     1060.6     1011.7     995.30     986.11     962.45     947.42
927.14     904.66     834.54
  806.62     737.58     635.70     609.86     594.32     461.71     330.90
282.41     230.96     137.54
  97.210
ZeroEnergy[kcal/mol]    12.422660419703661
 ElectronicLevels[1/cm]                  1
  0.0000000000000000       2.0000000000000000
End
!*********************************************
RRHO          !          15
Geometry[angstrom]          17
C    0.79439  -0.81736  -0.61014
C    0.79539  -0.81771   0.74498
C    1.96854  -0.81795   1.66210
C   -0.60310  -0.84045   1.20173
C   -1.41819  -0.85380   0.13235
C   -0.58650  -0.77280  -1.07476
H    1.66318  -0.81330  -1.24999
H    2.90676  -0.80163   1.11018
H    1.94328   0.04828   2.32703
H    1.96064  -1.70461   2.29957
H   -0.90375  -0.83753   2.23893
H   -2.49586  -0.85042   0.13606
H   -0.89217  -1.22265  -2.01345
H   -0.71636   0.54619  -1.37233
O   -0.69577   1.73432  -1.48248
O   -0.27874   2.17967  -0.26028
H    0.68278   2.10018  -0.30075
          Core          RigidRotor
     SymmetryFactor    1.5000000000000000
End
 Rotor                    Hindered
 Group    8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                    Hindered
 Group   16  17
 Axis           15         14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
```

Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.51 2.20 4.96 15.41 8.69 7.22 8.73 2.91 2.38 -0.23
1.02 4.49 12.18 7.36 4.41 2.15 0.62
End
Frequencies[1/cm] 41
3764.3 3256.7 3235.3 3224.1 3172.7 3135.9 3095.0
3039.5 1612.9 1567.5
1490.3 1483.7 1454.3 1447.1 1421.7 1394.5 1318.1
1270.7 1216.5 1127.9
1109.5 1059.5 1010.9 993.81 982.86 966.33 947.19
926.06 899.28 831.40
806.85 736.17 630.98 606.80 592.60 458.68 331.13
282.67 231.04 137.12
96.430
ZeroEnergy[kcal/mol] 12.096957371051090
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 16
Geometry[angstrom] 17
C 0.79420 -0.81724 -0.61041
C 0.79543 -0.81768 0.74508
C 1.96853 -0.81797 1.66206
C -0.60316 -0.84042 1.20179
C -1.41819 -0.85367 0.13221
C -0.58620 -0.77368 -1.07431
H 1.66307 -0.81340 -1.25009
H 2.90674 -0.80162 1.11018
H 1.94313 0.04829 2.32699
H 1.96058 -1.70460 2.29962
H -0.90378 -0.83769 2.23894
H -2.49584 -0.85050 0.13597
H -0.89243 -1.22015 -2.01432
H -0.71641 0.56176 -1.37350
O -0.69592 1.73354 -1.48284
O -0.27860 2.17976 -0.25991
H 0.68270 2.10047 -0.30080
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.29 0.98 1.39 1.02 0.33 0.00 0.26 0.94 1.39 1.00
0.29 -0.00 0.29 0.97 1.39 1.03 0.32
End
Rotor Hindered
Group 16 17
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18
0.00 0.35 1.21 1.95 2.25 2.32 2.37 2.45 2.49 2.46 2.36
2.15 1.84 1.51 1.28 1.16 0.86 0.26
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.51 2.20 4.96 15.41 8.69 7.22 8.73 2.91 2.38 -0.23
1.02 4.49 12.18 7.36 4.41 2.15 0.62
End
Frequencies[1/cm] 41
3767.2 3257.1 3235.7 3224.7 3174.4 3136.2 3094.9
3039.4 1609.2 1566.1
1489.5 1483.4 1464.6 1448.8 1421.4 1394.2 1315.8
1270.8 1213.1 1132.1
1109.8 1058.4 1010.5 994.03 979.65 970.34 946.34
925.49 894.12 827.01
806.99 734.30 626.53 603.91 589.99 455.18 331.24
280.73 228.29 135.95
95.260
ZeroEnergy[kcal/mol] 11.549753786796771
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 17
Geometry[angstrom] 17
C 0.79400 -0.81712 -0.61069
C 0.79548 -0.81764 0.74518
C 1.96852 -0.81799 1.66203
C -0.60322 -0.84040 1.20184
C -1.41819 -0.85354 0.13208
C -0.58590 -0.77460 -1.07384
H 1.66296 -0.81350 -1.25019
H 2.90672 -0.80161 1.11017
H 1.94297 0.04831 2.32695
H 1.96052 -1.70459 2.29966
H -0.90380 -0.83784 2.23895
H -2.49581 -0.85058 0.13588
H -0.89269 -1.21764 -2.01518
H -0.71648 0.57732 -1.37469
O -0.69608 1.73278 -1.48319
O -0.27846 2.17986 -0.25953
H 0.68261 2.10076 -0.30086
Core RigidRotor
SymmetryFactor 1.5000000000000000
End
Rotor Hindered
Group 8 9 10
Axis 3 2
Symmetry 1
Potential[kcal/mol] 18
0.00 0.29 0.98 1.39 1.02 0.33 0.00 0.26 0.94 1.39 1.00
0.29 -0.00 0.29 0.97 1.39 1.03 0.32
End
Rotor Hindered
Group 16 17
Axis 15 14
Symmetry 1
Potential[kcal/mol] 18
0.00 0.35 1.21 1.95 2.25 2.32 2.37 2.45 2.49 2.46 2.36
2.15 1.84 1.51 1.28 1.16 0.86 0.26
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.51 2.20 4.96 15.41 8.69 7.22 8.73 2.91 2.38 -0.23
1.02 4.49 12.18 7.36 4.41 2.15 0.62
End
Frequencies[1/cm] 41
3770.0 3257.4 3236.1 3225.3 3176.1 3136.5 3094.8
3039.3 1605.9 1564.7
1488.7 1483.1 1475.8 1449.8 1421.2 1394.0 1313.8
1271.0 1210.1 1138.7
1110.0 1057.4 1010.5 997.56 980.99 970.44 945.14
923.83 889.13 821.32
807.20 731.98 622.27 601.37 586.18 453.12 331.28
279.79 226.51 134.16
93.500
ZeroEnergy[kcal/mol] 11.004747601859123
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 18
Geometry[angstrom] 17
C 0.79380 -0.81699 -0.61097

```
C   0.79552  -0.81760   0.74529
C   1.96850  -0.81801   1.66199
C  -0.60327  -0.84038   1.20190
C  -1.41819  -0.85341   0.13194
C  -0.58558  -0.77555  -1.07337
H   1.66284  -0.81361  -1.25029
H   2.90670  -0.80160   1.11016
H   1.94282   0.04832   2.32691
H   1.96046  -1.70458   2.29970
H  -0.90383  -0.83800   2.23897
H  -2.49578  -0.85066   0.13579
H  -0.89296  -1.21508  -2.01606
H  -0.71657   0.59284  -1.37589
O  -0.69623   1.73204  -1.48356
O  -0.27833   2.17995  -0.25916
H   0.68254   2.10104  -0.30091
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                  Hindered
 Group   8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                  Hindered
 Group   16  17
 Axis           15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                  Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]          41
  3772.8     3257.7     3236.6     3225.8     3177.7     3136.7     3094.6
3039.2     1603.1     1563.2
  1488.2     1485.7     1482.8     1450.6     1420.9     1393.8     1312.2
1271.2     1207.6     1146.2
  1110.3     1056.4     1012.2     1005.0     984.09     965.75     943.30
918.86     882.83     814.26
  807.48     729.17     618.18     599.20     580.83     450.85     331.23
276.95     221.74     131.41
  90.840
ZeroEnergy[kcal/mol]    10.363525647139895
 ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
End
!*********************************************
RRHO          !          19
Geometry[angstrom]          17
C   0.79359  -0.81686  -0.61126
C   0.79557  -0.81757   0.74540
C   1.96849  -0.81803   1.66196
C  -0.60333  -0.84036   1.20196
C  -1.41819  -0.85328   0.13180
C  -0.58526  -0.77655  -1.07288
H   1.66273  -0.81372  -1.25040
H   2.90668  -0.80159   1.11015
H   1.94266   0.04833   2.32687
H   1.96039  -1.70457   2.29974
H  -0.90385  -0.83816   2.23899
H  -2.49576  -0.85075   0.13569
H  -0.89323  -1.21247  -2.01695
H  -0.71667   0.60832  -1.37710
O  -0.69639   1.73133  -1.48394
O  -0.27819   2.18005  -0.25877
H   0.68246   2.10132  -0.30097
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                  Hindered
 Group   8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                  Hindered
 Group   16  17
 Axis           15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                  Hindered
 Group   17
 Axis           16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]          41
  3775.6     3258.1     3236.9     3226.4     3179.3     3137.0     3094.5
3039.1     1600.7     1561.9
  1495.3     1487.2     1482.6     1451.3     1420.7     1394.0     1310.8
1271.5     1207.4     1160.6
  1110.6     1055.8     1027.9     1008.4     985.71     961.27     941.01
912.20     874.41     807.93
  806.03     725.82     614.56     597.29     573.72     451.98     331.11
273.91     219.49     127.28
  88.270
ZeroEnergy[kcal/mol]    9.6739921462555856
 ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
End
!*********************************************
RRHO          !          20
Geometry[angstrom]          17
C   0.79338  -0.81673  -0.61157
C   0.79561  -0.81754   0.74552
C   1.96848  -0.81805   1.66192
C  -0.60339  -0.84034   1.20202
C  -1.41819  -0.85315   0.13165
C  -0.58492  -0.77760  -1.07238
H   1.66261  -0.81384  -1.25052
H   2.90666  -0.80158   1.11014
H   1.94250   0.04834   2.32682
H   1.96033  -1.70455   2.29979
H  -0.90388  -0.83832   2.23901
H  -2.49573  -0.85084   0.13560
H  -0.89350  -1.20976  -2.01786
H  -0.71682   0.62374  -1.37829
O  -0.69655   1.73065  -1.48433
O  -0.27805   2.18016  -0.25838
H   0.68240   2.10160  -0.30104
          Core          RigidRotor
      SymmetryFactor    1.5000000000000000
End
 Rotor                  Hindered
 Group   8   9  10
 Axis           3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
```

```
 End
 Rotor                  Hindered
 Group   16  17
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                  Hindered
 Group   17
 Axis          16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
    Frequencies[1/cm]          41
  3778.3     3258.3     3237.3     3226.9     3180.8     3137.2     3094.3
3039.0     1598.7     1561.2
  1502.8     1486.9     1482.4     1452.0     1420.5     1395.0     1309.8
1272.6     1221.3     1182.3
  1110.9     1059.0     1049.2     1008.6     986.36     958.54     938.71
906.14     866.65     808.62
  797.71     722.18     612.07     595.48     565.45     456.86     330.95
271.91     214.87     122.88
  84.960
 ZeroEnergy[kcal/mol]    8.9826060047160041
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
 RRHO          !          21
 Geometry[angstrom]          17
 C    0.79315  -0.81660  -0.61189
 C    0.79566  -0.81750   0.74564
 C    1.96847  -0.81808   1.66188
 C   -0.60345  -0.84032   1.20209
 C   -1.41819  -0.85301   0.13150
 C   -0.58457  -0.77871  -1.07184
 H    1.66249  -0.81397  -1.25064
 H    2.90665  -0.80158   1.11014
 H    1.94233   0.04835   2.32678
 H    1.96026  -1.70454   2.29984
 H   -0.90391  -0.83848   2.23903
 H   -2.49571  -0.85094   0.13550
 H   -0.89378  -1.20693  -2.01880
 H   -0.71699   0.63906  -1.37946
 O   -0.69672   1.73001  -1.48474
 O   -0.27790   2.18027  -0.25797
 H    0.68235   2.10188  -0.30111
              Core          RigidRotor
        SymmetryFactor    1.5000000000000000
 End
 Rotor                  Hindered
 Group    8   9  10
 Axis          3          2
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.29    0.98    1.39    1.02    0.33    0.00    0.26    0.94    1.39    1.00
0.29   -0.00    0.29    0.97    1.39    1.03    0.32
 End
 Rotor                  Hindered
 Group   16  17
 Axis          15          14
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.35    1.21    1.95    2.25    2.32    2.37    2.45    2.49    2.46    2.36
2.15    1.84    1.51    1.28    1.16    0.86    0.26
 End
 Rotor                  Hindered
 Group   17
 Axis          16          15
 Symmetry          1
 Potential[kcal/mol]          18
  0.00    0.51    2.20    4.96   15.41    8.69    7.22    8.73    2.91    2.38   -0.23
1.02    4.49   12.18    7.36    4.41    2.15    0.62
 End
   Frequencies[1/cm]          41
  3781.0     3258.6     3237.6     3227.4     3182.2     3137.4     3094.2
3038.8     1597.1     1562.3
  1508.0     1487.5     1482.2     1452.5     1420.3     1399.5     1312.0
1299.5     1266.8     1189.9
  1111.3     1078.6     1052.2     1008.6     986.70     956.46     936.65
899.87     854.56     809.45
  789.15     718.07     611.19     593.60     555.98     468.21     330.75
269.75     210.82     118.30
  81.180
 ZeroEnergy[kcal/mol]    8.3364687099877557
 ElectronicLevels[1/cm]                    1
  0.0000000000000000       2.0000000000000000
 End
!**********************************************
      Tunneling    Eckart
      ImaginaryFrequency[1/cm]    1936.2500000000000
      WellDepth[kcal/mol]          17.90
      WellDepth[kcal/mol]          20.53
 End
End
End
```

```
!****************************************************
!             GLOBAL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
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]                     0.0001    1.0     10.   100.  1000. 10000.
!
!
EnergyStepOverTemperature              .2        ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature            30         ! [Highest barrier in the
model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]             400       ! Highest reference energy
used in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct     ! direct or low-eigenvalue
!
WellCutoff                            20        ! well truncation parameter : Max {
dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                 0.2       ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
!WellCutoff                          10
!ChemicalEigenvalueMin               1.e-6          #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!
AtomDistanceMin[bohr]                1.3
!!
RateOutput                            rate.out                    ! output file name for
rate coefficients
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!             MODEL SECTION
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                          ! Default collisional
energy relaxation kernel
    Exponential                                         ! Currently the only
possible energy relaxation model
      Factor[1/cm]              316                         ! (Delta_E_down)^(0)
@ standard T (300 K)
      Power                 0.535                        ! Power n in the
expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
      ExponentCutoff                10                           ! if (Delta_E) /
(Delta_E_down) > value  transition probability is zero
    End
!
  CollisionFrequency                                        ! Collision frequency
model
    LennardJones                                          ! Currently the only
possible collisional frequency model  based on LJ potential
      Epsilons[K]                90.58  281.367                ! Epsilon_1 and
Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K = x 1.4) Ar and c6h7 (from
Murakami & Jasper)
      Sigmas[angstrom]               3.54    4.694                 ! Sigma_1 and
Sigma_2 (from Murakami & Jasper)
      Masses[amu]                 39.948  79.05478              ! Masses of the
buffer gas molecule and of the complex (check order)
    End
!
```

```
!**************************************************
!
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!****************************************************
!  REACTANTS
!****************************************************


 Bimolecular REACS
 Fragment REAC1
 RRHO
 Geometry[angstrom]            14
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.34058
 C    1.17550   0.00000   2.25991
 C   -1.39560  -0.00008   1.80105
 C   -2.21870  -0.00003   0.74716
 C   -1.40657  -0.00007  -0.51024
 H    0.87312   0.00029  -0.63540
 H    2.11196   0.00080   1.70444
 H    1.16259   0.87759   2.90932
 H    1.16343  -0.87842   2.90820
 H   -1.69080  -0.00015   2.84114
 H   -3.29750  -0.00010   0.77029
 H   -1.62068  -0.87614  -1.13069
 H   -1.62069   0.87579  -1.13094
        Core    RigidRotor
            SymmetryFactor    1.0000000000000000
        End
 Rotor                         Hindered
 Group    8   9  10
 Axis            3           2
 Symmetry           3
 Potential[kcal/mol]          12
   0.00    0.08    0.32    0.66    1.03    1.33    1.44    1.32    1.03    0.66    0.32
0.08
 End
    Frequencies[1/cm]           35
   3241.0      3225.5      3207.9      3133.2      3100.2      3075.2      3043.9
3042.9      1708.1      1610.0
   1497.4      1487.3      1428.4      1422.7      1402.8      1311.9      1272.8
1227.8      1137.4      1111.0
   1073.3      1028.7      984.40      980.54      951.47      936.30      920.52
826.70      765.47      719.11
   624.46      583.63      368.96      327.69      231.38
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                     1
   0.0000000000000000        2.0000000000000000
 End
!************************************
 Fragment REACT2
 RRHO
 Geometry[angstrom]            3
 O    0.00000   0.00000   0.00000
 O    0.00000   0.00000   1.31234
 H    0.93494   0.00000   1.57303
        Core    RigidRotor
            SymmetryFactor    1.0000000000000000
        End
    Frequencies[1/cm]           3
   1234.9      1462.2      3683.2
  ZeroEnergy[kcal/mol]            0.
  ElectronicLevels[1/cm]                     1
   0.0000000000000000        2.0000000000000000
 End

 GroundEnergy[kcal/mol] 0.0
 End
!************************************
 Bimolecular PRODS
 Fragment PROD1
 RRHO
 Geometry[angstrom]            13
```

```
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.39409
C   1.09038   0.00000   2.23479
C  -1.41361  -0.00005   1.81740
C  -2.21408  -0.00003   0.75182
C  -1.40220  -0.00009  -0.51215
H   0.87980   0.00015  -0.62484
H   0.96884   0.00014   3.30847
H   2.09635   0.00011   1.83997
H  -1.72745  -0.00007   2.85132
H  -3.29354  -0.00010   0.76608
H  -1.61710  -0.87505  -1.13573
H  -1.61723   0.87450  -1.13618
     Core    RigidRotor
          SymmetryFactor    1.0000000000000000
     End
   Frequencies[1/cm]          33
  219.96     352.42     358.87     544.30     592.50     660.67     666.69
754.46     795.14     796.70
  925.16     926.06     951.77     962.74     984.98     1025.4     1111.8
1138.0     1259.1     1288.2
  1330.6     1389.7     1438.7     1448.7     1521.5     1659.2     3024.6
3049.1     3164.7     3213.4
  3231.7     3238.8     3260.5
 ZeroEnergy[kcal/mol]          0.
 ElectronicLevels[1/cm]                1
  0.0000000000000000      2.0000000000000000
End

!************************************
Fragment PROD2
RRHO
Geometry[angstrom]             4
O   0.00000   0.00000   0.00000
O   0.00000   0.00000   1.42622
H   0.94322   0.00000   1.61480
H  -0.34861  -0.87643  -0.18855
     Core    RigidRotor
          SymmetryFactor    2.0000000000000000
     End
Rotor                          Hindered
Group    4
Axis           1          2
Symmetry          1
Potential[kcal/mol]          18
   0.00    0.07    0.48    0.80    0.77    0.40    0.02    0.06    0.91    2.62    4.92
7.15    8.51    8.38    6.81    4.51    2.28    0.70
End
   Frequencies[1/cm]          5
  3840.9     3839.6     1465.2     1361.0     1016.3
 ZeroEnergy[kcal/mol]          0.
 ElectronicLevels[1/cm]                1
  0.0000000000000000      2.0000000000000000
End
GroundEnergy[kcal/mol]     0.78
End
!************************************
Well WR
Species
RRHO     ! transition state
Geometry[angstrom]            17
C  -0.00194   0.00030   0.00575
C  -0.00156   0.00058   1.34642
C   1.16502   0.00040   2.27418
C  -1.39942   0.02600   1.80183
C  -2.22308   0.05461   0.74283
C  -1.40480   0.02896  -0.51177
H   0.87186  -0.00513  -0.62826
H   2.10524  -0.03394   1.72689
H   1.15617   0.89945   2.89251
H   1.12798  -0.85810   2.94734
H  -1.69619   0.02223   2.84130
H  -3.30232   0.05506   0.76508
H  -1.64030  -0.85012  -1.11972
H  -1.59389   0.89835  -1.14993
O  -0.80439   3.12274   2.52519
O  -1.58504   3.11850   1.47373
H  -1.78900   2.16992   1.31409
     Core    RigidRotor
          SymmetryFactor   0.50000000000000000
     End
   Frequencies[1/cm]          45
  37.224     58.659     66.257     86.796     157.34     195.50     244.52
328.49     374.28     496.70
  586.45     625.89     740.61     774.38     828.34     919.78     943.77
950.85     985.61     991.51
  1031.7     1077.6     1112.1     1139.1     1229.2     1257.8     1275.3
1313.6     1402.5     1425.0
  1430.6     1487.7     1499.5     1515.5     1598.7     1706.9     3043.1
3047.4     3075.0     3108.7
  3139.6     3212.6     3229.8     3239.3     3450.2
 ZeroEnergy[kcal/mol]           -5.71
 ElectronicLevels[1/cm]                1
  0.0000000000000000      2.0000000000000000
End
End
!************************************
Well WP
Species
RRHO     ! transition state
Geometry[angstrom]            17
C  -0.00110   0.00050   0.00483
C   0.00008  -0.00065   1.39903
C   1.09064  -0.00189   2.24111
C  -1.41388   0.02807   1.82417
C  -2.21418   0.05253   0.75614
C  -1.40094   0.03807  -0.50738
H   0.87818  -0.00298  -0.62031
H   2.09659  -0.02975   1.84698
H   0.38752   2.48667   2.11917
H   0.96685  -0.00183   3.31468
H  -1.72648   0.03118   2.85820
H  -3.29376   0.06603   0.77088
H  -1.64068  -0.82560  -1.13676
H  -1.58601   0.92313  -1.12644
O  -0.31551   3.12045   2.31160
O  -1.00181   3.18759   1.06667
H  -1.65348   2.48143   1.16793
     Core    RigidRotor
          SymmetryFactor   0.50000000000000000
     End
   Frequencies[1/cm]          45
  37.602     59.796     80.035     116.80     136.89     225.41     291.49
352.59     362.72     541.19
  561.72     599.18     661.03     680.34     763.95     797.53     801.24
923.95     928.41     951.54
  962.80     991.91     1018.2     1027.3     1113.6     1141.7     1262.8
1291.2     1332.9     1390.3
  1428.3     1438.0     1446.4     1454.0     1522.0     1653.1     3028.3
3054.9     3164.3     3216.7
  3235.8     3240.0     3261.6     3754.7     3766.4
 ZeroEnergy[kcal/mol]           -1.03
 ElectronicLevels[1/cm]                1
  0.0000000000000000      2.0000000000000000
End
End
!************************************
Barrier        B1  REACS WR
  RRHO
    Stoichiometry  H9C6O2
    Core PhaseSpaceTheory
      FragmentGeometry[angstrom]            14
C   0.00000   0.00000   0.00000
C   0.00000   0.00000   1.34058
C   1.17550   0.00000   2.25991
C  -1.39560  -0.00008   1.80105
C  -2.21870  -0.00003   0.74716
C  -1.40657  -0.00007  -0.51024
```

```
H    0.87312   0.00029  -0.63540
H    2.11196   0.00080   1.70444
H    1.16259   0.87759   2.90932
H    1.16343  -0.87842   2.90820
H   -1.69080  -0.00015   2.84114
H   -3.29750  -0.00010   0.77029
H   -1.62068  -0.87614  -1.13069
H   -1.62069   0.87579  -1.13094
    FragmentGeometry[angstrom]            3
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.31234
H    0.93494   0.00000   1.57303
                        SymmetryFactor     1.0000000000000000
      PotentialPrefactor[au]          10.
      PotentialPowerExponent          6
              End
Rotor                    Hindered
Geometry[angstrom]          14
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.34058
C    1.17550   0.00000   2.25991
C   -1.39560  -0.00008   1.80105
C   -2.21870  -0.00003   0.74716
C   -1.40657  -0.00007  -0.51024
H    0.87312   0.00029  -0.63540
H    2.11196   0.00080   1.70444
H    1.16259   0.87759   2.90932
H    1.16343  -0.87842   2.90820
H   -1.69080  -0.00015   2.84114
H   -3.29750  -0.00010   0.77029
H   -1.62068  -0.87614  -1.13069
H   -1.62069   0.87579  -1.13094
Group    8   9  10
Axis         3        2
Symmetry         3
Potential[kcal/mol]       12
  0.0000     0.80000E-01 0.32000     0.66000     1.0300     1.3300     1.4400
1.3200     1.0300     0.66000
  0.32000     0.80000E-01
End
   Frequencies[1/cm]         38
  3241.0     3225.5     3207.9     3133.2     3100.2     3075.2     3043.9
3042.9     1708.1     1610.0
  1497.4     1487.3     1428.4     1422.7     1402.8     1311.9     1272.8
1227.8     1137.4     1111.0
  1073.3     1028.7     984.40     980.54     951.47     936.30     920.52
826.70     765.47     719.11
  624.46     583.63     368.96     327.69     231.38
  1234.9     1462.2     3683.2
 ZeroEnergy[kcal/mol]          0.
 ElectronicLevels[1/cm]              1
 0.0000000000000000      4.0000000000000000
End
!************************************
Barrier       B3  WP PRODS
  RRHO
   Stoichiometry  H9C6O2
   Core PhaseSpaceTheory
    FragmentGeometry[angstrom]           13
C    0.00000   0.00000   0.00000
C    0.00000   0.00000   1.39409
C    1.09038   0.00000   2.23479
C   -1.41361  -0.00005   1.81740
C   -2.21408  -0.00003   0.75182
C   -1.40220  -0.00009  -0.51215
H    0.87980   0.00015  -0.62484
H    0.96884   0.00014   3.30847
H    2.09635   0.00011   1.83997
H   -1.72745  -0.00007   2.85132
H   -3.29354  -0.00010   0.76608
H   -1.61710  -0.87505  -1.13573
H   -1.61723   0.87450  -1.13618
    FragmentGeometry[angstrom]            4
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.42622
H    0.94322   0.00000   1.61480
H   -0.34861  -0.87643  -0.18855
                        SymmetryFactor     2.0000000000000000
      PotentialPrefactor[au]          10.
      PotentialPowerExponent          6
              End
Rotor                    Hindered
Geometry[angstrom]          4
O    0.00000   0.00000   0.00000
O    0.00000   0.00000   1.42622
H    0.94322   0.00000   1.61480
H   -0.34861  -0.87643  -0.18855
Group    4
Axis         1        2
Symmetry         1
Potential[kcal/mol]       18
  0.0000     0.70000E-01 0.48000     0.80000     0.77000     0.40000
0.20000E-01 0.60000E-01 0.91000     2.6200
  4.9200     7.1500     8.5100     8.3800     6.8100     4.5100     2.2800
0.70000
End
   Frequencies[1/cm]         38
  219.96     352.42     358.87     544.30     592.50     660.67     666.69
754.46     795.14     796.70
  925.16     926.06     951.77     962.74     984.98     1025.4     1111.8
1138.0     1259.1     1288.2
  1330.6     1389.7     1438.7     1448.7     1521.5     1659.2     3024.6
3049.1     3164.7     3213.4
  3231.7     3238.8     3260.5
  3840.9     3839.6     1465.2     1361.0     1016.3
 ZeroEnergy[kcal/mol]          0.78069672555734915
 ElectronicLevels[1/cm]              1
 0.0000000000000000      4.0000000000000000
End
!************************************
Barrier B2 WR WP
Variational
RRHO         !         1
Geometry[angstrom]          17
C    0.10943  -0.84876  -1.21263
C    0.10643  -0.85011   0.13885
C    1.25990  -0.84272   1.02158
C   -1.28557  -0.72082   0.59305
C   -2.09862  -0.65534  -0.46632
C   -1.28868  -0.73656  -1.72403
H    0.98360  -0.90931  -1.84300
H    2.18386  -1.19983   0.57496
H    1.46092   0.26992   1.22181
H    1.09145  -1.24762   2.01700
H   -1.58350  -0.69352   1.63178
H   -3.17415  -0.56998  -0.44711
H   -1.57543  -1.59660  -2.33768
H   -1.42437   0.14580  -2.35800
O    1.51171   1.66942   1.26475
O    1.01161   2.05468   0.05675
H    0.05801   2.11502   0.20742
            Core          RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                    Hindered
 Group    8   9  10  15  16  17
 Axis         3        2
 Symmetry         3
 Potential[kcal/mol]       12
  0.00    0.23    0.84    1.82    3.11    4.63    6.29    4.51    2.97    1.68    0.73
0.16
 End
 Rotor                    Hindered
 Group   16  17
 Axis        15        9
 Symmetry         1
 Potential[kcal/mol]       18
```

```
 0.00  0.34  1.13  1.98  2.44  2.54  2.54  2.55  2.55  2.58  2.64
2.73  2.79  2.73  2.48  1.90  0.88  0.22
 End
 Rotor          Hindered
 Group  17
 Axis      16      15
 Symmetry      1
 Potential[kcal/mol]      18
 0.00  0.58  2.32  4.69  6.61  7.44  5.19  2.92  1.23  0.65  1.23
3.01  5.64  8.03  7.98  5.55  2.86  0.82
 End
   Frequencies[1/cm]      41
 3745.5   3241.9   3232.5   3211.3   3172.9   3093.8   3072.5
3042.5   1942.6   1654.8
 1585.6   1475.5   1447.8   1433.5   1423.1   1403.8   1352.3
1318.1   1274.0   1246.6
 1135.7   1111.7   1064.3   1037.5   984.23   981.69   953.81
943.52   925.84   915.23
 824.20   757.49   724.48   646.89   600.69   386.53   340.02
327.38   224.21   180.38
 94.170
 ZeroEnergy[kcal/mol]   12.770249244098919
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
 End
!**********************************************
RRHO      !      2
Geometry[angstrom]      17
C   0.10947  -0.84871  -1.21286
C   0.10682  -0.84990   0.13949
C   1.25935  -0.84293   1.02110
C  -1.28559  -0.72082   0.59312
C  -2.09851  -0.65537  -0.46626
C  -1.28866  -0.73658  -1.72407
H   0.98369  -0.90908  -1.84314
H   2.18479  -1.19665   0.57510
H   1.45988   0.28347   1.22052
H   1.09187  -1.24367   2.01822
H  -1.58356  -0.69342   1.63180
H  -3.17403  -0.56996  -0.44707
H  -1.57531  -1.59658  -2.33781
H  -1.42416   0.14580  -2.35806
O   1.51196   1.66792   1.26541
O   1.01131   2.05480   0.05607
H   0.05816   2.11578   0.20765
         Core      RigidRotor
     SymmetryFactor   0.50000000000000000
End
 Rotor          Hindered
 Group   8  9  10  15  16  17
 Axis      3      2
 Symmetry      3
 Potential[kcal/mol]      12
 0.00  0.23  0.84  1.82  3.11  4.63  6.29  4.51  2.97  1.68  0.73
0.16
 End
 Rotor          Hindered
 Group  16  17
 Axis      15      9
 Symmetry      1
 Potential[kcal/mol]      18
 0.00  0.34  1.13  1.98  2.44  2.54  2.54  2.55  2.55  2.58  2.64
2.73  2.79  2.73  2.48  1.90  0.88  0.22
 End
 Rotor          Hindered
 Group  17
 Axis      16      15
 Symmetry      1
 Potential[kcal/mol]      18
 0.00  0.58  2.32  4.69  6.61  7.44  5.19  2.92  1.23  0.65  1.23
3.01  5.64  8.03  7.98  5.55  2.86  0.82
 End
   Frequencies[1/cm]      41
 3748.9   3242.0   3232.9   3211.6   3175.1   3095.3   3072.4
3042.5   1794.3   1637.4
 1564.0   1474.5   1447.3   1432.3   1422.0   1403.7   1344.9
1317.9   1274.2   1244.6
 1135.8   1111.8   1063.6   1037.9   984.34   981.79   953.82
938.81   925.81   890.45
 823.28   756.21   725.19   648.06   603.38   393.78   347.06
328.44   239.28   206.30
 99.570
 ZeroEnergy[kcal/mol]   12.931101847707664
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
 End
!**********************************************
RRHO      !      3
Geometry[angstrom]      17
C   0.10950  -0.84867  -1.21310
C   0.10719  -0.84971   0.14010
C   1.25883  -0.84327   1.02065
C  -1.28562  -0.72082   0.59318
C  -2.09841  -0.65539  -0.46620
C  -1.28865  -0.73659  -1.72410
H   0.98377  -0.90888  -1.84327
H   2.18563  -1.19379   0.57522
H   1.45924   0.29763   1.21961
H   1.09222  -1.24012   2.01931
H  -1.58360  -0.69333   1.63182
H  -3.17393  -0.56994  -0.44704
H  -1.57521  -1.59657  -2.33794
H  -1.42397   0.14579  -2.35812
O   1.51219   1.66657   1.26602
O   1.01104   2.05491   0.05545
H   0.05831   2.11645   0.20785
         Core      RigidRotor
     SymmetryFactor   0.50000000000000000
End
 Rotor          Hindered
 Group   8  9  10  15  16  17
 Axis      3      2
 Symmetry      3
 Potential[kcal/mol]      12
 0.00  0.23  0.84  1.82  3.11  4.63  6.29  4.51  2.97  1.68  0.73
0.16
 End
 Rotor          Hindered
 Group  16  17
 Axis      15      9
 Symmetry      1
 Potential[kcal/mol]      18
 0.00  0.34  1.13  1.98  2.44  2.54  2.54  2.55  2.55  2.58  2.64
2.73  2.79  2.73  2.48  1.90  0.88  0.22
 End
 Rotor          Hindered
 Group  17
 Axis      16      15
 Symmetry      1
 Potential[kcal/mol]      18
 0.00  0.58  2.32  4.69  6.61  7.44  5.19  2.92  1.23  0.65  1.23
3.01  5.64  8.03  7.98  5.55  2.86  0.82
 End
   Frequencies[1/cm]      41
 3752.3   3242.2   3233.3   3211.9   3177.4   3096.9   3072.4
3042.5   1714.7   1616.9
 1505.5   1466.4   1445.0   1431.3   1417.9   1401.1   1336.2
1316.7   1274.3   1240.4
 1136.0   1111.9   1063.3   1038.3   984.47   981.84   953.86
937.23   925.99   853.55
 820.90   753.35   725.69   649.31   605.69   405.47   354.18
329.39   261.84   212.01
 103.16
 ZeroEnergy[kcal/mol]   13.085120373082985
 ElectronicLevels[1/cm]        1
 0.0000000000000000    2.0000000000000000
 End
```

```
!*********************************************
RRHO ! 4
Geometry[angstrom] 17
C 0.10953 -0.84864 -1.21332
C 0.10754 -0.84954 0.14069
C 1.25832 -0.84373 1.02020
C -1.28564 -0.72082 0.59322
C -2.09832 -0.65541 -0.46615
C -1.28864 -0.73660 -1.72414
H 0.98384 -0.90869 -1.84339
H 2.18640 -1.19120 0.57531
H 1.45890 0.31220 1.21901
H 1.09252 -1.23690 2.02029
H -1.58363 -0.69325 1.63183
H -3.17384 -0.56992 -0.44701
H -1.57512 -1.59655 -2.33805
H -1.42379 0.14578 -2.35818
O 1.51240 1.66534 1.26658
O 1.01079 2.05501 0.05488
H 0.05846 2.11705 0.20801
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.23 0.84 1.82 3.11 4.63 6.29 4.51 2.97 1.68 0.73
0.16
End
Rotor Hindered
Group 16 17
Axis 15 9
Symmetry 1
Potential[kcal/mol] 18
0.00 0.34 1.13 1.98 2.44 2.54 2.54 2.55 2.55 2.58 2.64
2.73 2.79 2.73 2.48 1.90 0.88 0.22
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.58 2.32 4.69 6.61 7.44 5.19 2.92 1.23 0.65 1.23
3.01 5.64 8.03 7.98 5.55 2.86 0.82
End
Frequencies[1/cm] 41
3755.6 3242.3 3233.8 3212.3 3179.7 3098.5 3072.3
3042.4 1689.3 1606.3
1484.1 1450.2 1433.1 1429.5 1409.3 1368.0 1326.4
1311.3 1274.3 1231.0
1136.2 1111.9 1062.9 1038.7 984.60 981.85 953.91
936.61 926.20 828.17
803.29 746.03 725.31 650.63 607.57 422.58 359.93
330.34 278.95 213.28
106.04
ZeroEnergy[kcal/mol] 13.354433133806166
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!*********************************************
RRHO ! 5
Geometry[angstrom] 17
C 0.10955 -0.84862 -1.21355
C 0.10787 -0.84937 0.14124
C 1.25783 -0.84427 1.01977
C -1.28567 -0.72082 0.59327
C -2.09823 -0.65543 -0.46610
C -1.28863 -0.73662 -1.72417
H 0.98391 -0.90851 -1.84349
H 2.18710 -1.18881 0.57538
H 1.45880 0.32707 1.21866
H 1.09279 -1.23396 2.02119
H -1.58366 -0.69317 1.63183
H -3.17375 -0.56990 -0.44699
H -1.57503 -1.59654 -2.33816
H -1.42363 0.14578 -2.35823
O 1.51260 1.66420 1.26710
O 1.01056 2.05511 0.05436
H 0.05862 2.11758 0.20814
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.23 0.84 1.82 3.11 4.63 6.29 4.51 2.97 1.68 0.73
0.16
End
Rotor Hindered
Group 16 17
Axis 15 9
Symmetry 1
Potential[kcal/mol] 18
0.00 0.34 1.13 1.98 2.44 2.54 2.54 2.55 2.55 2.58 2.64
2.73 2.79 2.73 2.48 1.90 0.88 0.22
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.58 2.32 4.69 6.61 7.44 5.19 2.92 1.23 0.65 1.23
3.01 5.64 8.03 7.98 5.55 2.86 0.82
End
Frequencies[1/cm] 41
3758.8 3242.4 3234.3 3212.6 3182.0 3100.2 3072.2
3042.4 1678.2 1600.1
1482.3 1449.0 1431.0 1426.9 1407.9 1333.9 1316.7
1290.5 1274.1 1210.2
1136.3 1112.0 1062.5 1039.0 984.72 981.80 953.96
936.32 926.43 824.75
778.88 733.38 716.13 651.93 608.84 443.07 363.85
331.31 290.58 213.41
108.41
ZeroEnergy[kcal/mol] 13.568994747613230
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!*********************************************
RRHO ! 6
Geometry[angstrom] 17
C 0.10958 -0.84860 -1.21376
C 0.10819 -0.84922 0.14178
C 1.25735 -0.84487 1.01935
C -1.28570 -0.72082 0.59330
C -2.09815 -0.65545 -0.46605
C -1.28862 -0.73663 -1.72420
H 0.98397 -0.90834 -1.84359
H 2.18775 -1.18662 0.57544
H 1.45891 0.34217 1.21848
H 1.09303 -1.23124 2.02202
H -1.58368 -0.69311 1.63184
H -3.17368 -0.56989 -0.44697
H -1.57495 -1.59653 -2.33826
H -1.42348 0.14577 -2.35828
O 1.51278 1.66315 1.26758
O 1.01034 2.05520 0.05387
H 0.05877 2.11807 0.20827
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17
Axis 3 2
```

```
 Symmetry 3
 Potential[kcal/mol] 12
  0.00 0.23 0.84 1.82 3.11 4.63 6.29 4.51 2.97 1.68 0.73
0.16
 End
 Rotor Hindered
 Group 16 17
 Axis 15 9
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.34 1.13 1.98 2.44 2.54 2.54 2.55 2.55 2.58 2.64
2.73 2.79 2.73 2.48 1.90 0.88 0.22
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.58 2.32 4.69 6.61 7.44 5.19 2.92 1.23 0.65 1.23
3.01 5.64 8.03 7.98 5.55 2.86 0.82
 End
   Frequencies[1/cm] 41
  3761.9 3242.6 3234.8 3213.0 3184.3 3101.8 3072.1
3042.4 1671.0 1594.6
  1482.2 1449.2 1430.6 1426.0 1407.8 1326.8 1306.2
1275.3 1266.6 1174.7
  1136.5 1111.8 1061.5 1038.8 984.80 981.59 954.00
936.15 926.59 823.51
  769.70 730.89 686.70 652.94 607.95 460.57 366.50
332.31 296.62 212.62
  110.22
 ZeroEnergy[kcal/mol] 13.775110493750601
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!**********************************************
RRHO ! 7
Geometry[angstrom] 17
C 0.10959 -0.84858 -1.21398
C 0.10850 -0.84908 0.14230
C 1.25689 -0.84552 1.01894
C -1.28573 -0.72082 0.59334
C -2.09808 -0.65547 -0.46601
C -1.28862 -0.73664 -1.72422
H 0.98403 -0.90819 -1.84368
H 2.18836 -1.18456 0.57549
H 1.45916 0.35741 1.21845
H 1.09325 -1.22870 2.02280
H -1.58369 -0.69305 1.63184
H -3.17360 -0.56987 -0.44695
H -1.57488 -1.59651 -2.33836
H -1.42333 0.14577 -2.35833
O 1.51295 1.66216 1.26804
O 1.01013 2.05529 0.05341
H 0.05892 2.11851 0.20837
         Core RigidRotor
     SymmetryFactor 0.50000000000000000
End
 Rotor Hindered
 Group 8 9 10 15 16 17
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
  0.00 0.23 0.84 1.82 3.11 4.63 6.29 4.51 2.97 1.68 0.73
0.16
 End
 Rotor Hindered
 Group 16 17
 Axis 15 9
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.34 1.13 1.98 2.44 2.54 2.54 2.55 2.55 2.58 2.64
2.73 2.79 2.73 2.48 1.90 0.88 0.22
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.58 2.32 4.69 6.61 7.44 5.19 2.92 1.23 0.65 1.23
3.01 5.64 8.03 7.98 5.55 2.86 0.82
 End
   Frequencies[1/cm] 41
  3764.8 3242.7 3235.3 3213.3 3186.6 3103.6 3072.0
3042.3 1666.1 1589.7
  1482.4 1450.3 1430.4 1425.8 1408.1 1325.4 1295.8
1274.4 1257.3 1148.1
  1136.8 1111.6 1060.4 1038.5 984.90 981.33 954.04
936.07 926.73 822.61
  766.18 730.98 663.50 651.42 605.72 479.87 368.44
333.36 302.11 211.72
  111.48
 ZeroEnergy[kcal/mol] 13.991795126985279
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
 End
!**********************************************
RRHO ! 8
Geometry[angstrom] 17
C 0.10961 -0.84857 -1.21419
C 0.10880 -0.84894 0.14280
C 1.25642 -0.84622 1.01854
C -1.28575 -0.72082 0.59337
C -2.09801 -0.65548 -0.46596
C -1.28861 -0.73664 -1.72425
H 0.98408 -0.90804 -1.84377
H 2.18893 -1.18261 0.57553
H 1.45950 0.37276 1.21851
H 1.09345 -1.22629 2.02353
H -1.58371 -0.69299 1.63184
H -3.17353 -0.56985 -0.44693
H -1.57482 -1.59650 -2.33845
H -1.42320 0.14577 -2.35837
O 1.51312 1.66122 1.26847
O 1.00994 2.05537 0.05298
H 0.05908 2.11894 0.20847
         Core RigidRotor
     SymmetryFactor 0.50000000000000000
End
 Rotor Hindered
 Group 8 9 10 15 16 17
 Axis 3 2
 Symmetry 3
 Potential[kcal/mol] 12
  0.00 0.23 0.84 1.82 3.11 4.63 6.29 4.51 2.97 1.68 0.73
0.16
 End
 Rotor Hindered
 Group 16 17
 Axis 15 9
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.34 1.13 1.98 2.44 2.54 2.54 2.55 2.55 2.58 2.64
2.73 2.79 2.73 2.48 1.90 0.88 0.22
 End
 Rotor Hindered
 Group 17
 Axis 16 15
 Symmetry 1
 Potential[kcal/mol] 18
  0.00 0.58 2.32 4.69 6.61 7.44 5.19 2.92 1.23 0.65 1.23
3.01 5.64 8.03 7.98 5.55 2.86 0.82
 End
   Frequencies[1/cm] 41
  3767.7 3242.9 3235.9 3213.7 3188.9 3105.3 3071.9
3042.2 1662.3 1584.7
  1482.8 1452.0 1430.3 1425.9 1408.5 1324.9 1287.4
1273.0 1249.6 1137.0
```

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  1128.2   1110.7   1059.4   1038.3   985.03   980.98   954.07
936.00   926.84   821.79
  764.14   731.39   658.85   639.98   599.69   498.34   369.77
334.35   302.74   210.10
  112.24
 ZeroEnergy[kcal/mol]   14.217749913012296
  ElectronicLevels[1/cm]          1
   0.0000000000000000    2.0000000000000000
 End
!***********************************************
 RRHO        !       9
 Geometry[angstrom]       17
 C    0.10963  -0.84855  -1.21439
 C    0.10910  -0.84881   0.14329
 C    1.25597  -0.84695   1.01814
 C   -1.28578  -0.72082   0.59339
 C   -2.09793  -0.65550  -0.46592
 C   -1.28861  -0.73665  -1.72428
 H    0.98413  -0.90789  -1.84385
 H    2.18947  -1.18075   0.57556
 H    1.45995   0.38819   1.21866
 H    1.09363  -1.22399   2.02423
 H   -1.58372  -0.69294   1.63183
 H   -3.17347  -0.56984  -0.44691
 H   -1.57475  -1.59649  -2.33854
 H   -1.42308   0.14576  -2.35842
 O    1.51327   1.66032   1.26889
 O    1.00976   2.05545   0.05256
 H    0.05923   2.11934   0.20857
            Core          RigidRotor
       SymmetryFactor   0.50000000000000000
 End
  Rotor                 Hindered
  Group   8  9  10  15  16  17
  Axis        3       2
  Symmetry       3
  Potential[kcal/mol]       12
   0.00   0.23   0.84   1.82   3.11   4.63   6.29   4.51   2.97   1.68   0.73
0.16
  End
  Rotor                 Hindered
  Group   16  17
  Axis        15       9
  Symmetry       1
  Potential[kcal/mol]       18
   0.00   0.34   1.13   1.98   2.44   2.54   2.54   2.55   2.55   2.58   2.64
2.73   2.79   2.73   2.48   1.90   0.88   0.22
  End
  Rotor                 Hindered
  Group   17
  Axis        16       15
  Symmetry       1
  Potential[kcal/mol]       18
   0.00   0.58   2.32   4.69   6.61   7.44   5.19   2.92   1.23   0.65   1.23
3.01   5.64   8.03   7.98   5.55   2.86   0.82
  End
    Frequencies[1/cm]       41
  3770.4   3243.0   3236.4   3214.1   3191.1   3106.9   3071.7
3042.1   1659.5   1579.7
  1483.4   1454.9   1430.3   1426.1   1408.9   1324.7   1282.4
1270.4   1241.6   1137.3
  1120.2   1109.1   1058.5   1038.2   985.19   980.61   954.10
935.93   926.95   820.98
  762.61   731.86   659.42   631.44   592.77   516.44   370.75
335.39   306.26   208.66
  112.36
 ZeroEnergy[kcal/mol]   14.397252321459204
  ElectronicLevels[1/cm]          1
   0.0000000000000000    2.0000000000000000
 End
!***********************************************
 RRHO        !       10
 Geometry[angstrom]       17
 C    0.10967  -0.84854  -1.21456
```

```
 C    0.10938  -0.84867   0.14374
 C    1.25550  -0.84771   1.01773
 C   -1.28584  -0.72081   0.59338
 C   -2.09784  -0.65551  -0.46585
 C   -1.28861  -0.73666  -1.72429
 H    0.98417  -0.90775  -1.84391
 H    2.18994  -1.17896   0.57563
 H    1.46048   0.40367   1.21885
 H    1.09381  -1.22175   2.02486
 H   -1.58373  -0.69289   1.63177
 H   -3.17336  -0.56983  -0.44688
 H   -1.57468  -1.59642  -2.33858
 H   -1.42295   0.14573  -2.35843
 O    1.51342   1.65946   1.26928
 O    1.00958   2.05552   0.05217
 H    0.05941   2.11976   0.20868
            Core          RigidRotor
       SymmetryFactor   0.50000000000000000
 End
  Rotor                 Hindered
  Group   8  9  10  15  16  17
  Axis        3       2
  Symmetry       3
  Potential[kcal/mol]       12
   0.00   0.23   0.84   1.82   3.11   4.63   6.29   4.51   2.97   1.68   0.73
0.16
  End
  Rotor                 Hindered
  Group   16  17
  Axis        15       9
  Symmetry       1
  Potential[kcal/mol]       18
   0.00   0.34   1.13   1.98   2.44   2.54   2.54   2.55   2.55   2.58   2.64
2.73   2.79   2.73   2.48   1.90   0.88   0.22
  End
  Rotor                 Hindered
  Group   17
  Axis        16       15
  Symmetry       1
  Potential[kcal/mol]       18
   0.00   0.58   2.32   4.69   6.61   7.44   5.19   2.92   1.23   0.65   1.23
3.01   5.64   8.03   7.98   5.55   2.86   0.82
  End
    Frequencies[1/cm]       41
  3773.4   3243.3   3237.1   3214.7   3193.8   3109.1   3072.1
3042.5   1657.2   1574.3
  1484.1   1459.0   1430.3   1426.3   1409.2   1324.5   1280.3
1267.0   1229.1   1137.4
  1115.2   1103.7   1056.4   1037.4   985.26   979.98   954.11
935.78   926.88   820.15
  761.18   732.23   660.33   627.06   583.54   529.24   371.10
336.21   305.95   207.11
  111.88
 ZeroEnergy[kcal/mol]   14.477550429866467
  ElectronicLevels[1/cm]          1
   0.0000000000000000    2.0000000000000000
 End
!***********************************************
 RRHO        !       11
 Geometry[angstrom]       17
 C    0.00000   0.00000   0.00000
 C    0.00000   0.00000   1.35897
 C    1.14538   0.00000   2.23208
 C   -1.39549   0.12772   1.80813
 C   -2.20738   0.19300   0.74895
 C   -1.39820   0.11185  -0.50958
 H    0.87455  -0.05908  -0.62919
 H    2.08080  -0.32867   1.79038
 H    1.35137   1.26773   2.43388
 H    0.98431  -0.37105   3.24025
 H   -1.69338   0.15570   2.84649
 H   -3.28289   0.27871   0.76789
 H   -1.68423  -0.74791  -1.12394
 H   -1.53245   0.99425  -1.14373
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O   1.40391   2.50724   2.48442
O   0.89976   2.90421   1.26656
H  -0.05007   2.96869   1.42353
             Core            RigidRotor
       SymmetryFactor   0.50000000000000000
End
 Rotor                       Hindered
 Group    8   9  10  15  16  17
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.23    0.84    1.82    3.11    4.63    6.29    4.51    2.97    1.68    0.73
0.16
 End
 Rotor                       Hindered
 Group   16  17
 Axis            15          9
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.34    1.13    1.98    2.44    2.54    2.54    2.55    2.55    2.58    2.64
2.73    2.79    2.73    2.48    1.90    0.88    0.22
 End
 Rotor                       Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.58    2.32    4.69    6.61    7.44    5.19    2.92    1.23    0.65    1.23
3.01    5.64    8.03    7.98    5.55    2.86    0.82
 End
    Frequencies[1/cm]          41
  3776.0      3243.5      3237.7      3215.0      3196.0      3110.8      3071.8
3042.3      1655.4      1569.1
  1485.3      1464.0      1430.5      1426.6      1409.5      1324.5      1279.7
1264.5      1216.9      1137.7
  1115.0      1102.7      1055.7      1037.1      985.44      979.48      954.12
935.66      926.91      819.33
  759.90      732.62      661.14      624.98      579.23      540.56      371.86
337.16      308.78      206.28
  111.27
 ZeroEnergy[kcal/mol]    14.504921651371346
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!*********************************************
RRHO          !           12
Geometry[angstrom]           17
C    0.10969  -0.84853  -1.21498
C    0.10997  -0.84841   0.14472
C    1.25459  -0.84936   1.01694
C   -1.28589  -0.72081   0.59345
C   -2.09772  -0.65554  -0.46577
C   -1.28860  -0.73668  -1.72436
H    0.98427  -0.90747  -1.84408
H    2.19097  -1.17544   0.57567
H    1.46159   0.43469   1.21942
H    1.09414  -1.21742   2.02617
H   -1.58376  -0.69279   1.63177
H   -3.17325  -0.56981  -0.44685
H   -1.57457  -1.59640  -2.33876
H   -1.42274   0.14572  -2.35853
O    1.51372   1.65782   1.27007
O    1.00924   2.05570   0.05140
H    0.05969   2.12044   0.20884
             Core            RigidRotor
       SymmetryFactor   0.50000000000000000
End
 Rotor                       Hindered
 Group    8   9  10  15  16  17
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.23    0.84    1.82    3.11    4.63    6.29    4.51    2.97    1.68    0.73
0.16
 End
 Rotor                       Hindered
 Group   16  17
 Axis            15          9
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.34    1.13    1.98    2.44    2.54    2.54    2.55    2.55    2.58    2.64
2.73    2.79    2.73    2.48    1.90    0.88    0.22
 End
 Rotor                       Hindered
 Group   17
 Axis            16          15
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.58    2.32    4.69    6.61    7.44    5.19    2.92    1.23    0.65    1.23
3.01    5.64    8.03    7.98    5.55    2.86    0.82
 End
    Frequencies[1/cm]          41
  3778.6      3243.6      3238.2      3215.3      3198.1      3112.3      3071.6
3042.2      1653.7      1563.2
  1487.3      1469.1      1430.8      1426.8      1409.7      1324.4      1279.5
1262.0      1202.9      1137.9
  1114.1      1099.0      1053.5      1036.4      985.61      978.85      954.13
935.51      926.84      818.47
  758.61      732.87      661.71      623.44      577.24      546.20      371.82
338.07      306.66      204.68
  109.81
 ZeroEnergy[kcal/mol]    14.404828115552091
  ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
 End
!*********************************************
RRHO          !           13
Geometry[angstrom]           17
C    0.10967  -0.84852  -1.21523
C    0.11027  -0.84830   0.14524
C    1.25415  -0.85022   1.01655
C   -1.28589  -0.72082   0.59350
C   -2.09768  -0.65555  -0.46575
C   -1.28860  -0.73669  -1.72440
H    0.98433  -0.90734  -1.84418
H    2.19154  -1.17373   0.57566
H    1.46221   0.45022   1.21978
H    1.09430  -1.21535   2.02685
H   -1.58378  -0.69275   1.63183
H   -3.17323  -0.56979  -0.44684
H   -1.57454  -1.59644  -2.33889
H   -1.42265   0.14575  -2.35861
O    1.51387   1.65705   1.27045
O    1.00908   2.05580   0.05102
H    0.05979   2.12072   0.20890
             Core            RigidRotor
       SymmetryFactor   0.50000000000000000
End
 Rotor                       Hindered
 Group    8   9  10  15  16  17
 Axis            3          2
 Symmetry           3
 Potential[kcal/mol]          12
  0.00    0.23    0.84    1.82    3.11    4.63    6.29    4.51    2.97    1.68    0.73
0.16
 End
 Rotor                       Hindered
 Group   16  17
 Axis            15          9
 Symmetry           1
 Potential[kcal/mol]          18
  0.00    0.34    1.13    1.98    2.44    2.54    2.54    2.55    2.55    2.58    2.64
2.73    2.79    2.73    2.48    1.90    0.88    0.22
 End
 Rotor                       Hindered
 Group   17
 Axis            16          15
 Symmetry           1
```

```
 Potential[kcal/mol]    18
  0.00   0.58   2.32   4.69   6.61   7.44   5.19   2.92   1.23   0.65   1.23
3.01   5.64   8.03   7.98   5.55   2.86   0.82
 End
   Frequencies[1/cm]    41
  3780.7    3243.5    3238.5    3215.3    3199.7    3113.5    3070.9
3041.6    1652.1    1557.1
  1490.8    1473.4    1431.1    1427.1    1409.9    1324.4    1279.5
1260.0    1188.3    1138.2
  1113.7    1096.6    1051.1    1035.5    985.82    978.25    954.16
935.38    926.77    817.59
  757.43    733.06    662.07    622.24    579.93    547.08    371.71
339.06    303.89    203.05
  107.80
 ZeroEnergy[kcal/mol]   14.205590363864856
  ElectronicLevels[1/cm]        1
  0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO      !      14
 Geometry[angstrom]     17
 C   0.10967  -0.84851  -1.21545
 C   0.11057  -0.84819  0.14573
 C   1.25370  -0.85110  1.01616
 C  -1.28591  -0.72082  0.59354
 C  -2.09762  -0.65556  -0.46572
 C  -1.28859  -0.73669  -1.72444
 H   0.98437  -0.90720  -1.84427
 H   2.19204  -1.17203  0.57567
 H   1.46290   0.46577  1.22013
 H   1.09445  -1.21328  2.02748
 H  -1.58379  -0.69271  1.63184
 H  -3.17318  -0.56977  -0.44682
 H  -1.57450  -1.59644  -2.33898
 H  -1.42256   0.14575  -2.35867
 O   1.51401   1.65631  1.27083
 O   1.00892   2.05588  0.05066
 H   0.05991   2.12101  0.20897
          Core        RigidRotor
      SymmetryFactor   0.50000000000000000
 End
  Rotor              Hindered
  Group   8  9  10  15  16  17
  Axis      3      2
  Symmetry     3
  Potential[kcal/mol]     12
  0.00   0.23   0.84   1.82   3.11   4.63   6.29   4.51   2.97   1.68   0.73
0.16
  End
  Rotor              Hindered
  Group   16  17
  Axis      15      9
  Symmetry     1
  Potential[kcal/mol]     18
  0.00   0.34   1.13   1.98   2.44   2.54   2.54   2.55   2.55   2.58   2.64
2.73   2.79   2.73   2.48   1.90   0.88   0.22
  End
  Rotor              Hindered
  Group   17
  Axis      16      15
  Symmetry     1
  Potential[kcal/mol]     18
  0.00   0.58   2.32   4.69   6.61   7.44   5.19   2.92   1.23   0.65   1.23
3.01   5.64   8.03   7.98   5.55   2.86   0.82
  End
   Frequencies[1/cm]    41
  3783.0    3243.6    3238.9    3215.6    3201.7    3115.0    3070.6
3041.3    1651.0    1551.2
  1496.5    1476.3    1431.5    1427.4    1410.0    1324.3    1279.6
1258.2    1174.4    1138.5
  1113.3    1095.5    1048.8    1034.4    985.97    977.57    954.16
935.18    926.62    816.70
  756.23    733.02    662.20    621.08    584.67    545.84    371.18
339.87    300.04    201.13
  105.16
 ZeroEnergy[kcal/mol]   13.976884997496539
  ElectronicLevels[1/cm]        1
  0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO      !      15
 Geometry[angstrom]     17
 C   0.10968  -0.84851  -1.21567
 C   0.11086  -0.84808  0.14622
 C   1.25324  -0.85202  1.01576
 C  -1.28594  -0.72082  0.59357
 C  -2.09757  -0.65557  -0.46568
 C  -1.28859  -0.73670  -1.72448
 H   0.98441  -0.90707  -1.84436
 H   2.19253  -1.17034  0.57568
 H   1.46363   0.48133  1.22050
 H   1.09461  -1.21121  2.02811
 H  -1.58381  -0.69267  1.63186
 H  -3.17313  -0.56976  -0.44681
 H  -1.57447  -1.59643  -2.33907
 H  -1.42247   0.14576  -2.35873
 O   1.51415   1.65560  1.27120
 O   1.00876   2.05596  0.05030
 H   0.06002   2.12130  0.20905
          Core        RigidRotor
      SymmetryFactor   0.50000000000000000
 End
  Rotor              Hindered
  Group   8  9  10  15  16  17
  Axis      3      2
  Symmetry     3
  Potential[kcal/mol]     12
  0.00   0.23   0.84   1.82   3.11   4.63   6.29   4.51   2.97   1.68   0.73
0.16
  End
  Rotor              Hindered
  Group   16  17
  Axis      15      9
  Symmetry     1
  Potential[kcal/mol]     18
  0.00   0.34   1.13   1.98   2.44   2.54   2.54   2.55   2.55   2.58   2.64
2.73   2.79   2.73   2.48   1.90   0.88   0.22
  End
  Rotor              Hindered
  Group   17
  Axis      16      15
  Symmetry     1
  Potential[kcal/mol]     18
  0.00   0.58   2.32   4.69   6.61   7.44   5.19   2.92   1.23   0.65   1.23
3.01   5.64   8.03   7.98   5.55   2.86   0.82
  End
   Frequencies[1/cm]    41
  3785.3    3243.7    3239.3    3215.8    3203.6    3116.5    3070.3
3041.1    1650.2    1546.3
  1503.7    1477.9    1432.0    1427.6    1410.1    1324.3    1279.8
1257.3    1161.5    1138.7
  1113.2    1097.9    1048.5    1033.8    986.13    976.92    954.16
934.94    926.49    815.86
  755.18    732.77    662.21    620.32    590.15    544.86    370.87
340.61    298.59    200.07
  102.24
 ZeroEnergy[kcal/mol]   13.663016626858463
  ElectronicLevels[1/cm]        1
  0.0000000000000000    2.0000000000000000
 End
!*********************************************
 RRHO      !      16
 Geometry[angstrom]     17
 C   0.10968  -0.84851  -1.21588
 C   0.11116  -0.84797  0.14671
 C   1.25277  -0.85298  1.01536
 C  -1.28596  -0.72082  0.59361
 C  -2.09751  -0.65558  -0.46565
```

C -1.28859 -0.73671 -1.72452
H 0.98445 -0.90693 -1.84446
H 2.19303 -1.16865 0.57570
H 1.46439 0.49687 1.22087
H 1.09477 -1.20912 2.02874
H -1.58383 -0.69263 1.63186
H -3.17309 -0.56974 -0.44679
H -1.57443 -1.59642 -2.33915
H -1.42240 0.14576 -2.35878
O 1.51430 1.65492 1.27158
O 1.00861 2.05605 0.04995
H 0.06013 2.12159 0.20913
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.23 0.84 1.82 3.11 4.63 6.29 4.51 2.97 1.68 0.73
0.16
End
Rotor Hindered
Group 16 17
Axis 15 9
Symmetry 1
Potential[kcal/mol] 18
0.00 0.34 1.13 1.98 2.44 2.54 2.54 2.55 2.55 2.58 2.64
2.73 2.79 2.73 2.48 1.90 0.88 0.22
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.58 2.32 4.69 6.61 7.44 5.19 2.92 1.23 0.65 1.23
3.01 5.64 8.03 7.98 5.55 2.86 0.82
End
Frequencies[1/cm] 41
3787.5 3243.8 3239.7 3216.0 3205.5 3118.0 3069.9
3040.9 1649.6 1542.3
1510.8 1478.8 1432.4 1427.8 1410.2 1324.4 1279.9
1257.5 1150.9 1138.8
1113.0 1100.9 1049.8 1033.1 986.27 976.25 954.16
934.68 926.36 815.05
754.31 732.28 662.21 619.52 594.47 545.27 370.45
341.31 296.65 199.09
98.980
ZeroEnergy[kcal/mol] 13.180238763559187
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 17
Geometry[angstrom] 17
C 0.10968 -0.84851 -1.21610
C 0.11147 -0.84786 0.14721
C 1.25229 -0.85398 1.01494
C -1.28599 -0.72082 0.59364
C -2.09745 -0.65560 -0.46561
C -1.28859 -0.73671 -1.72455
H 0.98450 -0.90680 -1.84456
H 2.19353 -1.16692 0.57571
H 1.46517 0.51238 1.22126
H 1.09493 -1.20700 2.02938
H -1.58386 -0.69259 1.63187
H -3.17304 -0.56973 -0.44677
H -1.57440 -1.59641 -2.33924
H -1.42232 0.14576 -2.35884
O 1.51444 1.65427 1.27196
O 1.00846 2.05613 0.04959
H 0.06023 2.12187 0.20922
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.23 0.84 1.82 3.11 4.63 6.29 4.51 2.97 1.68 0.73
0.16
End
Rotor Hindered
Group 16 17
Axis 15 9
Symmetry 1
Potential[kcal/mol] 18
0.00 0.34 1.13 1.98 2.44 2.54 2.54 2.55 2.55 2.58 2.64
2.73 2.79 2.73 2.48 1.90 0.88 0.22
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 18
0.00 0.58 2.32 4.69 6.61 7.44 5.19 2.92 1.23 0.65 1.23
3.01 5.64 8.03 7.98 5.55 2.86 0.82
End
Frequencies[1/cm] 41
3789.7 3243.9 3240.1 3216.2 3207.3 3119.4 3069.6
3040.6 1649.3 1539.9
1516.5 1479.3 1432.9 1428.0 1410.3 1324.8 1280.1
1259.2 1146.5 1139.0
1111.8 1101.3 1051.4 1031.7 986.37 975.50 954.16
934.40 926.17 814.31
753.66 731.52 662.46 618.55 596.73 547.91 369.98
341.95 293.62 197.97
95.340
ZeroEnergy[kcal/mol] 12.709906152961720
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 18
Geometry[angstrom] 17
C 0.10969 -0.84851 -1.21632
C 0.11178 -0.84776 0.14771
C 1.25179 -0.85503 1.01452
C -1.28601 -0.72082 0.59367
C -2.09739 -0.65560 -0.46557
C -1.28858 -0.73672 -1.72459
H 0.98454 -0.90666 -1.84466
H 2.19404 -1.16515 0.57572
H 1.46596 0.52782 1.22164
H 1.09510 -1.20481 2.03004
H -1.58389 -0.69256 1.63189
H -3.17298 -0.56972 -0.44675
H -1.57437 -1.59640 -2.33933
H -1.42225 0.14576 -2.35890
O 1.51459 1.65364 1.27234
O 1.00831 2.05622 0.04923
H 0.06032 2.12216 0.20931
Core RigidRotor
SymmetryFactor 0.50000000000000000
End
Rotor Hindered
Group 8 9 10 15 16 17
Axis 3 2
Symmetry 3
Potential[kcal/mol] 12
0.00 0.23 0.84 1.82 3.11 4.63 6.29 4.51 2.97 1.68 0.73
0.16
End
Rotor Hindered
Group 16 17
Axis 15 9

```
 Symmetry          1
 Potential[kcal/mol]        18
  0.00   0.34   1.13   1.98   2.44   2.54   2.54   2.55   2.55   2.58   2.64
2.73   2.79   2.73   2.48   1.90   0.88   0.22
 End
 Rotor                    Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]        18
  0.00   0.58   2.32   4.69   6.61   7.44   5.19   2.92   1.23   0.65   1.23
3.01   5.64   8.03   7.98   5.55   2.86   0.82
 End
   Frequencies[1/cm]        41
  3791.8     3243.9     3240.3     3216.4     3209.2     3120.8     3069.2
3040.4     1649.0     1539.7
  1519.7     1479.7     1433.4     1428.3     1410.4     1325.6     1280.3
1264.1     1155.1     1139.2
  1110.7     1094.6     1051.6     1028.9     986.41     974.62     954.17
934.10     925.90     813.64
  753.28     730.49     663.45     617.31     597.55     553.77     369.43
342.52     289.15     196.39
  91.430
 ZeroEnergy[kcal/mol]    12.189530763745053
 ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
 End
!********************************************
 RRHO          !          19
 Geometry[angstrom]          17
 C    0.10969  -0.84851  -1.21654
 C    0.11211  -0.84764   0.14823
 C    1.25127  -0.85614   1.01407
 C   -1.28603  -0.72082   0.59371
 C   -2.09733  -0.65562  -0.46553
 C   -1.28858  -0.73672  -1.72464
 H    0.98458  -0.90652  -1.84478
 H    2.19457  -1.16332   0.57574
 H    1.46677   0.54318   1.22201
 H    1.09527  -1.20254   2.03073
 H   -1.58392  -0.69252   1.63190
 H   -3.17293  -0.56970  -0.44673
 H   -1.57435  -1.59639  -2.33942
 H   -1.42218   0.14577  -2.35896
 O    1.51475   1.65306   1.27274
 O    1.00815   2.05631   0.04886
 H    0.06041   2.12246   0.20942
          Core          RigidRotor
       SymmetryFactor   0.50000000000000000
 End
 Rotor                    Hindered
 Group    8   9  10  15  16  17
 Axis          3          2
 Symmetry          3
 Potential[kcal/mol]        12
  0.00   0.23   0.84   1.82   3.11   4.63   6.29   4.51   2.97   1.68   0.73
0.16
 End
 Rotor                    Hindered
 Group   16  17
 Axis          15         9
 Symmetry          1
 Potential[kcal/mol]        18
  0.00   0.34   1.13   1.98   2.44   2.54   2.54   2.55   2.55   2.58   2.64
2.73   2.79   2.73   2.48   1.90   0.88   0.22
 End
 Rotor                    Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]        18
  0.00   0.58   2.32   4.69   6.61   7.44   5.19   2.92   1.23   0.65   1.23
3.01   5.64   8.03   7.98   5.55   2.86   0.82
 End
   Frequencies[1/cm]        41
  3793.8     3244.0     3240.6     3216.5     3210.9     3122.1     3068.8
3040.1     1649.0     1541.6
  1521.3     1480.0     1433.9     1428.7     1410.5     1328.5     1281.5
1278.2     1177.6     1139.3
  1110.6     1087.6     1049.3     1023.5     986.35     973.52     954.20
933.80     925.59     813.09
  753.20     729.29     666.16     616.23     598.72     563.45     369.02
343.02     284.90     194.89
  87.310
 ZeroEnergy[kcal/mol]    11.665129059505814
 ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
 End
!********************************************
 RRHO          !          20
 Geometry[angstrom]          17
 C    0.10970  -0.84851  -1.21677
 C    0.11245  -0.84753   0.14877
 C    1.25072  -0.85733   1.01360
 C   -1.28606  -0.72083   0.59374
 C   -2.09726  -0.65563  -0.46548
 C   -1.28858  -0.73673  -1.72468
 H    0.98463  -0.90638  -1.84490
 H    2.19512  -1.16140   0.57575
 H    1.46762   0.55843   1.22236
 H    1.09546  -1.20016   2.03144
 H   -1.58397  -0.69249   1.63191
 H   -3.17287  -0.56969  -0.44671
 H   -1.57432  -1.59638  -2.33952
 H   -1.42212   0.14577  -2.35902
 O    1.51491   1.65252   1.27315
 O    1.00800   2.05640   0.04848
 H    0.06048   2.12276   0.20953
          Core          RigidRotor
       SymmetryFactor   0.50000000000000000
 End
 Rotor                    Hindered
 Group    8   9  10  15  16  17
 Axis          3          2
 Symmetry          3
 Potential[kcal/mol]        12
  0.00   0.23   0.84   1.82   3.11   4.63   6.29   4.51   2.97   1.68   0.73
0.16
 End
 Rotor                    Hindered
 Group   16  17
 Axis          15         9
 Symmetry          1
 Potential[kcal/mol]        18
  0.00   0.34   1.13   1.98   2.44   2.54   2.54   2.55   2.55   2.58   2.64
2.73   2.79   2.73   2.48   1.90   0.88   0.22
 End
 Rotor                    Hindered
 Group   17
 Axis          16         15
 Symmetry          1
 Potential[kcal/mol]        18
  0.00   0.58   2.32   4.69   6.61   7.44   5.19   2.92   1.23   0.65   1.23
3.01   5.64   8.03   7.98   5.55   2.86   0.82
 End
   Frequencies[1/cm]        41
  3795.8     3244.1     3240.8     3216.6     3212.7     3123.5     3068.5
3039.8     1649.4     1544.8
  1526.4     1480.4     1434.4     1429.5     1410.9     1355.2     1309.9
1280.3     1203.9     1139.4
  1110.6     1085.1     1044.6     1013.1     986.11     971.86     954.23
933.49     925.22     812.76
  753.57     728.07     673.40     615.84     604.43     574.02     368.80
343.49     281.52     194.44
  83.050
 ZeroEnergy[kcal/mol]    11.205417652389697
 ElectronicLevels[1/cm]                1
  0.0000000000000000       2.0000000000000000
```

```
End
!********************************************
RRHO          !          21
Geometry[angstrom]          17
C    0.10971  -0.84852  -1.21701
C    0.11281  -0.84741   0.14933
C    1.25013  -0.85861   1.01311
C   -1.28608  -0.72083   0.59378
C   -2.09719  -0.65564  -0.46544
C   -1.28857  -0.73674  -1.72473
H    0.98468  -0.90622  -1.84503
H    2.19571  -1.15936   0.57577
H    1.46849   0.57350   1.22268
H    1.09566  -1.19763   2.03220
H   -1.58402  -0.69245   1.63193
H   -3.17281  -0.56968  -0.44668
H   -1.57431  -1.59636  -2.33962
H   -1.42207   0.14578  -2.35909
O    1.51508   1.65204   1.27359
O    1.00784   2.05651   0.04808
H    0.06055   2.12308   0.20966
            Core           RigidRotor
      SymmetryFactor   0.50000000000000000
End
 Rotor                       Hindered
 Group    8   9  10  15  16  17
 Axis           3          2
 Symmetry          3
 Potential[kcal/mol]          12
   0.00    0.23    0.84    1.82    3.11    4.63    6.29    4.51    2.97    1.68    0.73
0.16
 End
 Rotor                       Hindered
 Group   16  17
 Axis          15          9
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.34    1.13    1.98    2.44    2.54    2.54    2.55    2.55    2.58    2.64
2.73    2.79    2.73    2.48    1.90    0.88    0.22
 End
 Rotor                       Hindered
 Group   17
 Axis          16          15
 Symmetry          1
 Potential[kcal/mol]          18
   0.00    0.58    2.32    4.69    6.61    7.44    5.19    2.92    1.23    0.65    1.23
3.01    5.64    8.03    7.98    5.55    2.86    0.82
 End
   Frequencies[1/cm]          41
  3797.7     3244.1     3241.0     3216.6     3214.4     3124.8     3068.1
3039.5     1652.5     1581.3
  1539.4     1481.3     1452.8     1434.1     1425.2     1408.8     1318.3
1280.5     1218.1     1139.5
  1110.5     1085.5     1040.7     997.71     984.95     967.93     954.24
933.17     924.61     812.80
  755.10     727.42     691.83     622.78     612.06     577.47     368.84
343.97     278.77     197.42
  78.790
 ZeroEnergy[kcal/mol]    10.852697570125583
 ElectronicLevels[1/cm]                   1
  0.0000000000000000       2.0000000000000000
End
!********************************************
     Tunneling    Eckart
     ImaginaryFrequency[1/cm]    1947.0300000000000
     WellDepth[kcal/mol]          18.80
     WellDepth[kcal/mol]          14.12
End
End
End
```

A.2. Reaction Rate Constants Obtained From the MESS Calculations

Temperature [K]	0.001 atm	1 atm	10 atm	100 atm	1000 atm
300	6.99E-12	2.34E-14	2.72E-15	3.20E-17	8.09E-20
400	1.80E-11	1.33E-13	3.26E-14	7.72E-16	3.28E-18
500	3.20E-11	4.77E-13	1.71E-13	8.63E-15	6.30E-17
600	4.69E-11	1.48E-12	5.40E-13	5.51E-14	6.96E-16
700	6.22E-11	4.21E-12	1.30E-12	2.26E-13	4.98E-15
800	7.75E-11	1.05E-11	2.82E-12	6.64E-13	2.51E-14
900	9.24E-11	2.24E-11	5.89E-12	1.52E-12	9.33E-14
1000	1.06E-10	4.06E-11	1.17E-11	2.96E-12	2.64E-13
1100	1.19E-10	6.33E-11	2.16E-11	5.29E-12	6.72E-13
1200	1.29E-10	8.67E-11	3.59E-11	9.35E-12	1.35E-12
1300	1.37E-10	1.07E-10	5.37E-11	1.52E-11	2.37E-12
1400	1.42E-10	1.23E-10	7.27E-11	2.35E-11	3.79E-12
1500	1.45E-10	1.33E-10	9.04E-11	3.39E-11	5.48E-12
1600	1.46E-10	1.39E-10	1.05E-10	4.62E-11	1.05E-11
1700	1.45E-10	1.41E-10	1.15E-10	5.84E-11	1.46E-11
1800	1.42E-10	1.43E-10	1.23E-10	6.95E-11	1.94E-11
1900	1.38E-10	1.39E-10	1.25E-10	7.88E-11	2.76E-11
2000	1.34E-10	1.34E-10	1.36E-10	8.59E-11	3.34E-11
2100	1.28E-10	1.29E-10	1.30E-10	9.45E-11	3.88E-11
2200	1.23E-10	1.23E-10	1.24E-10	9.66E-11	4.44E-11
2300	1.17E-10	1.17E-10	1.18E-10	9.71E-11	4.94E-11
2400	1.12E-10	1.12E-10	1.12E-10	1.15E-10	5.37E-11
2500	1.06E-10	1.06E-10	1.07E-10	1.08E-10	6.25E-11

Table A.1: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Reaction of Fulvene + H $\rightarrow$ Benzene + H

Temperature [K]	W1 → W2	W2 → W1	W1 → W3	W3 → W1	W2 → W3	W3 → W2
300	2.24E-16	3.37E-15	3.09E-20	9.23E-04	2.75E-15	5.46E+00
400	1.97E-09	1.78E-08	6.86E-13	9.99E-01	1.71E-08	2.76E+03
500	4.15E-05	2.72E-04	4.78E-08	1.76E+02	2.67E-04	1.51E+05
600	3.53E-02	1.84E-01	1.03E-04	6.95E+03	1.82E-01	2.36E+06
700	4.60E+00	2.02E+01	2.71E-02	1.05E+05	2.01E+01	1.76E+07
800	1.84E+02	7.01E+02	1.86E+00	8.34E+05	6.98E+02	8.19E+07
900	3.30E+03	1.12E+04	5.14E+01	4.30E+06	1.12E+04	2.75E+08
1000	3.38E+04	1.04E+05	7.46E+02	1.63E+07	1.04E+05	7.35E+08
1100	2.29E+05	6.50E+05	6.75E+03	4.90E+07	6.48E+05	1.66E+09
1200	1.14E+06	3.00E+06	4.28E+04	1.24E+08	2.99E+06	3.30E+09
1300	4.46E+06	1.10E+07	2.06E+05	2.74E+08	1.10E+07	5.93E+09
1400	1.45E+07	3.35E+07	7.94E+05	5.43E+08	3.34E+07	9.86E+09
1500	4.02E+07	8.83E+07	2.58E+06	9.87E+08	8.81E+07	1.54E+10
1600	9.89E+07	2.06E+08	7.25E+06	1.67E+09	2.06E+08	2.28E+10
1700	2.19E+08	4.37E+08	1.81E+07	2.67E+09	4.37E+08	3.23E+10
1800	4.46E+08	8.54E+08	4.10E+07	4.07E+09	8.52E+08	4.42E+10
1900	8.45E+08	1.55E+09	8.53E+07	5.93E+09	1.55E+09	5.87E+10
2000	1.50E+09	2.67E+09	1.65E+08	8.35E+09	2.66E+09	7.59E+10
2100	2.54E+09	4.35E+09	3.02E+08	1.14E+10	4.34E+09	9.58E+10
2200	4.09E+09	6.78E+09	5.22E+08	1.52E+10	6.77E+09	1.19E+11
2300	6.34E+09	1.02E+10	8.63E+08	1.97E+10	1.02E+10	1.45E+11
2400	9.48E+09	1.48E+10	1.37E+09	2.51E+10	1.48E+10	1.73E+11
2500	1.37E+10	2.09E+10	2.09E+09	3.13E+10	2.08E+10	2.05E+11

Table A.2: Reaction Rate Constants in Units of s^{-1} for the Isomerization Reactions of the Decomposition of Methylcyclopentadienyl

Temperature [K]	W2 → W4	W4 → W2	W3 → W5	W5 → W3	W5 → W6	W6 → W5
300	2.26E-11	2.10E-07	1.59E+07	5.92E+02	1.98E+00	4.51E-14
400	9.34E-06	8.85E-03	2.44E+08	3.04E+05	3.60E+03	2.01E-07
500	3.52E-02	8.43E+00	1.29E+09	1.37E+07	3.49E+05	2.12E-03
600	9.56E+00	9.13E+02	4.02E+09	1.78E+08	7.53E+06	1.05E+00
700	5.49E+02	2.72E+04	9.15E+09	1.13E+09	6.83E+07	9.06E+01
800	1.18E+04	3.55E+05	1.72E+10	4.56E+09	3.59E+08	2.58E+03
900	1.29E+05	2.66E+06	2.82E+10	1.36E+10	1.31E+09	3.52E+04
1000	8.91E+05	1.34E+07	4.23E+10	3.25E+10	3.68E+09	2.85E+05
1100	4.35E+06	5.10E+07	5.92E+10	6.66E+10	8.59E+09	1.59E+06
1200	1.64E+07	1.56E+08	7.87E+10	1.21E+11	1.74E+10	6.63E+06
1300	5.05E+07	4.01E+08	1.00E+11	2.02E+11	3.17E+10	2.23E+07
1400	1.33E+08	9.06E+08	1.24E+11	3.12E+11	5.30E+10	6.30E+07
1500	3.08E+08	1.84E+09	1.50E+11	4.55E+11	8.28E+10	1.55E+08
1600	6.43E+08	3.42E+09	1.77E+11	6.34E+11	1.22E+11	3.42E+08
1700	1.23E+09	5.93E+09	2.05E+11	8.50E+11	1.73E+11	6.86E+08
1800	2.21E+09	9.67E+09	2.34E+11	1.10E+12	2.35E+11	1.27E+09
1900	3.71E+09	1.50E+10	2.64E+11	1.39E+12	3.09E+11	2.22E+09
2000	5.94E+09	2.23E+10	2.94E+11	1.72E+12	3.95E+11	3.65E+09
2100	9.08E+09	3.19E+10	3.26E+11	2.08E+12	4.94E+11	5.74E+09
2200	1.34E+10	4.42E+10	3.57E+11	2.47E+12	6.05E+11	8.65E+09
2300	1.90E+10	5.95E+10	3.89E+11	2.89E+12	7.29E+11	1.26E+10
2400	2.63E+10	7.82E+10	4.21E+11	3.34E+12	8.64E+11	1.78E+10
2500	3.55E+10	1.01E+11	4.53E+11	3.82E+12	1.01E+12	2.44E+10

Table A.2: Reaction Rate Constants in Units of s^{-1} for the Isomerization Reactions of the Decomposition of Methylcyclopentadienyl (Continued)

Temperature [K]	W1 → P1 + H	W2 → P1 + H	W3 → P1 + H	W4 → P1 + H	W6 → P2 + H
300	6.07E-25	4.07E-24	7.14E-11	2.72E-20	6.41E-07
400	1.55E-15	8.10E-15	2.74E-05	5.96E-12	4.29E-02
500	7.46E-10	3.32E-09	6.89E-02	6.51E-07	3.79E+01
600	4.85E-06	1.91E-05	1.36E+01	1.55E-03	3.68E+03
700	2.67E-03	9.51E-03	6.15E+02	4.09E-01	9.99E+04
800	3.13E-01	1.02E+00	1.10E+04	2.73E+01	1.21E+06
900	1.30E+01	3.89E+01	1.06E+05	7.21E+02	8.51E+06
1000	2.61E+02	7.24E+02	6.56E+05	9.97E+03	4.09E+07
1100	3.07E+03	7.98E+03	2.95E+06	8.61E+04	1.48E+08
1200	2.42E+04	5.92E+04	1.04E+07	5.21E+05	4.37E+08
1300	1.40E+05	3.25E+05	3.03E+07	2.40E+06	1.09E+09
1400	6.34E+05	1.40E+06	7.64E+07	8.92E+06	2.40E+09
1500	2.36E+06	4.98E+06	1.71E+08	2.79E+07	4.75E+09
1600	7.48E+06	1.51E+07	3.46E+08	7.58E+07	8.64E+09
1700	2.08E+07	4.05E+07	6.47E+08	1.84E+08	1.47E+10
1800	5.17E+07	9.72E+07	1.13E+09	4.03E+08	2.35E+10
1900	1.17E+08	2.13E+08	1.87E+09	8.16E+08	3.57E+10
2000	2.45E+08	4.32E+08	2.94E+09	1.54E+09	5.22E+10
2100	4.80E+08	8.19E+08	4.43E+09	2.74E+09	7.35E+10
2200	8.84E+08	1.47E+09	6.45E+09	4.63E+09	1.00E+11
2300	1.55E+09	2.50E+09	9.10E+09	7.48E+09	1.33E+11
2400	2.59E+09	4.08E+09	1.25E+10	1.16E+10	1.73E+11
2500	4.16E+09	6.39E+09	1.67E+10	1.74E+10	2.20E+11

Table A.3: Reaction Rate Constants in Units of s^{-1} for the Unimolecular Beta-Scission Reactions of the Decomposition of Methylcyclopentadienyl

Temperature [K]	$P1 + H \rightarrow W1$	$P1 + H \rightarrow W2$	$P1 + H \rightarrow W3$	$P1 + H \rightarrow W4$	$P2 + H \rightarrow W6$
300	6.89E-12	3.07E-12	2.71E-14	2.21E-12	3.11E-14
400	1.09E-11	6.30E-12	1.32E-13	4.90E-12	2.15E-13
500	1.52E-11	1.03E-11	3.81E-13	8.45E-12	7.68E-13
600	1.98E-11	1.50E-11	8.20E-13	1.27E-11	1.91E-12
700	2.47E-11	2.00E-11	1.47E-12	1.74E-11	3.80E-12
800	3.00E-11	2.54E-11	2.35E-12	2.26E-11	6.53E-12
900	3.55E-11	3.12E-11	3.45E-12	2.81E-11	1.01E-11
1000	4.14E-11	3.72E-11	4.77E-12	3.40E-11	1.47E-11
1100	4.76E-11	4.36E-11	6.29E-12	4.01E-11	2.01E-11
1200	5.41E-11	5.03E-11	8.00E-12	4.66E-11	2.63E-11
1300	6.08E-11	5.73E-11	9.90E-12	5.33E-11	3.34E-11
1400	6.78E-11	6.46E-11	1.20E-11	6.04E-11	4.13E-11
1500	7.51E-11	7.22E-11	1.42E-11	6.78E-11	4.99E-11
1600	8.26E-11	8.01E-11	1.65E-11	7.54E-11	5.92E-11
1700	9.04E-11	8.83E-11	1.90E-11	8.34E-11	6.91E-11
1800	9.84E-11	9.67E-11	2.17E-11	9.16E-11	7.96E-11
1900	1.07E-10	1.05E-10	2.44E-11	1.00E-10	9.07E-11
2000	1.15E-10	1.14E-10	2.73E-11	1.09E-10	1.02E-10
2100	1.24E-10	1.23E-10	3.03E-11	1.18E-10	1.14E-10
2200	1.33E-10	1.33E-10	3.34E-11	1.27E-10	1.27E-10
2300	1.42E-10	1.43E-10	3.65E-11	1.36E-10	1.40E-10
2400	1.51E-10	1.52E-10	3.98E-11	1.46E-10	1.54E-10
2500	1.60E-10	1.63E-10	4.32E-11	1.56E-10	1.67E-10

Table A.4: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Bimolecular Beta-Scission Reactions of the Decomposition of Methylcyclopentadienyl

Temperature [K]	$1MCPE + H \rightarrow R1 + H_2$	$R1 + H_2 \rightarrow 1MCPE + H$	$1MCPE + H \rightarrow R2 + H_2$	$R2 + H_2 \rightarrow 1MCPE + H$
500	1.29E-13	1.30E-24	5.28E-14	3.53E-24
600	3.12E-13	1.45E-22	1.40E-13	3.46E-22
700	6.20E-13	4.44E-21	3.02E-13	9.60E-21
800	1.08E-12	6.02E-20	5.60E-13	1.21E-19
900	1.70E-12	4.72E-19	9.35E-13	8.90E-19
1000	2.51E-12	2.51E-18	1.44E-12	4.50E-18
1100	3.50E-12	1.01E-17	2.09E-12	1.72E-17
1200	4.66E-12	3.26E-17	2.88E-12	5.35E-17
1300	5.99E-12	8.93E-17	3.82E-12	1.41E-16
1400	7.47E-12	2.14E-16	4.89E-12	3.27E-16
1500	9.06E-12	4.59E-16	6.08E-12	6.81E-16
1600	1.08E-11	9.01E-16	7.38E-12	1.30E-15
1700	1.25E-11	1.64E-15	8.77E-12	2.31E-15
1800	1.44E-11	2.82E-15	1.02E-11	3.86E-15
1900	1.63E-11	4.57E-15	1.18E-11	6.12E-15
2000	1.82E-11	7.10E-15	1.33E-11	9.30E-15
2100	2.01E-11	1.06E-14	1.50E-11	1.36E-14
2200	2.20E-11	1.53E-14	1.66E-11	1.92E-14
2300	2.40E-11	2.14E-14	1.82E-11	2.64E-14
2400	2.58E-11	2.92E-14	1.99E-11	3.53E-14
2500	2.77E-11	3.90E-14	2.15E-11	4.62E-14

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene

Temperature [K]	2MCPE + H → R3 + H_2	R3 + H_2 → 2MCPE + H	2MCPE + H → R4 + H_2	R4 + H_2 → 2MCPE + H
500	1.27E-13	1.52E-24	2.04E-14	3.77E-22
600	3.05E-13	1.63E-22	6.38E-14	1.67E-20
700	6.05E-13	4.86E-21	1.54E-13	2.65E-19
800	1.05E-12	6.46E-20	3.13E-13	2.20E-18
900	1.66E-12	4.99E-19	5.63E-13	1.17E-17
1000	2.45E-12	2.63E-18	9.21E-13	4.57E-17
1100	3.41E-12	1.05E-17	1.40E-12	1.42E-16
1200	4.55E-12	3.36E-17	2.02E-12	3.70E-16
1300	5.84E-12	9.14E-17	2.76E-12	8.40E-16
1400	7.28E-12	2.18E-16	3.65E-12	1.71E-15
1500	8.84E-12	4.65E-16	4.65E-12	3.19E-15
1600	1.05E-11	9.11E-16	5.78E-12	5.54E-15
1700	1.22E-11	1.66E-15	7.01E-12	9.03E-15
1800	1.40E-11	2.83E-15	8.33E-12	1.40E-14
1900	1.59E-11	4.58E-15	9.73E-12	2.08E-14
2000	1.78E-11	7.10E-15	1.12E-11	2.96E-14
2100	1.96E-11	1.06E-14	1.27E-11	4.10E-14
2200	2.15E-11	1.52E-14	1.43E-11	5.51E-14
2300	2.34E-11	2.13E-14	1.59E-11	7.24E-14
2400	2.52E-11	2.90E-14	1.75E-11	9.29E-14
2500	2.71E-11	3.86E-14	1.91E-11	1.17E-13

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	$5MCPE + H \rightarrow R5 + H_2$	$R5 + H_2 \rightarrow 5MCPE + H$	$1MCPE + CH_3 \rightarrow R1 + CH_4$
500	3.18E-13	1.06E-25	2.09E-16
600	6.18E-13	1.57E-23	8.16E-16
700	1.03E-12	5.83E-22	2.34E-15
800	1.57E-12	9.12E-21	5.44E-15
900	2.22E-12	7.99E-20	1.09E-14
1000	2.99E-12	4.65E-19	1.93E-14
1100	3.85E-12	2.01E-18	3.15E-14
1200	4.80E-12	6.90E-18	4.78E-14
1300	5.83E-12	1.99E-17	6.82E-14
1400	6.91E-12	4.97E-17	9.28E-14
1500	8.02E-12	1.11E-16	1.21E-13
1600	9.17E-12	2.25E-16	1.53E-13
1700	1.03E-11	4.22E-16	1.88E-13
1800	1.15E-11	7.43E-16	2.24E-13
1900	1.26E-11	1.24E-15	2.63E-13
2000	1.37E-11	1.96E-15	3.03E-13
2100	1.48E-11	2.98E-15	3.43E-13
2200	1.59E-11	4.37E-15	3.84E-13
2300	1.70E-11	6.22E-15	4.24E-13
2400	1.80E-11	8.60E-15	4.65E-13
2500	1.90E-11	1.16E-14	5.04E-13

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	R1 + CH_4 → 1MCPE + CH_3	1MCPE + CH_3 → R2 + CH_4	R2 + CH_4 → 1MCPE + CH_3
500	3.06E-26	1.03E-16	9.97E-26
600	6.49E-24	5.69E-16	2.38E-23
700	3.27E-22	2.17E-15	1.34E-21
800	6.56E-21	6.34E-15	2.94E-20
900	7.04E-20	1.53E-14	3.39E-19
1000	4.82E-19	3.19E-14	2.47E-18
1100	2.37E-18	5.93E-14	1.27E-17
1200	9.05E-18	1.01E-13	5.05E-17
1300	2.83E-17	1.59E-13	1.63E-16
1400	7.52E-17	2.36E-13	4.45E-16
1500	1.76E-16	3.33E-13	1.06E-15
1600	3.69E-16	4.49E-13	2.27E-15
1700	7.10E-16	5.85E-13	4.44E-15
1800	1.27E-15	7.40E-13	8.02E-15
1900	2.12E-15	9.10E-13	1.36E-14
2000	3.38E-15	1.10E-12	2.17E-14
2100	5.13E-15	1.29E-12	3.32E-14
2200	7.48E-15	1.50E-12	4.87E-14
2300	1.05E-14	1.72E-12	6.89E-14
2400	1.44E-14	1.94E-12	9.44E-14
2500	1.92E-14	2.17E-12	1.26E-13

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	2MCPE + CH_3 → R3 + CH_4	R3 + CH_4 → 2MCPE + CH_3	2MCPE + CH_3 → R4 + CH_4
500	2.45E-16	4.26E-26	4.67E-17
600	1.00E-15	9.12E-24	2.97E-16
700	2.99E-15	4.66E-22	1.25E-15
800	7.17E-15	9.47E-21	3.96E-15
900	1.47E-14	1.03E-19	1.01E-14
1000	2.68E-14	7.15E-19	2.22E-14
1100	4.44E-14	3.55E-18	4.28E-14
1200	6.85E-14	1.37E-17	7.51E-14
1300	9.92E-14	4.30E-17	1.22E-13
1400	1.37E-13	1.15E-16	1.85E-13
1500	1.81E-13	2.72E-16	2.67E-13
1600	2.31E-13	5.75E-16	3.67E-13
1700	2.86E-13	1.11E-15	4.87E-13
1800	3.45E-13	2.00E-15	6.24E-13
1900	4.08E-13	3.38E-15	7.80E-13
2000	4.73E-13	5.39E-15	9.51E-13
2100	5.40E-13	8.23E-15	1.14E-12
2200	6.08E-13	1.21E-14	1.33E-12
2300	6.76E-13	1.71E-14	1.54E-12
2400	7.44E-13	2.35E-14	1.75E-12
2500	8.12E-13	3.14E-14	1.97E-12

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	R4 + CH_4 → 2MCPE + CH_3	5MCPE + CH_3 → R5 + CH_4	R5 + CH_4 → 5MCPE + CH_3
500	1.25E-23	5.56E-16	2.66E-27
600	1.33E-21	1.77E-15	7.55E-25
700	4.18E-20	4.32E-15	4.67E-23
800	5.96E-19	8.84E-15	1.09E-21
900	4.91E-18	1.59E-14	1.32E-20
1000	2.73E-17	2.60E-14	9.98E-20
1100	1.13E-16	3.94E-14	5.30E-19
1200	3.72E-16	5.61E-14	2.16E-18
1300	1.03E-15	7.58E-14	7.10E-18
1400	2.45E-15	9.83E-14	1.98E-17
1500	5.22E-15	1.23E-13	4.82E-17
1600	1.01E-14	1.50E-13	1.05E-16
1700	1.81E-14	1.78E-13	2.09E-16
1800	3.02E-14	2.07E-13	3.83E-16
1900	4.77E-14	2.36E-13	6.60E-16
2000	7.18E-14	2.66E-13	1.07E-15
2100	1.04E-13	2.95E-13	1.67E-15
2200	1.44E-13	3.24E-13	2.48E-15
2300	1.94E-13	3.52E-13	3.56E-15
2400	2.55E-13	3.79E-13	4.94E-15
2500	3.26E-13	4.04E-13	6.68E-15

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	1MCPE + OH → R1 + H_2O	R1 + H_2O → 1MCPE + OH	1MCPE + OH → R2 + H_2O
500	9.71E-13	6.24E-04	5.46E-12
600	1.50E-12	8.21E-01	8.17E-12
700	2.10E-12	1.35E+02	1.15E-11
800	2.79E-12	6.15E+03	1.55E-11
900	3.57E-12	1.19E+05	2.02E-11
1000	4.48E-12	1.27E+06	2.57E-11
1100	5.49E-12	8.74E+06	3.20E-11
1200	6.63E-12	4.36E+07	3.91E-11
1300	7.89E-12	1.69E+08	4.70E-11
1400	9.28E-12	5.40E+08	5.58E-11
1500	1.08E-11	1.47E+09	6.54E-11
1600	1.24E-11	3.54E+09	7.59E-11
1700	1.42E-11	7.64E+09	8.74E-11
1800	1.62E-11	1.51E+10	9.97E-11
1900	1.82E-11	2.78E+10	1.13E-10
2000	2.04E-11	4.81E+10	1.27E-10
2100	2.27E-11	7.87E+10	1.42E-10
2200	2.52E-11	1.23E+11	1.58E-10
2300	2.78E-11	1.84E+11	1.75E-10
2400	3.05E-11	2.67E+11	1.93E-10
2500	3.34E-11	3.75E+11	2.12E-10

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	$R2 + H_2O \rightarrow 1MCPE + OH$	$2MCPE + OH \rightarrow R3 + H_2O$	$R3 + H_2O \rightarrow 2MCPE + OH$
500	3.61E-03	9.17E-13	1.29E-04
600	4.60E+00	1.42E-12	1.51E-01
700	7.62E+02	2.01E-12	2.32E+01
800	3.52E+04	2.69E-12	1.01E+03
900	6.92E+05	3.48E-12	1.89E+04
1000	7.48E+06	4.38E-12	1.96E+05
1100	5.23E+07	5.40E-12	1.33E+06
1200	2.64E+08	6.54E-12	6.51E+06
1300	1.04E+09	7.80E-12	2.49E+07
1400	3.33E+09	9.19E-12	7.87E+07
1500	9.16E+09	1.07E-11	2.12E+08
1600	2.21E+10	1.24E-11	5.05E+08
1700	4.81E+10	1.41E-11	1.08E+09
1800	9.58E+10	1.60E-11	2.13E+09
1900	1.77E+11	1.81E-11	3.89E+09
2000	3.07E+11	2.03E-11	6.68E+09
2100	5.05E+11	2.26E-11	1.09E+10
2200	7.93E+11	2.50E-11	1.69E+10
2300	1.19E+12	2.76E-11	2.53E+10
2400	1.74E+12	3.03E-11	3.64E+10
2500	2.45E+12	3.32E-11	5.10E+10

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	2MCPE + OH → R4 + H_2O	R4 + H_2O → 2MCPE + OH	5MCPE + OH → R5 + H_2O
500	6.15E-13	9.57E-05	6.41E-13
600	9.60E-13	1.40E-01	8.70E-13
700	1.39E-12	2.57E+01	1.14E-12
800	1.91E-12	1.29E+03	1.45E-12
900	2.52E-12	2.70E+04	1.80E-12
1000	3.24E-12	3.08E+05	2.19E-12
1100	4.06E-12	2.25E+06	2.63E-12
1200	5.00E-12	1.18E+07	3.11E-12
1300	6.05E-12	4.79E+07	3.63E-12
1400	7.21E-12	1.59E+08	4.20E-12
1500	8.49E-12	4.47E+08	4.82E-12
1600	9.89E-12	1.10E+09	5.48E-12
1700	1.14E-11	2.45E+09	6.18E-12
1800	1.31E-11	4.96E+09	6.92E-12
1900	1.48E-11	9.31E+09	7.71E-12
2000	1.67E-11	1.64E+10	8.55E-12
2100	1.88E-11	2.73E+10	9.43E-12
2200	2.09E-11	4.33E+10	1.04E-11
2300	2.32E-11	6.59E+10	1.13E-11
2400	2.56E-11	9.68E+10	1.23E-11
2500	2.82E-11	1.38E+11	1.34E-11

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	$R5 + H_2O \rightarrow 5MCPE + OH$	$1MCPE + OOH \rightarrow R1 + H_2O_2$	$R1 + H_2O_2 \rightarrow 1MCPE + OOH$
500	5.00E-05	4.18E-19	4.46E-22
600	6.91E-02	3.46E-18	9.80E-21
700	1.22E+01	1.88E-17	1.06E-19
800	5.99E+02	7.38E-17	6.91E-19
900	1.23E+04	2.28E-16	3.16E-18
1000	1.39E+05	5.87E-16	1.11E-17
1100	1.01E+06	1.30E-15	3.20E-17
1200	5.23E+06	2.59E-15	7.86E-17
1300	2.10E+07	4.67E-15	1.70E-16
1400	6.92E+07	7.82E-15	3.34E-16
1500	1.94E+08	1.23E-14	6.01E-16
1600	4.76E+08	1.83E-14	1.01E-15
1700	1.05E+09	2.61E-14	1.61E-15
1800	2.11E+09	3.58E-14	2.43E-15
1900	3.94E+09	4.75E-14	3.52E-15
2000	6.91E+09	6.14E-14	4.92E-15
2100	1.14E+10	7.73E-14	6.67E-15
2200	1.81E+10	9.54E-14	8.81E-15
2300	2.74E+10	1.16E-13	1.14E-14
2400	4.01E+10	1.38E-13	1.43E-14
2500	5.68E+10	1.62E-13	1.78E-14

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	1MCPE + OOH → R2 + H_2O_2	R2 + H_2O_2 → 1MCPE + OOH	2MCPE + OOH → R3 + H_2O_2
500	2.01E-19	2.26E-22	3.67E-19
600	1.85E-18	4.02E-21	3.17E-18
700	1.08E-17	3.62E-20	1.76E-17
800	4.47E-17	2.04E-19	7.06E-17
900	1.45E-16	8.20E-19	2.20E-16
1000	3.85E-16	2.57E-18	5.70E-16
1100	8.85E-16	6.68E-18	1.27E-15
1200	1.80E-15	1.50E-17	2.53E-15
1300	3.34E-15	2.99E-17	4.58E-15
1400	5.71E-15	5.44E-17	7.67E-15
1500	9.15E-15	9.14E-17	1.21E-14
1600	1.39E-14	1.44E-16	1.80E-14
1700	2.01E-14	2.16E-16	2.56E-14
1800	2.80E-14	3.08E-16	3.51E-14
1900	3.77E-14	4.24E-16	4.67E-14
2000	4.94E-14	5.65E-16	6.03E-14
2100	6.30E-14	7.32E-16	7.60E-14
2200	7.87E-14	9.25E-16	9.39E-14
2300	9.64E-14	1.14E-15	1.14E-13
2400	1.16E-13	1.39E-15	1.36E-13
2500	1.38E-13	1.66E-15	1.60E-13

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	R3 + H_2O_2 → 2MCPE + OOH	2MCPE + OOH → R4 + H_2O_2	R4 + H_2O_2 → 2MCPE + OOH
500	4.59E-22	5.47E-20	1.06E-19
600	1.02E-20	6.28E-19	9.90E-19
700	1.10E-19	4.30E-18	5.74E-18
800	7.19E-19	2.02E-17	2.35E-17
900	3.29E-18	7.21E-17	7.44E-17
1000	1.15E-17	2.08E-16	1.94E-16
1100	3.30E-17	5.11E-16	4.36E-16
1200	8.07E-17	1.10E-15	8.70E-16
1300	1.74E-16	2.14E-15	1.58E-15
1400	3.40E-16	3.80E-15	2.65E-15
1500	6.10E-16	6.31E-15	4.16E-15
1600	1.02E-15	9.87E-15	6.21E-15
1700	1.62E-15	1.47E-14	8.85E-15
1800	2.44E-15	2.10E-14	1.21E-14
1900	3.53E-15	2.89E-14	1.61E-14
2000	4.93E-15	3.85E-14	2.08E-14
2100	6.68E-15	5.00E-14	2.63E-14
2200	8.80E-15	6.35E-14	3.24E-14
2300	1.13E-14	7.89E-14	3.93E-14
2400	1.43E-14	9.63E-14	4.69E-14
2500	1.77E-14	1.16E-13	5.51E-14

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

Temperature [K]	$5MCPE + OOH \rightarrow R5 + H_2O_2$	$R5 + H_2O_2 \rightarrow 5MCPE + OOH$
500	1.45E-18	5.05E-23
600	9.81E-18	1.49E-21
700	4.48E-17	1.95E-20
800	1.53E-16	1.47E-19
900	4.20E-16	7.46E-19
1000	9.75E-16	2.84E-18
1100	1.99E-15	8.71E-18
1200	3.65E-15	2.25E-17
1300	6.14E-15	5.07E-17
1400	9.61E-15	1.02E-16
1500	1.42E-14	1.87E-16
1600	1.99E-14	3.19E-16
1700	2.68E-14	5.10E-16
1800	3.49E-14	7.76E-16
1900	4.42E-14	1.13E-15
2000	5.46E-14	1.58E-15
2100	6.61E-14	2.15E-15
2200	7.86E-14	2.85E-15
2300	9.21E-14	3.68E-15
2400	1.06E-13	4.65E-15
2500	1.22E-13	5.78E-15

Table A.5: Reaction Rate Constants in Units of $cm^3 \cdot s^{-1}$ for the Abstraction Reactions of Methylcyclopentadiene (Continued)

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List of Abbreviations

AITSTME	Ab initio transition state theory master equation simulations
aug	Augmented
CASSCF	Complete active space self-consistent field
CBS	Complete basis set
cc	Coupled-cluster
CCSD(T)	Coupled-cluster single and double substitutions with triple excitations
DF	Density fitted formalism
DFT	Density functional theory
GC	Gas chromatography
HF	Hartree-Fock method
HL	High-level
MCPE	Methylcyclopentadiene
MCSCF	Multi-configuration self-consistent field methods
MEL	Master equation lumping
MESS	Master equation system solver
MP2	Second-order Møller-Plesset perturbation theory
PES	Potential energy surface
pVQZ	Polarized valence quadruple zeta
pVTZ	Polarized valence triple zeta
RRKM	Rice-Ramsperger-Kassel-Marcus theory
SCF	Self-consistent field
SPI-MS	Single photon laser ionization mass spectrometry
SVUV-PIMS	Synchrotron vacuum ultraviolet photoionization mass spectrometry
TS	Transition state
TST	Transition state theory

Physical Constants

h	Planck's constant	6.626×10^{-34} J $\cdot$ s
k_B	Boltzmann's constant	1.381×10^{-23} J $\cdot$ K^{-1}
R	Universal gas constant	8.314 J $\cdot$ K^{-1} $\cdot$ mol^{-1}

List of Symbols

α	Exponent of temperature	-
$\beta_{i,j}$	Frequency of collision between the particles i and j	-
β_m	Basis functions	-
ϵ	Well depth	cm^{-1}
γ	Basis set	-
Ψ	Wave function	-
σ	Distance which the intermolecular potential is equal to zero	Å
ΔE_{down}	Transferred energy during deactivating collisions	cm^{-1}
ΔE^0_{down}	Transferred energy during deactivating collisions at the initial temperature	cm^{-1}
ΔG	Gibbs free energy difference	$J \cdot mol^{-1}$
ΔG_0	Gibbs free energy difference of the products	$J \cdot mol^{-1}$
$\Delta G^{\#}$	Gibbs free energy difference of the transition state	$J \cdot mol^{-1}$
$\Delta G^{\neq}$	Gibbs free energy difference of the transition state and the reactants	$J \cdot mol^{-1}$
θ	Weighting factor	-
a_m	Constants for the basis functions	-
Ar	Argon element	-
C	Carbon element	-
E	Energy of the system	J
E_a	Activation energy	$J \cdot mol^{-1}$
h	Planck's constant	$J \cdot s$
H	Hydrogen element	-
$\boldsymbol{H}$	Hamiltonian operator	J
k	Rate constant	s^{-1}

k_0	Pre-exponential factor	s^{-1}
k_B	Boltzmann's constant	$J \cdot K^{-1}$
m	Size of the basis set	-
M	Molecular size	-
n	Exponential of the equation of ΔE_{down}	-
N	Number of non-hydrogen (heavy) atoms	-
N_i	Number density of the particles with the size i	-
O	Oxygen element	-
P	Product	-
Q	Number of electrons	-
r	Distance between interacting particles	Å
R	Universal gas constant	$J \cdot K^{-1} \cdot mol^{-1}$
S	Number of species	-
$\tilde{S}$	Number of species after lumping	-
t	Time	s
T	Temperature	K
T^0	Initial temperature	K
V_{LJ}	Lennard-Jones potential	-
W	Well	-
x	Molar fraction	-

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